



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 02:17 AM EDT

PDB ID : 8RQP / pdb_00008rqp
Title : In meso structure of the alginate exporter, AlgE, from *Pseudomonas aeruginosa* in 7.10 monoacylglycerol
Authors : Smithers, L.; Boland, C.; Krawinski, P.; Caffrey, M.
Deposited on : 2024-01-19
Resolution : 1.45 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

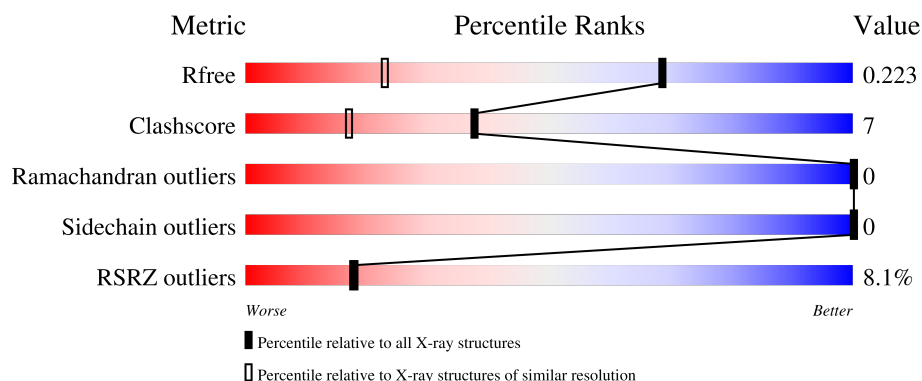
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 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	1756 (1.46-1.46)
Clashscore	190562	1795 (1.46-1.46)
Ramachandran outliers	187476	1776 (1.46-1.46)
Sidechain outliers	187428	1776 (1.46-1.46)
RSRZ outliers	180081	1756 (1.46-1.46)

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	479	8% 84% 12% .

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 4690 atoms, of which 455 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.

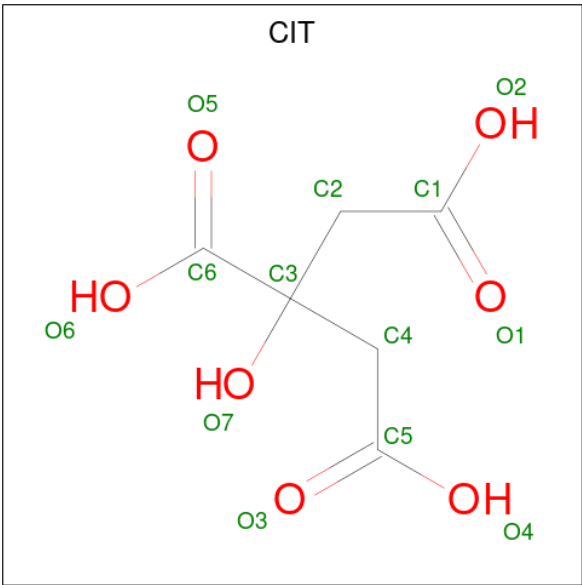
- Molecule 1 is a protein called Alginate production protein AlgE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total	C	N	O	S	13	14	0
			3697	2305	667	721	4			

There are 21 discrepancies between the modelled and reference sequences:

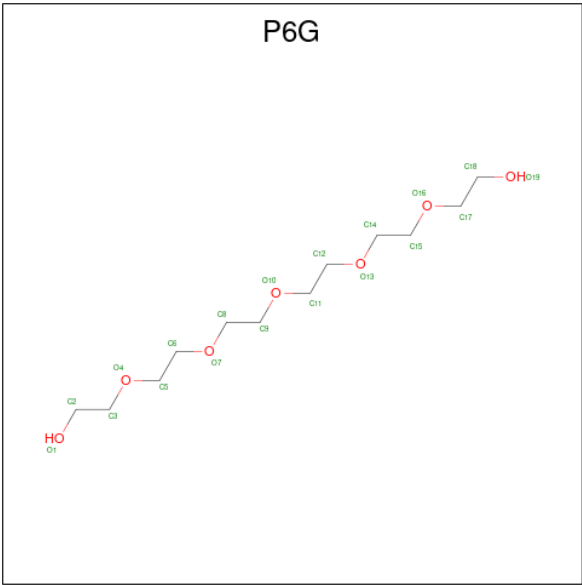
Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MET	-	initiating methionine	UNP P18895
A	13	GLY	-	expression tag	UNP P18895
A	14	SER	-	expression tag	UNP P18895
A	15	SER	-	expression tag	UNP P18895
A	16	HIS	-	expression tag	UNP P18895
A	17	HIS	-	expression tag	UNP P18895
A	18	HIS	-	expression tag	UNP P18895
A	19	HIS	-	expression tag	UNP P18895
A	20	HIS	-	expression tag	UNP P18895
A	21	HIS	-	expression tag	UNP P18895
A	22	SER	-	expression tag	UNP P18895
A	23	SER	-	expression tag	UNP P18895
A	24	GLY	-	expression tag	UNP P18895
A	25	LEU	-	expression tag	UNP P18895
A	26	VAL	-	expression tag	UNP P18895
A	27	PRO	-	expression tag	UNP P18895
A	28	ARG	-	expression tag	UNP P18895
A	29	GLY	-	expression tag	UNP P18895
A	30	SER	-	expression tag	UNP P18895
A	31	HIS	-	expression tag	UNP P18895
A	32	MET	-	expression tag	UNP P18895

- Molecule 2 is CITRIC ACID (CCD ID: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			18	6	5	7		

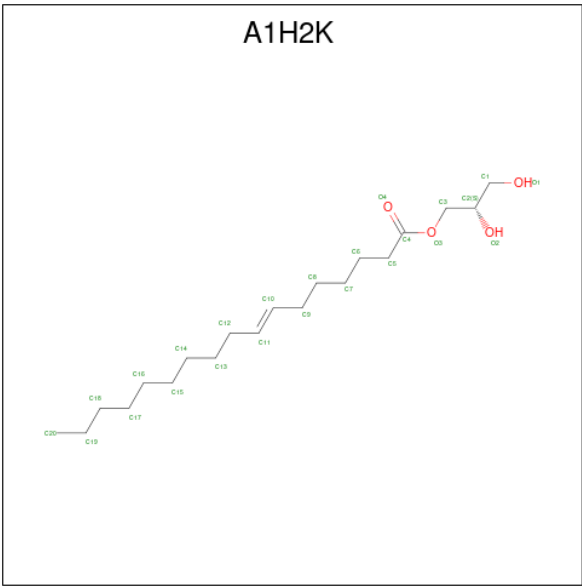
- Molecule 3 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			37	10	21	6		
3	A	1	Total	C	H	O	0	0
			23	6	13	4		

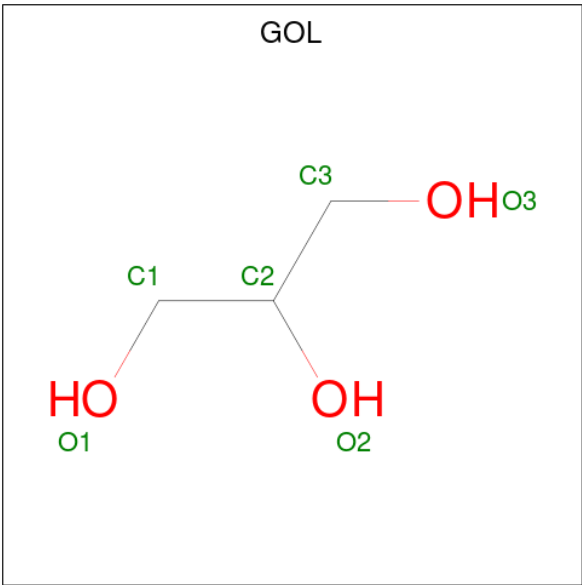
- Molecule 4 is 7.10 monoacylglycerol (S-form) (CCD ID: A1H2K) (formula: $C_{20}H_{38}O_4$) (la-

beled as "Ligand of Interest" by depositor).



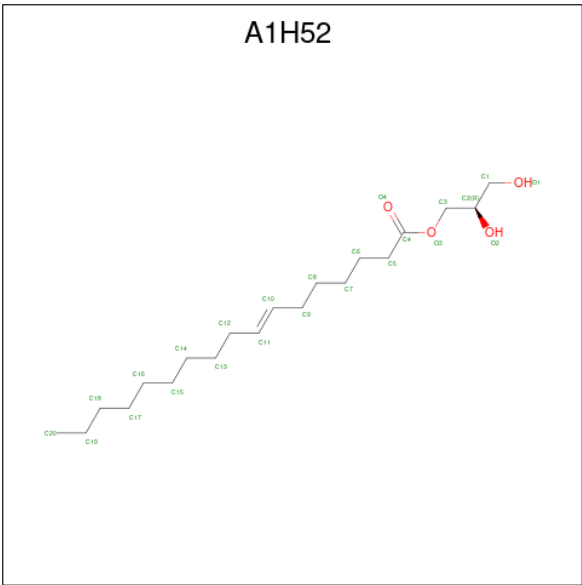
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H O 62 20 38 4	0	0
4	A	1	Total C H O 62 20 38 4	2	0
4	A	1	Total C H 44 15 29	0	0
4	A	1	Total C H O 62 20 38 4	2	0
4	A	1	Total C H O 62 20 38 4	2	0
4	A	1	Total C H O 62 20 38 4	2	0
4	A	1	Total C H 44 15 29	0	0
4	A	1	Total C H O 62 20 38 4	2	0
4	A	1	Total C H O 62 20 38 4	2	0

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 6 is 7.10 monoacylglycerol (R-form) (CCD ID: A1H52) (formula: C₂₀H₃₈O₄).

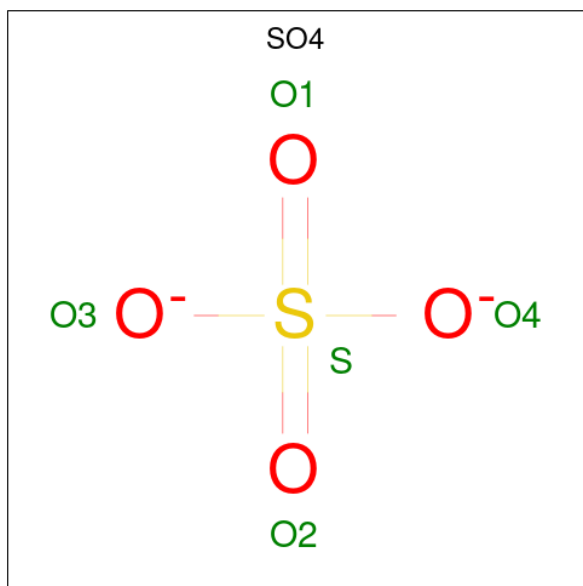


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	2	0
			62	20	38	4		
6	A	1	Total	C	H	O	2	0
			62	20	38	4		

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 9 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

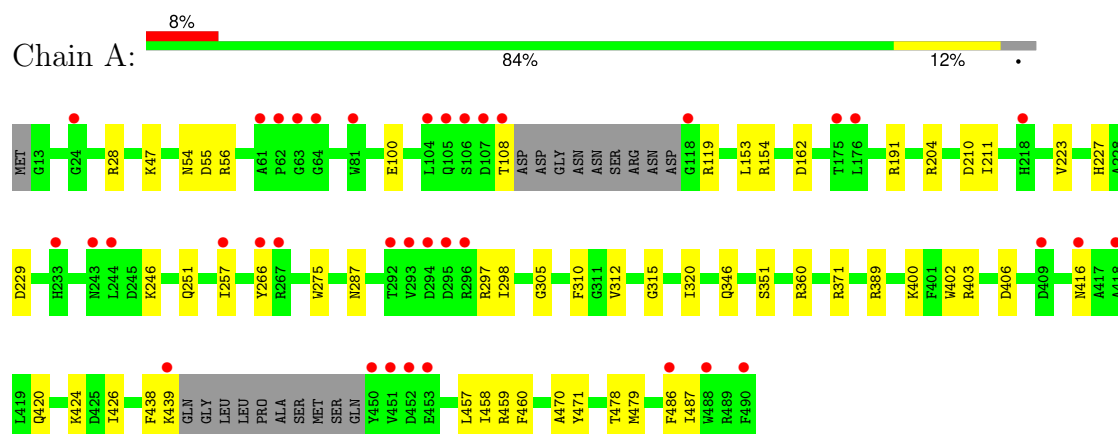
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	234	Total	O	0	0
			234	234		

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: Alginate production protein AlgE



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	57.36Å 74.55Å 115.91Å 90.00° 102.49° 90.00°	Depositor
Resolution (Å)	39.37 – 1.45 39.37 – 1.45	Depositor EDS
% Data completeness (in resolution range)	72.3 (39.37-1.45) 72.7 (39.37-1.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 1.45Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.190 , 0.223 0.190 , 0.223	Depositor DCC
R_{free} test set	3106 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	15.4	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4690	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.24% 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: CIT, A1H52, SO4, NA, CA, P6G, GOL, A1H2K

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	0.60	0/3795	0.69	2/5145 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	351	SER	CB-CA-C	-5.71	99.47	109.07
1	A	479	MET	CG-SD-CE	-5.37	89.09	100.90

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	3697	0	3427	52	0
2	A	13	5	5	0	0
3	A	26	34	34	5	0
4	A	198	324	0	3	0
5	A	12	16	16	0	0
6	A	48	76	0	0	0
7	A	1	0	0	0	0
8	A	5	0	0	0	0
9	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	A	234	0	0	6	1
All	All	4235	455	3482	52	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 7.

All (52) 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:458[A]:ILE:HD13	1:A:486:PHE:CD2	2.11	0.85
1:A:223:VAL:HG12	1:A:257[A]:ILE:HD12	1.64	0.77
1:A:420:GLN:HE21	1:A:471:TYR:C	2.00	0.69
1:A:420:GLN:HG2	1:A:470:ALA:O	1.95	0.66
1:A:210:ASP:C	1:A:211[A]:ILE:HD12	2.22	0.65
1:A:153:LEU:HD23	10:A:608:HOH:O	1.98	0.62
1:A:54:ASN:OD1	1:A:55:ASP:HB2	2.00	0.61
1:A:246[A]:LYS:HE3	10:A:743:HOH:O	2.00	0.61
1:A:223:VAL:HG12	1:A:257[A]:ILE:CD1	2.31	0.59
1:A:287:ASN:HD22	3:A:502:P6G:C9	2.16	0.59
1:A:56:ARG:HE	1:A:416:ASN:HD21	1.51	0.59
1:A:28:ARG:HG2	1:A:28:ARG:HH11	1.68	0.58
1:A:275:TRP:CZ2	1:A:315:GLY:HA3	2.38	0.57
1:A:56:ARG:NH2	10:A:601:HOH:O	2.24	0.56
1:A:406:ASP:HB3	1:A:424:LYS:HG2	1.88	0.56
1:A:287:ASN:HD22	3:A:502:P6G:H92	1.72	0.55
1:A:458[A]:ILE:HD13	1:A:486:PHE:CE2	2.41	0.55
1:A:229:ASP:C	1:A:229:ASP:OD2	2.50	0.54
1:A:310:PHE:CE2	1:A:312[B]:VAL:HG23	2.41	0.54
1:A:191:ARG:HD2	10:A:818:HOH:O	2.09	0.53
1:A:457:LEU:C	1:A:457:LEU:HD12	2.33	0.53
1:A:275:TRP:CE2	1:A:315:GLY:HA3	2.44	0.52
1:A:420:GLN:NE2	1:A:471:TYR:O	2.43	0.52
1:A:478:THR:HG21	4:A:508:A1H2K:C1	2.41	0.50
1:A:47:LYS:HZ3	1:A:487:ILE:HD11	1.77	0.49
1:A:47:LYS:NZ	1:A:487:ILE:HD11	2.29	0.48
1:A:305:GLY:HA3	3:A:502:P6G:H122	1.95	0.48
1:A:458[A]:ILE:HD13	1:A:486:PHE:CG	2.50	0.47
1:A:438:PHE:HD2	1:A:439:LYS:HG3	1.80	0.47
1:A:297:ARG:C	1:A:298:ILE:HD13	2.40	0.47
1:A:54:ASN:HA	1:A:55:ASP:HA	1.78	0.46
1:A:403:ARG:HG3	1:A:426:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ARG:HG2	1:A:416:ASN:ND2	2.31	0.46
1:A:56:ARG:NE	1:A:416:ASN:HD21	2.14	0.45
1:A:459:ARG:HD2	10:A:658:HOH:O	2.17	0.44
1:A:154[B]:ARG:HH11	1:A:162:ASP:CG	2.25	0.44
1:A:100:GLU:OE1	1:A:371:ARG:NH1	2.46	0.43
1:A:211[A]:ILE:HD12	1:A:211[A]:ILE:N	2.33	0.43
1:A:400:LYS:HD3	1:A:402:TRP:CZ2	2.54	0.42
1:A:227:HIS:CE1	1:A:251:GLN:HG2	2.54	0.42
1:A:56:ARG:CG	1:A:416:ASN:ND2	2.83	0.42
1:A:204:ARG:CZ	10:A:628:HOH:O	2.67	0.42
1:A:266[A]:TYR:CE2	1:A:360:ARG:HG2	2.55	0.42
1:A:346:GLN:HG2	3:A:506:P6G:H52	2.01	0.42
1:A:227:HIS:HE1	1:A:251:GLN:HG2	1.85	0.41
1:A:108:THR:HG22	1:A:119:ARG:NH2	2.35	0.41
1:A:56:ARG:HE	1:A:416:ASN:ND2	2.14	0.41
1:A:460:PHE:HZ	4:A:507:A1H2K:C8	2.34	0.41
1:A:211[B]:ILE:O	1:A:211[B]:ILE:HG13	2.20	0.40
1:A:287:ASN:HD22	3:A:502:P6G:H91	1.84	0.40
1:A:320:ILE:HD13	4:A:511:A1H2K:C20	2.50	0.40
1:A:389:ARG:HE	1:A:389:ARG:HB3	1.43	0.40

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)
10:A:803:HOH:O	10:A:803:HOH:O[2_655]	2.19	0.01

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	461/479 (96%)	446 (97%)	15 (3%)	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	379/388 (98%)	379 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	ASN
1	A	169	ASN
1	A	218	HIS
1	A	251	GLN
1	A	416	ASN
1	A	420	GLN

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 19 ligands modelled in this entry, 2 are monoatomic - leaving 17 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$
4	A1H2K	A	510	-	14,14,23	0.19	0	13,13,24	0.57	0
6	A1H52	A	513	-	23,23,23	0.38	0	24,24,24	0.92	0
4	A1H2K	A	505	-	14,14,23	0.17	0	13,13,24	0.27	0
4	A1H2K	A	507	-	23,23,23	0.28	0	24,24,24	0.39	0
5	GOL	A	514	-	5,5,5	1.02	0	5,5,5	1.00	0
3	P6G	A	506	-	9,9,18	0.19	0	8,8,17	0.60	0
4	A1H2K	A	508	-	23,23,23	0.34	0	24,24,24	0.48	0
4	A1H2K	A	511	-	23,23,23	0.30	0	24,24,24	0.56	0
4	A1H2K	A	515	-	23,23,23	0.29	0	24,24,24	0.54	0
4	A1H2K	A	503	-	23,23,23	0.26	0	24,24,24	0.42	0
5	GOL	A	512	-	5,5,5	0.67	0	5,5,5	1.08	0
3	P6G	A	502	-	15,15,18	0.22	0	14,14,17	0.63	0
4	A1H2K	A	509	-	23,23,23	0.28	0	24,24,24	0.61	0
6	A1H52	A	516	-	23,23,23	0.53	1 (4%)	24,24,24	0.96	2 (8%)
8	SO4	A	518	-	4,4,4	0.29	0	6,6,6	0.41	0
2	CIT	A	501	-	12,12,12	1.19	0	17,17,17	1.35	3 (17%)
4	A1H2K	A	504	-	23,23,23	0.21	0	24,24,24	0.47	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
4	A1H2K	A	510	-	-	2/12/12/23	-
6	A1H52	A	513	-	-	11/23/23/23	-
4	A1H2K	A	505	-	-	3/12/12/23	-
4	A1H2K	A	507	-	-	8/23/23/23	-
5	GOL	A	514	-	-	2/4/4/4	-
3	P6G	A	506	-	-	3/7/7/16	-
4	A1H2K	A	508	-	-	7/23/23/23	-
4	A1H2K	A	511	-	-	6/23/23/23	-
4	A1H2K	A	515	-	-	11/23/23/23	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	A1H2K	A	503	-	-	9/23/23/23	-
5	GOL	A	512	-	-	0/4/4/4	-
3	P6G	A	502	-	-	7/13/13/16	-
4	A1H2K	A	509	-	-	9/23/23/23	-
6	A1H52	A	516	-	-	8/23/23/23	-
2	CIT	A	501	-	-	0/16/16/16	-
4	A1H2K	A	504	-	-	7/23/23/23	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	516	A1H52	O2-C2	-2.34	1.36	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	516	A1H52	O2-C2-C3	3.04	120.19	109.70
2	A	501	CIT	O6-C6-C3	2.68	118.29	113.14
6	A	516	A1H52	O2-C2-C1	2.52	119.59	109.18
2	A	501	CIT	O2-C1-O1	-2.25	117.56	123.33
2	A	501	CIT	O4-C5-O3	-2.01	118.17	123.33

There are no chirality outliers.

All (93) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	507	A1H2K	O1-C1-C2-C3
4	A	508	A1H2K	O2-C2-C3-O3
4	A	515	A1H2K	O1-C1-C2-O2
4	A	515	A1H2K	C1-C2-C3-O3
4	A	515	A1H2K	O2-C2-C3-O3
4	A	515	A1H2K	O4-C4-O3-C3
4	A	515	A1H2K	C5-C4-O3-C3
5	A	514	GOL	C1-C2-C3-O3
6	A	513	A1H52	C1-C2-C3-O3
6	A	513	A1H52	O2-C2-C3-O3
6	A	513	A1H52	O4-C4-O3-C3
6	A	513	A1H52	C5-C4-O3-C3
6	A	516	A1H52	C1-C2-C3-O3
6	A	516	A1H52	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	A	504	A1H2K	C2-C3-O3-C4
4	A	503	A1H2K	C1-C2-C3-O3
6	A	516	A1H52	C16-C17-C18-C19
4	A	503	A1H2K	O2-C2-C3-O3
4	A	504	A1H2K	O2-C2-C3-O3
4	A	503	A1H2K	C4-C5-C6-C7
4	A	504	A1H2K	C1-C2-C3-O3
4	A	515	A1H2K	O1-C1-C2-C3
6	A	516	A1H52	O1-C1-C2-C3
3	A	502	P6G	O4-C5-C6-O7
3	A	502	P6G	O7-C8-C9-O10
4	A	511	A1H2K	C13-C14-C15-C16
5	A	514	GOL	O2-C2-C3-O3
6	A	516	A1H52	O1-C1-C2-O2
4	A	503	A1H2K	C6-C7-C8-C9
4	A	509	A1H2K	C16-C17-C18-C19
4	A	511	A1H2K	C11-C12-C13-C14
4	A	515	A1H2K	C14-C15-C16-C17
4	A	505	A1H2K	C11-C10-C9-C8
6	A	513	A1H52	C11-C12-C13-C14
4	A	508	A1H2K	C11-C10-C9-C8
3	A	502	P6G	O16-C17-C18-O19
6	A	513	A1H52	C6-C7-C8-C9
4	A	507	A1H2K	O1-C1-C2-O2
4	A	509	A1H2K	C9-C10-C11-C12
4	A	509	A1H2K	C7-C8-C9-C10
4	A	515	A1H2K	C7-C8-C9-C10
6	A	516	A1H52	C7-C8-C9-C10
4	A	509	A1H2K	C5-C6-C7-C8
4	A	508	A1H2K	C13-C14-C15-C16
4	A	507	A1H2K	C6-C7-C8-C9
4	A	507	A1H2K	C16-C17-C18-C19
4	A	509	A1H2K	C12-C13-C14-C15
4	A	511	A1H2K	C14-C15-C16-C17
4	A	509	A1H2K	C17-C18-C19-C20
4	A	508	A1H2K	C5-C6-C7-C8
4	A	510	A1H2K	C15-C16-C17-C18
4	A	511	A1H2K	C15-C16-C17-C18
4	A	505	A1H2K	C15-C16-C17-C18
4	A	508	A1H2K	C1-C2-C3-O3
3	A	506	P6G	O4-C5-C6-O7
4	A	507	A1H2K	C11-C10-C9-C8

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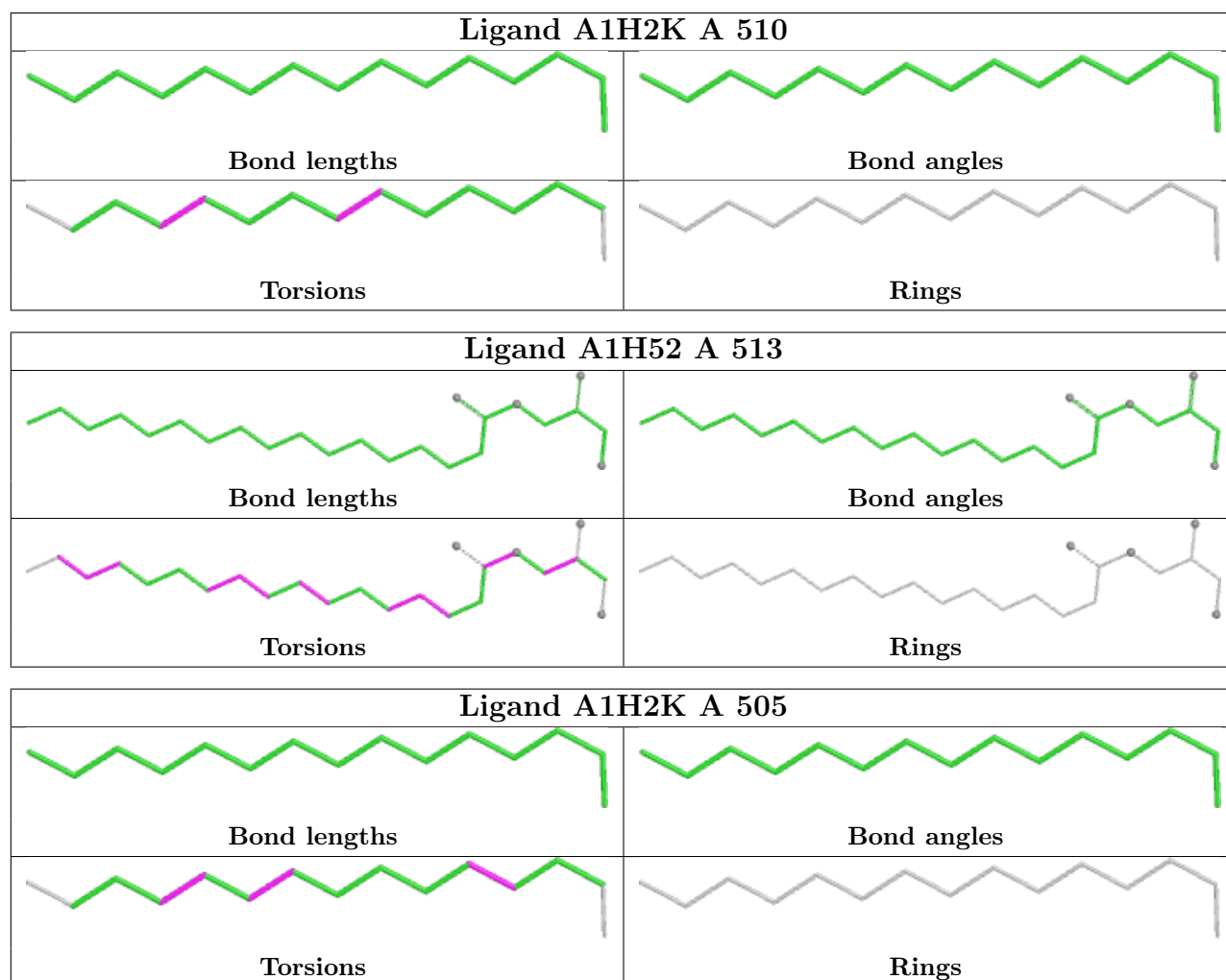
Mol	Chain	Res	Type	Atoms
4	A	508	A1H2K	C17-C18-C19-C20
4	A	503	A1H2K	O1-C1-C2-O2
4	A	503	A1H2K	C16-C17-C18-C19
6	A	513	A1H52	C17-C18-C19-C20
6	A	513	A1H52	C5-C6-C7-C8
4	A	511	A1H2K	C5-C6-C7-C8
3	A	506	P6G	C5-C6-O7-C8
4	A	507	A1H2K	C15-C16-C17-C18
3	A	502	P6G	C12-C11-O10-C9
4	A	510	A1H2K	C11-C12-C13-C14
3	A	502	P6G	C9-C8-O7-C6
3	A	502	P6G	C11-C12-O13-C14
6	A	513	A1H52	C12-C13-C14-C15
4	A	504	A1H2K	C13-C14-C15-C16
3	A	502	P6G	C14-C15-O16-C17
4	A	509	A1H2K	C15-C16-C17-C18
6	A	516	A1H52	C5-C6-C7-C8
4	A	507	A1H2K	C5-C6-C7-C8
4	A	515	A1H2K	C10-C11-C12-C13
4	A	515	A1H2K	C11-C10-C9-C8
6	A	513	A1H52	C9-C10-C11-C12
4	A	504	A1H2K	C7-C8-C9-C10
4	A	509	A1H2K	C11-C10-C9-C8
4	A	503	A1H2K	C7-C8-C9-C10
4	A	507	A1H2K	C11-C12-C13-C14
3	A	506	P6G	C2-C3-O4-C5
4	A	505	A1H2K	C13-C14-C15-C16
4	A	508	A1H2K	C10-C11-C12-C13
4	A	503	A1H2K	C11-C10-C9-C8
4	A	511	A1H2K	C12-C13-C14-C15
4	A	504	A1H2K	C17-C18-C19-C20
4	A	504	A1H2K	C12-C13-C14-C15
4	A	509	A1H2K	C6-C7-C8-C9
6	A	513	A1H52	C16-C17-C18-C19
6	A	516	A1H52	C14-C15-C16-C17
4	A	515	A1H2K	C6-C7-C8-C9
4	A	503	A1H2K	C17-C18-C19-C20

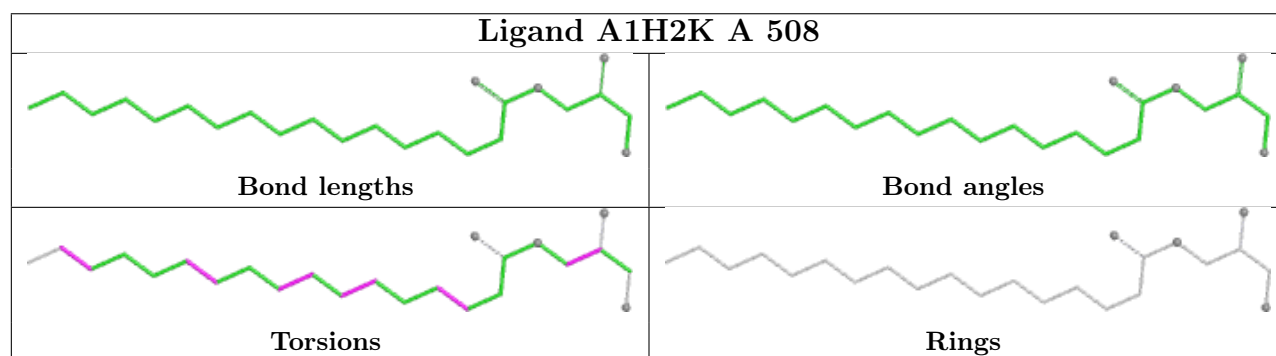
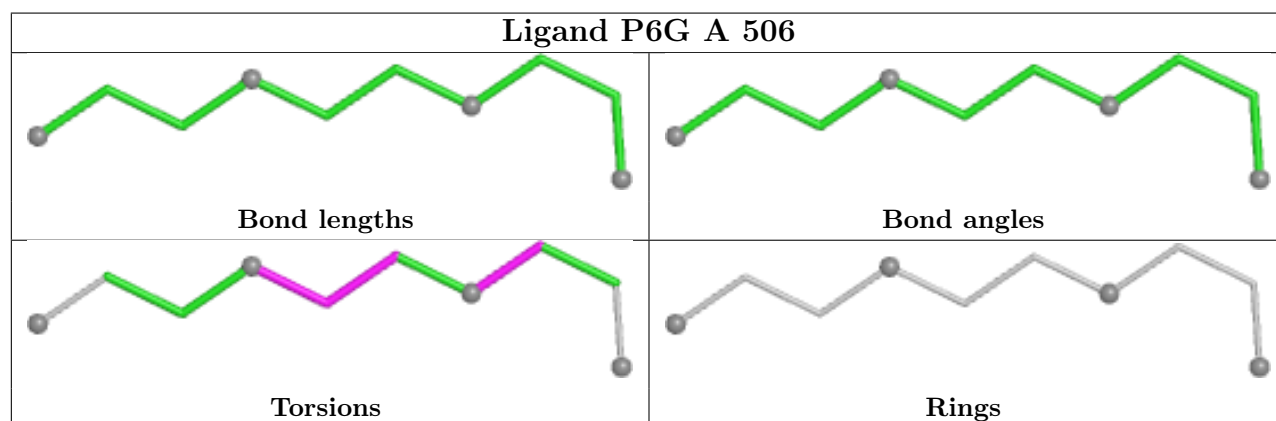
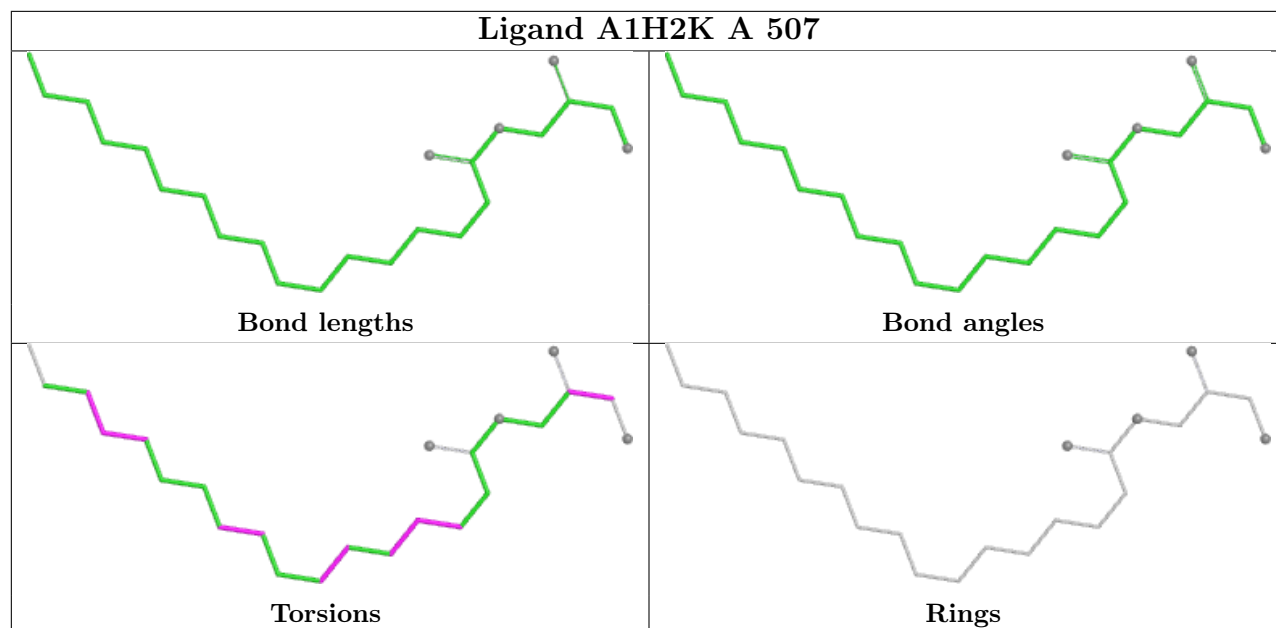
There are no ring outliers.

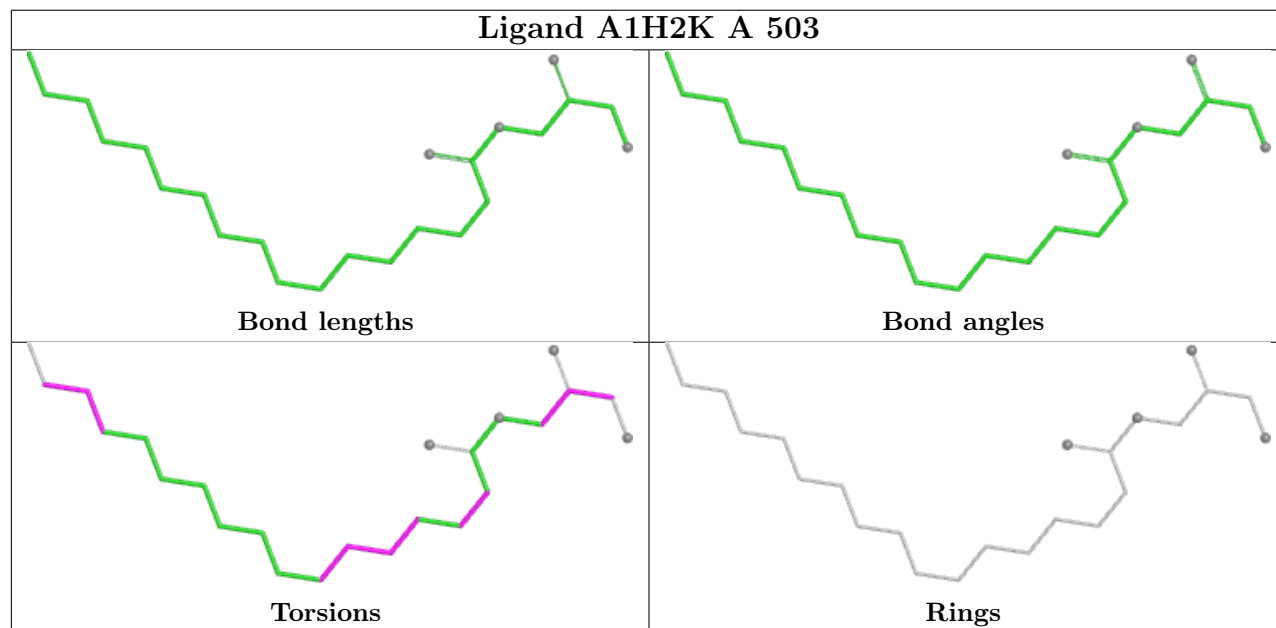
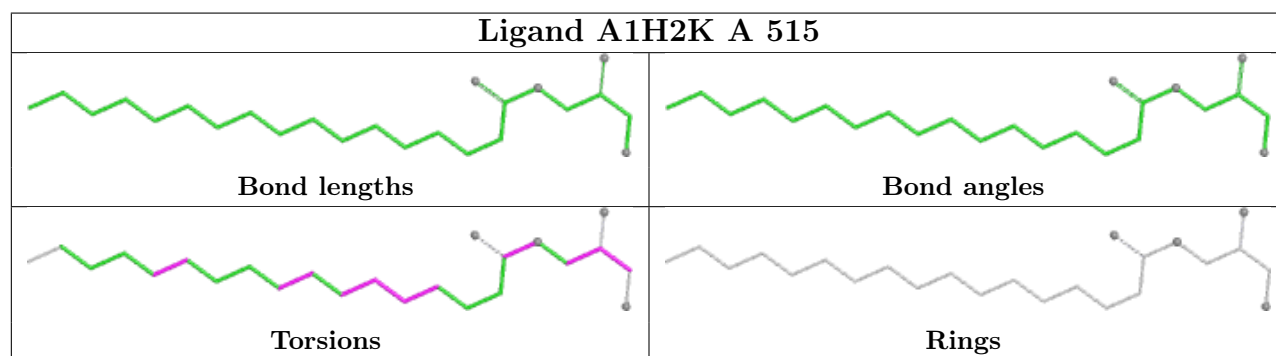
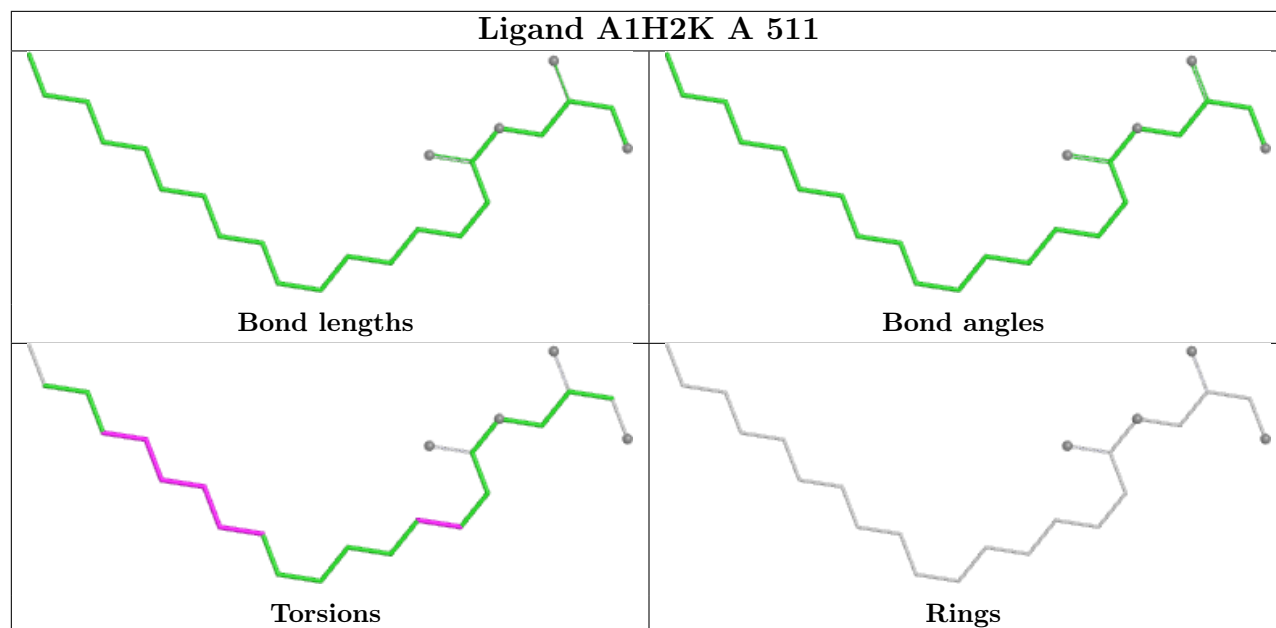
5 monomers are involved in 8 short contacts:

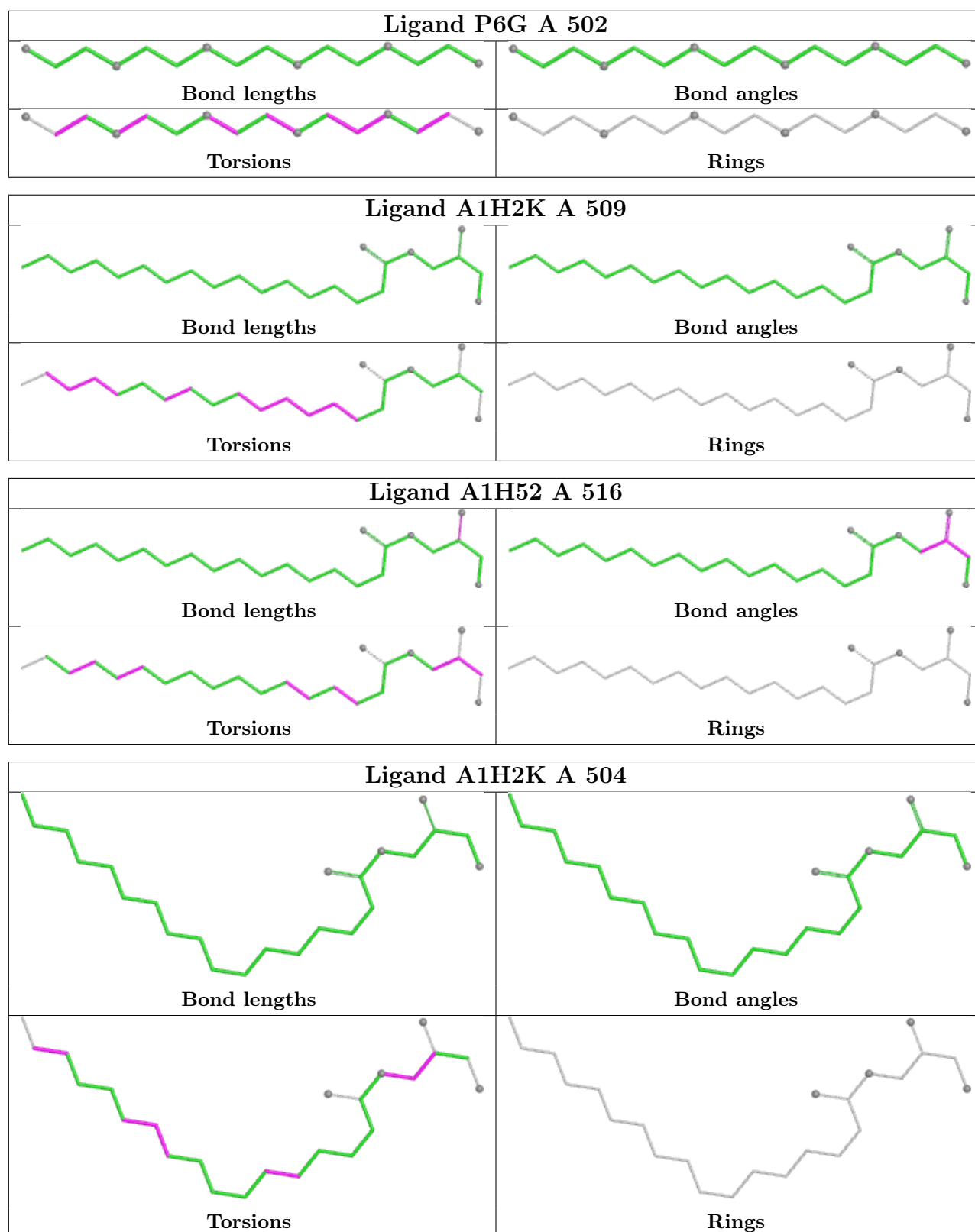
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	507	A1H2K	1	0
3	A	506	P6G	1	0
4	A	508	A1H2K	1	0
4	A	511	A1H2K	1	0
3	A	502	P6G	4	0

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 ⓘ

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	459/479 (95%)	0.39	37 (8%) 18 18	6, 18, 42, 86	43 (9%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	450	TYR	6.5
1	A	295	ASP	6.2
1	A	293	VAL	5.0
1	A	63	GLY	4.7
1	A	244	LEU	4.0
1	A	294	ASP	3.6
1	A	107	ASP	3.6
1	A	62	PRO	3.5
1	A	486	PHE	3.4
1	A	488	TRP	3.4
1	A	108	THR	3.3
1	A	451	VAL	3.1
1	A	105	GLN	3.1
1	A	176	LEU	3.1
1	A	106	SER	3.1
1	A	292	THR	3.0
1	A	81	TRP	3.0
1	A	439	LYS	3.0
1	A	64	GLY	3.0
1	A	243	ASN	2.9
1	A	104	LEU	2.8
1	A	266[A]	TYR	2.7
1	A	61	ALA	2.5
1	A	452	ASP	2.4
1	A	490	PHE	2.4
1	A	296	ARG	2.4
1	A	453	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	416	ASN	2.4
1	A	233	HIS	2.3
1	A	257[A]	ILE	2.3
1	A	409[A]	ASP	2.3
1	A	118	GLY	2.2
1	A	418	ALA	2.1
1	A	267	ARG	2.1
1	A	175	THR	2.0
1	A	24	GLY	2.0
1	A	218	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	A1H2K	A	507	24/24	0.66	0.19	40,56,80,84	2
6	A1H52	A	516	24/24	0.66	0.21	32,56,83,93	2
4	A1H2K	A	508	24/24	0.70	0.19	38,57,77,86	2
6	A1H52	A	513	24/24	0.71	0.16	31,57,80,96	2
4	A1H2K	A	510	15/24	0.75	0.17	27,42,62,62	0
4	A1H2K	A	503	24/24	0.77	0.16	27,50,67,83	0
4	A1H2K	A	515	24/24	0.78	0.15	24,47,59,64	2
4	A1H2K	A	511	24/24	0.79	0.15	25,48,61,66	2
4	A1H2K	A	504	24/24	0.79	0.14	20,46,67,83	2
4	A1H2K	A	505	15/24	0.80	0.17	24,39,59,59	0
4	A1H2K	A	509	24/24	0.83	0.15	25,41,61,63	2
5	GOL	A	512	6/6	0.85	0.17	28,34,40,48	14
5	GOL	A	514	6/6	0.85	0.11	36,45,54,55	0

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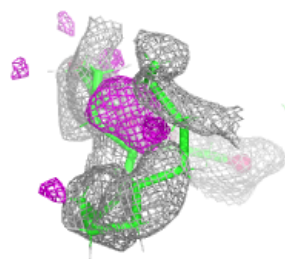
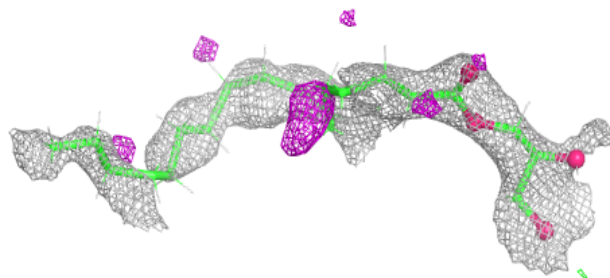
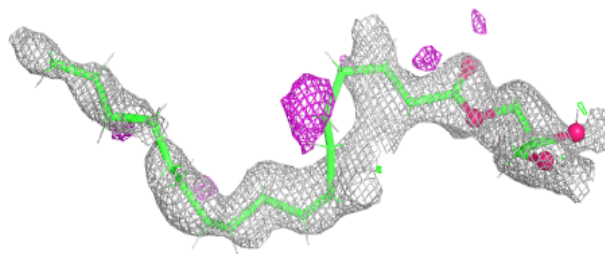
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	P6G	A	502	16/19	0.88	0.12	13,27,40,49	37
9	CA	A	519	1/1	0.90	0.17	68,68,68,68	0
3	P6G	A	506	10/19	0.91	0.16	7,22,31,36	23
2	CIT	A	501	13/13	0.92	0.09	17,22,27,33	6
8	SO4	A	518	5/5	0.98	0.06	13,14,16,16	5
7	NA	A	517	1/1	0.99	0.02	18,18,18,18	0

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

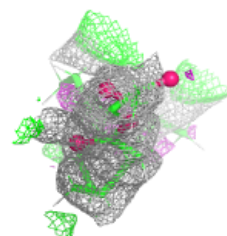
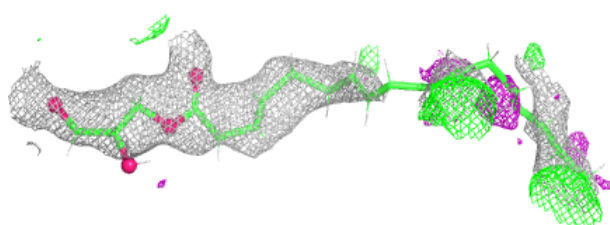
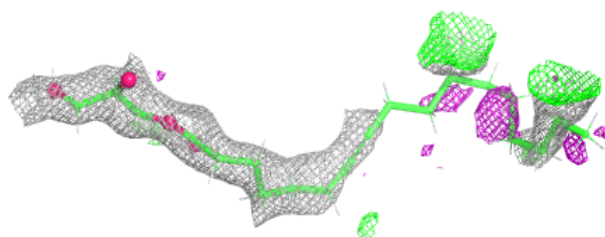
Electron density around A1H2K A 507:

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

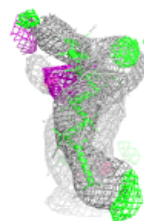
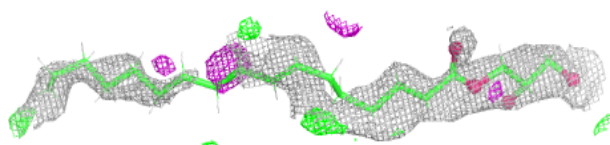
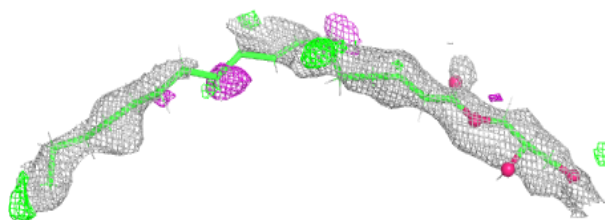


Electron density around A1H52 A 516:

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

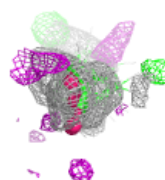
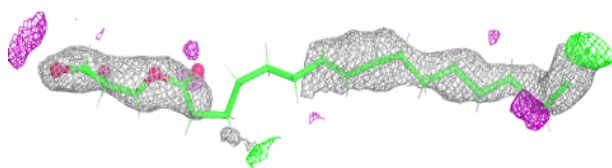
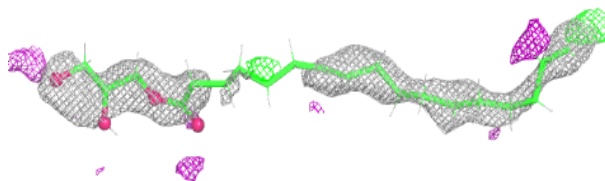
**Electron density around A1H2K A 508:**

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

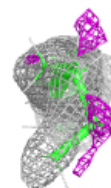
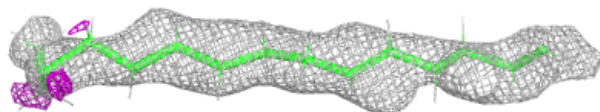
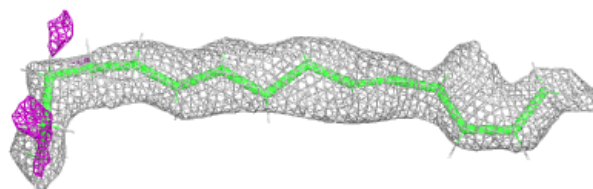


Electron density around A1H52 A 513:

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

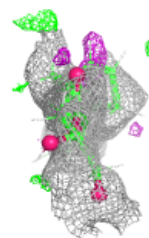
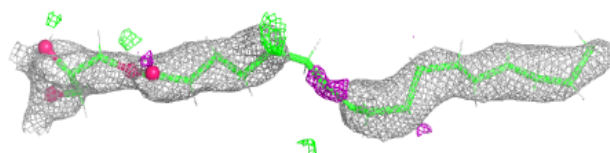
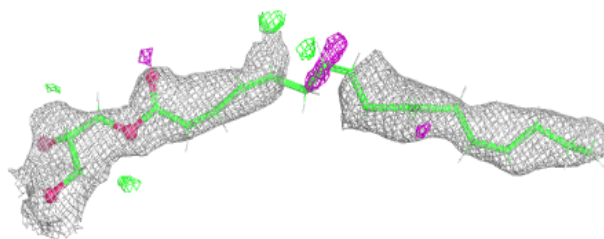
**Electron density around A1H2K A 510:**

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and green (positive)

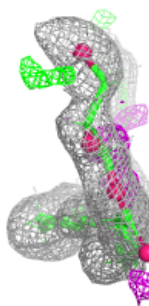
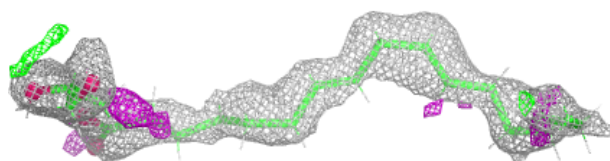
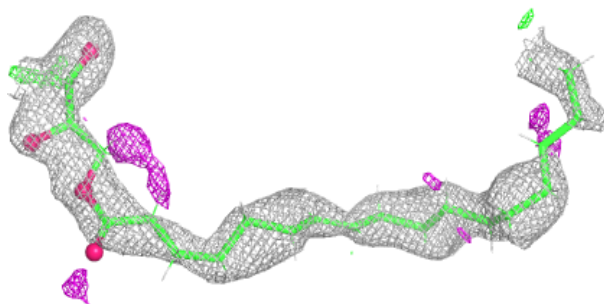


Electron density around A1H2K A 503:

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and green (positive)

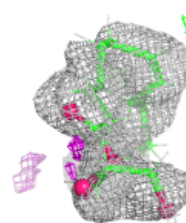
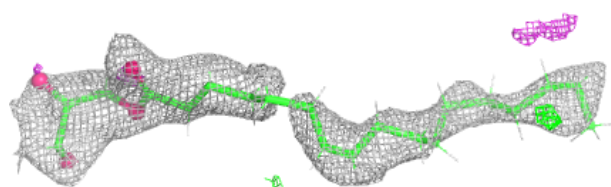
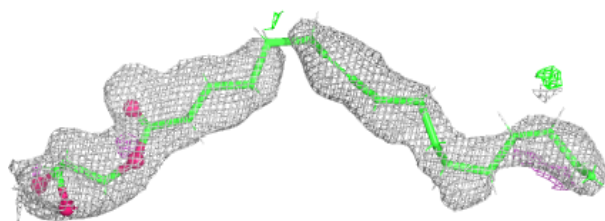
**Electron density around A1H2K A 515:**

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

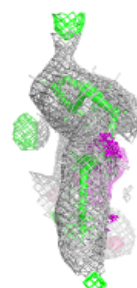
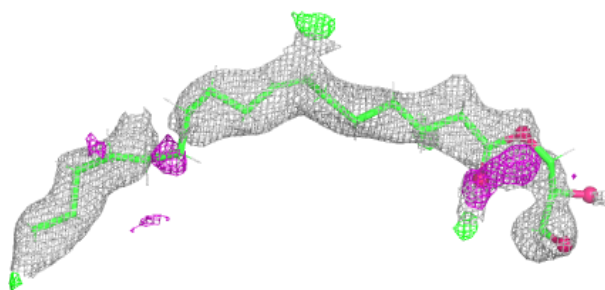


Electron density around A1H2K A 511:

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

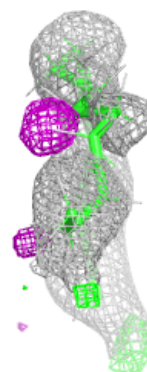
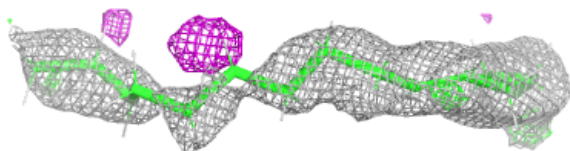
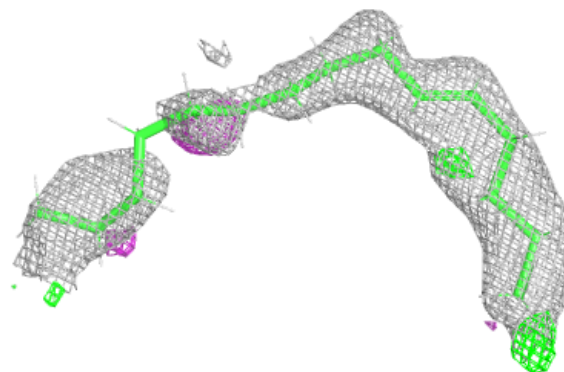
**Electron density around A1H2K A 504:**

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

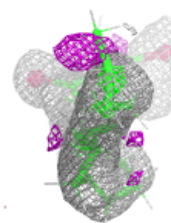
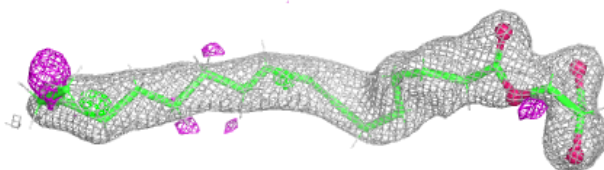
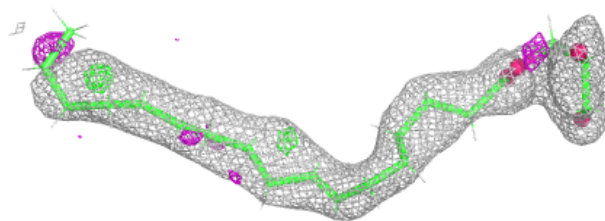


Electron density around A1H2K A 505:

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

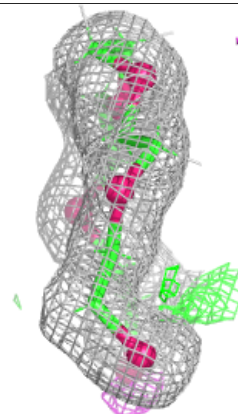
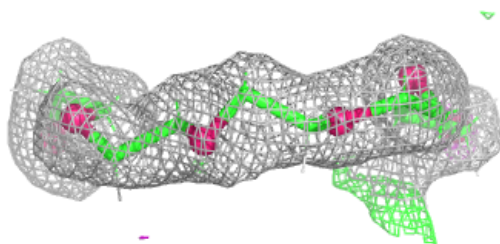
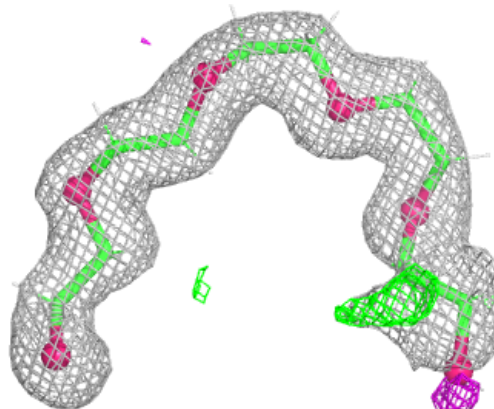
**Electron density around A1H2K A 509:**

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

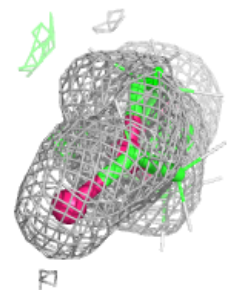
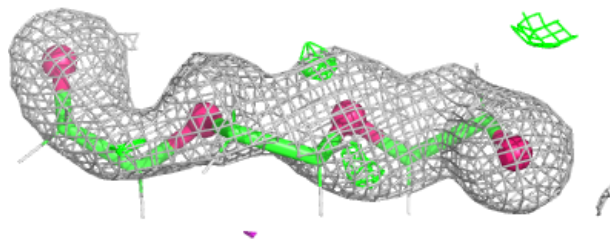
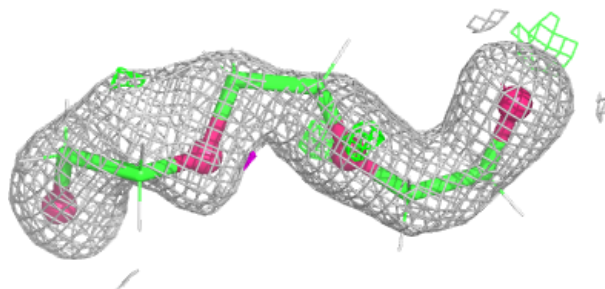


Electron density around P6G A 502:

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

**Electron density around P6G A 506:**

$2mF_o-DF_c$ (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.