



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 29, 2026 – 11:19 am BST

PDB ID : 9R83 / pdb_00009r83
Title : KOD-H4 DNA polymerase mutant in a ternary complex with HNA:DNA containing six HNA nucleotides and a 2',3'-dideoxycytidine at the 3'-end of the DNA primer complexed to a natural dATP in the active site
Authors : Gutfreund, C.; Betz, K.
Deposited on : 2025-05-15
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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)
Xtrriage (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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

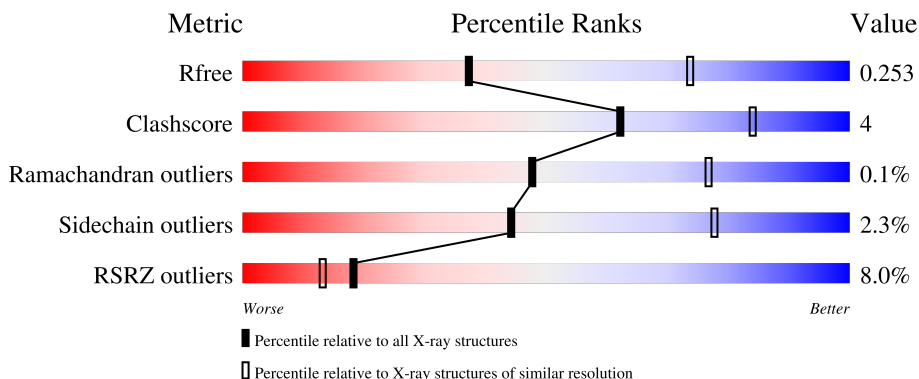
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	C	12	92% (green), 8% (yellow)
1	F	12	92% (green), 8% (yellow)
2	A	774	10% (red), 84% (green), 12% (yellow), 6% (grey)
2	B	774	6% (red), 85% (green), 11% (yellow), 1% (grey)

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Mol	Chain	Length	Quality of chain
3	D	16	
3	E	16	

2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 13577 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 DNA chain called DNA (5'-D(*GP*AP*CP*CP*AP*CP*GP*GP*CP*CP*AP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	F	12	Total 239	C 114	N 48	O 66	P 11	0	0	0
1	C	12	Total 239	C 114	N 48	O 66	P 11	0	0	0

- Molecule 2 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	748	Total 6142	C 3955	N 1041	O 1129	S 17	0	1	0
2	B	748	Total 6148	C 3955	N 1044	O 1132	S 17	0	2	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	93	GLN	VAL	engineered mutation	UNP D0VWU9
A	114	THR	ILE	engineered mutation	UNP D0VWU9
A	141	ALA	ASP	engineered mutation	UNP D0VWU9
A	143	ALA	GLU	engineered mutation	UNP D0VWU9
A	147	HIS	GLU	conflict	UNP D0VWU9
A	383	LYS	SER	engineered mutation	UNP D0VWU9
A	429	GLY	LYS	engineered mutation	UNP D0VWU9
A	445	LEU	PHE	engineered mutation	UNP D0VWU9
A	485	LEU	ALA	engineered mutation	UNP D0VWU9
A	493	VAL	TYR	engineered mutation	UNP D0VWU9
A	496	HIS	TYR	engineered mutation	UNP D0VWU9
A	497	MET	TYR	engineered mutation	UNP D0VWU9
A	499	PHE	TYR	engineered mutation	UNP D0VWU9
A	500	GLU	ALA	engineered mutation	UNP D0VWU9
A	501	ASN	ARG	engineered mutation	UNP D0VWU9

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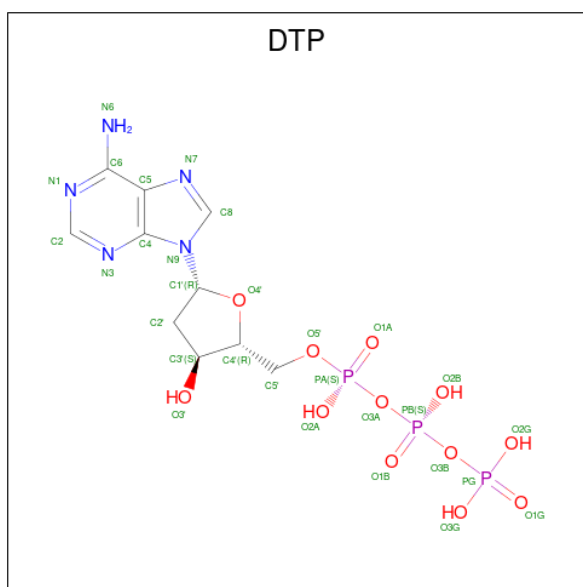
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Chain	Residue	Modelled	Actual	Comment	Reference
A	521	LEU	ILE	engineered mutation	UNP D0VWU9
A	584	LYS	GLU	conflict	UNP D0VWU9
A	664	LYS	GLU	engineered mutation	UNP D0VWU9
A	726	ARG	LYS	engineered mutation	UNP D0VWU9
A	735	LYS	ASN	engineered mutation	UNP D0VWU9
B	93	GLN	VAL	engineered mutation	UNP D0VWU9
B	114	THR	ILE	engineered mutation	UNP D0VWU9
B	141	ALA	ASP	engineered mutation	UNP D0VWU9
B	143	ALA	GLU	engineered mutation	UNP D0VWU9
B	147	HIS	GLU	conflict	UNP D0VWU9
B	383	LYS	SER	engineered mutation	UNP D0VWU9
B	429	GLY	LYS	engineered mutation	UNP D0VWU9
B	445	LEU	PHE	engineered mutation	UNP D0VWU9
B	485	LEU	ALA	engineered mutation	UNP D0VWU9
B	493	VAL	TYR	engineered mutation	UNP D0VWU9
B	496	HIS	TYR	engineered mutation	UNP D0VWU9
B	497	MET	TYR	engineered mutation	UNP D0VWU9
B	499	PHE	TYR	engineered mutation	UNP D0VWU9
B	500	GLU	ALA	engineered mutation	UNP D0VWU9
B	501	ASN	ARG	engineered mutation	UNP D0VWU9
B	521	LEU	ILE	engineered mutation	UNP D0VWU9
B	584	LYS	GLU	conflict	UNP D0VWU9
B	664	LYS	GLU	engineered mutation	UNP D0VWU9
B	726	ARG	LYS	engineered mutation	UNP D0VWU9
B	735	LYS	ASN	engineered mutation	UNP D0VWU9

- Molecule 3 is a DNA chain called DNA (5'-D(P*(6HA)P*(6HC)P*(6HT)P*(6HG)P*(6HT)P*GP*GP*CP*CP*GP*TP*GP*GP*TP*C)-3').

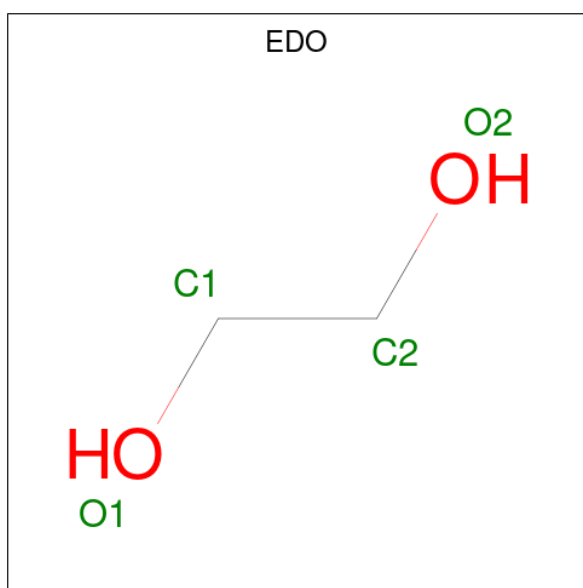
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	15	Total	C	N	O	P	0	0	0
			314	151	55	93	15			
3	E	15	Total	C	N	O	P	0	0	0
			314	151	55	93	15			

- Molecule 4 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (CCD ID: DTP) (formula: C₁₀H₁₆N₅O₁₂P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	A	1	Total	C	N	O	P	0	0
				30	10	5	12		
4	B	1	Total	C	N	O	P	0	0
				30	10	5	12		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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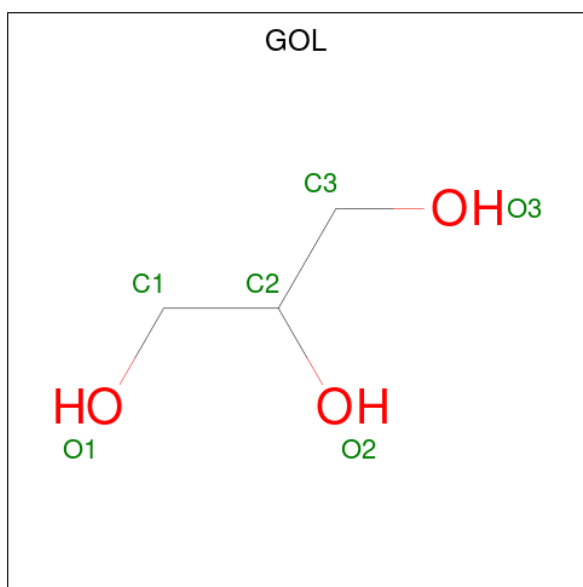
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Ca	0	0
			2	2		
6	B	2	Total	Ca	0	0
			2	2		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	29	Total	O	0	0
			29	29		
8	B	40	Total	O	0	0
			40	40		
8	D	1	Total	O	0	0
			1	1		
8	E	3	Total	O	0	0
			3	3		

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: DNA (5'-D(*GP*AP*CP*CP*AP*CP*GP*GP*CP*CP*AP*C)-3')

Chain F: 




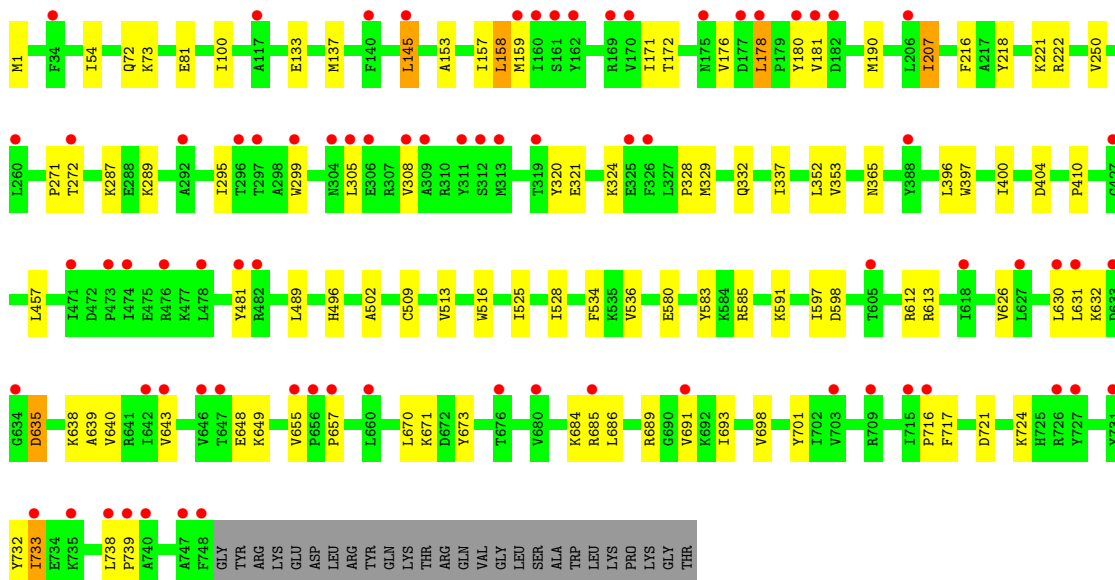
- Molecule 1: DNA (5'-D(*GP*AP*CP*CP*AP*CP*GP*GP*CP*CP*AP*C)-3')

Chain C: 




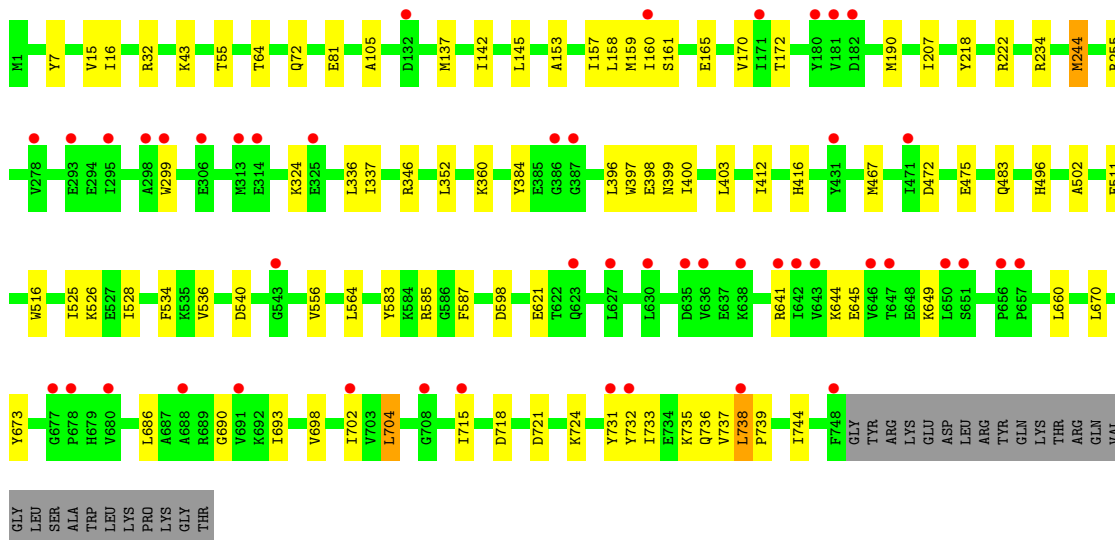
- Molecule 2: DNA polymerase

Chain A: 

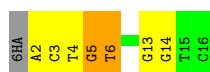


- Molecule 2: DNA polymerase

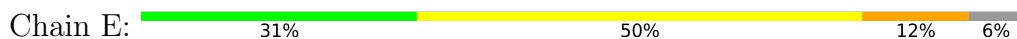
Chain B: 



● Molecule 3: DNA (5'-D(P*(6HA)P*(6HC)P*(6HT)P*(6HG)P*(6HT)P*GP*GP*CP*CP*GP*TP*GP*GP*TP*C)-3')



● Molecule 3: DNA (5'-D(P*(6HA)P*(6HC)P*(6HT)P*(6HG)P*(6HT)P*GP*GP*CP*CP*GP*TP*GP*GP*TP*C)-3')



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	108.99Å 142.00Å 149.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.12 – 2.80 45.12 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.1 (45.12-2.80) 97.4 (45.12-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.81Å)	Xtrriage
Refinement program	PHENIX 2.0_5936	Depositor
R, R_{free}	0.217 , 0.253 0.217 , 0.253	Depositor DCC
R_{free} test set	2726 reflections (2.46%)	wwPDB-VP
Wilson B-factor (Å ²)	58.2	Xtrriage
Anisotropy	0.403	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 66.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.000 for -h,l,k	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13577	wwPDB-VP
Average B, all atoms (Å ²)	83.0	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 76.73 % 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 9.8145e-07. 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 6HA, 6HG, CA, EDO, 6HC, DTP, 6HT

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	C	0.18	0/268	0.30	0/410
1	F	0.17	0/268	0.28	0/410
2	A	0.08	0/6279	0.24	0/8471
2	B	0.09	0/6283	0.26	1/8474 (0.0%)
3	D	0.24	0/231	0.41	0/355
3	E	0.21	0/231	0.42	0/355
All	All	0.10	0/13560	0.26	1/18475 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	540	ASP	CB-CA-C	-5.30	108.74	116.53

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	C	239	0	132	1	0
1	F	239	0	132	1	0
2	A	6142	0	6197	51	0
2	B	6148	0	6205	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	314	0	180	4	0
3	E	314	0	180	6	0
4	A	30	0	10	0	0
4	B	30	0	10	1	0
5	A	8	0	12	0	0
5	B	16	0	24	1	0
5	D	4	0	6	0	0
5	E	4	0	6	0	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
7	B	6	0	8	0	0
7	D	6	0	8	0	0
8	A	29	0	0	0	0
8	B	40	0	0	0	0
8	D	1	0	0	0	0
8	E	3	0	0	0	0
All	All	13577	0	13110	110	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 4.

The worst 5 of 110 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)
2:A:321:GLU:HA	2:A:324:LYS:HD3	1.70	0.73
2:A:635:ASP:HB3	2:A:638:LYS:HB2	1.73	0.68
2:B:145:LEU:HB2	2:B:158:LEU:HD21	1.75	0.67
2:A:337:ILE:HG13	2:A:352:LEU:HD22	1.76	0.67
2:A:404:ASP:HB3	2:A:580:GLU:HG3	1.78	0.65

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	
2	A	747/774 (96%)	708 (95%)	38 (5%)	1 (0%)	48	77
2	B	748/774 (97%)	710 (95%)	37 (5%)	1 (0%)	48	77
All	All	1495/1548 (97%)	1418 (95%)	75 (5%)	2 (0%)	48	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	738	LEU
2	A	693	ILE

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	
2	A	652/673 (97%)	633 (97%)	19 (3%)	37	73
2	B	653/673 (97%)	642 (98%)	11 (2%)	53	83
All	All	1305/1346 (97%)	1275 (98%)	30 (2%)	44	78

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	689	ARG
2	B	733	ILE
2	A	732	TYR
2	B	738	LEU
2	B	698	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	59	HIS

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Mol	Chain	Res	Type
2	B	72	GLN
2	B	339	GLN
2	B	399	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](#)

10 non-standard protein/DNA/RNA residues are modelled in this entry.

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	6HT	E	4	3	19,22,23	4.01	10 (52%)	24,31,34	2.20	7 (29%)
3	6HT	E	6	3,1	19,22,23	3.96	11 (57%)	24,31,34	2.21	8 (33%)
3	6HC	E	3	3	18,21,22	3.44	11 (61%)	21,29,32	1.89	4 (19%)
3	6HG	E	5	3,1	22,25,26	2.80	12 (54%)	28,36,39	2.38	11 (39%)
3	6HA	E	2	3	21,24,25	1.83	6 (28%)	27,34,37	3.04	11 (40%)
3	6HT	D	4	3	19,22,23	4.00	10 (52%)	24,31,34	2.24	9 (37%)
3	6HC	D	3	3	18,21,22	3.44	11 (61%)	21,29,32	1.93	4 (19%)
3	6HG	D	5	3,1	22,25,26	2.81	11 (50%)	28,36,39	2.37	11 (39%)
3	6HT	D	6	3,1	19,22,23	3.97	10 (52%)	24,31,34	2.31	8 (33%)
3	6HA	D	2	3	21,24,25	1.82	6 (28%)	27,34,37	3.02	11 (40%)

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	6HT	E	4	3	-	3/7/22/23	0/2/2/2
3	6HT	E	6	3,1	-	2/7/22/23	0/2/2/2
3	6HC	E	3	3	-	0/7/22/23	0/2/2/2
3	6HG	E	5	3,1	-	0/7/22/23	0/3/3/3
3	6HA	E	2	3	-	3/7/22/23	0/3/3/3
3	6HT	D	4	3	-	3/7/22/23	0/2/2/2
3	6HC	D	3	3	-	0/7/22/23	0/2/2/2
3	6HG	D	5	3,1	-	0/7/22/23	0/3/3/3
3	6HT	D	6	3,1	-	2/7/22/23	0/2/2/2
3	6HA	D	2	3	-	3/7/22/23	0/3/3/3

The worst 5 of 98 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	4	6HT	C6-C5	9.16	1.49	1.34
3	D	4	6HT	C6-C5	9.08	1.49	1.34
3	D	6	6HT	C6-C5	9.03	1.49	1.34
3	E	6	6HT	C6-C5	8.98	1.49	1.34
3	D	6	6HT	C2-N1	7.92	1.51	1.38

The worst 5 of 84 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2	6HA	N6-C6-N1	-7.04	102.93	118.35
3	D	2	6HA	N6-C6-N1	-7.02	102.98	118.35
3	E	2	6HA	C5-C6-N6	6.28	137.09	123.43
3	D	2	6HA	C5-C6-N6	6.25	137.03	123.43
3	D	3	6HC	C3'-C2'-C1'	6.10	119.54	112.39

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	2	6HA	O4'-C4'-C5'-O5'
3	D	2	6HA	C3'-C4'-C5'-O5'
3	E	2	6HA	O4'-C4'-C5'-O5'
3	E	2	6HA	C3'-C4'-C5'-O5'
3	D	4	6HT	O4'-C4'-C5'-O5'

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	6	6HT	3	0
3	E	5	6HG	3	0
3	D	5	6HG	3	0
3	D	6	6HT	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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$
5	EDO	B	805	-	3,3,3	0.47	0	2,2,2	0.33	0
5	EDO	A	802	-	3,3,3	0.47	0	2,2,2	0.31	0
4	DTP	B	806	6	28,32,32	3.04	9 (32%)	42,50,50	2.44	15 (35%)
7	GOL	D	102	-	5,5,5	0.34	0	5,5,5	0.38	0
5	EDO	D	101	-	3,3,3	0.48	0	2,2,2	0.32	0
4	DTP	A	801	6	28,32,32	3.04	9 (32%)	42,50,50	2.44	15 (35%)
5	EDO	B	803	-	3,3,3	0.47	0	2,2,2	0.32	0
5	EDO	B	802	-	3,3,3	0.47	0	2,2,2	0.34	0
5	EDO	B	804	-	3,3,3	0.48	0	2,2,2	0.28	0
7	GOL	B	801	-	5,5,5	0.32	0	5,5,5	0.40	0
5	EDO	E	101	-	3,3,3	0.47	0	2,2,2	0.34	0
5	EDO	A	803	-	3,3,3	0.48	0	2,2,2	0.34	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
5	EDO	B	805	-	-	1/1/1/1	-
5	EDO	A	802	-	-	1/1/1/1	-
4	DTP	B	806	6	-	8/22/34/34	0/3/3/3
7	GOL	D	102	-	-	0/4/4/4	-
5	EDO	D	101	-	-	0/1/1/1	-
4	DTP	A	801	6	-	7/22/34/34	0/3/3/3
5	EDO	B	803	-	-	0/1/1/1	-
5	EDO	B	802	-	-	1/1/1/1	-
5	EDO	B	804	-	-	0/1/1/1	-
7	GOL	B	801	-	-	1/4/4/4	-
5	EDO	E	101	-	-	1/1/1/1	-
5	EDO	A	803	-	-	1/1/1/1	-

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	806	DTP	C2'-C3'	-11.43	1.22	1.52
4	A	801	DTP	C2'-C3'	-11.40	1.22	1.52
4	A	801	DTP	O4'-C1'	-4.95	1.31	1.42
4	B	806	DTP	O4'-C1'	-4.89	1.31	1.42
4	A	801	DTP	C6-N6	4.52	1.45	1.34

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	801	DTP	C1'-N9-C8	-5.84	105.51	126.52
4	A	801	DTP	N3-C2-N1	-5.74	119.62	128.60
4	B	806	DTP	C1'-N9-C8	-5.72	105.97	126.52
4	B	806	DTP	N3-C2-N1	-5.70	119.69	128.60
4	A	801	DTP	N9-C8-N7	-4.96	107.13	113.91

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

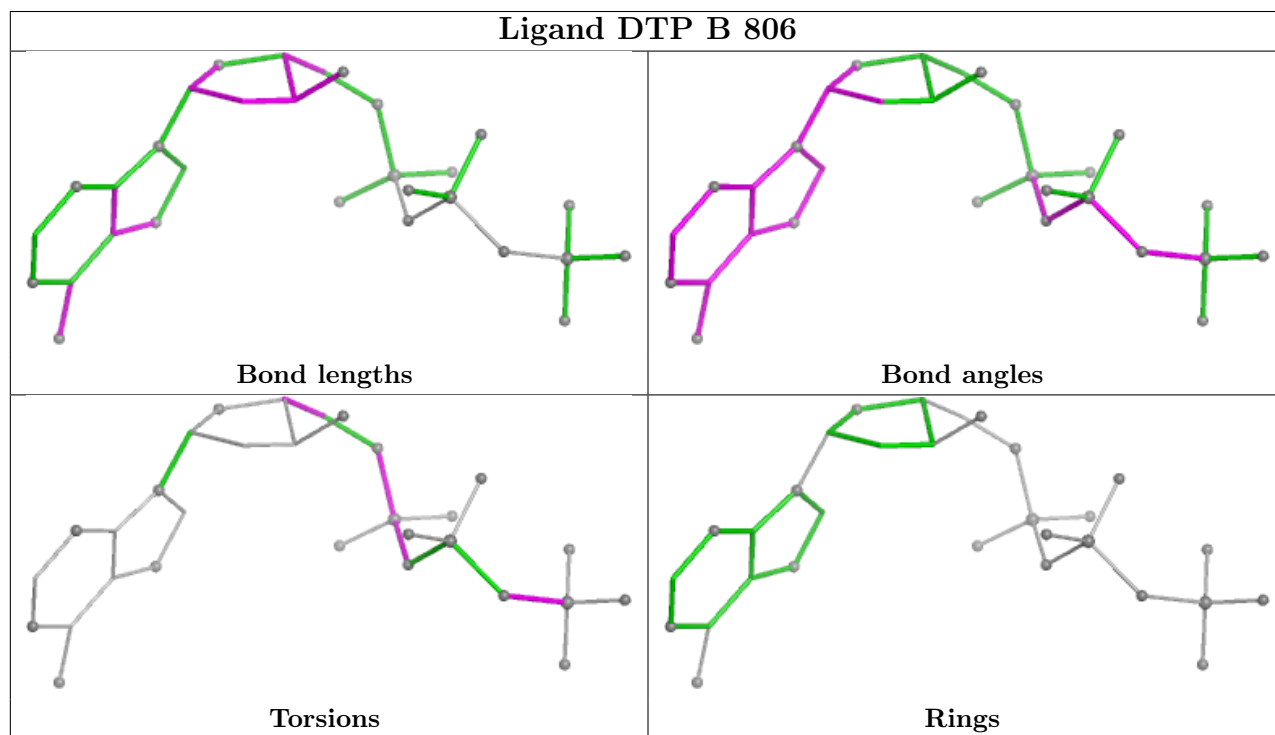
Mol	Chain	Res	Type	Atoms
4	A	801	DTP	PB-O3B-PG-O3G
4	A	801	DTP	C5'-O5'-PA-O2A
4	B	806	DTP	PB-O3B-PG-O3G
4	B	806	DTP	C5'-O5'-PA-O2A
4	A	801	DTP	O4'-C4'-C5'-O5'

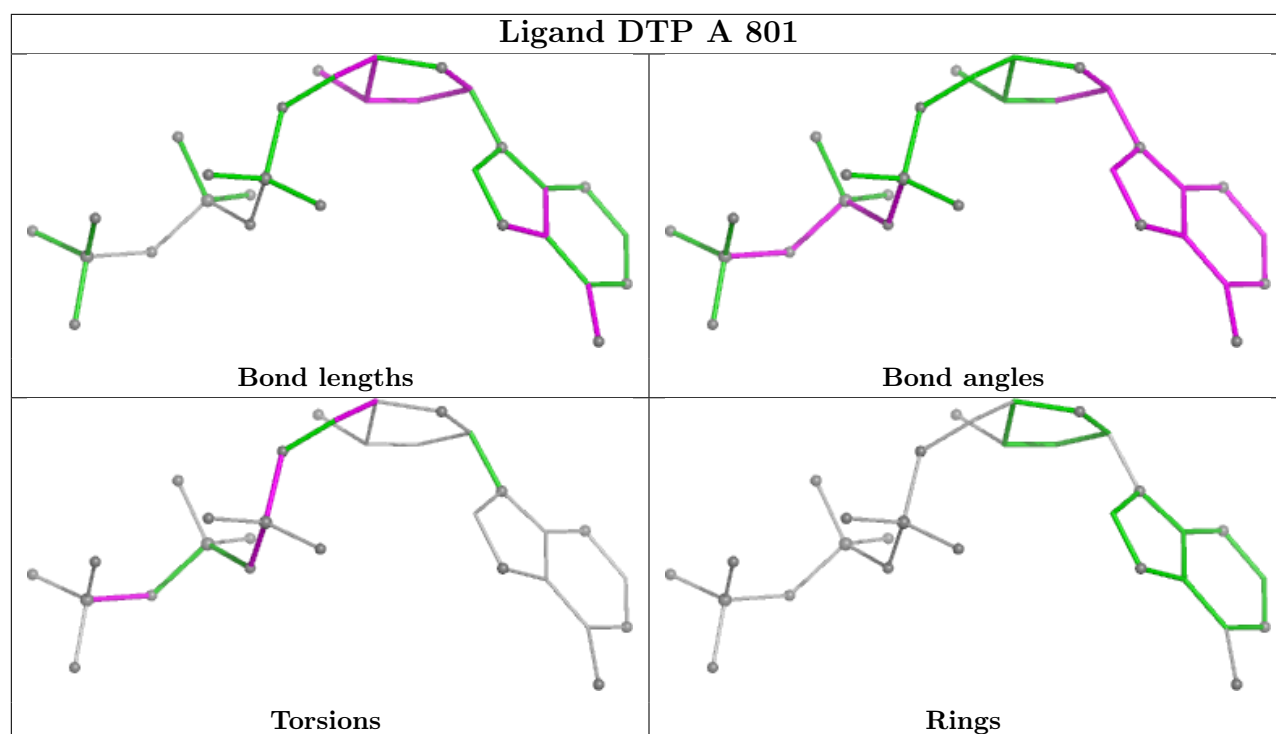
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	805	EDO	1	0
4	B	806	DTP	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	C	12/12 (100%)	-0.13	0 100 100	60, 87, 124, 129	0
1	F	12/12 (100%)	0.13	0 100 100	65, 98, 133, 141	0
2	A	748/774 (96%)	0.65	76 (10%) 12 9	24, 81, 161, 252	1 (0%)
2	B	748/774 (96%)	0.38	47 (6%) 26 19	23, 66, 151, 261	2 (0%)
3	D	10/16 (62%)	0.26	0 100 100	83, 104, 126, 131	0
3	E	10/16 (62%)	0.20	0 100 100	76, 113, 131, 133	0
All	All	1540/1604 (96%)	0.50	123 (7%) 18 13	23, 74, 158, 261	3 (0%)

The worst 5 of 123 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	312	SER	7.1
2	A	308	VAL	6.3
2	A	309	ALA	5.9
2	B	635	ASP	5.6
2	A	181	VAL	4.9

6.2 Non-standard residues in protein, DNA, RNA chains [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	6HA	D	2	22/23	0.72	0.12	77,104,126,130	0
3	6HA	E	2	22/23	0.72	0.12	87,107,124,137	0
3	6HC	E	3	20/21	0.85	0.13	63,87,103,107	0
3	6HC	D	3	20/21	0.87	0.12	70,77,88,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	6HT	E	4	21/22	0.94	0.09	42,49,68,80	0
3	6HG	E	5	23/24	0.94	0.10	42,50,62,73	0
3	6HT	D	6	21/22	0.94	0.11	45,56,67,73	0
3	6HT	E	6	21/22	0.94	0.12	39,54,64,66	0
3	6HG	D	5	23/24	0.95	0.09	41,51,62,68	0
3	6HT	D	4	21/22	0.96	0.09	36,48,68,79	0

6.3 Carbohydrates [i](#)

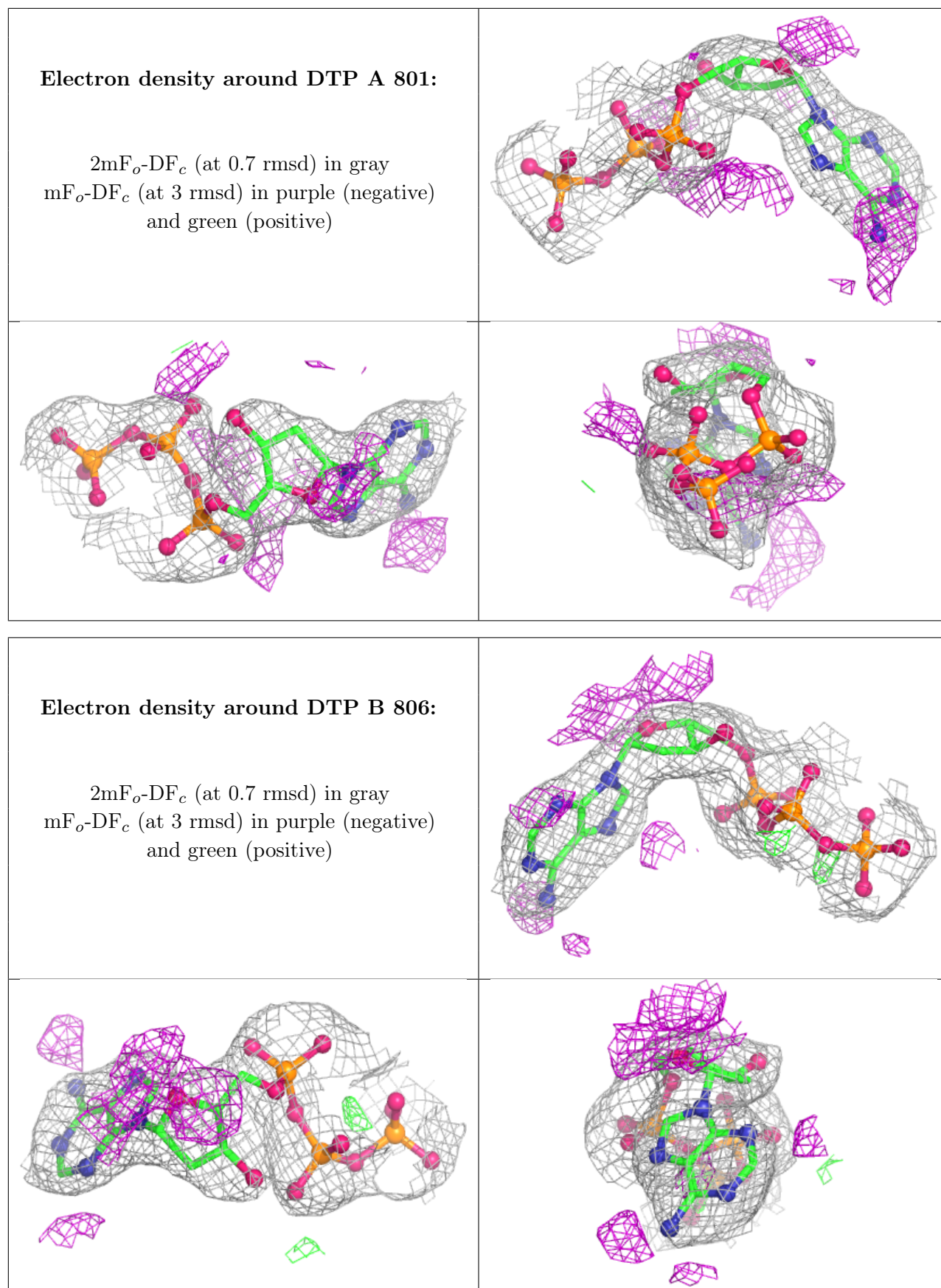
There are no oligosaccharides in this entry.

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.

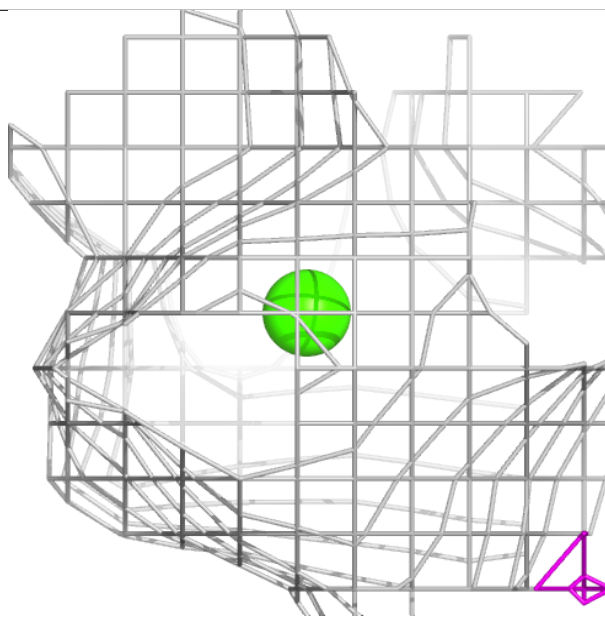
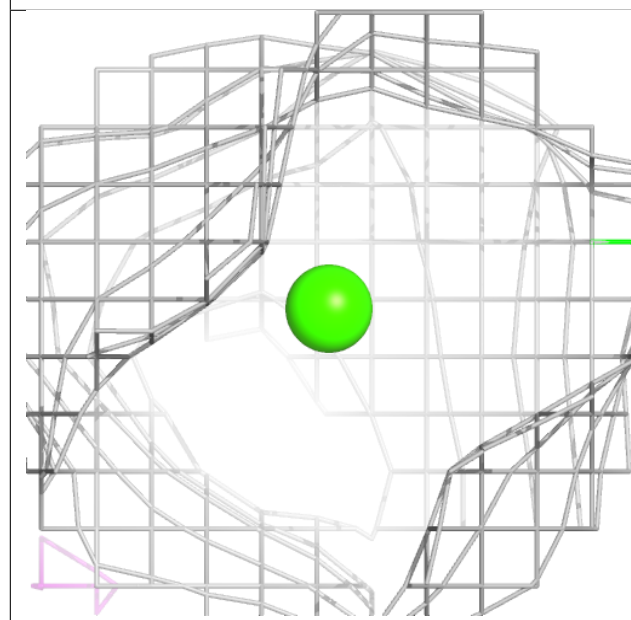
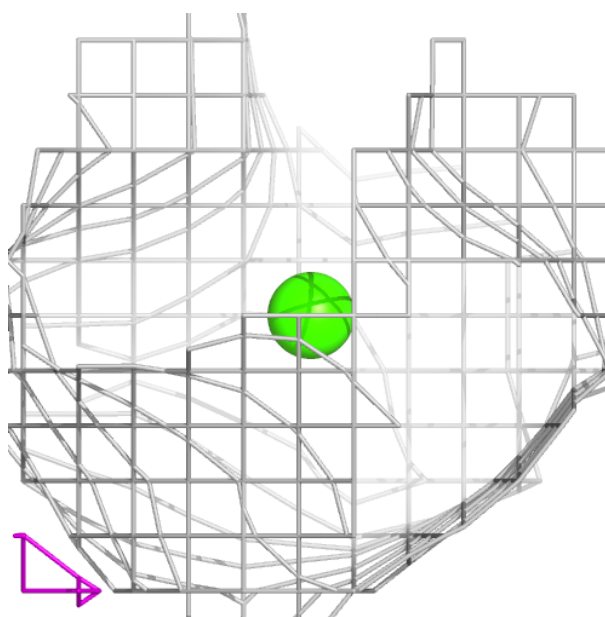
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	EDO	A	803	4/4	0.68	0.29	75,81,85,94	0
5	EDO	D	101	4/4	0.68	0.18	73,76,79,95	0
7	GOL	B	801	6/6	0.74	0.15	56,61,74,83	0
7	GOL	D	102	6/6	0.76	0.18	65,87,91,94	0
5	EDO	E	101	4/4	0.77	0.16	81,87,88,91	0
5	EDO	B	802	4/4	0.82	0.21	62,63,76,85	0
5	EDO	B	805	4/4	0.82	0.16	58,71,84,85	0
5	EDO	B	804	4/4	0.89	0.15	43,46,51,65	0
5	EDO	B	803	4/4	0.91	0.15	57,64,78,83	0
5	EDO	A	802	4/4	0.92	0.15	43,58,58,66	0
4	DTP	A	801	30/30	0.95	0.09	37,49,62,70	0
4	DTP	B	806	30/30	0.95	0.10	37,47,59,73	0
6	CA	B	808	1/1	0.96	0.05	71,71,71,71	0
6	CA	A	805	1/1	0.98	0.04	60,60,60,60	0
6	CA	B	807	1/1	0.99	0.02	64,64,64,64	0
6	CA	A	804	1/1	0.99	0.02	61,61,61,61	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.



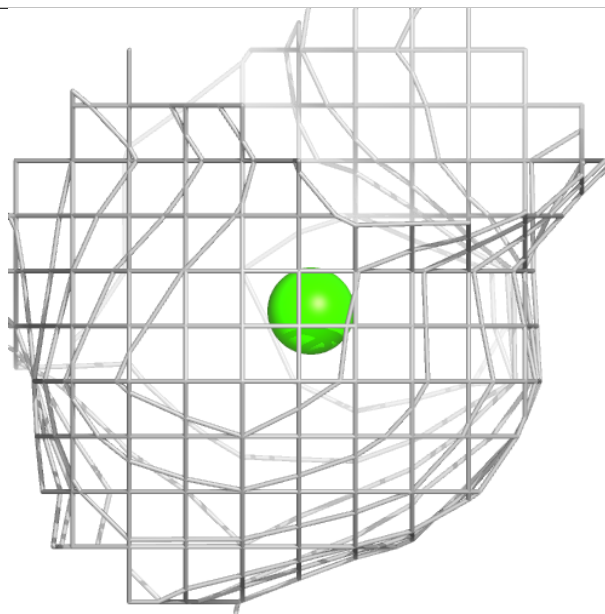
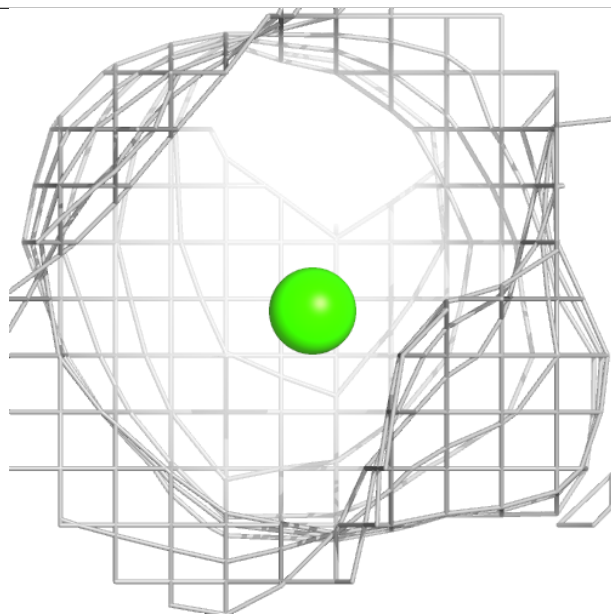
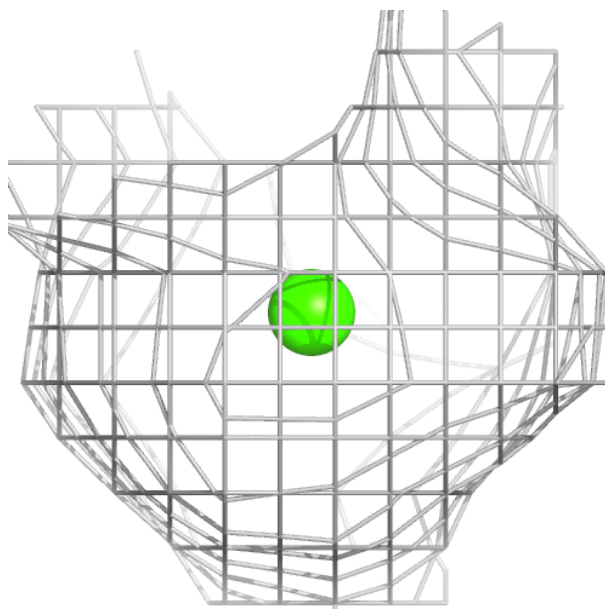
Electron density around CA B 808:

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



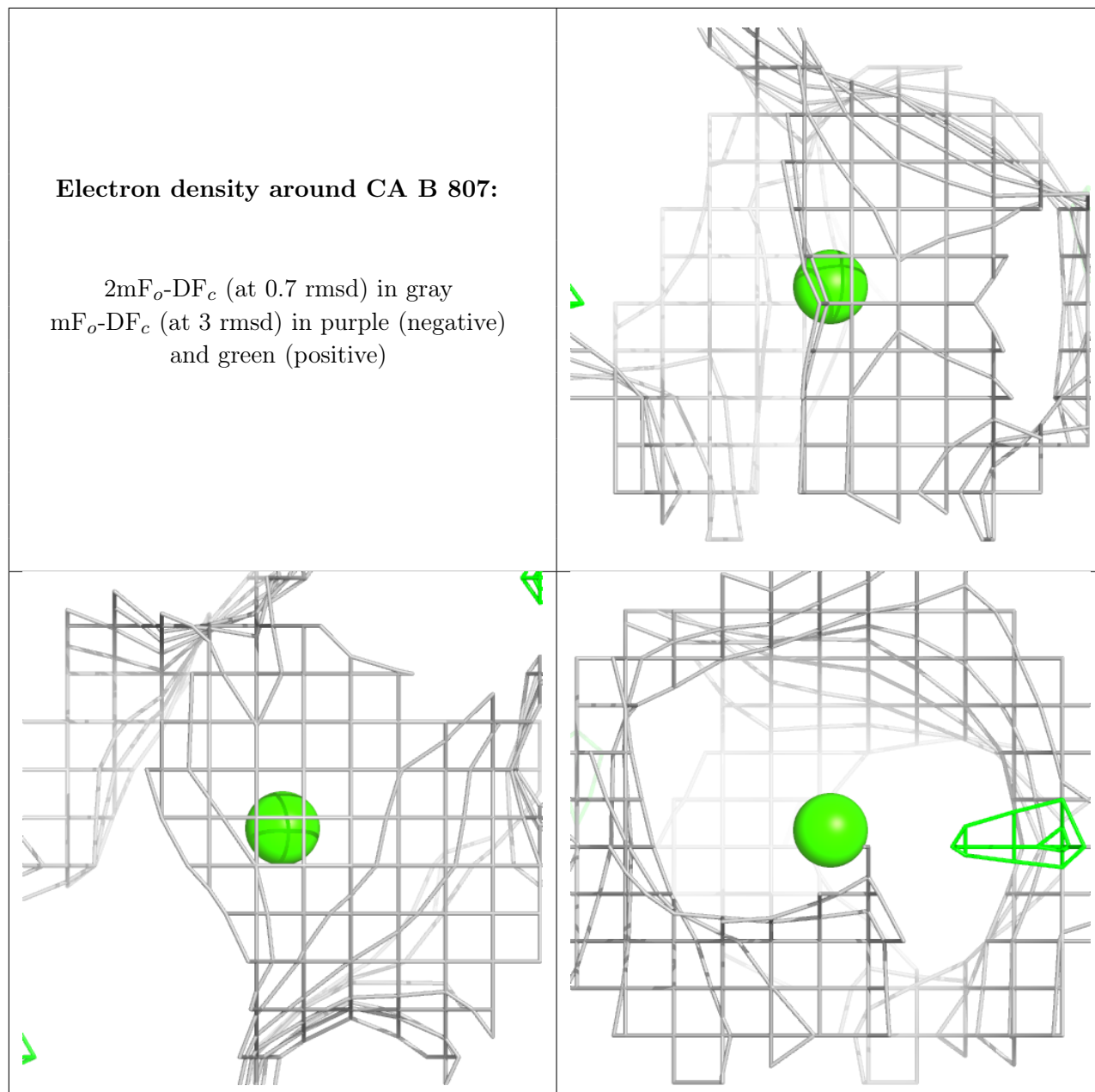
Electron density around CA A 805:

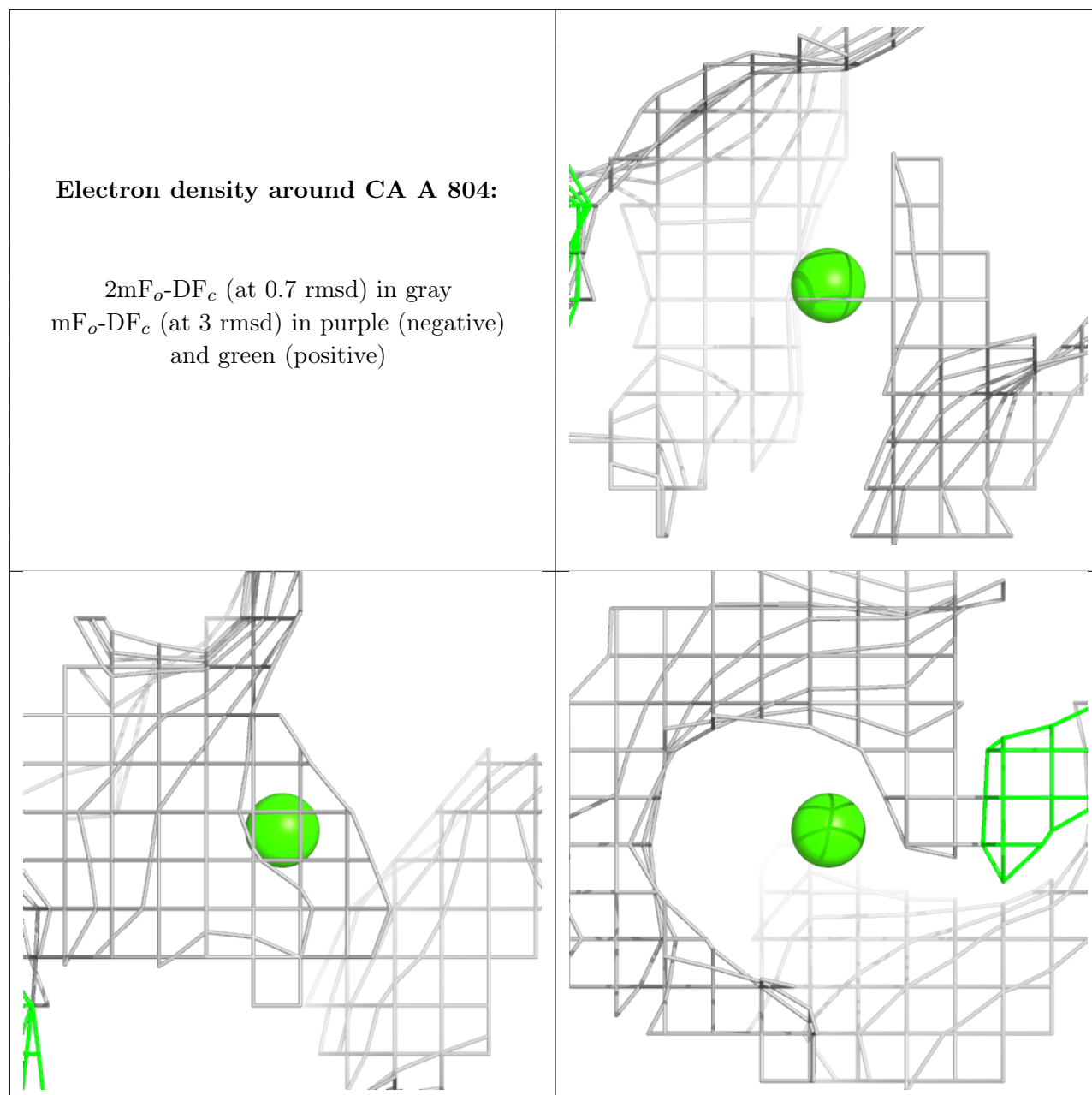
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CA B 807:

$2mF_o-DF_c$ (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.