



Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2026 – 10:37 am BST

PDB ID : 9RUI / pdb_00009rui
Title : Apo state of the CdmB methyltransferase involved in the anaerobic dehalogenation of haloalkanes
Authors : Wagner, T.; Lemaire, O.N.
Deposited on : 2025-07-04
Resolution : 1.57 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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

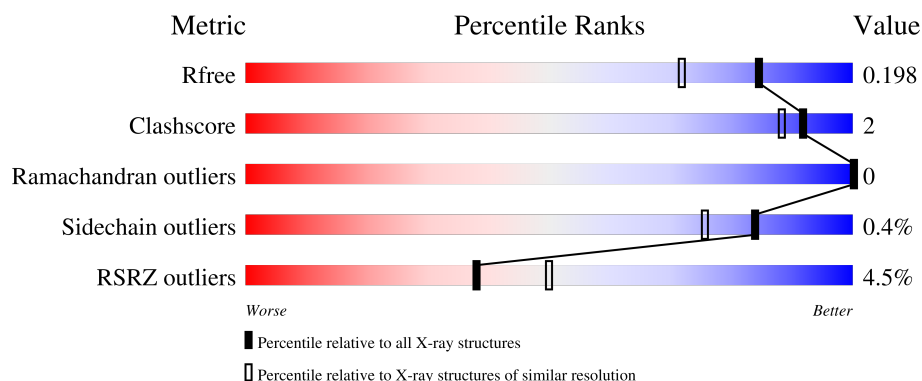
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.57 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	1094 (1.58-1.58)
Clashscore	190562	1105 (1.58-1.58)
Ramachandran outliers	187476	1082 (1.58-1.58)
Sidechain outliers	187428	1081 (1.58-1.58)
RSRZ outliers	180081	1094 (1.58-1.58)

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	429	<div> <div>4%</div> <div>96%</div> <div>..</div> </div>
1	B	429	<div> <div>5%</div> <div>90%</div> <div>6% .</div> </div>

2 Entry composition [i](#)

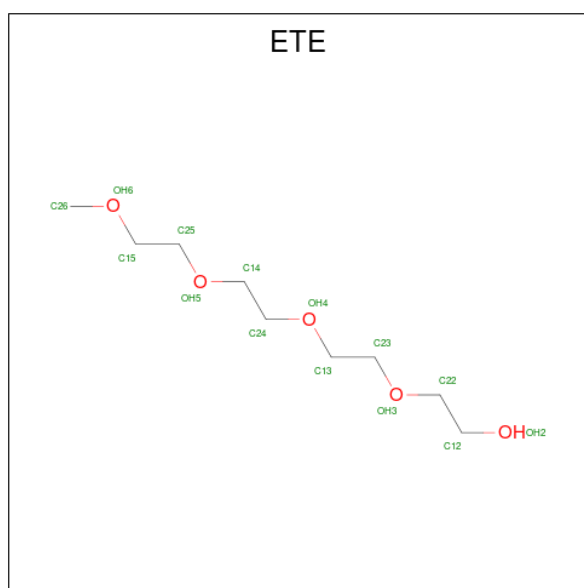
There are 10 unique types of molecules in this entry. The entry contains 7447 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CdmB from *Acetobacterium malicum* subsp. dehalogenans.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	423	Total	C	N	O	S	0	4	0
			3389	2198	554	625	12			
1	B	415	Total	C	N	O	S	0	3	0
			3310	2150	538	611	11			

- Molecule 2 is 2-{2-[2-2-(METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (CCD ID: ETE) (formula: C₉H₂₀O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			14	9	5		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	1
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

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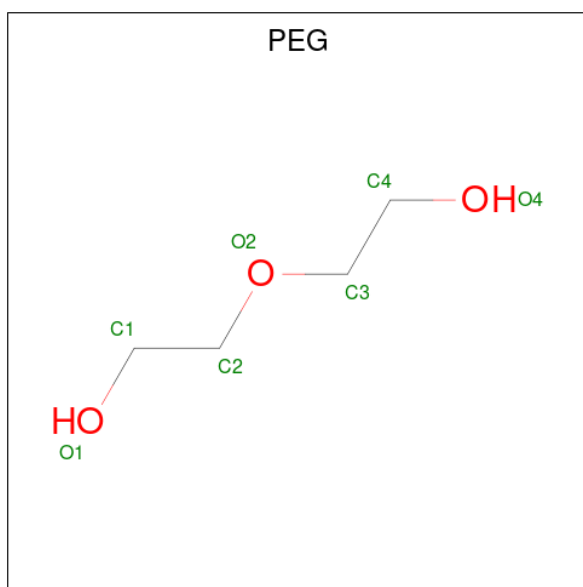
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	1
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



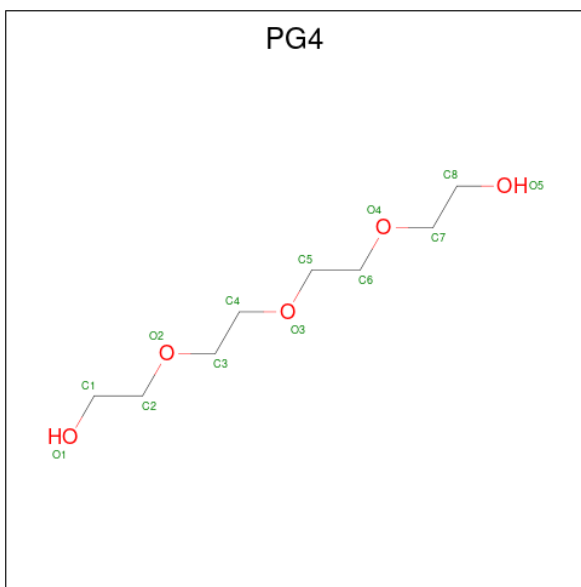
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).

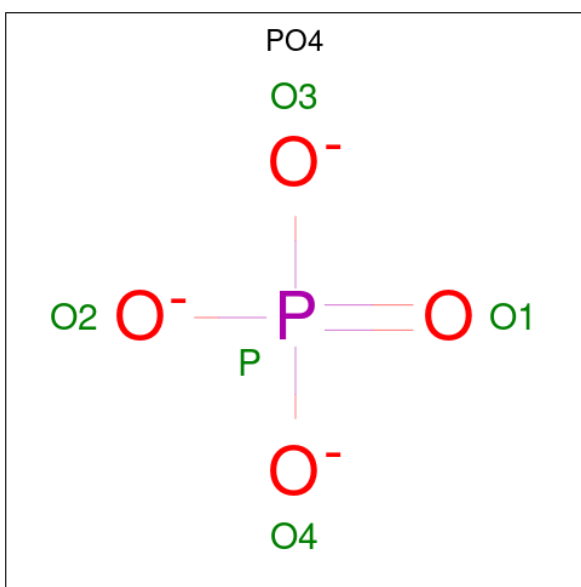


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	1
			13	8	5		

- Molecule 7 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	K	0	0
			2	2		
7	B	1	Total	K	0	0
			1	1		

- Molecule 8 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	P	0	1
			5	4	1		
8	A	1	Total	O	P	0	1
			5	4	1		
8	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 9 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Na	0	0
			1	1		

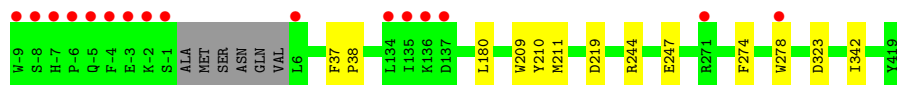
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	342	Total	O	0	0
			342	342		
10	B	160	Total	O	0	1
			160	160		

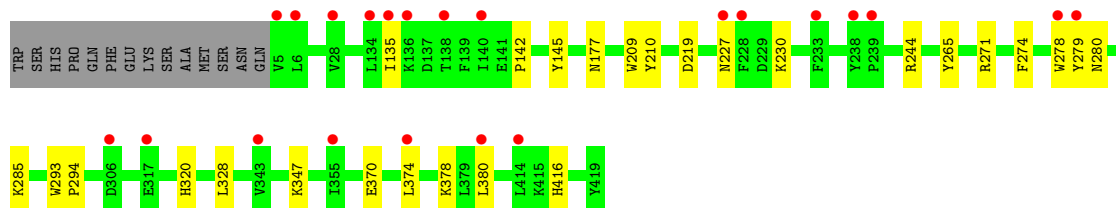
3 Residue-property plots [i](#)

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: CdmB from *Acetobacterium malicum* subsp. dehalogenans



- Molecule 1: CdmB from *Acetobacterium malicum* subsp. dehalogenans



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	69.51Å 85.79Å 155.80Å 90.00° 99.05° 90.00°	Depositor
Resolution (Å)	27.88 – 1.57 27.88 – 1.57	Depositor EDS
% Data completeness (in resolution range)	65.4 (27.88-1.57) 65.4 (27.88-1.57)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 1.57Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.173 , 0.195 0.180 , 0.198	Depositor DCC
R_{free} test set	4232 reflections (3.36%)	wwPDB-VP
Wilson B-factor (Å ²)	24.9	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 53.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7447	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, NA, GOL, K, EDO, PG4, ETE, PO4

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	0/3478	0.62	0/4716
1	B	0.48	0/3397	0.66	2/4611 (0.0%)
All	All	0.45	0/6875	0.64	2/9327 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	279	TYR	N-CA-CB	-7.08	100.30	110.57
1	B	209	TRP	N-CA-C	-6.83	103.76	111.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3389	0	3373	7	0
1	B	3310	0	3299	16	0
2	A	14	0	20	0	0
3	A	64	0	96	0	0
3	B	44	0	66	0	0
4	A	18	0	24	0	0
4	B	18	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	49	0	70	1	0
5	B	7	0	10	0	0
6	A	13	0	18	0	0
7	A	2	0	0	0	0
7	B	1	0	0	0	0
8	A	15	0	0	0	0
9	A	1	0	0	0	0
10	A	342	0	0	0	0
10	B	160	0	0	0	0
All	All	7447	0	7000	22	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 2.

All (22) 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:219:ASP:HB3	1:B:278[A]:TRP:CE3	2.44	0.53
1:A:244:ARG:NH1	1:A:247:GLU:OE1	2.46	0.49
1:A:180:LEU:HD13	1:B:177:ASN:HA	1.96	0.47
1:B:142:PRO:HA	1:B:145:TYR:CD2	2.50	0.47
1:B:370:GLU:H	1:B:370:GLU:CD	2.22	0.47
1:B:280:ASN:OD1	1:B:280:ASN:N	2.48	0.45
1:B:293:TRP:CZ2	1:B:328:LEU:HD21	2.53	0.43
1:B:374:LEU:HD11	1:B:378:LYS:CE	2.48	0.43
1:B:374:LEU:HD11	1:B:378:LYS:HE3	1.99	0.43
1:A:219:ASP:HB3	1:A:278:TRP:CE3	2.54	0.43
1:B:285:LYS:HE2	1:B:320:HIS:HB2	2.01	0.43
1:A:210:TYR:CD2	1:A:274:PHE:HB2	2.54	0.43
1:B:265:TYR:HD1	1:B:271:ARG:HG3	1.84	0.43
1:B:347:LYS:HE3	1:B:347:LYS:HB3	1.90	0.43
1:B:210:TYR:CD2	1:B:274:PHE:HB2	2.54	0.42
1:B:244:ARG:HD2	1:B:244:ARG:HA	1.80	0.42
1:A:323:ASP:OD1	1:A:323:ASP:C	2.63	0.42
1:B:227:ASN:HB3	1:B:230:LYS:HD2	2.02	0.42
1:A:342:ILE:HG12	5:A:510:PEG:H42	2.02	0.41
1:B:293:TRP:N	1:B:294:PRO:CD	2.83	0.41
1:A:37:PHE:HB3	1:A:38:PRO:HD3	2.02	0.40
1:B:380:LEU:HD23	1:B:416:HIS:C	2.47	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	423/429 (99%)	412 (97%)	11 (3%)	0	100	100
1	B	416/429 (97%)	405 (97%)	11 (3%)	0	100	100
All	All	839/858 (98%)	817 (97%)	22 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	367/368 (100%)	364 (99%)	3 (1%)	73	57
1	B	358/368 (97%)	357 (100%)	1 (0%)	86	79
All	All	725/736 (98%)	721 (99%)	4 (1%)	84	65

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	209	TRP
1	A	211[A]	MET
1	A	211[B]	MET
1	B	135	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	ASN
1	A	216	ASN
1	A	405	ASN
1	B	55	GLN
1	B	91	ASN
1	B	199	GLN
1	B	205	ASN
1	B	375	HIS
1	B	405	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 50 ligands modelled in this entry, 4 are monoatomic - leaving 46 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	$\# Z > 2$
3	EDO	A	505	-	3,3,3	0.49	0	2,2,2	0.32	0
3	EDO	A	524	-	3,3,3	0.07	0	2,2,2	0.24	0
3	EDO	B	511[B]	-	3,3,3	0.06	0	2,2,2	0.19	0
3	EDO	A	523	-	3,3,3	0.14	0	2,2,2	0.29	0
3	EDO	B	510	-	3,3,3	0.05	0	2,2,2	0.18	0
2	ETE	A	501	9	13,13,13	0.34	0	12,12,12	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PEG	A	506	-	6,6,6	0.10	0	5,5,5	0.09	0
5	PEG	B	507	-	6,6,6	0.12	0	5,5,5	0.08	0
3	EDO	A	528	-	3,3,3	0.06	0	2,2,2	0.20	0
3	EDO	B	508	-	3,3,3	0.06	0	2,2,2	0.26	0
3	EDO	A	514	-	3,3,3	0.48	0	2,2,2	0.34	0
3	EDO	A	512	-	3,3,3	0.48	0	2,2,2	0.46	0
3	EDO	B	505	-	3,3,3	0.54	0	2,2,2	0.21	0
4	GOL	B	503	-	5,5,5	0.09	0	5,5,5	0.33	0
8	PO4	A	533	-	4,4,4	0.77	0	6,6,6	0.52	0
4	GOL	A	503	-	5,5,5	0.62	0	5,5,5	1.09	0
3	EDO	B	515	-	3,3,3	0.07	0	2,2,2	0.19	0
3	EDO	B	512	-	3,3,3	0.06	0	2,2,2	0.19	0
5	PEG	A	516	-	6,6,6	0.11	0	5,5,5	0.09	0
3	EDO	A	518	-	3,3,3	0.05	0	2,2,2	0.18	0
8	PO4	A	532[B]	7	4,4,4	1.10	0	6,6,6	0.72	0
3	EDO	B	513	-	3,3,3	0.05	0	2,2,2	0.25	0
3	EDO	A	519	-	3,3,3	0.05	0	2,2,2	0.23	0
3	EDO	B	506	-	3,3,3	0.47	0	2,2,2	0.32	0
3	EDO	A	527	-	3,3,3	0.07	0	2,2,2	0.21	0
3	EDO	B	514	-	3,3,3	0.05	0	2,2,2	0.17	0
8	PO4	A	531[A]	7	4,4,4	0.69	0	6,6,6	0.43	0
5	PEG	A	510	-	6,6,6	0.11	0	5,5,5	0.07	0
5	PEG	A	515	-	6,6,6	0.11	0	5,5,5	0.15	0
4	GOL	A	521	-	5,5,5	0.09	0	5,5,5	0.32	0
4	GOL	B	501	-	5,5,5	0.74	0	5,5,5	0.99	0
3	EDO	A	520	-	3,3,3	0.08	0	2,2,2	0.33	0
5	PEG	A	517	-	6,6,6	0.11	0	5,5,5	0.08	0
3	EDO	A	513	-	3,3,3	0.47	0	2,2,2	0.40	0
3	EDO	A	504	-	3,3,3	0.52	0	2,2,2	0.25	0
4	GOL	A	509	-	5,5,5	0.81	0	5,5,5	0.82	0
6	PG4	A	511[A]	-	12,12,12	0.15	0	11,11,11	0.21	0
3	EDO	A	502	-	3,3,3	0.65	0	2,2,2	0.20	0
3	EDO	B	502	-	3,3,3	0.47	0	2,2,2	0.33	0
3	EDO	A	508[A]	-	3,3,3	0.51	0	2,2,2	0.31	0
5	PEG	A	507	-	6,6,6	0.18	0	5,5,5	0.07	0
5	PEG	A	526	-	6,6,6	0.13	0	5,5,5	0.08	0
3	EDO	A	525	-	3,3,3	0.06	0	2,2,2	0.18	0
4	GOL	B	504	-	5,5,5	0.79	0	5,5,5	0.91	0
3	EDO	A	522	-	3,3,3	0.06	0	2,2,2	0.18	0
3	EDO	B	509	-	3,3,3	0.05	0	2,2,2	0.20	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
3	EDO	A	505	-	-	1/1/1/1	-
3	EDO	A	524	-	-	1/1/1/1	-
3	EDO	B	511[B]	-	-	0/1/1/1	-
3	EDO	A	523	-	-	1/1/1/1	-
3	EDO	B	510	-	-	1/1/1/1	-
2	ETE	A	501	9	-	1/11/11/11	-
5	PEG	A	506	-	-	0/4/4/4	-
5	PEG	B	507	-	-	1/4/4/4	-
3	EDO	A	528	-	-	1/1/1/1	-
3	EDO	B	508	-	-	1/1/1/1	-
3	EDO	A	514	-	-	0/1/1/1	-
3	EDO	A	512	-	-	1/1/1/1	-
3	EDO	B	505	-	-	0/1/1/1	-
4	GOL	B	503	-	-	3/4/4/4	-
4	GOL	A	503	-	-	0/4/4/4	-
3	EDO	B	515	-	-	1/1/1/1	-
3	EDO	B	512	-	-	1/1/1/1	-
5	PEG	A	516	-	-	2/4/4/4	-
3	EDO	A	518	-	-	0/1/1/1	-
3	EDO	B	513	-	-	1/1/1/1	-
3	EDO	A	519	-	-	1/1/1/1	-
3	EDO	B	506	-	-	1/1/1/1	-
3	EDO	A	527	-	-	0/1/1/1	-
3	EDO	B	514	-	-	1/1/1/1	-
5	PEG	A	510	-	-	3/4/4/4	-
5	PEG	A	515	-	-	1/4/4/4	-
4	GOL	A	521	-	-	2/4/4/4	-
4	GOL	B	501	-	-	4/4/4/4	-
3	EDO	A	520	-	-	1/1/1/1	-
5	PEG	A	517	-	-	3/4/4/4	-
3	EDO	A	513	-	-	1/1/1/1	-
3	EDO	A	504	-	-	1/1/1/1	-
4	GOL	A	509	-	-	2/4/4/4	-
6	PG4	A	511[A]	-	-	7/10/10/10	-
3	EDO	A	502	-	-	1/1/1/1	-
3	EDO	B	502	-	-	1/1/1/1	-
3	EDO	A	508[A]	-	-	0/1/1/1	-
5	PEG	A	507	-	-	3/4/4/4	-
5	PEG	A	526	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	525	-	-	1/1/1/1	-
4	GOL	B	504	-	-	1/4/4/4	-
3	EDO	A	522	-	-	1/1/1/1	-
3	EDO	B	509	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	509	GOL	O1-C1-C2-C3
4	B	501	GOL	O1-C1-C2-C3
4	B	501	GOL	C1-C2-C3-O3
4	B	503	GOL	C1-C2-C3-O3
5	A	507	PEG	O2-C3-C4-O4
6	A	511[A]	PG4	O1-C1-C2-O2
3	B	515	EDO	O1-C1-C2-O2
5	A	526	PEG	O1-C1-C2-O2
6	A	511[A]	PG4	O4-C7-C8-O5
4	A	521	GOL	O1-C1-C2-C3
6	A	511[A]	PG4	O2-C3-C4-O3
4	B	501	GOL	O1-C1-C2-O2
4	B	503	GOL	O2-C2-C3-O3
3	A	519	EDO	O1-C1-C2-O2
3	A	528	EDO	O1-C1-C2-O2
3	B	502	EDO	O1-C1-C2-O2
5	A	516	PEG	O1-C1-C2-O2
4	A	521	GOL	O1-C1-C2-O2
5	A	517	PEG	O2-C3-C4-O4
3	A	505	EDO	O1-C1-C2-O2
3	B	509	EDO	O1-C1-C2-O2
4	A	509	GOL	O1-C1-C2-O2
4	B	504	GOL	O2-C2-C3-O3
3	A	502	EDO	O1-C1-C2-O2
3	A	522	EDO	O1-C1-C2-O2
3	A	525	EDO	O1-C1-C2-O2
3	B	506	EDO	O1-C1-C2-O2
3	B	510	EDO	O1-C1-C2-O2
3	B	512	EDO	O1-C1-C2-O2
3	B	513	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	A	507	PEG	O1-C1-C2-O2
5	A	516	PEG	O2-C3-C4-O4
6	A	511[A]	PG4	C5-C6-O4-C7
5	A	517	PEG	C4-C3-O2-C2
5	B	507	PEG	C1-C2-O2-C3
6	A	511[A]	PG4	C4-C3-O2-C2
6	A	511[A]	PG4	C6-C5-O3-C4
4	B	501	GOL	O2-C2-C3-O3
5	A	510	PEG	O1-C1-C2-O2
3	A	523	EDO	O1-C1-C2-O2
3	A	524	EDO	O1-C1-C2-O2
5	A	517	PEG	C1-C2-O2-C3
5	A	507	PEG	C4-C3-O2-C2
5	A	510	PEG	C4-C3-O2-C2
5	A	510	PEG	C1-C2-O2-C3
2	A	501	ETE	C15-C25-OH5-C14
3	B	508	EDO	O1-C1-C2-O2
5	A	526	PEG	O2-C3-C4-O4
3	A	504	EDO	O1-C1-C2-O2
3	A	512	EDO	O1-C1-C2-O2
3	A	513	EDO	O1-C1-C2-O2
3	A	520	EDO	O1-C1-C2-O2
4	B	503	GOL	O1-C1-C2-O2
6	A	511[A]	PG4	C8-C7-O4-C6
5	A	515	PEG	O1-C1-C2-O2
3	B	514	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	510	PEG	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	423/429 (98%)	0.04	16 (3%) 44 55	11, 26, 41, 95	4 (0%)
1	B	415/429 (96%)	0.60	22 (5%) 32 43	15, 43, 67, 100	3 (0%)
All	All	838/858 (97%)	0.32	38 (4%) 38 50	11, 32, 63, 100	7 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	5	VAL	6.0
1	A	-6	PRO	5.6
1	A	134	LEU	5.6
1	A	-9	TRP	5.4
1	A	135	ILE	5.2
1	A	-4	PHE	4.8
1	B	279	TYR	4.6
1	B	278[A]	TRP	4.5
1	A	137	ASP	4.3
1	A	278	TRP	3.9
1	A	-2	LYS	3.7
1	B	228	PHE	3.7
1	A	6	LEU	3.5
1	A	-5	GLN	3.5
1	A	-7	HIS	3.4
1	B	135	ILE	3.3
1	B	28	VAL	3.2
1	A	136	LYS	3.0
1	A	-1	SER	3.0
1	A	-8	SER	2.9
1	B	140	ILE	2.6
1	B	238	TYR	2.5
1	A	-3	GLU	2.5
1	A	271[A]	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	355	ILE	2.5
1	B	138	THR	2.5
1	B	306	ASP	2.5
1	B	136	LYS	2.4
1	B	374	LEU	2.4
1	B	233	PHE	2.4
1	B	343	VAL	2.4
1	B	227	ASN	2.4
1	B	239	PRO	2.3
1	B	134	LEU	2.3
1	B	414	LEU	2.2
1	B	317	GLU	2.2
1	B	6	LEU	2.1
1	B	380	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EDO	A	520	4/4	0.64	0.17	56,58,60,65	0
3	EDO	A	522	4/4	0.65	0.19	59,60,66,67	0
4	GOL	B	504	6/6	0.68	0.16	61,69,75,77	0
3	EDO	A	527	4/4	0.70	0.17	51,51,52,57	0
3	EDO	A	518	4/4	0.70	0.16	60,61,62,72	0
3	EDO	B	508	4/4	0.72	0.19	43,46,50,63	0
4	GOL	A	521	6/6	0.72	0.17	39,53,54,59	0
3	EDO	A	525	4/4	0.72	0.13	53,55,60,62	0
5	PEG	A	507	7/7	0.72	0.18	47,48,56,57	0

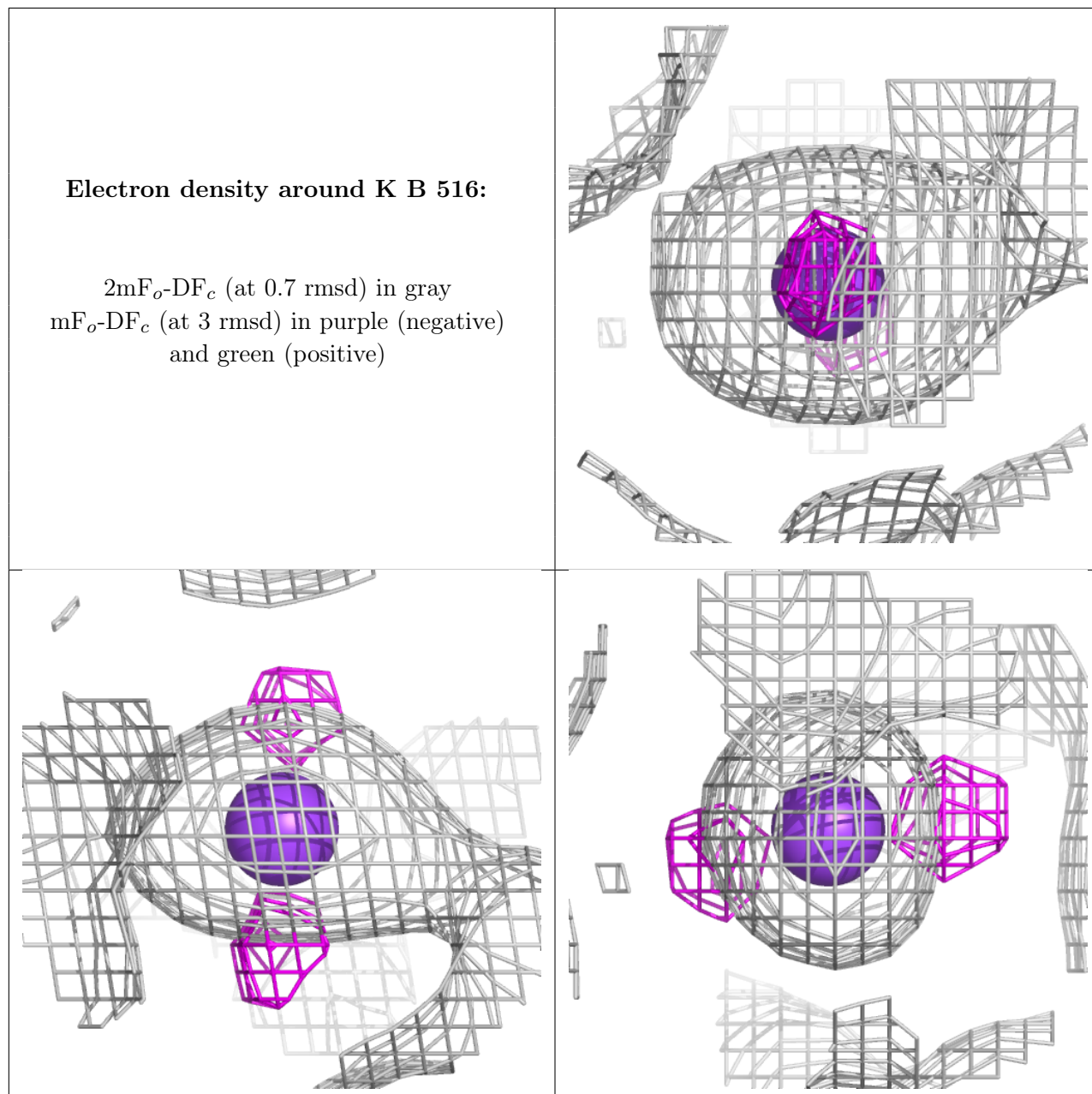
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	PEG	A	510	7/7	0.72	0.18	39,42,59,61	0
3	EDO	A	528	4/4	0.73	0.18	54,55,59,65	0
3	EDO	B	515	4/4	0.74	0.16	58,60,63,67	0
3	EDO	B	506	4/4	0.75	0.17	54,58,60,72	0
3	EDO	B	512	4/4	0.75	0.16	58,60,60,61	0
4	GOL	B	503	6/6	0.75	0.18	42,48,49,60	0
5	PEG	A	526	7/7	0.75	0.17	50,57,70,74	0
3	EDO	A	523	4/4	0.76	0.14	56,60,61,67	0
3	EDO	B	514	4/4	0.77	0.15	56,57,57,62	0
3	EDO	B	513	4/4	0.78	0.16	51,54,61,63	0
3	EDO	A	512	4/4	0.79	0.17	49,51,53,54	0
3	EDO	B	509	4/4	0.79	0.13	57,59,59,68	0
3	EDO	A	524	4/4	0.80	0.15	37,51,52,55	0
3	EDO	B	511[B]	4/4	0.81	0.13	53,55,60,61	0
3	EDO	B	502	4/4	0.82	0.20	50,53,63,72	0
5	PEG	A	516	7/7	0.82	0.13	46,47,58,59	0
4	GOL	A	509	6/6	0.82	0.13	40,48,57,57	0
5	PEG	A	517	7/7	0.83	0.17	36,44,53,55	0
5	PEG	A	515	7/7	0.84	0.12	50,51,53,56	0
3	EDO	B	510	4/4	0.84	0.13	61,63,64,66	0
8	PO4	A	533	5/5	0.84	0.10	37,48,60,61	0
5	PEG	A	506	7/7	0.85	0.13	38,46,50,58	0
3	EDO	A	505	4/4	0.85	0.12	45,46,59,60	0
3	EDO	A	502	4/4	0.86	0.16	29,37,46,46	0
5	PEG	B	507	7/7	0.86	0.12	48,55,55,57	0
6	PG4	A	511[A]	13/13	0.86	0.11	32,35,41,44	13
3	EDO	A	514	4/4	0.86	0.12	49,55,60,60	0
3	EDO	A	519	4/4	0.87	0.13	46,49,52,56	0
3	EDO	A	508[A]	4/4	0.87	0.14	52,54,54,55	4
4	GOL	B	501	6/6	0.87	0.13	26,40,48,49	0
3	EDO	A	513	4/4	0.87	0.12	36,37,39,42	0
8	PO4	A	531[A]	5/5	0.87	0.12	34,35,41,49	5
4	GOL	A	503	6/6	0.87	0.16	22,36,45,54	0
2	ETE	A	501	14/14	0.89	0.10	24,31,40,44	0
3	EDO	B	505	4/4	0.89	0.11	43,46,50,51	0
3	EDO	A	504	4/4	0.90	0.12	52,55,55,58	0
8	PO4	A	532[B]	5/5	0.93	0.09	31,33,36,46	5
7	K	B	516	1/1	0.96	0.07	34,34,34,34	0
7	K	A	529	1/1	0.97	0.04	23,23,23,23	0
9	NA	A	534	1/1	0.98	0.03	21,21,21,21	0
7	K	A	530	1/1	0.99	0.02	18,18,18,18	0

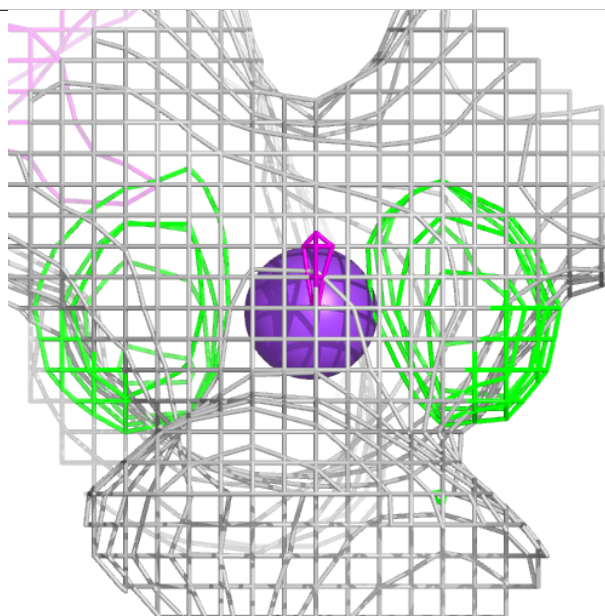
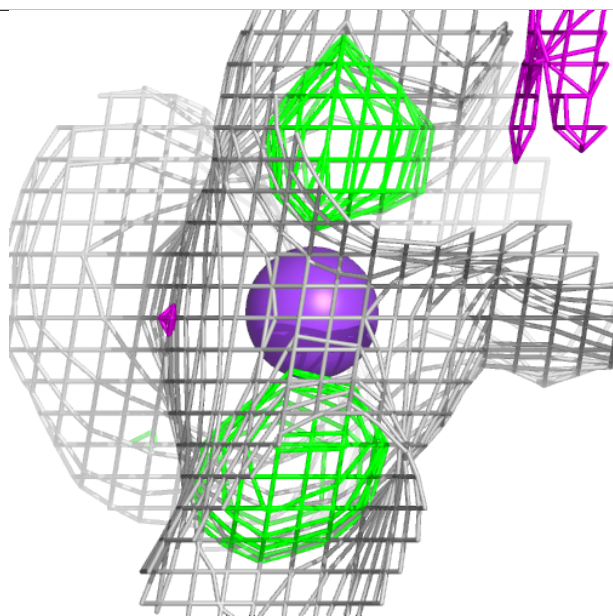
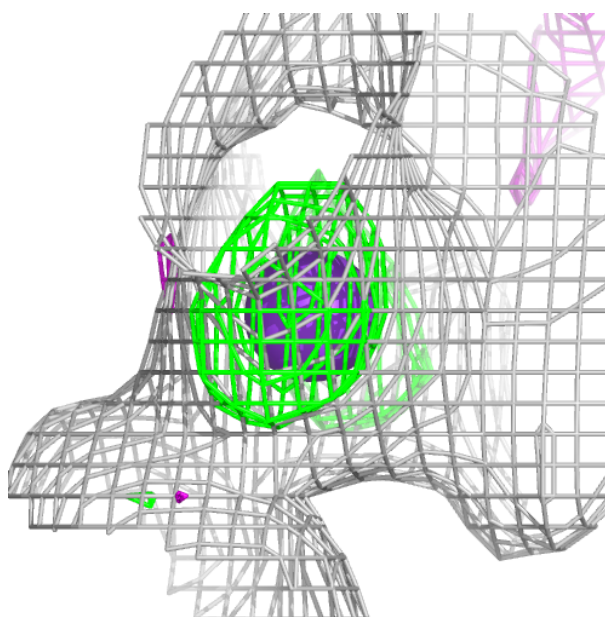
The following is a graphical depiction of the model fit to experimental electron density of all

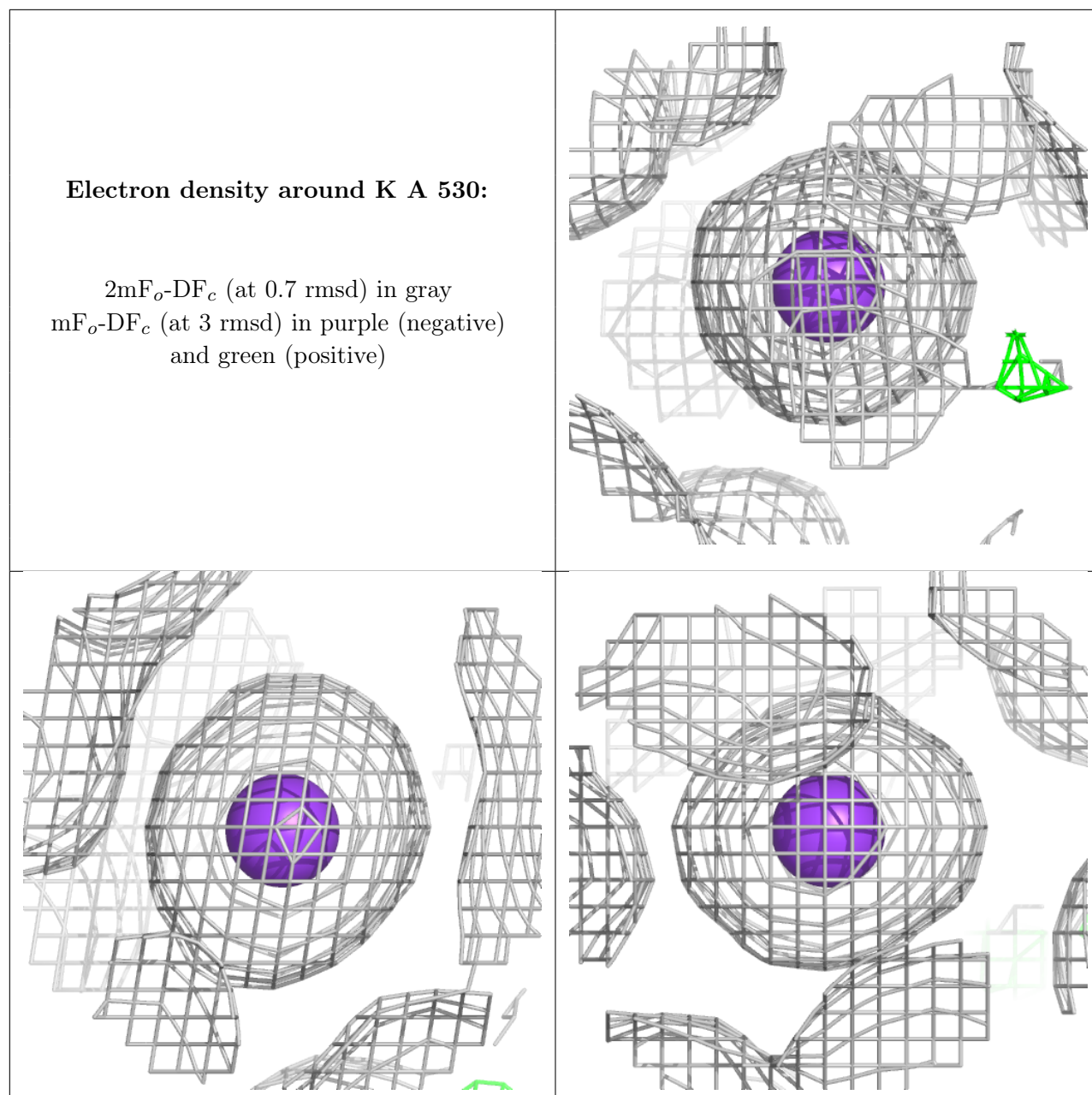
instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around K A 529:

$2mF_o-DF_c$ (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.