



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:30 PM UTC

PDB ID : 7CNT / pdb_00007cnt
Title : Structure of 2,5-dihydroxypridine Dioxygenase from *Pseudomonas putida* KT2440 in complex with product N-formylmaleamic acid formed via in crystallo reaction with 2,5-dihydroxypridine
Authors : Liu, G.Q.; Tang, H.Z.
Deposited on : 2020-08-03
Resolution : 2.28 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

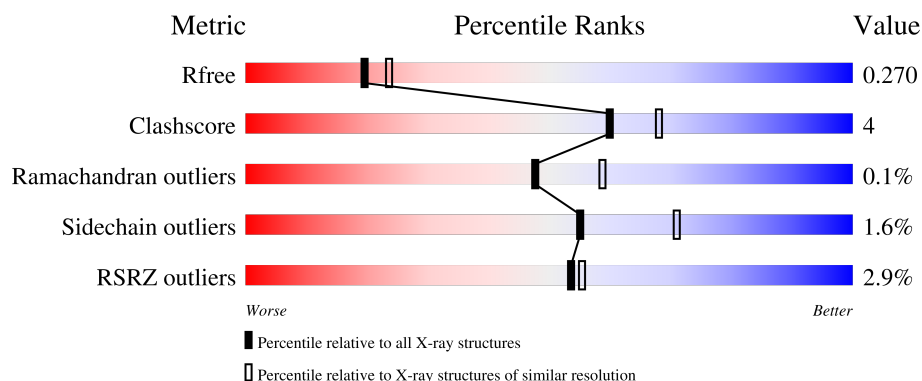
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	3% 85% 10% ..
1	B	363	3% 81% 14% ..
1	C	363	2% 85% 11% .
1	D	363	2% 87% 8% ..
1	E	363	3% 85% 11% .

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Mol	Chain	Length	Quality of chain
1	F	363	3% 87% 9% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16612 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-dihydroxypyridine 5,6-dioxygenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	348	Total	C	N	O	S	Se	0	1	0
			2734	1726	476	516	5	11			
1	B	348	Total	C	N	O	S	Se	0	1	0
			2731	1725	473	516	5	12			
1	C	348	Total	C	N	O	S	Se	0	0	0
			2723	1720	472	515	5	11			
1	D	348	Total	C	N	O	S	Se	0	1	0
			2731	1724	474	517	5	11			
1	E	348	Total	C	N	O	S	Se	0	0	0
			2723	1720	472	515	5	11			
1	F	348	Total	C	N	O	S	Se	0	0	0
			2723	1720	472	515	5	11			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	initiating methionine	UNP Q88FY1
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	1	MSE	-	initiating methionine	UNP Q88FY1
B	351	LYS	-	expression tag	UNP Q88FY1
B	352	LEU	-	expression tag	UNP Q88FY1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	353	ALA	-	expression tag	UNP Q88FY1
B	354	ALA	-	expression tag	UNP Q88FY1
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	1	MSE	-	initiating methionine	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	1	MSE	-	initiating methionine	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	1	MSE	-	initiating methionine	UNP Q88FY1
E	351	LYS	-	expression tag	UNP Q88FY1
E	352	LEU	-	expression tag	UNP Q88FY1

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	1	MSE	-	initiating methionine	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

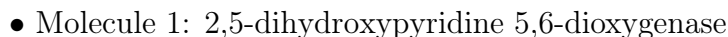
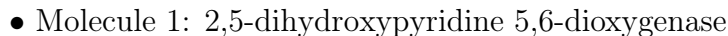
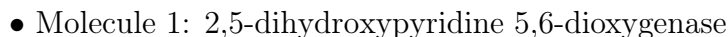
- Molecule 2 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

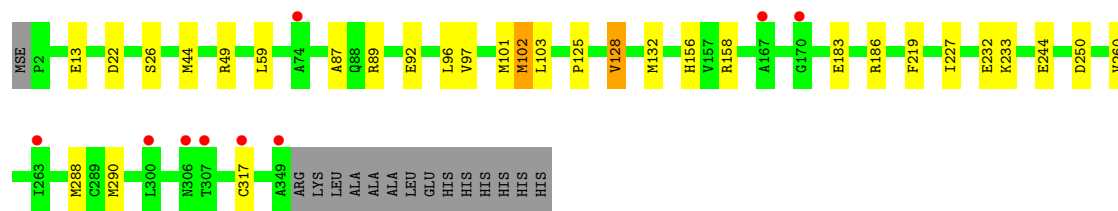
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe 1 1	0	0
2	B	1	Total Fe 1 1	0	0
2	C	1	Total Fe 1 1	0	0
2	D	1	Total Fe 1 1	0	0
2	E	1	Total Fe 1 1	0	0
2	F	1	Total Fe 1 1	0	0

- Molecule 3 is water.

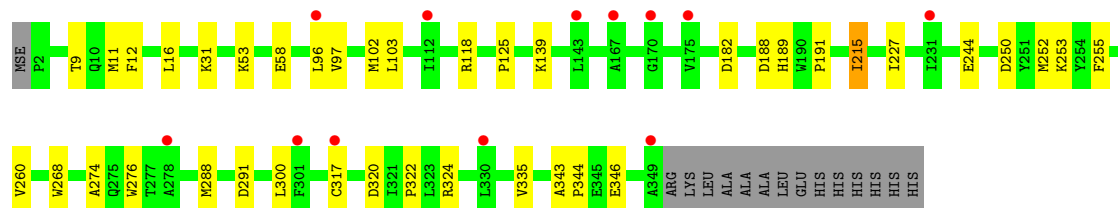
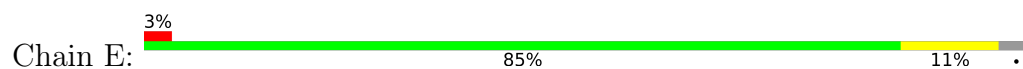
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	39	Total 39	O 39	0	0
3	B	39	Total 39	O 39	0	0
3	C	38	Total 38	O 38	0	0
3	D	40	Total 40	O 40	0	0
3	E	36	Total 36	O 36	0	0
3	F	49	Total 49	O 49	0	0

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

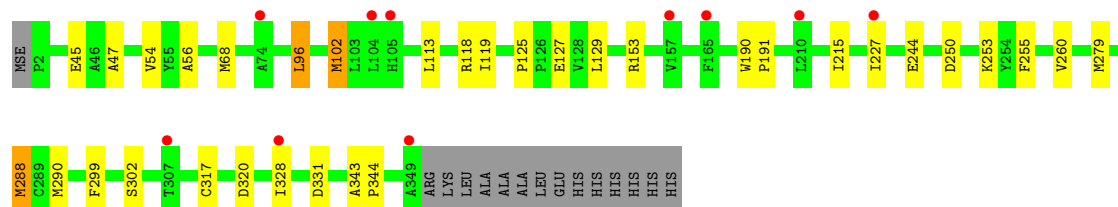
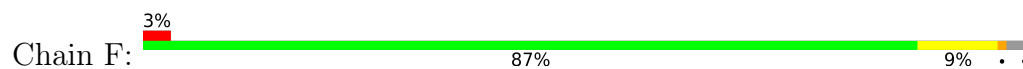




- Molecule 1: 2,5-dihydroxypyridine 5,6-dioxygenase



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	118.89Å 125.92Å 144.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.28 30.00 – 2.28	Depositor EDS
% Data completeness (in resolution range)	99.0 (30.00-2.28) 98.9 (30.00-2.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.211 , 0.267 0.220 , 0.270	Depositor DCC
R_{free} test set	4900 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	52.6	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 20.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	16612	wwPDB-VP
Average B, all atoms (Å ²)	67.0	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 49.86 % 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 7.0282e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FE2

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	0.98	1/2788 (0.0%)	1.02	1/3769 (0.0%)
1	B	1.05	4/2785 (0.1%)	1.06	4/3765 (0.1%)
1	C	0.99	2/2777 (0.1%)	1.03	4/3755 (0.1%)
1	D	0.98	1/2785 (0.0%)	1.01	3/3766 (0.1%)
1	E	0.93	2/2777 (0.1%)	1.07	4/3755 (0.1%)
1	F	0.99	2/2777 (0.1%)	1.05	2/3755 (0.1%)
All	All	0.99	12/16689 (0.1%)	1.04	18/22565 (0.1%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	125	PRO	CA-C	13.89	1.59	1.51
1	C	125	PRO	CA-C	9.29	1.56	1.51
1	E	125	PRO	CA-C	7.46	1.55	1.51
1	B	221	ASN	CA-C	-6.41	1.45	1.52
1	F	125	PRO	CA-C	5.69	1.55	1.52
1	F	45	GLU	C-O	-5.54	1.17	1.24
1	A	118	ARG	CA-C	5.37	1.59	1.52
1	B	177	GLU	CA-C	-5.07	1.47	1.52
1	E	118	ARG	CA-C	5.06	1.59	1.52
1	B	156	HIS	CA-C	5.04	1.58	1.52
1	B	164	ASP	C-O	-5.04	1.18	1.23
1	C	125	PRO	C-O	-5.00	1.20	1.25

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	138	ASP	N-CA-C	-6.57	104.20	111.36
1	F	102	MSE	N-CA-C	6.19	118.16	110.91
1	E	11	MSE	N-CA-C	-5.92	104.41	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	11	MSE	N-CA-C	-5.66	105.20	111.36
1	B	31	LYS	N-CA-C	5.49	116.62	108.60
1	A	147	THR	N-CA-C	-5.45	104.37	111.02
1	E	9	THR	N-CA-C	-5.45	105.26	111.14
1	F	288	MSE	N-CA-CB	-5.43	102.31	110.73
1	C	110	GLU	N-CA-C	-5.37	105.59	111.82
1	C	125	PRO	N-CA-C	5.24	115.50	110.47
1	D	97	VAL	CB-CA-C	-5.24	103.03	110.83
1	D	44	MSE	CB-CA-C	-5.15	102.79	110.88
1	D	128	VAL	N-CA-C	-5.12	105.72	110.53
1	E	215	ILE	N-CA-C	5.10	115.25	108.11
1	B	87	ALA	N-CA-C	-5.07	105.83	111.36
1	E	252	MSE	CA-CB-CG	-5.06	103.98	114.10
1	C	91	LEU	CA-C-N	5.05	127.75	120.38
1	C	91	LEU	C-N-CA	5.05	127.75	120.38

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	2734	0	2665	24	0
1	B	2731	0	2662	38	0
1	C	2723	0	2654	27	0
1	D	2731	0	2659	19	0
1	E	2723	0	2654	18	0
1	F	2723	0	2654	21	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	39	0	0	2	0
3	B	39	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	38	0	0	2	0
3	D	40	0	0	2	0
3	E	36	0	0	1	0
3	F	49	0	0	0	0
All	All	16612	0	15948	140	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 4.

All (140) 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:102:MSE:HE1	1:C:288:MSE:SE	1.91	1.19
1:E:102:MSE:HE1	1:E:288:MSE:SE	2.03	1.08
1:F:102:MSE:HE1	1:F:288:MSE:SE	2.05	1.06
1:A:288:MSE:HE2	1:A:290:MSE:SE	2.07	1.05
1:B:102[A]:MSE:O	1:B:102[A]:MSE:HG3	1.60	1.01
1:C:102:MSE:CE	1:C:288:MSE:SE	2.63	0.96
1:B:288:MSE:HE2	1:B:290:MSE:SE	2.21	0.90
1:D:158:ARG:HD3	3:D:638:HOH:O	1.84	0.77
1:F:153:ARG:HG2	1:F:331:ASP:OD1	1.87	0.75
1:F:227:ILE:HD11	1:F:244:GLU:HB3	1.70	0.74
1:B:186:ARG:HH11	1:B:186:ARG:HG3	1.52	0.73
1:B:102[A]:MSE:HE1	1:B:288:MSE:SE	2.38	0.73
1:D:102:MSE:CE	1:D:288:MSE:SE	2.88	0.71
1:C:38:ARG:HD3	3:C:626:HOH:O	1.91	0.70
1:B:227:ILE:HD11	1:B:244:GLU:HB3	1.74	0.69
1:C:227:ILE:HD11	1:C:244:GLU:HB3	1.74	0.68
1:F:102:MSE:O	1:F:102:MSE:HG3	1.92	0.68
1:E:227:ILE:HD11	1:E:244:GLU:HB3	1.77	0.67
1:B:8:LEU:HD12	1:B:11:MSE:HE2	1.77	0.65
1:A:288:MSE:CE	1:A:290:MSE:SE	2.92	0.64
1:B:108:GLU:HG2	3:B:602:HOH:O	1.99	0.62
1:D:227:ILE:HD11	1:D:244:GLU:HB3	1.80	0.62
1:A:20[A]:ARG:CZ	3:A:603:HOH:O	2.49	0.61
1:C:244:GLU:HB2	3:C:629:HOH:O	2.00	0.60
1:B:102[A]:MSE:CE	1:B:288:MSE:SE	2.99	0.60
1:A:132:MSE:SE	1:A:274:ALA:HB2	2.52	0.59
1:B:260:VAL:HG12	1:B:317:CYS:HB3	1.85	0.59
1:A:227:ILE:HD11	1:A:244:GLU:HB3	1.85	0.58
1:A:20[A]:ARG:NH2	3:A:603:HOH:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:53:LYS:HD3	3:E:635:HOH:O	2.03	0.57
1:E:188:ASP:OD1	1:E:189:HIS:N	2.35	0.57
1:B:186:ARG:HG3	1:B:186:ARG:NH1	2.14	0.57
1:B:156:HIS:HB2	3:B:630:HOH:O	2.04	0.57
1:A:96:LEU:HD23	1:A:118:ARG:HG3	1.86	0.56
1:D:156:HIS:CE1	3:D:628:HOH:O	2.57	0.56
1:F:260:VAL:HG12	1:F:317:CYS:HB3	1.87	0.56
1:A:276:TRP:CD1	1:A:324:ARG:HD2	2.42	0.55
1:A:13:GLU:OE2	1:A:49:ARG:NH1	2.40	0.55
1:A:260:VAL:HG12	1:A:317:CYS:HB3	1.89	0.54
1:F:227:ILE:HD11	1:F:244:GLU:CB	2.37	0.54
1:B:92:GLU:HG3	1:B:112:ILE:HG12	1.90	0.53
1:D:102:MSE:HE1	1:D:288:MSE:SE	2.58	0.53
1:D:13:GLU:OE2	1:D:49:ARG:NH1	2.41	0.53
1:D:288:MSE:HE2	1:D:290:MSE:SE	2.59	0.53
1:B:260:VAL:CG1	1:B:317:CYS:HB3	2.39	0.53
1:A:155:LEU:HB2	1:A:169:LEU:HD11	1.92	0.51
1:E:300:LEU:HD11	1:E:320:ASP:HB3	1.93	0.51
1:A:148:LEU:HD11	1:A:333:LYS:NZ	2.26	0.50
1:B:49:ARG:NH1	1:C:49:ARG:HD3	2.26	0.50
1:B:102[A]:MSE:HA	1:B:121:LEU:HD11	1.94	0.50
1:F:47:ALA:HB3	1:F:54:VAL:HG11	1.92	0.50
1:D:13:GLU:OE2	1:D:49:ARG:CZ	2.60	0.49
1:F:113:LEU:HD21	1:F:119:ILE:HD12	1.95	0.49
1:A:335:VAL:HG23	1:A:336:VAL:HG23	1.94	0.49
1:C:242:GLY:O	1:C:245:ALA:HB3	2.13	0.49
1:C:265:HIS:CE1	1:C:302:SER:HB2	2.48	0.48
1:B:102[B]:MSE:HA	1:B:121:LEU:HD11	1.95	0.48
1:F:96:LEU:HD23	1:F:118:ARG:HG3	1.96	0.48
1:A:64:HIS:CG	1:A:75:TYR:CD1	3.02	0.48
1:F:343:ALA:HA	1:F:344:PRO:C	2.39	0.48
1:D:128:VAL:HG13	1:D:132:MSE:CE	2.44	0.48
1:A:148:LEU:HD22	1:A:344:PRO:HG3	1.96	0.47
1:F:129:LEU:HB3	1:F:190:TRP:CZ2	2.49	0.47
1:A:118:ARG:HD2	1:A:181:ALA:O	2.13	0.47
1:B:277:THR:OG1	1:F:68:MSE:HE1	2.15	0.47
1:B:295:PHE:CE2	1:B:298:ASN:HB3	2.50	0.47
1:B:326:CYS:HB2	3:B:622:HOH:O	2.15	0.47
1:B:215:ILE:HB	1:B:322:PRO:HG2	1.97	0.47
1:E:268:TRP:CH2	1:E:335:VAL:HG11	2.49	0.47
1:B:159:SER:OG	1:B:163:SER:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:ALA:HB3	1:C:54:VAL:HG11	1.98	0.46
1:E:96:LEU:HD12	1:E:97:VAL:N	2.31	0.46
1:C:210:LEU:HD22	1:C:227:ILE:HD12	1.97	0.46
1:C:128:VAL:CG1	1:C:132:MSE:HE3	2.46	0.46
1:F:288:MSE:HE2	1:F:290:MSE:SE	2.66	0.46
1:D:260:VAL:HG12	1:D:317:CYS:HB3	1.98	0.45
1:D:101:MSE:O	1:D:102:MSE:HB3	2.16	0.45
1:B:276:TRP:CD2	1:B:324:ARG:HD2	2.51	0.45
1:B:316:PRO:HD2	3:B:606:HOH:O	2.15	0.45
1:A:215:ILE:HB	1:A:322:PRO:HG2	1.98	0.45
1:D:22:ASP:OD1	1:D:22:ASP:C	2.59	0.45
1:E:274:ALA:HB1	1:E:291:ASP:HA	1.98	0.45
1:A:276:TRP:CG	1:A:324:ARG:HD2	2.52	0.45
1:C:31:LYS:O	1:C:58:GLU:HA	2.15	0.45
1:E:12:PHE:O	1:E:16:LEU:HG	2.17	0.45
1:A:148:LEU:HD12	1:A:148:LEU:HA	1.81	0.45
1:F:215:ILE:HG23	1:F:279:MSE:HE1	1.98	0.45
1:B:49:ARG:NE	1:C:49:ARG:CZ	2.80	0.45
1:E:31:LYS:O	1:E:58:GLU:HA	2.16	0.44
1:A:49:ARG:HD3	1:D:49:ARG:NH1	2.32	0.44
1:C:259:GLU:HB3	1:C:313:ARG:HD2	2.00	0.44
1:B:274:ALA:HB1	1:B:291:ASP:HA	1.99	0.44
1:E:102:MSE:O	1:E:102:MSE:HG3	2.17	0.44
1:B:240:HIS:ND1	3:B:601:HOH:O	2.36	0.44
1:C:138:ASP:O	1:C:142:VAL:HG23	2.17	0.44
1:C:298:ASN:OD1	1:C:298:ASN:C	2.61	0.44
1:F:299:PHE:HB2	1:F:328:ILE:HD11	2.00	0.44
1:E:139:LYS:NZ	1:E:182:ASP:OD2	2.50	0.44
1:E:276:TRP:CD1	1:E:324:ARG:HD2	2.53	0.43
1:E:215:ILE:O	1:E:322:PRO:HD2	2.18	0.43
1:C:276:TRP:CE2	1:C:324:ARG:HD2	2.54	0.43
1:B:49:ARG:CZ	1:C:49:ARG:NE	2.81	0.43
1:D:232:GLU:O	1:D:233:LYS:C	2.62	0.43
1:B:343:ALA:HA	1:B:344:PRO:C	2.43	0.43
1:D:219:PHE:N	1:D:219:PHE:CD1	2.87	0.43
1:E:255:PHE:CD2	1:E:317:CYS:HB2	2.54	0.42
1:E:260:VAL:HG12	1:E:317:CYS:HB3	2.00	0.42
1:C:64:HIS:HB2	1:C:67:ALA:HB2	2.01	0.42
1:C:59:LEU:HD21	1:C:87:ALA:HB1	2.01	0.42
1:B:49:ARG:HD3	1:C:49:ARG:NH1	2.35	0.42
1:B:306:ASN:CG	1:B:311:GLY:HA3	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:255:PHE:CG	1:F:317:CYS:HB2	2.55	0.42
1:A:105:HIS:HB3	1:A:308:GLU:HG2	2.02	0.41
1:F:127:GLU:H	1:F:127:GLU:CD	2.28	0.41
1:A:20[A]:ARG:NH1	1:A:182:ASP:O	2.54	0.41
1:B:73:THR:HG23	1:B:102[A]:MSE:HE3	2.02	0.41
1:B:186:ARG:NH1	1:B:186:ARG:CG	2.80	0.41
1:D:89:ARG:NH1	1:D:92:GLU:OE1	2.53	0.41
1:F:127:GLU:CD	1:F:127:GLU:N	2.79	0.41
1:F:190:TRP:HA	1:F:191:PRO:HA	1.92	0.41
1:B:41:ASN:O	1:B:45:GLU:HG2	2.20	0.41
1:D:59:LEU:HD21	1:D:87:ALA:HB1	2.03	0.41
1:D:183:GLU:O	1:D:186:ARG:HB3	2.21	0.41
1:C:260:VAL:HG12	1:C:317:CYS:HB3	2.01	0.41
1:C:288:MSE:HE2	1:C:290:MSE:SE	2.70	0.41
1:B:64:HIS:CG	1:B:75:TYR:CD1	3.08	0.41
1:B:96:LEU:HD12	1:B:118:ARG:HG3	2.01	0.41
1:B:255:PHE:O	1:B:256:ASN:C	2.63	0.41
1:E:343:ALA:HA	1:E:344:PRO:C	2.46	0.41
1:A:260:VAL:CG1	1:A:317:CYS:HB3	2.50	0.41
1:A:306:ASN:CG	1:A:311:GLY:HA3	2.46	0.41
1:C:276:TRP:NE1	1:C:324:ARG:HD2	2.36	0.41
1:F:302:SER:HB2	1:F:320:ASP:OD1	2.21	0.41
1:C:101:MSE:O	1:C:102:MSE:HB3	2.20	0.40
1:B:103:LEU:HD23	1:B:103:LEU:HA	1.98	0.40
1:D:128:VAL:HG13	1:D:132:MSE:HE3	2.04	0.40
1:B:290:MSE:SE	1:B:293:ARG:HD2	2.71	0.40
1:C:58:GLU:HB3	1:F:56:ALA:HB3	2.04	0.40
1:C:219:PHE:N	1:C:219:PHE:CD1	2.88	0.40
1:E:103:LEU:HD23	1:E:103:LEU:HA	1.97	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	347/363 (96%)	330 (95%)	16 (5%)	1 (0%)	36	44
1	B	347/363 (96%)	328 (94%)	18 (5%)	1 (0%)	36	44
1	C	346/363 (95%)	333 (96%)	12 (4%)	1 (0%)	36	44
1	D	347/363 (96%)	333 (96%)	14 (4%)	0	100	100
1	E	346/363 (95%)	324 (94%)	22 (6%)	0	100	100
1	F	346/363 (95%)	328 (95%)	18 (5%)	0	100	100
All	All	2079/2178 (96%)	1976 (95%)	100 (5%)	3 (0%)	48	59

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	192	SER
1	A	192	SER
1	C	192	SER

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	288/287 (100%)	280 (97%)	8 (3%)	38	53
1	B	288/287 (100%)	286 (99%)	2 (1%)	76	86
1	C	287/287 (100%)	282 (98%)	5 (2%)	53	70
1	D	288/287 (100%)	283 (98%)	5 (2%)	53	70
1	E	287/287 (100%)	283 (99%)	4 (1%)	59	74
1	F	287/287 (100%)	284 (99%)	3 (1%)	68	81
All	All	1725/1722 (100%)	1698 (98%)	27 (2%)	55	71

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	GLU
1	A	53	LYS

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Mol	Chain	Res	Type
1	A	54	VAL
1	A	96	LEU
1	A	250	ASP
1	A	253	LYS
1	A	308	GLU
1	A	309	VAL
1	B	54	VAL
1	B	333	LYS
1	C	26	SER
1	C	54	VAL
1	C	140	ARG
1	C	186	ARG
1	C	250	ASP
1	D	26	SER
1	D	96	LEU
1	D	102	MSE
1	D	103	LEU
1	D	250	ASP
1	E	191	PRO
1	E	250	ASP
1	E	253	LYS
1	E	346	GLU
1	F	96	LEU
1	F	250	ASP
1	F	253	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	GLN
1	A	156	HIS
1	A	166	HIS
1	A	265	HIS
1	B	48	GLN
1	B	166	HIS
1	B	282	HIS
1	C	33	HIS
1	C	88	GLN
1	C	265	HIS
1	C	282	HIS
1	D	63	ASN
1	D	64	HIS

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Mol	Chain	Res	Type
1	D	240	HIS
1	D	265	HIS
1	D	282	HIS
1	E	33	HIS
1	E	70	ASN
1	F	33	HIS
1	F	265	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 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	337/363 (92%)	0.38	11 (3%)	49	51	33, 62, 105, 131	1 (0%)
1	B	337/363 (92%)	0.25	10 (2%)	52	54	40, 57, 102, 145	0
1	C	337/363 (92%)	0.22	7 (2%)	63	65	39, 62, 103, 127	0
1	D	337/363 (92%)	0.36	9 (2%)	56	58	29, 63, 100, 128	1 (0%)
1	E	337/363 (92%)	0.49	12 (3%)	46	48	45, 69, 104, 138	0
1	F	337/363 (92%)	0.24	10 (2%)	52	54	39, 60, 90, 120	0
All	All	2022/2178 (92%)	0.32	59 (2%)	53	55	29, 62, 101, 145	2 (0%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	328	ILE	5.2
1	C	305	PRO	4.1
1	A	43	ALA	3.6
1	E	317	CYS	3.6
1	F	349	ALA	3.6
1	F	104	LEU	3.5
1	F	210	LEU	3.4
1	A	74	ALA	3.4
1	C	338	ALA	3.2
1	A	104	LEU	3.2
1	B	349	ALA	3.2
1	E	96	LEU	3.2
1	B	76	CYS	3.1
1	E	301	PHE	3.1
1	B	104	LEU	3.1
1	F	165	PHE	3.1
1	A	75	TYR	3.1
1	C	349	ALA	3.1
1	E	330	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	75	TYR	3.0
1	D	307	THR	2.9
1	B	74	ALA	2.9
1	E	170	GLY	2.8
1	E	143	LEU	2.8
1	F	157	VAL	2.8
1	F	227	ILE	2.7
1	A	105	HIS	2.7
1	E	167	ALA	2.7
1	C	309	VAL	2.7
1	D	263	ILE	2.6
1	A	333	LYS	2.6
1	A	349	ALA	2.5
1	D	74	ALA	2.5
1	D	317	CYS	2.5
1	F	74	ALA	2.5
1	A	65	PRO	2.5
1	E	175	VAL	2.4
1	D	300	LEU	2.4
1	C	306	ASN	2.3
1	F	307	THR	2.3
1	B	307	THR	2.3
1	C	65	PRO	2.3
1	D	170	GLY	2.3
1	D	167	ALA	2.3
1	E	231	ILE	2.3
1	A	12	PHE	2.2
1	B	258	PRO	2.2
1	D	306	ASN	2.2
1	C	304	GLY	2.2
1	B	73	THR	2.2
1	D	349	ALA	2.1
1	B	105	HIS	2.1
1	B	282	HIS	2.1
1	F	105	HIS	2.1
1	A	317	CYS	2.1
1	E	112	ILE	2.1
1	A	20[A]	ARG	2.1
1	E	278	ALA	2.0
1	E	349	ALA	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

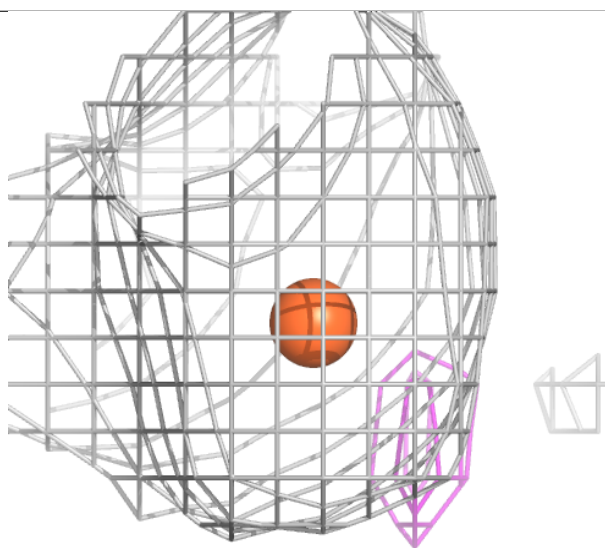
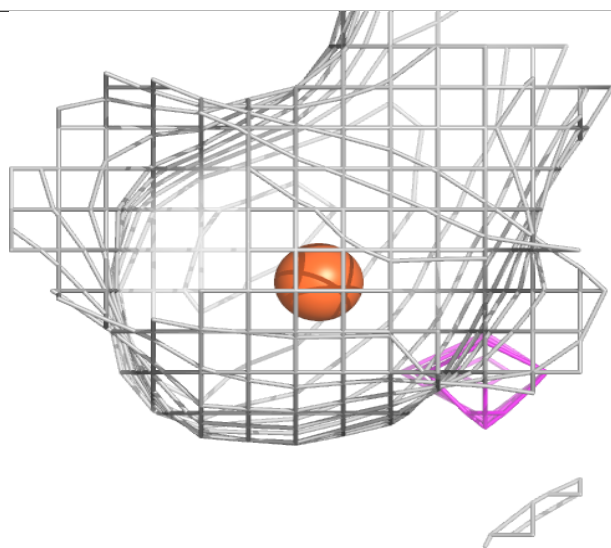
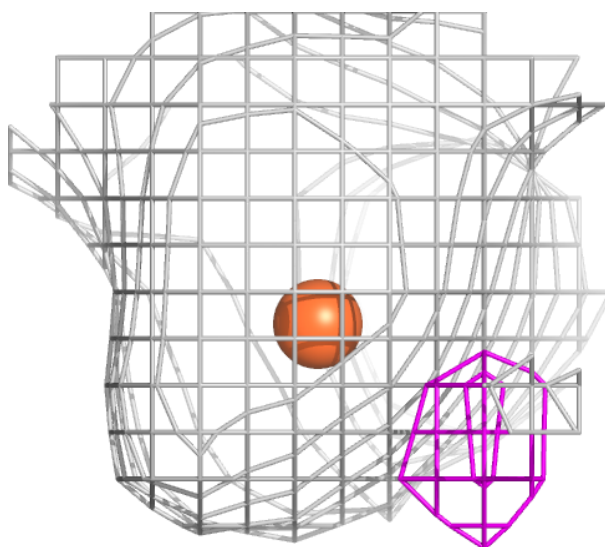
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FE2	B	501	1/1	0.87	0.10	112,112,112,112	0
2	FE2	A	501	1/1	0.90	0.09	110,110,110,110	0
2	FE2	C	501	1/1	0.92	0.07	103,103,103,103	0
2	FE2	D	501	1/1	0.97	0.08	93,93,93,93	0
2	FE2	E	501	1/1	0.98	0.03	89,89,89,89	0
2	FE2	F	501	1/1	0.99	0.05	72,72,72,72	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.

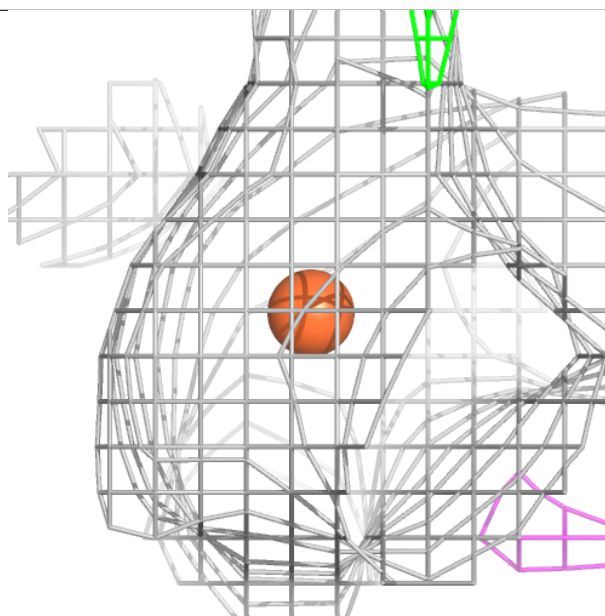
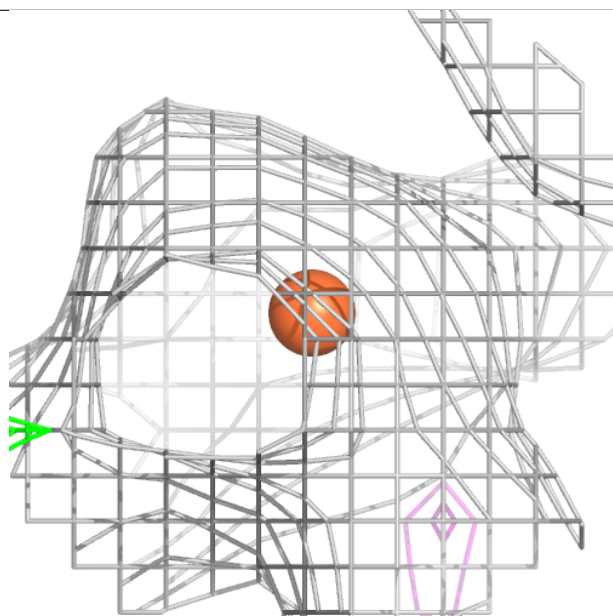
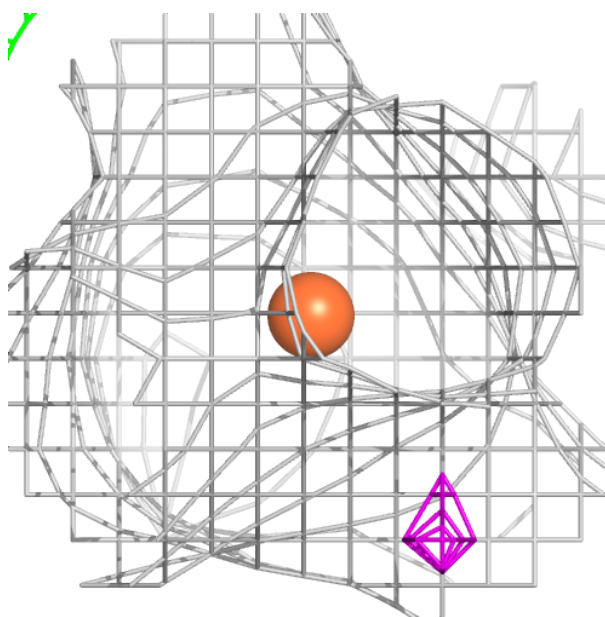
Electron density around FE2 B 501:

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



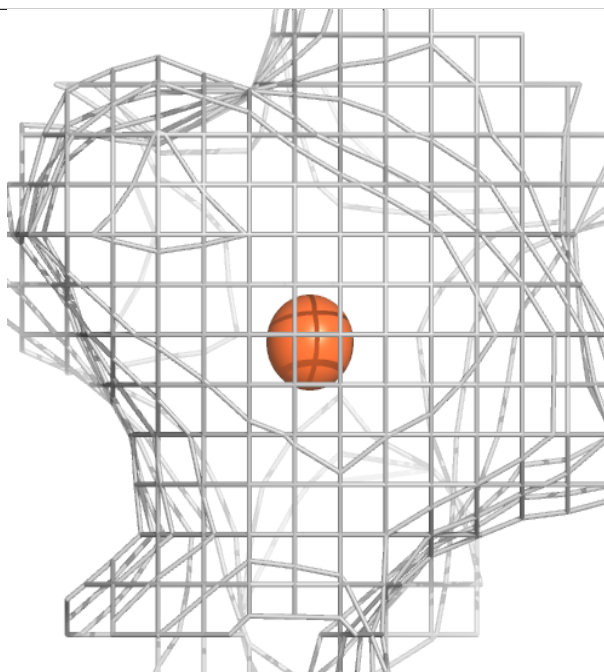
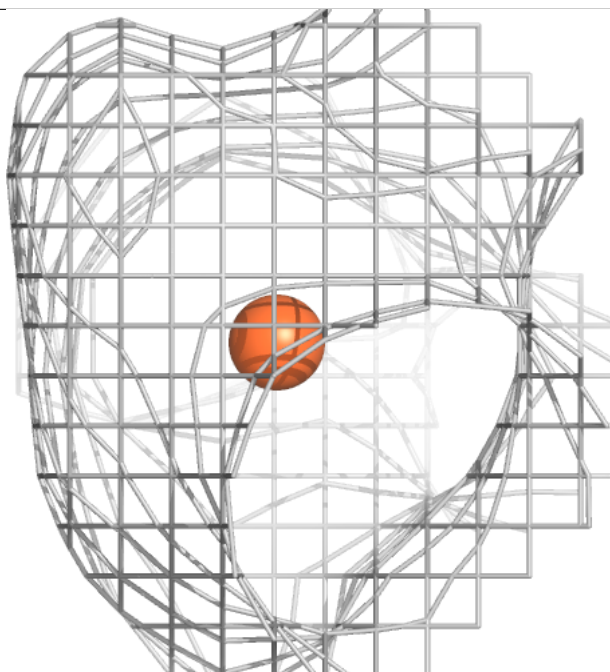
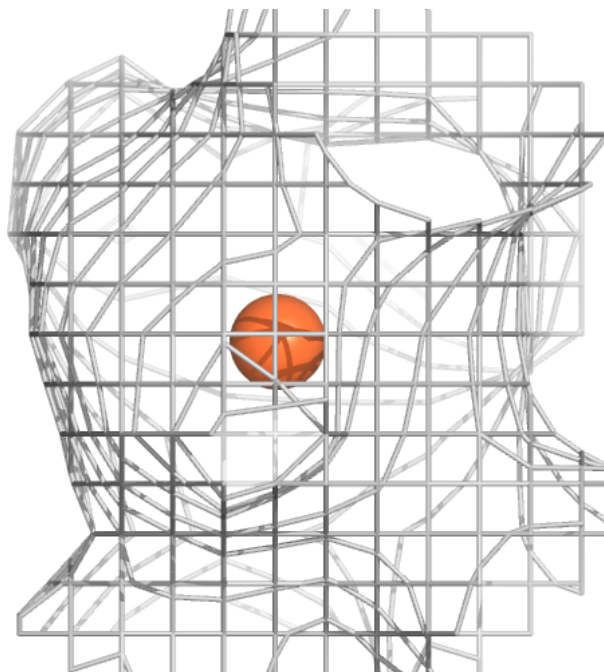
Electron density around FE2 A 501:

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



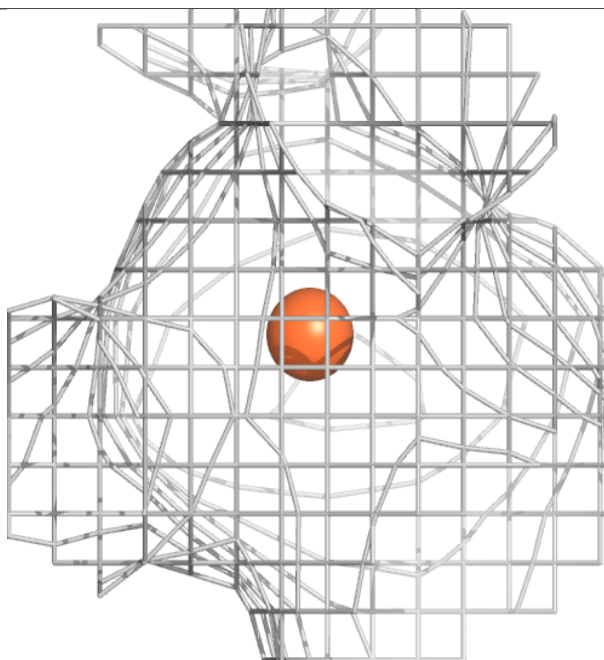
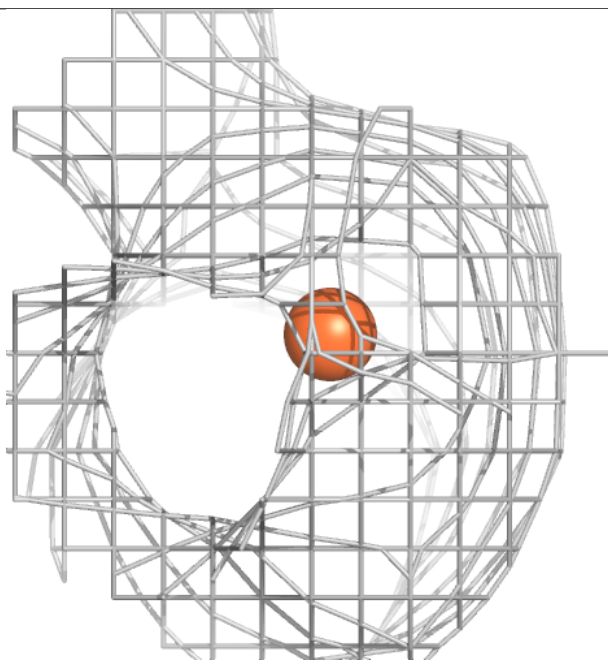
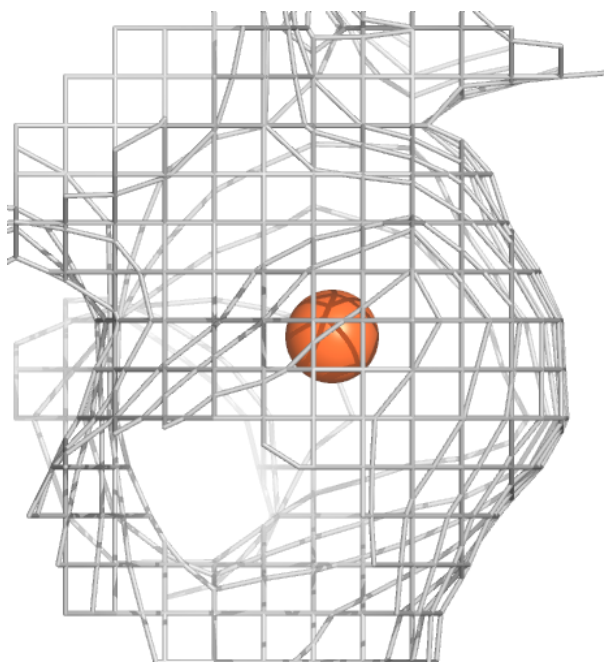
Electron density around FE2 C 501:

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



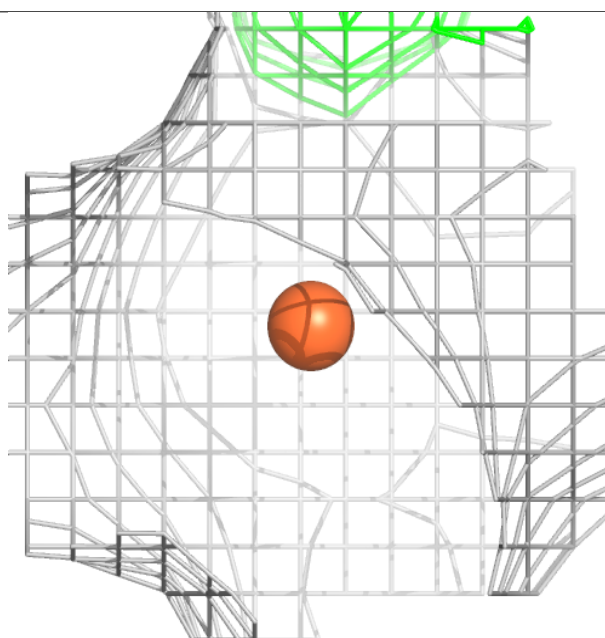
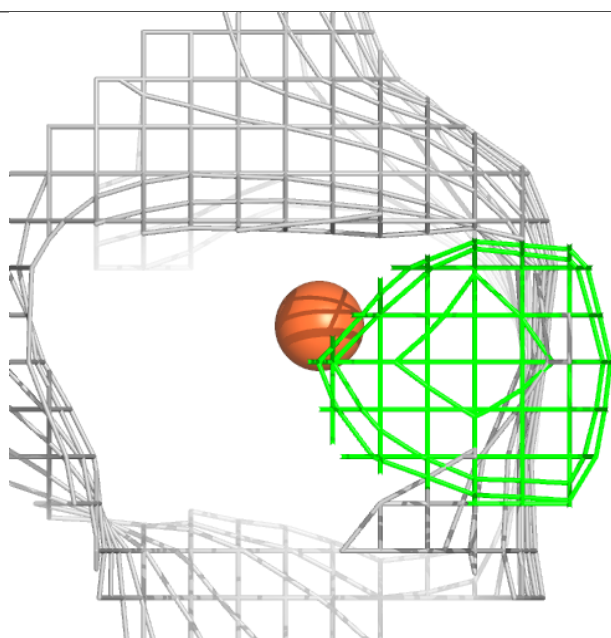
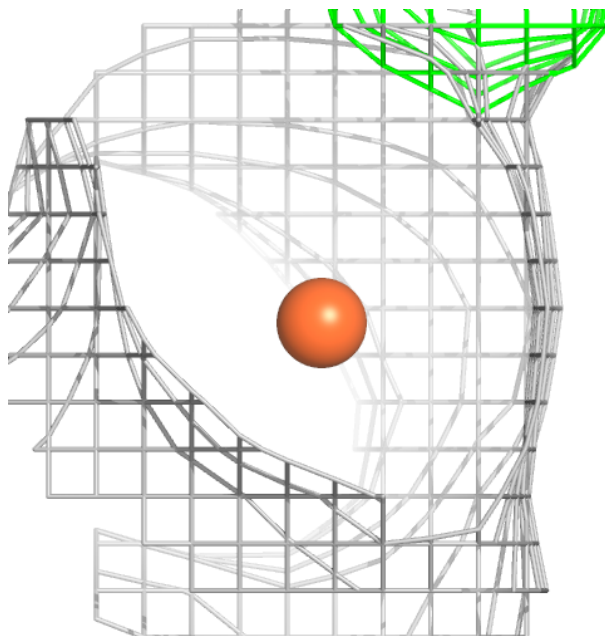
Electron density around FE2 D 501:

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



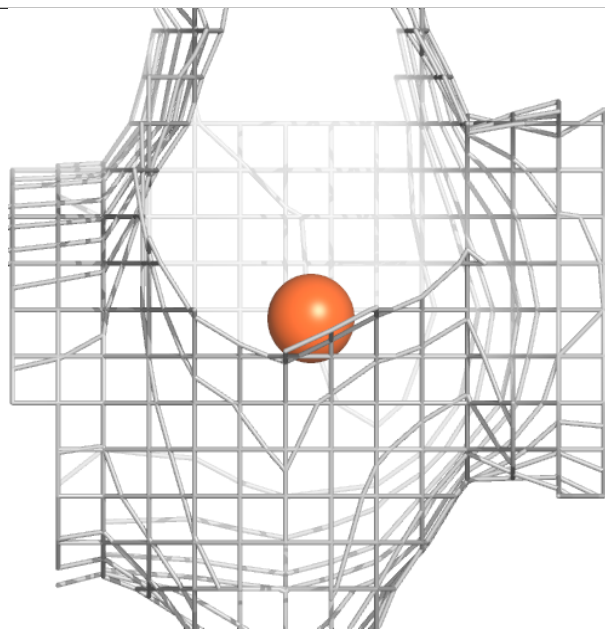
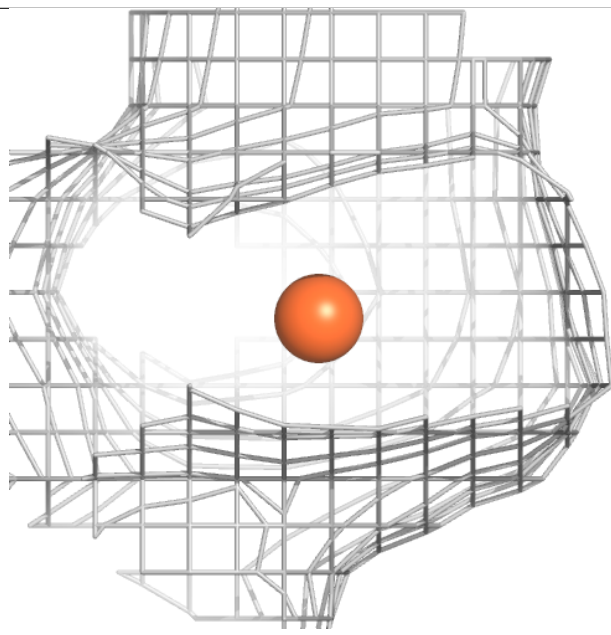
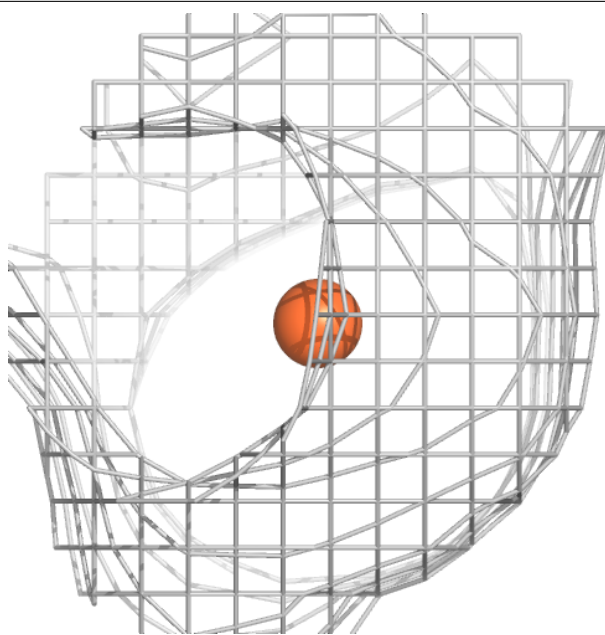
Electron density around FE2 E 501:

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



Electron density around FE2 F 501:

$2mF_o - DF_c$ (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.