



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 19, 2020 – 09:33 AM BST

PDB ID : 6VK5
Title : Crystal Structure of Methylosinus trichosporium OB3b Soluble Methane Monooxygenase Hydroxylase and Regulatory Component Complex
Authors : Jones, J.C.; Banerjee, R.; Shi, K.; Aihara, H.; Lipscomb, J.D.
Deposited on : 2020-01-18
Resolution : 1.86 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.6
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.6

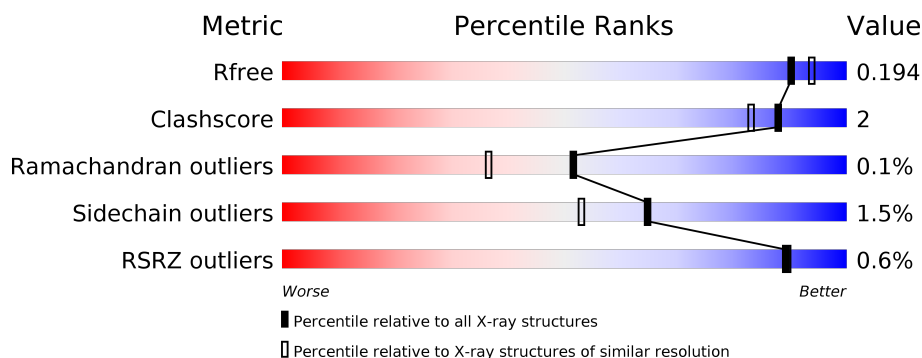
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.86 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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 on 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	526	<div> <div>91%</div> <div>6%</div> </div>
1	E	526	<div> <div>93%</div> <div>...</div> </div>
2	B	395	<div> <div>95%</div> <div>...</div> </div>
2	F	395	<div> <div>94%</div> <div>5%</div> </div>
3	C	169	<div> <div>%</div> <div>96%</div> <div>...</div> </div>
3	G	169	<div> <div>95%</div> <div>...</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	138	<div><div></div><div>2%</div><div>90%</div><div>5%</div><div>• •</div></div>
4	H	138	<div><div></div><div>4%</div><div>91%</div><div>7%</div><div>• •</div></div>

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 40070 atoms, of which 19003 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 Methane monooxygenase component A alpha chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	515	Total	C	H	N	O	S	0	0	0
			8145	2676	3970	723	764	12			
1	E	515	Total	C	H	N	O	S	0	2	0
			8164	2682	3981	724	765	12			

- Molecule 2 is a protein called Methane monooxygenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	392	Total	C	H	N	O	S	0	0	0
			6196	2033	3010	556	592	5			
2	F	392	Total	C	H	N	O	S	0	3	0
			6224	2040	3024	559	596	5			

- Molecule 3 is a protein called Methane monooxygenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	168	Total	C	H	N	O	S	0	0	0
			2762	874	1400	234	253	1			
3	G	168	Total	C	H	N	O	S	0	0	0
			2762	874	1400	234	253	1			

- Molecule 4 is a protein called Methane monooxygenase regulatory protein B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	132	Total	C	H	N	O	S	0	0	0
			1997	639	995	162	198	3			
4	H	137	Total	C	H	N	O	S	0	0	0
			2071	662	1033	167	206	3			

- Molecule 5 is FE (III) ION (three-letter code: FE) (formula: Fe) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Fe	0	0
			2	2		
5	E	2	Total	Fe	0	0
			2	2		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



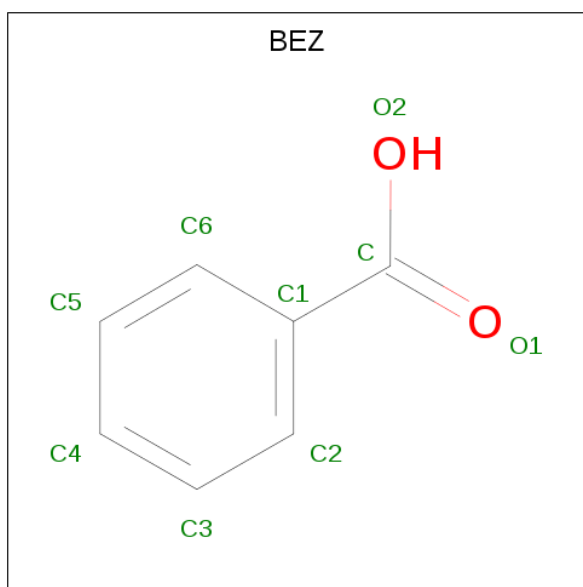
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	A	1	Total	C	H	O	0	0
			10	2	6	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	H	O	0	0
			10	2	6	2		
6	B	1	Total	C	H	O	0	0
			10	2	6	2		
6	B	1	Total	C	H	O	0	0
			10	2	6	2		
6	C	1	Total	C	H	O	0	0
			10	2	6	2		
6	D	1	Total	C	H	O	0	0
			10	2	6	2		
6	D	1	Total	C	H	O	0	0
			10	2	6	2		
6	E	1	Total	C	H	O	0	0
			10	2	6	2		
6	E	1	Total	C	H	O	0	0
			10	2	6	2		
6	E	1	Total	C	H	O	0	0
			10	2	6	2		
6	E	1	Total	C	H	O	0	0
			10	2	6	2		
6	E	1	Total	C	H	O	0	0
			10	2	6	2		
6	E	1	Total	C	H	O	0	0
			10	2	6	2		
6	E	1	Total	C	H	O	0	0
			10	2	6	2		
6	F	1	Total	C	H	O	0	0
			10	2	6	2		
6	F	1	Total	C	H	O	0	0
			10	2	6	2		
6	F	1	Total	C	H	O	0	0
			10	2	6	2		
6	F	1	Total	C	H	O	0	0
			10	2	6	2		
6	G	1	Total	C	H	O	0	0
			10	2	6	2		
6	G	1	Total	C	H	O	0	0
			10	2	6	2		
6	H	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 7 is BENZOIC ACID (three-letter code: BEZ) (formula: C₇H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			14	7	5	2		
7	E	1	Total	C	H	O	0	0
			14	7	5	2		

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	E	1	Total	Cl	0	0
			1	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	293	Total	O	0	0
			293	293		
9	B	257	Total	O	0	1
			258	258		
9	C	105	Total	O	0	0
			105	105		
9	D	40	Total	O	0	0
			40	40		
9	E	296	Total	O	0	0
			296	296		
9	F	257	Total	O	0	1
			258	258		

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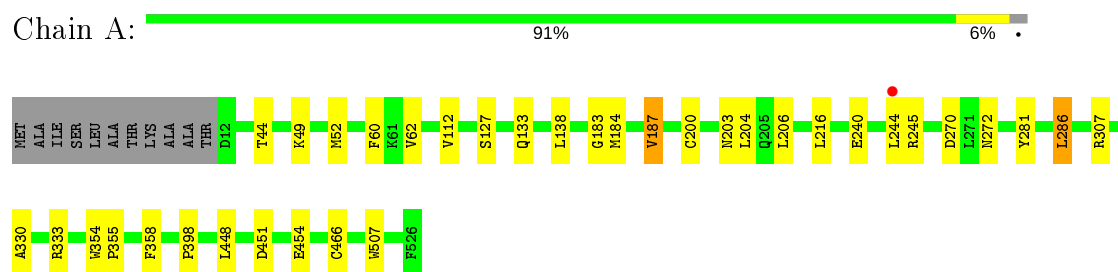
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	G	111	Total 111	O 111	0	0
9	H	55	Total 55	O 55	0	0

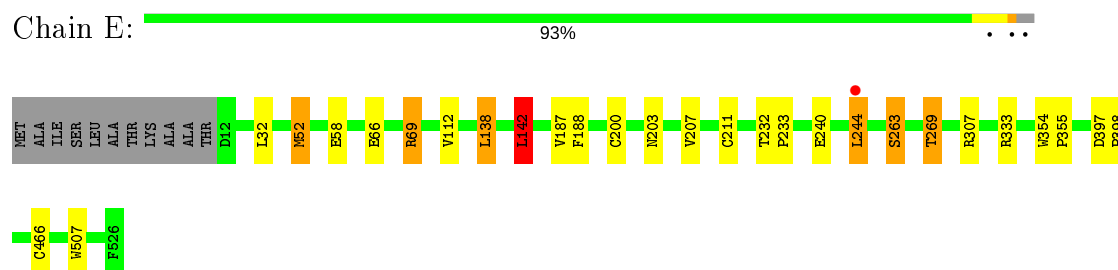
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

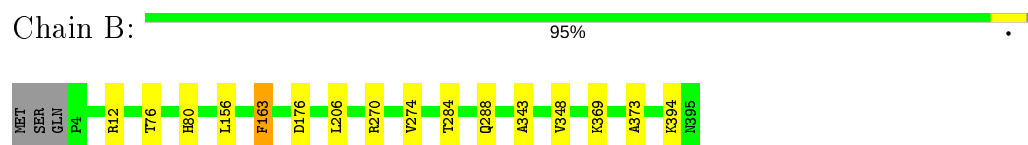
- Molecule 1: Methane monooxygenase component A alpha chain



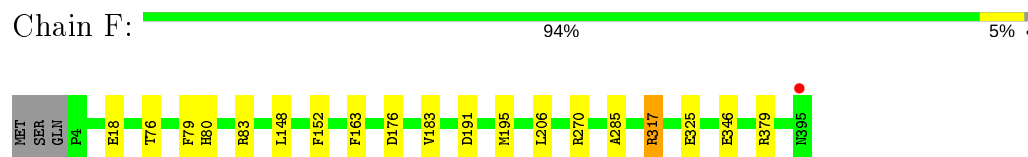
- Molecule 1: Methane monooxygenase component A alpha chain



- Molecule 2: Methane monooxygenase



- Molecule 2: Methane monooxygenase



- Molecule 3: Methane monooxygenase





- Molecule 3: Methane monooxygenase

Chain G: 95% ..



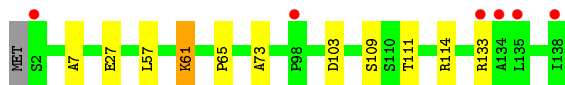
- Molecule 4: Methane monooxygenase regulatory protein B

Chain D: 90% 5% ..



- Molecule 4: Methane monooxygenase regulatory protein B

Chain H: 91% 7% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	102.61Å 105.46Å 299.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.54 – 1.86 99.47 – 1.86	Depositor EDS
% Data completeness (in resolution range)	99.7 (73.54-1.86) 99.7 (99.47-1.86)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 1.86Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.170 , 0.193 0.172 , 0.194	Depositor DCC
R_{free} test set	13531 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	28.8	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 34.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.030 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	40070	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BEZ, CL, EDO, 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	0.42	0/4305	0.59	1/5850 (0.0%)
1	E	0.40	0/4329	0.58	1/5884 (0.0%)
2	B	0.40	0/3279	0.55	0/4457
2	F	0.40	0/3298	0.57	2/4483 (0.0%)
3	C	0.38	0/1388	0.56	0/1877
3	G	0.39	0/1388	0.54	0/1877
4	D	0.39	0/1018	0.55	0/1376
4	H	0.39	0/1054	0.55	0/1426
All	All	0.40	0/20059	0.57	4/27230 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	286	LEU	CA-CB-CG	-6.03	101.43	115.30
2	F	317	ARG	NE-CZ-NH1	6.03	123.31	120.30
2	F	317	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	E	142	LEU	CA-CB-CG	5.21	127.28	115.30

There are no chirality outliers.

There are no planarity outliers.

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	4175	3970	3972	28	0
1	E	4183	3981	3973	23	1
2	B	3186	3010	3025	9	0
2	F	3200	3024	3030	12	1
3	C	1362	1400	1400	4	0
3	G	1362	1400	1400	5	0
4	D	1002	995	995	5	0
4	H	1038	1033	1033	8	0
5	A	2	0	0	0	0
5	E	2	0	0	0	0
6	A	40	60	60	7	0
6	B	12	18	18	0	0
6	C	4	6	6	0	0
6	D	8	12	12	2	0
6	E	28	42	42	0	0
6	F	16	24	24	2	0
6	G	8	12	12	0	0
6	H	4	6	6	0	0
7	A	9	5	5	0	0
7	E	9	5	5	0	0
8	E	1	0	0	0	0
9	A	293	0	0	2	0
9	B	258	0	0	0	0
9	C	105	0	0	0	0
9	D	40	0	0	0	0
9	E	296	0	0	4	1
9	F	258	0	0	3	1
9	G	111	0	0	2	0
9	H	55	0	0	1	0
All	All	21067	19003	19018	78	2

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 2.

All (78) 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:E:69:ARG:NH2	4:H:103:ASP:OD1	2.03	0.92
3:G:158:LYS:NZ	9:G:301:HOH:O	2.08	0.86
1:E:58:GLU:OE1	9:E:901:HOH:O	1.95	0.82
4:H:7:ALA:O	9:H:301:HOH:O	2.00	0.77
1:E:269:THR:HG23	9:E:1095:HOH:O	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:138:LEU:HD22	1:E:142:LEU:HD22	1.71	0.72
2:F:346:GLU:HG3	6:F:404:EDO:H22	1.72	0.71
1:E:269:THR:HG21	9:G:397:HOH:O	1.99	0.63
1:A:272:ASN:HB2	6:A:810:EDO:H12	1.81	0.62
3:G:154:GLU:O	3:G:158:LYS:HD2	2.00	0.60
1:E:244:LEU:CD1	4:H:111:THR:HG23	2.30	0.60
1:E:333:ARG:NH2	4:H:27:GLU:OE2	2.34	0.60
1:E:66:GLU:OE2	1:E:69:ARG:NH1	2.40	0.55
2:F:325:GLU:OE1	9:F:501:HOH:O	2.18	0.54
1:A:187:VAL:HG21	1:A:281:TYR:CD1	2.42	0.54
1:A:138:LEU:HD22	2:B:163:PHE:CE1	2.43	0.54
1:E:333:ARG:NH1	9:E:906:HOH:O	2.42	0.53
1:E:269:THR:HG22	9:E:1184:HOH:O	2.09	0.52
2:B:80:HIS:CD2	3:C:141:MET:HG2	2.45	0.51
1:E:354:TRP:CG	1:E:355:PRO:HD3	2.45	0.51
1:A:454:GLU:OE1	3:C:157:ARG:HD2	2.11	0.51
2:B:343:ALA:HB2	2:B:394:LYS:HD2	1.93	0.51
1:E:187:VAL:HG13	1:E:188:PHE:N	2.27	0.49
1:A:216:LEU:HD13	1:A:286:LEU:CD1	2.41	0.49
1:A:62:VAL:HG11	1:A:245:ARG:NH2	2.28	0.49
1:A:133:GLN:OE1	9:A:901:HOH:O	2.19	0.48
1:E:142:LEU:HD13	2:F:183:VAL:HG12	1.96	0.48
1:A:451:ASP:HB3	6:A:812:EDO:H12	1.96	0.48
1:A:240:GLU:HG3	4:D:109:SER:O	2.14	0.48
1:E:240:GLU:HG3	4:H:109:SER:O	2.13	0.48
3:G:67:VAL:O	3:G:71:GLU:HG2	2.14	0.48
1:E:200:CYS:HA	1:E:203:ASN:OD1	2.14	0.47
2:F:80:HIS:CD2	3:G:141:MET:HG2	2.49	0.47
2:F:285:ALA:HB2	6:F:401:EDO:H12	1.97	0.47
1:A:49:LYS:NZ	1:A:270:ASP:OD2	2.41	0.46
1:A:354:TRP:HA	6:A:808:EDO:H22	1.96	0.46
1:E:244:LEU:HD11	4:H:111:THR:HG23	1.97	0.46
1:E:52:MET:HB3	1:E:263:SER:OG	2.16	0.46
1:A:358:PHE:CE1	6:A:807:EDO:H22	2.49	0.46
1:A:333:ARG:NH2	4:D:27:GLU:OE2	2.46	0.46
1:A:187:VAL:HG13	1:A:281:TYR:HB3	1.98	0.46
1:A:203:ASN:OD1	1:A:204:LEU:N	2.48	0.46
1:A:244:LEU:HD12	1:A:245:ARG:N	2.30	0.46
1:A:330:ALA:H	6:A:810:EDO:C1	2.28	0.45
4:H:61:LYS:NZ	4:H:65:PRO:O	2.49	0.45
6:A:808:EDO:H21	9:A:1090:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:163:LYS:HD2	3:G:165:LEU:HD21	1.98	0.45
3:C:163:LYS:HD2	3:C:165:LEU:HD21	2.00	0.43
1:E:142:LEU:HD13	2:F:183:VAL:CG1	2.47	0.43
1:A:60:PHE:CZ	1:A:244:LEU:HD13	2.53	0.43
1:E:207:VAL:O	1:E:211:CYS:HB3	2.18	0.43
1:A:451:ASP:HB3	6:A:812:EDO:C1	2.48	0.43
2:B:274:VAL:HG11	2:B:348:VAL:HG11	2.00	0.43
1:E:466:CYS:HB2	2:F:76:THR:HA	2.00	0.43
1:A:44:THR:HB	1:A:127:SER:HA	2.01	0.43
1:A:200:CYS:HA	1:A:203:ASN:OD1	2.19	0.43
1:E:244:LEU:CD1	4:H:111:THR:CG2	2.96	0.42
2:F:79:PHE:HB2	2:F:83:ARG:HB3	2.00	0.42
2:B:369:LYS:HA	2:B:373:ALA:HB3	2.01	0.42
2:F:317:ARG:NH2	9:F:509:HOH:O	2.51	0.42
1:A:354:TRP:CG	1:A:355:PRO:HD3	2.54	0.41
1:A:448:LEU:HD22	1:A:448:LEU:N	2.35	0.41
3:C:168:GLN:O	3:C:169:ALA:HB3	2.21	0.41
1:A:240:GLU:CG	4:D:109:SER:O	2.68	0.41
2:F:18:GLU:HG2	9:F:678:HOH:O	2.19	0.41
1:A:466:CYS:HB2	2:B:76:THR:HA	2.03	0.41
1:E:232:THR:HB	1:E:233:PRO:HD3	2.02	0.41
1:A:183:GLY:O	1:A:187:VAL:HG22	2.20	0.41
2:B:12:ARG:HH12	6:D:202:EDO:C2	2.34	0.41
4:D:72:LYS:O	4:D:73:ALA:HB3	2.21	0.41
2:B:156:LEU:C	2:B:156:LEU:HD12	2.42	0.41
2:B:284:THR:O	2:B:288:GLN:HG2	2.21	0.40
2:F:148:LEU:O	2:F:152:PHE:HB3	2.22	0.40
1:A:184:MET:HA	1:A:187:VAL:HG23	2.04	0.40
1:A:398:PRO:HA	1:A:507:TRP:CE2	2.56	0.40
2:F:191:ASP:O	2:F:195:MET:HG2	2.21	0.40
4:D:99:PHE:HE1	6:D:201:EDO:C2	2.35	0.40
1:E:398:PRO:HA	1:E:507:TRP:CE2	2.57	0.40

All (2) 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)
9:E:1151:HOH:O	9:F:718:HOH:O[3_555]	2.17	0.03
1:E:397:ASP:OD2	2:F:379:ARG:HH21[3_555]	1.59	0.01

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	513/526 (98%)	495 (96%)	18 (4%)	0	100	100
1	E	515/526 (98%)	497 (96%)	18 (4%)	0	100	100
2	B	390/395 (99%)	380 (97%)	10 (3%)	0	100	100
2	F	393/395 (100%)	382 (97%)	11 (3%)	0	100	100
3	C	166/169 (98%)	164 (99%)	2 (1%)	0	100	100
3	G	166/169 (98%)	164 (99%)	2 (1%)	0	100	100
4	D	130/138 (94%)	125 (96%)	4 (3%)	1 (1%)	19	7
4	H	135/138 (98%)	129 (96%)	5 (4%)	1 (1%)	22	9
All	All	2408/2456 (98%)	2336 (97%)	70 (3%)	2 (0%)	51	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	73	ALA
4	H	73	ALA

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	426/433 (98%)	421 (99%)	5 (1%)	71	62
1	E	428/433 (99%)	418 (98%)	10 (2%)	50	34
2	B	324/327 (99%)	320 (99%)	4 (1%)	71	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	326/327 (100%)	322 (99%)	4 (1%)	71	62
3	C	145/146 (99%)	145 (100%)	0	100	100
3	G	145/146 (99%)	144 (99%)	1 (1%)	84	79
4	D	105/110 (96%)	102 (97%)	3 (3%)	42	26
4	H	109/110 (99%)	105 (96%)	4 (4%)	34	17
All	All	2008/2032 (99%)	1977 (98%)	31 (2%)	65	53

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	MET
1	A	112	VAL
1	A	187	VAL
1	A	206	LEU
1	A	307	ARG
2	B	163	PHE
2	B	176	ASP
2	B	206	LEU
2	B	270	ARG
4	D	61	LYS
4	D	101	VAL
4	D	114	ARG
1	E	32	LEU
1	E	52	MET
1	E	69	ARG
1	E	112	VAL
1	E	138	LEU
1	E	142	LEU
1	E	244	LEU
1	E	263	SER
1	E	269	THR
1	E	307	ARG
2	F	163	PHE
2	F	176	ASP
2	F	206	LEU
2	F	270	ARG
3	G	158	LYS
4	H	57	LEU
4	H	61	LYS
4	H	114	ARG

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Mol	Chain	Res	Type
4	H	133	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 37 ligands modelled in this entry, 5 are monoatomic - leaving 32 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	$\# Z > 2$
6	EDO	G	202	-	3,3,3	0.39	0	2,2,2	0.49	0
7	BEZ	A	813	5	7,9,9	2.91	1 (14%)	8,11,11	0.52	0
7	BEZ	E	810	5	7,9,9	2.78	1 (14%)	8,11,11	0.65	0
6	EDO	A	803	-	3,3,3	0.39	0	2,2,2	0.37	0
6	EDO	E	803	-	3,3,3	0.56	0	2,2,2	0.44	0
6	EDO	E	809	-	3,3,3	0.68	0	2,2,2	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	EDO	A	812	-	3,3,3	0.52	0	2,2,2	0.37	0
6	EDO	D	202	-	3,3,3	0.51	0	2,2,2	0.10	0
6	EDO	F	402	-	3,3,3	0.49	0	2,2,2	0.32	0
6	EDO	F	401	-	3,3,3	0.55	0	2,2,2	0.24	0
6	EDO	B	401	-	3,3,3	0.57	0	2,2,2	0.31	0
6	EDO	C	201	-	3,3,3	0.37	0	2,2,2	0.47	0
6	EDO	A	807	-	3,3,3	0.41	0	2,2,2	0.40	0
6	EDO	G	201	-	3,3,3	0.55	0	2,2,2	0.25	0
6	EDO	A	805	-	3,3,3	0.47	0	2,2,2	0.39	0
6	EDO	B	403	-	3,3,3	0.67	0	2,2,2	0.35	0
6	EDO	A	806	-	3,3,3	0.65	0	2,2,2	0.15	0
6	EDO	A	811	-	3,3,3	0.51	0	2,2,2	0.41	0
6	EDO	D	201	-	3,3,3	0.61	0	2,2,2	0.33	0
6	EDO	H	201	-	3,3,3	0.55	0	2,2,2	0.11	0
6	EDO	A	810	-	3,3,3	0.51	0	2,2,2	0.18	0
6	EDO	A	809	-	3,3,3	0.47	0	2,2,2	0.24	0
6	EDO	E	808	-	3,3,3	0.55	0	2,2,2	0.31	0
6	EDO	F	403	-	3,3,3	0.48	0	2,2,2	0.21	0
6	EDO	A	804	-	3,3,3	0.54	0	2,2,2	0.39	0
6	EDO	E	805	-	3,3,3	0.51	0	2,2,2	0.24	0
6	EDO	E	806	-	3,3,3	0.46	0	2,2,2	0.42	0
6	EDO	A	808	-	3,3,3	0.38	0	2,2,2	0.50	0
6	EDO	E	807	-	3,3,3	0.48	0	2,2,2	0.61	0
6	EDO	F	404	-	3,3,3	0.40	0	2,2,2	0.53	0
6	EDO	E	804	-	3,3,3	0.51	0	2,2,2	0.30	0
6	EDO	B	402	-	3,3,3	0.41	0	2,2,2	0.38	0

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
6	EDO	G	202	-	-	0/1/1/1	-
7	BEZ	A	813	5	-	0/0/4/4	0/1/1/1
7	BEZ	E	810	5	-	0/0/4/4	0/1/1/1
6	EDO	A	803	-	-	0/1/1/1	-
6	EDO	E	803	-	-	1/1/1/1	-
6	EDO	E	809	-	-	1/1/1/1	-
6	EDO	A	812	-	-	0/1/1/1	-
6	EDO	D	202	-	-	0/1/1/1	-
6	EDO	F	402	-	-	0/1/1/1	-
6	EDO	F	401	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	B	401	-	-	0/1/1/1	-
6	EDO	C	201	-	-	0/1/1/1	-
6	EDO	A	807	-	-	0/1/1/1	-
6	EDO	G	201	-	-	0/1/1/1	-
6	EDO	A	805	-	-	0/1/1/1	-
6	EDO	B	403	-	-	0/1/1/1	-
6	EDO	A	806	-	-	0/1/1/1	-
6	EDO	A	811	-	-	1/1/1/1	-
6	EDO	D	201	-	-	1/1/1/1	-
6	EDO	H	201	-	-	1/1/1/1	-
6	EDO	A	810	-	-	0/1/1/1	-
6	EDO	A	809	-	-	1/1/1/1	-
6	EDO	E	808	-	-	0/1/1/1	-
6	EDO	F	403	-	-	1/1/1/1	-
6	EDO	A	804	-	-	0/1/1/1	-
6	EDO	E	805	-	-	1/1/1/1	-
6	EDO	E	806	-	-	0/1/1/1	-
6	EDO	A	808	-	-	1/1/1/1	-
6	EDO	E	807	-	-	0/1/1/1	-
6	EDO	F	404	-	-	1/1/1/1	-
6	EDO	E	804	-	-	1/1/1/1	-
6	EDO	B	402	-	-	1/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	813	BEZ	C1-C	-7.66	1.40	1.47
7	E	810	BEZ	C1-C	-7.29	1.40	1.47

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	F	403	EDO	O1-C1-C2-O2
6	F	401	EDO	O1-C1-C2-O2
6	D	201	EDO	O1-C1-C2-O2
6	E	805	EDO	O1-C1-C2-O2
6	A	809	EDO	O1-C1-C2-O2
6	E	803	EDO	O1-C1-C2-O2
6	E	809	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
6	F	404	EDO	O1-C1-C2-O2
6	A	808	EDO	O1-C1-C2-O2
6	A	811	EDO	O1-C1-C2-O2
6	H	201	EDO	O1-C1-C2-O2
6	E	804	EDO	O1-C1-C2-O2
6	B	402	EDO	O1-C1-C2-O2

There are no ring outliers.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	812	EDO	2	0
6	D	202	EDO	1	0
6	F	401	EDO	1	0
6	A	807	EDO	1	0
6	D	201	EDO	1	0
6	A	810	EDO	2	0
6	A	808	EDO	2	0
6	F	404	EDO	1	0

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, 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	515/526 (97%)	-0.07	1 (0%) 95 94	21, 26, 37, 58	0
1	E	515/526 (97%)	-0.08	1 (0%) 95 94	21, 26, 37, 55	0
2	B	392/395 (99%)	-0.12	0 100 100	21, 26, 35, 51	0
2	F	392/395 (99%)	-0.11	1 (0%) 94 93	22, 26, 35, 57	0
3	C	168/169 (99%)	-0.13	2 (1%) 79 79	25, 30, 39, 53	0
3	G	168/169 (99%)	-0.17	0 100 100	23, 31, 39, 48	0
4	D	132/138 (95%)	0.03	3 (2%) 60 59	25, 31, 41, 85	0
4	H	137/138 (99%)	0.08	6 (4%) 34 33	25, 32, 44, 75	0
All	All	2419/2456 (98%)	-0.08	14 (0%) 89 89	21, 27, 38, 85	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	169	ALA	4.6
4	H	135	LEU	4.5
4	H	2	SER	3.6
4	D	133	ARG	3.4
4	D	2	SER	3.3
4	H	133	ARG	3.3
3	C	2	ALA	3.1
2	F	395	ASN	2.9
4	H	134	ALA	2.9
4	H	98	PRO	2.3
4	H	138	ILE	2.1
1	A	244	LEU	2.1
1	E	244	LEU	2.1
4	D	118	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	EDO	A	810	4/4	0.81	0.40	33,40,48,52	0
6	EDO	A	808	4/4	0.81	0.61	31,38,45,48	0
6	EDO	A	809	4/4	0.82	0.28	38,46,50,51	0
6	EDO	B	403	4/4	0.82	0.21	31,37,42,44	0
6	EDO	D	201	4/4	0.83	0.21	33,40,45,49	0
6	EDO	E	809	4/4	0.84	0.27	38,46,49,49	0
6	EDO	A	806	4/4	0.86	0.18	33,39,42,42	0
6	EDO	F	403	4/4	0.87	0.20	43,51,53,56	0
6	EDO	H	201	4/4	0.87	0.21	38,46,48,48	0
6	EDO	F	401	4/4	0.88	0.12	28,34,38,43	0
6	EDO	E	805	4/4	0.88	0.20	42,63,80,80	0
6	EDO	B	401	4/4	0.88	0.17	31,37,43,49	0
6	EDO	F	404	4/4	0.88	0.11	41,50,56,58	0
6	EDO	E	808	4/4	0.90	0.13	32,38,43,43	0
6	EDO	E	804	4/4	0.90	0.15	37,44,52,52	0
6	EDO	E	807	4/4	0.91	0.18	32,38,45,45	0
6	EDO	E	803	4/4	0.91	0.18	34,41,43,50	0
6	EDO	A	807	4/4	0.91	0.27	28,33,43,52	0
6	EDO	A	812	4/4	0.92	0.18	32,39,44,47	0
6	EDO	A	804	4/4	0.93	0.11	29,35,39,41	0
6	EDO	D	202	4/4	0.93	0.17	33,40,40,42	0
6	EDO	A	811	4/4	0.93	0.11	33,40,40,42	0
6	EDO	G	202	4/4	0.94	0.17	39,47,51,53	0
6	EDO	A	805	4/4	0.95	0.16	25,30,35,39	0
6	EDO	B	402	4/4	0.95	0.14	30,37,44,45	0
6	EDO	E	806	4/4	0.96	0.15	29,35,40,42	0
8	CL	E	811	1/1	0.96	0.04	55,55,55,55	0

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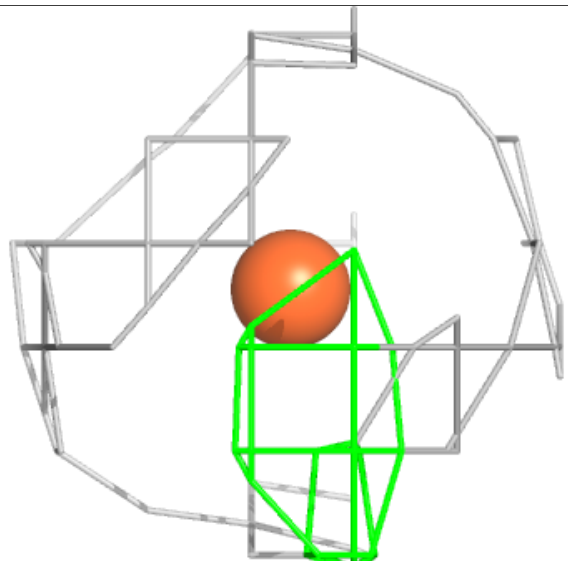
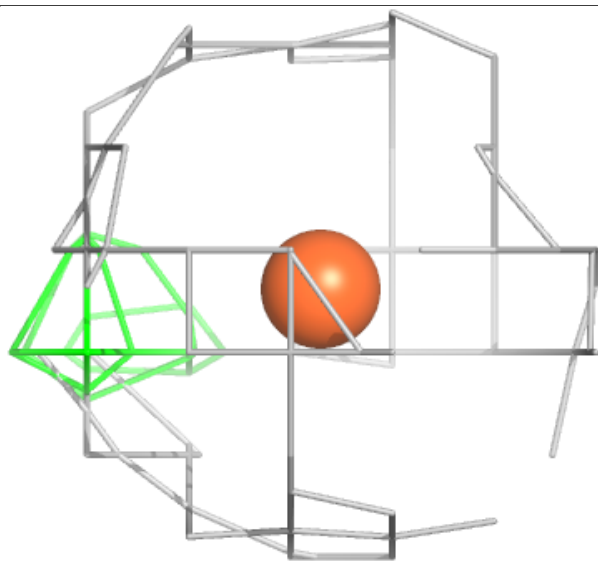
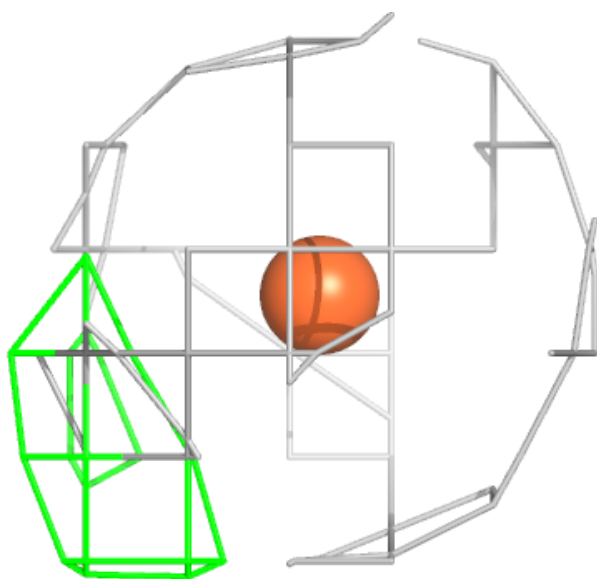
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	EDO	C	201	4/4	0.96	0.11	27,32,33,35	0
6	EDO	F	402	4/4	0.97	0.14	30,36,40,41	0
7	BEZ	A	813	9/9	0.97	0.10	24,26,30,32	0
6	EDO	G	201	4/4	0.97	0.12	28,33,35,35	0
6	EDO	A	803	4/4	0.98	0.14	30,36,38,40	0
7	BEZ	E	810	9/9	0.98	0.11	23,25,30,30	0
5	FE	A	801	1/1	1.00	0.13	24,24,24,24	0
5	FE	E	802	1/1	1.00	0.13	24,24,24,24	0
5	FE	A	802	1/1	1.00	0.12	25,25,25,25	0
5	FE	E	801	1/1	1.00	0.12	23,23,23,23	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.

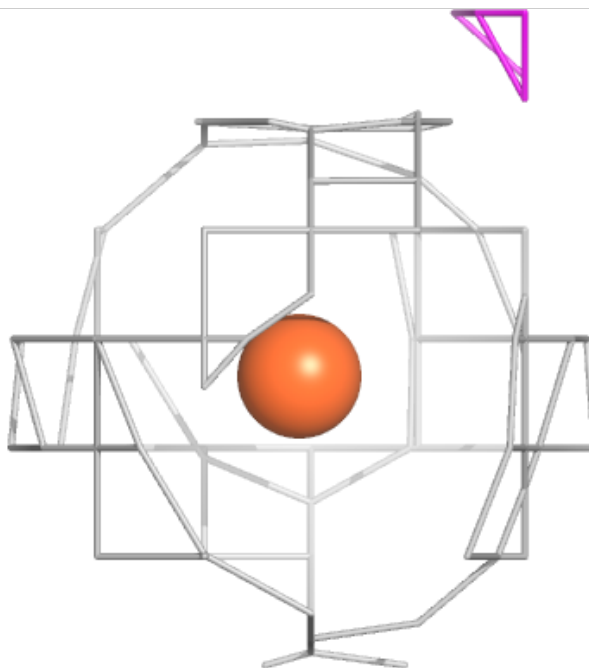
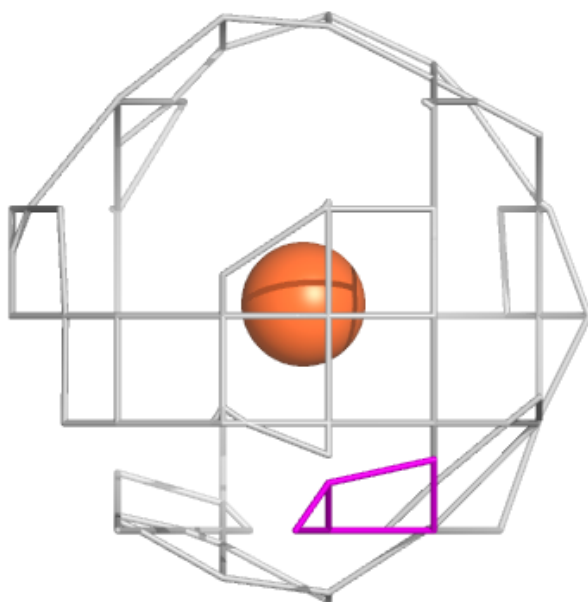
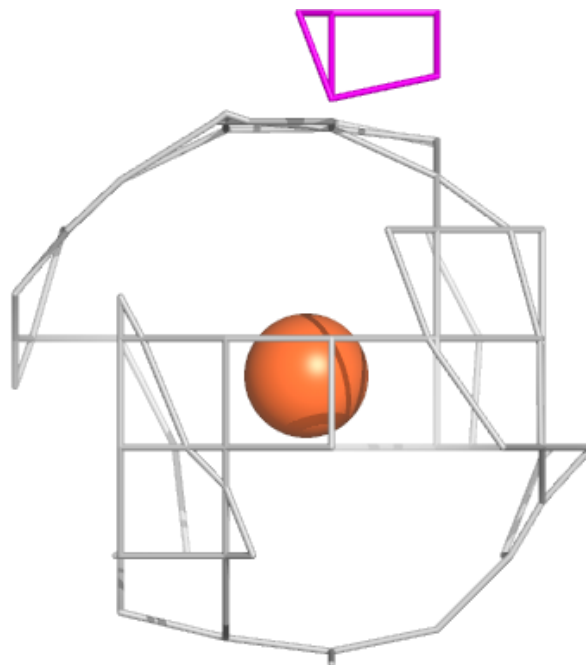
Electron density around FE A 801:

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



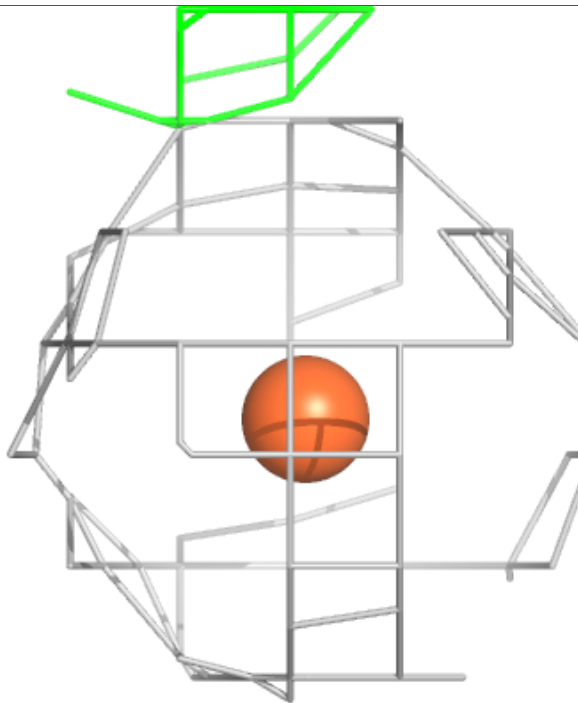
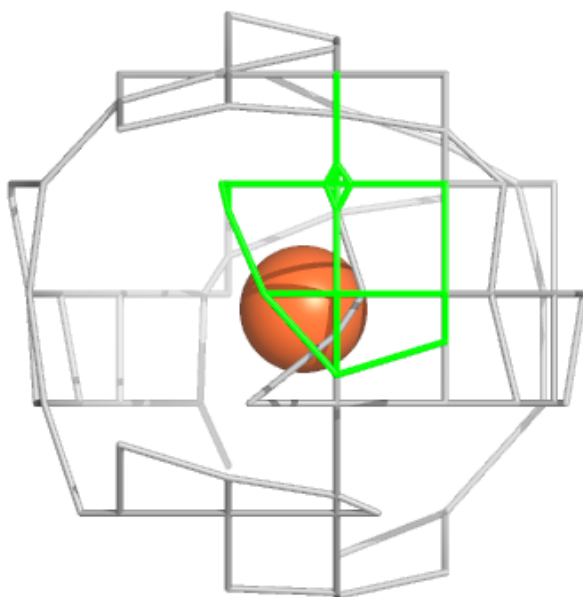
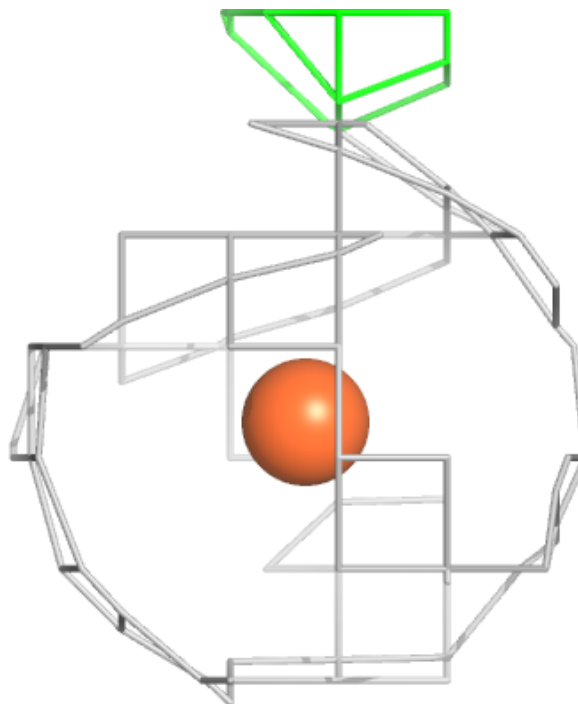
Electron density around FE E 802:

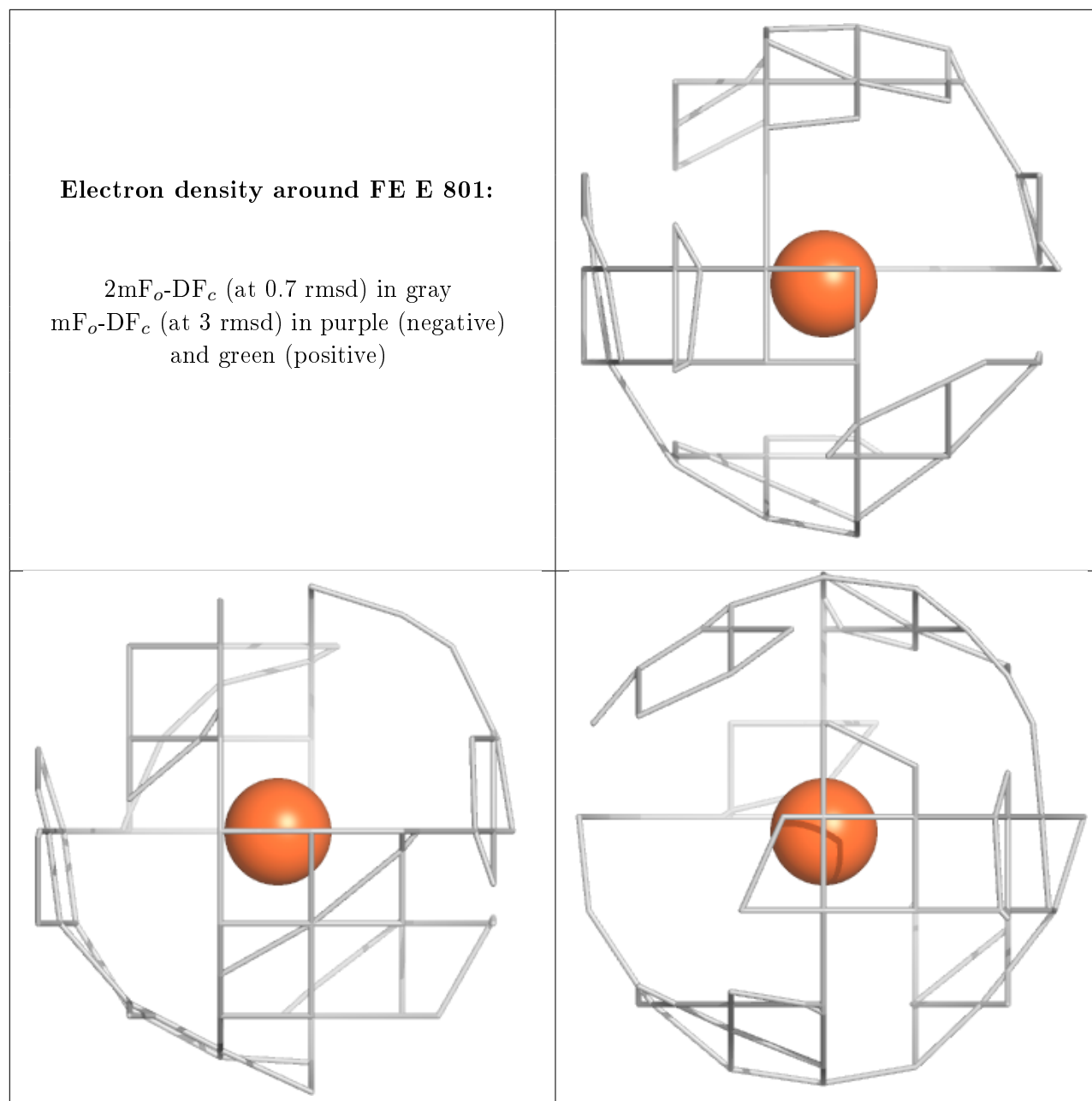
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FE A 802:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.