



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2026 – 01:42 PM EDT

PDB ID : 4OSD / pdb_00004osd
Title : Dimer of a C-terminal fragment of phage T4 gp5 beta-helix
Authors : Buth, S.A.; Leiman, P.G.; Shneider, M.M.
Deposited on : 2014-02-12
Resolution : 1.96 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 : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

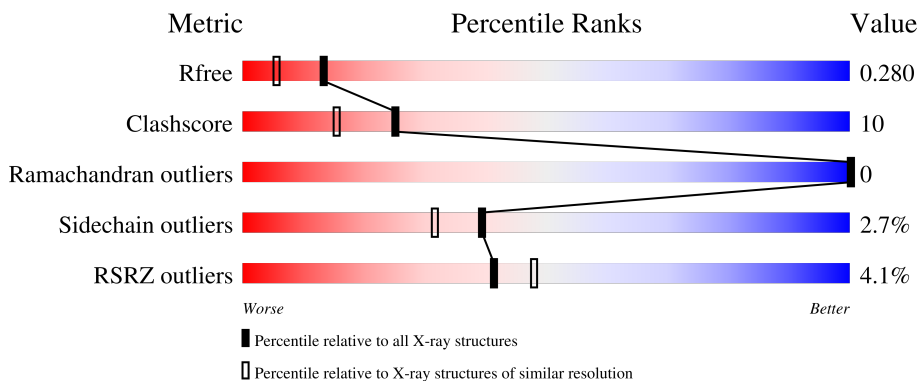
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	95	 4% 81% 17%
1	B	95	 4% 78% 20%
1	C	95	 4% 77% 19%
1	D	95	 2% 76% 21%
1	E	95	 5% 73% 24%

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Mol	Chain	Length	Quality of chain
1	F	95	<p>4% 80% 16% ..</p>
1	G	95	<p>7% 85% 12% ..</p>
1	H	95	<p>5% 84% 13% ..</p>
1	I	95	<p>5% 81% 16% .</p>
1	J	95	<p>3% 80% 18% .</p>
1	K	95	<p>2% 77% 21% .</p>
1	L	95	<p>2% 78% 18% ..</p>
1	M	95	<p>3% 80% 17% ..</p>
1	N	95	<p>5% 76% 21% ..</p>
1	O	95	<p>3% 79% 18% ..</p>
1	P	95	<p>4% 78% 20% .</p>
1	Q	95	<p>3% 67% 29% ..</p>
1	R	95	<p>3% 79% 18% ..</p>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13209 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 Tail-associated lysozyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	93	676	411	113	150	2	0	0	0
1	B	93	684	417	114	151	2	0	1	0
1	C	93	676	411	113	150	2	0	0	0
1	D	93	684	417	114	151	2	0	1	0
1	E	93	685	417	115	151	2	0	1	0
1	F	93	682	414	114	152	2	0	1	0
1	G	93	676	411	113	150	2	0	0	0
1	H	93	685	417	115	151	2	0	1	0
1	I	92	670	408	112	148	2	0	0	0
1	J	93	676	411	113	150	2	0	0	0
1	K	93	676	411	113	150	2	0	0	0
1	L	92	679	413	113	151	2	0	1	0
1	M	93	676	411	113	150	2	0	0	0
1	N	93	682	414	114	152	2	0	1	0
1	O	93	676	411	113	150	2	0	0	0
1	P	93	682	414	114	152	2	0	1	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	Q	93	676	411	113	150	2	0	0	0
1	R	93	676	411	113	150	2	0	0	0

There are 54 discrepancies between the modelled and reference sequences:

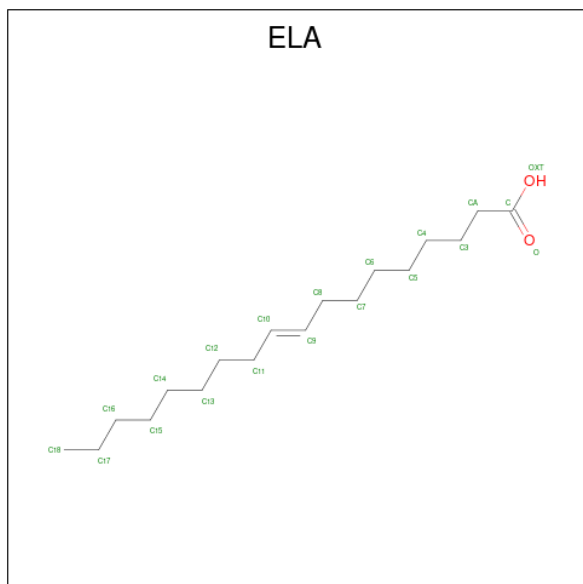
Chain	Residue	Modelled	Actual	Comment	Reference
A	481	SER	-	expression tag	UNP P16009
A	482	GLY	-	expression tag	UNP P16009
A	483	SER	-	expression tag	UNP P16009
B	481	SER	-	expression tag	UNP P16009
B	482	GLY	-	expression tag	UNP P16009
B	483	SER	-	expression tag	UNP P16009
C	481	SER	-	expression tag	UNP P16009
C	482	GLY	-	expression tag	UNP P16009
C	483	SER	-	expression tag	UNP P16009
D	481	SER	-	expression tag	UNP P16009
D	482	GLY	-	expression tag	UNP P16009
D	483	SER	-	expression tag	UNP P16009
E	481	SER	-	expression tag	UNP P16009
E	482	GLY	-	expression tag	UNP P16009
E	483	SER	-	expression tag	UNP P16009
F	481	SER	-	expression tag	UNP P16009
F	482	GLY	-	expression tag	UNP P16009
F	483	SER	-	expression tag	UNP P16009
G	481	SER	-	expression tag	UNP P16009
G	482	GLY	-	expression tag	UNP P16009
G	483	SER	-	expression tag	UNP P16009
H	481	SER	-	expression tag	UNP P16009
H	482	GLY	-	expression tag	UNP P16009
H	483	SER	-	expression tag	UNP P16009
I	481	SER	-	expression tag	UNP P16009
I	482	GLY	-	expression tag	UNP P16009
I	483	SER	-	expression tag	UNP P16009
J	481	SER	-	expression tag	UNP P16009
J	482	GLY	-	expression tag	UNP P16009
J	483	SER	-	expression tag	UNP P16009
K	481	SER	-	expression tag	UNP P16009
K	482	GLY	-	expression tag	UNP P16009
K	483	SER	-	expression tag	UNP P16009
L	481	SER	-	expression tag	UNP P16009

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Chain	Residue	Modelled	Actual	Comment	Reference
L	482	GLY	-	expression tag	UNP P16009
L	483	SER	-	expression tag	UNP P16009
M	481	SER	-	expression tag	UNP P16009
M	482	GLY	-	expression tag	UNP P16009
M	483	SER	-	expression tag	UNP P16009
N	481	SER	-	expression tag	UNP P16009
N	482	GLY	-	expression tag	UNP P16009
N	483	SER	-	expression tag	UNP P16009
O	481	SER	-	expression tag	UNP P16009
O	482	GLY	-	expression tag	UNP P16009
O	483	SER	-	expression tag	UNP P16009
P	481	SER	-	expression tag	UNP P16009
P	482	GLY	-	expression tag	UNP P16009
P	483	SER	-	expression tag	UNP P16009
Q	481	SER	-	expression tag	UNP P16009
Q	482	GLY	-	expression tag	UNP P16009
Q	483	SER	-	expression tag	UNP P16009
R	481	SER	-	expression tag	UNP P16009
R	482	GLY	-	expression tag	UNP P16009
R	483	SER	-	expression tag	UNP P16009

- Molecule 2 is Elaidic acid (CCD ID: ELA) (formula: $C_{18}H_{34}O_2$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
2	A	1	Total	C	O	0	0
			20	18	2		

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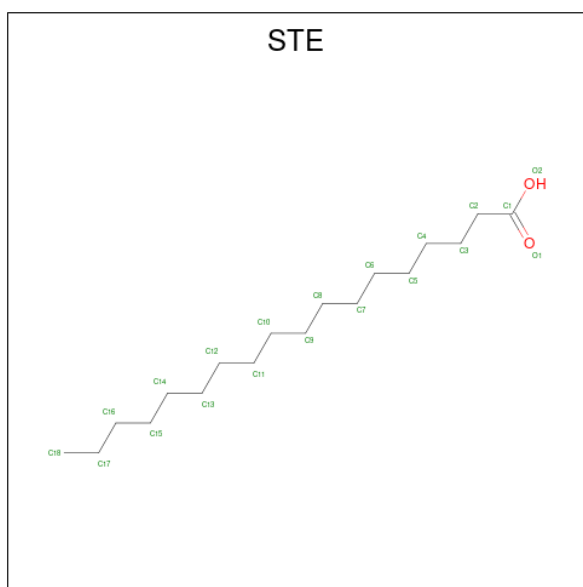
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			18	16	2		
2	F	1	Total	C	O	0	0
			20	18	2		
2	G	1	Total	C	O	0	0
			20	18	2		
2	J	1	Total	C	O	0	0
			20	18	2		
2	M	1	Total	C	O	0	0
			20	18	2		
2	P	1	Total	C	O	0	0
			20	18	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

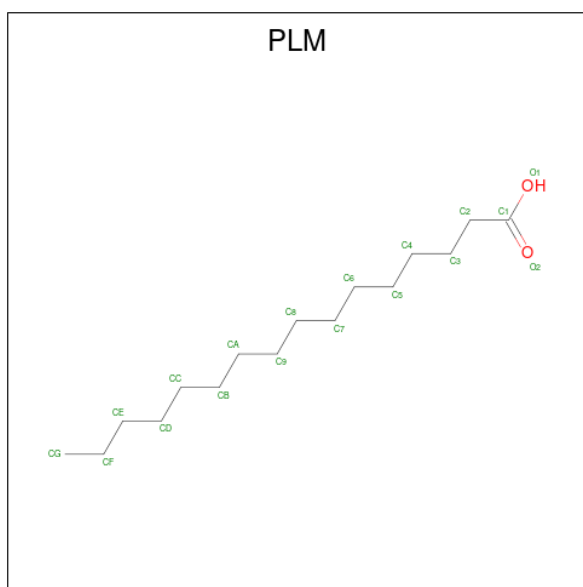
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		
3	H	1	Total	Mg	0	0
			1	1		
3	L	1	Total	Mg	0	0
			1	1		
3	O	1	Total	Mg	0	0
			1	1		
3	Q	1	Total	Mg	0	0
			1	1		

- Molecule 4 is STEARIC ACID (CCD ID: STE) (formula: C₁₈H₃₆O₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	C O	0	0
			20	18 2		
4	F	1	Total	C O	0	0
			20	18 2		
4	G	1	Total	C O	0	0
			20	18 2		
4	K	1	Total	C O	0	0
			20	18 2		
4	O	1	Total	C O	0	0
			20	18 2		
4	P	1	Total	C O	0	0
			20	18 2		

- Molecule 5 is PALMITIC ACID (CCD ID: PLM) (formula: C₁₆H₃₂O₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	C O	0	0
			18	16 2		
5	H	1	Total	C O	0	0
			18	16 2		
5	K	1	Total	C O	0	0
			18	16 2		
5	N	1	Total	C O	0	0
			18	16 2		
5	Q	1	Total	C O	0	0
			18	16 2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	36	Total	O	0	0
			36	36		
6	B	38	Total	O	0	0
			38	38		
6	C	41	Total	O	0	0
			41	41		
6	D	38	Total	O	0	0
			38	38		
6	E	36	Total	O	0	0
			36	36		
6	F	42	Total	O	0	0
			42	42		
6	G	28	Total	O	0	0
			28	28		

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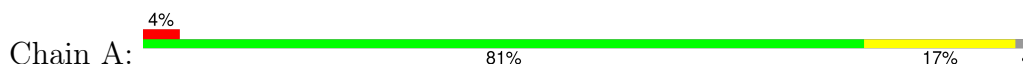
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	21	Total 21	O 21	0	0
6	I	20	Total 20	O 20	0	0
6	J	46	Total 46	O 46	0	0
6	K	32	Total 32	O 32	0	0
6	L	37	Total 37	O 37	0	0
6	M	21	Total 21	O 21	0	0
6	N	22	Total 22	O 22	0	0
6	O	34	Total 34	O 34	0	0
6	P	45	Total 45	O 45	0	0
6	Q	44	Total 44	O 44	0	0
6	R	57	Total 57	O 57	0	0

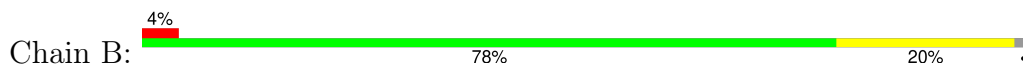
3 Residue-property plots [i](#)

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.

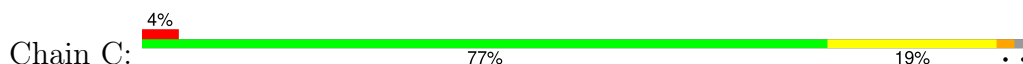
- Molecule 1: Tail-associated lysozyme



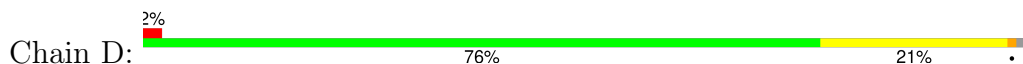
- Molecule 1: Tail-associated lysozyme



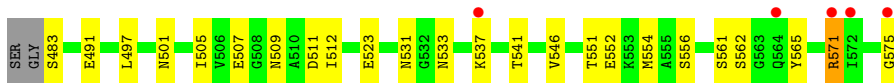
- Molecule 1: Tail-associated lysozyme



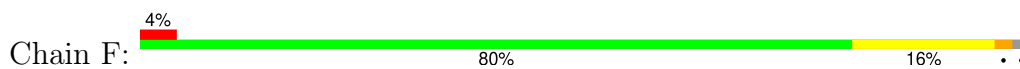
- Molecule 1: Tail-associated lysozyme



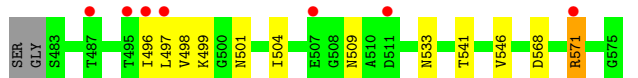
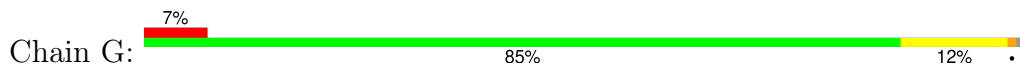
- Molecule 1: Tail-associated lysozyme



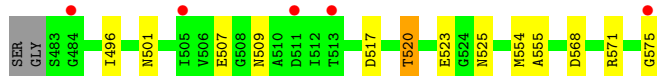
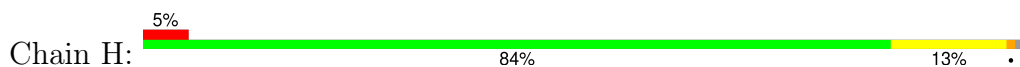
- Molecule 1: Tail-associated lysozyme



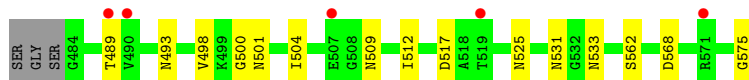
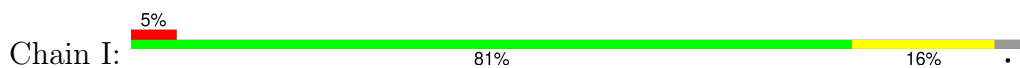
- Molecule 1: Tail-associated lysozyme



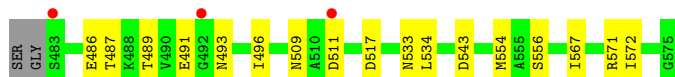
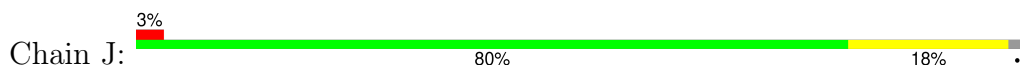
- Molecule 1: Tail-associated lysozyme



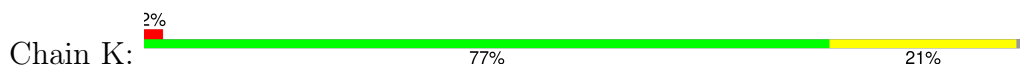
- Molecule 1: Tail-associated lysozyme



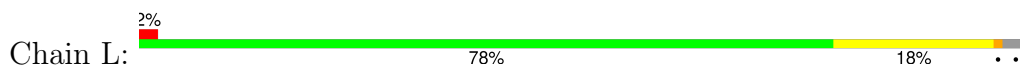
- Molecule 1: Tail-associated lysozyme



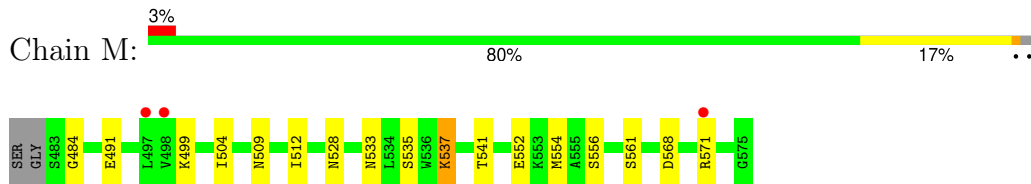
- Molecule 1: Tail-associated lysozyme



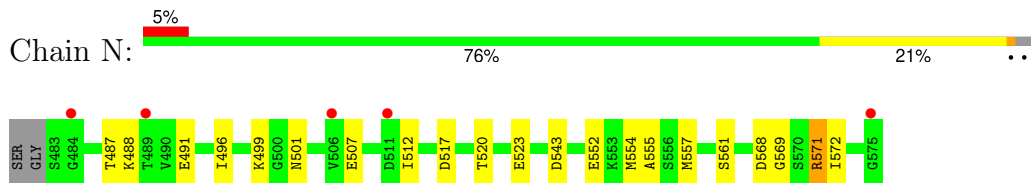
- Molecule 1: Tail-associated lysozyme



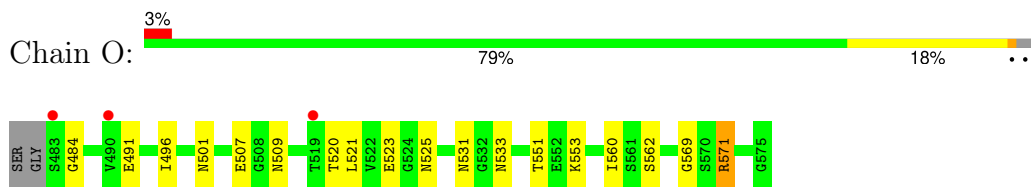
- Molecule 1: Tail-associated lysozyme



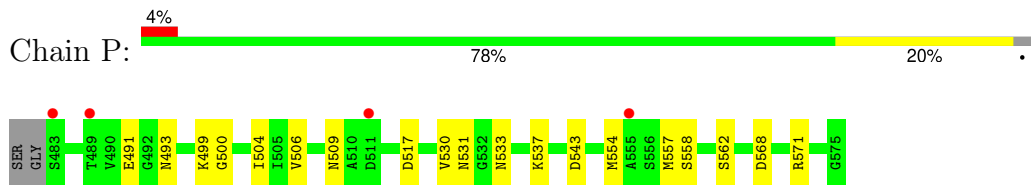
- Molecule 1: Tail-associated lysozyme



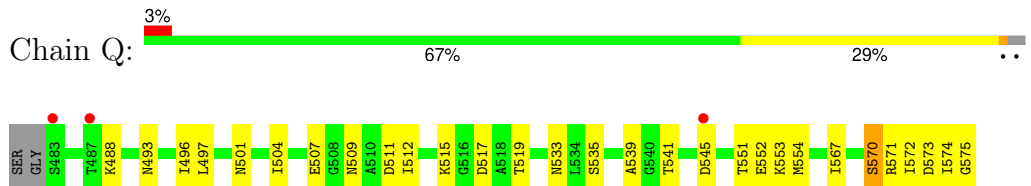
- Molecule 1: Tail-associated lysozyme



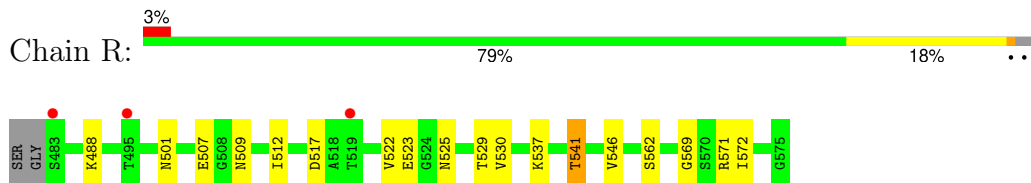
- Molecule 1: Tail-associated lysozyme



- Molecule 1: Tail-associated lysozyme



- Molecule 1: Tail-associated lysozyme



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	110.29Å 73.79Å 111.60Å 90.00° 113.39° 90.00°	Depositor
Resolution (Å)	59.87 – 1.96 59.87 – 1.97	Depositor EDS
% Data completeness (in resolution range)	99.1 (59.87-1.96) 99.1 (59.87-1.97)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.02 (at 1.97Å)	Xtrriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.219 , 0.279 0.225 , 0.280	Depositor DCC
R_{free} test set	5818 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	26.9	Xtrriage
Anisotropy	0.214	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 25.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.022 for l,-k,h	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13209	wwPDB-VP
Average B, all atoms (Å ²)	35.0	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 45.87 % 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 1.2412e-04. 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: ELA, MG, PLM, STE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.31	0/682	1.16	0/925
1	B	1.32	2/690 (0.3%)	1.10	0/936
1	C	1.42	1/682 (0.1%)	1.12	1/925 (0.1%)
1	D	1.35	4/690 (0.6%)	1.15	1/936 (0.1%)
1	E	1.31	1/691 (0.1%)	1.07	1/936 (0.1%)
1	F	1.35	2/688 (0.3%)	1.12	0/933
1	G	1.11	0/682	1.07	0/925
1	H	1.17	1/691 (0.1%)	1.05	0/936
1	I	1.18	0/676	1.06	0/917
1	J	1.38	1/682 (0.1%)	1.13	1/925 (0.1%)
1	K	1.45	1/682 (0.1%)	1.12	2/925 (0.2%)
1	L	1.33	2/685 (0.3%)	1.10	0/929
1	M	1.18	0/682	1.07	0/925
1	N	1.14	0/688	1.01	0/933
1	O	1.23	0/682	1.04	0/925
1	P	1.49	4/688 (0.6%)	1.13	1/933 (0.1%)
1	Q	1.51	6/682 (0.9%)	1.14	0/925
1	R	1.49	5/682 (0.7%)	1.18	0/925
All	All	1.32	30/12325 (0.2%)	1.10	7/16714 (0.0%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	539	ALA	N-CA	7.71	1.55	1.46
1	Q	545	ASP	CA-C	7.27	1.61	1.52
1	R	569	GLY	N-CA	6.87	1.51	1.44
1	J	534	LEU	N-CA	6.53	1.53	1.46
1	Q	519	THR	CA-C	6.27	1.60	1.52

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	570	SER	N-CA-C	-6.83	103.76	111.14
1	C	570	SER	N-CA-C	-6.26	104.54	111.36
1	E	562	SER	N-CA-C	-5.95	104.92	111.82
1	J	572	ILE	CB-CA-C	-5.82	102.47	110.96
1	K	511	ASP	CB-CA-C	-5.70	101.01	110.14

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	676	0	651	22	0
1	B	684	0	661	24	0
1	C	676	0	651	26	1
1	D	684	0	661	23	0
1	E	685	0	663	29	0
1	F	682	0	655	22	0
1	G	676	0	651	20	0
1	H	685	0	663	17	0
1	I	670	0	646	20	0
1	J	676	0	651	19	0
1	K	676	0	651	31	0
1	L	679	0	651	24	0
1	M	676	0	651	20	0
1	N	682	0	655	20	0
1	O	676	0	651	17	0
1	P	682	0	655	19	0
1	Q	676	0	651	30	0
1	R	676	0	651	20	0
2	A	38	0	59	7	0
2	F	20	0	33	0	0
2	G	20	0	33	1	0
2	J	20	0	33	1	0
2	M	20	0	33	0	0
2	P	20	0	33	2	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	1	0	0	0	0
3	H	1	0	0	0	0
3	L	1	0	0	0	0
3	O	1	0	0	0	0
3	Q	1	0	0	0	0
4	C	20	0	35	2	0
4	F	20	0	35	2	0
4	G	20	0	35	1	0
4	K	20	0	35	3	0
4	O	20	0	35	1	0
4	P	20	0	35	1	0
5	D	18	0	31	4	0
5	H	18	0	31	2	0
5	K	18	0	31	3	0
5	N	18	0	31	2	0
5	Q	18	0	31	5	0
6	A	36	0	0	3	0
6	B	38	0	0	1	0
6	C	41	0	0	0	0
6	D	38	0	0	1	0
6	E	36	0	0	3	0
6	F	42	0	0	2	0
6	G	28	0	0	0	0
6	H	21	0	0	0	0
6	I	20	0	0	0	0
6	J	46	0	0	1	0
6	K	32	0	0	1	0
6	L	37	0	0	2	0
6	M	21	0	0	0	0
6	N	22	0	0	0	0
6	O	34	0	0	2	1
6	P	45	0	0	4	0
6	Q	44	0	0	0	0
6	R	57	0	0	1	0
All	All	13209	0	12358	241	1

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 10.

The worst 5 of 241 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:J:511:ASP:OD1	1:K:519:THR:HB	1.64	0.96
1:K:512:ILE:HD11	5:K:602:PLM:H31	1.47	0.94
1:P:493:ASN:HD22	1:Q:501:ASN:H	1.22	0.85
1:G:499:LYS:HA	1:H:507:GLU:HG3	1.59	0.84
1:M:499:LYS:HA	1:N:507:GLU:HG3	1.60	0.83

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:483:SER:N	6:O:706:HOH:O[2_556]	1.99	0.21

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	91/95 (96%)	91 (100%)	0	0	100	100
1	B	92/95 (97%)	92 (100%)	0	0	100	100
1	C	91/95 (96%)	91 (100%)	0	0	100	100
1	D	92/95 (97%)	92 (100%)	0	0	100	100
1	E	92/95 (97%)	92 (100%)	0	0	100	100
1	F	92/95 (97%)	92 (100%)	0	0	100	100
1	G	91/95 (96%)	91 (100%)	0	0	100	100
1	H	92/95 (97%)	90 (98%)	2 (2%)	0	100	100
1	I	90/95 (95%)	90 (100%)	0	0	100	100
1	J	91/95 (96%)	90 (99%)	1 (1%)	0	100	100
1	K	91/95 (96%)	90 (99%)	1 (1%)	0	100	100
1	L	91/95 (96%)	90 (99%)	1 (1%)	0	100	100
1	M	91/95 (96%)	91 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	92/95 (97%)	92 (100%)	0	0	100	100
1	O	91/95 (96%)	91 (100%)	0	0	100	100
1	P	92/95 (97%)	92 (100%)	0	0	100	100
1	Q	91/95 (96%)	91 (100%)	0	0	100	100
1	R	91/95 (96%)	90 (99%)	1 (1%)	0	100	100
All	All	1644/1710 (96%)	1638 (100%)	6 (0%)	0	100	100

There are no Ramachandran outliers to report.

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	75/76 (99%)	73 (97%)	2 (3%)	39	32
1	B	76/76 (100%)	75 (99%)	1 (1%)	61	58
1	C	75/76 (99%)	71 (95%)	4 (5%)	20	9
1	D	76/76 (100%)	76 (100%)	0	100	100
1	E	76/76 (100%)	73 (96%)	3 (4%)	28	18
1	F	76/76 (100%)	74 (97%)	2 (3%)	40	33
1	G	75/76 (99%)	73 (97%)	2 (3%)	39	32
1	H	76/76 (100%)	74 (97%)	2 (3%)	40	33
1	I	74/76 (97%)	74 (100%)	0	100	100
1	J	75/76 (99%)	74 (99%)	1 (1%)	61	58
1	K	75/76 (99%)	75 (100%)	0	100	100
1	L	75/76 (99%)	71 (95%)	4 (5%)	20	9
1	M	75/76 (99%)	72 (96%)	3 (4%)	28	17
1	N	76/76 (100%)	73 (96%)	3 (4%)	28	18
1	O	75/76 (99%)	71 (95%)	4 (5%)	20	9
1	P	76/76 (100%)	75 (99%)	1 (1%)	61	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	75/76 (99%)	72 (96%)	3 (4%)	28	17
1	R	75/76 (99%)	72 (96%)	3 (4%)	28	17
All	All	1356/1368 (99%)	1318 (97%)	38 (3%)	39	30

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	553	LYS
1	R	512	ILE
1	O	560	ILE
1	Q	496	ILE
1	R	562	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 85 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	528	ASN
1	P	528	ASN
1	N	501	ASN
1	O	526	GLN
1	Q	501	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 24 ligands modelled in this entry, 6 are monoatomic - leaving 18 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	ELA	F	603	-	19,19,19	1.25	1 (5%)	19,19,19	1.57	4 (21%)
5	PLM	Q	602	-	17,17,17	1.11	1 (5%)	17,17,17	1.11	1 (5%)
2	ELA	P	602	-	19,19,19	1.28	2 (10%)	19,19,19	1.50	2 (10%)
5	PLM	D	601	-	17,17,17	0.63	0	17,17,17	1.68	2 (11%)
5	PLM	K	602	-	17,17,17	0.97	1 (5%)	17,17,17	1.22	0
2	ELA	G	602	-	19,19,19	1.08	1 (5%)	19,19,19	1.55	2 (10%)
2	ELA	A	601	-	19,19,19	1.30	1 (5%)	19,19,19	1.29	1 (5%)
4	STE	C	601	-	19,19,19	0.66	0	19,19,19	0.62	0
2	ELA	A	602	-	17,17,19	1.34	1 (5%)	17,17,19	1.04	1 (5%)
4	STE	O	602	-	19,19,19	0.64	0	19,19,19	0.69	0
4	STE	F	602	-	19,19,19	0.63	0	19,19,19	0.67	0
2	ELA	M	601	-	19,19,19	1.06	1 (5%)	19,19,19	1.35	4 (21%)
5	PLM	H	602	-	17,17,17	0.75	0	17,17,17	1.47	1 (5%)
5	PLM	N	601	-	17,17,17	0.78	0	17,17,17	1.42	3 (17%)
4	STE	K	601	-	19,19,19	0.57	0	19,19,19	0.82	0
4	STE	P	601	-	19,19,19	0.76	0	19,19,19	0.54	0
4	STE	G	601	-	19,19,19	0.71	0	19,19,19	0.44	0
2	ELA	J	601	-	19,19,19	1.26	2 (10%)	19,19,19	1.20	1 (5%)

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	ELA	F	603	-	-	10/17/17/17	-
5	PLM	Q	602	-	-	6/15/15/15	-
2	ELA	P	602	-	-	5/17/17/17	-
5	PLM	D	601	-	-	6/15/15/15	-
5	PLM	K	602	-	-	3/15/15/15	-
2	ELA	G	602	-	-	5/17/17/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ELA	A	601	-	-	8/17/17/17	-
4	STE	C	601	-	-	10/17/17/17	-
2	ELA	A	602	-	-	6/15/15/17	-
4	STE	O	602	-	-	7/17/17/17	-
4	STE	F	602	-	-	7/17/17/17	-
2	ELA	M	601	-	-	5/17/17/17	-
5	PLM	H	602	-	-	9/15/15/15	-
5	PLM	N	601	-	-	3/15/15/15	-
4	STE	K	601	-	-	8/17/17/17	-
4	STE	P	601	-	-	7/17/17/17	-
4	STE	G	601	-	-	9/17/17/17	-
2	ELA	J	601	-	-	4/17/17/17	-

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	ELA	C10-C9	4.56	1.57	1.31
2	F	603	ELA	C10-C9	4.52	1.57	1.31
2	A	602	ELA	C10-C9	4.37	1.56	1.31
2	P	602	ELA	C10-C9	4.21	1.55	1.31
2	M	601	ELA	C10-C9	3.97	1.54	1.31

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	602	PLM	C3-C2-C1	-3.83	104.50	114.51
2	G	602	ELA	C3-CA-C	-3.72	104.80	114.51
5	D	601	PLM	C3-C2-C1	-3.70	104.84	114.51
2	F	603	ELA	C3-CA-C	-3.57	105.20	114.51
2	P	602	ELA	C3-CA-C	-2.75	107.32	114.51

There are no chirality outliers.

5 of 118 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	Q	602	PLM	C1-C2-C3-C4
5	H	602	PLM	C1-C2-C3-C4
4	K	601	STE	C1-C2-C3-C4
2	F	603	ELA	C4-C3-CA-C

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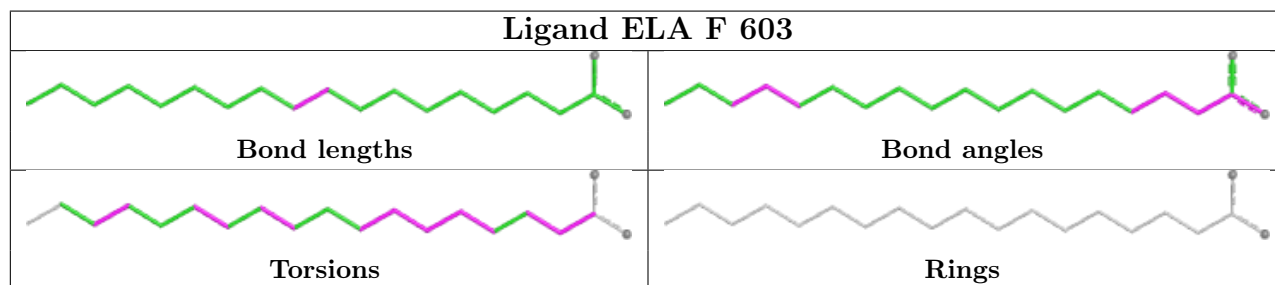
Mol	Chain	Res	Type	Atoms
4	G	601	STE	C5-C6-C7-C8

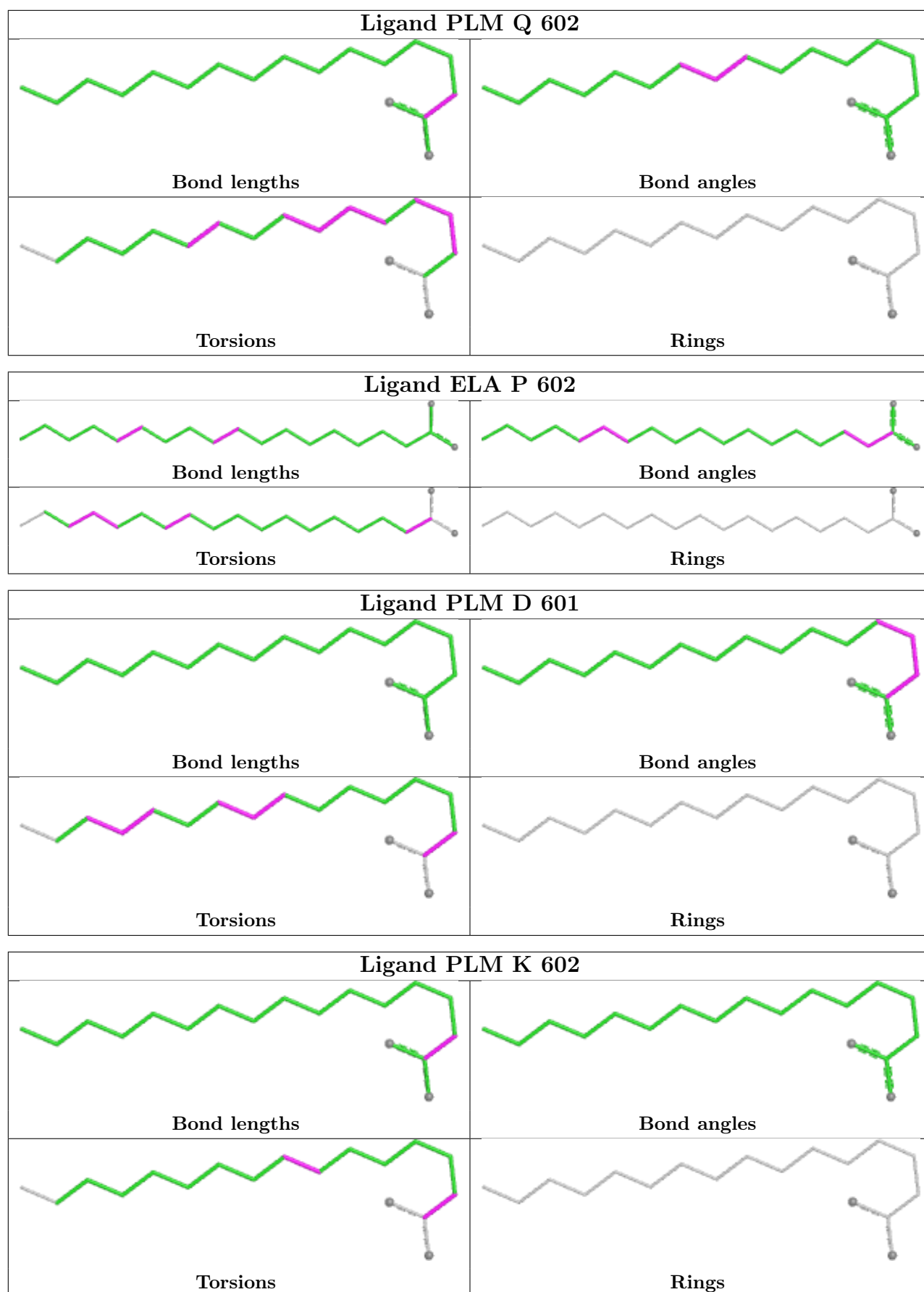
There are no ring outliers.

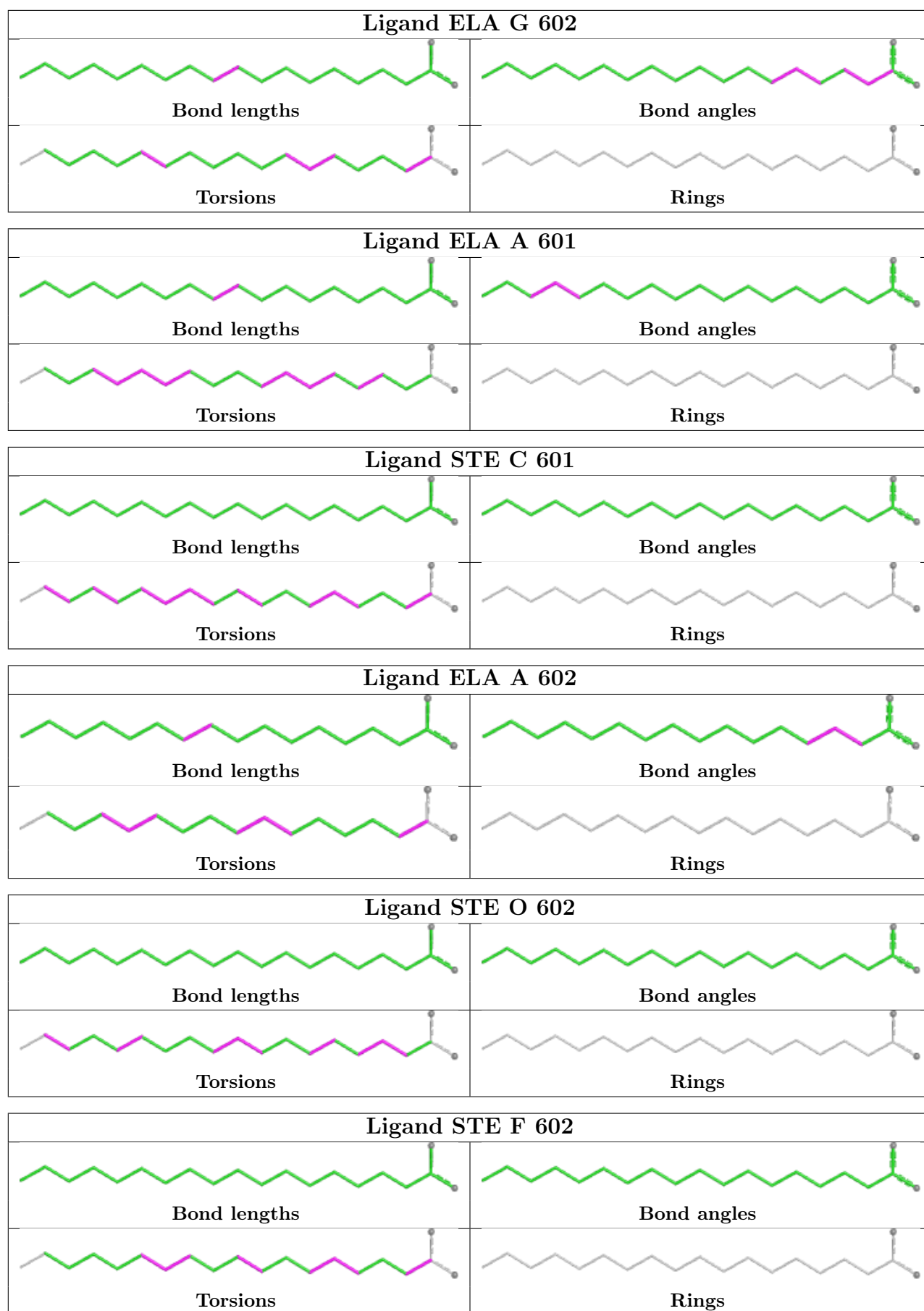
16 monomers are involved in 36 short contacts:

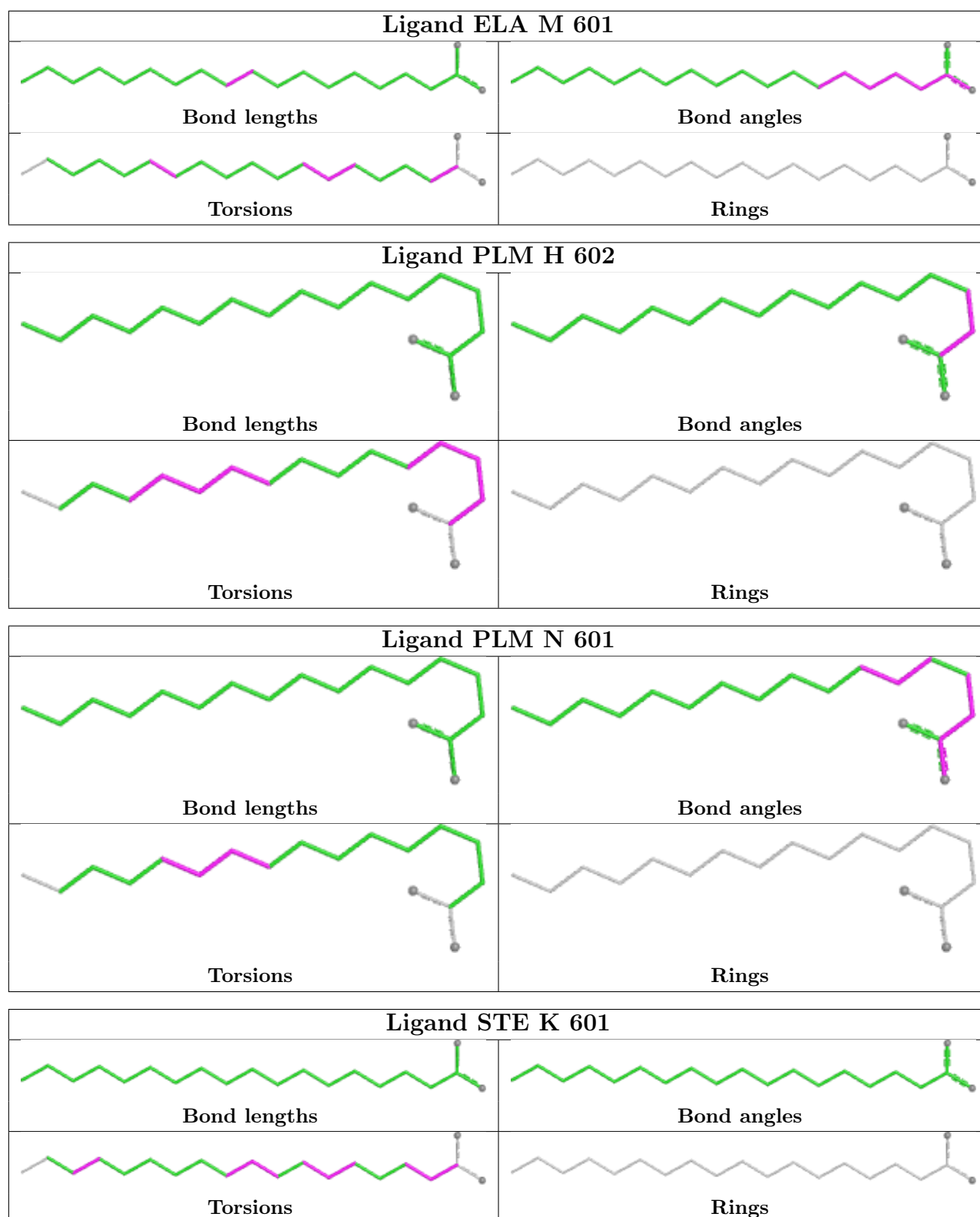
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	Q	602	PLM	5	0
2	P	602	ELA	2	0
5	D	601	PLM	4	0
5	K	602	PLM	3	0
2	G	602	ELA	1	0
2	A	601	ELA	6	0
4	C	601	STE	2	0
2	A	602	ELA	1	0
4	O	602	STE	1	0
4	F	602	STE	2	0
5	H	602	PLM	2	0
5	N	601	PLM	2	0
4	K	601	STE	3	0
4	P	601	STE	1	0
4	G	601	STE	1	0
2	J	601	ELA	1	0

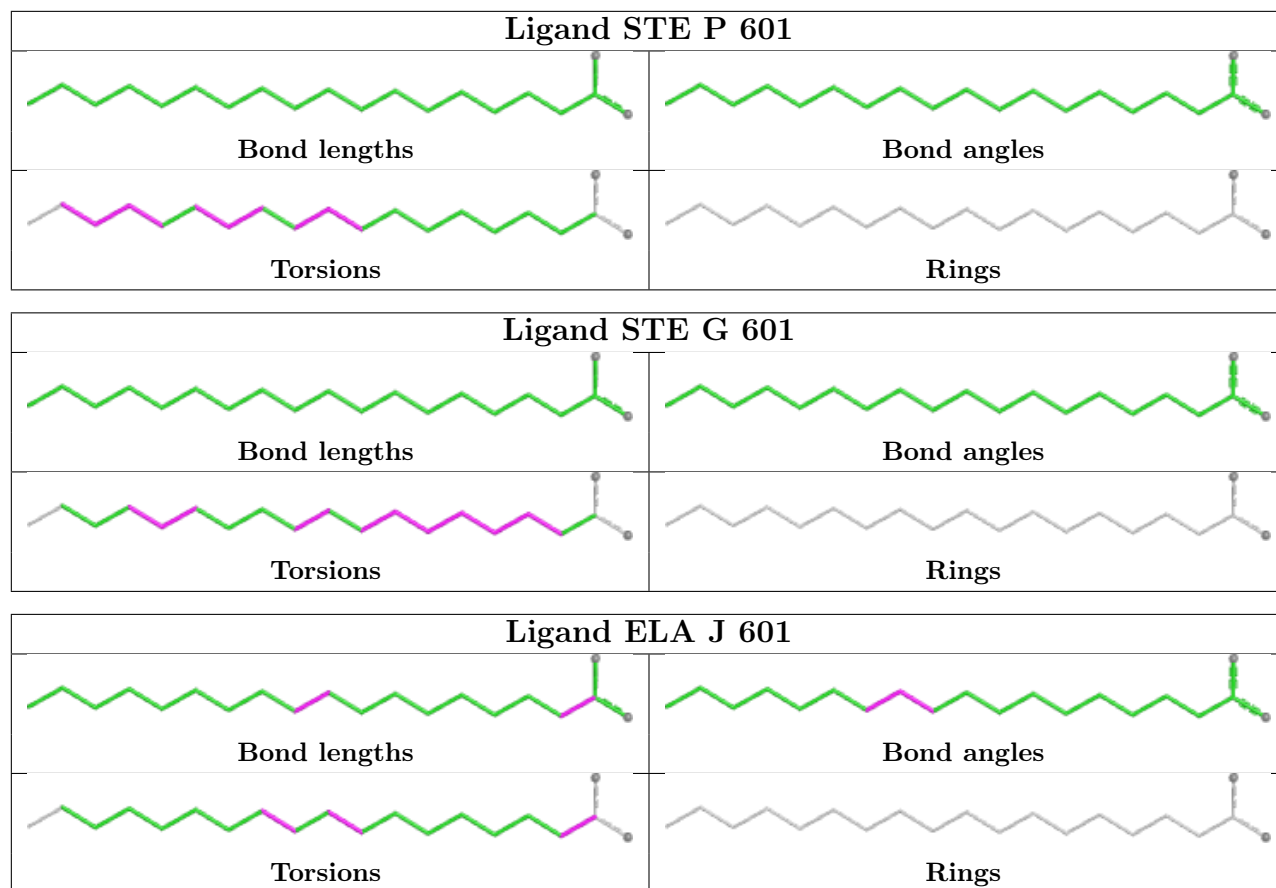
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	93/95 (97%)	0.44	4 (4%) 40 46	20, 30, 48, 76	0
1	B	93/95 (97%)	0.40	4 (4%) 40 46	14, 30, 53, 75	1 (1%)
1	C	93/95 (97%)	0.38	4 (4%) 40 46	17, 30, 46, 71	1 (1%)
1	D	93/95 (97%)	0.37	2 (2%) 62 69	18, 30, 49, 79	1 (1%)
1	E	93/95 (97%)	0.36	5 (5%) 31 37	15, 30, 49, 72	1 (1%)
1	F	93/95 (97%)	0.46	4 (4%) 40 46	13, 30, 45, 75	2 (2%)
1	G	93/95 (97%)	0.65	7 (7%) 20 23	24, 37, 59, 69	0
1	H	93/95 (97%)	0.58	5 (5%) 31 37	22, 35, 57, 83	1 (1%)
1	I	92/95 (96%)	0.62	5 (5%) 31 37	25, 36, 60, 69	1 (1%)
1	J	93/95 (97%)	0.34	3 (3%) 50 56	21, 30, 44, 51	0
1	K	93/95 (97%)	0.35	2 (2%) 62 69	21, 30, 49, 75	0
1	L	92/95 (96%)	0.46	2 (2%) 62 69	21, 30, 48, 61	2 (2%)
1	M	93/95 (97%)	0.52	3 (3%) 50 56	24, 35, 59, 72	0
1	N	93/95 (97%)	0.52	5 (5%) 31 37	14, 36, 60, 90	1 (1%)
1	O	93/95 (97%)	0.62	3 (3%) 50 56	25, 35, 62, 76	1 (1%)
1	P	93/95 (97%)	0.34	4 (4%) 40 46	13, 30, 43, 51	1 (1%)
1	Q	93/95 (97%)	0.44	3 (3%) 50 56	20, 29, 45, 69	0
1	R	93/95 (97%)	0.45	3 (3%) 50 56	19, 30, 46, 58	1 (1%)
All	All	1672/1710 (97%)	0.46	68 (4%) 41 48	13, 32, 54, 90	14 (0%)

The worst 5 of 68 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	571	ARG	4.8
1	B	575	GLY	4.3
1	E	575	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
1	E	572	ILE	4.1
1	D	572	ILE	4.0

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.

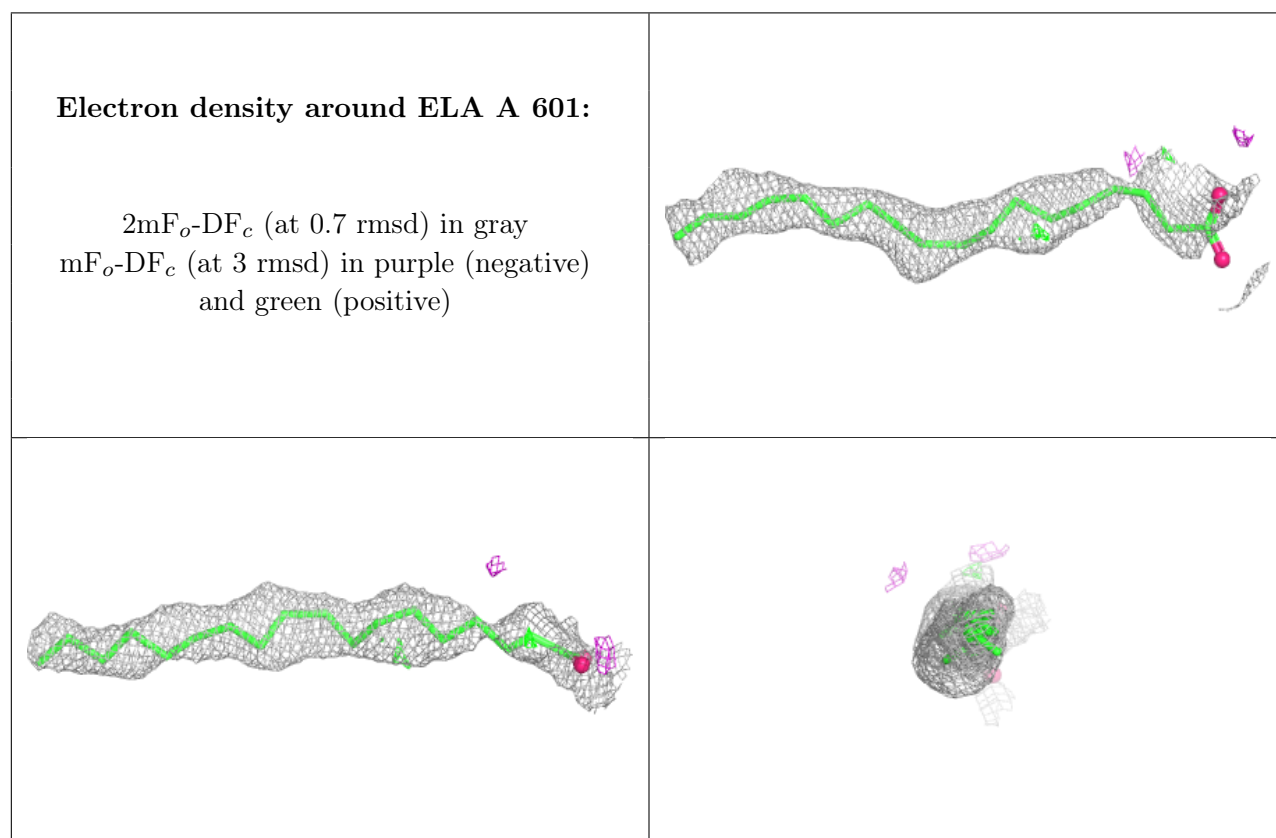
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ELA	A	601	20/20	0.81	0.18	53,67,89,98	0
2	ELA	G	602	20/20	0.81	0.20	79,101,108,110	0
4	STE	C	601	20/20	0.81	0.19	52,58,81,81	0
4	STE	O	602	20/20	0.81	0.22	75,88,97,98	0
5	PLM	K	602	18/18	0.81	0.25	62,68,76,77	0
5	PLM	N	601	18/18	0.81	0.27	60,102,110,111	0
5	PLM	Q	602	18/18	0.81	0.24	59,69,83,86	0
4	STE	P	601	20/20	0.82	0.21	63,71,77,78	0
4	STE	K	601	20/20	0.82	0.20	54,63,69,72	0
2	ELA	P	602	20/20	0.83	0.23	76,80,83,85	0
5	PLM	H	602	18/18	0.83	0.24	72,85,90,90	0
2	ELA	F	603	20/20	0.83	0.18	62,70,80,83	0
2	ELA	A	602	18/20	0.83	0.23	56,63,76,76	0
2	ELA	J	601	20/20	0.83	0.20	60,68,73,74	0
4	STE	F	602	20/20	0.84	0.17	54,62,73,80	0
5	PLM	D	601	18/18	0.84	0.21	51,62,71,73	0
2	ELA	M	601	20/20	0.85	0.20	73,83,87,88	0
4	STE	G	601	20/20	0.85	0.20	66,78,91,94	0
3	MG	F	601	1/1	0.98	0.06	40,40,40,40	0
3	MG	H	601	1/1	0.98	0.04	46,46,46,46	0
3	MG	L	601	1/1	0.98	0.08	35,35,35,35	0

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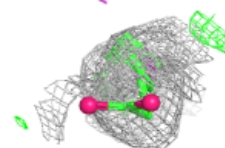
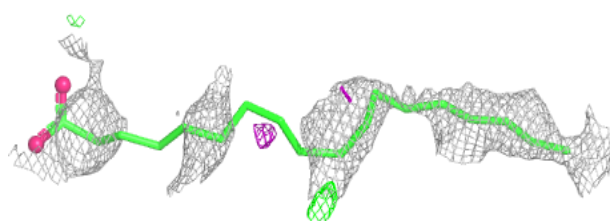
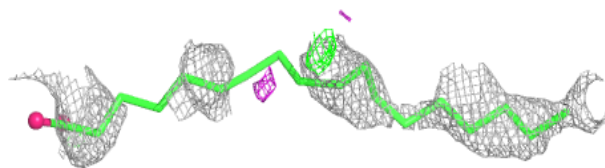
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	Q	601	1/1	0.98	0.04	43,43,43,43	0
3	MG	B	601	1/1	0.98	0.04	41,41,41,41	0
3	MG	O	601	1/1	0.99	0.04	40,40,40,40	0

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.

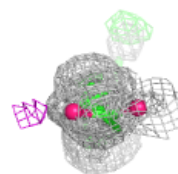
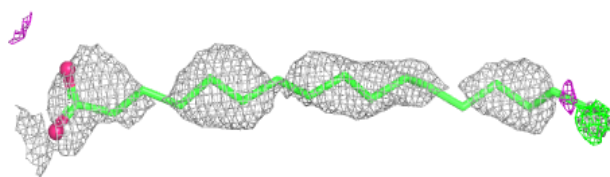
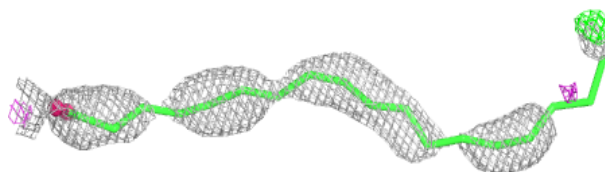


Electron density around ELA G 602:

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

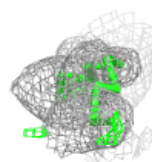
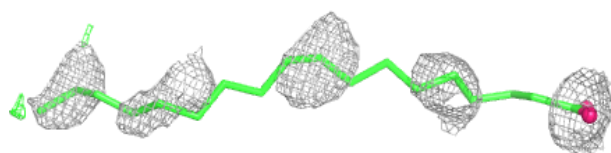
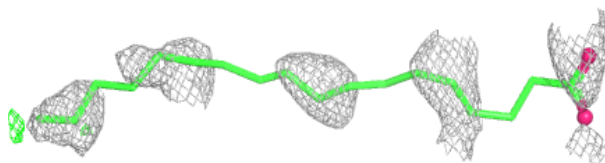
**Electron density around STE C 601:**

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

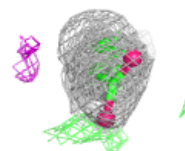
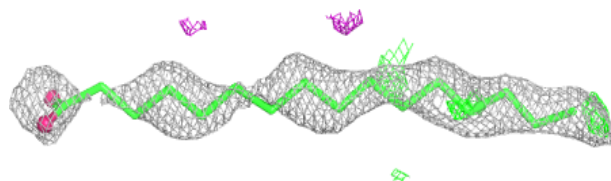
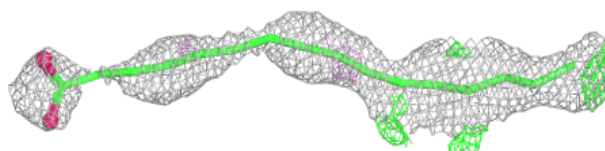


Electron density around STE O 602:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

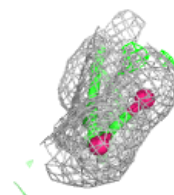
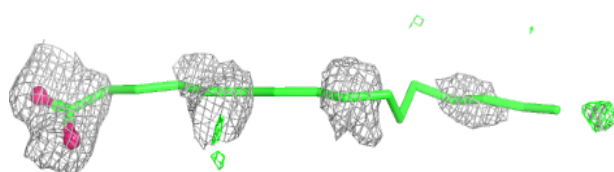
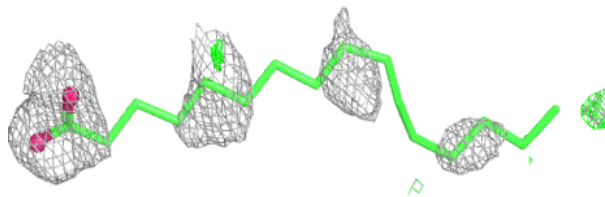
**Electron density around PLM K 602:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

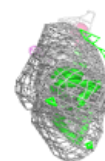
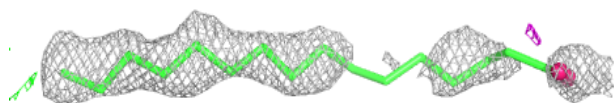
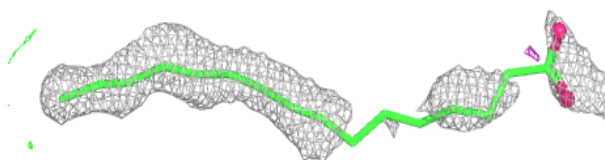


Electron density around PLM N 601:

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

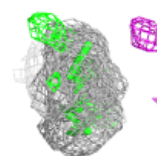
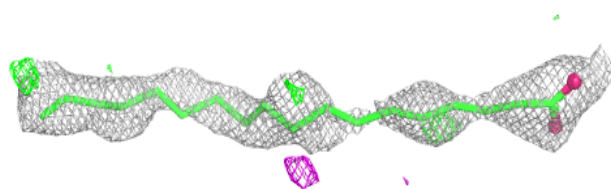
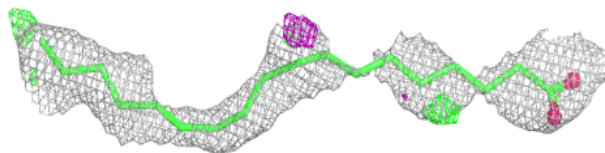
**Electron density around PLM Q 602:**

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

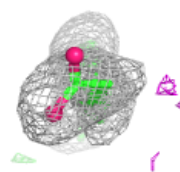
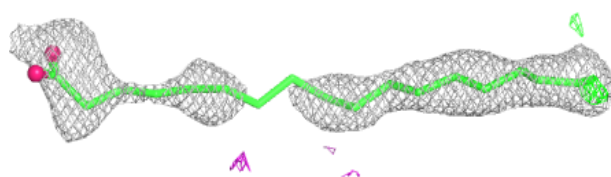
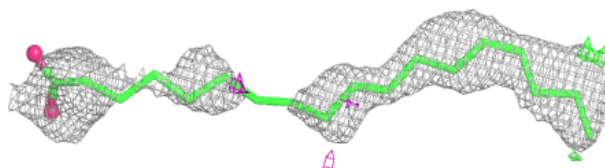


Electron density around STE P 601:

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

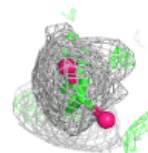
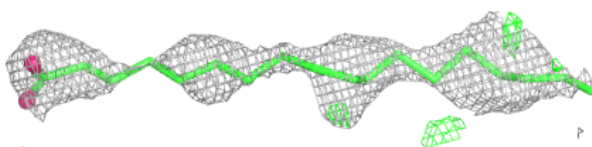
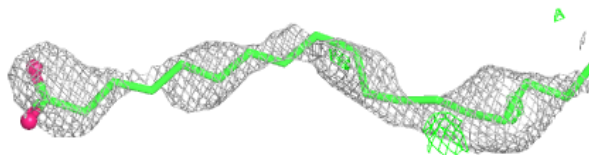
**Electron density around STE K 601:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

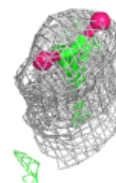
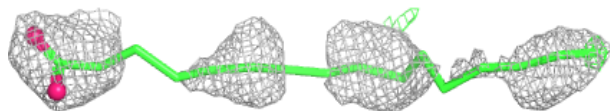
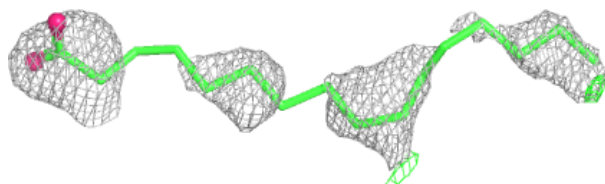


Electron density around ELA P 602:

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

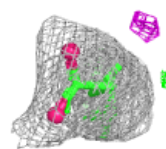
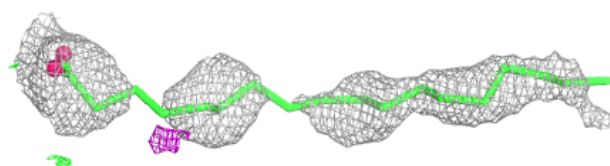
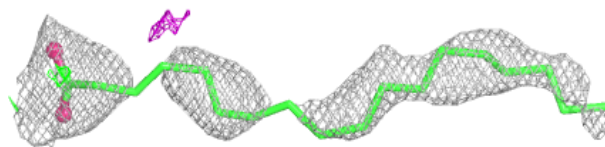
**Electron density around PLM H 602:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

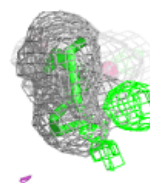
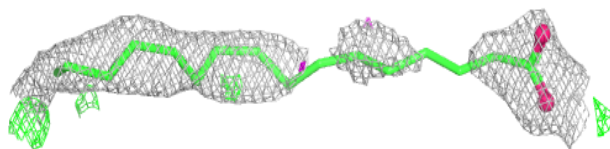
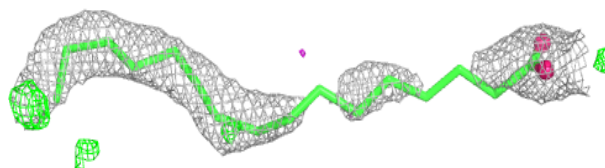


Electron density around ELA F 603:

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

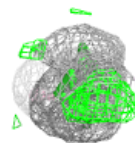
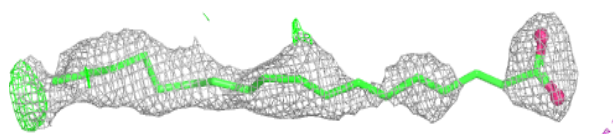
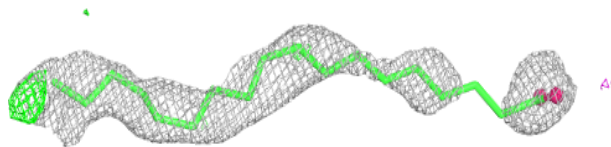
**Electron density around ELA A 602:**

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

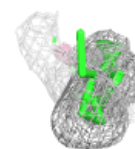
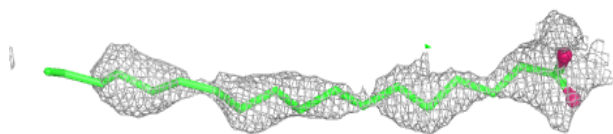
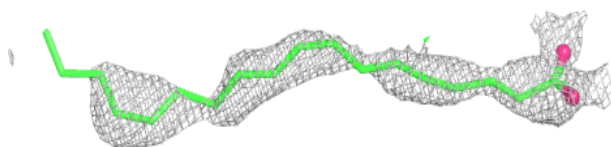


Electron density around ELA J 601:

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

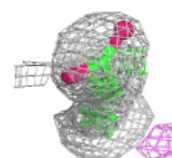
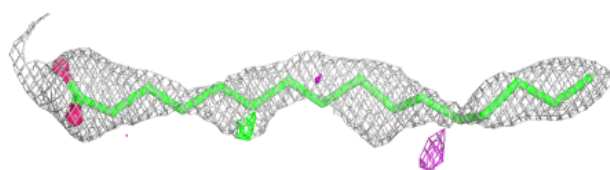
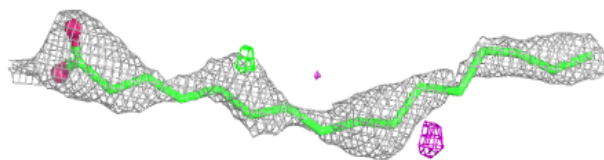
**Electron density around STE F 602:**

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

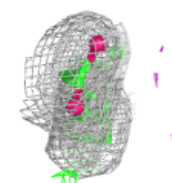
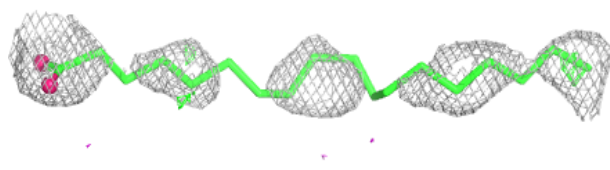
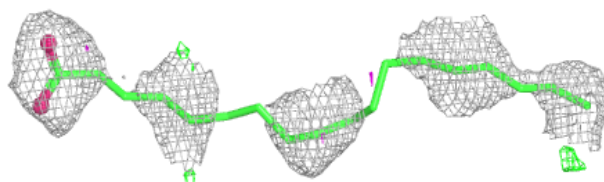


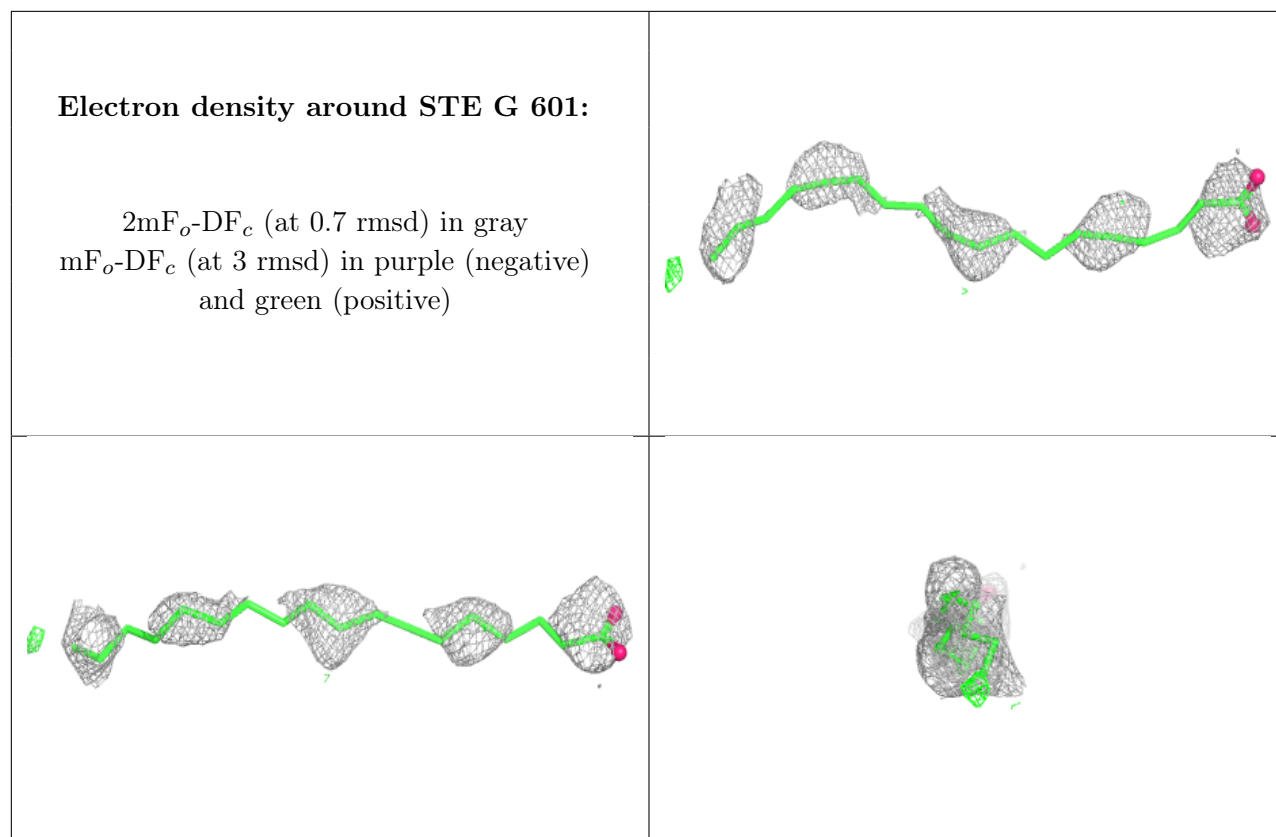
Electron density around PLM D 601:

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

**Electron density around ELA M 601:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.