



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:56 AM UTC

PDB ID : 5W7F / pdb_00005w7f
Title : Murine acyloxyacyl hydrolase (AOAH), S262A mutant, with lipid A
Authors : Gorelik, A.; Illes, K.; Nagar, B.
Deposited on : 2017-06-19
Resolution : 2.80 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

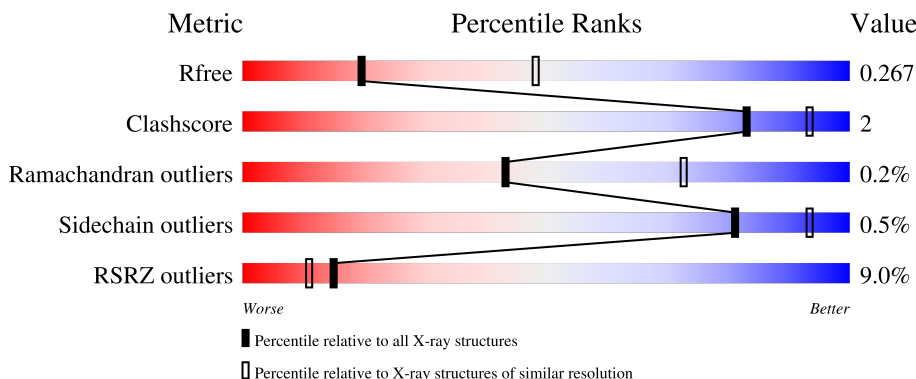
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

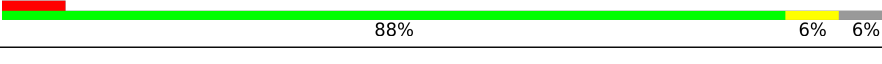
The reported resolution of this entry is 2.80 Å.

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	A	562	 10% 86% 6% 7%
1	B	562	 7% 88% 6% 6%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16778 atoms, of which 8258 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 Acyloxyacyl hydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	522	Total	C	H	N	O	S	0	0	0
			8214	2648	4037	728	777	24			
1	B	528	Total	C	H	N	O	S	0	0	0
			8303	2674	4083	738	784	24			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	ASP	-	expression tag	UNP O35298
A	14	ARG	-	expression tag	UNP O35298
A	15	HIS	-	expression tag	UNP O35298
A	16	HIS	-	expression tag	UNP O35298
A	17	HIS	-	expression tag	UNP O35298
A	18	HIS	-	expression tag	UNP O35298
A	19	HIS	-	expression tag	UNP O35298
A	20	HIS	-	expression tag	UNP O35298
A	21	LYS	-	expression tag	UNP O35298
A	22	LEU	-	expression tag	UNP O35298
A	152	ARG	PRO	conflict	UNP O35298
A	184	VAL	ILE	conflict	UNP O35298
A	262	ALA	SER	engineered mutation	UNP O35298
B	13	ASP	-	expression tag	UNP O35298
B	14	ARG	-	expression tag	UNP O35298
B	15	HIS	-	expression tag	UNP O35298
B	16	HIS	-	expression tag	UNP O35298
B	17	HIS	-	expression tag	UNP O35298
B	18	HIS	-	expression tag	UNP O35298
B	19	HIS	-	expression tag	UNP O35298
B	20	HIS	-	expression tag	UNP O35298
B	21	LYS	-	expression tag	UNP O35298
B	22	LEU	-	expression tag	UNP O35298
B	152	ARG	PRO	conflict	UNP O35298
B	184	VAL	ILE	conflict	UNP O35298

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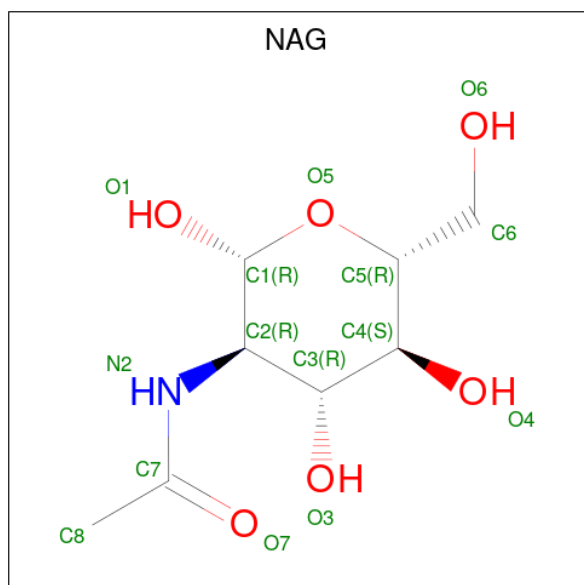
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Chain	Residue	Modelled	Actual	Comment	Reference
B	262	ALA	SER	engineered mutation	UNP O35298

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

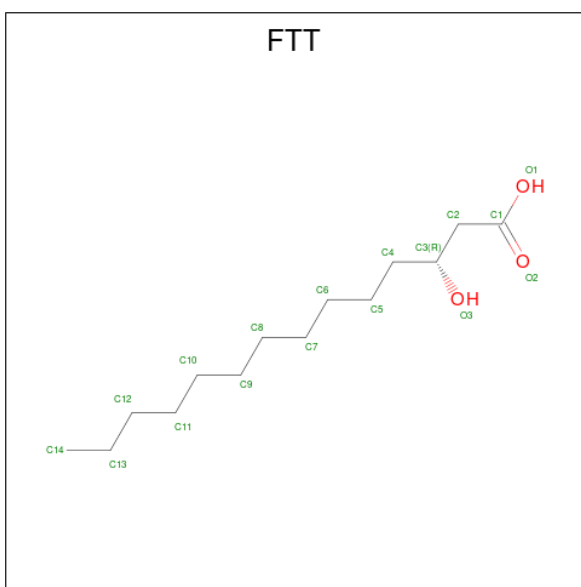
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total Ca 3 3	0	0
2	B	3	Total Ca 3 3	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



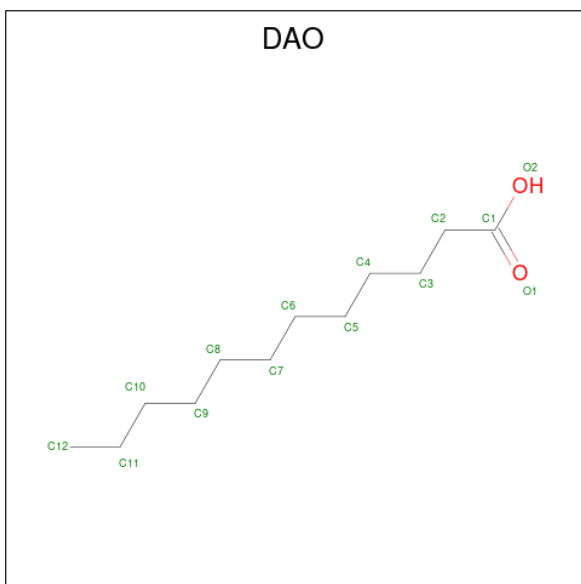
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H N O 28 8 14 1 5	0	0
3	B	1	Total C H N O 28 8 14 1 5	0	0

- Molecule 4 is 3-HYDROXY-TETRADECANOIC ACID (CCD ID: FTT) (formula: C₁₄H₂₈O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			42	14	26	2		
4	B	1	Total	C	H	O	0	0
			42	14	26	2		

- Molecule 5 is LAURIC ACID (CCD ID: DAO) (formula: $C_{12}H_{24}O_2$) (labeled as "Ligand of Interest" by depositor).



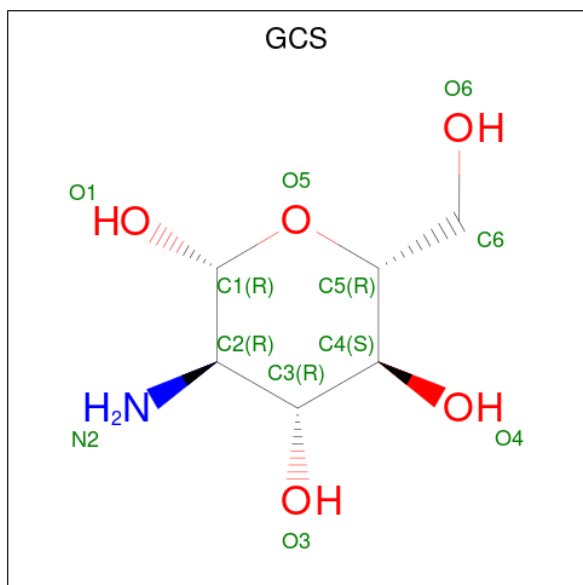
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			36	12	23	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	H	O	0	0
			36	12	23	1		

- Molecule 6 is 2-amino-2-deoxy-beta-D-glucopyranose (CCD ID: GCS) (formula: $C_6H_{13}NO_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	H	N	O	0	0
			24	6	12	1	5		

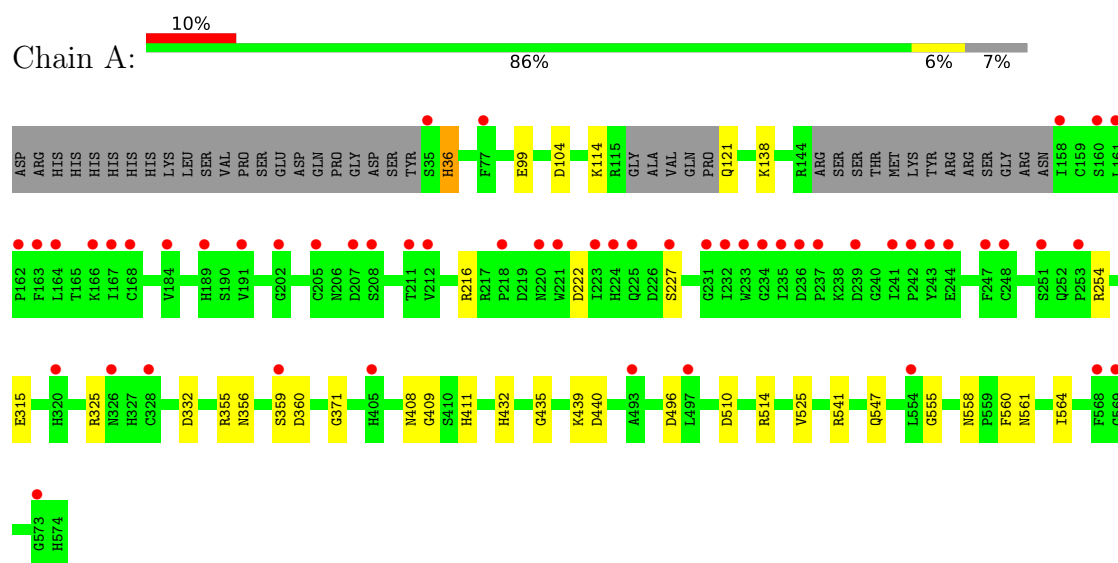
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	11	Total	O	0	0
			11	11		
7	B	8	Total	O	0	0
			8	8		

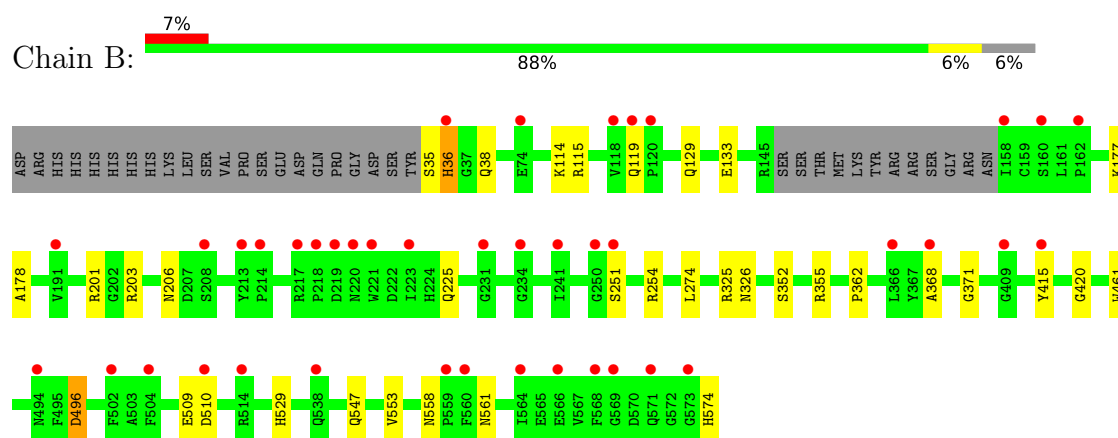
3 Residue-property plots [i](#)

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: Acyloxyacyl hydrolase



• Molecule 1: Acyloxyacyl hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.80Å 88.35Å 93.45Å 90.00° 103.01° 90.00°	Depositor
Resolution (Å)	46.22 – 2.80 46.22 – 2.80	Depositor EDS
% Data completeness (in resolution range)	63.0 (46.22-2.80) 82.9 (46.22-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, R_{free}	0.216 , 0.265 0.216 , 0.267	Depositor DCC
R_{free} test set	1409 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 26.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	16778	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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: FTT, NAG, DAO, CA, GCS

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	0.12	0/4285	0.28	0/5814
1	B	0.12	0/4330	0.29	0/5877
All	All	0.12	0/8615	0.29	0/11691

There are no bond length outliers.

There are no bond angle outliers.

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	4177	4037	4037	20	0
1	B	4220	4083	4083	19	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	14	14	13	0	0
3	B	14	14	13	0	0
4	A	16	26	26	0	0
4	B	16	26	26	1	0
5	A	13	23	23	0	0
5	B	13	23	23	0	0
6	B	12	12	10	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	11	0	0	0	0
7	B	8	0	0	1	0
All	All	8520	8258	8254	40	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 (40) 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:A:315:GLU:OE2	1:A:514:ARG:NH2	2.11	0.82
1:A:216:ARG:NH1	1:A:359:SER:OG	2.18	0.77
1:B:251:SER:OG	1:B:326:ASN:ND2	2.19	0.75
1:B:119:GLN:N	1:B:119:GLN:OE1	2.21	0.74
1:B:206:ASN:ND2	1:B:225:GLN:OE1	2.26	0.67
1:A:325:ARG:NH2	1:A:547:GLN:OE1	2.31	0.64
1:B:35:SER:OG	1:B:38:GLN:OE1	2.15	0.63
1:B:325:ARG:NH2	1:B:547:GLN:OE1	2.32	0.63
1:A:121:GLN:N	1:A:121:GLN:OE1	2.37	0.57
1:B:274:LEU:O	7:B:701:HOH:O	2.18	0.57
1:A:408:ASN:OD1	1:A:409:GLY:N	2.38	0.57
1:A:558:ASN:O	1:A:561:ASN:ND2	2.38	0.56
1:B:115:ARG:NH1	1:B:133:GLU:OE1	2.39	0.56
1:A:325:ARG:NH1	1:A:555:GLY:O	2.43	0.52
1:B:558:ASN:O	1:B:561:ASN:ND2	2.44	0.50
1:A:432:HIS:NE2	1:A:525:VAL:O	2.40	0.49
1:A:411:HIS:ND1	1:A:496:ASP:OD1	2.41	0.48
1:A:99:GLU:OE1	1:A:138:LYS:NZ	2.27	0.48
6:B:607:GCS:O1	6:B:607:GCS:O6	2.25	0.47
1:B:203:ARG:NH2	1:B:574:HIS:O	2.44	0.46
1:B:178:ALA:O	1:B:201:ARG:NH2	2.49	0.46
1:A:356:ASN:N	1:A:360:ASP:OD2	2.40	0.46
1:A:36:HIS:HB2	1:A:114:LYS:HE2	1.99	0.45
1:B:177:LYS:O	1:B:352:SER:HB3	2.17	0.45
1:B:509:GLU:HG3	1:B:510:ASP:N	2.32	0.45
1:B:36:HIS:CB	1:B:114:LYS:HE2	2.48	0.44
1:A:104:ASP:N	1:A:104:ASP:OD1	2.50	0.43
1:A:440:ASP:OD1	1:A:440:ASP:N	2.51	0.43
1:A:560:PHE:O	1:A:564:ILE:N	2.45	0.43
1:B:420:GLY:HA3	1:B:461:TRP:CD2	2.54	0.43
1:B:529:HIS:CE1	4:B:605:FTT:H42	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ASP:OD1	1:A:227:SER:OG	2.37	0.42
1:A:510:ASP:OD2	1:A:541:ARG:NH1	2.49	0.42
1:B:355:ARG:NH2	1:B:362:PRO:O	2.46	0.42
1:A:496:ASP:OD1	1:A:496:ASP:N	2.44	0.42
1:A:332:ASP:OD2	1:A:355:ARG:NH1	2.49	0.41
1:B:254:ARG:NH1	1:B:553:VAL:O	2.49	0.41
1:B:368:ALA:HA	1:B:415:TYR:HB2	2.03	0.41
1:B:496:ASP:OD1	1:B:496:ASP:N	2.43	0.41
1:A:435:GLY:O	1:A:439:LYS:N	2.55	0.40

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	
1	A	516/562 (92%)	499 (97%)	16 (3%)	1 (0%)	43	72
1	B	524/562 (93%)	507 (97%)	16 (3%)	1 (0%)	43	72
All	All	1040/1124 (92%)	1006 (97%)	32 (3%)	2 (0%)	43	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	371	GLY
1	B	371	GLY

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	464/500 (93%)	462 (100%)	2 (0%)	84	94
1	B	468/500 (94%)	465 (99%)	3 (1%)	78	92
All	All	932/1000 (93%)	927 (100%)	5 (0%)	81	93

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	254	ARG
1	B	36	HIS
1	B	129	GLN
1	B	496	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	121	GLN
1	A	123	HIS
1	A	206	ASN
1	A	282	ASN
1	A	320	HIS
1	A	329	ASN
1	A	438	ASN
1	A	512	GLN
1	B	199	HIS
1	B	206	ASN
1	B	225	GLN
1	B	326	ASN
1	B	357	GLN
1	B	390	GLN
1	B	438	ASN
1	B	454	GLN
1	B	494	ASN
1	B	529	HIS
1	B	538	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 6 are monoatomic - leaving 7 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	DAO	A	606	4	11,12,13	0.46	0	10,11,13	0.93	0
4	FTT	A	605	5	14,15,16	0.61	0	15,15,17	0.92	0
5	DAO	B	606	4	11,12,13	0.42	0	10,11,13	0.96	0
3	NAG	A	604	1	14,14,15	0.28	0	17,19,21	0.55	0
4	FTT	B	605	6,5	14,15,16	0.59	0	15,15,17	1.04	1 (6%)
6	GCS	B	607	4	12,12,12	1.77	2 (16%)	16,17,17	0.94	1 (6%)
3	NAG	B	604	1	14,14,15	0.23	0	17,19,21	0.48	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	DAO	A	606	4	-	3/10/10/11	-
4	FTT	A	605	5	-	8/14/14/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DAO	B	606	4	-	5/10/10/11	-
3	NAG	A	604	1	-	0/6/23/26	0/1/1/1
4	FTT	B	605	6,5	-	7/14/14/15	-
6	GCS	B	607	4	-	2/2/22/22	0/1/1/1
3	NAG	B	604	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	607	GCS	C3-C2	-4.08	1.48	1.53
6	B	607	GCS	O5-C1	3.47	1.51	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	607	GCS	O5-C1-C2	2.68	112.64	109.51
4	B	605	FTT	C3-C2-C1	-2.17	109.00	112.70

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	605	FTT	C1-C2-C3-C4
4	A	605	FTT	C1-C2-C3-O3
4	B	605	FTT	C2-C3-C4-C5
5	B	606	DAO	O1-C1-C2-C3
6	B	607	GCS	O5-C5-C6-O6
6	B	607	GCS	C4-C5-C6-O6
4	B	605	FTT	O3-C3-C4-C5
4	A	605	FTT	C6-C7-C8-C9
4	A	605	FTT	C4-C5-C6-C7
5	B	606	DAO	C2-C3-C4-C5
4	A	605	FTT	C9-C10-C11-C12
4	B	605	FTT	C5-C6-C7-C8
5	A	606	DAO	C2-C3-C4-C5
4	B	605	FTT	C6-C7-C8-C9
4	B	605	FTT	C4-C5-C6-C7
4	A	605	FTT	C11-C12-C13-C14
4	B	605	FTT	C11-C10-C9-C8
5	B	606	DAO	C3-C4-C5-C6

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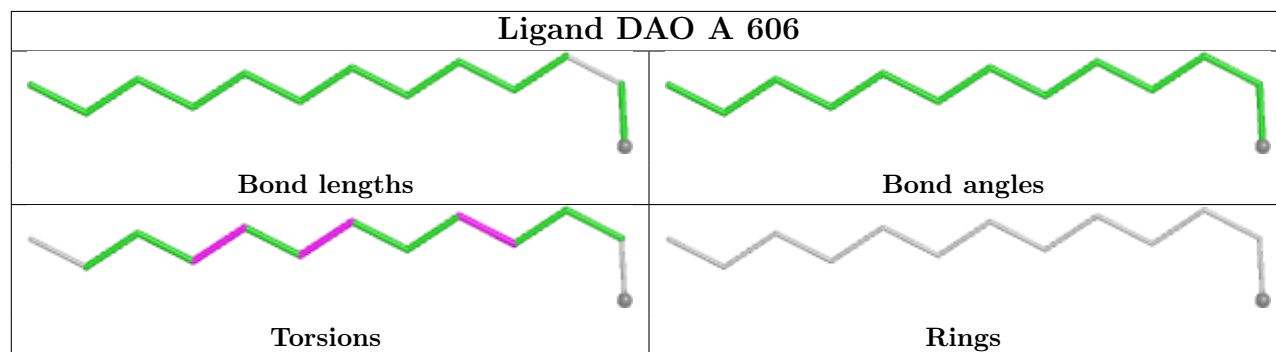
Mol	Chain	Res	Type	Atoms
4	A	605	FTT	C5-C6-C7-C8
4	B	605	FTT	C7-C8-C9-C10
5	B	606	DAO	C11-C10-C9-C8
5	A	606	DAO	C5-C6-C7-C8
5	A	606	DAO	C7-C8-C9-C10
5	B	606	DAO	C7-C8-C9-C10
4	A	605	FTT	C7-C8-C9-C10

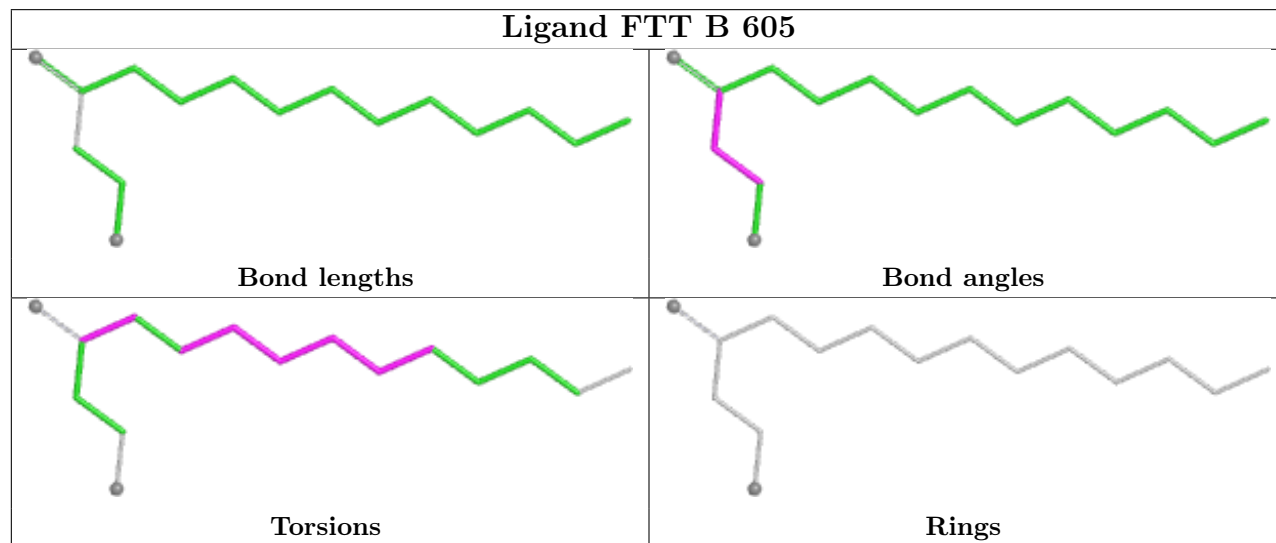
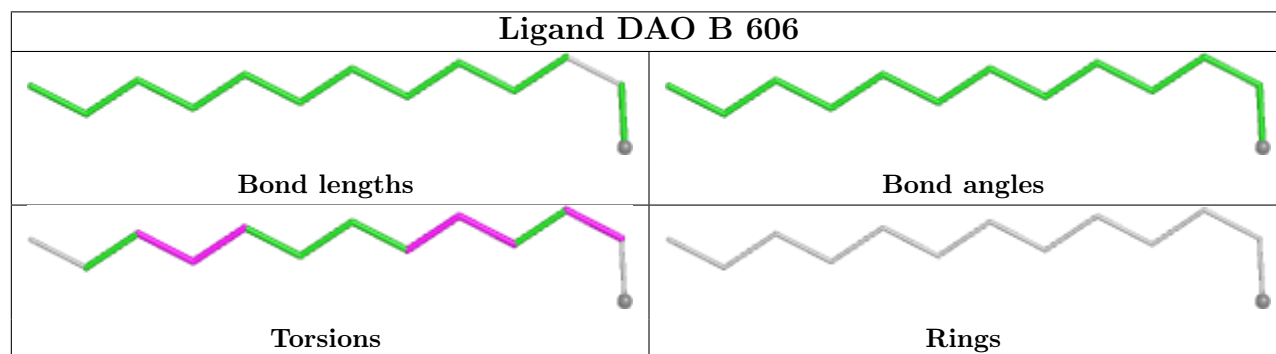
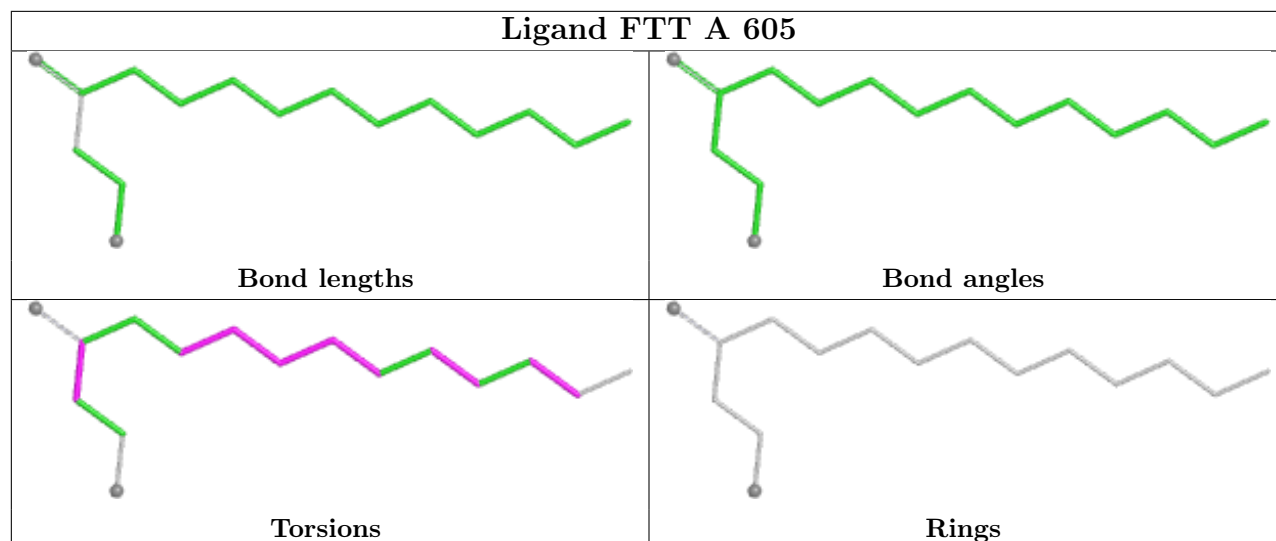
There are no ring outliers.

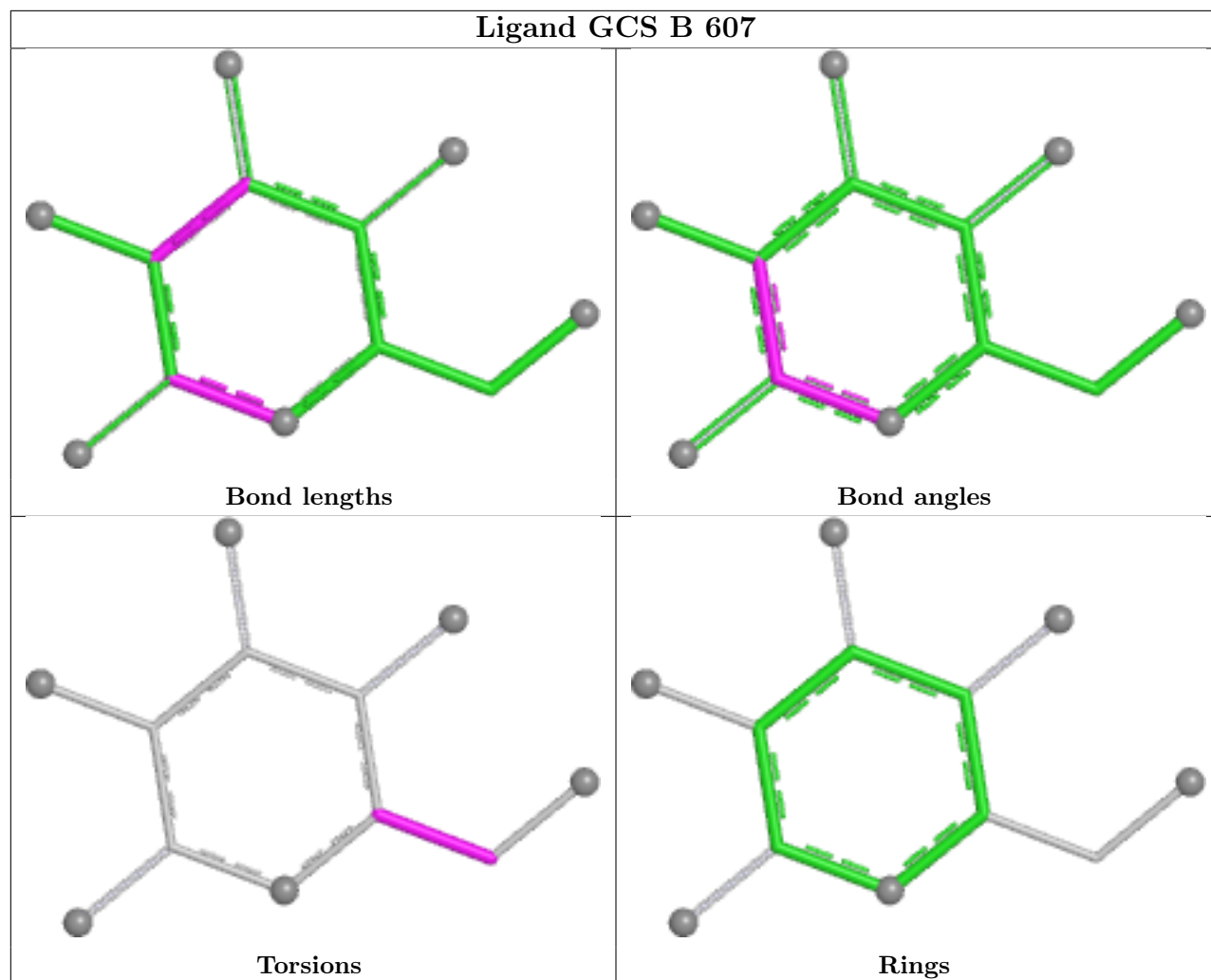
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	605	FTT	1	0
6	B	607	GCS	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

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	522/562 (92%)	0.54	54 (10%) 12 9	12, 43, 108, 141	0
1	B	528/562 (93%)	0.58	41 (7%) 19 14	14, 45, 105, 125	0
All	All	1050/1124 (93%)	0.56	95 (9%) 15 11	12, 44, 107, 141	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	231	GLY	6.4
1	A	242	PRO	5.1
1	B	366	LEU	5.0
1	B	415	TYR	4.8
1	A	233	TRP	4.8
1	A	161	LEU	4.3
1	B	218	PRO	4.2
1	A	163	PHE	4.2
1	A	158	ILE	4.1
1	B	160	SER	3.9
1	A	164	LEU	3.9
1	B	538	GLN	3.7
1	B	231	GLY	3.7
1	A	162	PRO	3.7
1	B	504	PHE	3.6
1	A	224	HIS	3.6
1	B	573	GLY	3.5
1	B	120	PRO	3.5
1	B	118	VAL	3.4
1	A	221	TRP	3.4
1	A	234	GLY	3.4
1	B	221	TRP	3.4
1	A	239	ASP	3.4
1	A	248	CYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	244	GLU	3.3
1	A	223	ILE	3.3
1	B	219	ASP	3.2
1	A	227	SER	3.2
1	A	569	GLY	3.2
1	B	559	PRO	3.0
1	A	573	GLY	2.9
1	B	250	GLY	2.9
1	A	320	HIS	2.9
1	A	243	TYR	2.8
1	A	253	PRO	2.8
1	A	191	VAL	2.8
1	A	241	ILE	2.8
1	A	160	SER	2.8
1	B	162	PRO	2.7
1	A	328	CYS	2.7
1	B	213	TYR	2.7
1	A	568	PHE	2.7
1	A	235	ILE	2.6
1	A	554	LEU	2.7
1	A	211	THR	2.6
1	B	119	GLN	2.6
1	B	571	GLN	2.6
1	B	368	ALA	2.6
1	B	241	ILE	2.6
1	B	409	GLY	2.5
1	A	497	LEU	2.5
1	A	202	GLY	2.5
1	A	35	SER	2.4
1	B	158	ILE	2.4
1	A	359	SER	2.4
1	B	74	GLU	2.4
1	B	564	ILE	2.3
1	B	191	VAL	2.3
1	A	225	GLN	2.3
1	A	251	SER	2.3
1	B	510	ASP	2.3
1	B	220	ASN	2.3
1	B	36	HIS	2.3
1	A	208	SER	2.3
1	B	560	PHE	2.2
1	B	494	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	232	ILE	2.2
1	A	218	PRO	2.2
1	B	251	SER	2.2
1	B	568	PHE	2.2
1	B	514	ARG	2.2
1	B	208	SER	2.2
1	B	566	GLU	2.2
1	B	569	GLY	2.2
1	A	493	ALA	2.2
1	A	189	HIS	2.1
1	A	237	PRO	2.1
1	B	234	GLY	2.1
1	B	223	ILE	2.1
1	A	326	ASN	2.1
1	A	166	LYS	2.1
1	B	502	PHE	2.1
1	A	205	CYS	2.1
1	A	184	VAL	2.1
1	A	220	ASN	2.1
1	B	217	ARG	2.1
1	A	167	ILE	2.1
1	A	168	CYS	2.1
1	A	405	HIS	2.1
1	B	214	PRO	2.1
1	A	247	PHE	2.1
1	A	207	ASP	2.1
1	A	236	ASP	2.1
1	A	212	VAL	2.0
1	A	77	PHE	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 oligosaccharides in this entry.

6.4 Ligands

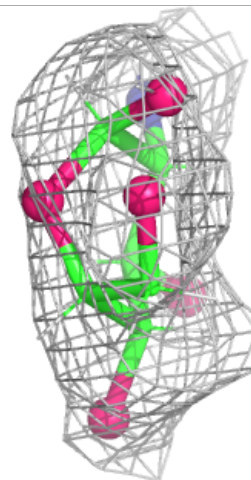
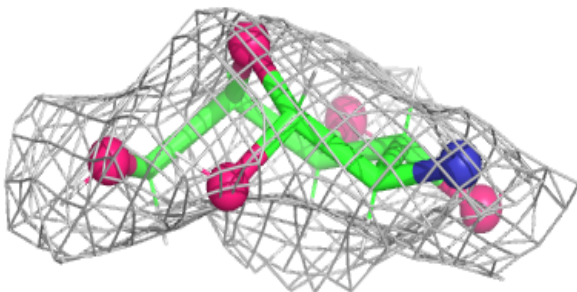
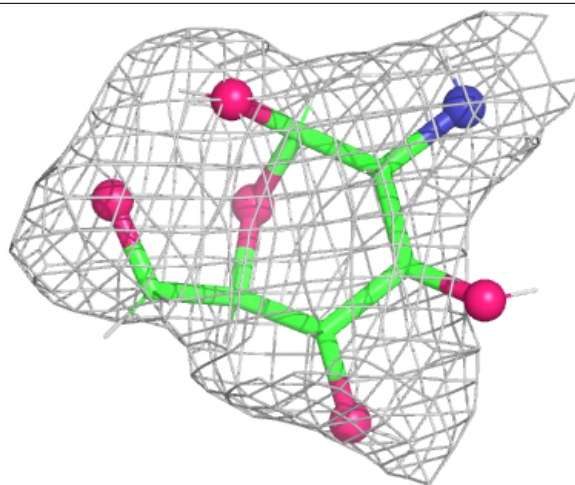
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	GCS	B	607	12/12	0.78	0.14	54,82,97,102	0
4	FTT	A	605	16/17	0.84	0.14	20,31,55,66	0
3	NAG	B	604	14/15	0.86	0.11	40,55,66,66	0
5	DAO	A	606	13/14	0.88	0.15	19,31,40,42	0
4	FTT	B	605	16/17	0.88	0.12	22,34,62,75	0
5	DAO	B	606	13/14	0.90	0.13	28,37,50,55	0
2	CA	A	603	1/1	0.91	0.08	78,78,78,78	0
2	CA	B	602	1/1	0.91	0.09	77,77,77,77	0
3	NAG	A	604	14/15	0.91	0.09	18,28,41,47	0
2	CA	A	601	1/1	0.92	0.07	64,64,64,64	0
2	CA	B	601	1/1	0.93	0.06	64,64,64,64	0
2	CA	A	602	1/1	0.96	0.10	83,83,83,83	0
2	CA	B	603	1/1	0.98	0.08	89,89,89,89	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.

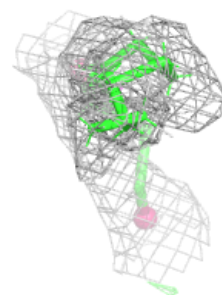
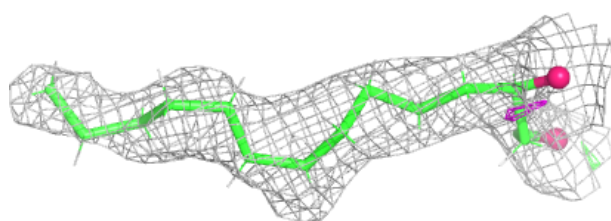
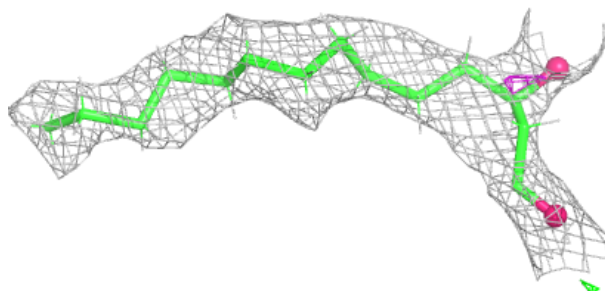
Electron density around GCS B 607:

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

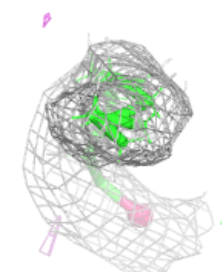
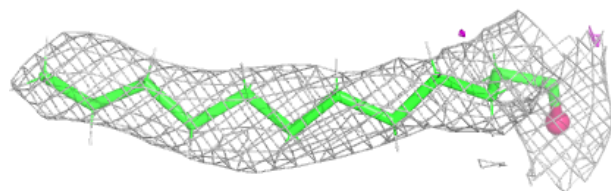
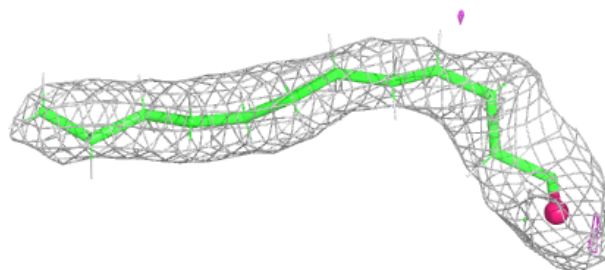


Electron density around FTT A 605:

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

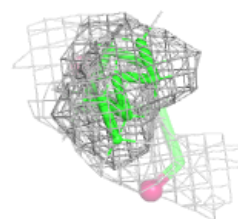
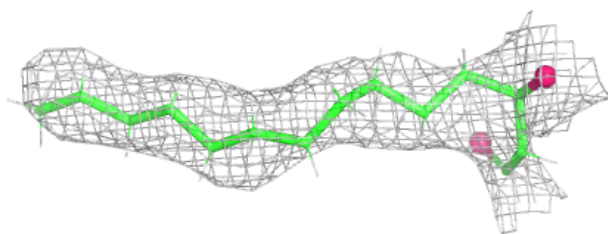
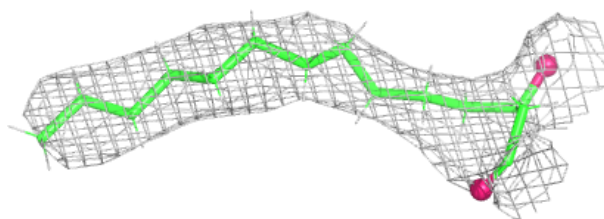
**Electron density around DAO A 606:**

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

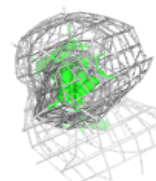
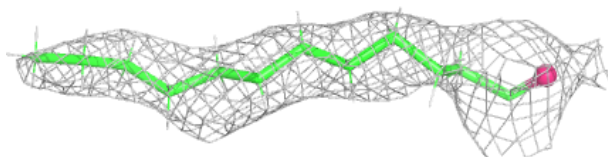
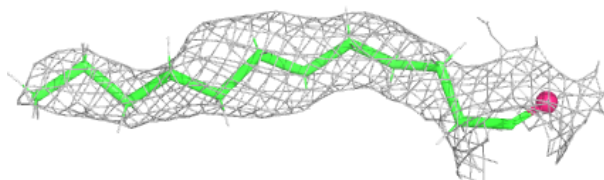


Electron density around FTT B 605:

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

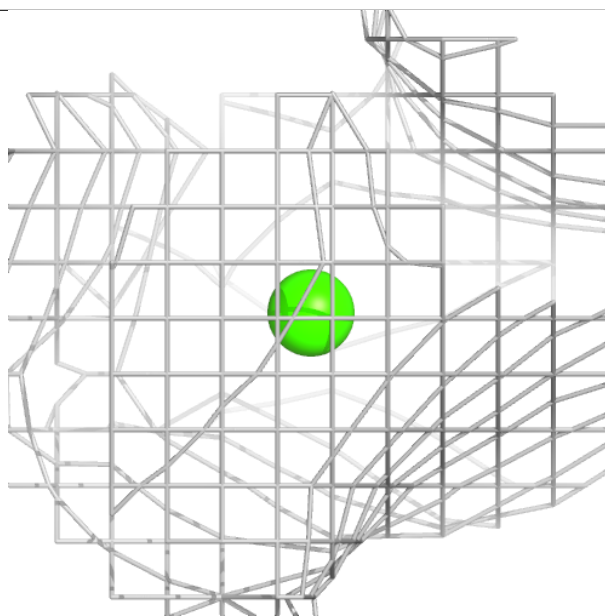
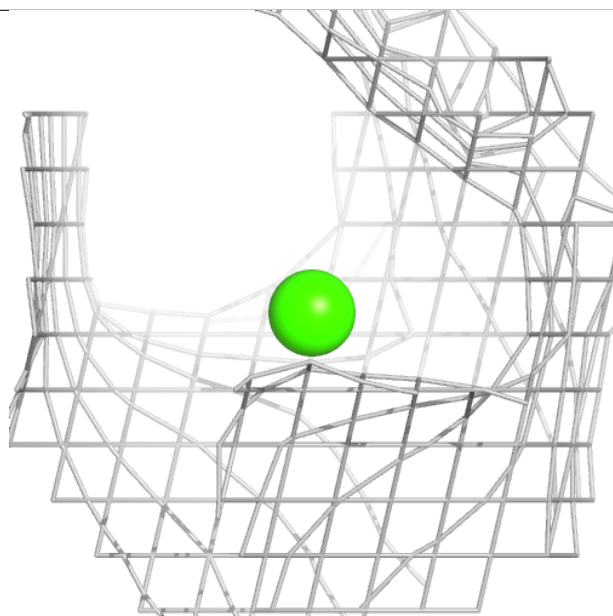
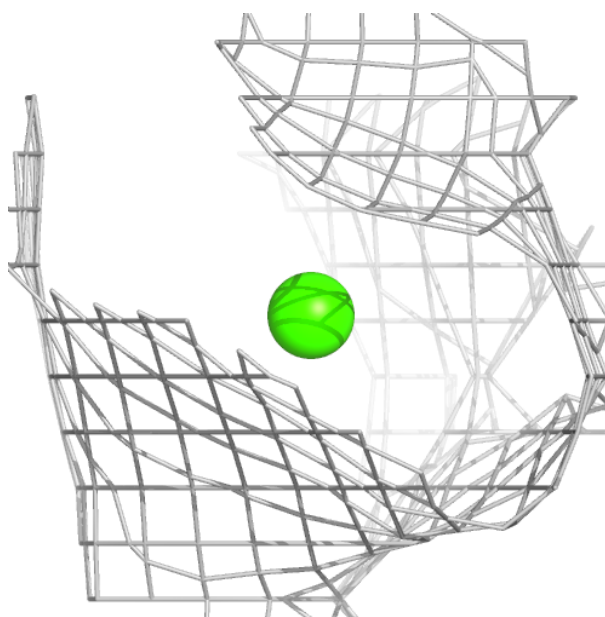
**Electron density around DAO B 606:**

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



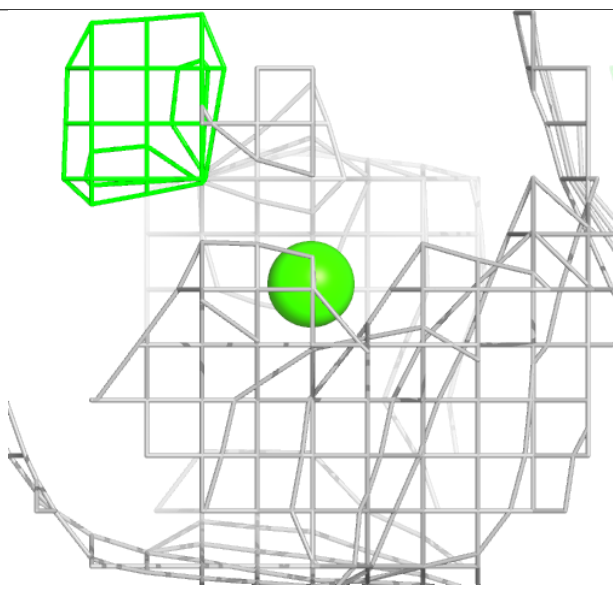
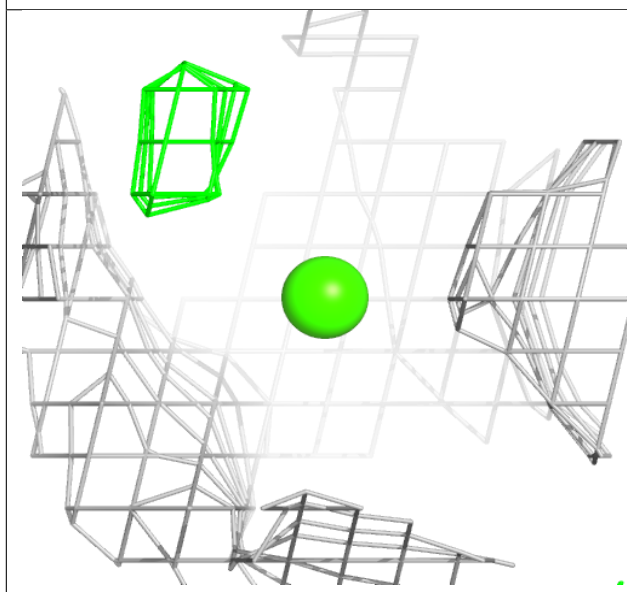
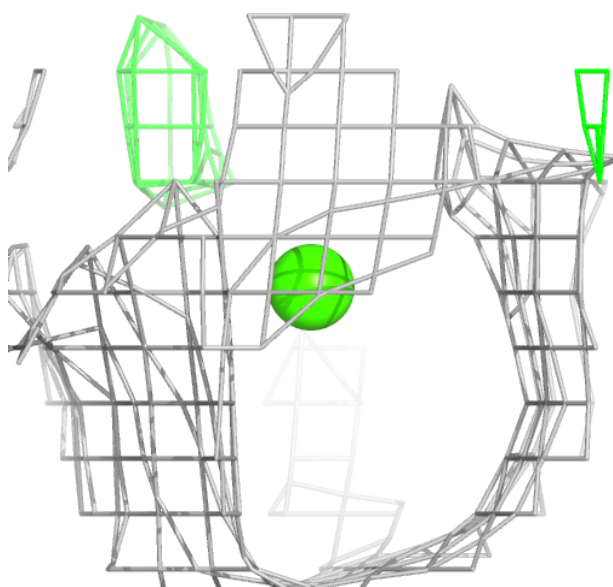
Electron density around CA A 603:

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



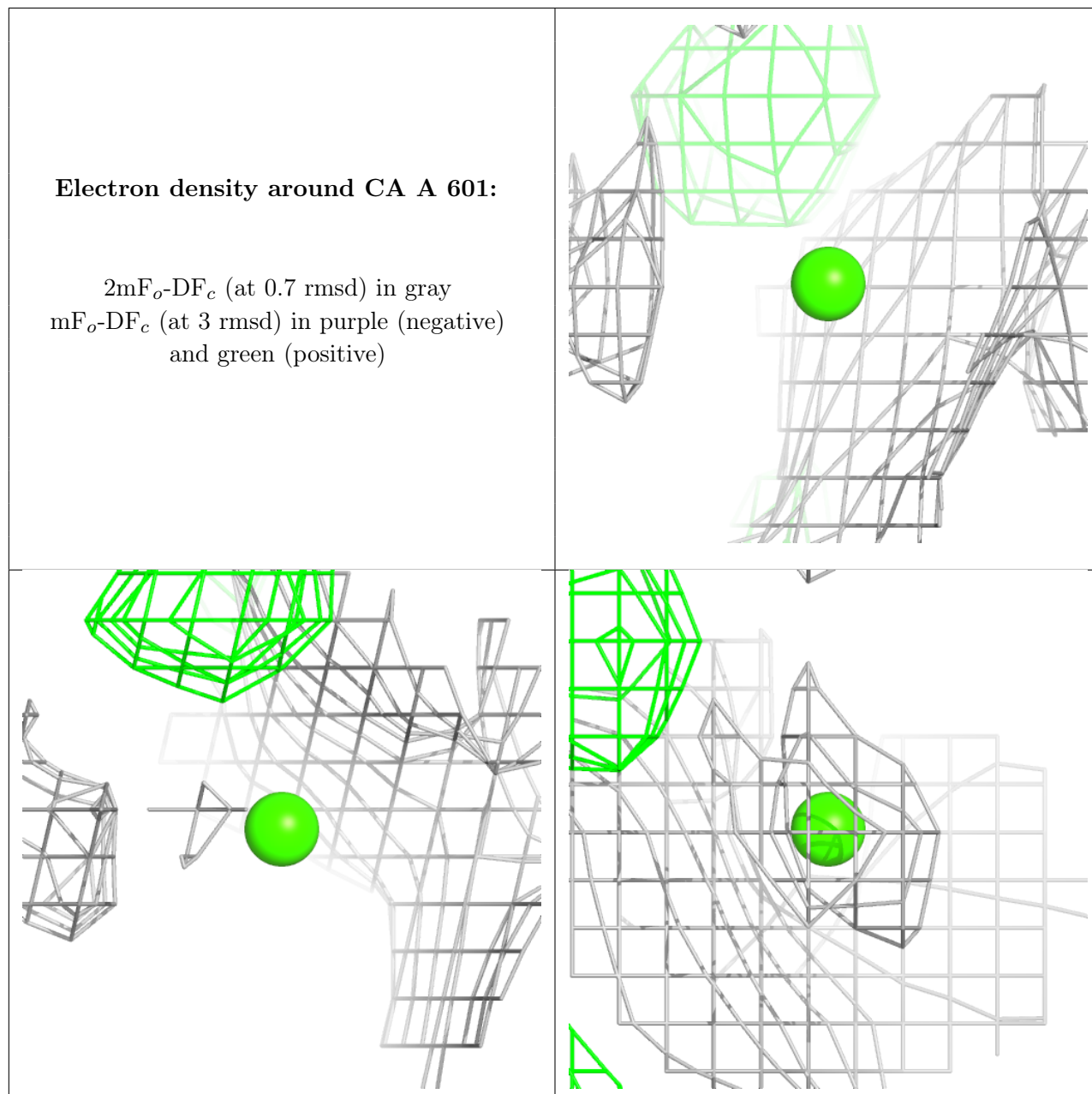
Electron density around CA B 602:

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



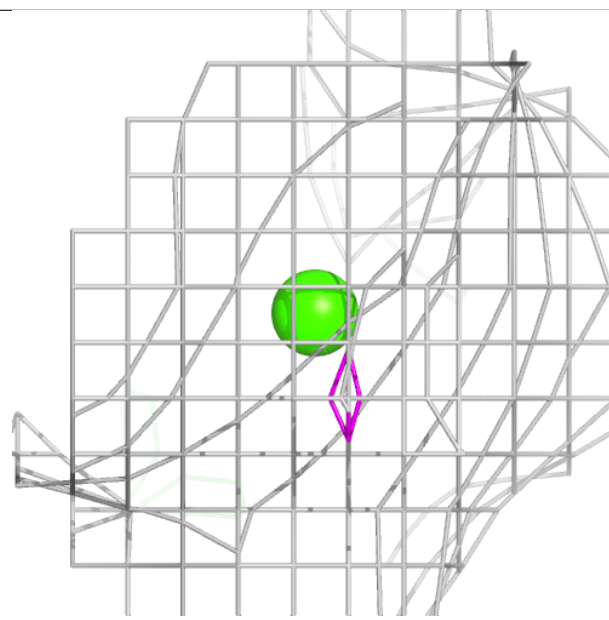
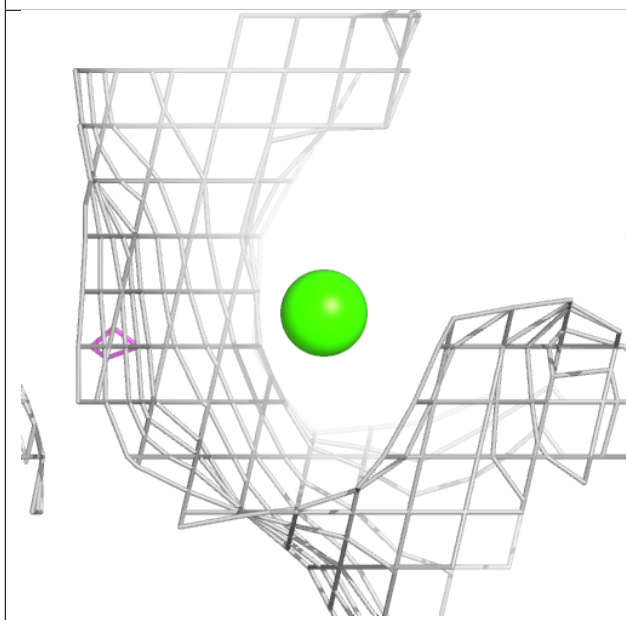
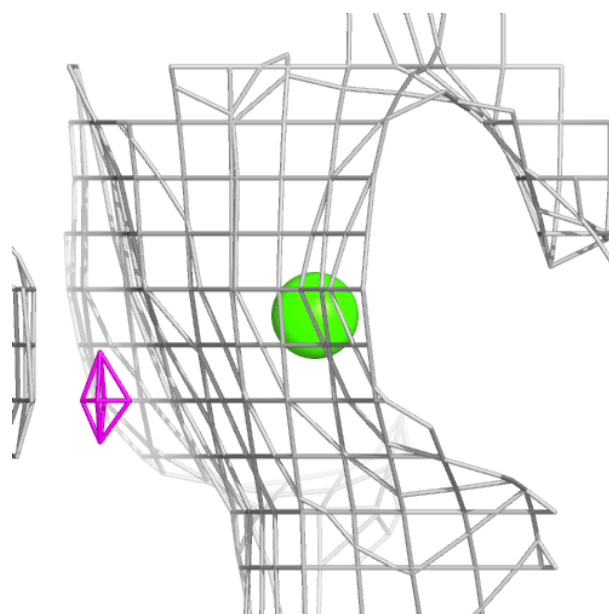
Electron density around CA A 601:

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



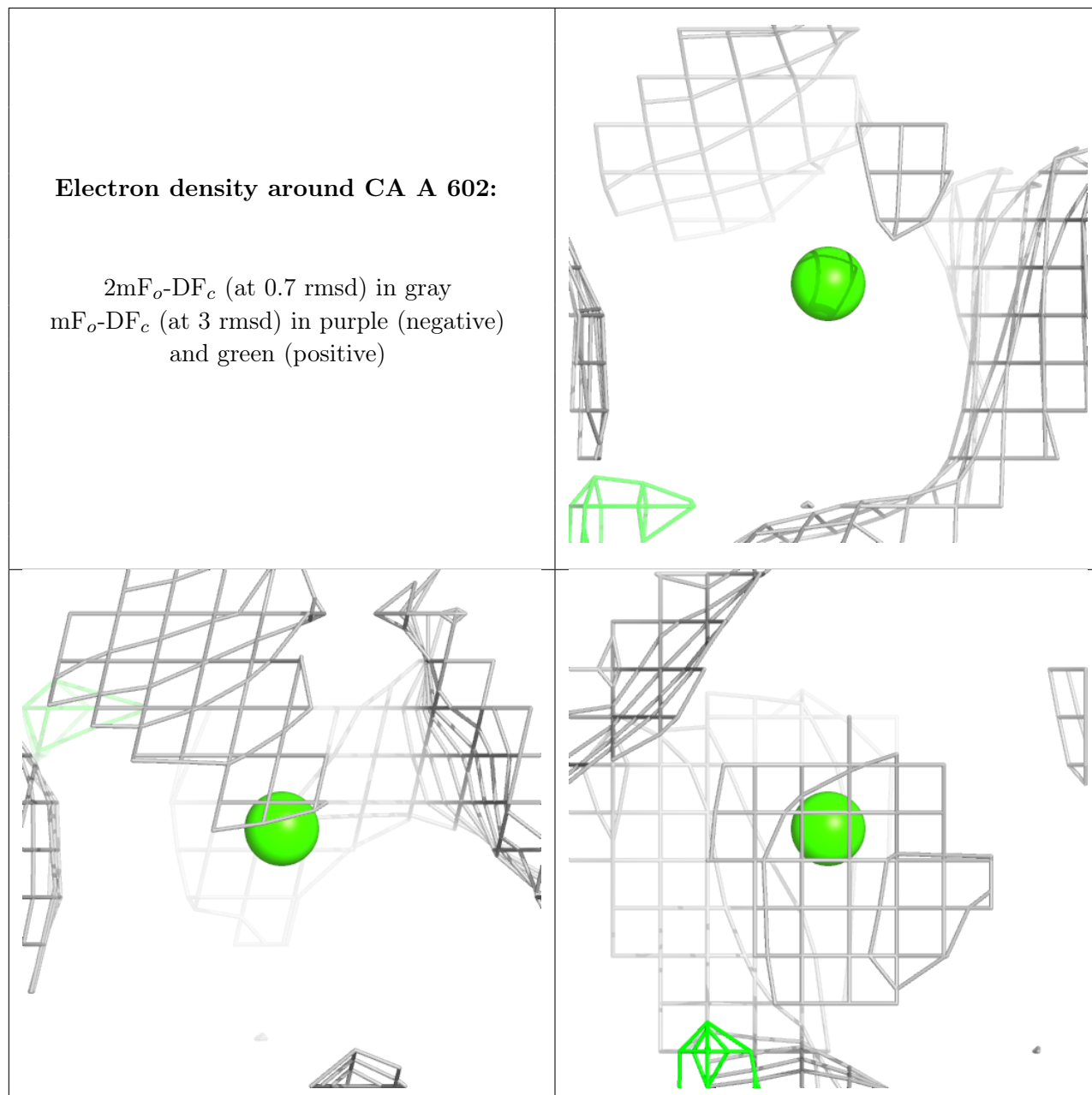
Electron density around CA B 601:

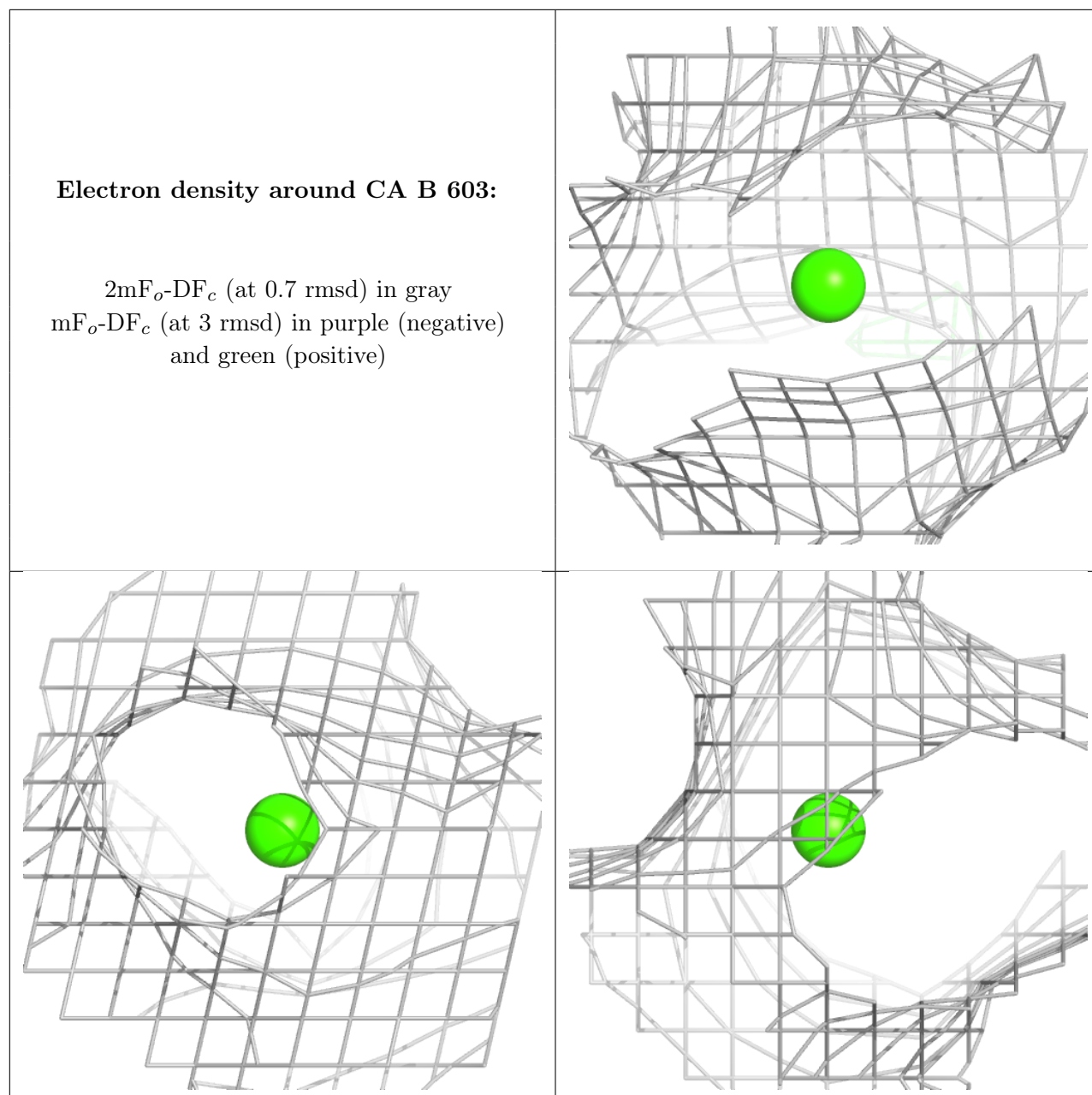
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CA A 602:

$2mF_o-DF_c$ (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.