



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 2, 2025 – 04:31 PM JST

PDB ID : 9M2A / pdb\_00009m2a  
Title : The crystal structure of the trypanosome alternative oxidase complexed with a trypanocidal phosphonium derivative (compound1)  
Authors : Ebiloma, G.U.; Balogun, E.O.; Dardonville, C.; De Koning, H.P.; Shiba, T.  
Deposited on : 2025-02-27  
Resolution : 3.01 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

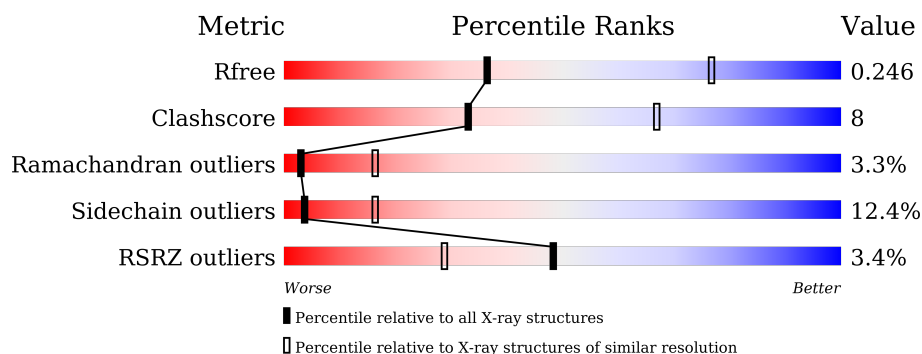
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.01 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	2927 (3.04-3.00)
Clashscore	180529	3300 (3.04-3.00)
Ramachandran outliers	177936	3188 (3.04-3.00)
Sidechain outliers	177891	3191 (3.04-3.00)
RSRZ outliers	164620	2939 (3.04-3.00)

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  $\geq 3$ , 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	272	<div> <div>2%</div> <div> <div></div> <div>65%</div> <div>29%</div> <div>• •</div> </div> </div>
1	B	272	<div> <div>4%</div> <div> <div></div> <div>70%</div> <div>25%</div> <div>• •</div> </div> </div>
1	C	272	<div> <div>5%</div> <div> <div></div> <div>71%</div> <div>24%</div> <div>•</div> </div> </div>
1	D	272	<div> <div>3%</div> <div> <div></div> <div>68%</div> <div>27%</div> <div>• •</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8805 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 Alternative oxidase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			2175	1393	387	385	10			
1	B	268	Total	C	N	O	S	0	0	0
			2175	1393	387	385	10			
1	C	271	Total	C	N	O	S	0	0	0
			2198	1406	390	392	10			
1	D	271	Total	C	N	O	S	0	0	0
			2201	1408	390	392	11			

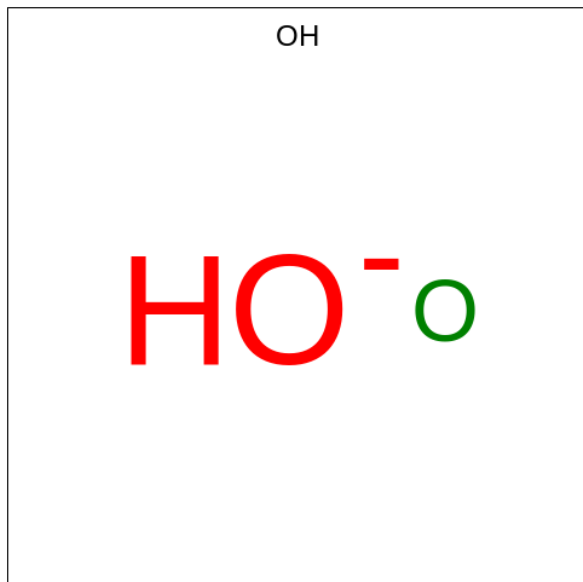
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	ALA	-	expression tag	UNP Q26710
A	31	ALA	-	expression tag	UNP Q26710
B	30	ALA	-	expression tag	UNP Q26710
B	31	ALA	-	expression tag	UNP Q26710
C	30	ALA	-	expression tag	UNP Q26710
C	31	ALA	-	expression tag	UNP Q26710
D	30	ALA	-	expression tag	UNP Q26710
D	31	ALA	-	expression tag	UNP Q26710

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

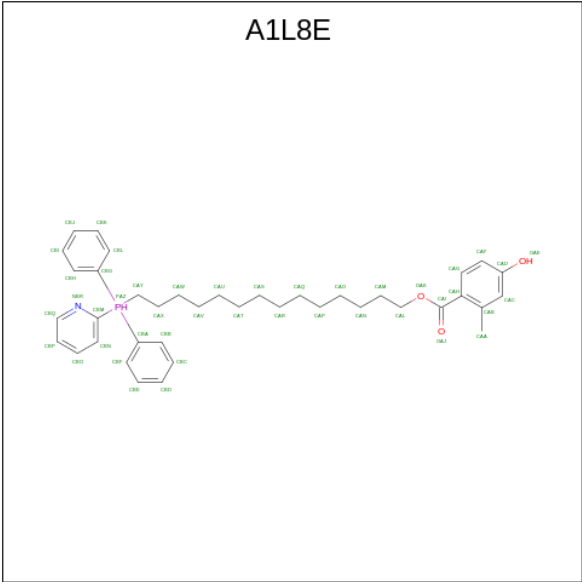
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Fe	0	0
			2	2		
2	B	2	Total	Fe	0	0
			2	2		
2	C	2	Total	Fe	0	0
			2	2		
2	D	2	Total	Fe	0	0
			2	2		

- Molecule 3 is HYDROXIDE ION (CCD ID: OH) (formula: HO) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O	0	0
			1	1		
3	B	1	Total	O	0	0
			1	1		
3	C	1	Total	O	0	0
			1	1		
3	D	1	Total	O	0	0
			1	1		

- Molecule 4 is 14-[diphenyl(pyridin-2-yl)- $\lambda^5$ -phosphanyl]tetradecyl 2-methyl-4-oxidan-yl-benzoate (CCD ID: A1L8E) (formula: C<sub>39</sub>H<sub>50</sub>NO<sub>3</sub>P) (labeled as "Ligand of Interest" by depositor).

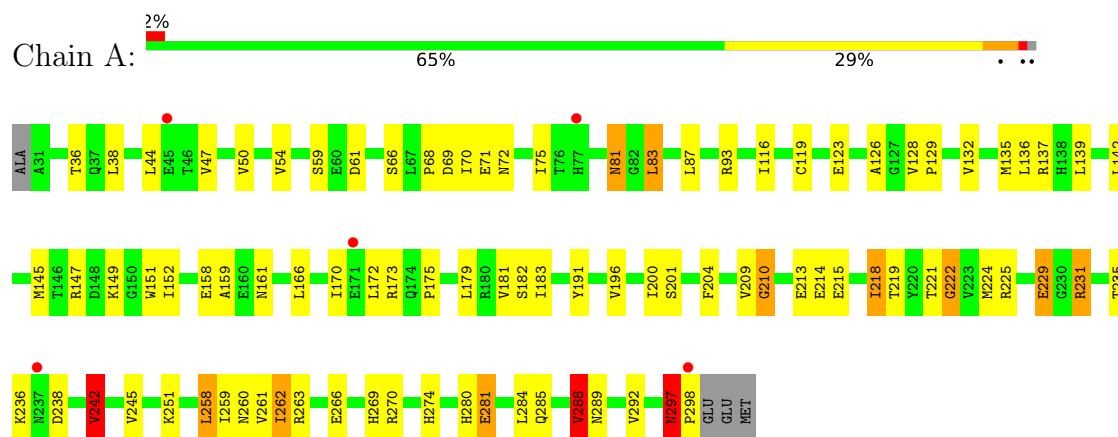


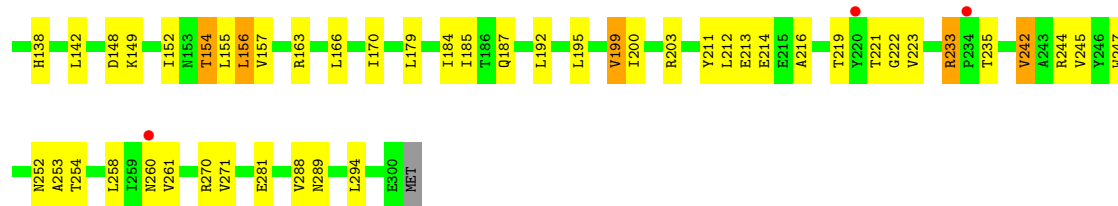
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			44	39	1	3	1		

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

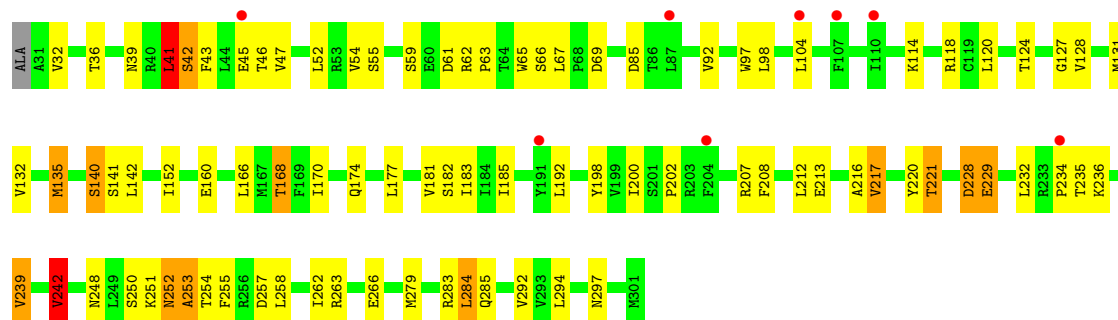
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Alternative oxidase, mitochondrial





● Molecule 1: Alternative oxidase, mitochondrial



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	151.37Å 221.73Å 62.85Å 90.00° 114.50° 90.00°	Depositor
Resolution (Å)	44.96 – 3.01 44.96 – 3.01	Depositor EDS
% Data completeness (in resolution range)	81.8 (44.96-3.01) 81.8 (44.96-3.01)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.16 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, $R_{free}$	0.195 , 0.254 0.193 , 0.246	Depositor DCC
$R_{free}$ test set	1495 reflections (4.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	70.7	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 57.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.166 for -h-2*k,l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	8805	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.82% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE, A1L8E, OH

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	0.74	0/2225	1.06	2/3023 (0.1%)
1	B	0.75	0/2225	1.09	4/3023 (0.1%)
1	C	0.71	0/2248	1.05	2/3054 (0.1%)
1	D	0.70	0/2251	1.08	4/3057 (0.1%)
All	All	0.72	0/8949	1.07	12/12157 (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	B	0	2
1	D	0	1
All	All	0	3

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	252	ASN	N-CA-C	7.14	118.71	111.07
1	D	228	ASP	N-CA-C	-6.26	101.41	110.24
1	D	217	VAL	N-CA-C	-6.15	104.34	110.30
1	D	41	LEU	N-CA-C	-5.91	103.62	111.24
1	C	132	VAL	N-CA-CB	5.62	117.77	110.57
1	C	242	VAL	CB-CA-C	-5.58	104.61	112.14
1	A	288	VAL	N-CA-CB	5.46	117.74	110.26
1	A	200	ILE	N-CA-C	5.25	115.39	110.30
1	B	296	LYS	N-CA-C	5.17	119.59	113.12
1	B	260	ASN	N-CA-C	5.16	116.99	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	228	ASP	N-CA-C	-5.08	102.39	109.96
1	B	37	GLN	N-CA-C	-5.07	104.70	111.24

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	237	ASN	Peptide
1	B	40	ARG	Peptide
1	D	235	THR	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2175	0	2206	47	0
1	B	2175	0	2206	31	0
1	C	2198	0	2223	37	0
1	D	2201	0	2227	40	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	44	0	0	0	0
All	All	8805	0	8862	136	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 8.

All (136) 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:221:THR:HG22	1:B:263:ARG:HE	1.36	0.88
1:A:135:MET:HE2	1:B:135:MET:HE2	1.61	0.82
1:A:183:ILE:HD13	1:B:145:MET:HE1	1.72	0.71
1:B:217:VAL:O	1:B:221:THR:HG23	1.94	0.67
1:B:161:ASN:ND2	1:B:246:TYR:OH	2.25	0.64
1:C:154:THR:OG1	1:C:289:ASN:ND2	2.33	0.62
1:D:55:SER:O	1:D:62:ARG:NH2	2.35	0.59
1:A:81:ASN:N	1:A:81:ASN:HD22	2.00	0.59
1:A:221:THR:O	1:A:224:MET:N	2.38	0.57
1:A:149:LYS:HB3	1:A:288:VAL:HA	1.86	0.57
1:A:218:ILE:O	1:A:219:THR:C	2.47	0.57
1:A:69:ASP:OD1	1:B:35:HIS:ND1	2.38	0.56
1:A:262:ILE:O	1:A:266:GLU:HG2	2.05	0.56
1:A:183:ILE:HD13	1:B:145:MET:CE	2.35	0.56
1:B:112:GLU:O	1:B:116:ILE:HD12	2.04	0.56
1:D:221:THR:HG22	1:D:263:ARG:HE	1.70	0.56
1:D:59:SER:N	1:D:160:GLU:OE2	2.39	0.56
1:A:38:LEU:HD11	1:B:65:TRP:CZ3	2.41	0.55
1:C:38:LEU:HD11	1:D:65:TRP:CH2	2.42	0.55
1:A:224:MET:SD	1:A:263:ARG:NH2	2.80	0.54
1:A:137:ARG:NE	1:A:151:TRP:HB2	2.24	0.53
1:C:124:THR:HA	1:D:142:LEU:HD22	1.91	0.53
1:B:85:ASP:HA	1:B:207:ARG:HG2	1.91	0.53
1:D:221:THR:HG22	1:D:263:ARG:NE	2.24	0.53
1:D:207:ARG:O	1:D:208:PHE:C	2.53	0.52
1:A:229:GLU:OE2	1:A:231:ARG:CZ	2.58	0.52
1:B:228:ASP:O	1:B:229:GLU:CB	2.59	0.51
1:B:168:THR:CG2	1:B:243:ALA:HB2	2.41	0.50
1:B:228:ASP:O	1:B:229:GLU:HB2	2.12	0.49
1:B:161:ASN:HA	1:B:246:TYR:OH	2.12	0.49
1:A:214:GLU:HG2	1:A:270:ARG:HD2	1.95	0.49
1:D:66:SER:O	1:D:67:LEU:C	2.56	0.48
1:A:123:GLU:HA	1:A:126:ALA:HB3	1.95	0.48
1:A:137:ARG:HE	1:A:151:TRP:HB2	1.79	0.48
1:B:151:TRP:CD1	1:B:289:ASN:HB2	2.48	0.48
1:A:54:VAL:HG13	1:A:245:VAL:HG21	1.96	0.48
1:A:93:ARG:NH2	1:A:215:GLU:OE2	2.47	0.47
1:A:181:VAL:O	1:A:182:SER:C	2.57	0.47
1:D:228:ASP:O	1:D:229:GLU:HG3	2.14	0.47
1:D:239:VAL:HG21	1:D:253:ALA:HB3	1.96	0.47
1:C:152:ILE:HG22	1:C:156:LEU:HD22	1.97	0.47
1:C:213:GLU:O	1:C:216:ALA:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:140:SER:O	1:D:141:SER:C	2.58	0.47
1:C:138:HIS:HA	1:C:152:ILE:HD11	1.96	0.46
1:A:72:ASN:ND2	1:D:41:LEU:HD21	2.31	0.46
1:A:128:VAL:O	1:A:129:PRO:C	2.58	0.46
1:D:198:TYR:CE1	1:D:202:PRO:HB3	2.50	0.46
1:C:31:ALA:HA	1:C:32:VAL:HB	1.96	0.46
1:D:42:SER:OG	1:D:43:PHE:N	2.49	0.46
1:B:89:TYR:O	1:B:93:ARG:HG2	2.16	0.46
1:A:258:LEU:O	1:A:261:VAL:HG22	2.16	0.46
1:A:213:GLU:OE2	1:A:269:HIS:HB2	2.14	0.46
1:B:198:TYR:O	1:B:199:VAL:C	2.57	0.46
1:C:57:GLU:OE2	1:C:163:ARG:NH2	2.45	0.45
1:A:54:VAL:CG2	1:A:242:VAL:HG13	2.46	0.45
1:A:289:ASN:O	1:A:292:VAL:HG22	2.17	0.45
1:C:92:VAL:HG21	1:C:211:TYR:HB2	1.96	0.45
1:C:103:SER:O	1:C:104:LEU:HD22	2.17	0.45
1:B:47:VAL:N	1:B:48:PRO:CD	2.80	0.45
1:D:258:LEU:CD2	1:D:262:ILE:HD11	2.46	0.45
1:A:209:VAL:O	1:A:210:GLY:C	2.60	0.44
1:A:142:LEU:HD23	1:B:166:LEU:HD12	1.98	0.44
1:B:168:THR:HG23	1:B:243:ALA:HB2	1.98	0.44
1:D:120:LEU:HD12	1:D:166:LEU:HD23	1.99	0.44
1:A:145:MET:HG2	1:B:166:LEU:HD21	1.98	0.44
1:C:72:ASN:O	1:D:39:ASN:ND2	2.42	0.44
1:A:75:ILE:HB	1:C:75:ILE:HB	1.99	0.44
1:C:76:THR:OG1	1:C:270:ARG:CZ	2.66	0.44
1:C:184:ILE:O	1:C:187:GLN:N	2.51	0.44
1:B:280:HIS:CD2	1:B:285:GLN:HG3	2.53	0.44
1:C:35:HIS:ND1	1:D:69:ASP:OD1	2.51	0.44
1:A:172:LEU:HD22	1:A:236:LYS:CB	2.48	0.44
1:A:213:GLU:HG3	1:A:269:HIS:HB2	2.00	0.44
1:C:75:ILE:HD12	1:C:75:ILE:N	2.33	0.43
1:A:119:CYS:O	1:A:123:GLU:HG2	2.18	0.43
1:C:123:GLU:OE2	1:C:123:GLU:HA	2.18	0.43
1:C:135:MET:HE2	1:D:135:MET:HE2	2.00	0.43
1:C:118:ARG:HE	1:C:219:THR:HG21	1.82	0.43
1:A:175:PRO:CB	1:A:179:LEU:HD12	2.49	0.43
1:B:190:MET:O	1:B:191:TYR:C	2.60	0.43
1:A:280:HIS:O	1:A:281:GLU:C	2.61	0.43
1:D:216:ALA:O	1:D:220:TYR:CD2	2.71	0.43
1:D:250:SER:O	1:D:252:ASN:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:254:THR:N	1:D:257:ASP:OD1	2.51	0.43
1:A:139:LEU:HD11	1:B:191:TYR:CE2	2.54	0.43
1:B:140:SER:HA	1:B:143:ARG:HG2	2.01	0.43
1:D:120:LEU:HD12	1:D:166:LEU:CD2	2.49	0.43
1:A:59:SER:O	1:A:61:ASP:N	2.50	0.43
1:D:168:THR:HG21	1:D:258:LEU:HD21	2.01	0.43
1:A:158:GLU:O	1:A:159:ALA:C	2.62	0.43
1:A:201:SER:O	1:A:204:PHE:N	2.51	0.43
1:D:92:VAL:HG13	1:D:212:LEU:HD23	2.01	0.43
1:C:233:ARG:HG2	1:C:235:THR:HG23	2.01	0.42
1:A:258:LEU:O	1:A:259:ILE:C	2.61	0.42
1:D:254:THR:O	1:D:257:ASP:N	2.52	0.42
1:B:282:LYS:O	1:B:283:ARG:C	2.62	0.42
1:C:135:MET:CE	1:D:135:MET:HE2	2.49	0.42
1:C:138:HIS:CE1	1:D:131:MET:HE3	2.55	0.42
1:C:203:ARG:NH1	1:C:281:GLU:OE2	2.52	0.42
1:C:148:ASP:CG	1:C:152:ILE:HD12	2.44	0.42
1:C:105:TYR:CD2	1:C:105:TYR:C	2.97	0.42
1:C:115:VAL:O	1:C:118:ARG:HG2	2.19	0.42
1:A:70:ILE:HD12	1:A:260:ASN:O	2.20	0.42
1:B:138:HIS:NE2	1:B:142:LEU:HD11	2.34	0.42
1:B:213:GLU:OE1	1:B:266:GLU:OE2	2.37	0.42
1:D:124:THR:HG22	1:D:166:LEU:HD11	2.00	0.42
1:D:217:VAL:O	1:D:221:THR:HG23	2.19	0.42
1:A:158:GLU:O	1:A:161:ASN:N	2.53	0.42
1:D:252:ASN:O	1:D:253:ALA:C	2.62	0.41
1:A:137:ARG:NE	1:A:151:TRP:CB	2.83	0.41
1:C:247:TRP:CG	1:C:261:VAL:HG21	2.55	0.41
1:D:213:GLU:OE2	1:D:266:GLU:OE2	2.38	0.41
1:A:116:ILE:HG21	1:A:173:ARG:HB3	2.03	0.41
1:A:181:VAL:O	1:A:183:ILE:N	2.53	0.41
1:B:62:ARG:HB3	1:B:63:PRO:HD2	2.02	0.41
1:C:195:LEU:O	1:C:199:VAL:HG23	2.19	0.41
1:C:222:GLY:O	1:C:223:VAL:C	2.63	0.41
1:D:181:VAL:O	1:D:182:SER:C	2.62	0.41
1:D:54:VAL:HG21	1:D:242:VAL:HA	2.03	0.41
1:A:68:PRO:O	1:A:71:GLU:HB3	2.20	0.41
1:B:65:TRP:NE1	1:B:265:ASP:OD1	2.46	0.41
1:D:174:GLN:N	1:D:174:GLN:OE1	2.53	0.41
1:C:138:HIS:NE2	1:D:127:GLY:O	2.52	0.41
1:A:221:THR:O	1:A:222:GLY:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:GLU:OE1	1:C:213:GLU:HA	2.20	0.40
1:C:214:GLU:HG2	1:C:270:ARG:HD2	2.02	0.40
1:D:234:PRO:CB	1:D:255:PHE:HB3	2.52	0.40
1:B:85:ASP:CG	1:B:207:ARG:HE	2.30	0.40
1:C:75:ILE:HD11	1:C:221:THR:HG21	2.03	0.40
1:C:142:LEU:HD13	1:D:124:THR:O	2.22	0.40
1:D:239:VAL:O	1:D:239:VAL:CG1	2.69	0.40
1:D:279:MET:O	1:D:284:LEU:N	2.54	0.40
1:A:297:ASN:HD22	1:A:298:PRO:HD3	1.86	0.40
1:C:43:PHE:O	1:C:44:LEU:C	2.63	0.40
1:C:70:ILE:HD12	1:C:260:ASN:O	2.22	0.40
1:C:149:LYS:HB3	1:C:288:VAL:HA	2.02	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	266/272 (98%)	217 (82%)	40 (15%)	9 (3%)	3	16
1	B	266/272 (98%)	234 (88%)	24 (9%)	8 (3%)	3	18
1	C	269/272 (99%)	223 (83%)	39 (14%)	7 (3%)	4	21
1	D	269/272 (99%)	225 (84%)	33 (12%)	11 (4%)	2	12
All	All	1070/1088 (98%)	899 (84%)	136 (13%)	35 (3%)	3	16

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	229	GLU
1	A	242	VAL
1	B	104	LEU

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Mol	Chain	Res	Type
1	B	229	GLU
1	C	60	GLU
1	C	103	SER
1	C	252	ASN
1	D	229	GLU
1	D	242	VAL
1	D	251	LYS
1	A	83	LEU
1	B	45	GLU
1	B	126	ALA
1	C	32	VAL
1	C	45	GLU
1	D	200	ILE
1	D	253	ALA
1	B	230	GLY
1	B	231	ARG
1	D	135	MET
1	D	283	ARG
1	A	152	ILE
1	A	222	GLY
1	B	283	ARG
1	D	183	ILE
1	A	191	TYR
1	A	218	ILE
1	C	253	ALA
1	D	128	VAL
1	A	210	GLY
1	D	152	ILE
1	C	200	ILE
1	A	297	ASN
1	B	32	VAL
1	D	63	PRO

### 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	242/245 (99%)	214 (88%)	28 (12%)	4	18
1	B	242/245 (99%)	212 (88%)	30 (12%)	4	16
1	C	244/245 (100%)	214 (88%)	30 (12%)	4	16
1	D	245/245 (100%)	212 (86%)	33 (14%)	3	13
All	All	973/980 (99%)	852 (88%)	121 (12%)	4	16

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	THR
1	A	44	LEU
1	A	47	VAL
1	A	50	VAL
1	A	66	SER
1	A	81	ASN
1	A	83	LEU
1	A	87	LEU
1	A	132	VAL
1	A	136	LEU
1	A	147	ARG
1	A	166	LEU
1	A	170	ILE
1	A	196	VAL
1	A	225	ARG
1	A	231	ARG
1	A	235	THR
1	A	238	ASP
1	A	242	VAL
1	A	251	LYS
1	A	258	LEU
1	A	262	ILE
1	A	274	HIS
1	A	281	GLU
1	A	284	LEU
1	A	285	GLN
1	A	288	VAL
1	A	297	ASN
1	B	44	LEU
1	B	46	THR
1	B	47	VAL
1	B	52	LEU
1	B	54	VAL

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Mol	Chain	Res	Type
1	B	60	GLU
1	B	66	SER
1	B	69	ASP
1	B	81	ASN
1	B	83	LEU
1	B	86	THR
1	B	87	LEU
1	B	96	ARG
1	B	98	LEU
1	B	104	LEU
1	B	132	VAL
1	B	145	MET
1	B	154	THR
1	B	156	LEU
1	B	166	LEU
1	B	168	THR
1	B	171	GLU
1	B	174	GLN
1	B	179	LEU
1	B	185	ILE
1	B	212	LEU
1	B	245	VAL
1	B	258	LEU
1	B	284	LEU
1	B	292	VAL
1	C	32	VAL
1	C	47	VAL
1	C	49	VAL
1	C	55	SER
1	C	81	ASN
1	C	104	LEU
1	C	105	TYR
1	C	111	THR
1	C	116	ILE
1	C	118	ARG
1	C	132	VAL
1	C	154	THR
1	C	155	LEU
1	C	156	LEU
1	C	157	VAL
1	C	166	LEU
1	C	170	ILE

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Mol	Chain	Res	Type
1	C	179	LEU
1	C	185	ILE
1	C	192	LEU
1	C	199	VAL
1	C	212	LEU
1	C	233	ARG
1	C	242	VAL
1	C	244	ARG
1	C	245	VAL
1	C	254	THR
1	C	258	LEU
1	C	271	VAL
1	C	294	LEU
1	D	32	VAL
1	D	36	THR
1	D	41	LEU
1	D	42	SER
1	D	45	GLU
1	D	46	THR
1	D	47	VAL
1	D	52	LEU
1	D	61	ASP
1	D	85	ASP
1	D	97	TRP
1	D	98	LEU
1	D	104	LEU
1	D	114	LYS
1	D	118	ARG
1	D	132	VAL
1	D	140	SER
1	D	168	THR
1	D	170	ILE
1	D	177	LEU
1	D	185	ILE
1	D	192	LEU
1	D	221	THR
1	D	232	LEU
1	D	236	LYS
1	D	239	VAL
1	D	242	VAL
1	D	248	ASN
1	D	284	LEU

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Mol	Chain	Res	Type
1	D	285	GLN
1	D	292	VAL
1	D	294	LEU
1	D	297	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	81	ASN
1	A	153	ASN
1	A	187	GLN
1	A	260	ASN
1	A	274	HIS
1	A	297	ASN
1	B	81	ASN
1	B	153	ASN
1	B	174	GLN
1	B	206	HIS
1	B	248	ASN
1	B	273	ASN
1	B	280	HIS
1	B	297	ASN
1	C	248	ASN
1	C	260	ASN
1	C	289	ASN
1	D	72	ASN
1	D	81	ASN
1	D	187	GLN
1	D	248	ASN
1	D	260	ASN

### 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 [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 8 are monoatomic and 4 are modelled with single atom - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	A1L8E	A	504	-	47,47,47	1.85	8 (17%)	59,60,60	1.95	8 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	A1L8E	A	504	-	-	13/41/41/41	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	504	A1L8E	CAA-CAB	-5.85	1.39	1.51
4	A	504	A1L8E	PAZ-CBA	5.60	1.89	1.79
4	A	504	A1L8E	PAZ-CAY	4.82	1.90	1.80
4	A	504	A1L8E	CAH-CAI	-4.59	1.40	1.50
4	A	504	A1L8E	PAZ-CBG	3.43	1.85	1.79
4	A	504	A1L8E	PAZ-CBM	3.18	1.84	1.81
4	A	504	A1L8E	CBQ-NBR	2.35	1.39	1.34
4	A	504	A1L8E	OAK-CAI	2.18	1.39	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	504	A1L8E	CAY-PAZ-CBA	-7.39	94.09	109.59
4	A	504	A1L8E	CAY-PAZ-CBG	-6.68	95.57	109.59
4	A	504	A1L8E	CBM-PAZ-CBG	5.44	122.99	109.18
4	A	504	A1L8E	CBM-PAZ-CBA	3.91	119.10	109.18
4	A	504	A1L8E	CBG-PAZ-CBA	3.83	116.48	109.26
4	A	504	A1L8E	PAZ-CAY-CAX	-3.39	105.61	114.43
4	A	504	A1L8E	CAC-CAB-CAH	3.30	120.54	118.03
4	A	504	A1L8E	CBN-CBM-NBR	-2.22	117.92	122.09

There are no chirality outliers.

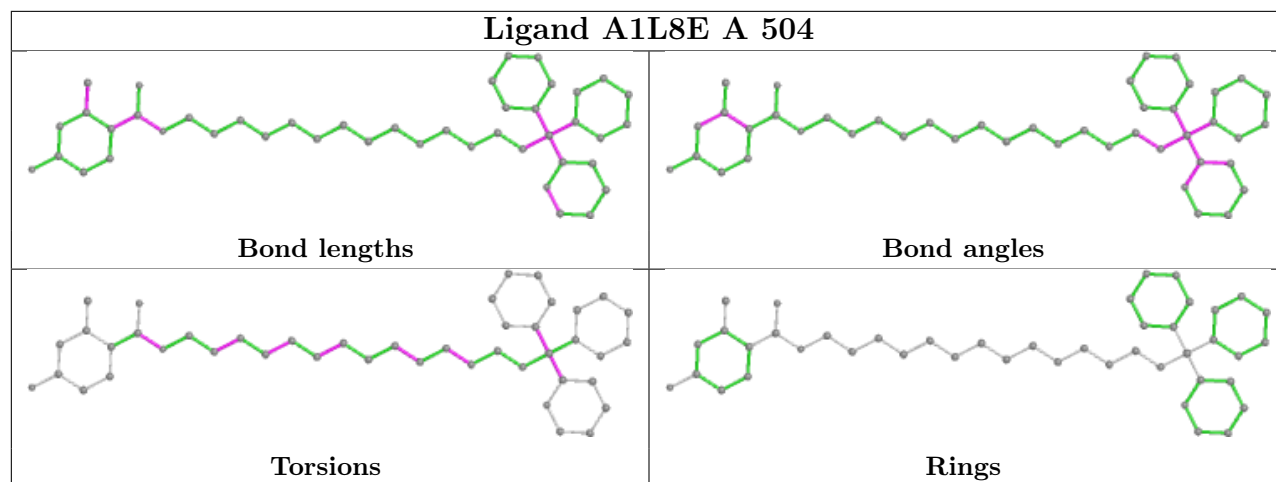
All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	504	A1L8E	NBR-CBM-PAZ-CBG
4	A	504	A1L8E	CBN-CBM-PAZ-CAY
4	A	504	A1L8E	CAH-CAI-OAK-CAL
4	A	504	A1L8E	OAJ-CAI-OAK-CAL
4	A	504	A1L8E	CAN-CAO-CAP-CAQ
4	A	504	A1L8E	CAP-CAQ-CAR-CAS
4	A	504	A1L8E	CAU-CAV-CAW-CAX
4	A	504	A1L8E	CBF-CBA-PAZ-CBM
4	A	504	A1L8E	CAS-CAT-CAU-CAV
4	A	504	A1L8E	CBN-CBM-PAZ-CBA
4	A	504	A1L8E	CBN-CBM-PAZ-CBG
4	A	504	A1L8E	CBB-CBA-PAZ-CBM
4	A	504	A1L8E	CAL-CAM-CAN-CAO

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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	268/272 (98%)	0.09	5 (1%) 66 44	34, 56, 86, 128	0
1	B	268/272 (98%)	0.27	10 (3%) 45 27	38, 58, 87, 112	0
1	C	271/272 (99%)	0.40	14 (5%) 34 19	46, 70, 121, 141	0
1	D	271/272 (99%)	0.23	8 (2%) 52 32	47, 72, 117, 166	0
All	All	1078/1088 (99%)	0.25	37 (3%) 48 29	34, 64, 108, 166	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	171	GLU	5.1
1	C	260	ASN	4.4
1	D	110	ILE	4.1
1	C	99	PHE	4.0
1	C	104	LEU	3.9
1	D	191	TYR	3.6
1	C	110	ILE	3.6
1	B	281	GLU	3.5
1	C	66	SER	3.1
1	D	87	LEU	3.1
1	C	119	CYS	3.1
1	D	234	PRO	2.9
1	C	60	GLU	2.8
1	A	45	GLU	2.8
1	D	104	LEU	2.7
1	C	39	ASN	2.7
1	C	220	TYR	2.7
1	B	290	PRO	2.6
1	A	298	PRO	2.5
1	B	104	LEU	2.4
1	C	31	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	237	ASN	2.4
1	D	204	PHE	2.3
1	C	97	TRP	2.3
1	B	174	GLN	2.3
1	B	32	VAL	2.3
1	D	45	GLU	2.3
1	C	114	LYS	2.2
1	C	234	PRO	2.2
1	B	170	ILE	2.1
1	B	45	GLU	2.1
1	B	218	ILE	2.1
1	D	107	PHE	2.1
1	C	30	ALA	2.0
1	B	298	PRO	2.0
1	B	273	ASN	2.0
1	A	77	HIS	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	A1L8E	A	504	44/44	0.83	0.20	63,74,90,93	0
3	OH	C	503	1/1	0.95	0.06	25,25,25,25	0
3	OH	A	503	1/1	0.97	0.05	11,11,11,11	0
2	FE	C	502	1/1	0.98	0.06	49,49,49,49	0
3	OH	B	503	1/1	0.98	0.12	28,28,28,28	0
2	FE	A	502	1/1	0.99	0.03	43,43,43,43	0
2	FE	D	502	1/1	0.99	0.02	39,39,39,39	0

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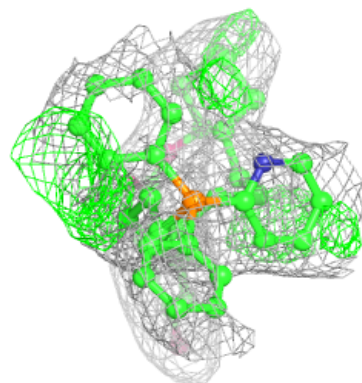
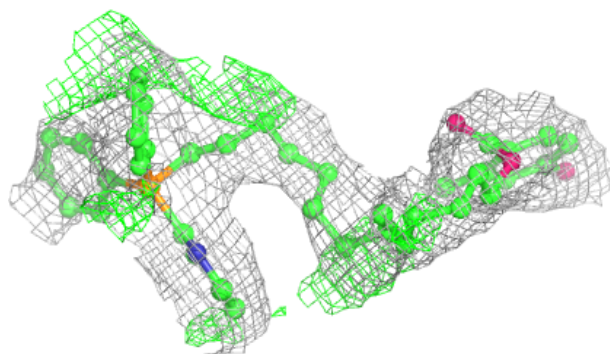
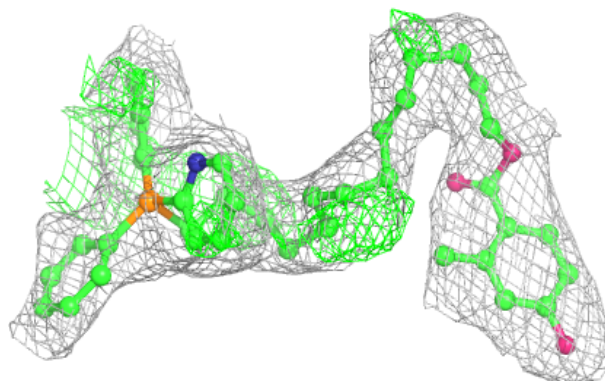
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	OH	D	503	1/1	0.99	0.03	20,20,20,20	0
2	FE	B	502	1/1	0.99	0.05	60,60,60,60	0
2	FE	B	501	1/1	1.00	0.03	45,45,45,45	0
2	FE	D	501	1/1	1.00	0.01	47,47,47,47	0
2	FE	A	501	1/1	1.00	0.01	45,45,45,45	0
2	FE	C	501	1/1	1.00	0.02	51,51,51,51	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.

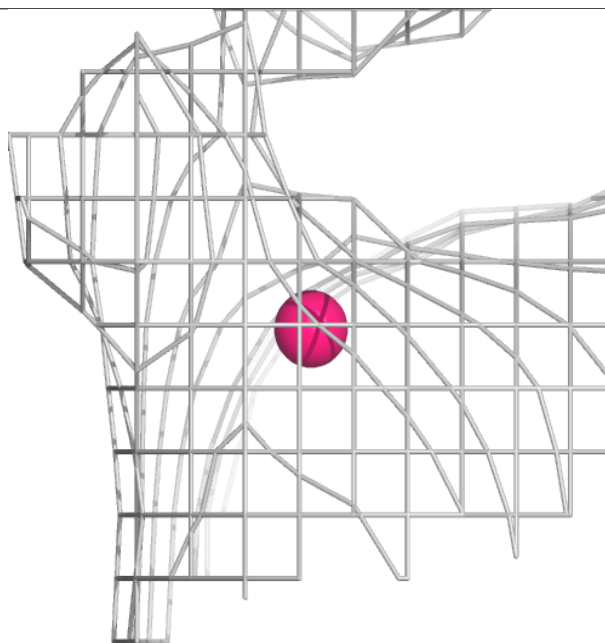
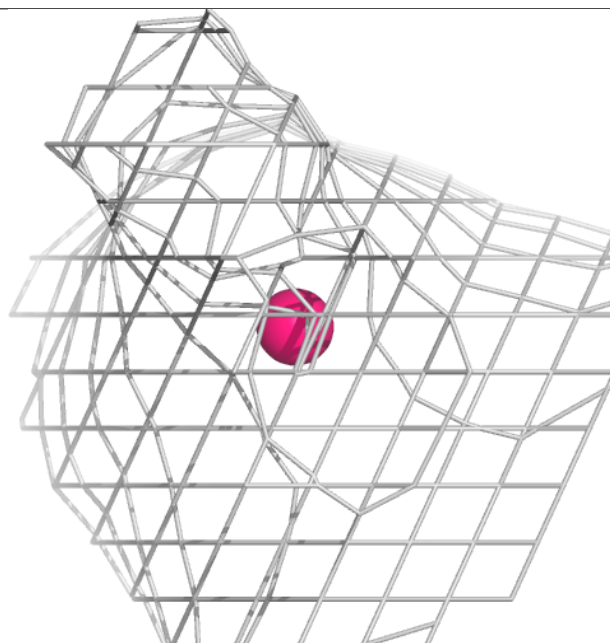
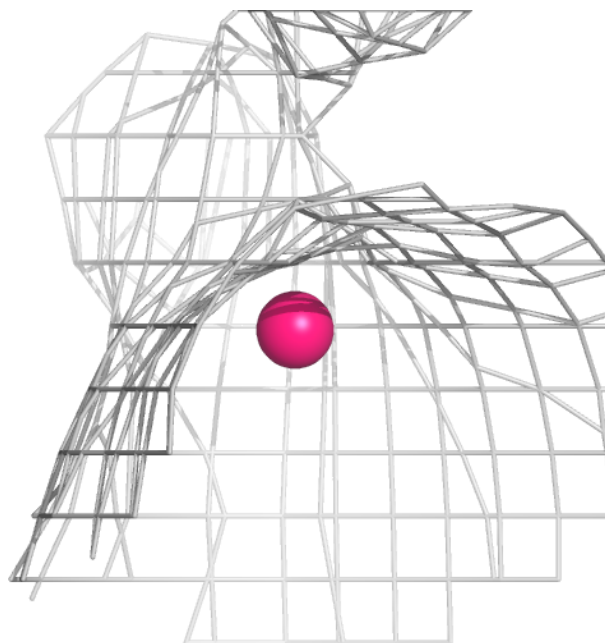
**Electron density around A1L8E A 504:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



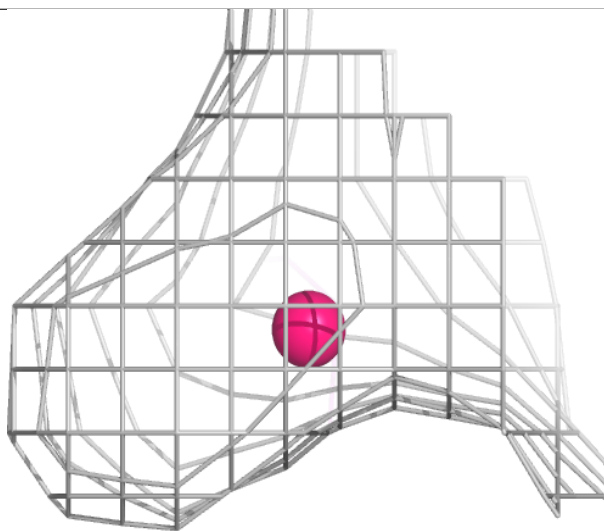
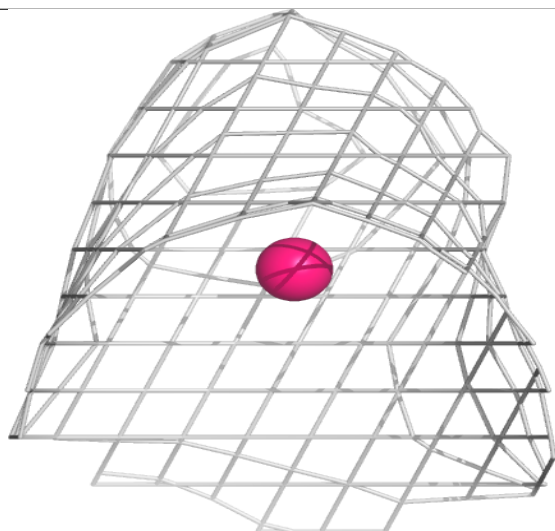
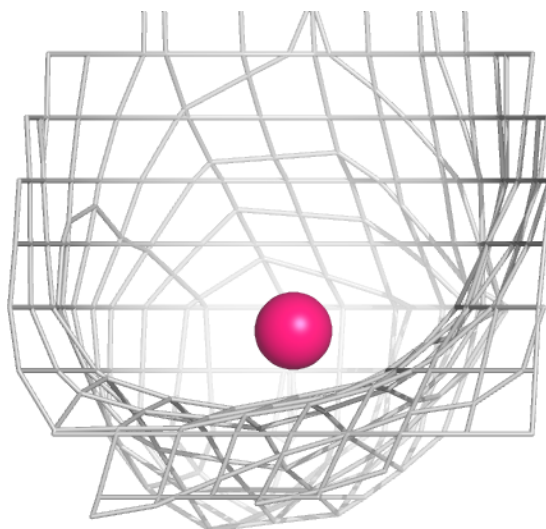
**Electron density around OH C 503:**

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



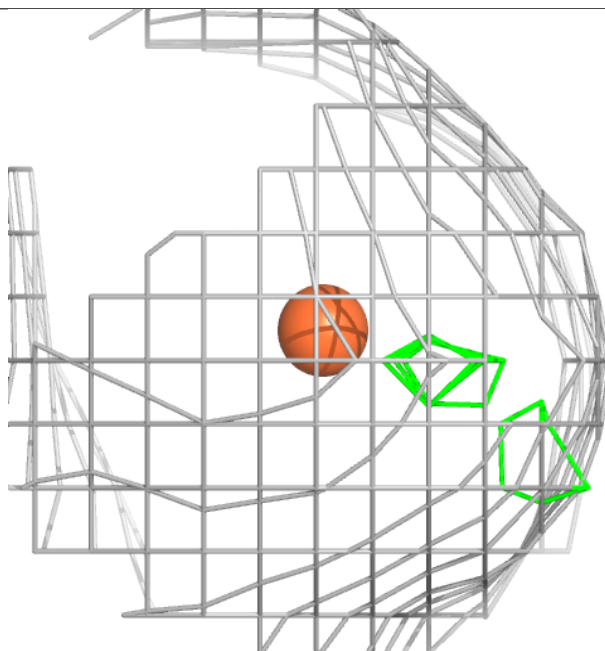
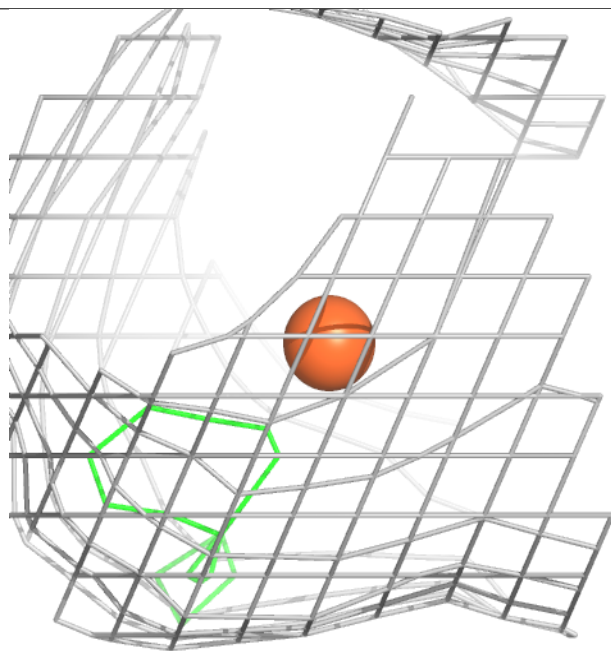
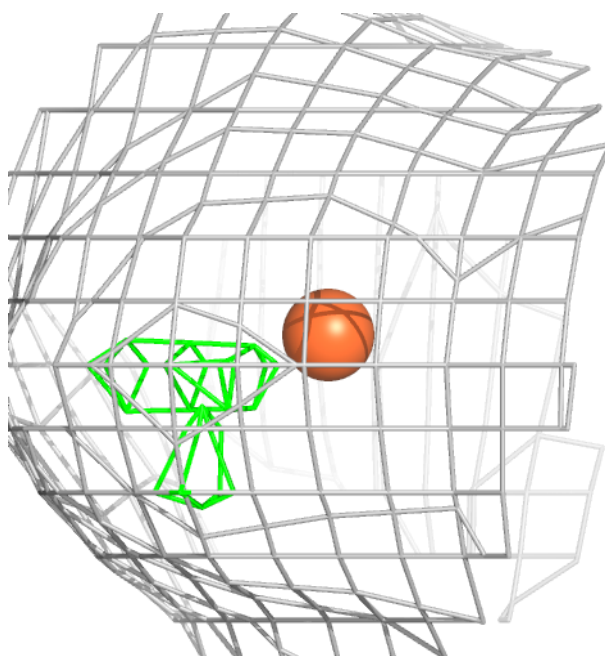
**Electron density around OH A 503:**

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



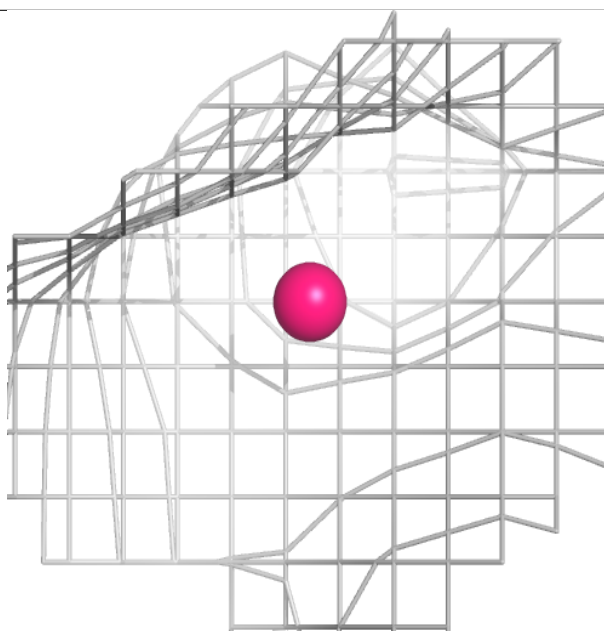
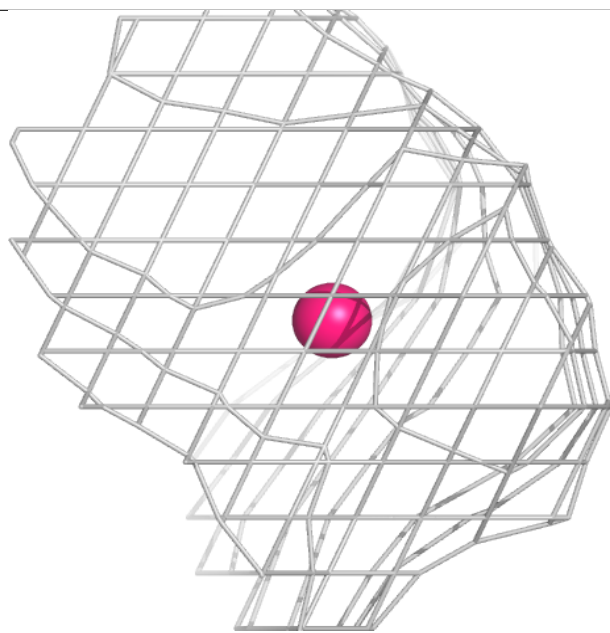
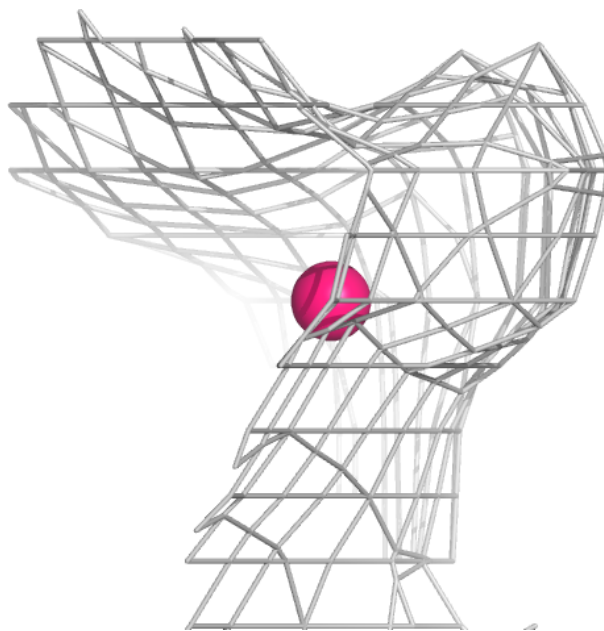
**Electron density around FE C 502:**

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



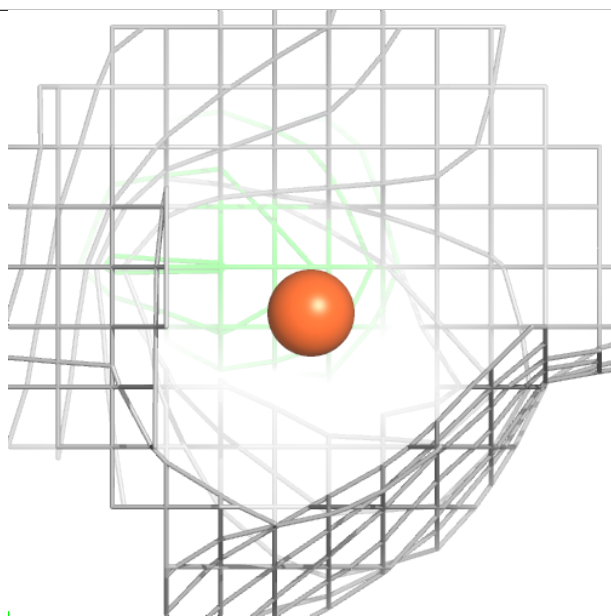
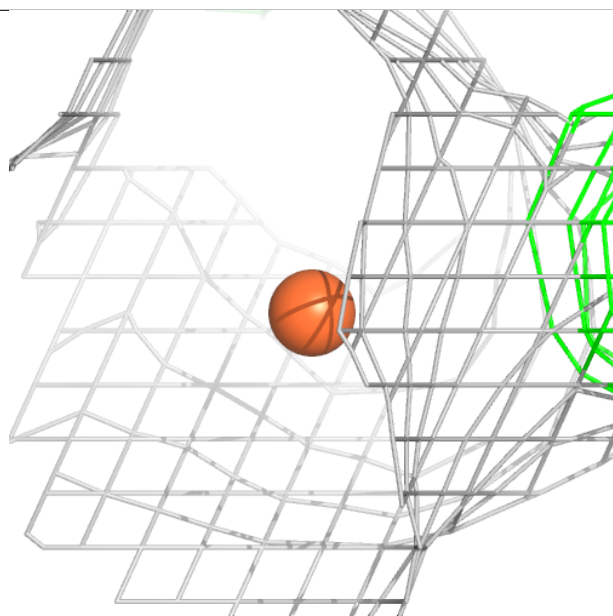
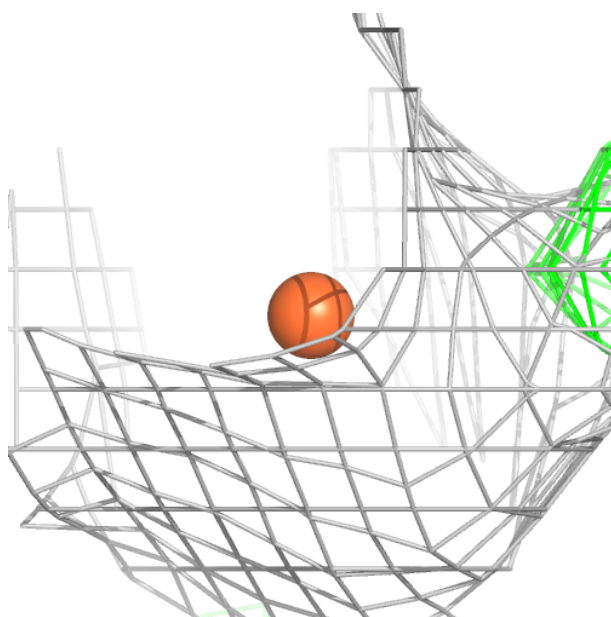
**Electron density around OH B 503:**

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



**Electron density around FE A 502:**

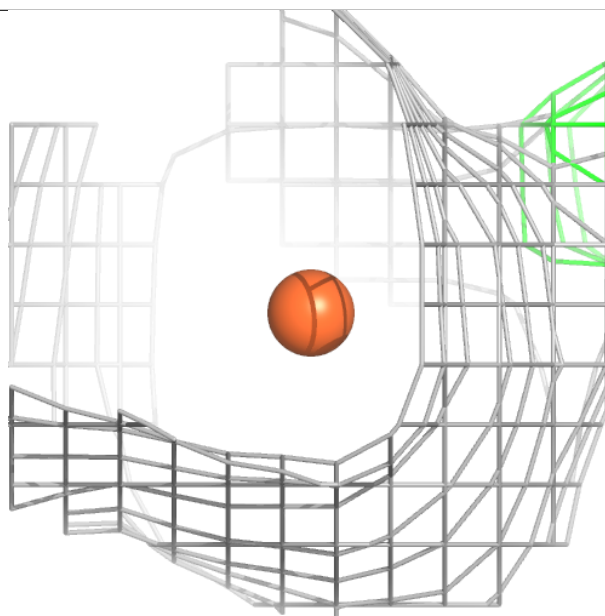
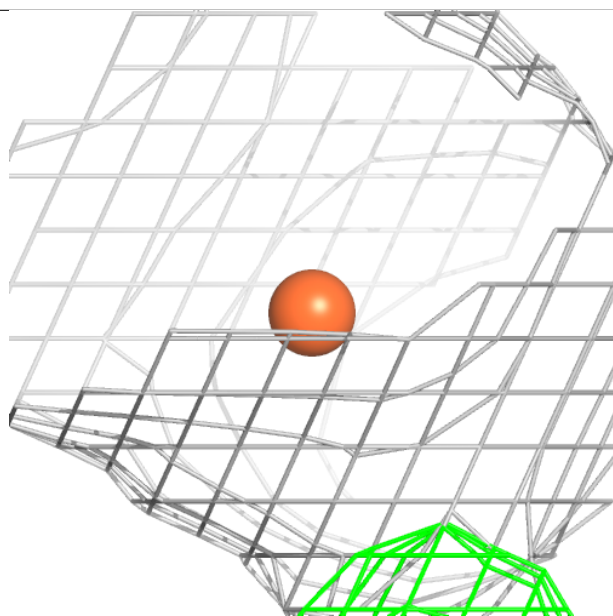
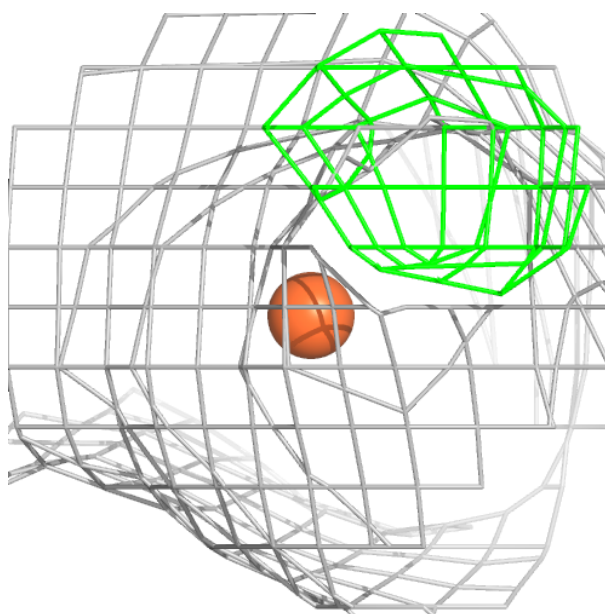
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





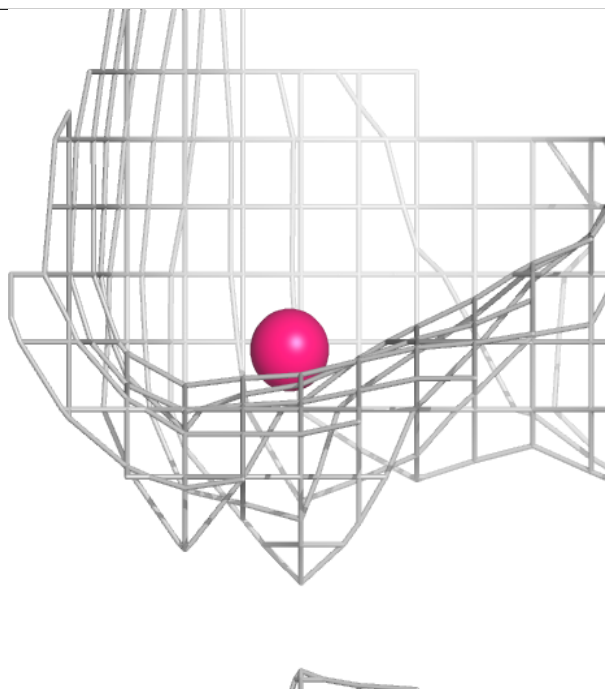
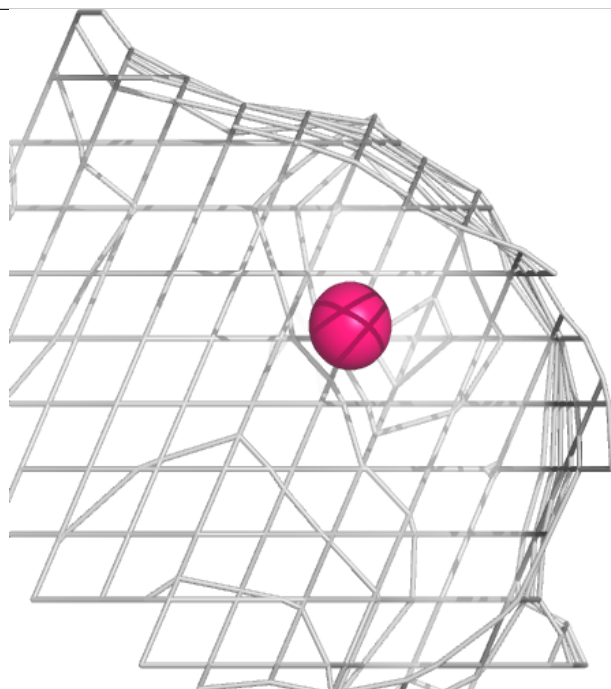
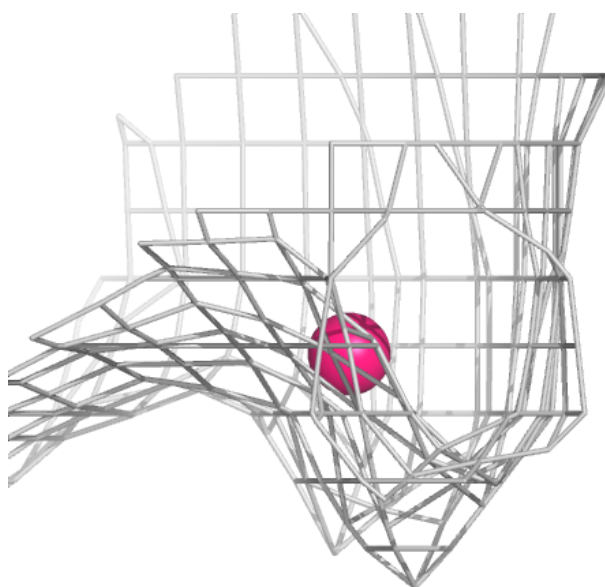
**Electron density around FE D 502:**

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



**Electron density around OH D 503:**

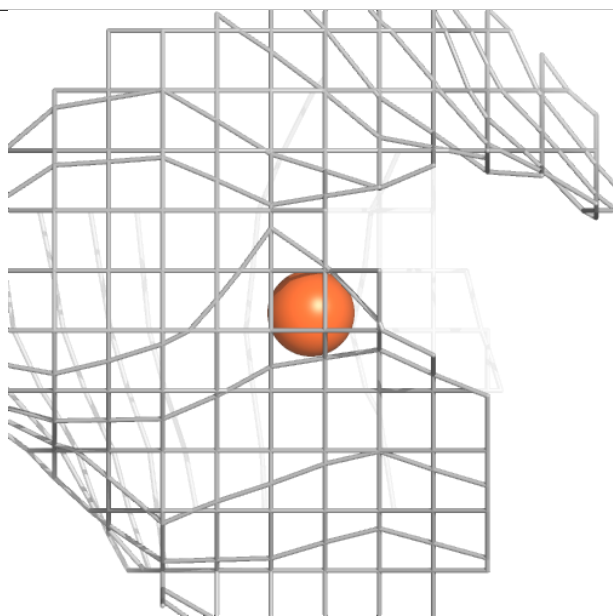
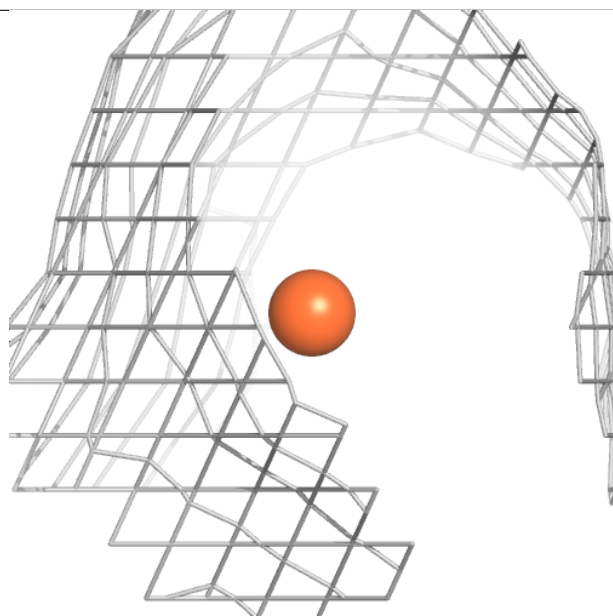
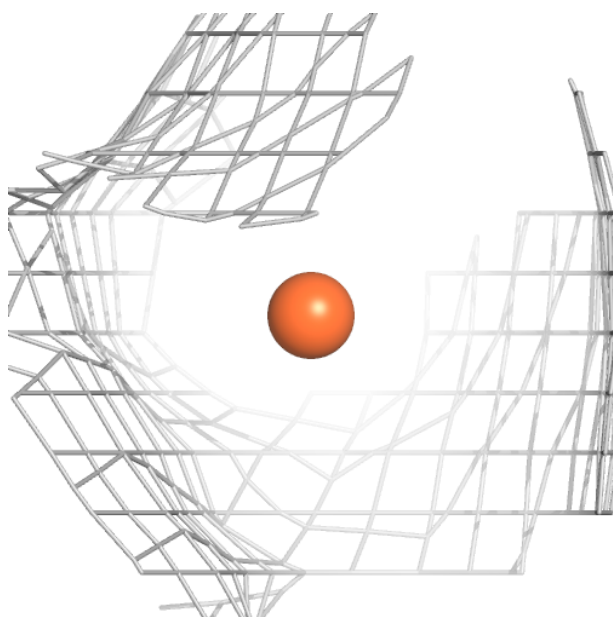
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





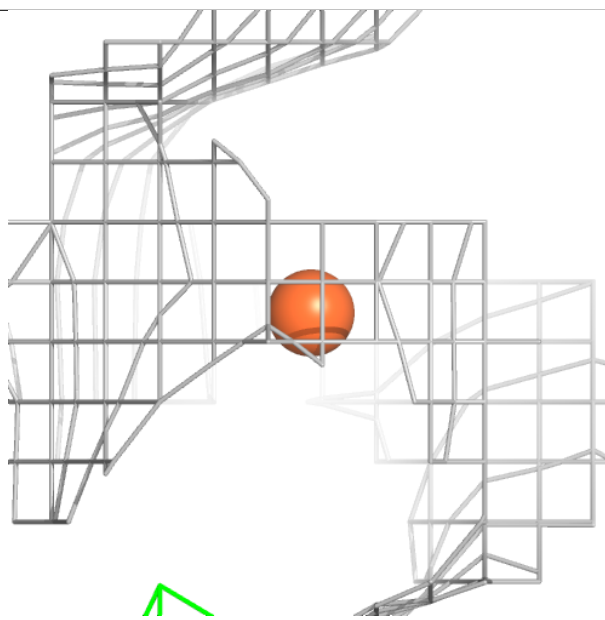
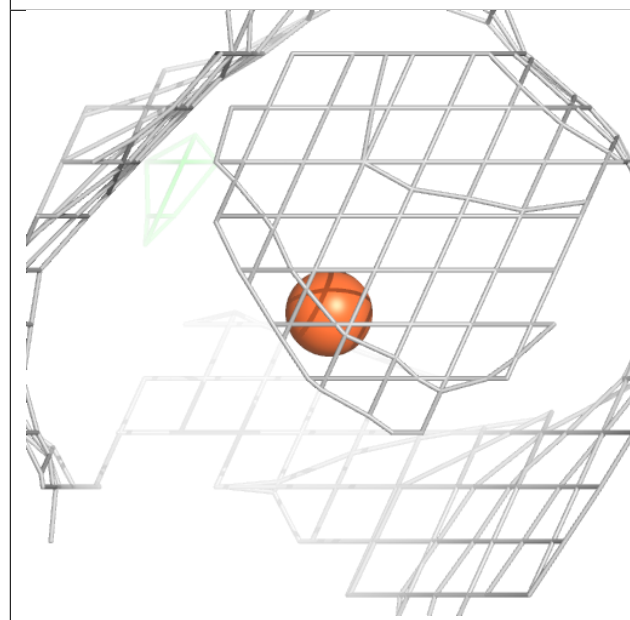
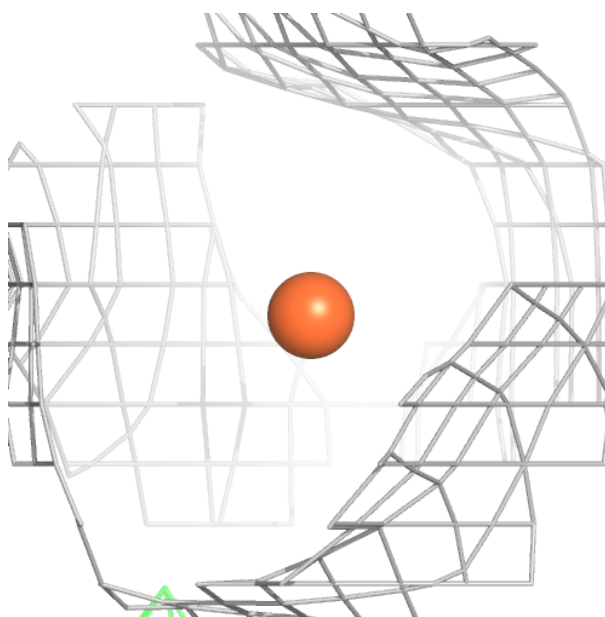
**Electron density around FE B 502:**

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



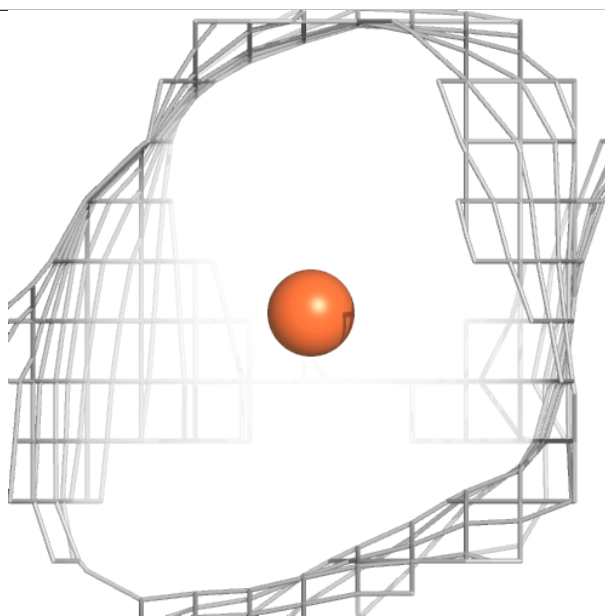
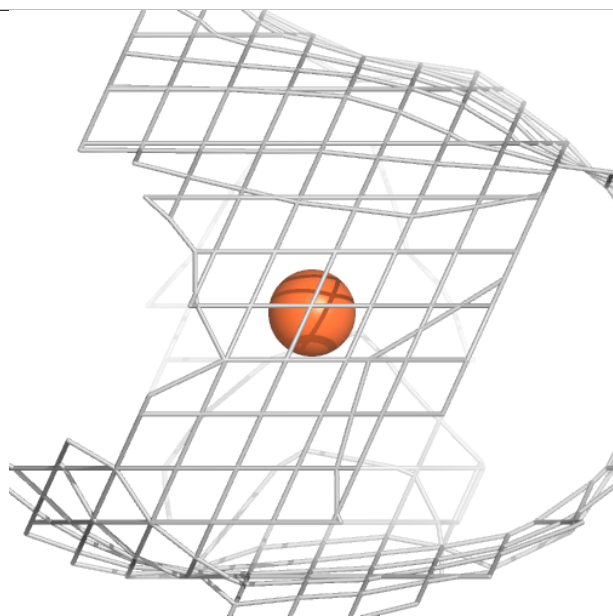
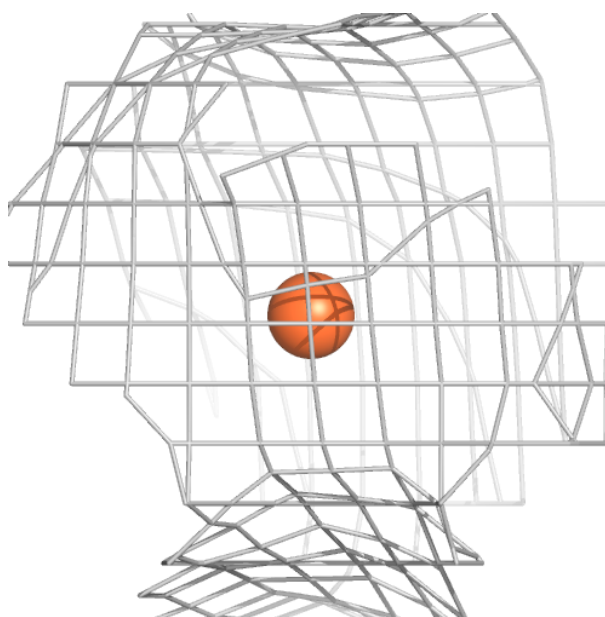
**Electron density around FE B 501:**

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



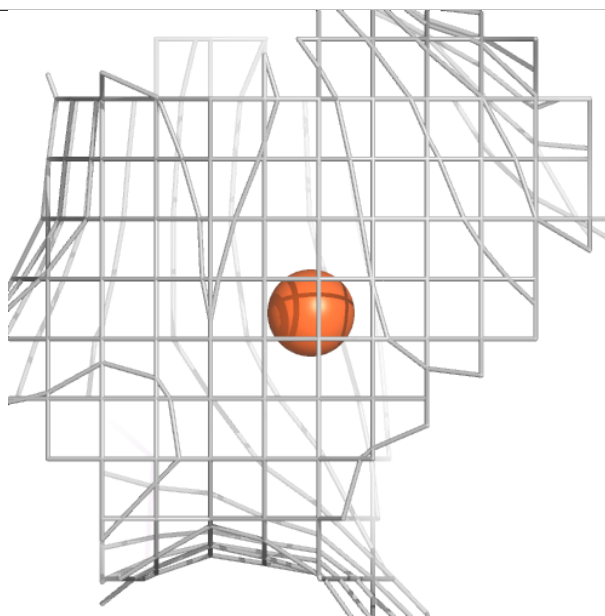
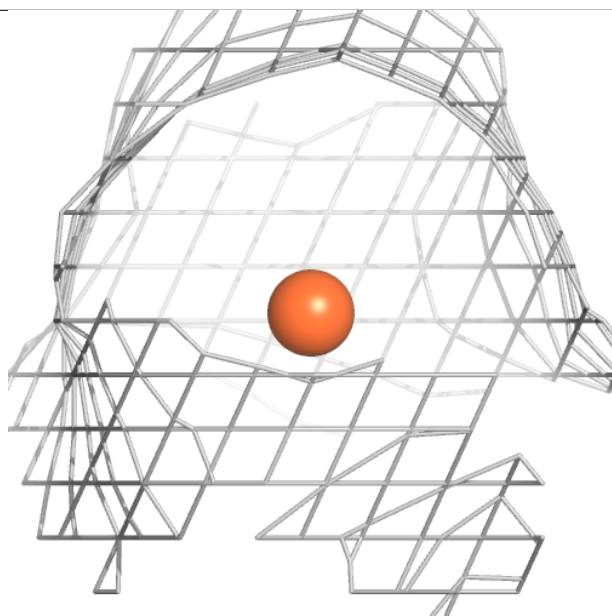
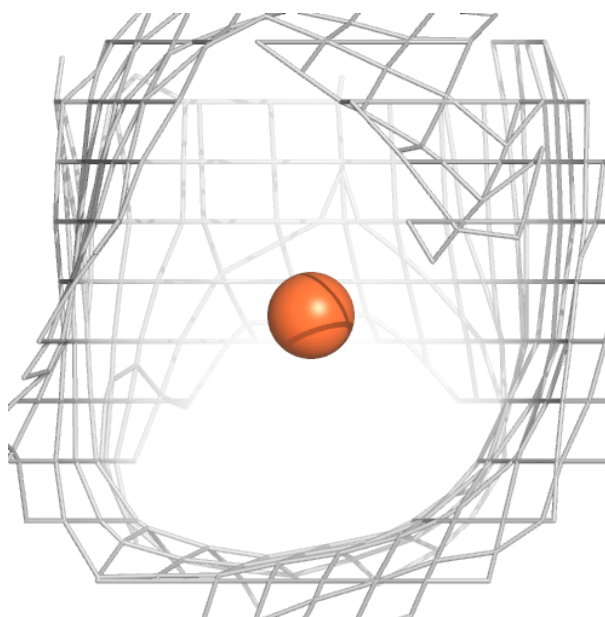
**Electron density around FE D 501:**

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



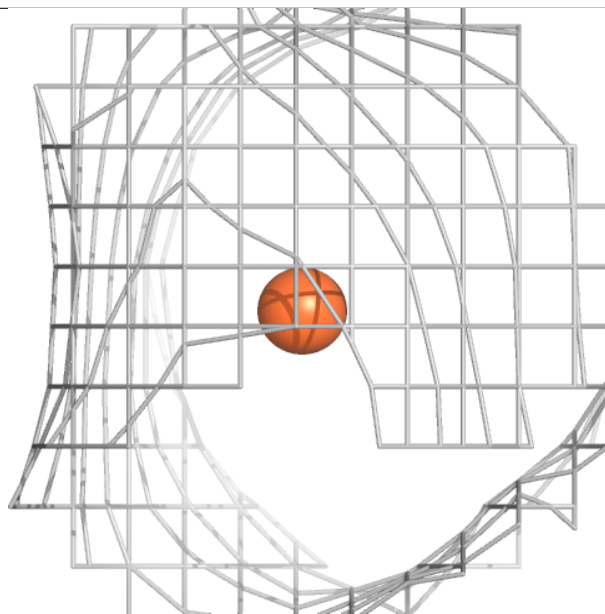
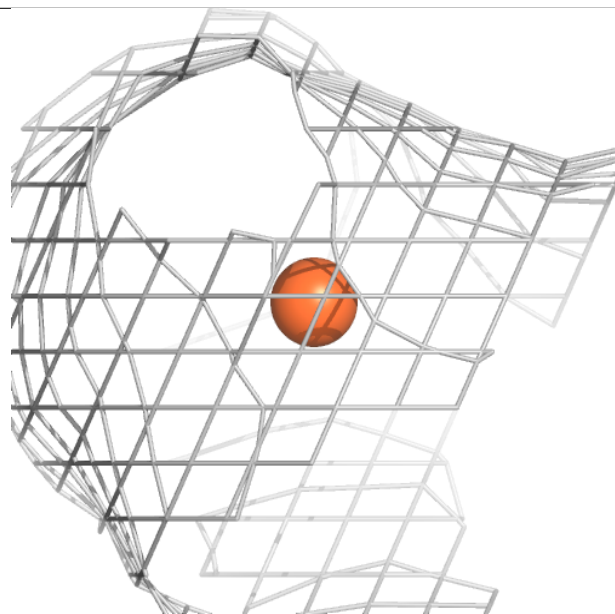
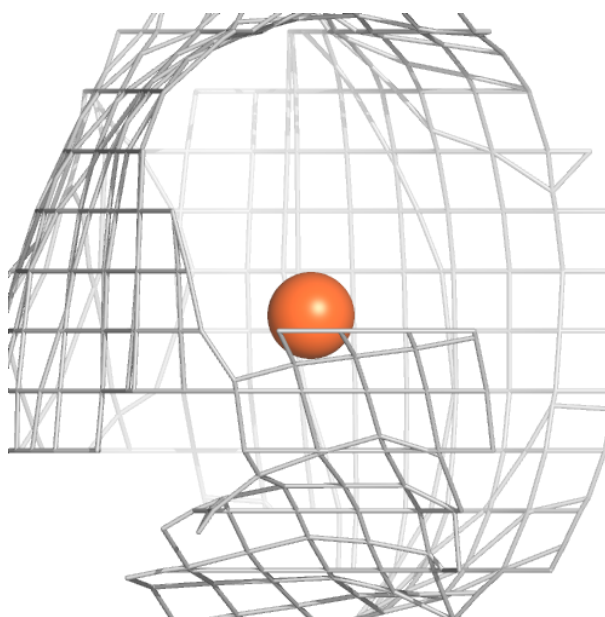
**Electron density around FE A 501:**

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



**Electron density around FE 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.