



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:28 AM UTC

PDB ID : 7E06 / pdb_00007e06
Title : Trans-3/4-proline-hydroxylase H11 with AKG
Authors : Gong, W.G.; Yang, L.Y.
Deposited on : 2021-01-27
Resolution : 1.97 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

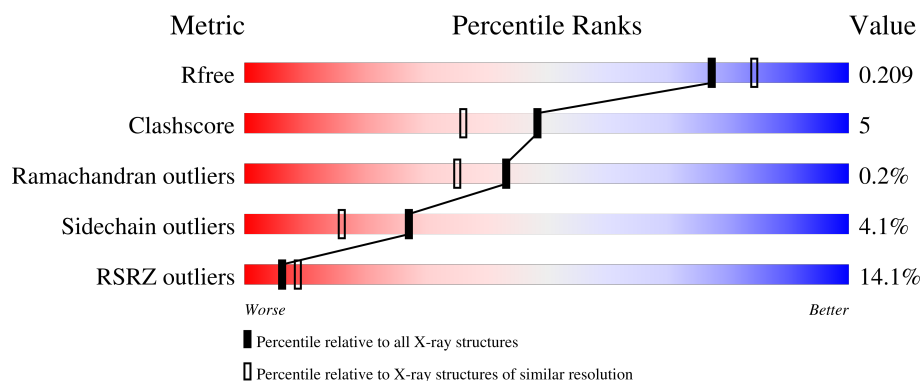
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	268	10% 82% 10% 6%
1	B	268	17% 77% 18% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4572 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.

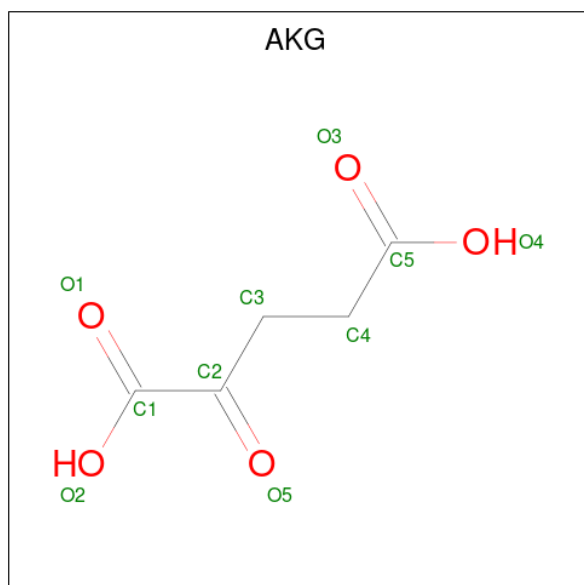
- Molecule 1 is a protein called Phytanoyl-CoA dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	S	0	1	0
			2000	1270	357	367	6			
1	B	261	Total	C	N	O	S	0	1	0
			2079	1321	368	384	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLN	-	expression tag	UNP S5TUM1
A	0	ILE	-	expression tag	UNP S5TUM1
B	-1	GLN	-	expression tag	UNP S5TUM1
B	0	ILE	-	expression tag	UNP S5TUM1

- Molecule 2 is 2-OXOGLUTARIC ACID (CCD ID: AKG) (formula: C₅H₆O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	5	5		
2	B	1	Total	C	O	0	0
			10	5	5		

- Molecule 3 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Fe	0	0
			1	1		
3	B	1	Total	Fe	0	0
			1	1		

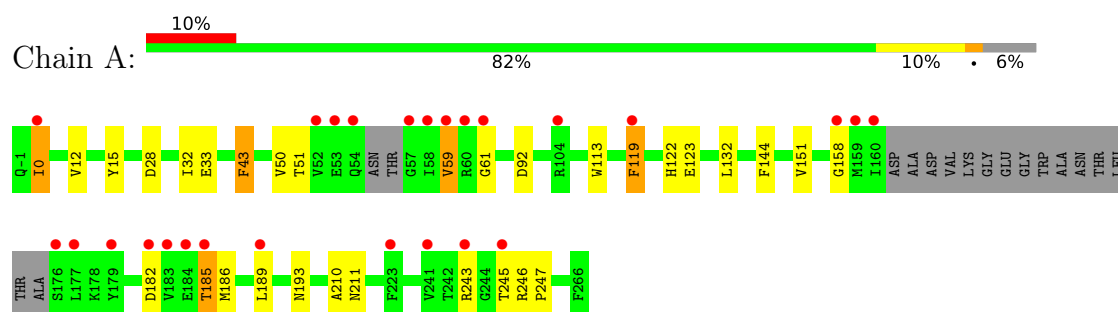
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	256	Total	O	0	0
			256	256		
4	B	215	Total	O	0	0
			215	215		

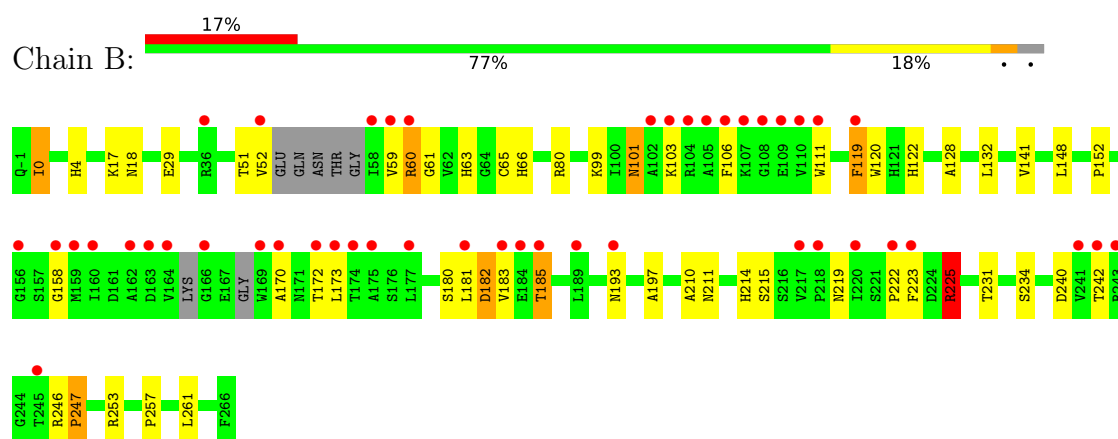
3 Residue-property plots [i](#)

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: Phytanoyl-CoA dioxygenase



• Molecule 1: Phytanoyl-CoA dioxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	106.76Å 106.76Å 144.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	85.76 – 1.97 85.76 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.2 (85.76-1.97) 99.2 (85.76-1.98)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	10.49 (at 1.98Å)	Xtrriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.169 , 0.204 (Not available) , 0.209	Depositor DCC
R_{free} test set	2882 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	28.3	Xtrriage
Anisotropy	0.022	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4572	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.75 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.1213e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: AKG, 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	1.55	14/2052 (0.7%)	1.22	7/2784 (0.3%)
1	B	1.58	19/2132 (0.9%)	1.32	13/2896 (0.4%)
All	All	1.56	33/4184 (0.8%)	1.27	20/5680 (0.4%)

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	12	VAL	N-CA	-6.67	1.38	1.46
1	B	257	PRO	CA-C	-6.53	1.44	1.52
1	B	152	PRO	N-CA	-6.29	1.39	1.47
1	B	103	LYS	N-CA	5.95	1.53	1.46
1	B	225	ARG	CD-NE	-5.85	1.38	1.46
1	B	247	PRO	CA-C	5.59	1.59	1.52
1	B	17	LYS	N-CA	5.58	1.52	1.46
1	B	128	ALA	N-CA	-5.58	1.40	1.45
1	A	28	ASP	N-CA	5.55	1.52	1.45
1	B	141	VAL	CA-C	5.55	1.59	1.52
1	B	103	LYS	CA-C	5.53	1.60	1.52
1	A	92	ASP	N-CA	-5.47	1.39	1.45
1	A	61	GLY	N-CA	5.42	1.51	1.45
1	B	214	HIS	CA-C	-5.41	1.46	1.52
1	B	122	HIS	CA-C	-5.38	1.45	1.52
1	A	245	THR	CA-C	5.36	1.59	1.52
1	B	141	VAL	C-O	-5.36	1.18	1.24
1	A	32	ILE	CA-C	-5.36	1.46	1.52
1	A	193	ASN	N-CA	5.35	1.53	1.45
1	B	210	ALA	C-O	-5.35	1.17	1.24
1	B	18	ASN	CA-C	-5.29	1.45	1.52
1	A	15	TYR	CA-CB	5.23	1.61	1.53
1	B	66	HIS	C-O	-5.22	1.17	1.24
1	B	80	ARG	CD-NE	-5.22	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	210	ALA	CA-C	5.19	1.59	1.52
1	A	151	VAL	CA-C	-5.15	1.49	1.53
1	B	215	SER	C-O	-5.15	1.18	1.23
1	A	119	PHE	N-CA	-5.09	1.40	1.46
1	A	122	HIS	CA-C	-5.08	1.46	1.52
1	B	4	HIS	C-O	5.08	1.29	1.23
1	A	43	PHE	C-O	-5.07	1.18	1.24
1	B	197	ALA	C-O	-5.02	1.19	1.24
1	A	247	PRO	CA-C	5.01	1.58	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	80	ARG	NE-CZ-NH1	-10.92	110.58	121.50
1	B	80	ARG	NE-CZ-NH2	10.65	128.78	119.20
1	B	80	ARG	CD-NE-CZ	8.89	136.85	124.40
1	B	80	ARG	CB-CG-CD	8.70	131.31	111.30
1	B	80	ARG	CG-CD-NE	-8.39	93.55	112.00
1	B	101	ASN	CA-C-N	6.29	128.95	120.65
1	B	101	ASN	C-N-CA	6.29	128.95	120.65
1	B	59	VAL	CB-CA-C	6.01	118.11	111.08
1	A	246	ARG	CA-C-N	-5.95	114.50	120.21
1	A	246	ARG	C-N-CA	-5.95	114.50	120.21
1	A	246	ARG	N-CA-C	5.79	116.79	110.13
1	A	144	PHE	N-CA-C	5.75	121.01	113.30
1	B	29	GLU	N-CA-C	5.70	117.50	111.28
1	B	101	ASN	O-C-N	5.47	130.34	123.12
1	B	261	LEU	CB-CA-C	-5.41	100.40	109.65
1	A	33	GLU	N-CA-C	5.39	117.16	111.28
1	A	245	THR	CB-CA-C	5.37	119.21	110.24
1	B	119	PHE	CB-CA-C	-5.30	102.56	110.88
1	A	0	ILE	CB-CA-C	5.21	119.82	110.65
1	B	65	CYS	N-CA-C	5.04	117.51	111.71

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	2000	0	1927	12	0
1	B	2079	0	2004	32	0
2	A	10	0	4	0	0
2	B	10	0	4	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	256	0	0	5	0
4	B	215	0	0	4	0
All	All	4572	0	3939	44	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (44) 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:225:ARG:O	1:B:225:ARG:HD2	1.83	0.79
1:A:0:ILE:HG22	4:A:803:HOH:O	1.86	0.75
1:A:0:ILE:CG2	4:A:803:HOH:O	2.38	0.71
1:B:111:TRP:CZ3	1:B:172:THR:O	2.47	0.67
1:A:50:VAL:HG11	1:A:59:VAL:HG12	1.81	0.62
1:B:240:ASP:OD1	1:B:242:THR:HB	1.99	0.62
1:B:111:TRP:CH2	1:B:172:THR:O	2.52	0.61
1:A:132:LEU:C	1:A:132:LEU:HD12	2.25	0.61
1:B:63:HIS:ND1	4:B:601:HOH:O	2.30	0.59
1:B:101:ASN:OD1	1:B:173:LEU:CD2	2.50	0.59
1:A:119:PHE:CE1	1:A:123:GLU:HG3	2.38	0.58
1:A:158:GLY:C	1:A:211:ASN:HD21	2.11	0.58
4:A:628:HOH:O	1:B:0:ILE:HG23	2.04	0.57
1:B:158:GLY:C	1:B:211:ASN:HD21	2.13	0.56
1:B:61:GLY:HA3	1:B:173:LEU:HD13	1.87	0.56
1:B:158:GLY:HA2	1:B:211:ASN:HD21	1.74	0.53
1:B:101:ASN:OD1	1:B:173:LEU:HD21	2.10	0.51
1:B:158:GLY:CA	1:B:211:ASN:HD21	2.24	0.51
1:B:253:ARG:NH1	4:B:604:HOH:O	2.44	0.50
1:B:101:ASN:OD1	1:B:173:LEU:HD22	2.10	0.50
1:B:158:GLY:HA2	1:B:211:ASN:ND2	2.27	0.49
1:B:106:PHE:CE2	1:B:222:PRO:HA	2.47	0.48
1:B:99:LYS:HE3	2:B:501:AKG:O1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:628:HOH:O	1:B:0:ILE:CG2	2.61	0.47
1:B:132:LEU:C	1:B:132:LEU:HD12	2.39	0.47
1:B:111:TRP:CH2	1:B:172:THR:C	2.93	0.46
1:B:172:THR:HG21	4:B:725:HOH:O	2.17	0.45
1:B:119:PHE:CD2	1:B:170:ALA:HB1	2.52	0.45
1:A:113:TRP:CD2	1:A:186:MET:HE2	2.51	0.45
1:B:111:TRP:HH2	1:B:173:LEU:HD23	1.82	0.45
1:A:43:PHE:HB3	1:A:59:VAL:HG21	2.00	0.44
1:A:59:VAL:O	1:A:59:VAL:HG23	2.18	0.43
1:B:219:ASN:ND2	1:B:223:PHE:O	2.27	0.43
1:B:51:THR:HG23	4:B:601:HOH:O	2.19	0.43
1:B:111:TRP:CH2	1:B:173:LEU:HD23	2.54	0.42
1:A:50:VAL:HG12	1:A:51:THR:N	2.34	0.42
1:A:243:ARG:NH2	4:A:603:HOH:O	2.45	0.42
1:B:99:LYS:CE	2:B:501:AKG:O1	2.68	0.42
1:B:182:ASP:OD2	1:B:185:THR:OG1	2.34	0.42
1:A:182:ASP:OD1	1:A:185:THR:N	2.40	0.41
1:B:120:TRP:CH2	1:B:231:THR:HG21	2.55	0.41
1:B:111:TRP:CH2	1:B:173:LEU:HA	2.56	0.40
1:B:60:ARG:HD3	1:B:173:LEU:HB3	2.03	0.40
1:B:246:ARG:HB3	1:B:247:PRO:HD2	2.03	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	246/268 (92%)	242 (98%)	3 (1%)	1 (0%)	30	20
1	B	254/268 (95%)	245 (96%)	9 (4%)	0	100	100
All	All	500/536 (93%)	487 (97%)	12 (2%)	1 (0%)	43	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	125/225 (56%)	123 (98%)	2 (2%)	55	50
1	B	219/225 (97%)	207 (94%)	12 (6%)	19	8
All	All	344/450 (76%)	330 (96%)	14 (4%)	27	16

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	185	THR
1	A	189	LEU
1	B	0	ILE
1	B	52	VAL
1	B	60	ARG
1	B	148	LEU
1	B	180	SER
1	B	181	LEU
1	B	182	ASP
1	B	183	VAL
1	B	185	THR
1	B	193	ASN
1	B	225	ARG
1	B	234	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	GLN
1	A	101	ASN

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Mol	Chain	Res	Type
1	A	211	ASN
1	B	41	GLN
1	B	63	HIS
1	B	97	GLN
1	B	193	ASN
1	B	211	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z > 2$
2	AKG	B	501	3	9,9,9	1.84	1 (11%)	11,11,11	2.97	5 (45%)
2	AKG	A	501	3	9,9,9	2.14	2 (22%)	11,11,11	2.73	5 (45%)

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
2	AKG	B	501	3	-	0/9/9/9	-
2	AKG	A	501	3	-	0/9/9/9	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	AKG	C2-C1	-4.44	1.46	1.53
2	A	501	AKG	C2-C1	-4.15	1.47	1.53
2	A	501	AKG	O1-C1	3.75	1.31	1.22

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	AKG	O1-C1-C2	-7.57	112.39	121.81
2	A	501	AKG	O5-C2-C1	-6.10	110.96	119.67
2	A	501	AKG	C3-C2-C1	3.95	122.57	115.86
2	B	501	AKG	O2-C1-C2	3.79	124.11	113.59
2	A	501	AKG	O1-C1-C2	-3.25	117.76	121.81
2	A	501	AKG	C4-C3-C2	2.78	118.12	112.91
2	B	501	AKG	O4-C5-C4	2.58	122.14	114.00
2	B	501	AKG	C3-C2-C1	2.52	120.14	115.86
2	A	501	AKG	O5-C2-C3	2.38	126.27	121.17
2	B	501	AKG	C4-C3-C2	2.05	116.76	112.91

There are no chirality outliers.

There are no torsion outliers.

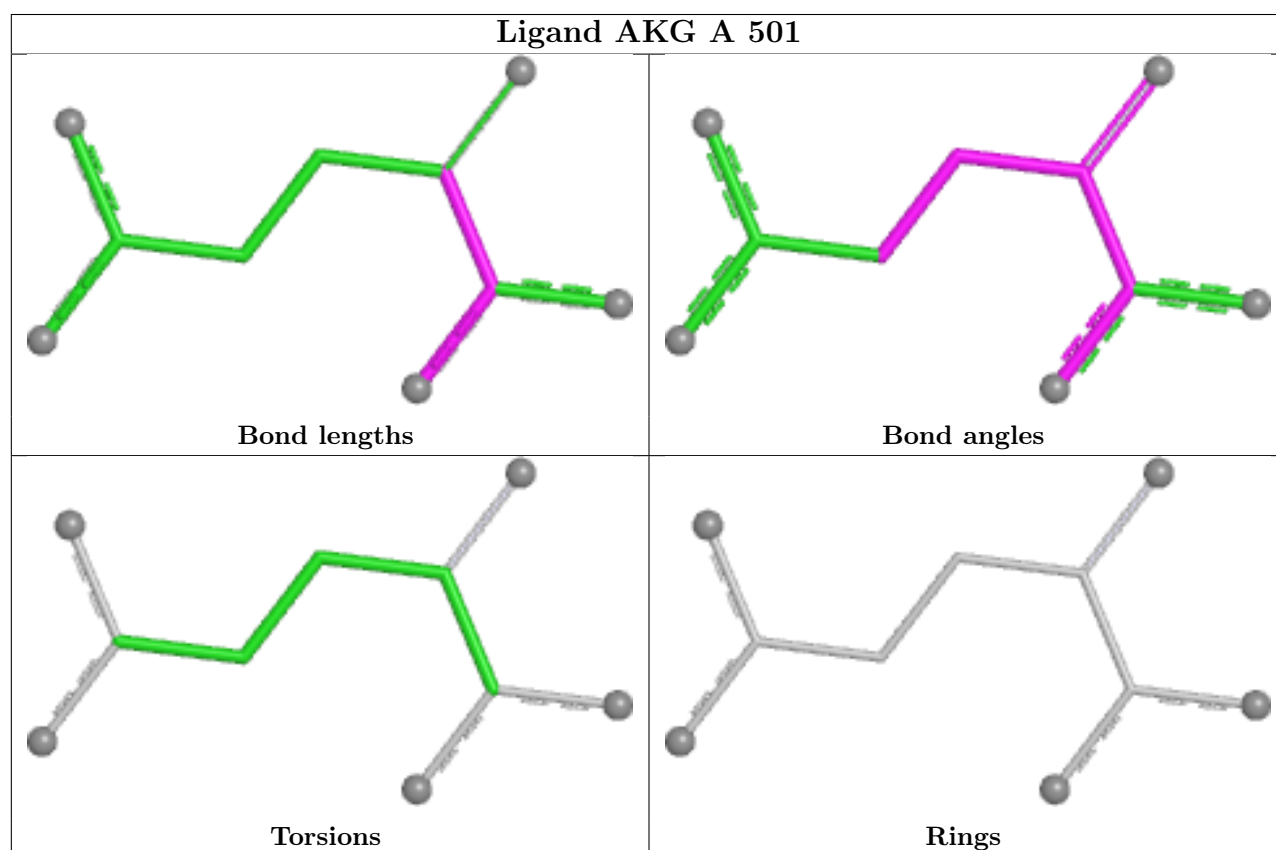
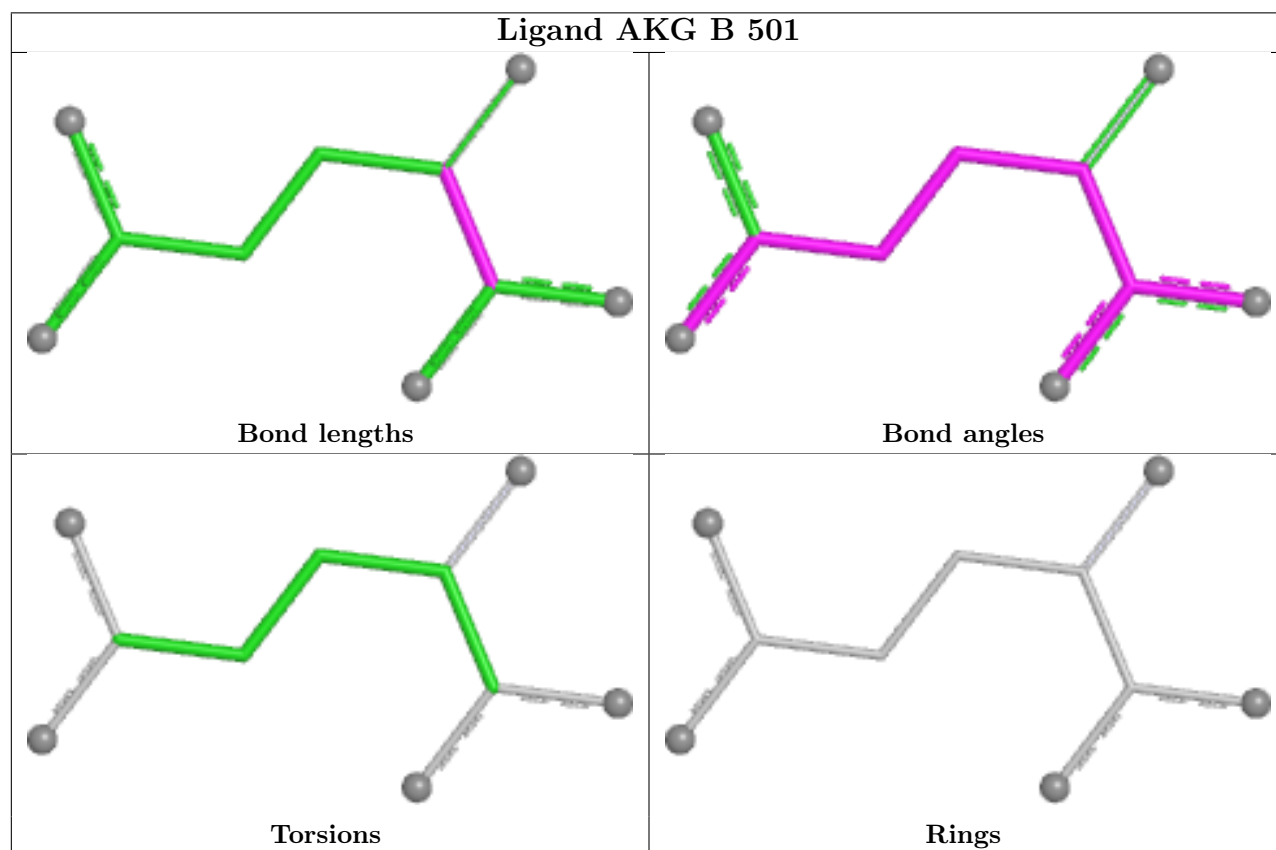
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	AKG	2	0

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, 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	251/268 (93%)	0.39	26 (10%)	11 16	12, 30, 77, 104	1 (0%)
1	B	261/268 (97%)	0.73	46 (17%)	4 4	14, 33, 86, 114	1 (0%)
All	All	512/536 (95%)	0.56	72 (14%)	6 9	12, 31, 83, 114	2 (0%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	58	ILE	7.0
1	B	52	VAL	6.6
1	B	110	VAL	6.1
1	A	58	ILE	6.0
1	B	172	THR	5.7
1	A	160	ILE	5.5
1	A	183	VAL	5.3
1	B	183	VAL	5.2
1	B	106	PHE	5.2
1	B	173	LEU	5.2
1	B	175	ALA	5.0
1	B	164	VAL	4.9
1	B	169	TRP	4.8
1	B	105	ALA	4.8
1	B	102	ALA	4.5
1	B	59	VAL	4.5
1	A	177	LEU	4.4
1	B	220	ILE	4.4
1	B	174	THR	4.4
1	B	107	LYS	4.3
1	B	170	ALA	4.1
1	A	54	GLN	4.1
1	B	160	ILE	4.0
1	A	59	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	52	VAL	3.7
1	A	158	GLY	3.6
1	A	245	THR	3.6
1	B	111	TRP	3.5
1	B	104	ARG	3.5
1	A	159	MET	3.4
1	B	166	GLY	3.3
1	B	217	VAL	3.3
1	B	223	PHE	3.3
1	A	57	GLY	3.3
1	A	53	GLU	3.2
1	A	182	ASP	3.2
1	A	185	THR	3.0
1	B	185	THR	3.0
1	A	241	VAL	2.9
1	B	222	PRO	2.8
1	B	243	ARG	2.8
1	A	119	PHE	2.7
1	A	243	ARG	2.6
1	A	223	PHE	2.6
1	B	119	PHE	2.6
1	A	176	SER	2.6
1	A	104	ARG	2.6
1	B	163	ASP	2.6
1	B	177	LEU	2.6
1	B	162	ALA	2.6
1	B	60	ARG	2.5
1	B	108	GLY	2.5
1	A	60	ARG	2.5
1	B	218	PRO	2.5
1	B	181	LEU	2.5
1	B	159	MET	2.5
1	A	179	TYR	2.4
1	A	184	GLU	2.4
1	B	36[A]	ARG	2.4
1	A	189	LEU	2.3
1	B	109	GLU	2.3
1	A	61	GLY	2.3
1	B	193	ASN	2.3
1	B	245	THR	2.2
1	B	242	THR	2.2
1	B	103	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	184	GLU	2.2
1	A	0	ILE	2.1
1	B	158	GLY	2.1
1	B	241	VAL	2.1
1	B	189	LEU	2.1
1	B	156	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

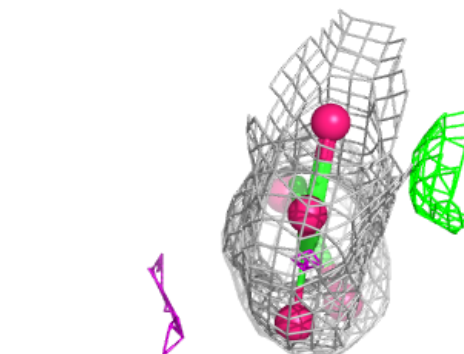
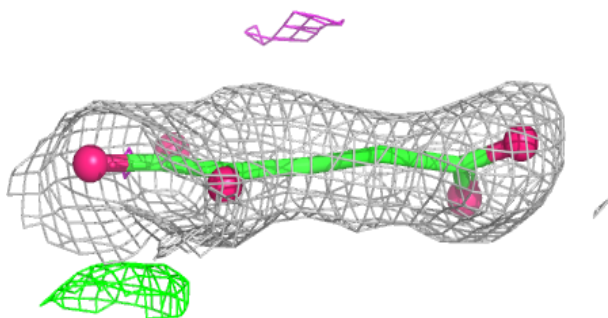
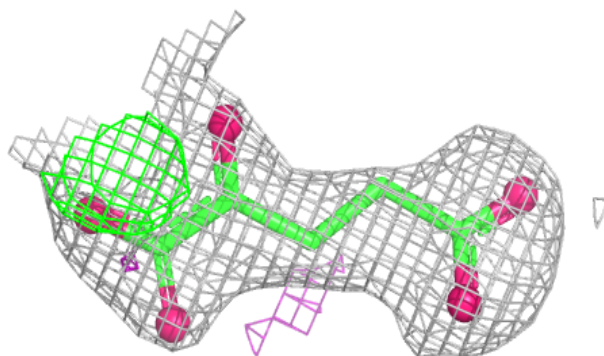
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	AKG	B	501	10/10	0.88	0.12	43,61,66,66	0
2	AKG	A	501	10/10	0.97	0.06	34,40,44,47	0
3	FE	A	502	1/1	0.99	0.05	18,18,18,18	1
3	FE	B	502	1/1	0.99	0.06	34,34,34,34	1

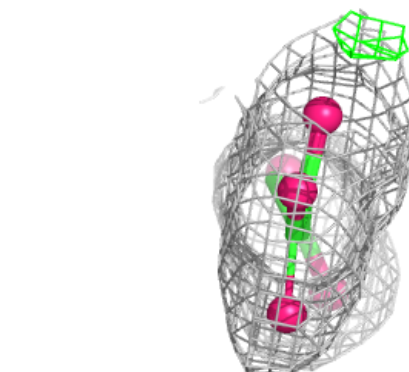
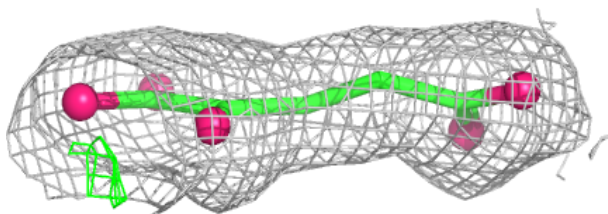
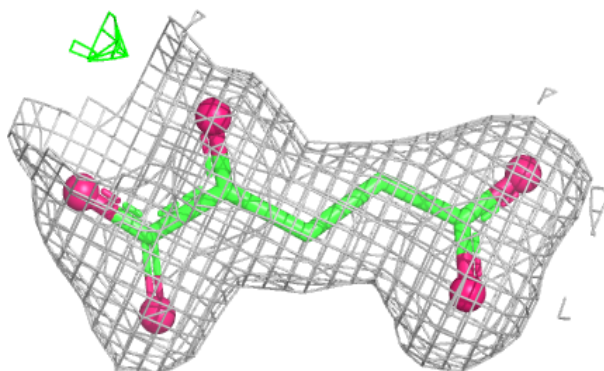
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around AKG 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)

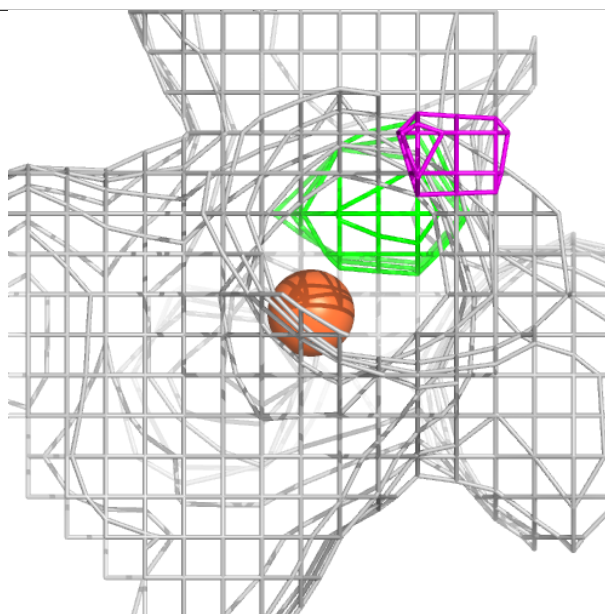
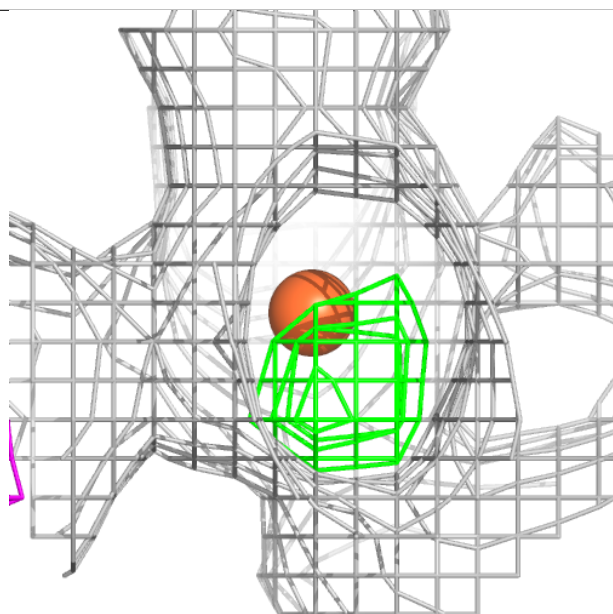
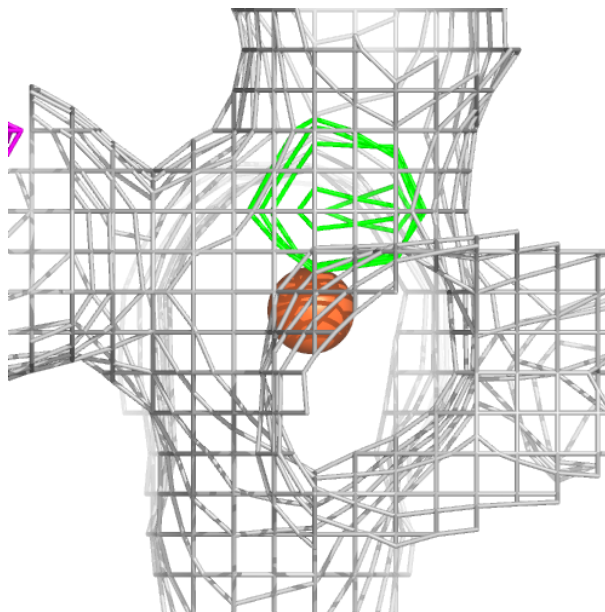
**Electron density around AKG A 501:**

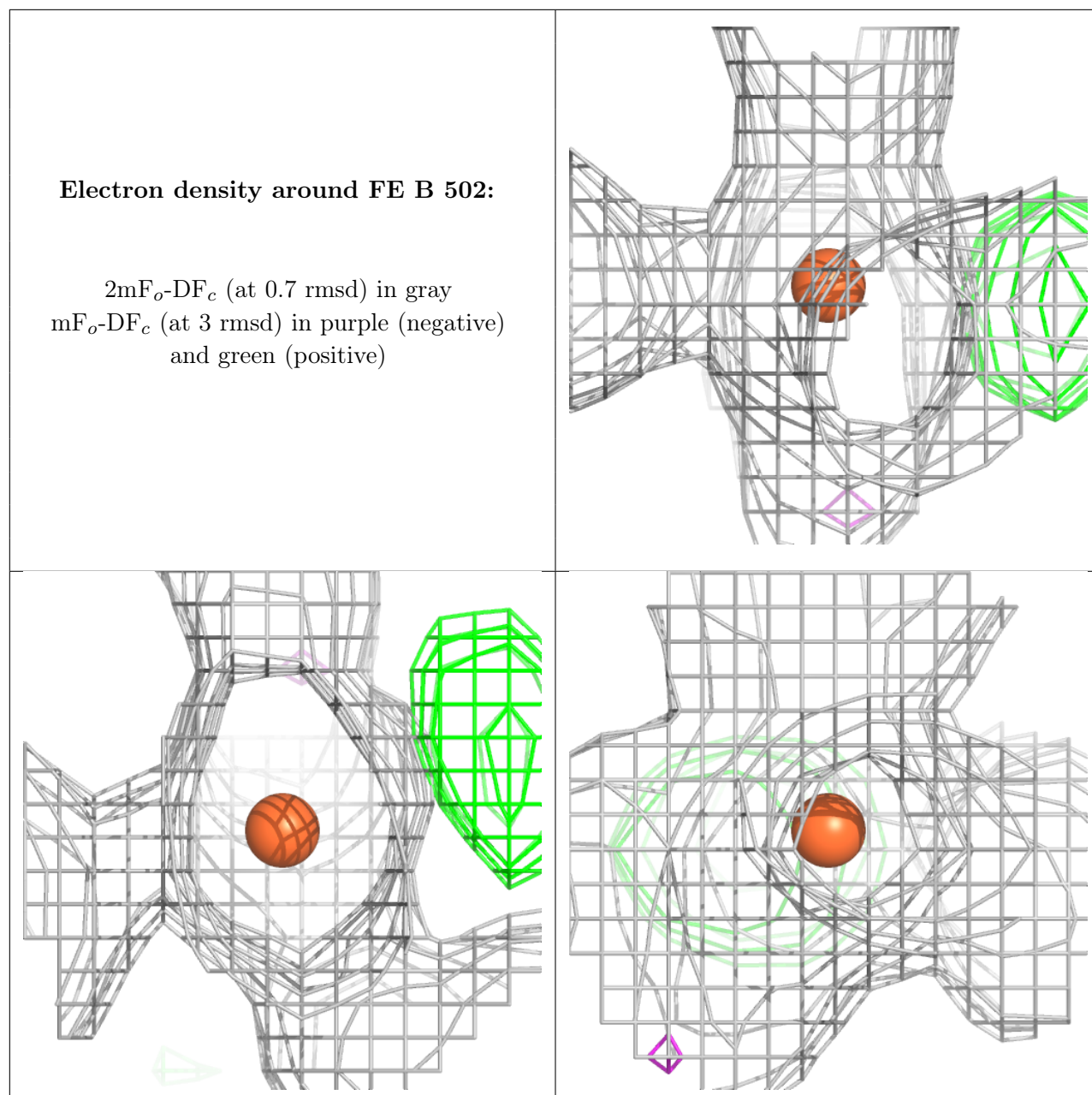
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FE 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.