WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Nov 6, 2023 – 10:19 AM EST

PDB ID	:	7MDE
Title	:	Full-length S95A ClbP
Authors	:	Velilla, J.A.; Volpe, M.R.; Gaudet, R.
Deposited on	:	2021-04-04
Resolution	:	2.70 Å(reported)

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

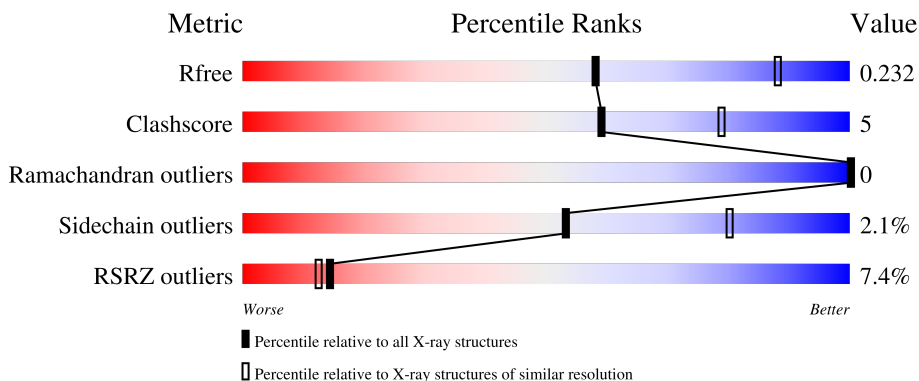|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.70 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	Percentile Ranks	Value
Rfree		0.232
Clashscore		5
Ramachandran outliers		0
Sidechain outliers		2.1%
RSRZ outliers		7.4%

Worse　　　　　　　　　　　　　　　　*Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	480	7% (upper bar); 82% / 10% / · / 7%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 3605 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 Beta-lactamase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	446	3341	2146	572	609	3	11	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	95	ALA	SER	engineered mutation	UNP Q0P7K6
A	454	MSE	LEU	engineered mutation	UNP Q0P7K6
A	478	MSE	ILE	engineered mutation	UNP Q0P7K6
A	505	HIS	-	expression tag	UNP Q0P7K6
A	506	HIS	-	expression tag	UNP Q0P7K6
A	507	HIS	-	expression tag	UNP Q0P7K6
A	508	HIS	-	expression tag	UNP Q0P7K6
A	509	HIS	-	expression tag	UNP Q0P7K6
A	510	HIS	-	expression tag	UNP Q0P7K6

- Molecule 2 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: $C_{21}H_{40}O_4$).

OLC

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 19	C 15	O 4	0	0
2	A	1	Total 11	C 10	O 1	0	0

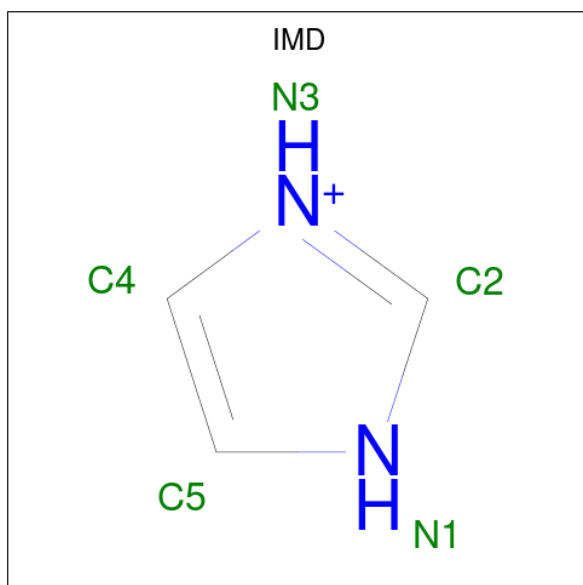- Molecule 3 is NONAETHYLENE GLYCOL (three-letter code: 2PE) (formula: $C_{18}H_{38}O_{10}$).

2PE

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 14	C 9	O 5	0	0
3	A	1	Total 7	C 4	O 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 11	C 7	O 4	0	0
3	A	1	Total 7	C 4	O 3	0	0

- Molecule 4 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 5	C 3	N 2	0	0

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).

DMS

C2

S

C1 — S

O

O

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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

SO4

O1

O

O3 O⁻ — S — O⁻ O4

S

O

O2

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
6	A	1	5	4	1	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	3	Total 3	Cl 3	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	178	Total 178	O 178	0	0

3 Residue-property plots ⓘ

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: Beta-lactamase
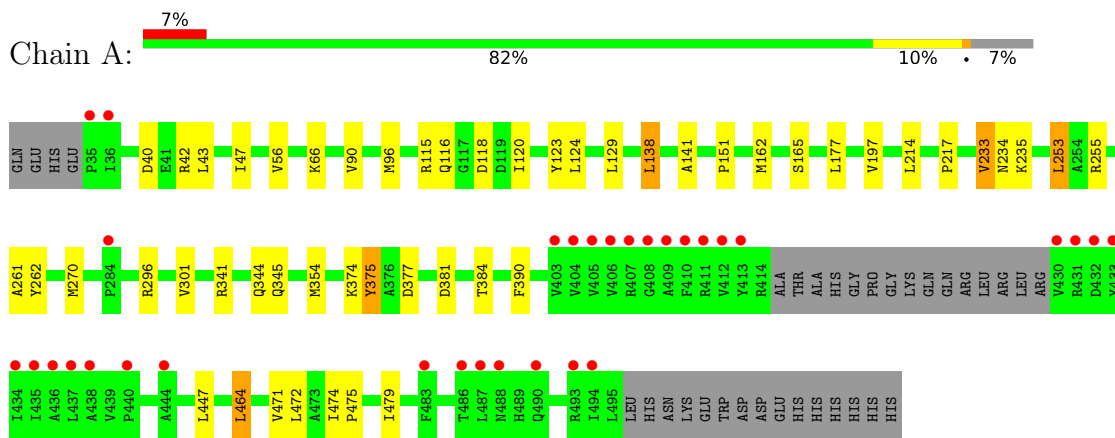
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	97.47Å 97.47Å 183.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.74 – 2.70 48.74 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.74-2.70) 87.2 (48.74-2.70)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.99 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.195 , 0.235 0.199 , 0.232	Depositor DCC
R_{free} test set	753 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å^2)	38.1	Xtriage
Anisotropy	0.863	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 53.2	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	3605	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.72% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: DMS, IMD, OLC, 2PE, SO4, CL

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	0.40	0/3403	0.62	1/4625 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	375	TYR	O-C-N	-13.60	100.94	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	375	TYR	Mainchain

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	3341	0	3283	31	0
2	A	30	0	40	1	0
3	A	39	0	48	1	0
4	A	5	0	5	0	0
5	A	4	0	6	0	0
6	A	5	0	0	0	0
7	A	3	0	0	0	0
8	A	178	0	0	3	0
All	All	3605	0	3382	32	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 (32) 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:261:ALA:HB2	2:A:601:OLC:H22	1.82	0.61
1:A:42:ARG:NH1	8:A:702:HOH:O	2.26	0.59
1:A:151:PRO:HA	1:A:177:LEU:HD11	1.89	0.53
1:A:56:VAL:HG12	1:A:354:MSE:HB3	1.91	0.52
1:A:255:ARG:NH1	8:A:703:HOH:O	2.42	0.50
1:A:214:LEU:C	1:A:217:PRO:HD2	2.32	0.48
1:A:96:MSE:CE	1:A:270:MSE:HE2	2.44	0.48
1:A:390:PHE:CE2	1:A:471:VAL:HG23	2.48	0.48
1:A:447:LEU:HD12	1:A:479:ILE:HD11	1.95	0.47
1:A:253:LEU:HD13	1:A:262:TYR:CG	2.49	0.47
1:A:341:ARG:HG2	1:A:344:GLN:OE1	2.15	0.47
1:A:66:LYS:HG2	1:A:345:GLN:HB2	1.96	0.47
1:A:475:PRO:O	1:A:479:ILE:HG12	2.15	0.47
1:A:233:VAL:O	1:A:234:ASN:HB2	2.15	0.46
1:A:116:GLN:HG2	1:A:141:ALA:HB2	1.97	0.46
1:A:381:ASP:HB3	1:A:384:THR:HG22	1.96	0.46
1:A:214:LEU:O	1:A:217:PRO:HD2	2.17	0.44
1:A:115:ARG:HB2	1:A:118:ASP:OD1	2.18	0.44
1:A:90:VAL:HB	1:A:235:LYS:HA	1.98	0.44
1:A:120:ILE:HD12	1:A:120:ILE:HA	1.87	0.43
1:A:296:ARG:HE	1:A:296:ARG:HB2	1.57	0.43
1:A:129:LEU:HD12	1:A:138:LEU:HD13	2.00	0.43
1:A:120:ILE:HD11	1:A:197:VAL:HG21	2.01	0.42
1:A:474:ILE:HB	1:A:475:PRO:HD3	2.01	0.42
1:A:234:ASN:N	8:A:706:HOH:O	2.35	0.42
1:A:447:LEU:HD13	1:A:475:PRO:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:606:2PE:H21	3:A:606:2PE:H52	1.74	0.42
1:A:40:ASP:HB3	1:A:43:LEU:HB2	2.01	0.41
1:A:43:LEU:O	1:A:47:ILE:HG13	2.20	0.41
1:A:162:MSE:HB3	1:A:165:SER:HB3	2.03	0.40
1:A:123:TYR:C	1:A:124:LEU:HD12	2.42	0.40
1:A:464:LEU:HG	1:A:472:LEU:HD11	2.02	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	442/480 (92%)	427 (97%)	15 (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	336/381 (88%)	329 (98%)	7 (2%)	53 80

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	LEU
1	A	233	VAL
1	A	253	LEU
1	A	301	VAL
1	A	374	LYS
1	A	377	ASP
1	A	464	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 3 are monoatomic - leaving 9 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	OLC	A	602	-	10,10,24	0.51	0	9,9,25	0.72	0
3	2PE	A	607	-	6,6,27	0.48	0	5,5,26	0.28	0
6	SO4	A	609	-	4,4,4	0.20	0	6,6,6	0.21	0
3	2PE	A	603	-	13,13,27	0.52	0	12,12,26	0.27	0
5	DMS	A	608	-	3,3,3	0.70	0	3,3,3	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	OLC	A	601	-	18,18,24	0.88	1 (5%)	18,19,25	1.03	1 (5%)
3	2PE	A	606	-	10,10,27	0.54	0	9,9,26	0.36	0
4	IMD	A	605	-	3,5,5	0.45	0	4,5,5	0.48	0
3	2PE	A	604	-	6,6,27	0.52	0	5,5,26	0.30	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
2	OLC	A	602	-	-	3/7/8/24	-
3	2PE	A	607	-	-	1/4/4/25	-
3	2PE	A	603	-	-	8/11/11/25	-
2	OLC	A	601	-	-	8/18/18/24	-
3	2PE	A	606	-	-	5/8/8/25	-
4	IMD	A	605	-	-	-	0/1/1/1
3	2PE	A	604	-	-	2/4/4/25	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	OLC	O20-C1	2.48	1.40	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	OLC	O20-C1-C2	2.49	119.71	111.91

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	OLC	C9-C10-C11-C12
2	A	601	OLC	O20-C21-C22-O23
3	A	606	2PE	C2-C3-O4-C5
2	A	601	OLC	C2-C1-O20-C21
2	A	601	OLC	O19-C1-O20-C21
3	A	603	2PE	O25-C26-C27-O28
3	A	603	2PE	O22-C23-C24-O25

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Mol	Chain	Res	Type	Atoms
2	A	601	OLC	O20-C21-C22-C24
3	A	606	2PE	O7-C8-C9-O10
3	A	603	2PE	O19-C20-C21-O22
3	A	607	2PE	C2-C3-O4-C5
3	A	603	2PE	C24-C23-O22-C21
3	A	606	2PE	C5-C6-O7-C8
2	A	601	OLC	O20-C1-C2-C3
3	A	603	2PE	C23-C24-O25-C26
3	A	603	2PE	C20-C21-O22-C23
3	A	604	2PE	C2-C3-O4-C5
2	A	602	OLC	C6-C7-C8-C9
3	A	606	2PE	C8-C9-O10-C11
3	A	604	2PE	O1-C2-C3-O4
3	A	606	2PE	O4-C5-C6-O7
2	A	601	OLC	C4-C5-C6-C7
3	A	603	2PE	C17-C18-O19-C20
2	A	602	OLC	C3-C4-C5-C6
3	A	603	2PE	O16-C17-C18-O19
2	A	601	OLC	O19-C1-C2-C3
2	A	602	OLC	C7-C8-C9-C10

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	OLC	1	0
3	A	606	2PE	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 then 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.

Ligand OLC A 602

Bond lengths

Bond angles

Torsions

Rings

Ligand 2PE A 607

Bond lengths

Bond angles

Torsions

Rings

Ligand 2PE A 603

Bond lengths

Bond angles

Torsions

Rings

Ligand OLC A 601

Bond lengths

Bond angles

Torsions

Rings

Ligand 2PE A 606

Bond lengths

Bond angles

Torsions

Rings

Ligand 2PE A 604

Bond lengths

Bond angles

Torsions

Rings
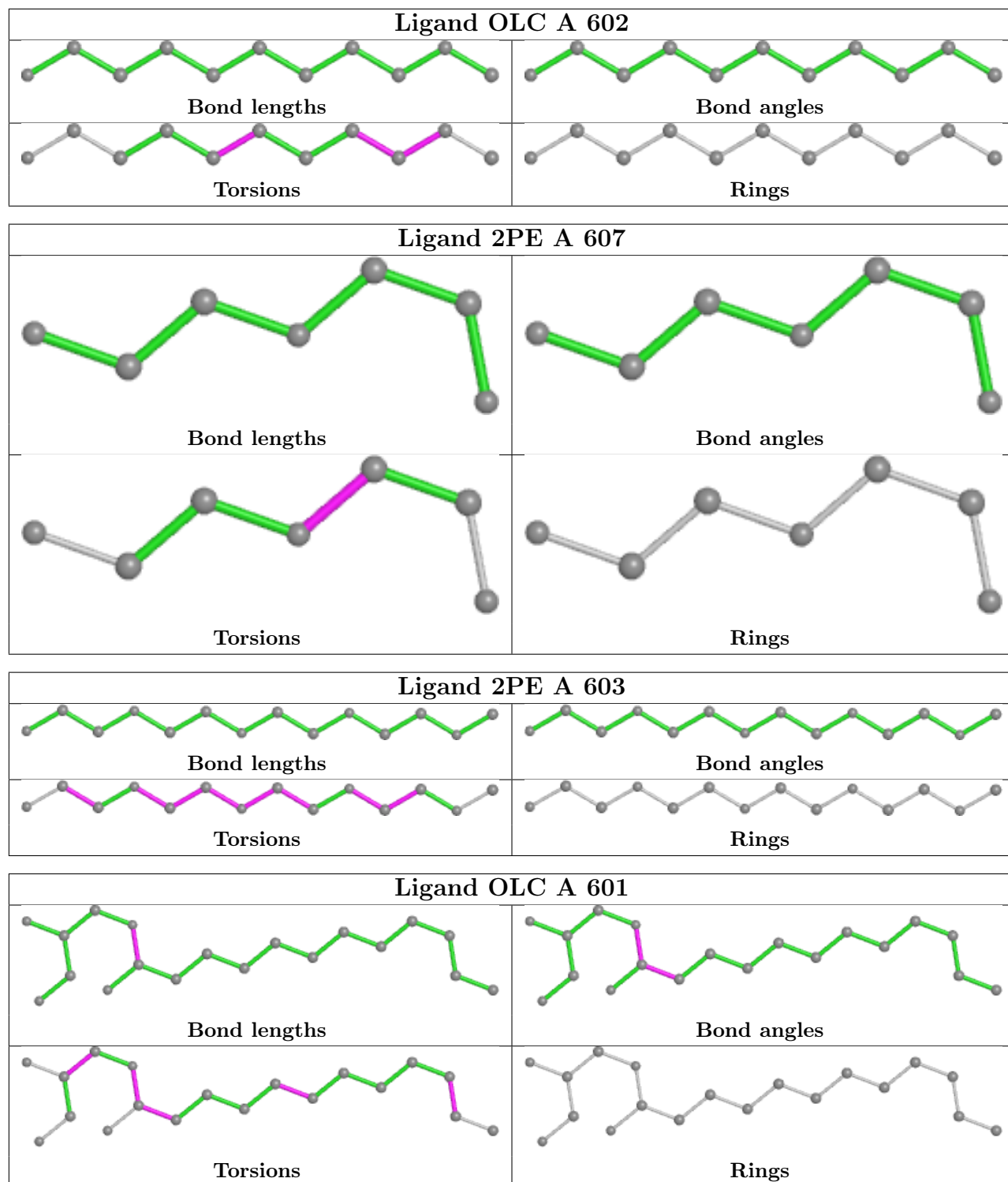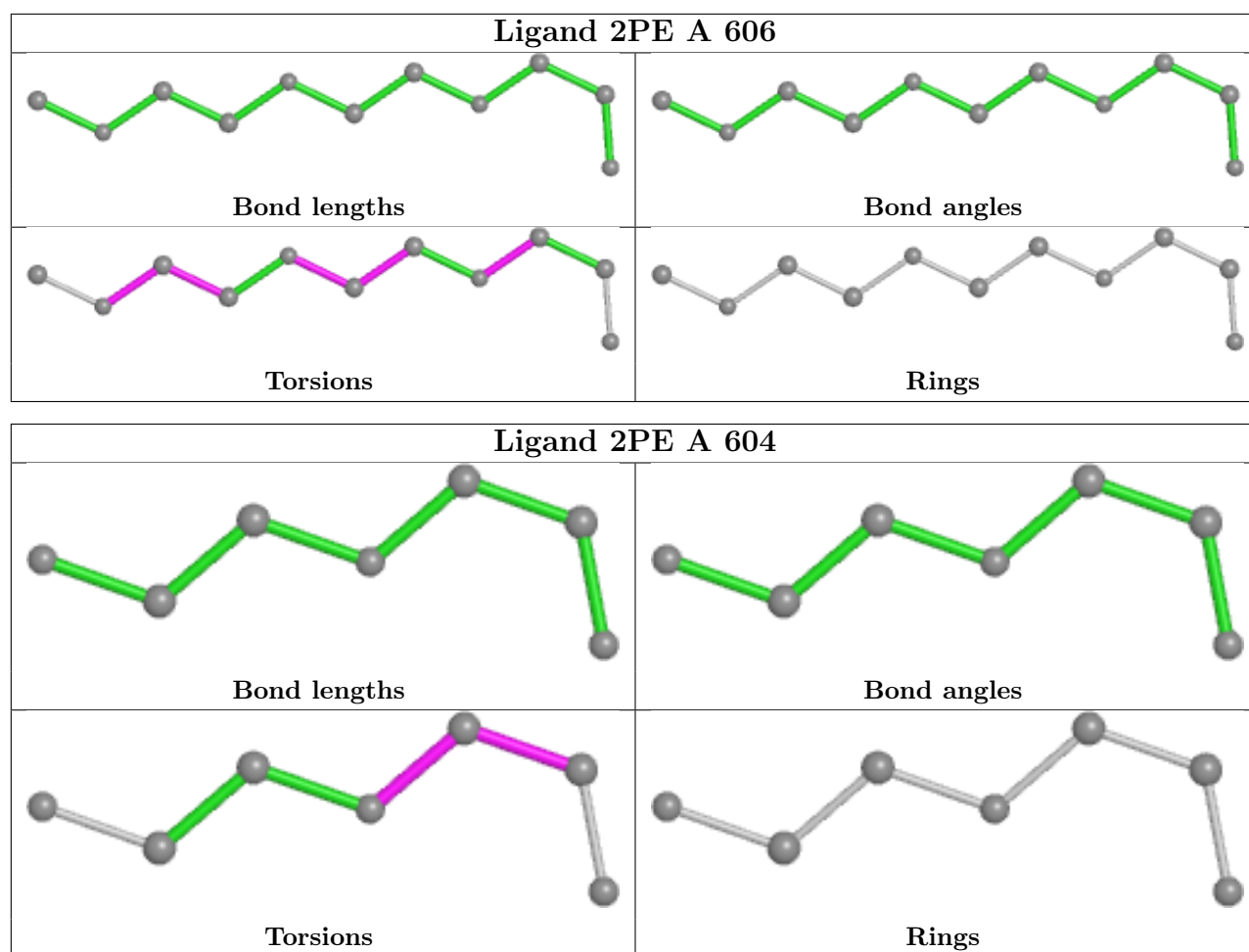
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	435/480 (90%)	0.02	32 (7%)	14	12	38, 55, 149, 184	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	434	ILE	7.9
1	A	430	VAL	5.1
1	A	412	VAL	4.9
1	A	413	TYR	4.9
1	A	436	ALA	4.6
1	A	406	VAL	4.5
1	A	409	ALA	4.5
1	A	486	THR	4.3
1	A	431	ARG	4.1
1	A	36	ILE	4.0
1	A	408	GLY	3.9
1	A	403	VAL	3.8
1	A	433	TYR	3.4
1	A	410	PHE	3.4
1	A	432	ASP	3.4
1	A	440	PRO	3.3
1	A	405	VAL	3.1
1	A	35	PRO	3.1
1	A	435	ILE	3.1
1	A	490	GLN	3.0
1	A	494	ILE	2.9
1	A	483	PHE	2.8
1	A	438	ALA	2.7
1	A	437	LEU	2.6
1	A	488	ASN	2.6
1	A	487	LEU	2.6
1	A	411	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	404	VAL	2.2
1	A	493	ARG	2.1
1	A	407	ARG	2.1
1	A	284	PRO	2.1
1	A	444	ALA	2.1

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	2PE	A	603	14/28	0.83	0.36	74,82,90,106	0
2	OLC	A	602	11/25	0.86	0.20	76,84,95,95	0
3	2PE	A	604	7/28	0.86	0.25	74,76,81,82	0
3	2PE	A	606	11/28	0.86	0.22	69,82,97,100	0
4	IMD	A	605	5/5	0.86	0.32	83,85,91,92	0
3	2PE	A	607	7/28	0.88	0.26	63,69,76,84	0
7	CL	A	611	1/1	0.89	0.10	80,80,80,80	0
2	OLC	A	601	19/25	0.91	0.26	39,54,68,76	0
7	CL	A	610	1/1	0.95	0.06	77,77,77,77	0
7	CL	A	612	1/1	0.96	0.28	55,55,55,55	0
6	SO4	A	609	5/5	0.97	0.13	85,85,85,90	0
5	DMS	A	608	4/4	0.97	0.18	59,64,70,74	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 2PE A 603:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
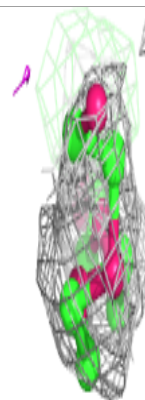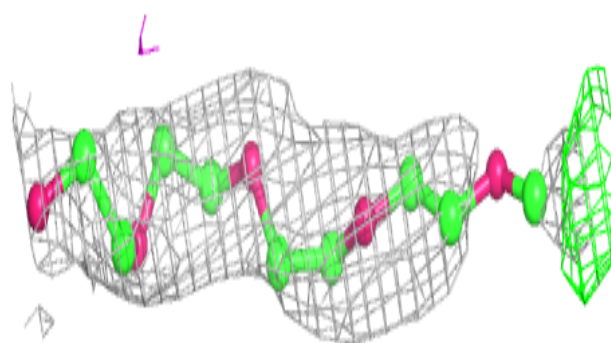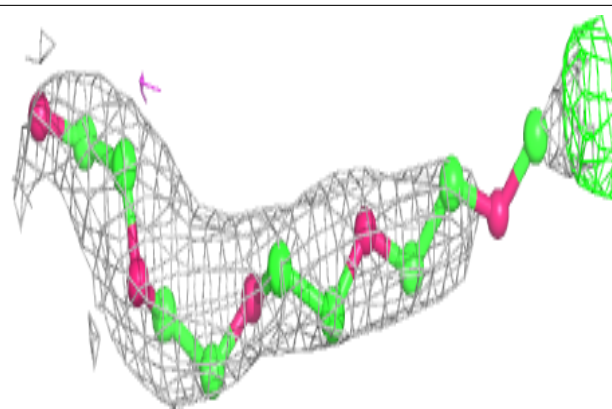
Electron density around OLC A 602:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
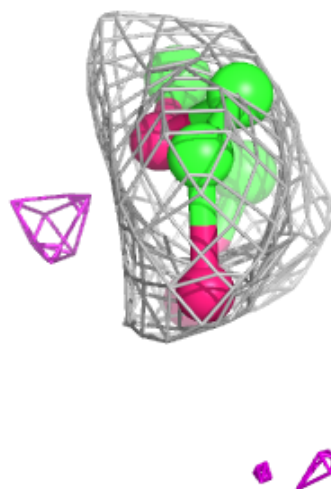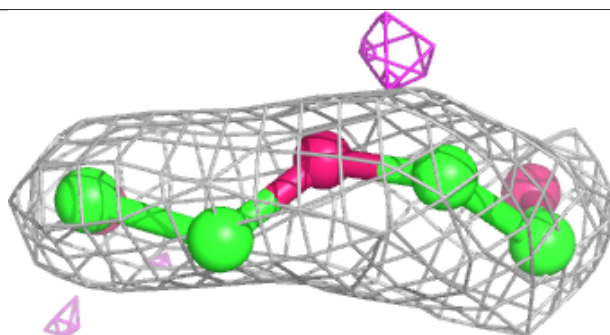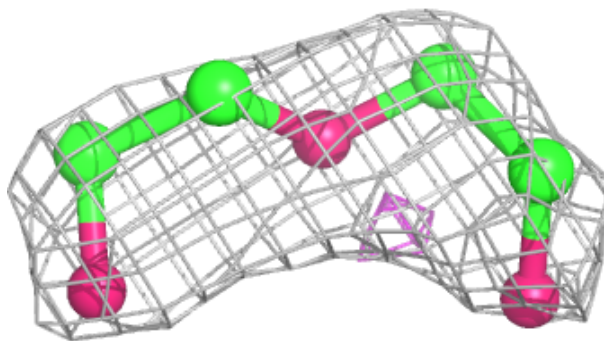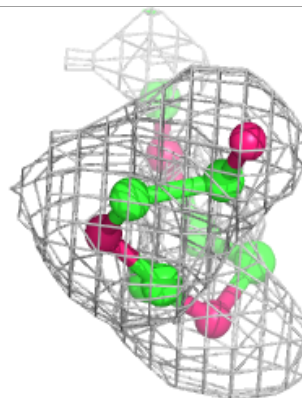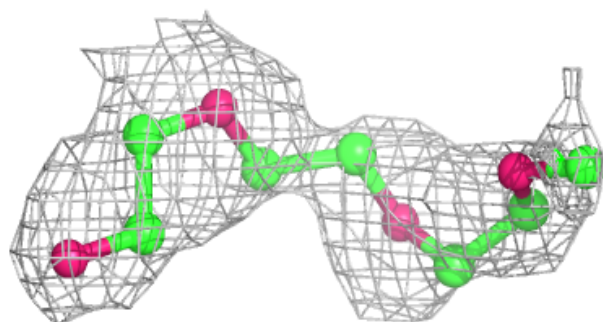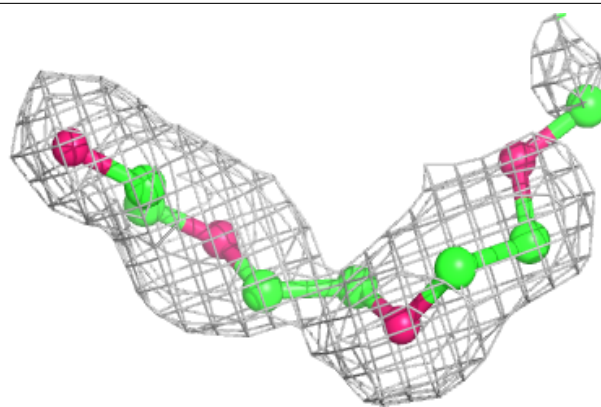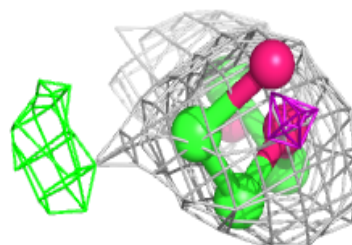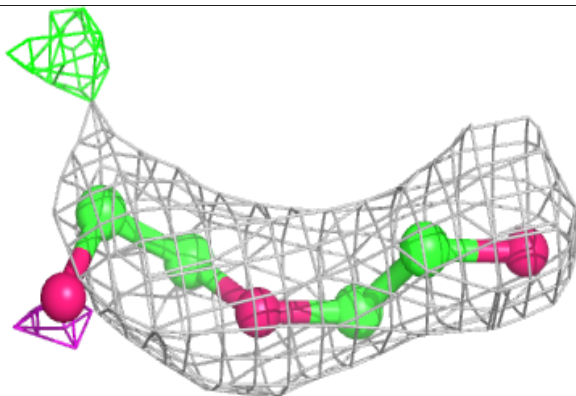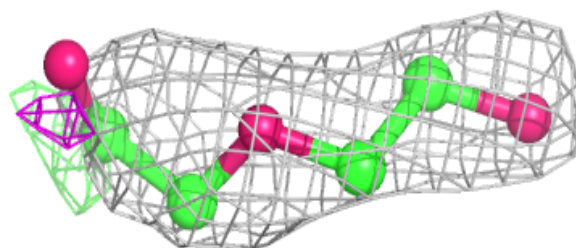$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
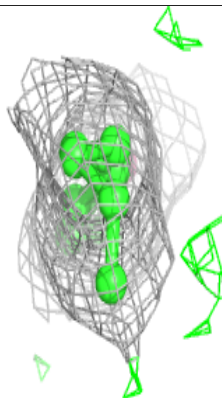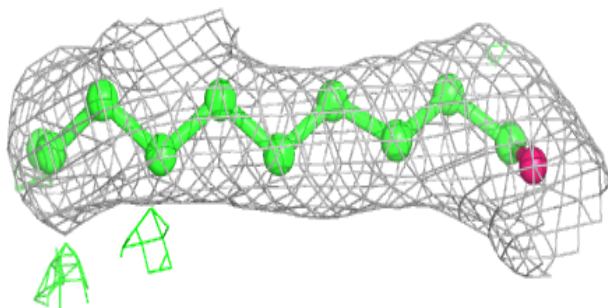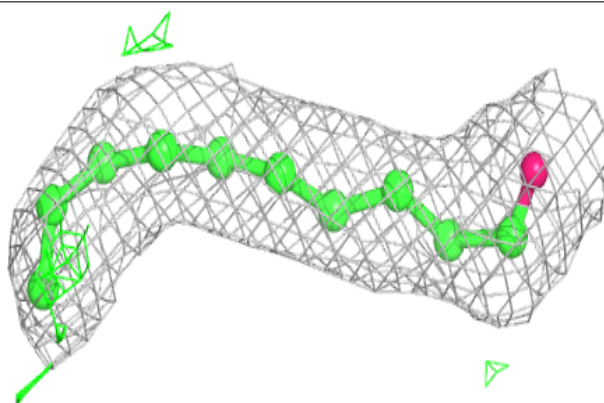
Electron density around 2PE A 604:

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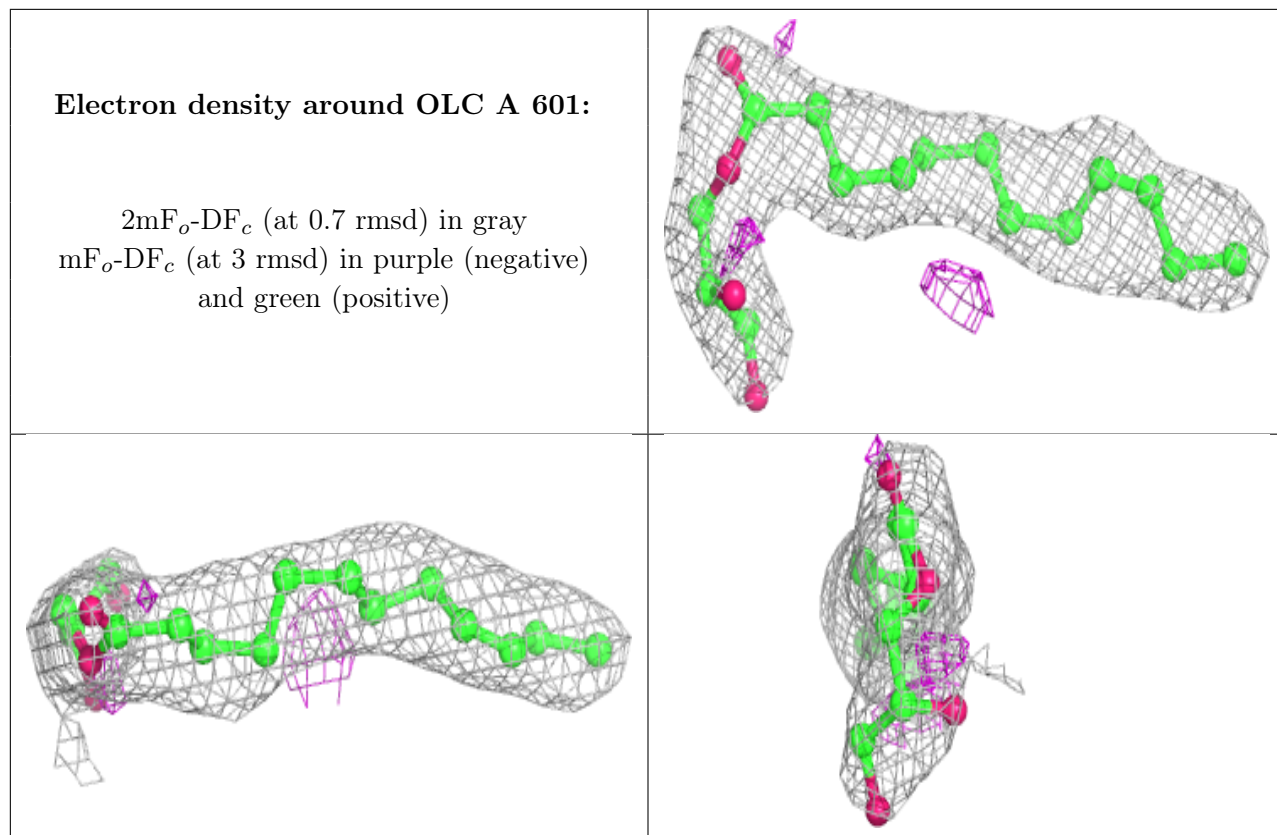mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around 2PE 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 2PE A 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 OLC A 601:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.