



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:10 AM UTC

PDB ID : 7ACG / pdb_00007acg
Title : In meso structure of the alginate exporter, AlgE, from *Pseudomonas aeruginosa* in 9.8 monoacylglycerol
Authors : Smithers, L.; van Dalsen, L.; Boland, C.; Caffrey, M.
Deposited on : 2020-09-10
Resolution : 1.85 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

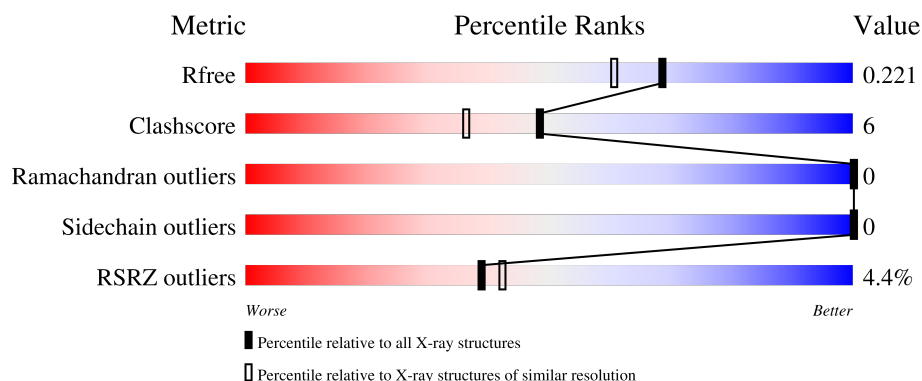
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LH9	A	504	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LH9	A	506	X	-	-	-
2	LH9	A	513	X	-	-	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 7922 atoms, of which 3847 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.

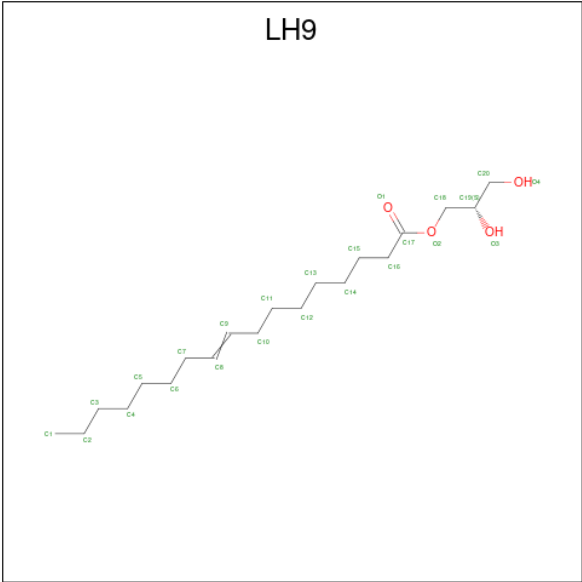
- Molecule 1 is a protein called Alginate biosynthesis protein AlgE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	457	Total	C	H	N	O	S	0	10	0
			7053	2279	3397	659	713	5			

There are 21 discrepancies between the modelled and reference sequences:

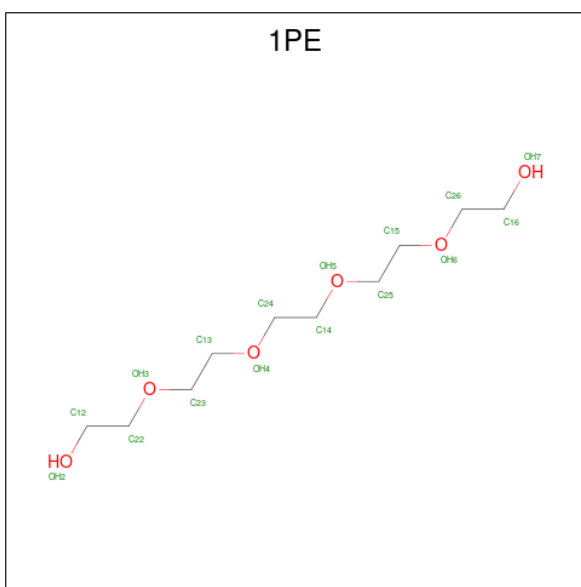
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0A080VSR9
A	-18	GLY	-	expression tag	UNP A0A080VSR9
A	-17	SER	-	expression tag	UNP A0A080VSR9
A	-16	SER	-	expression tag	UNP A0A080VSR9
A	-15	HIS	-	expression tag	UNP A0A080VSR9
A	-14	HIS	-	expression tag	UNP A0A080VSR9
A	-13	HIS	-	expression tag	UNP A0A080VSR9
A	-12	HIS	-	expression tag	UNP A0A080VSR9
A	-11	HIS	-	expression tag	UNP A0A080VSR9
A	-10	HIS	-	expression tag	UNP A0A080VSR9
A	-9	SER	-	expression tag	UNP A0A080VSR9
A	-8	SER	-	expression tag	UNP A0A080VSR9
A	-7	GLY	-	expression tag	UNP A0A080VSR9
A	-6	LEU	-	expression tag	UNP A0A080VSR9
A	-5	VAL	-	expression tag	UNP A0A080VSR9
A	-4	PRO	-	expression tag	UNP A0A080VSR9
A	-3	ARG	-	expression tag	UNP A0A080VSR9
A	-2	GLY	-	expression tag	UNP A0A080VSR9
A	-1	SER	-	expression tag	UNP A0A080VSR9
A	0	HIS	-	expression tag	UNP A0A080VSR9
A	1	MET	-	expression tag	UNP A0A080VSR9

- Molecule 2 is [(2 {S})-2,3-bis(oxidanyl)propyl] heptadec-9-enoate (CCD ID: LH9) (formula: C₂₀H₃₈O₄) (labeled as "Ligand of Interest" by depositor).



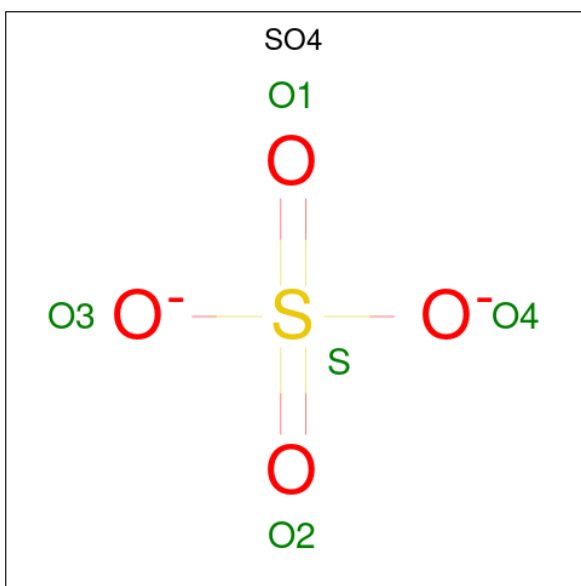
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			62	20	38	4		
2	A	1	Total	C	H	O	0	0
			62	20	38	4		
2	A	1	Total	C	H	O	0	0
			62	20	38	4		
2	A	1	Total	C	H	O	0	0
			62	20	38	4		
2	A	1	Total	C	H	O	0	0
			62	20	38	4		
2	A	1	Total	C	H	O	0	0
			62	20	38	4		
2	A	1	Total	C	H	O	0	0
			62	20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

- Molecule 3 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



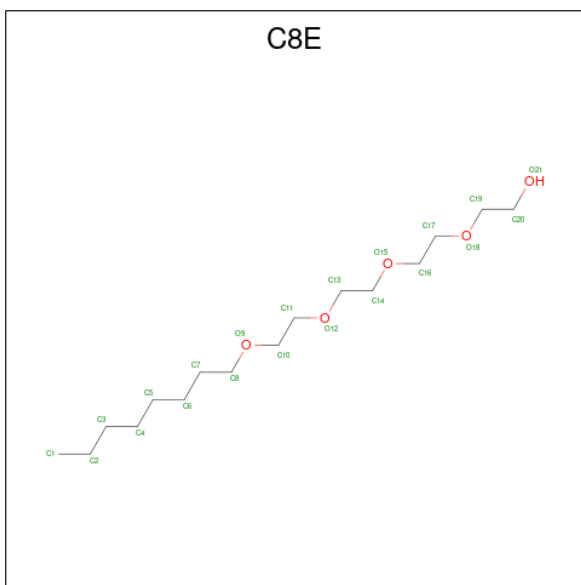
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			37	10	21	6		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



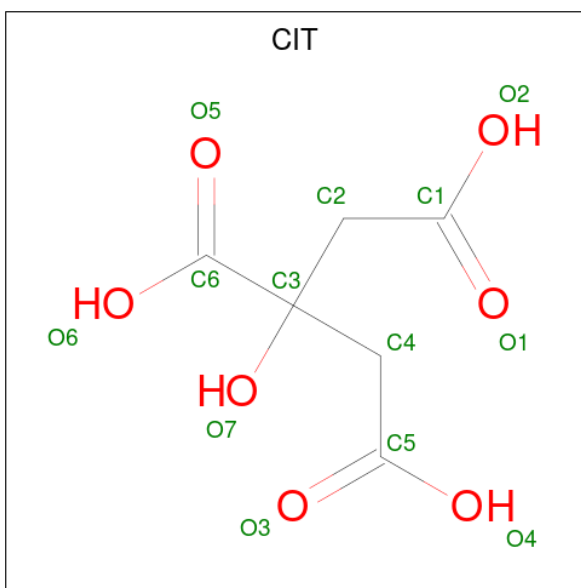
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (CCD ID: C8E) (formula: C₁₆H₃₄O₅).



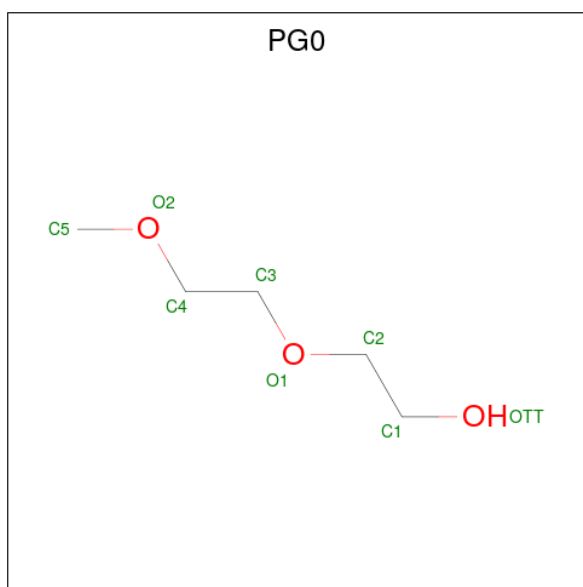
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			55	16	34	5		

- Molecule 6 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



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

- Molecule 7 is 2-(2-METHOXYETHOXY)ETHANOL (CCD ID: PG0) (formula: $C_5H_{12}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			18	5	10	3		

- Molecule 8 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	2	Total	Na	0	0
			2	2		

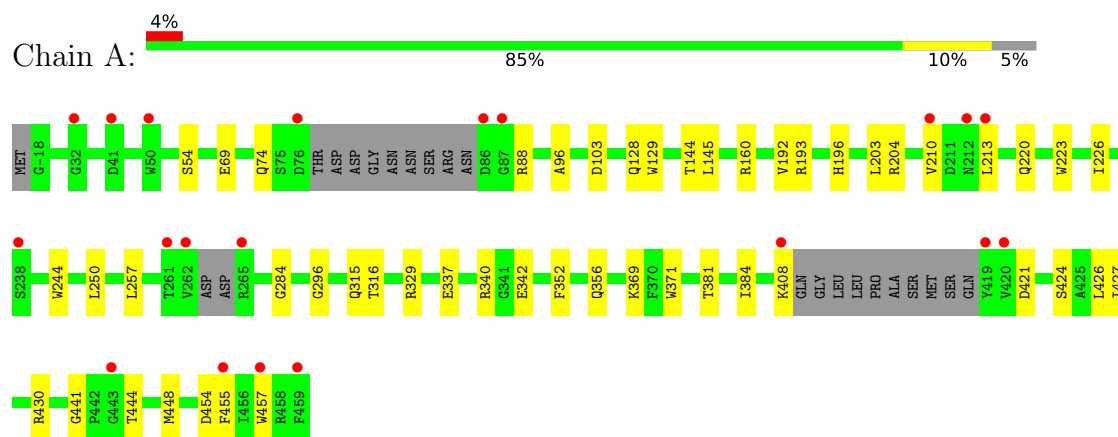
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	114	Total	O	0	0
			114	114		

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 biosynthesis 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	56.75Å 74.19Å 114.99Å 90.00° 102.73° 90.00°	Depositor
Resolution (Å)	44.37 – 1.85 44.37 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.1 (44.37-1.85) 99.1 (44.37-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 1.86Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.184 , 0.220 0.188 , 0.221	Depositor DCC
R_{free} test set	1986 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	25.9	Xtriage
Anisotropy	0.377	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.011 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7922	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.10% 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: PG0, C8E, LH9, 1PE, NA, SO4, CIT

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	0.29	0/3802	0.56	0/5149

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3656	3397	3346	38	0
2	A	240	380	0	2	0
3	A	16	21	22	0	0
4	A	5	0	0	0	0
5	A	21	34	34	0	0
6	A	13	5	5	0	0
7	A	8	10	12	5	0
8	A	2	0	0	0	0
9	A	114	0	0	1	0
All	All	4075	3847	3419	41	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 6.

All (41) 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:316:THR:HG23	7:A:512:PG0:H51	1.47	0.97
1:A:427:ILE:HD13	1:A:455:PHE:CD1	2.24	0.72
1:A:337[B]:GLU:OE1	1:A:430:ARG:NH1	2.23	0.72
1:A:128:GLN:O	7:A:512:PG0:H53	1.90	0.71
1:A:315:GLN:HA	7:A:512:PG0:H52	1.76	0.66
1:A:144:THR:HG22	1:A:145:LEU:CD1	2.27	0.65
1:A:144:THR:HG22	1:A:145:LEU:HD12	1.83	0.61
1:A:204:ARG:HG3	1:A:210:VAL:HG22	1.83	0.61
1:A:88:ARG:CG	1:A:213:LEU:HD11	2.35	0.56
1:A:203:LEU:HB3	1:A:257:LEU:HD13	1.89	0.55
1:A:441:GLY:O	1:A:444:THR:HG23	2.08	0.54
1:A:192:VAL:HG12	1:A:226[A]:ILE:HG22	1.89	0.53
1:A:315:GLN:CA	7:A:512:PG0:H52	2.38	0.53
2:A:501:LH9:O1	2:A:501:LH9:O3	2.29	0.51
1:A:427:ILE:HD12	1:A:454:ASP:O	2.11	0.50
1:A:369:LYS:HD3	1:A:371:TRP:CZ2	2.48	0.49
2:A:504:LH9:C4	2:A:504:LH9:C8	2.90	0.49
1:A:210:VAL:HG21	1:A:257:LEU:HD21	1.96	0.47
1:A:244:TRP:CZ2	1:A:284:GLY:HA3	2.50	0.47
1:A:421:ASP:N	1:A:421:ASP:OD1	2.47	0.47
1:A:54:SER:OG	1:A:103:ASP:HB3	2.16	0.46
1:A:427:ILE:HD13	1:A:455:PHE:CG	2.50	0.46
1:A:342:GLU:OE1	1:A:381:THR:HG23	2.17	0.45
1:A:69:GLU:OE1	1:A:340:ARG:NH1	2.44	0.44
1:A:427:ILE:HD13	1:A:455:PHE:CE1	2.51	0.44
1:A:88:ARG:HG3	1:A:213:LEU:HD11	1.99	0.43
1:A:315:GLN:CB	7:A:512:PG0:H52	2.48	0.43
1:A:408:LYS:HB3	1:A:424:SER:OG	2.18	0.43
1:A:74:GLN:NE2	1:A:160:ARG:HH11	2.17	0.43
1:A:129:TRP:CE2	1:A:193:ARG:HD2	2.54	0.43
1:A:96:ALA:HB2	1:A:160:ARG:HG2	2.01	0.42
1:A:329:ARG:H	1:A:356:GLN:HE22	1.65	0.42
1:A:384:ILE:CD1	1:A:448:MET:HE3	2.48	0.42
1:A:426:LEU:HD12	1:A:426:LEU:C	2.44	0.42
1:A:196:HIS:CE1	1:A:220:GLN:HG2	2.54	0.42
1:A:455:PHE:HB3	1:A:457:TRP:CH2	2.55	0.41
1:A:223:TRP:CE2	1:A:250:LEU:HD13	2.56	0.41
1:A:337[B]:GLU:CD	1:A:430:ARG:NH1	2.79	0.40
1:A:296:GLY:HA3	1:A:352:PHE:CZ	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	459/479 (96%)	445 (97%)	14 (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 (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 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	LH9	A	504	-	23,23,23	1.31	2 (8%)	24,24,24	1.27	2 (8%)
3	1PE	A	503	-	15,15,15	0.54	0	14,14,14	0.31	0
2	LH9	A	501	-	23,23,23	1.15	3 (13%)	24,24,24	1.04	0
2	LH9	A	507	-	23,23,23	1.15	2 (8%)	24,24,24	0.98	1 (4%)
2	LH9	A	514	-	23,23,23	1.25	2 (8%)	24,24,24	0.95	1 (4%)
2	LH9	A	506	-	23,23,23	1.15	2 (8%)	24,24,24	1.07	1 (4%)
2	LH9	A	505	-	23,23,23	1.13	2 (8%)	24,24,24	1.23	1 (4%)
2	LH9	A	510	-	23,23,23	1.17	3 (13%)	24,24,24	0.84	0
2	LH9	A	517	-	23,23,23	1.13	2 (8%)	24,24,24	1.27	2 (8%)
7	PG0	A	512	-	7,7,7	0.52	0	6,6,6	0.37	0
6	CIT	A	511	-	12,12,12	1.03	0	17,17,17	1.36	1 (5%)
2	LH9	A	513	-	23,23,23	1.11	2 (8%)	24,24,24	1.13	1 (4%)
2	LH9	A	502	-	23,23,23	1.15	3 (13%)	24,24,24	1.23	2 (8%)
5	C8E	A	509	-	20,20,20	0.43	0	19,19,19	0.31	0
4	SO4	A	508	-	4,4,4	0.24	0	6,6,6	0.20	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	LH9	A	504	-	1/1/4/4	12/23/23/23	-
3	1PE	A	503	-	-	7/13/13/13	-
2	LH9	A	501	-	-	9/23/23/23	-
2	LH9	A	507	-	-	7/23/23/23	-
2	LH9	A	514	-	-	14/23/23/23	-
2	LH9	A	506	-	1/1/4/4	10/23/23/23	-
2	LH9	A	505	-	-	15/23/23/23	-
2	LH9	A	510	-	-	14/23/23/23	-
2	LH9	A	517	-	-	8/23/23/23	-
7	PG0	A	512	-	-	3/5/5/5	-
6	CIT	A	511	-	-	0/16/16/16	-
2	LH9	A	513	-	1/1/4/4	13/23/23/23	-
2	LH9	A	502	-	-	7/23/23/23	-
5	C8E	A	509	-	-	8/18/18/18	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	504	LH9	C9-C8	4.13	1.55	1.31
2	A	514	LH9	C9-C8	4.05	1.54	1.31
2	A	510	LH9	C9-C8	3.91	1.53	1.31
2	A	501	LH9	C9-C8	3.91	1.53	1.31
2	A	506	LH9	C9-C8	3.85	1.53	1.31
2	A	513	LH9	C9-C8	3.85	1.53	1.31
2	A	517	LH9	C9-C8	3.79	1.53	1.31
2	A	507	LH9	C9-C8	3.77	1.53	1.31
2	A	505	LH9	C9-C8	3.73	1.52	1.31
2	A	502	LH9	C9-C8	3.64	1.52	1.31
2	A	504	LH9	O2-C17	2.99	1.42	1.33
2	A	514	LH9	O2-C17	2.85	1.41	1.33
2	A	502	LH9	O2-C18	-2.81	1.38	1.45
2	A	505	LH9	O2-C17	2.65	1.41	1.33
2	A	507	LH9	O2-C17	2.63	1.41	1.33
2	A	506	LH9	O2-C17	2.54	1.40	1.33
2	A	517	LH9	O2-C17	2.42	1.40	1.33
2	A	513	LH9	O2-C17	2.40	1.40	1.33
2	A	510	LH9	O2-C17	2.38	1.40	1.33
2	A	501	LH9	O2-C18	-2.32	1.40	1.45
2	A	502	LH9	O2-C17	2.21	1.39	1.33
2	A	510	LH9	O2-C18	-2.21	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	LH9	O2-C17	2.12	1.39	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	504	LH9	O2-C17-C16	3.69	123.08	111.83
6	A	511	CIT	O6-C6-C3	3.54	119.94	113.14
2	A	517	LH9	O2-C17-C16	3.46	122.39	111.83
2	A	513	LH9	O2-C17-C16	2.98	120.92	111.83
2	A	506	LH9	O2-C17-C16	2.90	120.69	111.83
2	A	502	LH9	C15-C16-C17	-2.87	103.17	113.69
2	A	507	LH9	O2-C17-C16	2.78	120.31	111.83
2	A	514	LH9	O2-C17-C16	2.78	120.30	111.83
2	A	505	LH9	O2-C17-C16	2.52	119.52	111.83
2	A	517	LH9	C14-C15-C16	-2.45	104.12	113.13
2	A	504	LH9	O2-C18-C19	2.31	116.73	105.85
2	A	502	LH9	C10-C9-C8	-2.05	109.48	124.83

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	504	LH9	C19
2	A	506	LH9	C19
2	A	513	LH9	C19

All (127) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	LH9	C18-C19-C20-O4
2	A	502	LH9	O2-C18-C19-C20
2	A	504	LH9	O2-C18-C19-C20
2	A	504	LH9	O2-C18-C19-O3
2	A	505	LH9	C18-C19-C20-O4
2	A	506	LH9	O2-C18-C19-C20
2	A	506	LH9	O2-C18-C19-O3
2	A	513	LH9	C18-C19-C20-O4
2	A	513	LH9	O3-C19-C20-O4
2	A	514	LH9	C18-C19-C20-O4
2	A	514	LH9	O3-C19-C20-O4
2	A	505	LH9	O1-C17-O2-C18
2	A	505	LH9	C16-C17-O2-C18
2	A	514	LH9	C16-C17-O2-C18

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Mol	Chain	Res	Type	Atoms
2	A	517	LH9	C16-C17-O2-C18
2	A	505	LH9	C7-C8-C9-C10
2	A	504	LH9	O1-C17-O2-C18
2	A	514	LH9	O1-C17-O2-C18
2	A	517	LH9	O1-C17-O2-C18
2	A	504	LH9	C16-C17-O2-C18
2	A	502	LH9	O2-C18-C19-O3
2	A	510	LH9	C16-C17-O2-C18
2	A	502	LH9	C7-C8-C9-C10
2	A	506	LH9	C7-C8-C9-C10
2	A	510	LH9	C7-C8-C9-C10
2	A	506	LH9	C16-C17-O2-C18
2	A	510	LH9	O1-C17-O2-C18
3	A	503	1PE	OH6-C15-C25-OH5
3	A	503	1PE	OH2-C12-C22-OH3
2	A	501	LH9	C14-C15-C16-C17
2	A	506	LH9	O1-C17-O2-C18
2	A	513	LH9	C14-C15-C16-C17
3	A	503	1PE	OH7-C16-C26-OH6
7	A	512	PG0	OTT-C1-C2-O1
2	A	514	LH9	C14-C15-C16-C17
2	A	507	LH9	C7-C8-C9-C10
2	A	510	LH9	C18-C19-C20-O4
2	A	517	LH9	C18-C19-C20-O4
2	A	510	LH9	C2-C3-C4-C5
2	A	514	LH9	C3-C4-C5-C6
2	A	502	LH9	C12-C13-C14-C15
2	A	501	LH9	O3-C19-C20-O4
2	A	501	LH9	C13-C14-C15-C16
2	A	506	LH9	C10-C11-C12-C13
2	A	505	LH9	C9-C10-C11-C12
2	A	506	LH9	C3-C4-C5-C6
2	A	517	LH9	C2-C3-C4-C5
2	A	501	LH9	C12-C13-C14-C15
2	A	513	LH9	C3-C4-C5-C6
2	A	502	LH9	C9-C10-C11-C12
2	A	510	LH9	C9-C10-C11-C12
5	A	509	C8E	C3-C4-C5-C6
2	A	505	LH9	C14-C15-C16-C17
2	A	510	LH9	C5-C6-C7-C8
2	A	513	LH9	C13-C14-C15-C16
5	A	509	C8E	O18-C19-C20-O21

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Mol	Chain	Res	Type	Atoms
2	A	505	LH9	O3-C19-C20-O4
2	A	517	LH9	O3-C19-C20-O4
2	A	502	LH9	C13-C14-C15-C16
2	A	507	LH9	C5-C6-C7-C8
2	A	513	LH9	C16-C17-O2-C18
2	A	506	LH9	C13-C14-C15-C16
2	A	514	LH9	C7-C8-C9-C10
2	A	514	LH9	C9-C10-C11-C12
2	A	501	LH9	C10-C11-C12-C13
2	A	505	LH9	C11-C12-C13-C14
2	A	504	LH9	C5-C6-C7-C8
2	A	505	LH9	C10-C11-C12-C13
2	A	502	LH9	C11-C12-C13-C14
2	A	514	LH9	C1-C2-C3-C4
2	A	513	LH9	O1-C17-O2-C18
2	A	504	LH9	C1-C2-C3-C4
2	A	513	LH9	C1-C2-C3-C4
2	A	514	LH9	C2-C3-C4-C5
7	A	512	PG0	C3-C4-O2-C5
2	A	504	LH9	C3-C4-C5-C6
2	A	513	LH9	O2-C18-C19-O3
2	A	510	LH9	C4-C5-C6-C7
2	A	510	LH9	O3-C19-C20-O4
2	A	506	LH9	C12-C13-C14-C15
5	A	509	C8E	O12-C13-C14-O15
3	A	503	1PE	C23-C13-OH4-C24
2	A	517	LH9	C4-C5-C6-C7
2	A	501	LH9	C6-C7-C8-C9
2	A	517	LH9	C7-C8-C9-C10
2	A	504	LH9	C12-C13-C14-C15
3	A	503	1PE	C16-C26-OH6-C15
2	A	505	LH9	C3-C4-C5-C6
2	A	517	LH9	C11-C10-C9-C8
5	A	509	C8E	C11-C10-O9-C8
5	A	509	C8E	C14-C13-O12-C11
2	A	510	LH9	C13-C14-C15-C16
2	A	514	LH9	C10-C11-C12-C13
2	A	505	LH9	C13-C14-C15-C16
2	A	507	LH9	O2-C18-C19-O3
2	A	501	LH9	C11-C10-C9-C8
2	A	514	LH9	C5-C6-C7-C8
3	A	503	1PE	C24-C14-OH5-C25

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Mol	Chain	Res	Type	Atoms
2	A	506	LH9	O3-C19-C20-O4
2	A	504	LH9	C11-C10-C9-C8
2	A	501	LH9	C19-C18-O2-C17
3	A	503	1PE	OH5-C14-C24-OH4
2	A	510	LH9	C6-C7-C8-C9
2	A	505	LH9	C5-C6-C7-C8
2	A	513	LH9	C10-C11-C12-C13
2	A	507	LH9	C14-C15-C16-C17
2	A	507	LH9	C4-C5-C6-C7
5	A	509	C8E	C17-C16-O15-C14
2	A	510	LH9	C11-C10-C9-C8
2	A	507	LH9	C18-C19-C20-O4
2	A	504	LH9	C6-C7-C8-C9
2	A	505	LH9	C4-C5-C6-C7
2	A	514	LH9	C11-C10-C9-C8
7	A	512	PG0	C1-C2-O1-C3
2	A	510	LH9	O2-C18-C19-C20
2	A	505	LH9	C11-C10-C9-C8
2	A	514	LH9	C12-C13-C14-C15
2	A	513	LH9	C6-C7-C8-C9
2	A	504	LH9	C15-C16-C17-O2
2	A	513	LH9	C15-C16-C17-O2
5	A	509	C8E	C4-C5-C6-C7
2	A	504	LH9	C15-C16-C17-O1
2	A	513	LH9	C15-C16-C17-O1
2	A	507	LH9	C1-C2-C3-C4
2	A	510	LH9	C11-C12-C13-C14
5	A	509	C8E	C2-C3-C4-C5
2	A	505	LH9	C15-C16-C17-O2

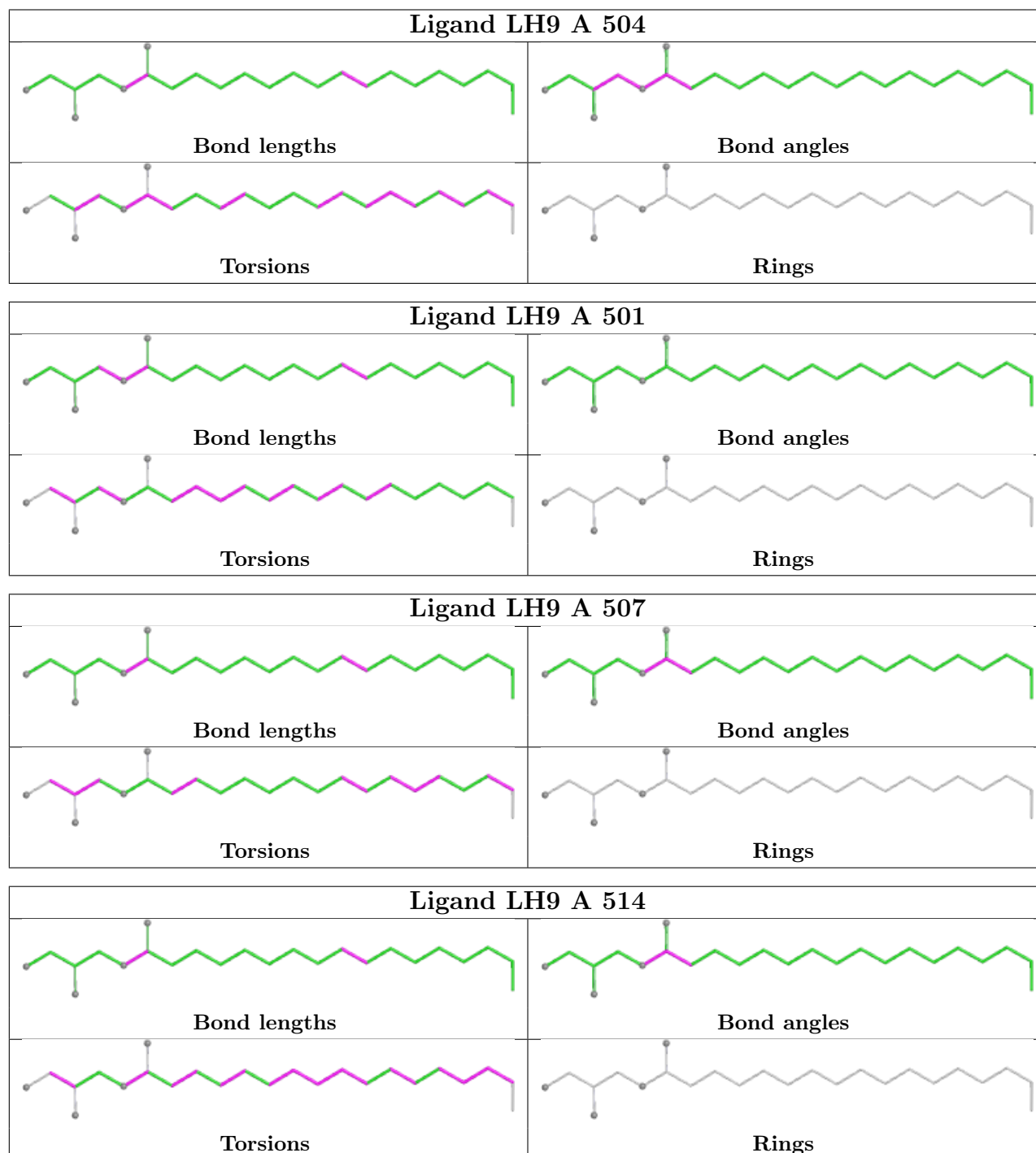
There are no ring outliers.

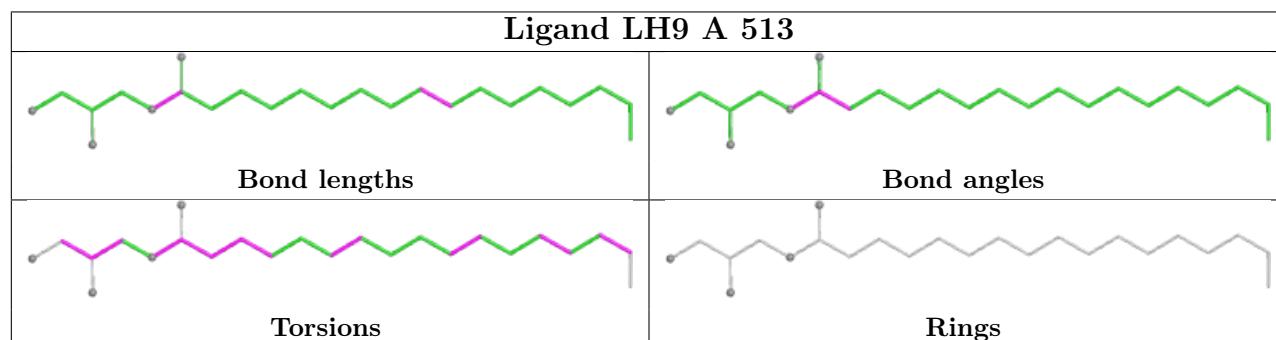
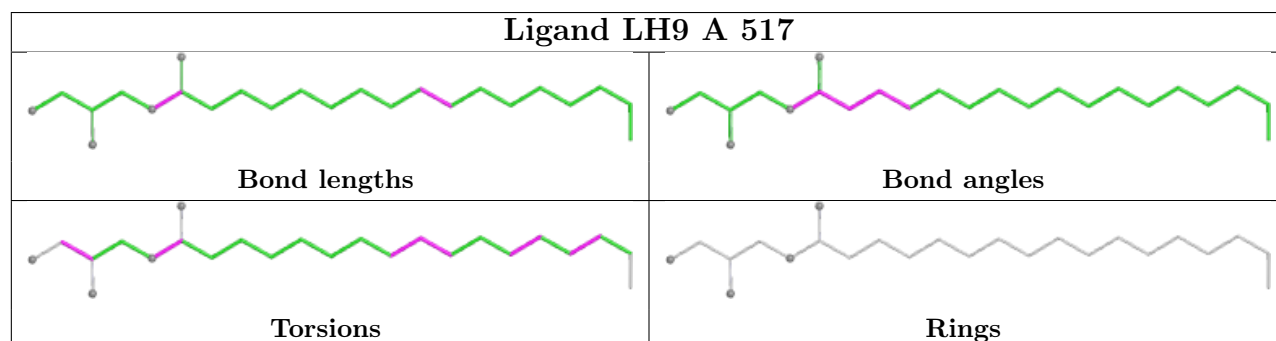
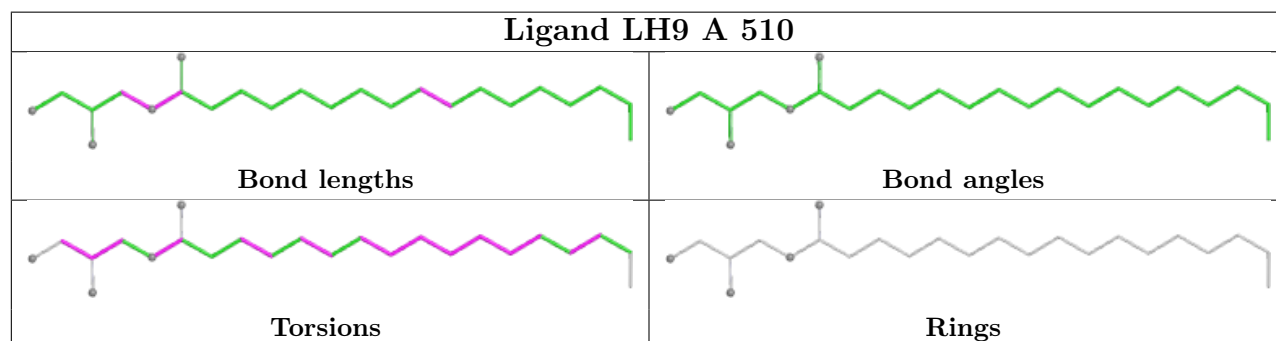
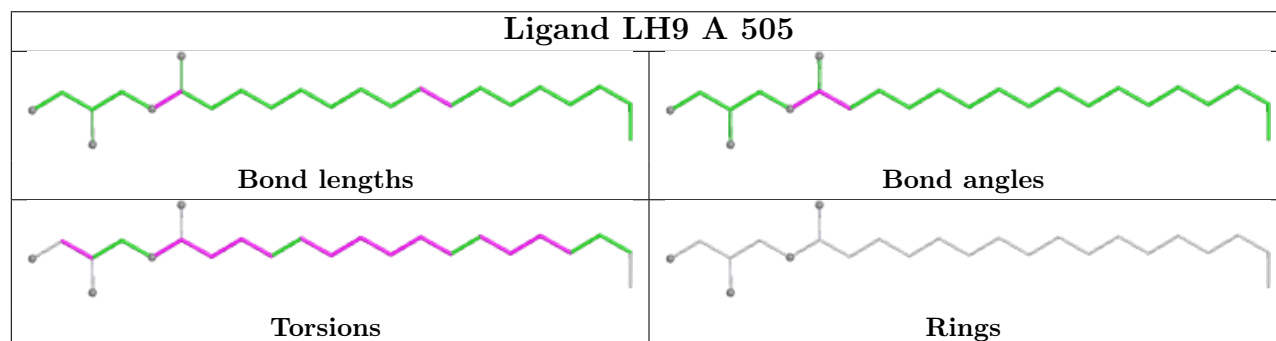
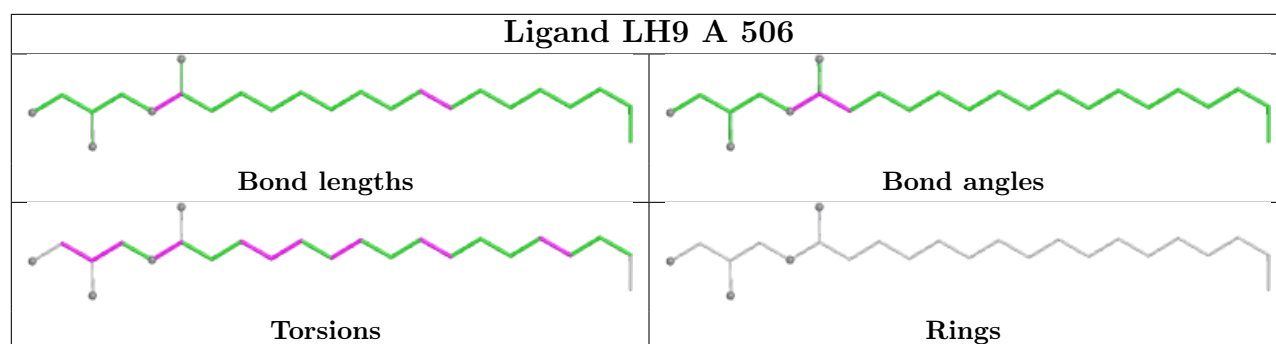
3 monomers are involved in 7 short contacts:

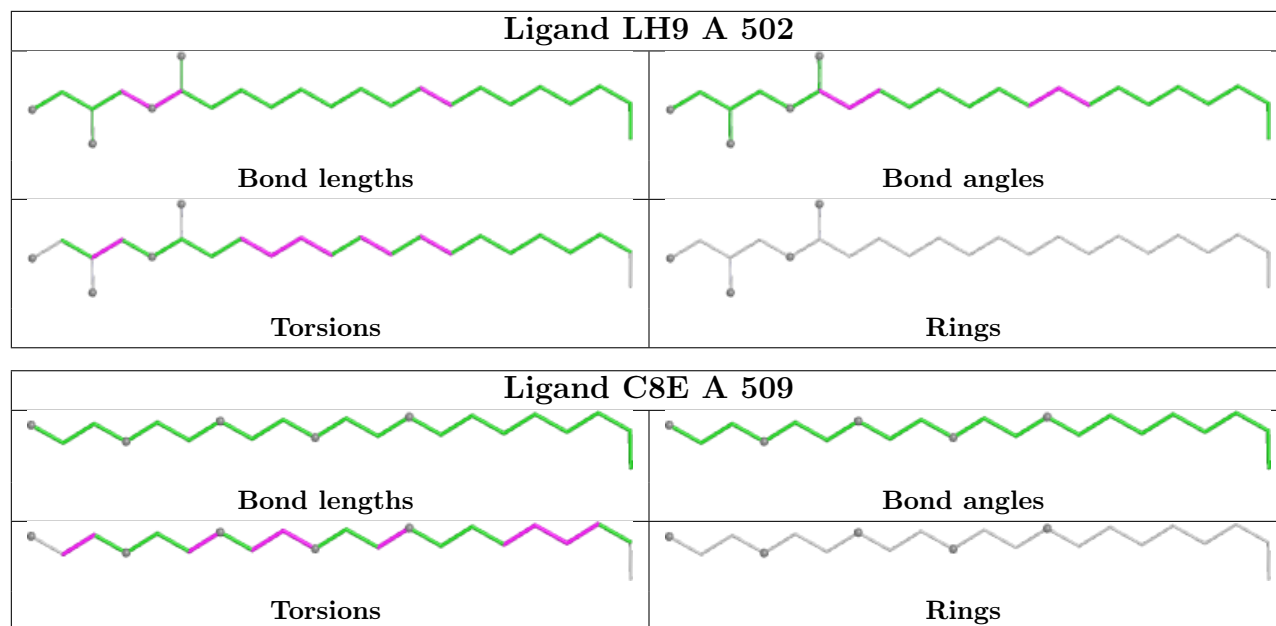
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	504	LH9	1	0
2	A	501	LH9	1	0
7	A	512	PG0	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	457/479 (95%)	0.22	20 (4%)	39 42	15, 35, 66, 119	5 (1%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	262	VAL	4.4
1	A	455	PHE	4.3
1	A	213	LEU	4.1
1	A	419	TYR	4.0
1	A	265	ARG	3.4
1	A	457	TRP	3.1
1	A	261	THR	3.0
1	A	212	ASN	2.9
1	A	76	ASP	2.6
1	A	87	GLY	2.6
1	A	210	VAL	2.6
1	A	86	ASP	2.4
1	A	50	TRP	2.4
1	A	459	PHE	2.3
1	A	408	LYS	2.3
1	A	420	VAL	2.3
1	A	41	ASP	2.3
1	A	238	SER	2.3
1	A	443	GLY	2.1
1	A	32	GLY	2.1

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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

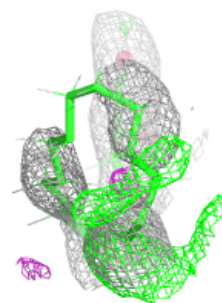
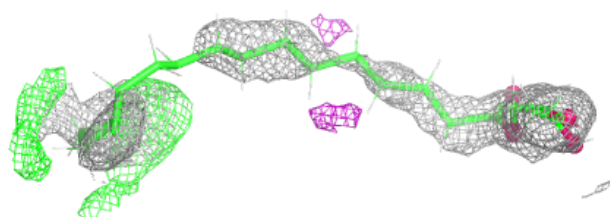
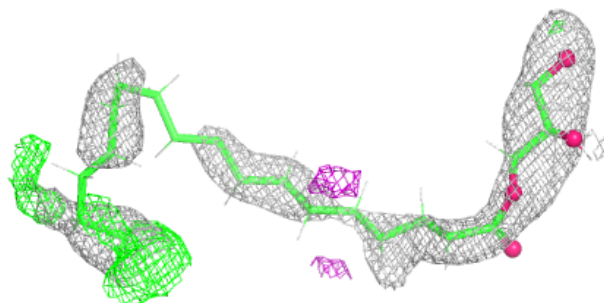
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	LH9	A	504	24/24	0.68	0.24	48,69,83,99	0
2	LH9	A	514	24/24	0.77	0.17	55,72,85,87	0
2	LH9	A	506	24/24	0.79	0.17	35,60,79,94	0
2	LH9	A	501	24/24	0.80	0.16	35,48,100,114	0
2	LH9	A	505	24/24	0.80	0.19	39,61,76,82	0
2	LH9	A	517	24/24	0.80	0.15	37,58,73,83	0
5	C8E	A	509	21/21	0.80	0.18	49,68,82,93	0
2	LH9	A	510	24/24	0.81	0.18	46,75,101,105	0
2	LH9	A	507	24/24	0.82	0.20	40,58,76,90	0
2	LH9	A	513	24/24	0.85	0.16	49,75,97,99	0
2	LH9	A	502	24/24	0.86	0.13	34,57,78,83	0
6	CIT	A	511	13/13	0.87	0.09	30,42,48,50	0
3	1PE	A	503	16/16	0.89	0.11	32,56,85,86	0
7	PG0	A	512	8/8	0.91	0.10	13,35,56,56	0
8	NA	A	516	1/1	0.91	0.11	54,54,54,54	0
8	NA	A	515	1/1	0.98	0.04	30,30,30,30	0
4	SO4	A	508	5/5	0.98	0.07	27,28,35,35	0

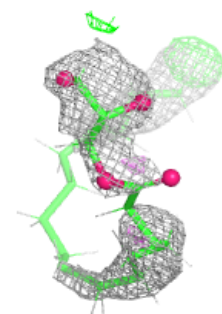
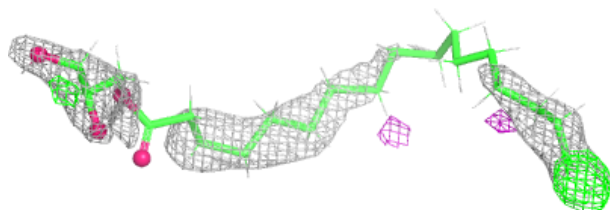
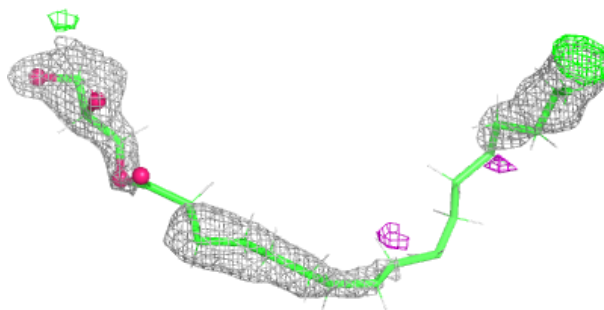
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LH9 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)

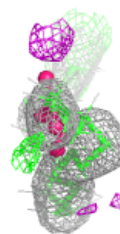
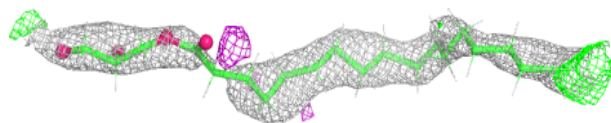
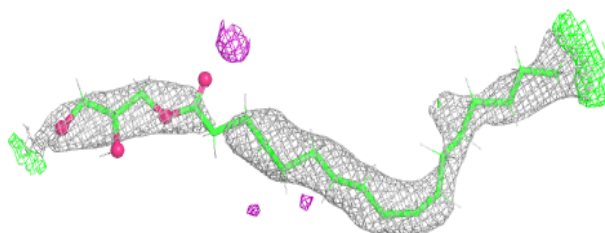
**Electron density around LH9 A 514:**

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

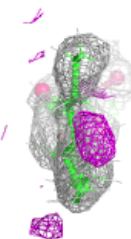
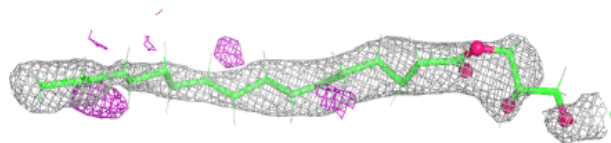
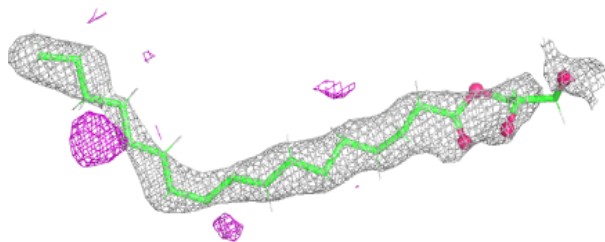


Electron density around LH9 A 506:

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

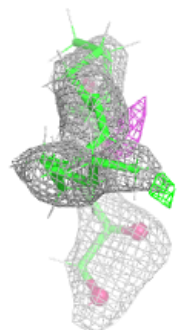
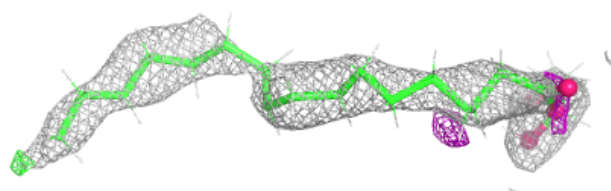
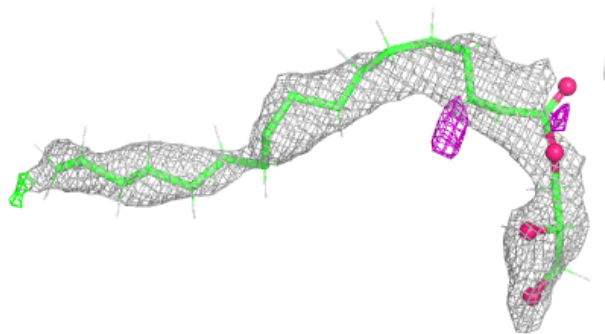
**Electron density around LH9 A 501:**

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

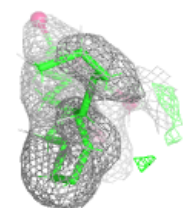
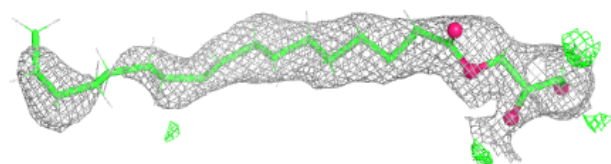
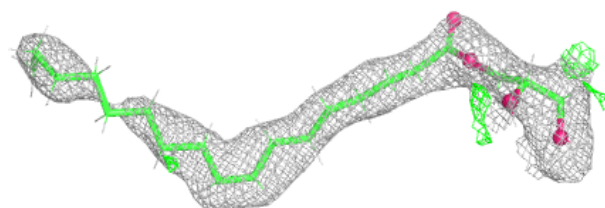


Electron density around LH9 A 505:

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and green (positive)

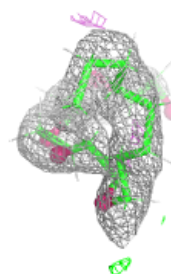
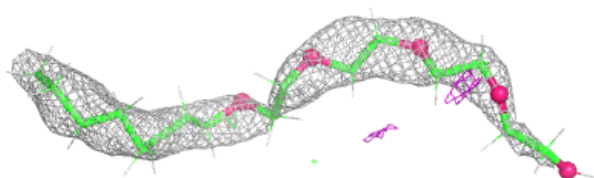
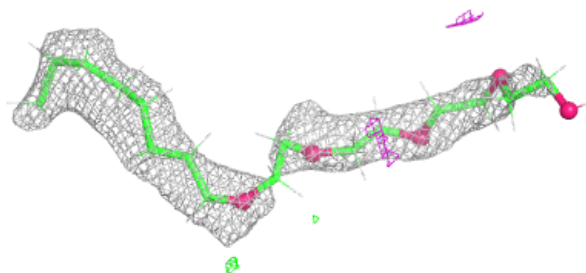
**Electron density around LH9 A 517:**

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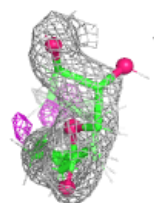
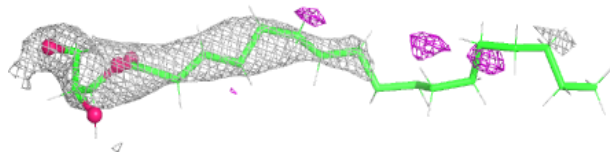
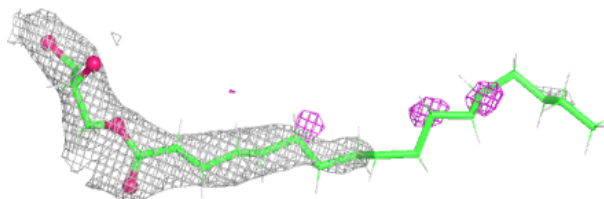


Electron density around C8E A 509:

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

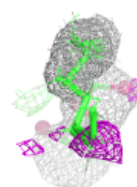
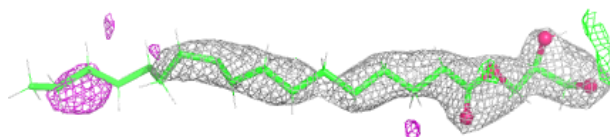
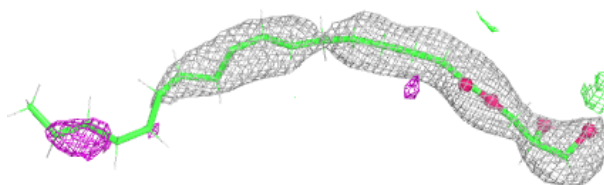
**Electron density around LH9 A 510:**

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

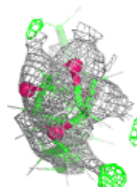
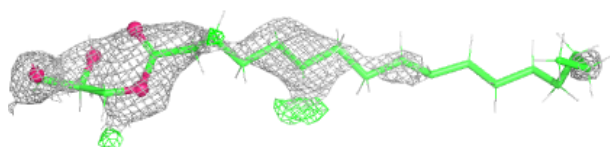
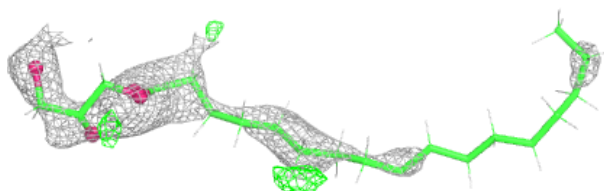


Electron density around LH9 A 507:

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

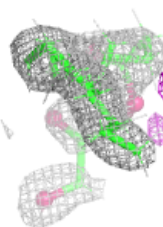
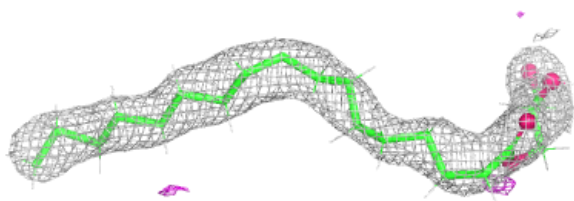
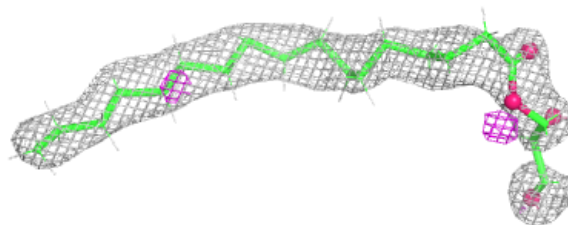
**Electron density around LH9 A 513:**

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



Electron density around LH9 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.