



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 22, 2022 – 12:16 PM EDT

PDB ID : 7MDF
Title : Full-length S95A ClbP bound to N-acyl-D-asparagine analog
Authors : Velilla, J.A.; Volpe, M.R.; Gaudet, R.
Deposited on : 2021-04-04
Resolution : 2.30 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.29
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.29

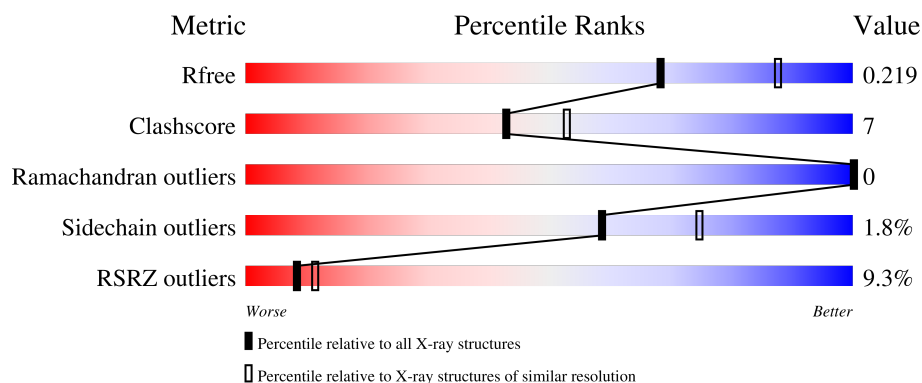
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	480	

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
5	2PE	A	707	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	97N	A	711	-	-	-	X
7	97N	A	712	-	-	-	X

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 3935 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

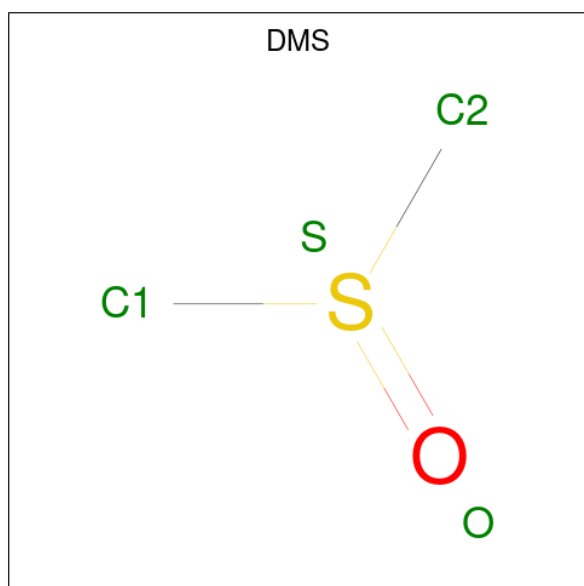
- Molecule 1 is a protein called Beta-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	453	3431	2200	594	623	14	0	6	0

There are 9 discrepancies between the modelled and reference sequences:

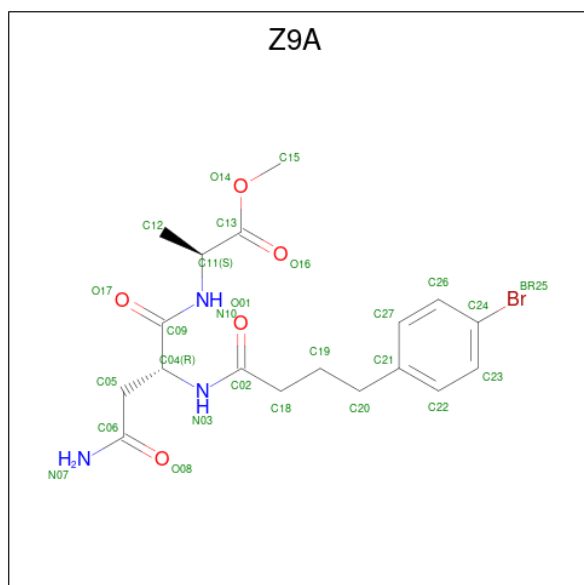
Chain	Residue	Modelled	Actual	Comment	Reference
A	95	ALA	SER	engineered mutation	UNP Q0P7K6
A	454	MET	LEU	engineered mutation	UNP Q0P7K6
A	478	MET	ILE	engineered mutation	UNP Q0P7K6
A	505	HIS	-	expression tag	UNP Q0P7K6
A	506	HIS	-	expression tag	UNP Q0P7K6
A	507	HIS	-	expression tag	UNP Q0P7K6
A	508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

- Molecule 2 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



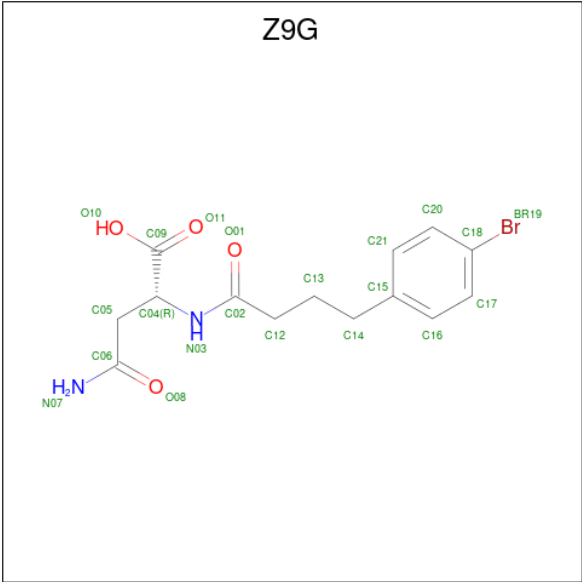
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	A	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 3 is methyl N 2 -[4-(4-bromophenyl)butanoyl]-D-asparaginy-L-alaninate (three-letter code: Z9A) (formula: C₁₈H₂₄BrN₃O₅).



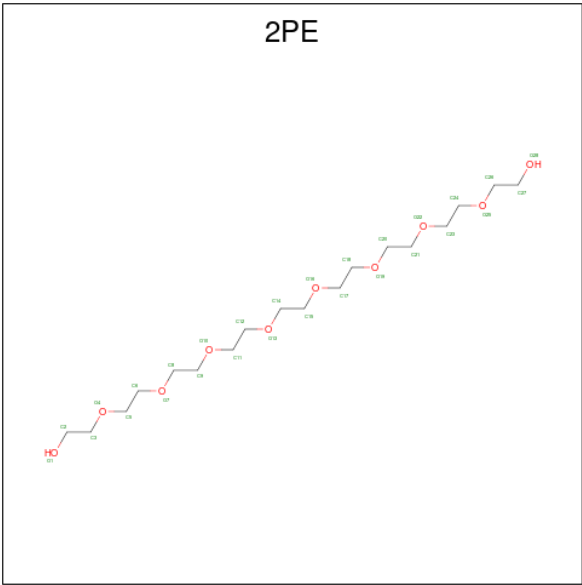
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	Br	C	N	O	0	0
			27	1	18	3	5		

- Molecule 4 is N 2 -[4-(4-bromophenyl)butanoyl]-D-asparagine (three-letter code: Z9G) (formula: C₁₄H₁₇BrN₂O₄) (labeled as "Ligand of Interest" by depositor).

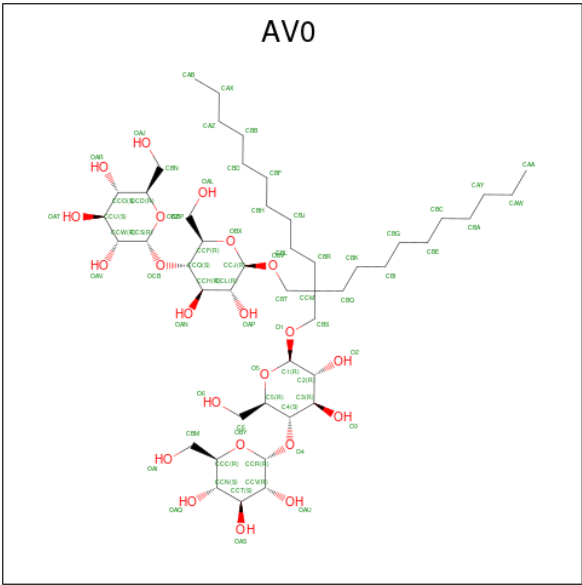


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	Br	C	N	O		
4	A	1	21	1	14	2	4	0	0

- Molecule 5 is NONAETHYLENE GLYCOL (three-letter code: 2PE) (formula: C₁₈H₃₈O₁₀).

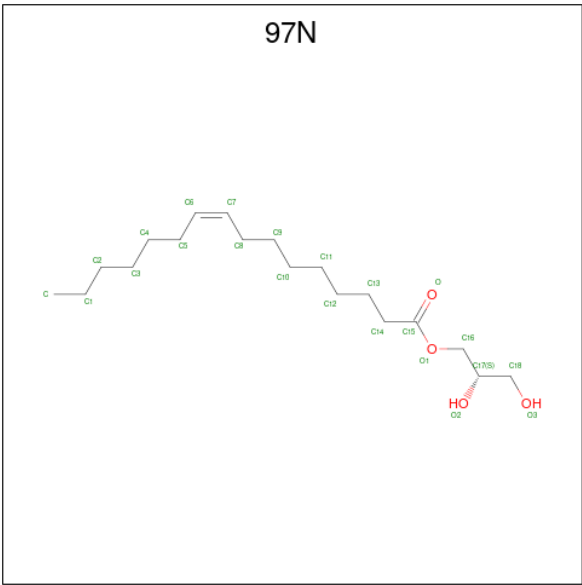


- Molecule 6 is 2-decyl-2-[[[(4-O-alpha-D-glucopyranosyl-beta-D-glucopyranosyl)oxy]methyl]dodecyl 4-O-alpha-D-glucopyranosyl-beta-D-glucopyranoside (three-letter code: AV0) (formula: C₄₇H₈₈O₂₂).



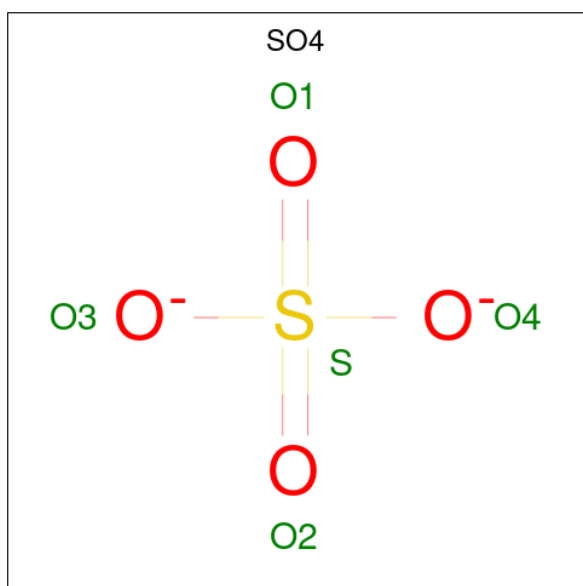
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			32	26	6		

- Molecule 7 is (2S)-2,3-dihydroxypropyl (9Z)-hexadec-9-enoate (three-letter code: 97N) (formula: C₁₉H₃₆O₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 17 13 4	0	0
7	A	1	Total C O 18 14 4	0	0
7	A	1	Total C O 17 13 4	0	0
7	A	1	Total C 11 11	0	0
7	A	1	Total C 4 4	0	0

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

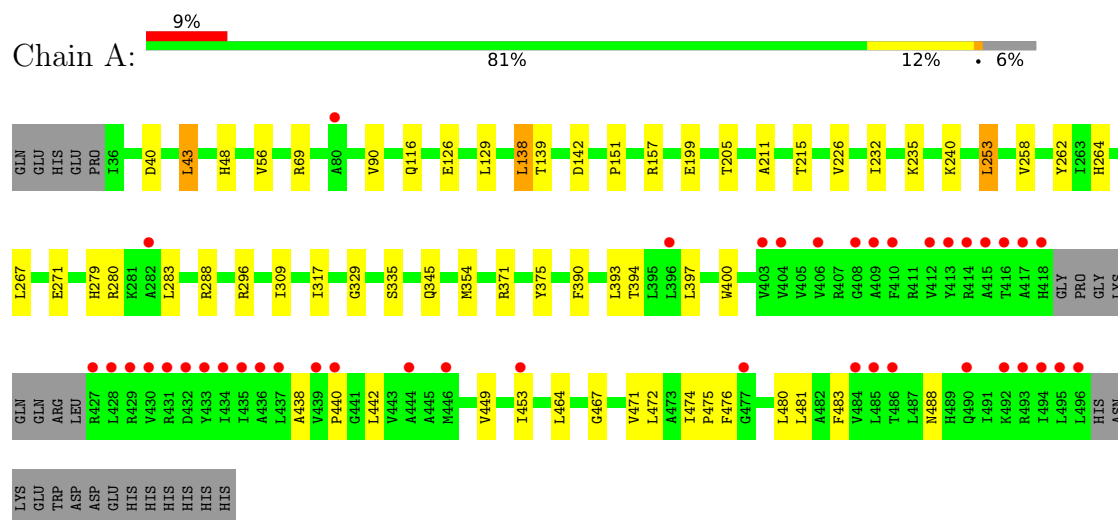
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	309	Total 309	O 309	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: Beta-lactamase



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	96.69Å 96.69Å 182.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.74 – 2.30 48.34 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.74-2.30) 85.5 (48.34-2.30)	Depositor EDS
R_{merge}	0.36	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.91 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.191 , 0.219 0.191 , 0.219	Depositor DCC
R_{free} test set	1965 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	26.8	Xtriage
Anisotropy	0.751	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 62.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3935	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.12% 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: 2PE, 97N, Z9G, DMS, SO4, AV0, CL, Z9A

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	0.39	0/3520	0.59	0/4801

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	375	TYR	Mainchain

5.2 Too-close contacts [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	3431	0	3387	45	0
2	A	8	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	27	0	0	0	0
4	A	21	0	0	0	0
5	A	32	0	39	3	0
6	A	32	0	0	0	0
7	A	67	0	0	0	0
8	A	5	0	0	1	0
9	A	3	0	0	0	0
10	A	309	0	0	7	2
All	All	3935	0	3438	48	2

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 (48) 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:69:ARG:NH1	8:A:714:SO4:O4	1.98	0.96
1:A:199:GLU:OE2	10:A:801:HOH:O	1.97	0.82
1:A:390:PHE:HE2	1:A:471:VAL:HG12	1.56	0.70
1:A:464:LEU:HD21	1:A:472:LEU:HD13	1.75	0.68
1:A:139[B]:THR:HG23	1:A:142:ASP:H	1.59	0.68
1:A:390:PHE:CE2	1:A:471:VAL:HG12	2.36	0.60
1:A:129:LEU:HD12	1:A:138:LEU:HD13	1.87	0.56
1:A:126:GLU:OE1	10:A:802:HOH:O	2.18	0.56
1:A:400:TRP:HD1	1:A:481:LEU:HD11	1.73	0.54
1:A:157:ARG:NH2	10:A:809:HOH:O	2.41	0.54
1:A:139[B]:THR:HG22	1:A:142:ASP:OD2	2.08	0.53
1:A:390:PHE:O	1:A:394:THR:HG23	2.09	0.53
1:A:258:VAL:HA	1:A:262:TYR:HB2	1.91	0.53
1:A:56:VAL:HG12	1:A:354:MET:HB3	1.91	0.51
1:A:40:ASP:HB3	1:A:43:LEU:HB2	1.92	0.51
1:A:69:ARG:HD3	1:A:271:GLU:OE2	2.11	0.51
1:A:440:PRO:HG3	1:A:483:PHE:HD1	1.75	0.51
1:A:400:TRP:CD1	1:A:481:LEU:HD11	2.45	0.51
1:A:69:ARG:HD3	1:A:271:GLU:CD	2.32	0.50
1:A:329:GLY:O	1:A:335:SER:HA	2.12	0.50
1:A:400:TRP:CD1	1:A:481:LEU:HD21	2.48	0.49
1:A:267:LEU:O	1:A:271:GLU:HG3	2.13	0.49
1:A:226:VAL:HG11	1:A:232:ILE:HD11	1.94	0.48
1:A:116:GLN:O	1:A:139[B]:THR:OG1	2.32	0.48
1:A:240:LYS:HD3	1:A:467:GLY:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:HIS:HD2	10:A:1072:HOH:O	1.98	0.47
1:A:280:ARG:HA	1:A:283:LEU:HG	1.98	0.46
1:A:253:LEU:HD13	1:A:262:TYR:CD2	2.50	0.46
1:A:90:VAL:HB	1:A:235:LYS:HA	1.97	0.46
1:A:280:ARG:O	1:A:288:ARG:NH1	2.49	0.45
1:A:139[B]:THR:HG21	10:A:1012:HOH:O	2.16	0.44
1:A:232:ILE:HD13	1:A:264:HIS:CD2	2.53	0.44
1:A:440:PRO:HB3	1:A:483:PHE:HB2	2.00	0.44
1:A:309:ILE:HG23	1:A:317:ILE:O	2.19	0.43
1:A:440:PRO:HG3	1:A:483:PHE:CD1	2.53	0.43
1:A:438:ALA:O	1:A:442:LEU:N	2.51	0.43
1:A:139[B]:THR:HG23	1:A:142:ASP:N	2.31	0.42
1:A:205:THR:HG23	10:A:811:HOH:O	2.18	0.42
1:A:371:ARG:HD2	10:A:805:HOH:O	2.20	0.42
1:A:279:HIS:NE2	1:A:345:GLN:OE1	2.52	0.42
5:A:706:2PE:H82	5:A:706:2PE:H111	1.80	0.41
1:A:393:LEU:O	1:A:397:LEU:HG	2.20	0.41
1:A:211:ALA:HA	1:A:215:THR:OG1	2.21	0.41
5:A:706:2PE:H52	5:A:706:2PE:H81	1.58	0.41
1:A:474:ILE:HB	1:A:475:PRO:HD3	2.02	0.41
5:A:706:2PE:H52	5:A:706:2PE:H21	1.91	0.41
1:A:476:PHE:O	1:A:480:LEU:HB2	2.20	0.40
1:A:449:VAL:HG12	1:A:453:ILE:HG13	2.02	0.40

All (2) 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:828:HOH:O	10:A:828:HOH:O[2_565]	1.88	0.32
10:A:815:HOH:O	10:A:916:HOH:O[6_455]	2.18	0.02

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

The Analysed column shows the number of residues for which the backbone conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	455/480 (95%)	438 (96%)	17 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	347/392 (88%)	341 (98%)	6 (2%)	60	76

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	LEU
1	A	138	LEU
1	A	151	PRO
1	A	253	LEU
1	A	296	ARG
1	A	488	ASN

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 3 are monoatomic - leaving 14 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
3	Z9A	A	703	-	27,27,27	2.00	6 (22%)	35,35,35	1.51	7 (20%)
7	97N	A	710	-	17,17,22	0.98	1 (5%)	18,18,23	0.99	1 (5%)
2	DMS	A	701	-	3,3,3	0.70	0	3,3,3	0.40	0
7	97N	A	709	-	16,16,22	0.99	2 (12%)	17,17,23	0.95	1 (5%)
7	97N	A	711	-	16,16,22	1.01	1 (6%)	17,17,23	1.02	1 (5%)
5	2PE	A	705	-	6,6,27	0.47	0	5,5,26	0.39	0
8	SO4	A	714	-	4,4,4	0.13	0	6,6,6	0.29	0
4	Z9G	A	704	-	21,21,21	1.65	2 (9%)	27,27,27	1.26	3 (11%)
7	97N	A	712	-	10,10,22	0.34	0	9,9,23	0.71	0
6	AV0	A	708	-	32,32,72	1.23	4 (12%)	37,38,98	1.27	3 (8%)
7	97N	A	713	-	3,3,22	0.43	0	2,2,23	0.71	0
5	2PE	A	706	-	13,13,27	0.52	0	12,12,26	0.26	0
5	2PE	A	707	-	10,10,27	0.50	0	9,9,26	0.20	0
2	DMS	A	702	-	3,3,3	0.66	0	3,3,3	0.61	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
3	Z9A	A	703	-	-	1/28/28/28	0/1/1/1
7	97N	A	710	-	-	9/17/17/22	-
7	97N	A	709	-	-	6/16/16/22	-
7	97N	A	711	-	-	12/16/16/22	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	2PE	A	705	-	-	3/4/4/25	-
4	Z9G	A	704	-	-	1/18/18/18	0/1/1/1
7	97N	A	712	-	-	5/8/8/22	-
6	AV0	A	708	-	-	17/25/45/130	0/1/1/4
7	97N	A	713	-	-	1/1/1/22	-
5	2PE	A	706	-	-	8/11/11/25	-
5	2PE	A	707	-	-	4/8/8/25	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	703	Z9A	C09-N10	5.89	1.47	1.34
4	A	704	Z9G	C02-N03	5.45	1.45	1.34
3	A	703	Z9A	C02-N03	5.16	1.45	1.34
3	A	703	Z9A	C06-N07	3.95	1.45	1.32
4	A	704	Z9G	C06-N07	3.90	1.45	1.32
3	A	703	Z9A	O14-C13	2.94	1.40	1.33
7	A	711	97N	O1-C15	2.61	1.40	1.33
7	A	710	97N	O1-C15	2.60	1.40	1.33
6	A	708	AV0	CBS-CCM	2.58	1.60	1.51
7	A	709	97N	O1-C15	2.51	1.40	1.33
6	A	708	AV0	O5-C1	2.46	1.48	1.41
3	A	703	Z9A	O01-C02	-2.20	1.18	1.23
6	A	708	AV0	O3-C3	2.09	1.47	1.43
7	A	709	97N	O1-C16	-2.03	1.40	1.45
6	A	708	AV0	O5-C5	2.01	1.49	1.44
3	A	703	Z9A	O14-C15	-2.00	1.40	1.45

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	708	AV0	CBJ-CBL-CBR	4.97	131.20	113.62
3	A	703	Z9A	C05-C04-N03	-3.36	104.02	110.60
3	A	703	Z9A	O14-C13-C11	3.25	119.65	111.28
6	A	708	AV0	O5-C5-C4	2.95	115.05	109.69
4	A	704	Z9G	C14-C13-C12	-2.82	105.05	114.34
7	A	711	97N	O1-C15-C14	2.82	120.75	111.91
3	A	703	Z9A	C04-C05-C06	2.64	117.48	112.24
3	A	703	Z9A	C18-C02-N03	2.61	120.36	115.83
7	A	710	97N	O1-C15-C14	2.52	119.81	111.91
3	A	703	Z9A	O01-C02-N03	-2.44	118.84	122.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	709	97N	O1-C15-C14	2.36	119.32	111.91
6	A	708	AV0	C3-C4-C5	2.34	114.41	110.24
3	A	703	Z9A	C20-C19-C18	-2.23	107.00	114.34
4	A	704	Z9G	O10-C09-C04	2.22	120.79	113.40
3	A	703	Z9A	C27-C21-C22	2.18	121.60	118.17
4	A	704	Z9G	O10-C09-O11	-2.03	119.48	124.09

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	708	AV0	O5-C1-O1-CBS
6	A	708	AV0	CBK-CBQ-CCM-CBS
6	A	708	AV0	O1-CBS-CCM-CBR
7	A	710	97N	O1-C16-C17-O2
7	A	711	97N	O2-C17-C18-O3
7	A	713	97N	C-C1-C2-C3
5	A	705	2PE	C23-C24-O25-C26
7	A	709	97N	C14-C15-O1-C16
7	A	710	97N	C14-C15-O1-C16
7	A	710	97N	O-C15-O1-C16
7	A	711	97N	C11-C10-C9-C8
6	A	708	AV0	O5-C5-C6-O6
7	A	709	97N	O-C15-O1-C16
7	A	710	97N	C11-C12-C13-C14
6	A	708	AV0	C4-C5-C6-O6
6	A	708	AV0	CBE-CBG-CBI-CBK
5	A	707	2PE	O4-C5-C6-O7
7	A	711	97N	O1-C16-C17-C18
5	A	706	2PE	O4-C5-C6-O7
7	A	711	97N	O1-C16-C17-O2
7	A	711	97N	C12-C13-C14-C15
7	A	709	97N	C10-C11-C12-C13
6	A	708	AV0	CBJ-CBL-CBR-CCM
7	A	709	97N	O1-C16-C17-O2
5	A	707	2PE	O7-C8-C9-O10
5	A	706	2PE	O1-C2-C3-O4
5	A	707	2PE	O1-C2-C3-O4
7	A	710	97N	C10-C11-C12-C13
7	A	710	97N	O1-C16-C17-C18
5	A	706	2PE	C5-C6-O7-C8
7	A	710	97N	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
7	A	711	97N	C16-C17-C18-O3
5	A	706	2PE	C2-C3-O4-C5
7	A	709	97N	C9-C10-C11-C12
6	A	708	AV0	O1-CBS-CCM-CBQ
7	A	711	97N	C9-C10-C11-C12
7	A	712	97N	C4-C5-C6-C7
7	A	712	97N	C3-C4-C5-C6
6	A	708	AV0	CBA-CBC-CBE-CBG
7	A	711	97N	C11-C12-C13-C14
6	A	708	AV0	CBF-CBH-CBJ-CBL
6	A	708	AV0	CAA-CAW-CAY-CBA
6	A	708	AV0	C2-C1-O1-CBS
7	A	712	97N	C-C1-C2-C3
7	A	712	97N	C6-C7-C8-C9
7	A	711	97N	C14-C15-O1-C16
3	A	703	Z9A	N03-C04-C05-C06
7	A	711	97N	O-C15-O1-C16
6	A	708	AV0	CAW-CAY-CBA-CBC
5	A	706	2PE	C8-C9-O10-C11
7	A	711	97N	C7-C8-C9-C10
6	A	708	AV0	CBK-CBQ-CCM-CBR
4	A	704	Z9G	C02-C12-C13-C14
6	A	708	AV0	CBC-CBE-CBG-CBI
5	A	706	2PE	C12-C11-O10-C9
6	A	708	AV0	CAY-CBA-CBC-CBE
5	A	707	2PE	C5-C6-O7-C8
6	A	708	AV0	CBD-CBF-CBH-CBJ
7	A	711	97N	C6-C7-C8-C9
7	A	712	97N	C1-C2-C3-C4
7	A	710	97N	C13-C14-C15-O1
7	A	709	97N	C7-C8-C9-C10
5	A	706	2PE	O10-C11-C12-O13
7	A	710	97N	C13-C14-C15-O
5	A	705	2PE	O25-C26-C27-O28
5	A	706	2PE	O7-C8-C9-O10
5	A	705	2PE	O22-C23-C24-O25

There are no ring outliers.

2 monomers are involved in 4 short contacts:

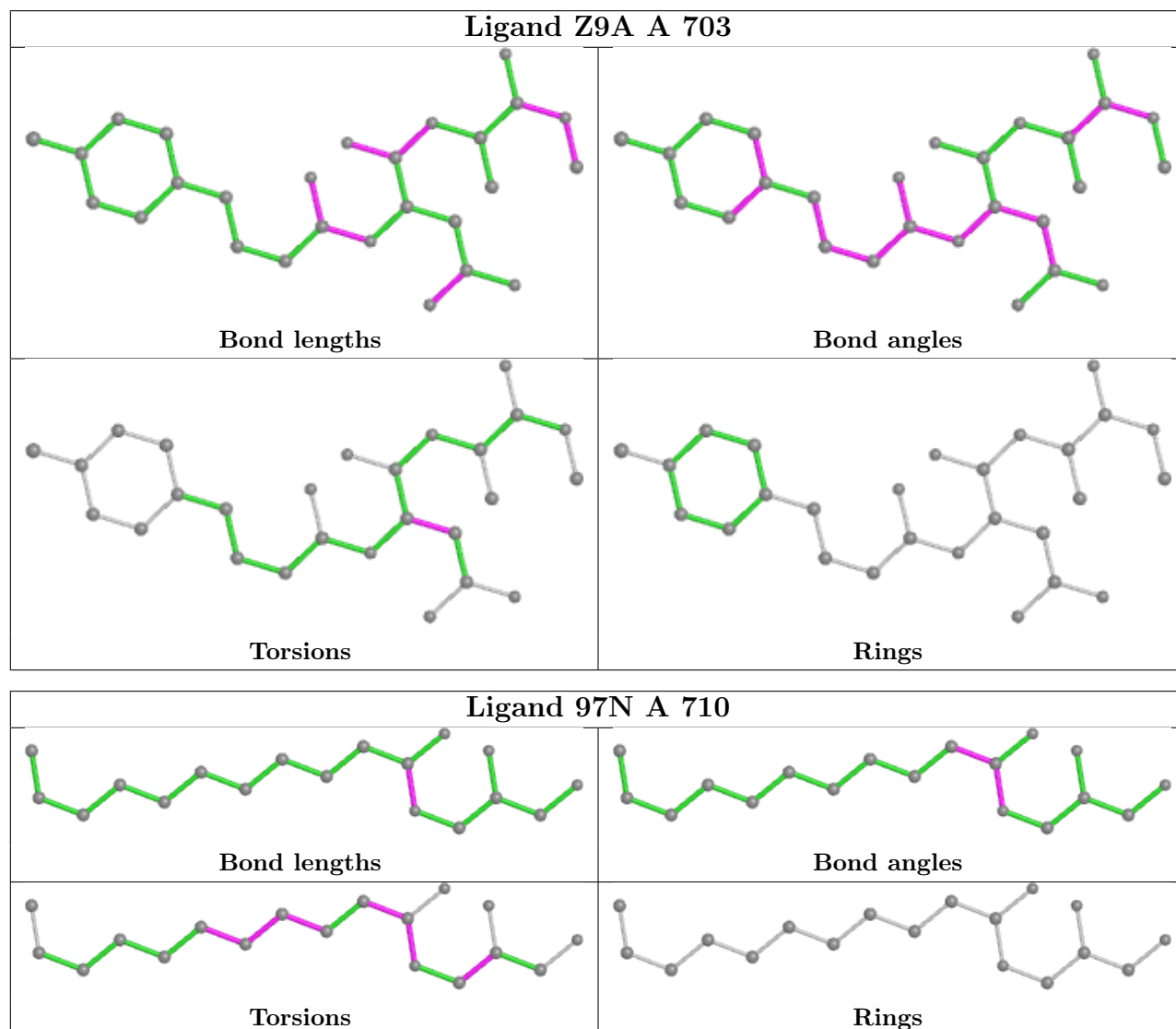
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	714	SO4	1	0

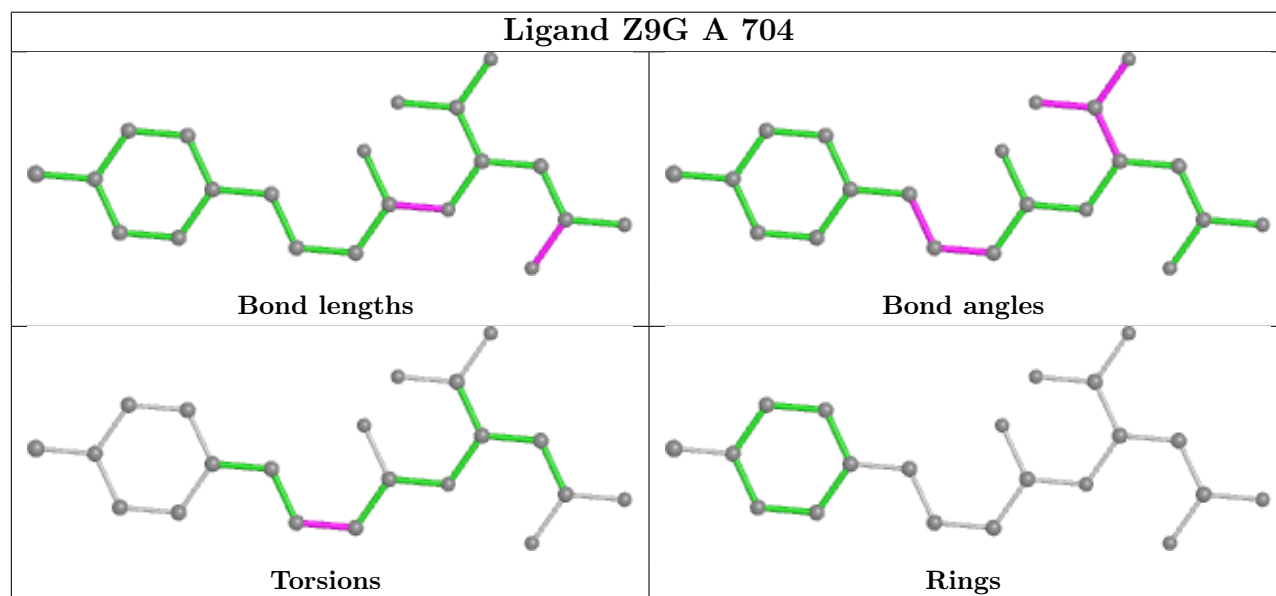
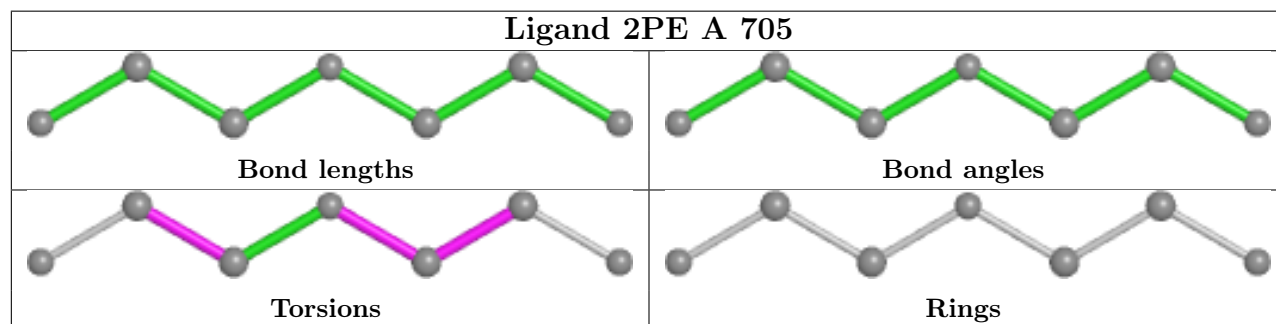
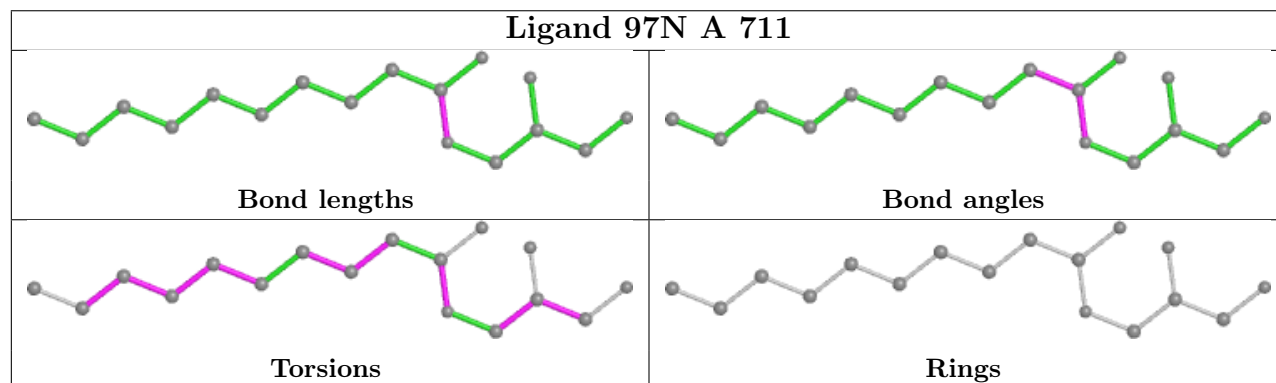
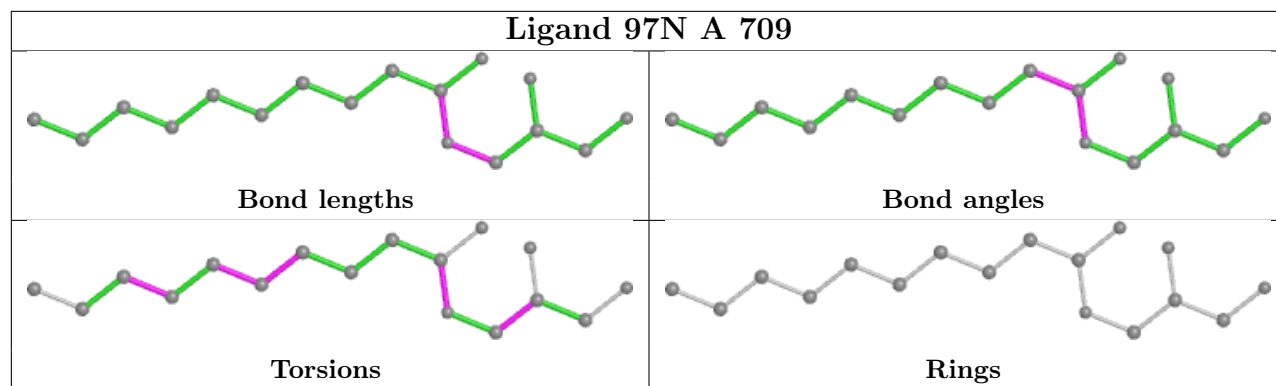
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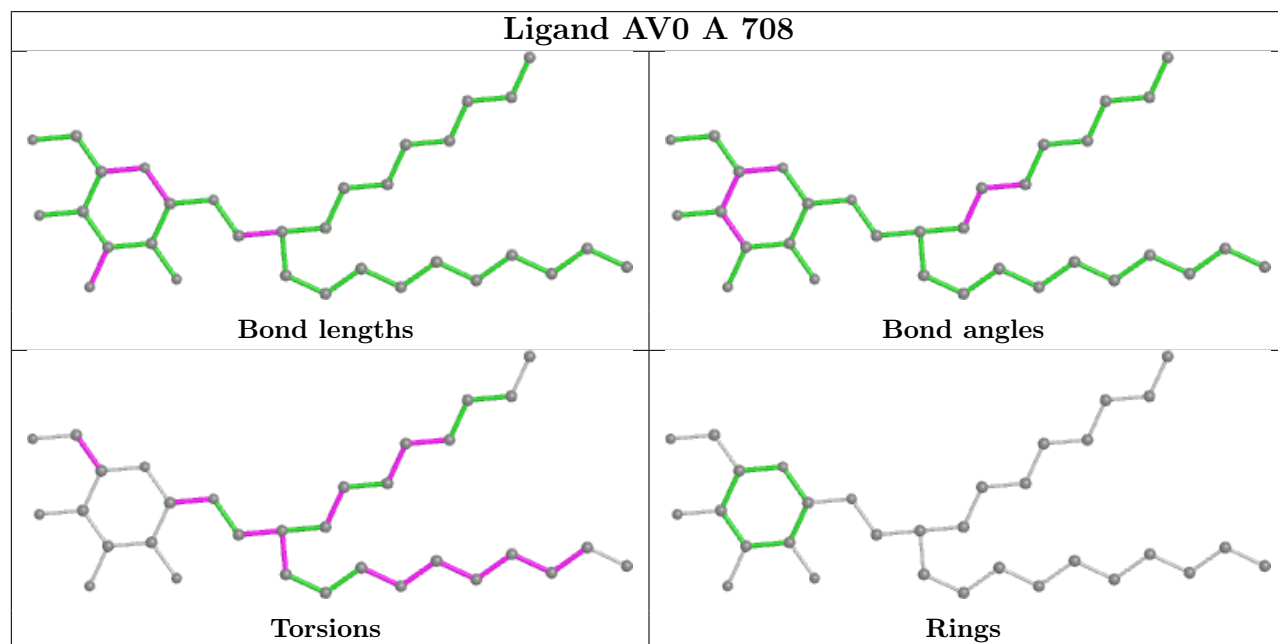
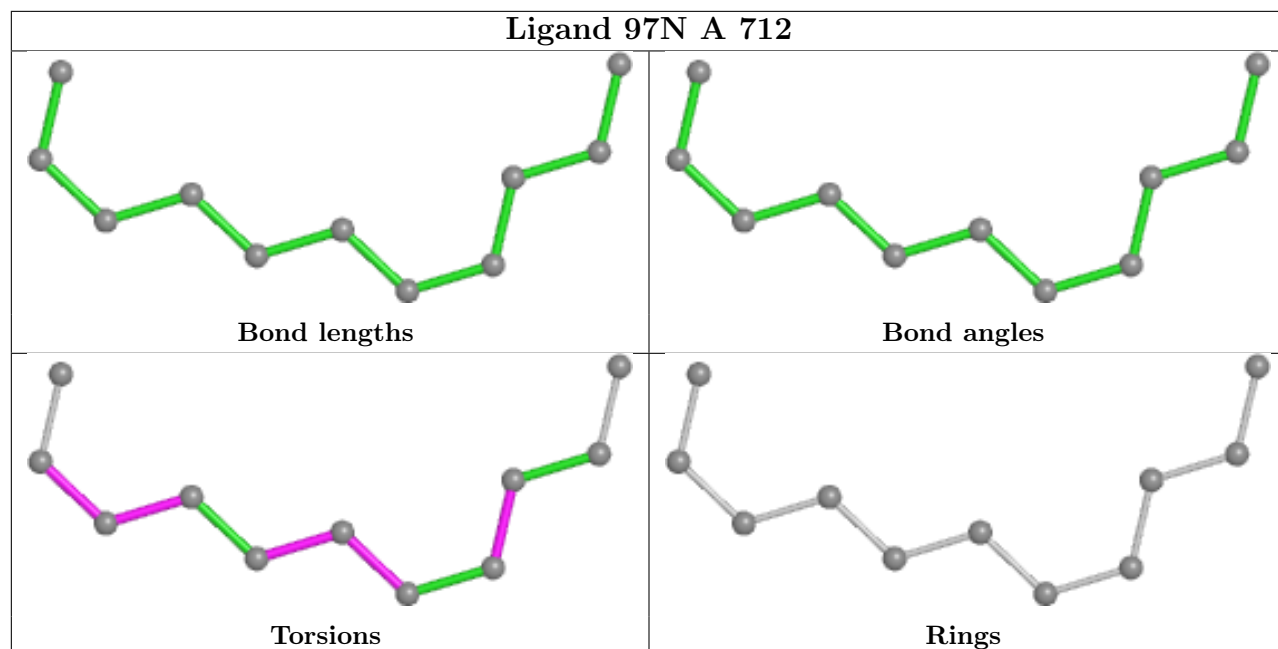
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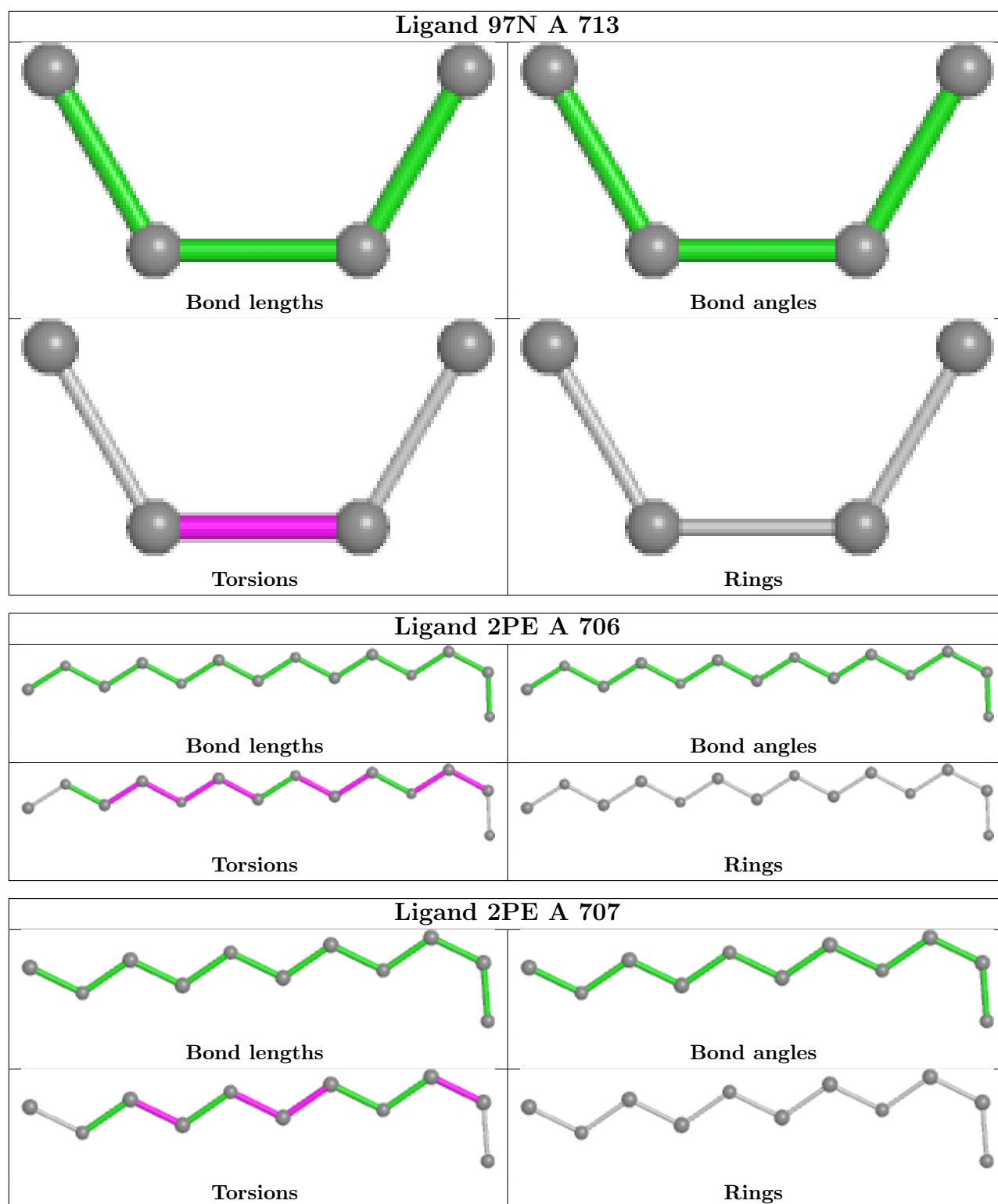
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	706	2PE	3	0

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 ⓘ

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	453/480 (94%)	0.27	42 (9%) 8 11	26, 43, 150, 208	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	428	LEU	11.5
1	A	418	HIS	11.3
1	A	416	THR	10.9
1	A	410	PHE	8.4
1	A	413	TYR	7.8
1	A	417	ALA	7.4
1	A	427	ARG	6.7
1	A	436	ALA	6.7
1	A	415	ALA	6.2
1	A	430	VAL	5.4
1	A	406	VAL	4.5
1	A	496	LEU	4.4
1	A	429	ARG	4.4
1	A	412	VAL	3.8
1	A	435	ILE	3.8
1	A	431	ARG	3.7
1	A	403	VAL	3.7
1	A	485	LEU	3.7
1	A	434	ILE	3.6
1	A	282	ALA	3.4
1	A	453	ILE	3.4
1	A	494	ILE	3.4
1	A	432	ASP	3.3
1	A	495	LEU	3.3
1	A	486	THR	3.2
1	A	414	ARG	3.2
1	A	437	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	439	VAL	2.8
1	A	484	VAL	2.8
1	A	409	ALA	2.7
1	A	440	PRO	2.6
1	A	446	MET	2.4
1	A	80	ALA	2.4
1	A	404	VAL	2.4
1	A	493	ARG	2.4
1	A	492	LYS	2.3
1	A	477	GLY	2.2
1	A	408	GLY	2.2
1	A	396	LEU	2.2
1	A	490	GLN	2.1
1	A	444	ALA	2.1
1	A	433	TYR	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 monosaccharides 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
5	2PE	A	707	11/28	0.64	0.41	99,112,118,123	0
7	97N	A	713	4/23	0.65	0.17	100,100,109,117	0
7	97N	A	712	11/23	0.66	0.47	90,98,102,102	0
7	97N	A	711	17/23	0.67	0.45	91,100,127,127	0
9	CL	A	716	1/1	0.69	0.15	115,115,115,115	0
7	97N	A	710	18/23	0.76	0.36	78,104,118,118	0
7	97N	A	709	17/23	0.77	0.31	77,99,118,121	0
6	AV0	A	708	32/69	0.79	0.25	45,92,112,117	0

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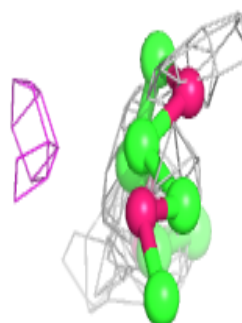
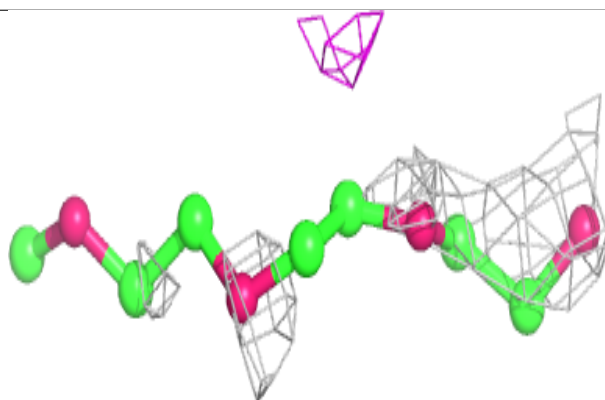
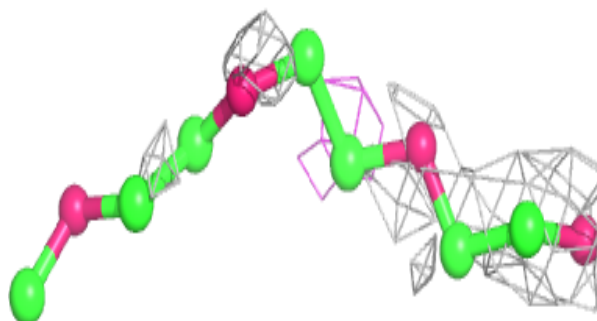
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	CL	A	715	1/1	0.81	0.09	76,76,76,76	0
3	Z9A	A	703	27/27	0.82	0.17	38,58,70,79	1
5	2PE	A	706	14/28	0.84	0.24	69,89,108,112	0
5	2PE	A	705	7/28	0.89	0.26	52,68,83,85	0
4	Z9G	A	704	21/21	0.93	0.14	32,41,56,63	1
9	CL	A	717	1/1	0.96	0.08	71,71,71,71	0
8	SO4	A	714	5/5	0.97	0.08	61,80,87,88	0
2	DMS	A	702	4/4	0.97	0.17	38,48,49,52	0
2	DMS	A	701	4/4	0.99	0.18	26,28,39,55	0

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

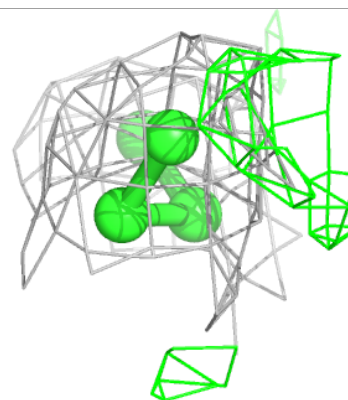
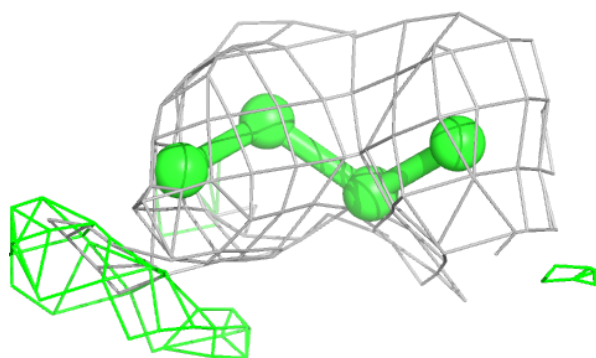
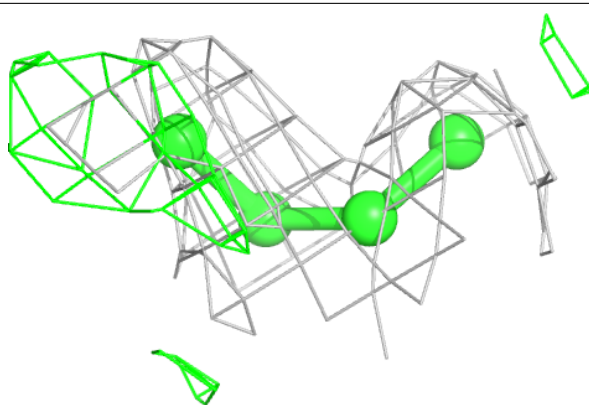
Electron density around 2PE A 707:

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

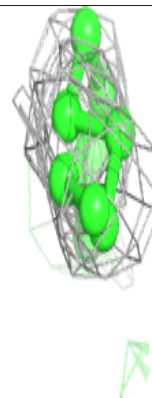
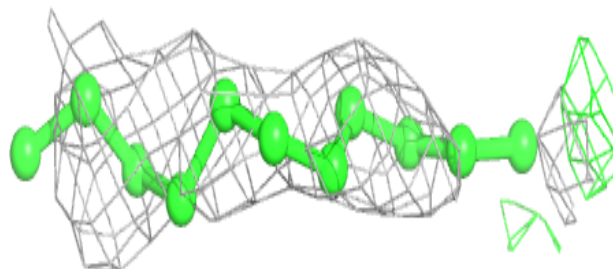
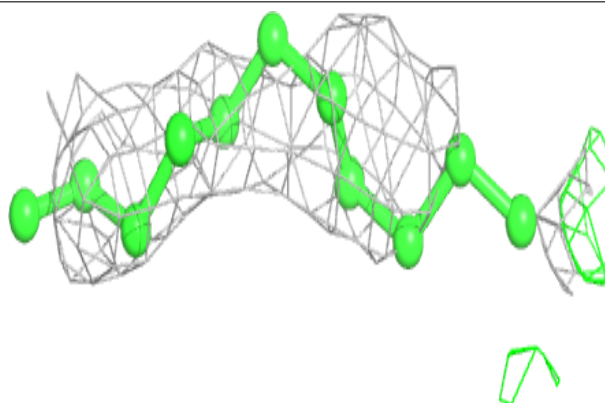


Electron density around 97N A 713:

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

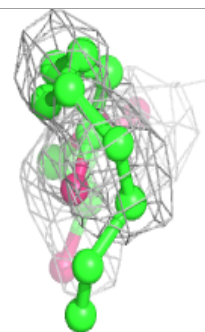
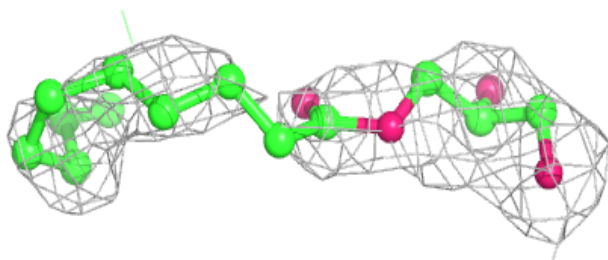
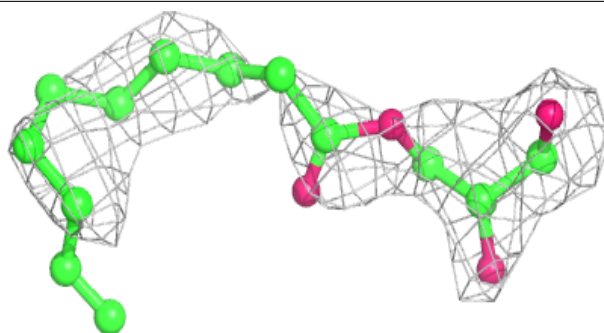
**Electron density around 97N A 712:**

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

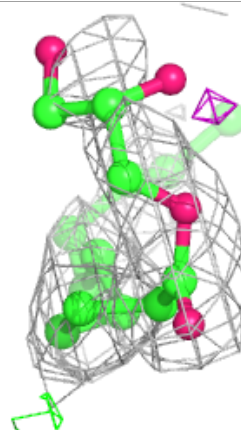
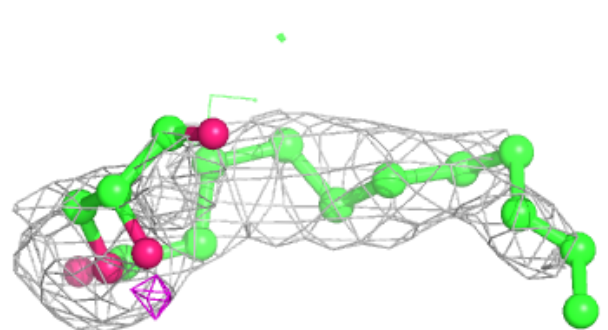
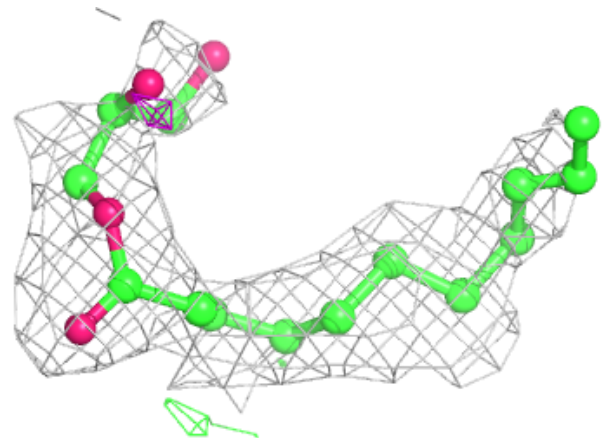


Electron density around 97N A 711:

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

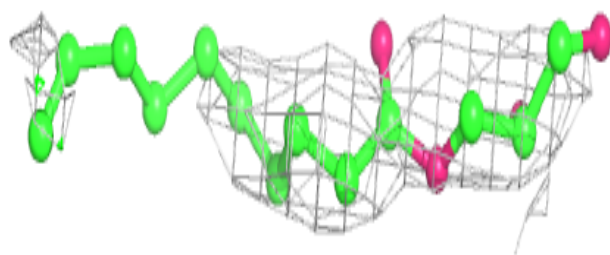
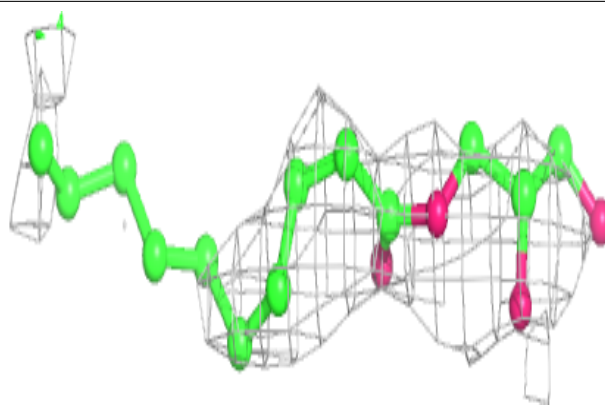
**Electron density around 97N A 710:**

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

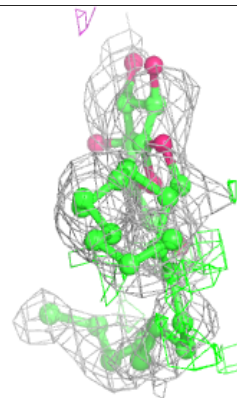
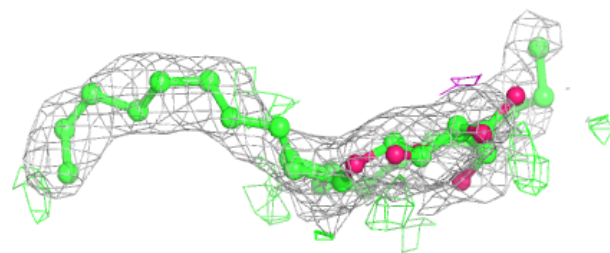
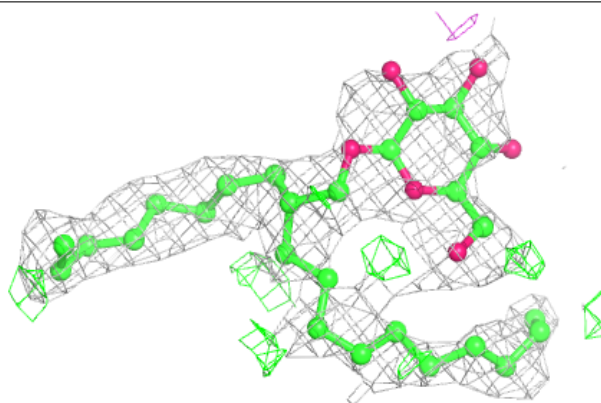


Electron density around 97N A 709:

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

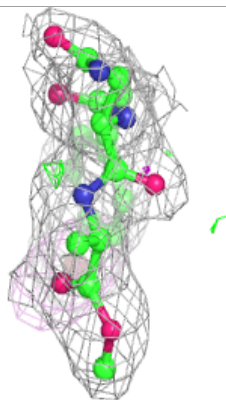
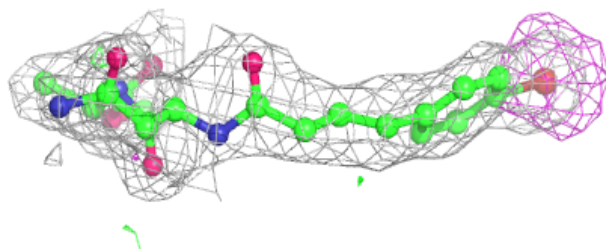
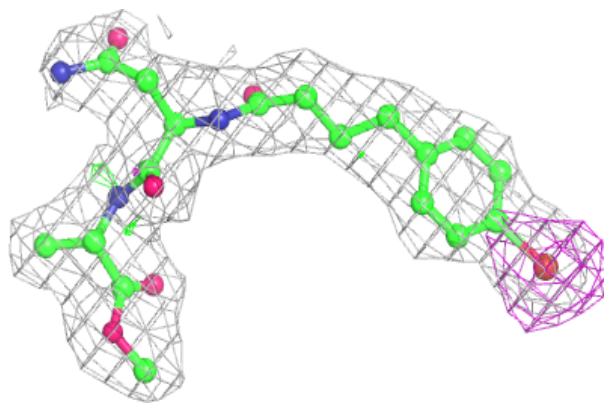
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$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

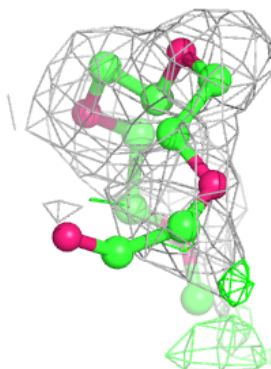
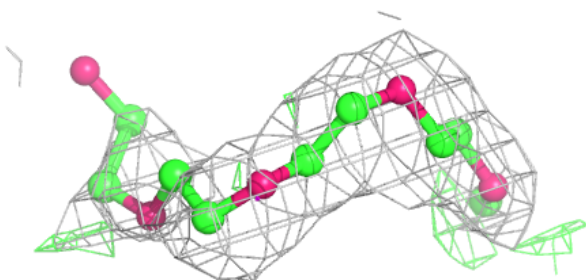
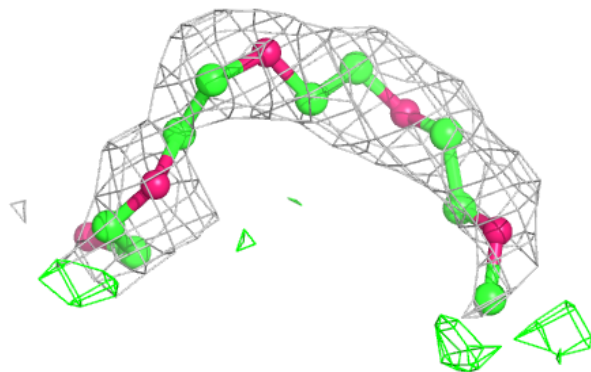


Electron density around Z9A A 703:

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and green (positive)

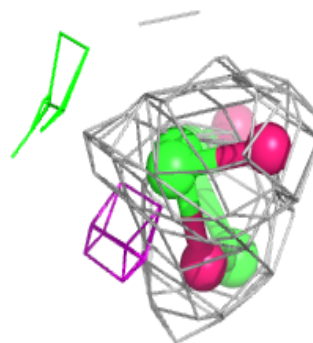
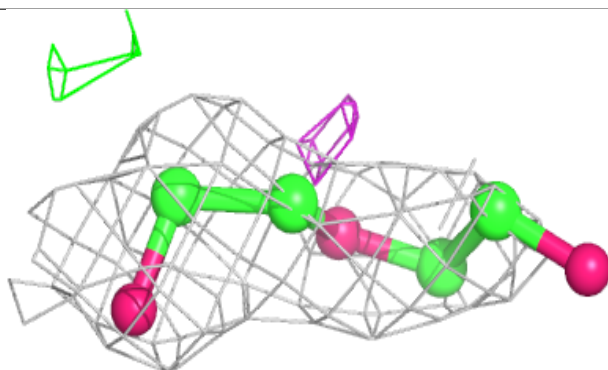
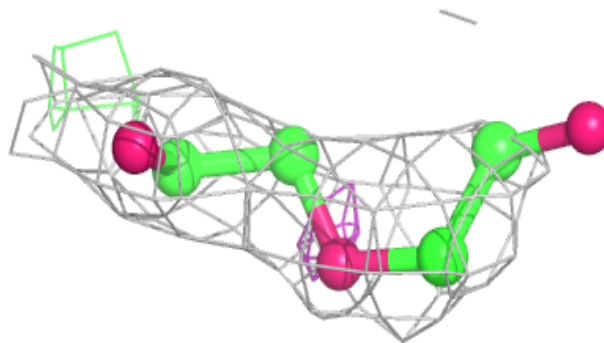
**Electron density around 2PE A 706:**

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and green (positive)

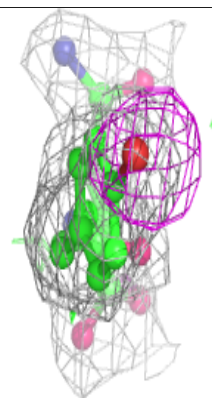
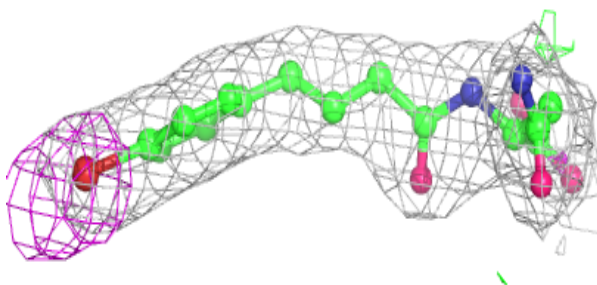
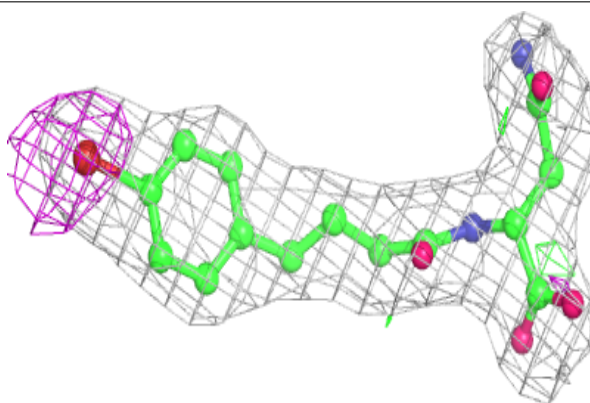


Electron density around 2PE A 705:

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

**Electron density around Z9G A 704:**

$2mF_o-DF_c$ (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.