



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:26 PM UTC

PDB ID : 9N43 / pdb_00009n43
Title : Crystal structure of none-heme iron enzyme (TqaM) from *Trichoderma atroviride* bound with iron
Authors : Liu, S.; Zheng, Y.-C.; Chang, W.-C.
Deposited on : 2025-02-01
Resolution : 2.60 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
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

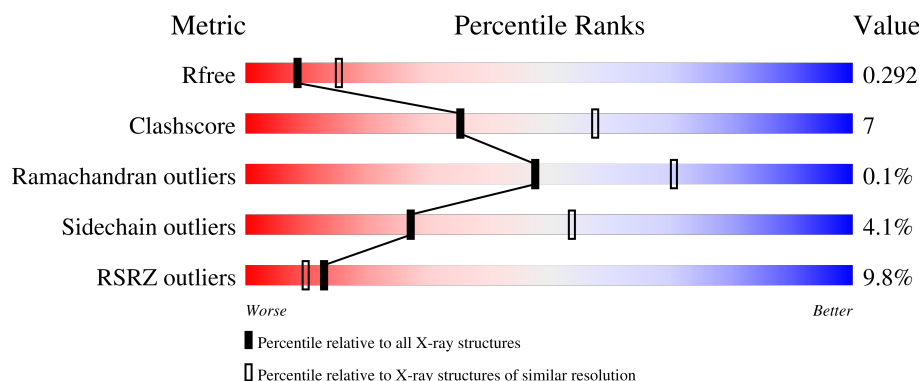
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	283	6% 84% 14% ..
1	B	283	8% 80% 18% .
1	C	283	12% 78% 19% ..
1	D	283	12% 83% 16% .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8977 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 Class II aldolase/adducin N-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	0	0
			2172	1373	391	395	13			
1	B	283	Total	C	N	O	S	0	0	0
			2186	1381	393	398	14			
1	C	279	Total	C	N	O	S	0	1	0
			2166	1369	390	394	13			
1	D	283	Total	C	N	O	S	0	1	0
			2199	1389	395	401	14			

- 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	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		
2	D	1	Total	Fe	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	66	Total	O	0	0
			66	66		
3	B	70	Total	O	0	0
			70	70		
3	C	59	Total	O	0	0
			59	59		

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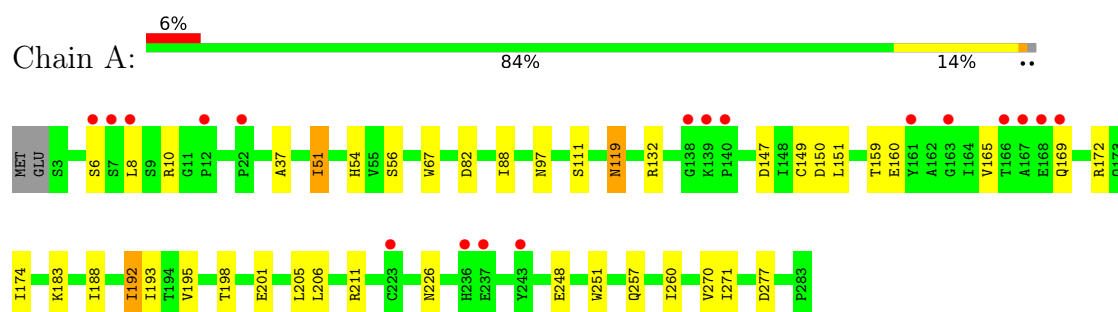
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	55	Total	O	0	0
			55	55		

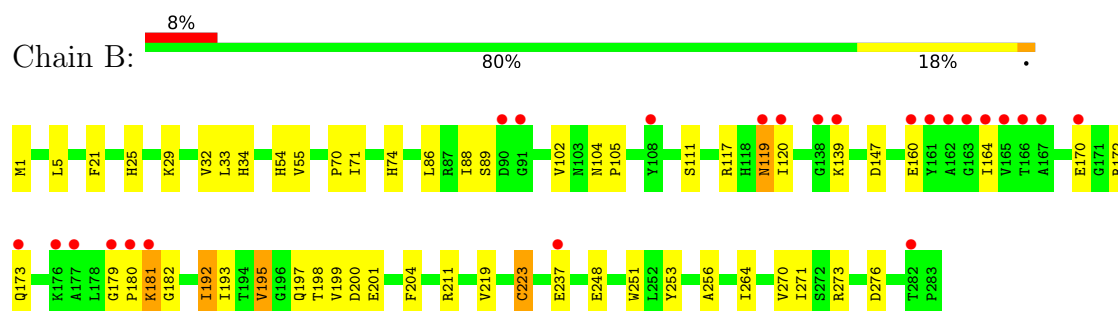
3 Residue-property plots

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.

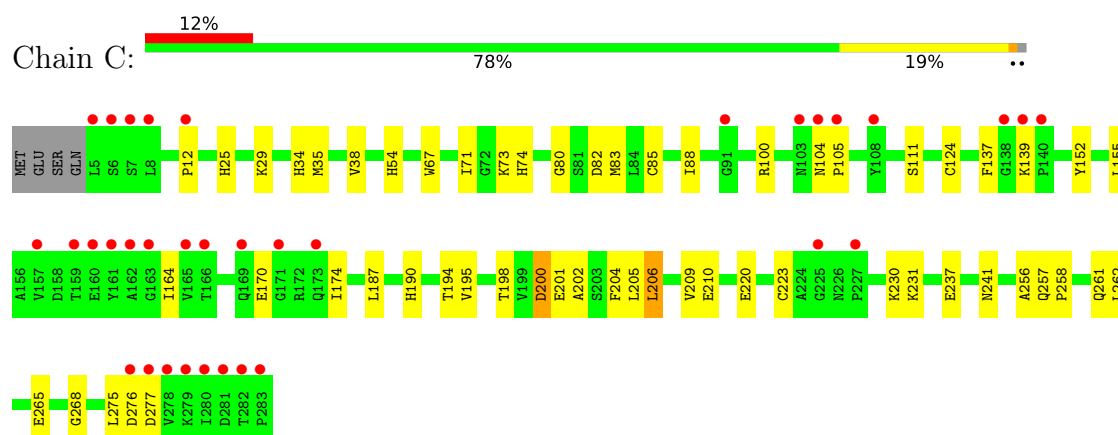
- Molecule 1: Class II aldolase/adducin N-terminal domain-containing protein



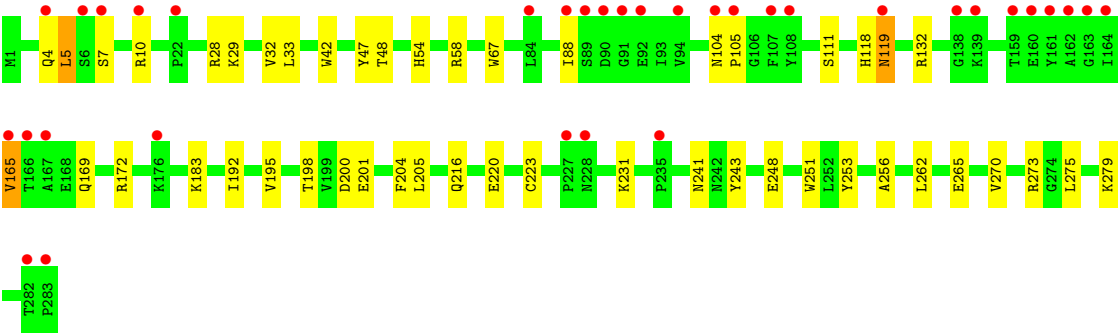
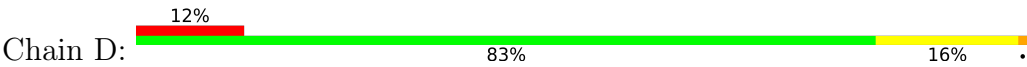
- Molecule 1: Class II aldolase/adducin N-terminal domain-containing protein



- Molecule 1: Class II aldolase/adducin N-terminal domain-containing protein



- Molecule 1: Class II aldolase/adducin N-terminal domain-containing protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	114.51Å 124.97Å 187.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.25 – 2.60 18.25 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.5 (18.25-2.60) 97.5 (18.25-2.60)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.38 (at 2.59Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.260 , 0.292 0.261 , 0.292	Depositor DCC
R_{free} test set	2045 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	1.3	Xtriage
Anisotropy	5.298	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 60.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.77	EDS
Total number of atoms	8977	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

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	0.11	0/2224	0.25	0/3013
1	B	0.11	0/2238	0.26	0/3031
1	C	0.09	0/2218	0.25	0/3006
1	D	0.10	0/2251	0.26	0/3048
All	All	0.10	0/8931	0.26	0/12098

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	2172	0	2148	32	0
1	B	2186	0	2165	37	0
1	C	2166	0	2144	37	0
1	D	2199	0	2182	32	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
3	A	66	0	0	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	70	0	0	11	1
3	C	59	0	0	10	1
3	D	55	0	0	4	0
All	All	8977	0	8639	128	1

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 7.

All (128) 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:A:160:GLU:OE1	3:A:401:HOH:O	1.83	0.96
1:A:6:SER:O	3:A:402:HOH:O	1.95	0.83
1:A:37:ALA:HB3	1:A:260:ILE:HG23	1.61	0.81
1:C:164:ILE:HG21	1:D:241:ASN:HD22	1.46	0.81
1:C:71:ILE:O	3:C:401:HOH:O	2.00	0.80
1:D:279:LYS:NZ	3:D:402:HOH:O	2.14	0.80
1:A:277:ASP:OD1	3:A:403:HOH:O	2.00	0.79
1:B:70:PRO:O	3:B:401:HOH:O	1.99	0.78
1:C:82:ASP:O	3:C:403:HOH:O	2.03	0.77
1:B:199:VAL:N	3:B:402:HOH:O	2.06	0.76
1:A:82:ASP:OD1	3:A:404:HOH:O	2.04	0.75
1:C:12:PRO:O	3:C:402:HOH:O	2.02	0.75
1:B:270:VAL:O	3:B:403:HOH:O	2.06	0.73
1:A:10:ARG:HB2	1:D:104:ASN:HB3	1.70	0.73
1:C:202:ALA:O	3:C:404:HOH:O	2.07	0.72
1:C:206:LEU:HB3	3:C:404:HOH:O	1.90	0.71
1:A:51:ILE:O	3:A:405:HOH:O	2.09	0.71
1:B:5:LEU:O	3:B:404:HOH:O	2.09	0.71
1:A:169:GLN:HG2	1:A:172:ARG:HH21	1.57	0.70
1:B:119:ASN:O	1:B:197:GLN:NE2	2.23	0.70
1:B:198:THR:HG23	1:B:201:GLU:H	1.58	0.68
1:B:21:PHE:O	3:B:405:HOH:O	2.10	0.68
1:A:226:ASN:O	3:A:406:HOH:O	2.10	0.68
1:B:119:ASN:N	1:B:119:ASN:OD1	2.27	0.68
1:C:204:PHE:HB2	1:C:256:ALA:HB2	1.75	0.68
1:C:88:ILE:O	3:C:405:HOH:O	2.12	0.67
1:D:118:HIS:O	3:D:401:HOH:O	2.12	0.66
1:C:241:ASN:OD1	3:C:407:HOH:O	2.14	0.65
1:B:211:ARG:NH2	3:B:412:HOH:O	2.28	0.65
1:B:160:GLU:HB3	1:B:173:GLN:HE22	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:TYR:O	3:C:406:HOH:O	2.13	0.65
1:A:37:ALA:CB	1:A:260:ILE:HG23	2.27	0.65
1:A:132:ARG:NH1	1:B:147:ASP:OD2	2.28	0.65
1:B:273:ARG:HB2	3:B:403:HOH:O	1.97	0.64
1:B:170:GLU:OE2	3:B:406:HOH:O	2.14	0.64
1:A:260:ILE:HB	3:A:411:HOH:O	1.97	0.64
1:D:119:ASN:OD1	1:D:119:ASN:N	2.31	0.63
1:C:268:GLY:O	3:C:408:HOH:O	2.16	0.63
1:A:183:LYS:HD2	3:A:412:HOH:O	1.97	0.63
1:A:198:THR:HG23	1:A:201:GLU:H	1.64	0.62
1:D:204:PHE:HB2	1:D:256:ALA:HB2	1.80	0.61
1:C:198:THR:HG23	1:C:201:GLU:H	1.65	0.61
1:D:198:THR:HG23	1:D:201:GLU:H	1.67	0.59
1:C:100:ARG:NH1	3:C:414:HOH:O	2.35	0.59
1:B:88:ILE:HG23	1:B:111:SER:HB2	1.84	0.59
1:A:149:CYS:SG	3:A:458:HOH:O	2.43	0.58
1:B:33:LEU:HD11	1:B:271:ILE:HD12	1.85	0.58
1:D:88:ILE:HG23	1:D:111:SER:HB2	1.86	0.58
1:B:172:ARG:NH1	3:B:417:HOH:O	2.36	0.58
1:D:165:VAL:HG13	1:D:169:GLN:HB2	1.84	0.58
1:B:25:HIS:NE2	1:B:276:ASP:OD1	2.33	0.58
1:B:86:LEU:HD21	1:B:102:VAL:HG21	1.86	0.57
1:A:88:ILE:HG23	1:A:111:SER:HB2	1.87	0.56
1:D:104:ASN:CG	1:D:105:PRO:HD3	2.29	0.56
1:A:248:GLU:HG3	1:A:251:TRP:H	1.73	0.54
1:D:28:ARG:HD3	1:D:67:TRP:HZ2	1.74	0.53
1:C:104[A]:ASN:ND2	1:D:7:SER:O	2.40	0.53
1:D:33:LEU:HB2	1:D:275:LEU:HD11	1.91	0.52
1:A:159:THR:HG23	1:A:188:ILE:HD12	1.91	0.52
1:A:147:ASP:OD2	1:D:132:ARG:NH1	2.38	0.52
1:C:170:GLU:O	1:C:174:ILE:HG12	2.10	0.52
1:B:117:ARG:NH1	1:B:182:GLY:O	2.33	0.52
1:C:88:ILE:HG23	1:C:111:SER:HB2	1.92	0.52
1:D:169:GLN:HG2	1:D:172:ARG:HH12	1.75	0.51
1:A:119:ASN:N	1:A:119:ASN:OD1	2.43	0.51
1:B:71:ILE:O	3:B:408:HOH:O	2.19	0.50
1:D:58:ARG:NH2	3:D:412:HOH:O	2.44	0.50
1:B:198:THR:HG21	1:B:253:TYR:HD1	1.77	0.50
1:B:117:ARG:HD2	1:B:179:GLY:O	2.12	0.50
1:A:270:VAL:N	3:A:415:HOH:O	2.33	0.49
1:A:150:ASP:O	3:A:408:HOH:O	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:HIS:CE1	1:D:262:LEU:HD22	2.47	0.49
1:A:271:ILE:O	3:A:409:HOH:O	2.20	0.49
1:C:73:LYS:HB2	1:C:100:ARG:NH1	2.28	0.49
1:C:80:GLY:HA3	1:C:275:LEU:HD21	1.95	0.49
1:C:187:LEU:HB2	1:C:190:HIS:HB3	1.95	0.48
1:C:104[A]:ASN:CG	1:C:105:PRO:HD3	2.39	0.48
1:A:211:ARG:NH2	3:A:417:HOH:O	2.33	0.48
1:C:220:GLU:OE2	1:C:231:LYS:NZ	2.35	0.47
1:C:230:LYS:HD3	1:C:230:LYS:HA	1.71	0.47
1:B:248:GLU:HG3	1:B:251:TRP:H	1.80	0.47
1:C:35:MET:HB3	1:C:83:MET:HE3	1.97	0.47
1:B:204:PHE:HB2	1:B:256:ALA:HB2	1.96	0.47
1:C:206:LEU:O	1:C:210:GLU:HB2	2.15	0.47
1:A:174:ILE:HG21	1:A:193:ILE:HD13	1.97	0.47
1:C:25:HIS:O	1:C:29:LYS:HG3	2.15	0.47
1:B:29:LYS:HA	1:B:32:VAL:HG22	1.96	0.46
1:B:74:HIS:CE1	1:C:262:LEU:HD22	2.50	0.46
1:B:180:PRO:HB2	1:B:181:LYS:HD3	1.97	0.46
1:D:243:TYR:OH	3:D:403:HOH:O	2.18	0.46
1:C:205:LEU:O	1:C:209:VAL:HG23	2.15	0.46
1:C:34:HIS:O	1:C:38:VAL:HG23	2.16	0.46
1:A:260:ILE:N	3:A:411:HOH:O	2.46	0.46
1:A:257:GLN:C	3:A:411:HOH:O	2.59	0.46
1:C:104[A]:ASN:HB3	1:D:10:ARG:CB	2.47	0.45
1:D:220:GLU:OE2	1:D:231:LYS:NZ	2.36	0.45
1:B:198:THR:HA	3:B:402:HOH:O	2.16	0.45
1:B:34:HIS:ND1	1:B:200:ASP:OD2	2.44	0.44
1:D:5:LEU:HD22	1:D:5:LEU:H	1.81	0.44
1:C:200:ASP:OD1	1:C:200:ASP:N	2.51	0.44
1:A:165:VAL:HG22	1:A:169:GLN:HB2	2.00	0.44
1:D:198:THR:HG21	1:D:253:TYR:HD1	1.82	0.43
1:D:183:LYS:HE3	1:D:205:LEU:HD11	2.00	0.43
1:C:124:CYS:HB2	1:C:194:THR:OG1	2.19	0.43
1:C:137:PHE:HE1	1:D:223:CYS:SG	2.42	0.43
1:A:10:ARG:CB	1:D:104:ASN:HB3	2.46	0.43
1:C:104[A]:ASN:ND2	1:C:105:PRO:HD3	2.34	0.42
1:D:28:ARG:HD3	1:D:67:TRP:CZ2	2.53	0.42
1:D:29:LYS:HA	1:D:32:VAL:HG22	2.01	0.42
1:B:192:ILE:HG12	1:B:193:ILE:N	2.35	0.42
1:B:1:MET:HE3	1:B:1:MET:HB2	1.98	0.42
1:B:104:ASN:HB3	1:B:105:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:LYS:HE2	1:D:275:LEU:O	2.20	0.42
1:D:42:TRP:HB3	1:D:47:TYR:HB2	2.00	0.42
1:D:248:GLU:HG3	1:D:251:TRP:H	1.85	0.42
1:B:29:LYS:HE2	1:B:276:ASP:HA	2.01	0.41
1:A:192:ILE:HD11	1:A:206:LEU:HA	2.02	0.41
1:B:5:LEU:HD23	1:B:5:LEU:HA	1.86	0.41
1:B:219:VAL:O	1:B:223:CYS:HB2	2.20	0.41
1:C:67:TRP:CZ3	1:C:85:CYS:HB2	2.56	0.41
1:B:120:ILE:HD13	1:B:195:VAL:HG21	2.02	0.41
1:A:56:SER:HA	1:A:67:TRP:O	2.20	0.41
1:C:257:GLN:N	1:C:258:PRO:HD2	2.36	0.41
1:B:264:ILE:HG23	1:B:271:ILE:HD11	2.03	0.41
1:D:200:ASP:OD1	1:D:200:ASP:N	2.54	0.41
1:D:270:VAL:HG22	1:D:273:ARG:NH2	2.35	0.41
1:C:29:LYS:NZ	1:C:276:ASP:OD1	2.39	0.40
1:A:151:LEU:HD21	1:A:205:LEU:HD22	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:447:HOH:O	3:C:453:HOH:O[8_445]	2.13	0.07

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	279/283 (99%)	271 (97%)	8 (3%)	0	100	100
1	B	281/283 (99%)	274 (98%)	7 (2%)	0	100	100
1	C	278/283 (98%)	271 (98%)	7 (2%)	0	100	100
1	D	282/283 (100%)	271 (96%)	10 (4%)	1 (0%)	30	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1120/1132 (99%)	1087 (97%)	32 (3%)	1 (0%)	48 70

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	4	GLN

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	229/232 (99%)	222 (97%)	7 (3%)	35 63
1	B	231/232 (100%)	220 (95%)	11 (5%)	23 47
1	C	229/232 (99%)	218 (95%)	11 (5%)	23 47
1	D	233/232 (100%)	224 (96%)	9 (4%)	28 55
All	All	922/928 (99%)	884 (96%)	38 (4%)	27 54

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	51	ILE
1	A	54	HIS
1	A	97	ASN
1	A	119	ASN
1	A	192	ILE
1	A	195	VAL
1	B	54	HIS
1	B	55	VAL
1	B	89	SER
1	B	119	ASN
1	B	139	LYS
1	B	164	ILE
1	B	181	LYS

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Mol	Chain	Res	Type
1	B	192	ILE
1	B	195	VAL
1	B	223	CYS
1	B	237	GLU
1	C	54	HIS
1	C	139	LYS
1	C	155	LEU
1	C	195	VAL
1	C	200	ASP
1	C	206	LEU
1	C	223	CYS
1	C	237	GLU
1	C	261	GLN
1	C	265	GLU
1	C	277	ASP
1	D	5	LEU
1	D	48	THR
1	D	54	HIS
1	D	119	ASN
1	D	165	VAL
1	D	192	ILE
1	D	195	VAL
1	D	216	GLN
1	D	265	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	241	ASN
1	B	146	GLN
1	B	173	GLN
1	B	189	ASN
1	C	41	ASN
1	C	189	ASN
1	D	104	ASN
1	D	241	ASN
1	D	257	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 [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	281/283 (99%)	0.61	18 (6%)	25 20	5, 15, 35, 80	0
1	B	283/283 (100%)	0.70	24 (8%)	16 13	5, 13, 35, 99	0
1	C	279/283 (98%)	0.83	34 (12%)	8 6	7, 14, 38, 141	1 (0%)
1	D	283/283 (100%)	0.93	34 (12%)	9 7	5, 19, 42, 66	1 (0%)
All	All	1126/1132 (99%)	0.77	110 (9%)	13 10	5, 15, 38, 141	2 (0%)

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	282	THR	8.8
1	C	139	LYS	7.3
1	B	166	THR	6.3
1	B	161	TYR	6.2
1	B	165	VAL	6.1
1	B	162	ALA	5.9
1	A	138	GLY	5.7
1	A	139	LYS	5.6
1	D	282	THR	5.5
1	C	140	PRO	5.5
1	B	163	GLY	5.4
1	D	161	TYR	5.4
1	D	162	ALA	5.4
1	B	139	LYS	5.3
1	C	138	GLY	5.3
1	D	104	ASN	5.1
1	D	139[A]	LYS	4.9
1	C	104[A]	ASN	4.9
1	A	7	SER	4.8
1	D	163	GLY	4.8
1	D	166	THR	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	166	THR	4.5
1	B	167	ALA	4.5
1	D	6	SER	4.3
1	C	165	VAL	4.2
1	C	225	GLY	4.2
1	D	167	ALA	4.1
1	C	278	VAL	4.1
1	D	283	PRO	4.0
1	C	276	ASP	3.8
1	D	165	VAL	3.8
1	C	277	ASP	3.7
1	D	89	SER	3.7
1	A	12	PRO	3.7
1	B	164	ILE	3.6
1	D	108	TYR	3.5
1	A	140	PRO	3.4
1	B	282	THR	3.3
1	C	105	PRO	3.3
1	B	138	GLY	3.3
1	C	12	PRO	3.2
1	D	227	PRO	3.2
1	D	4	GLN	3.2
1	B	170	GLU	3.2
1	D	91	GLY	3.2
1	B	120	ILE	3.1
1	C	7	SER	3.1
1	C	5	LEU	3.0
1	C	103	ASN	3.0
1	C	108	TYR	2.9
1	D	22	PRO	2.9
1	D	105	PRO	2.9
1	D	164	ILE	2.9
1	D	235	PRO	2.8
1	C	162	ALA	2.8
1	D	176	LYS	2.8
1	C	163	GLY	2.8
1	D	7	SER	2.8
1	D	88	ILE	2.7
1	C	160	GLU	2.7
1	D	92	GLU	2.7
1	A	167	ALA	2.7
1	C	283	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	281	ASP	2.7
1	A	8	LEU	2.6
1	A	168	GLU	2.6
1	A	237	GLU	2.6
1	C	171	GLY	2.6
1	B	179	GLY	2.5
1	C	173	GLN	2.5
1	C	161	TYR	2.5
1	A	169	GLN	2.5
1	C	279	LYS	2.5
1	A	161	TYR	2.5
1	A	163	GLY	2.5
1	B	180	PRO	2.5
1	C	227	PRO	2.5
1	B	160	GLU	2.5
1	D	107	PHE	2.4
1	B	177	ALA	2.4
1	D	84	LEU	2.4
1	D	138	GLY	2.4
1	C	91	GLY	2.4
1	B	119	ASN	2.3
1	A	6	SER	2.3
1	D	159	THR	2.3
1	D	90	ASP	2.3
1	C	169	GLN	2.3
1	A	22	PRO	2.3
1	C	280	ILE	2.3
1	C	166	THR	2.2
1	B	237	GLU	2.2
1	B	90	ASP	2.2
1	C	8	LEU	2.2
1	A	236	HIS	2.2
1	B	176	LYS	2.2
1	D	228	ASN	2.2
1	B	91	GLY	2.1
1	D	160	GLU	2.1
1	D	10	ARG	2.1
1	B	181	LYS	2.1
1	B	173	GLN	2.1
1	A	223	CYS	2.1
1	C	157	VAL	2.1
1	C	6	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	108	TYR	2.0
1	D	94	VAL	2.0
1	C	159	THR	2.0
1	D	119	ASN	2.0
1	A	243	TYR	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](#)

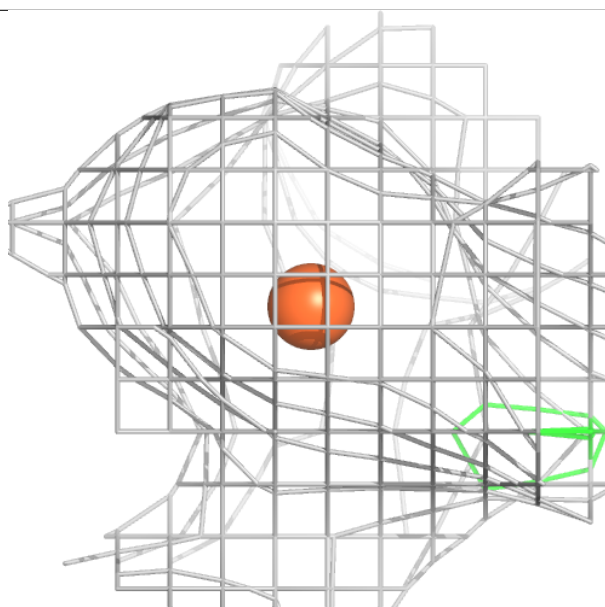
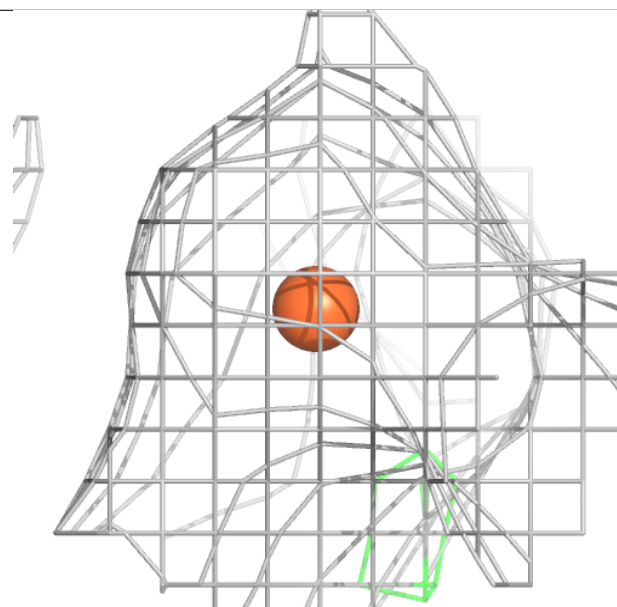
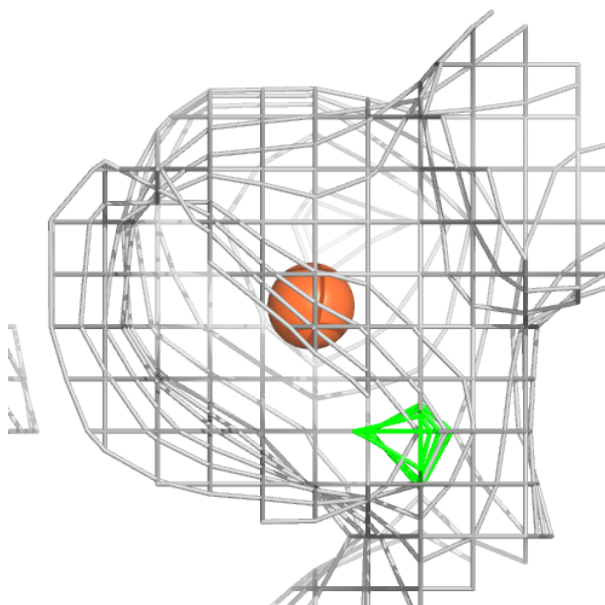
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FE	A	301	1/1	0.81	0.11	56,56,56,56	0
2	FE	B	301	1/1	0.82	0.08	50,50,50,50	0
2	FE	C	301	1/1	0.92	0.07	43,43,43,43	0
2	FE	D	301	1/1	0.97	0.03	27,27,27,27	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.

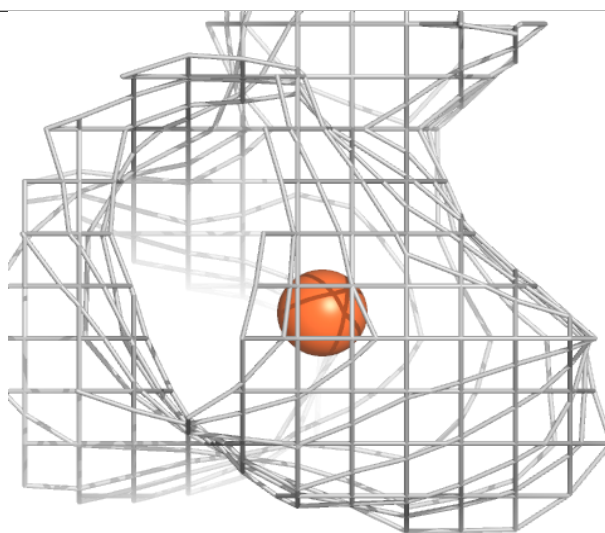
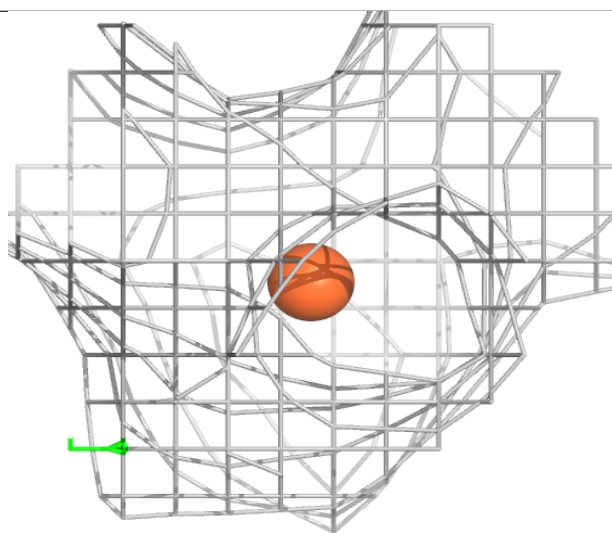
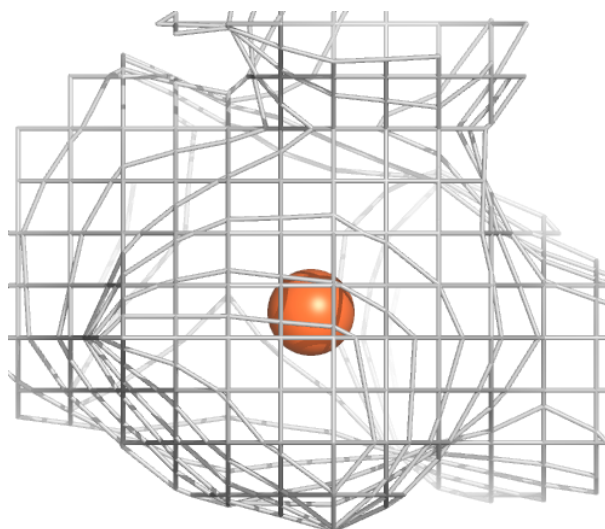
Electron density around FE A 301:

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



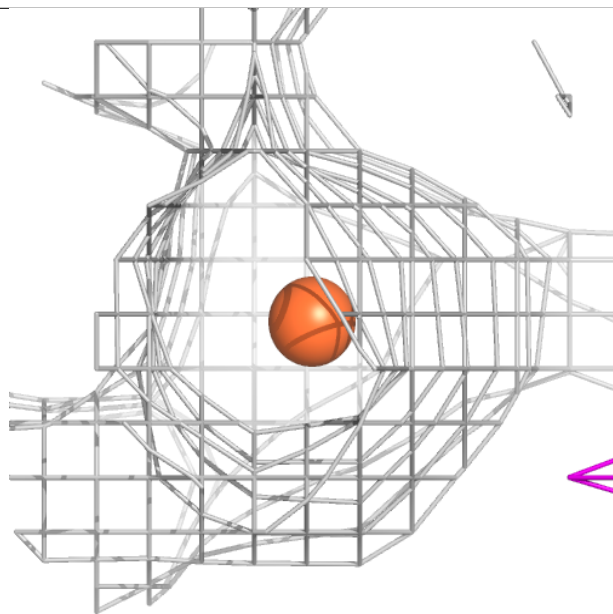
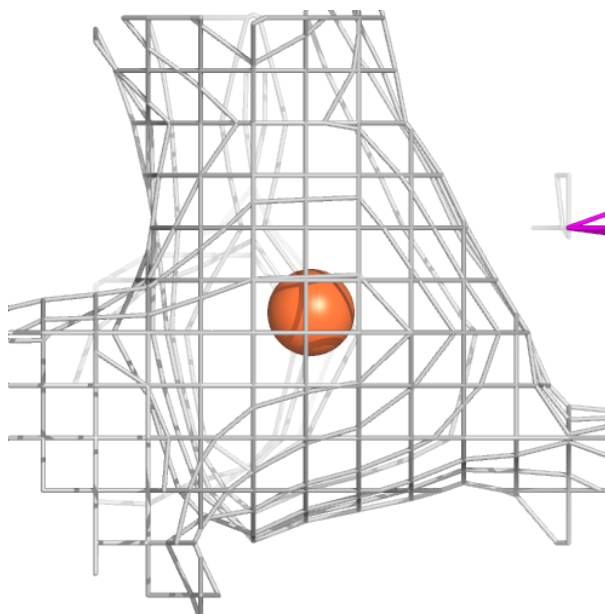
Electron density around FE B 301:

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



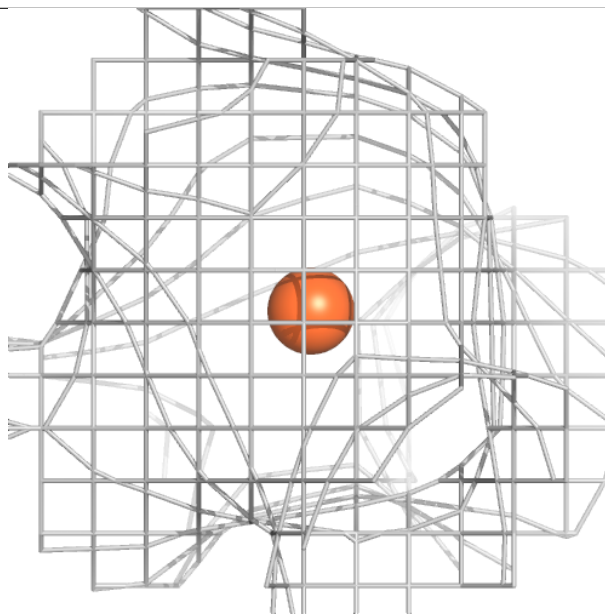
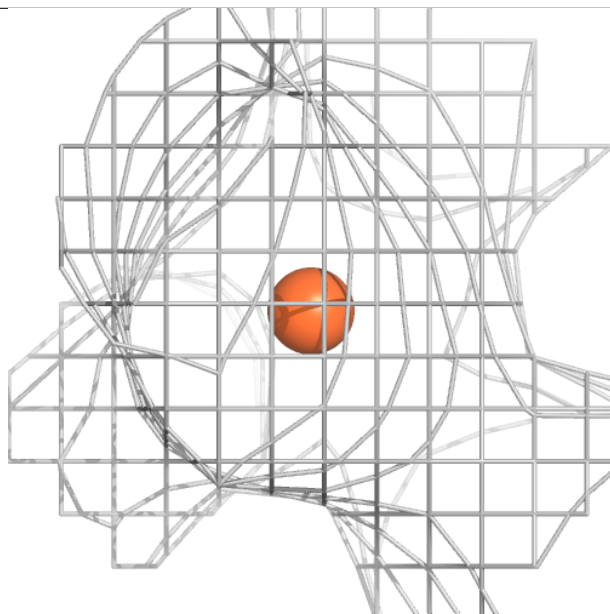
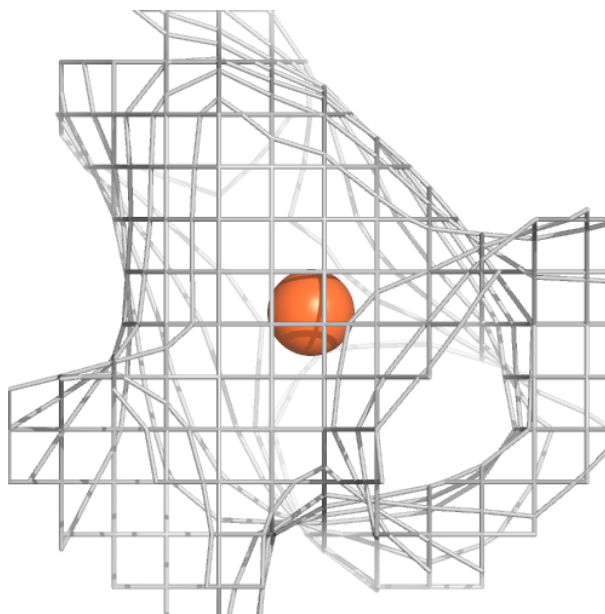
Electron density around FE C 301:

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



Electron density around FE D 301:

$2mF_o-DF_c$ (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.