



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 03:15 AM UTC

PDB ID : 1GNJ / pdb_00001gnj
Title : HUMAN SERUM ALBUMIN COMPLEXED WITH cis-5,8,11,14-EICOSAT
ETRAENOIC ACID (ARACHIDONIC ACID)
Authors : Petitpas, I.; Gruene, T.; Bhattacharya, A.A.; Curry, S.
Deposited on : 2001-10-05
Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

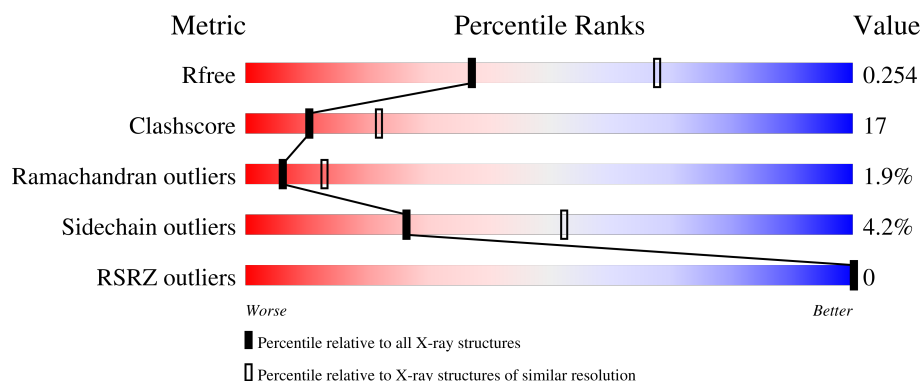
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	585	 65% 30% . .

2 Entry composition [i](#)

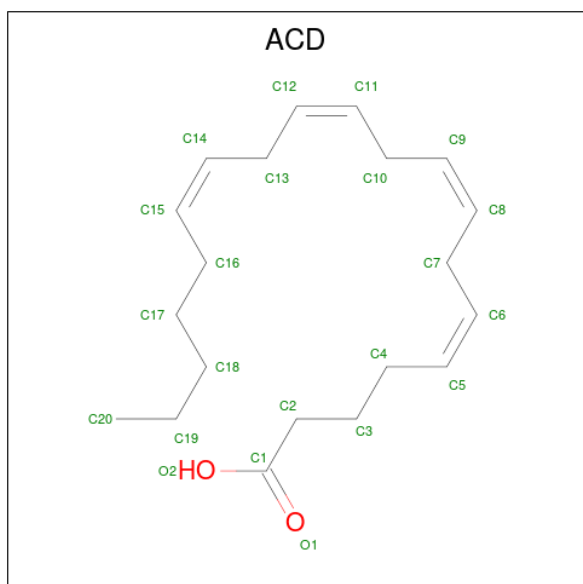
There are 3 unique types of molecules in this entry. The entry contains 4679 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SERUM ALBUMIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	582	Total	C	N	O	S	0	0	0
			4520	2858	762	859	41			

- Molecule 2 is ARACHIDONIC ACID (CCD ID: ACD) (formula: $C_{20}H_{32}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			22	20	2		
2	A	1	Total	C	O	0	0
			22	20	2		
2	A	1	Total	C	O	0	0
			22	20	2		
2	A	1	Total	C	O	0	0
			22	20	2		
2	A	1	Total	C	O	0	0
			22	20	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 22 20 2	0	0
2	A	1	Total C 13 13	0	0
2	A	1	Total C O 5 3 2	0	0

- Molecule 3 is water.

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

- Molecule 1: SERUM ALBUMIN

K557	A449	Y370	D256			ASP
C558	E450	A371	R257			ALA
C559	L453	K372	L260			H3
A561	L457	F374	A261			V7
D562	M458	K378	K262			
D563	K459	P379	V263			R10
K564	L460	L380				
E565	C461	V381	E266			L14
T566						
C567	V469	K382	K281			L139
F568		K383	P282			L31
A582	E479	P384	L283			K32
L583	S480	K385	L284			Q33
G584	L482	K386				
LEU	L481	L387	S287			F36
	N483	K388	A291			E37
	R484	K389	E292			D38
	P486	Q390				H39
		E393	E297			F49
		L394	N298			
	Y497	F395	P299			T52
			A300			
F509		L398	D301			A59
H510		G399	L302			E60
A511		A400	F303			N61
D512		Y401	S304			C62
E513		K402	L305			D63
C514		F403				K64
T515		Q404	K313			L69
L516		L407	D314			
E517		L408	V315			S193
K519		Y409	K323			K73
E520		R410				L74
R521		Y411	K329			C75
S522		L412	F330			T76
I523		K413	L331			V77
		K414	Y332			R81
Q526		V415	E333			
		F416				Y84
K536		Y417	K336			G85
T540		Y418	K337			
K541		S419	P338			D89
E542			K339			
Q543		L423	V344			E95
L544		V424	K348			P96
K545		E425				E97
A546		V426	K348			R98
V547		S427	K351			
M548		R428				F102
		Y429	C360			L103
		L430				
F551		A552	A364			R114
A553		V433	D365			L115
F554		G434	K366			V116
V555		S435	H367			R117
F556						P118
						F119

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	190.22Å 38.97Å 96.24Å 90.00° 105.75° 90.00°	Depositor
Resolution (Å)	29.62 – 2.60 29.62 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.9 (29.62-2.60) 95.0 (29.62-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 2.61Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.194 , 0.245 0.212 , 0.254	Depositor DCC
R_{free} test set	971 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	61.0	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4679	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.64% 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: ACD

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	0.48	0/4610	0.96	21/6241 (0.3%)

There are no bond length outliers.

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	298	MET	CA-C-N	7.74	129.52	119.84
1	A	298	MET	C-N-CA	7.74	129.52	119.84
1	A	313	LYS	N-CA-C	-7.16	101.08	110.53
1	A	323	LYS	N-CA-C	6.89	119.38	111.11
1	A	206	PHE	N-CA-C	6.40	120.19	112.38

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	4520	0	4326	154	0
2	A	150	0	204	10	0
3	A	9	0	0	3	0
All	All	4679	0	4530	155	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 17.

The worst 5 of 155 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:558:CYS:HB3	1:A:568:PHE:CE1	2.13	0.82
1:A:424:VAL:O	1:A:428:ARG:HG3	1.79	0.80
1:A:479:GLU:HG3	1:A:483:ASN:HB2	1.66	0.77
1:A:73:LYS:O	1:A:76:THR:HB	1.86	0.74
1:A:351:LYS:O	1:A:351:LYS:HE3	1.88	0.73

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	580/585 (99%)	526 (91%)	43 (7%)	11 (2%)	6 13

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	565	GLU
1	A	367	HIS
1	A	557	LYS
1	A	564	LYS
1	A	205	LYS

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	477/511 (93%)	457 (96%)	20 (4%)	26	52

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	408	LEU
1	A	453	LEU
1	A	482	VAL
1	A	460	LEU
1	A	185	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	267	ASN
1	A	268	GLN
1	A	458	ASN
1	A	390	GLN
1	A	105	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

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	ACD	A	1005	-	21,21,21	0.97	0	21,21,21	0.55	0
2	ACD	A	1008	-	4,4,21	0.99	0	4,4,21	0.65	0
2	ACD	A	1007	-	12,12,21	0.97	0	11,11,21	0.31	0
2	ACD	A	1002	-	21,21,21	0.95	0	21,21,21	0.48	0
2	ACD	A	1003	-	21,21,21	0.94	0	21,21,21	0.50	0
2	ACD	A	1004	-	21,21,21	0.97	1 (4%)	21,21,21	0.55	0
2	ACD	A	1006	-	21,21,21	0.99	0	21,21,21	0.45	0
2	ACD	A	1001	-	21,21,21	0.94	0	21,21,21	0.53	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	ACD	A	1005	-	-	5/19/19/19	-
2	ACD	A	1008	-	-	2/2/2/19	-
2	ACD	A	1007	-	-	3/10/10/19	-
2	ACD	A	1002	-	-	5/19/19/19	-
2	ACD	A	1003	-	-	9/19/19/19	-
2	ACD	A	1004	-	-	6/19/19/19	-
2	ACD	A	1006	-	-	9/19/19/19	-
2	ACD	A	1001	-	-	11/19/19/19	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1004	ACD	C12-C11	2.05	1.43	1.31

There are no bond angle outliers.

There are no chirality outliers.

5 of 50 torsion outliers are listed below:

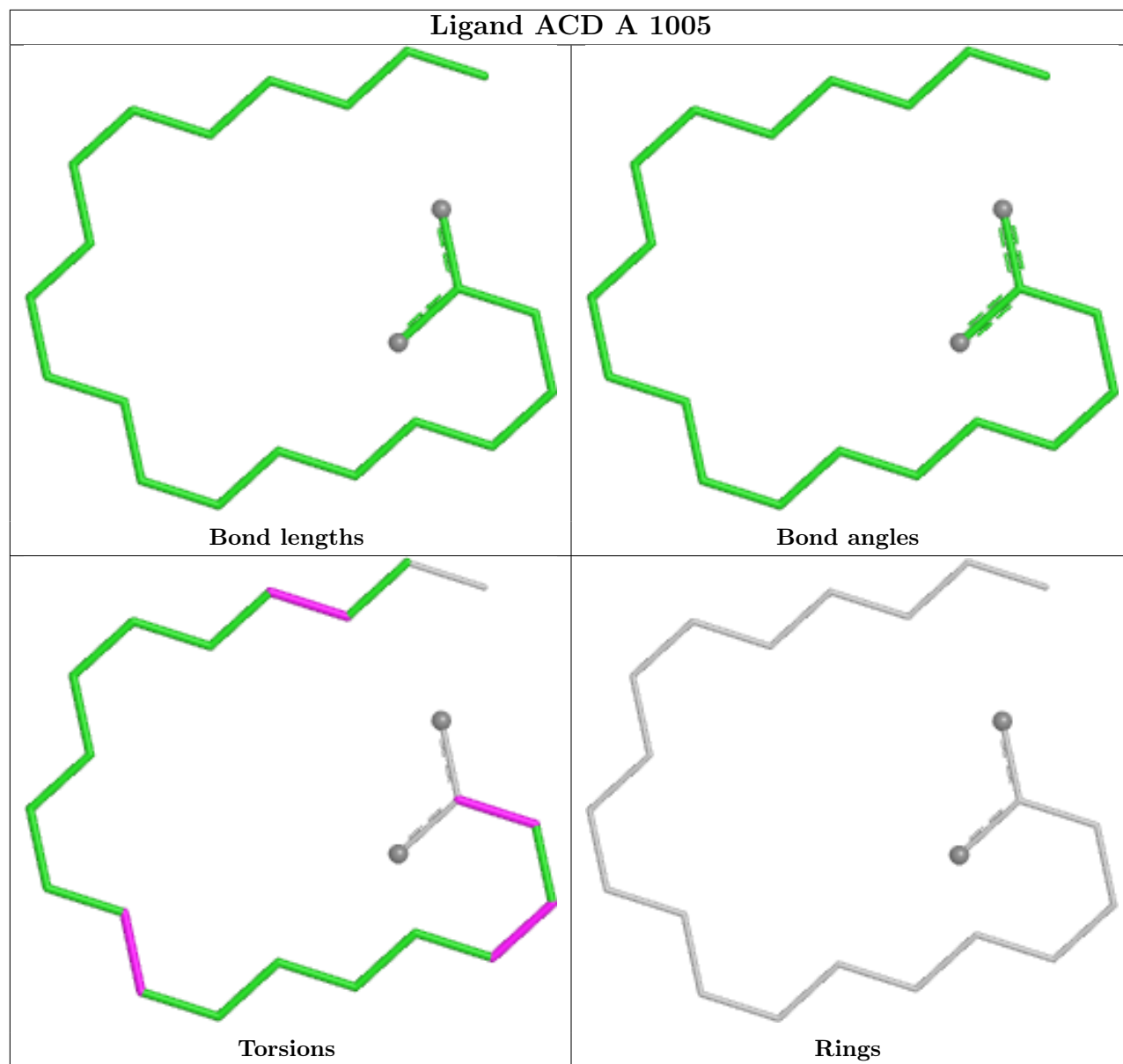
Mol	Chain	Res	Type	Atoms
2	A	1007	ACD	C11-C10-C9-C8
2	A	1002	ACD	C1-C2-C3-C4
2	A	1001	ACD	C1-C2-C3-C4
2	A	1006	ACD	C1-C2-C3-C4
2	A	1004	ACD	C16-C17-C18-C19

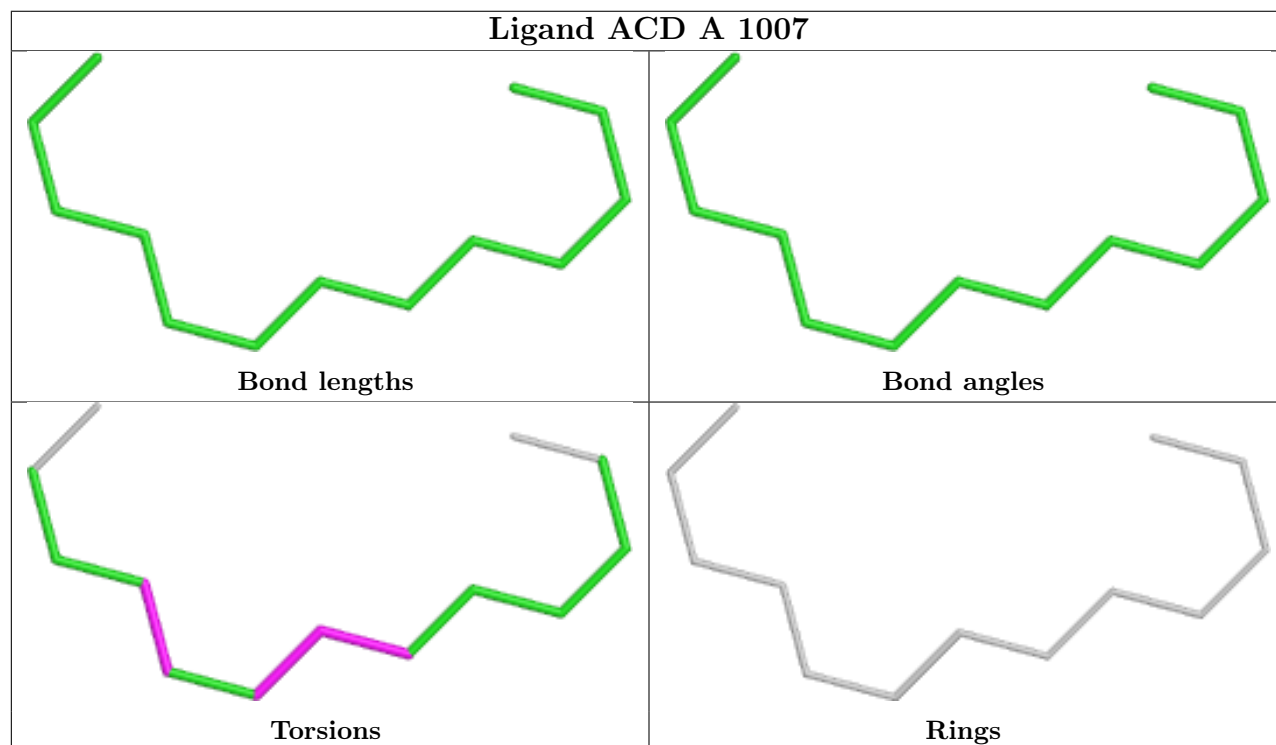
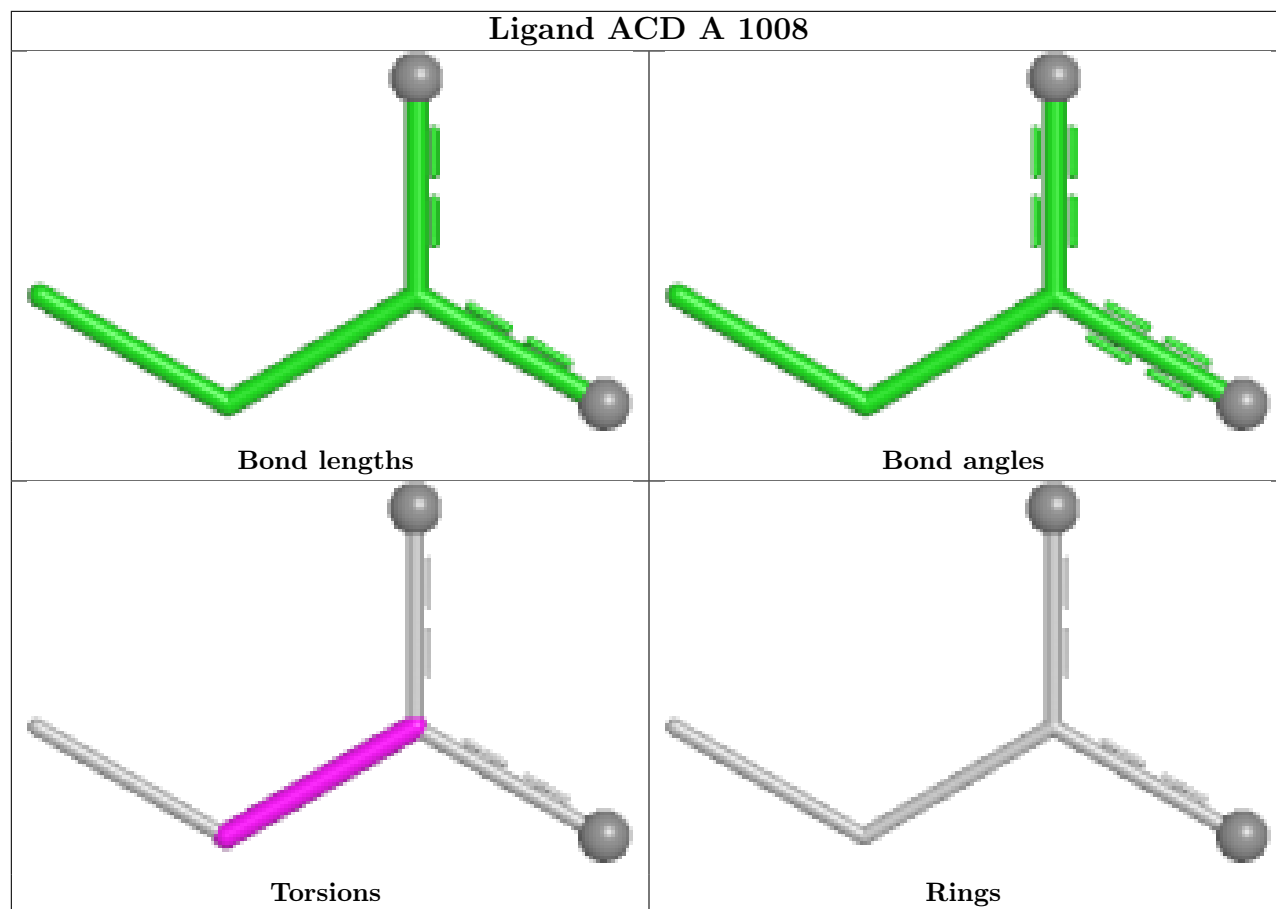
There are no ring outliers.

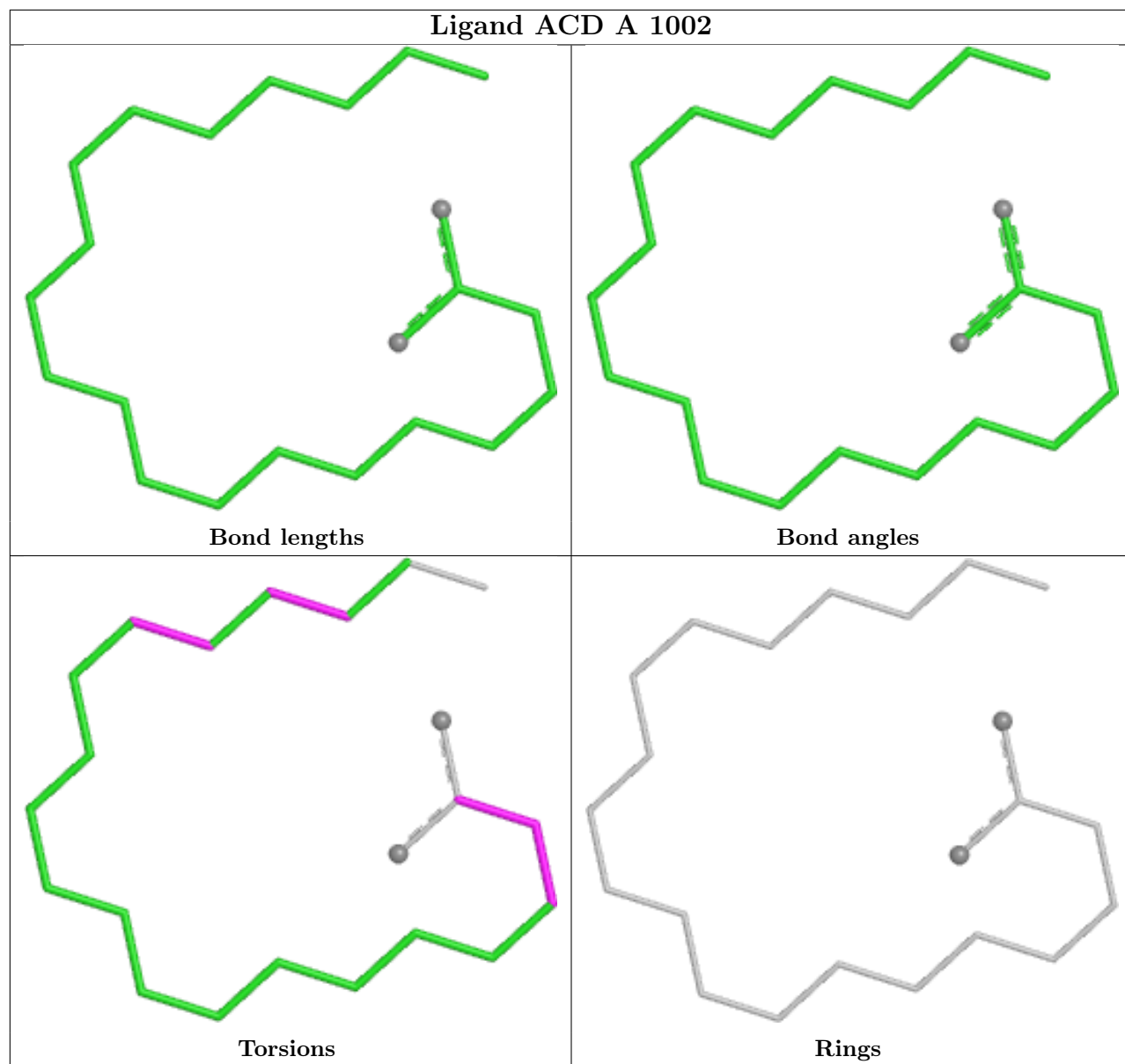
7 monomers are involved in 10 short contacts:

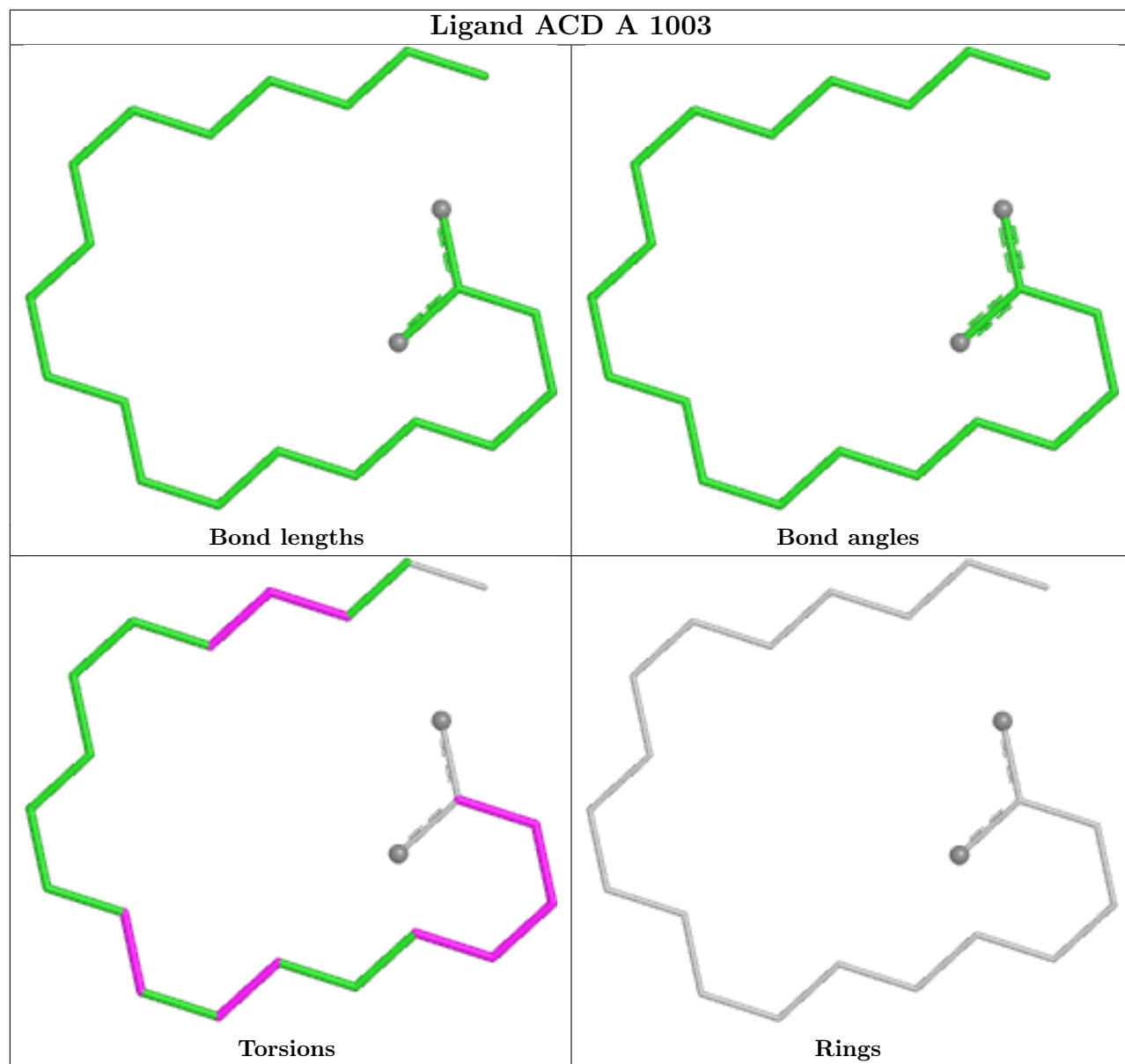
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1005	ACD	1	0
2	A	1008	ACD	1	0
2	A	1007	ACD	1	0
2	A	1002	ACD	2	0
2	A	1003	ACD	2	0
2	A	1004	ACD	1	0
2	A	1001	ACD	2	0

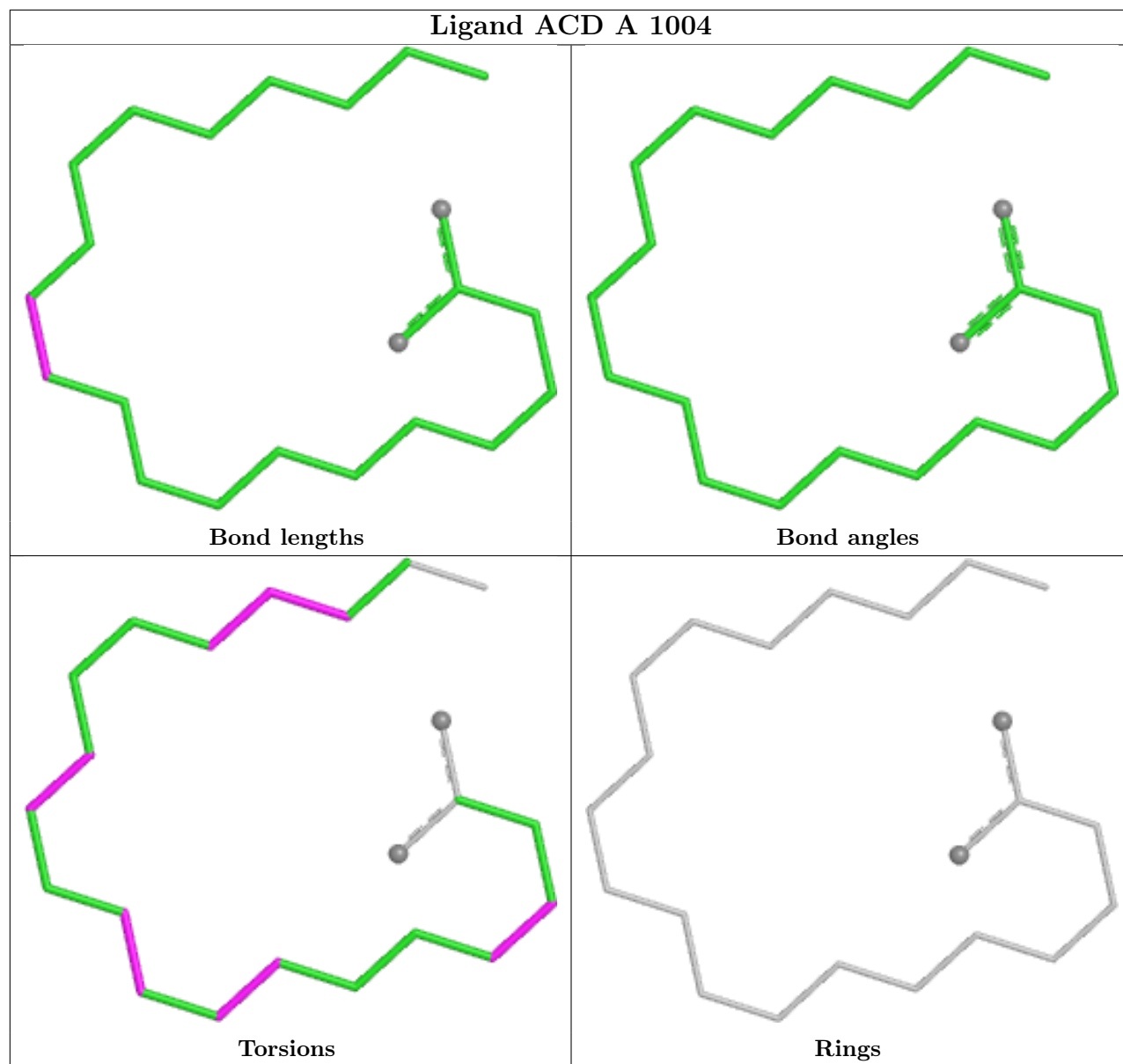
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

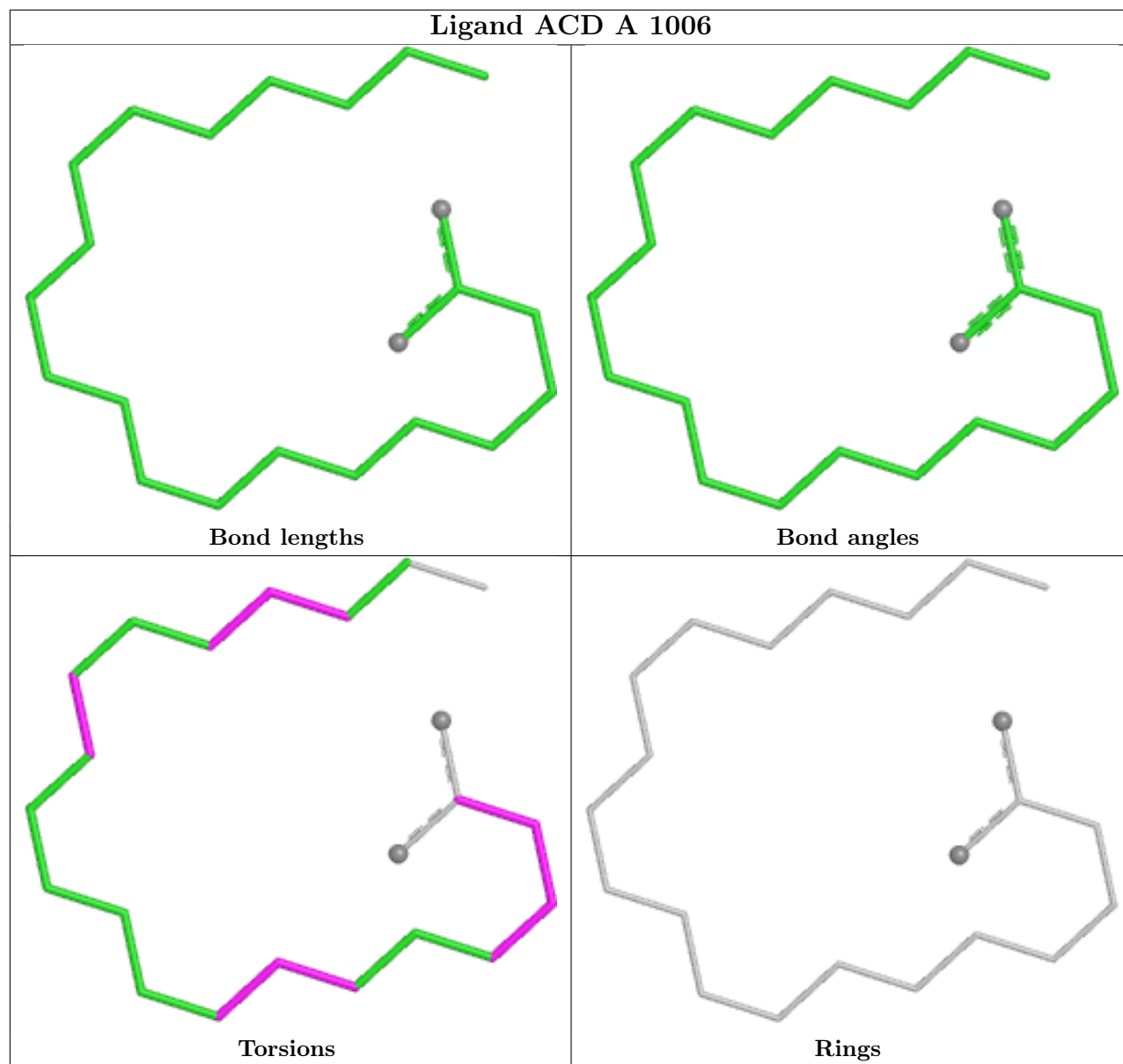


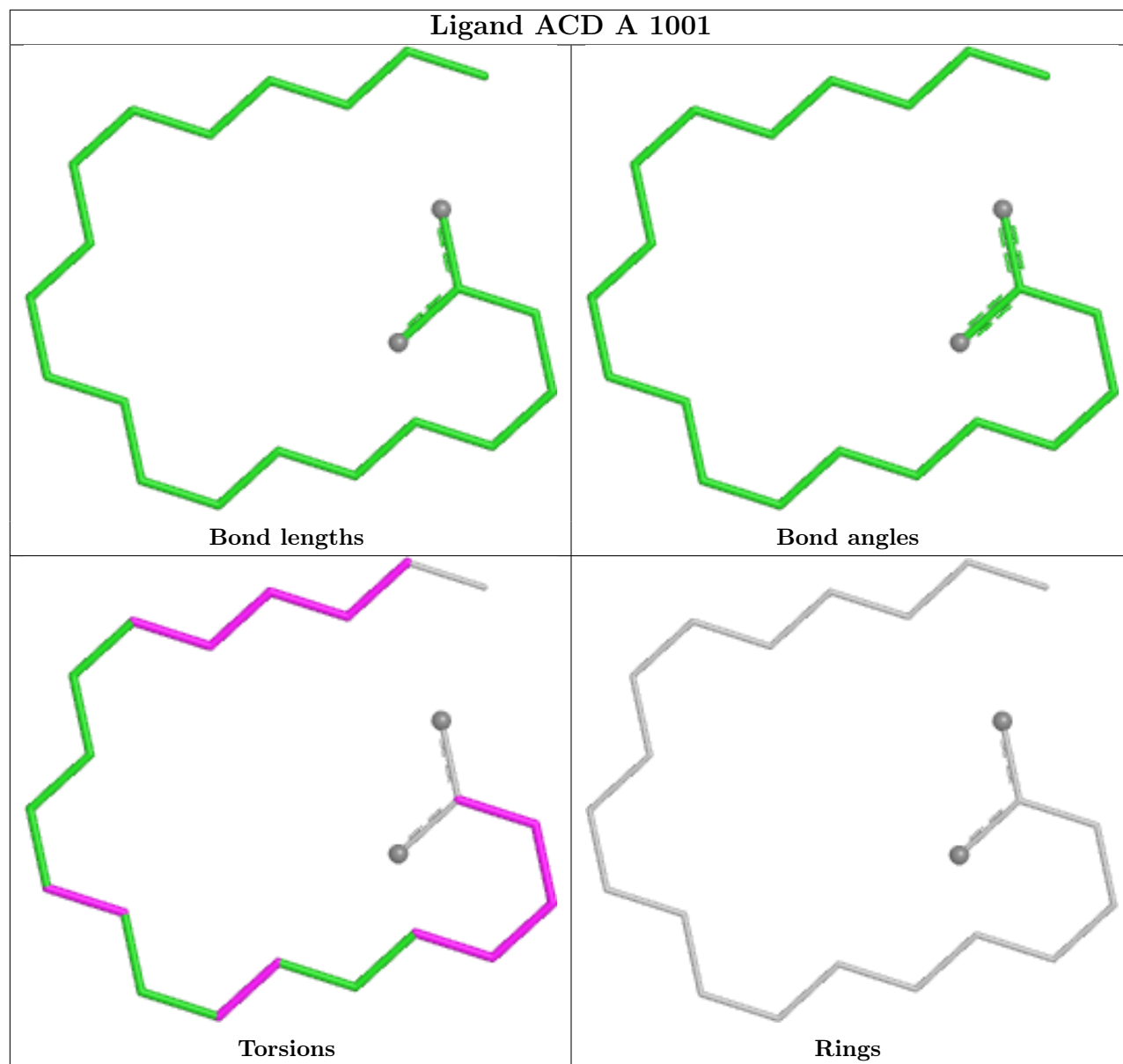












5.7 Other polymers [i](#)

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	582/585 (99%)	-0.48	0 100 100	34, 60, 89, 108	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

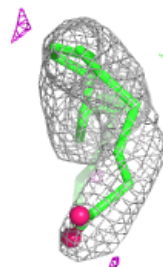
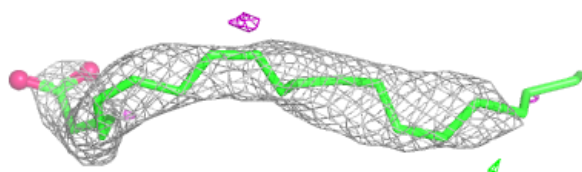
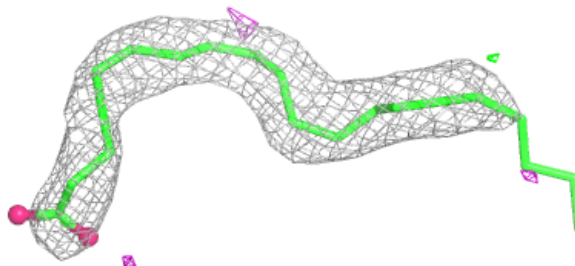
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ACD	A	1006	22/22	0.89	0.16	66,70,84,86	0
2	ACD	A	1007	13/22	0.89	0.15	66,69,72,73	0
2	ACD	A	1004	22/22	0.90	0.18	75,85,93,94	0
2	ACD	A	1005	22/22	0.90	0.15	72,79,93,94	0
2	ACD	A	1001	22/22	0.91	0.12	64,71,82,82	0
2	ACD	A	1008	5/22	0.92	0.13	94,94,96,97	0
2	ACD	A	1002	22/22	0.93	0.15	60,74,90,91	0
2	ACD	A	1003	22/22	0.95	0.12	51,60,62,64	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.

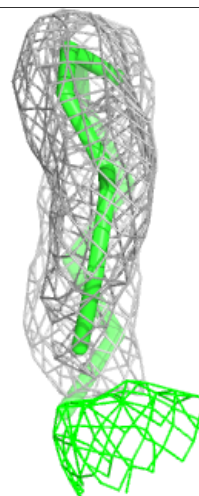
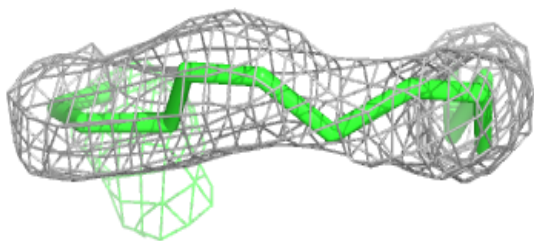
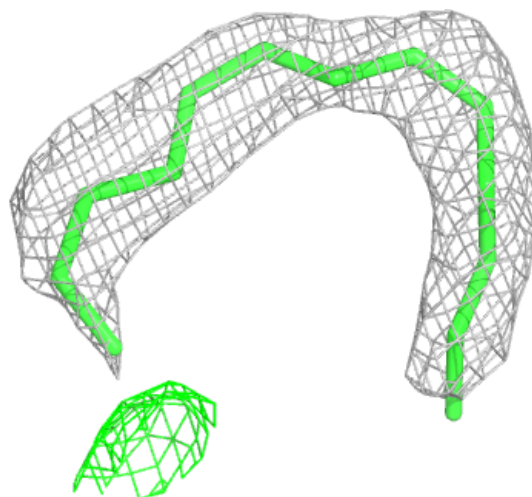
Electron density around ACD A 1006:

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



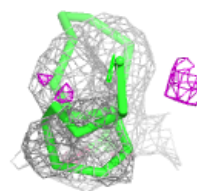
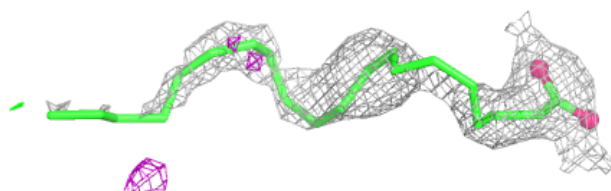
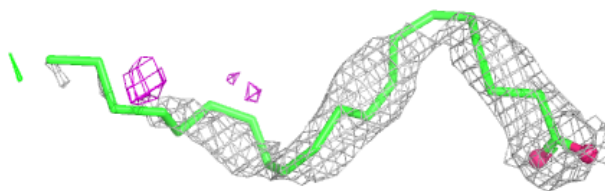
Electron density around ACD A 1007:

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

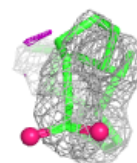
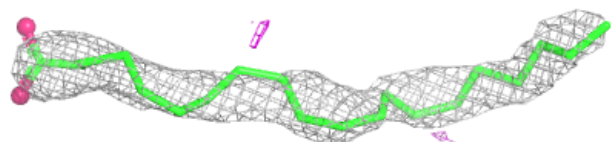
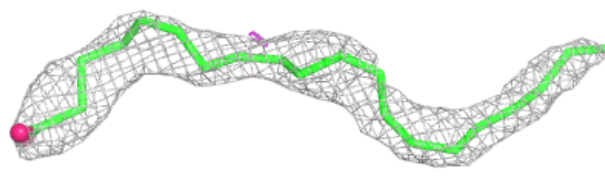


Electron density around ACD A 1004:

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

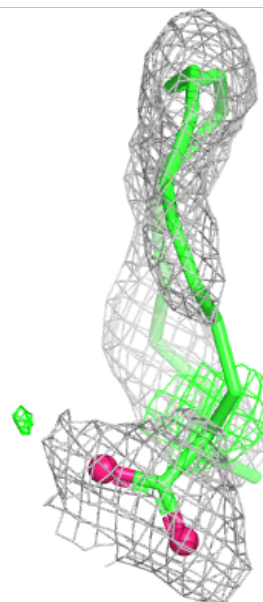
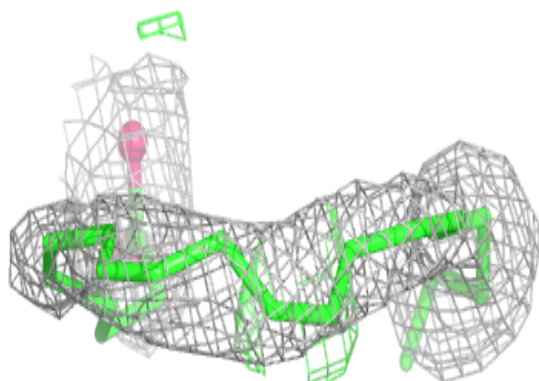
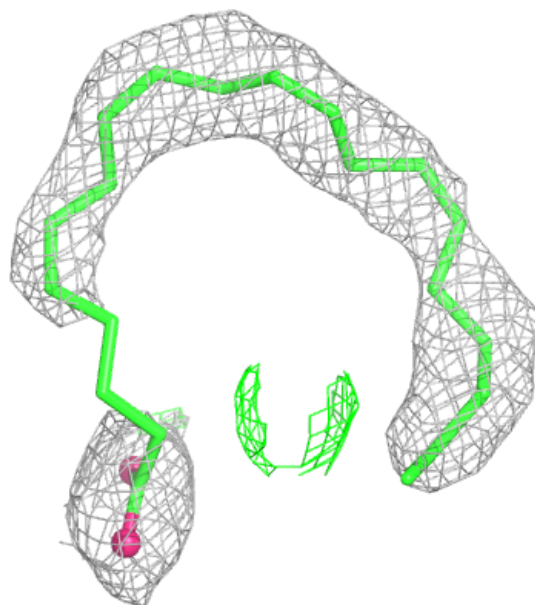
**Electron density around ACD A 1005:**

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



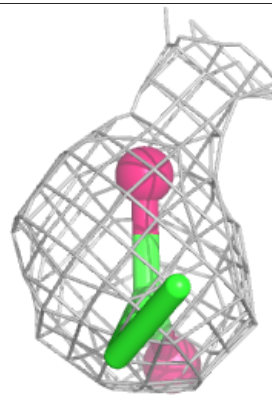
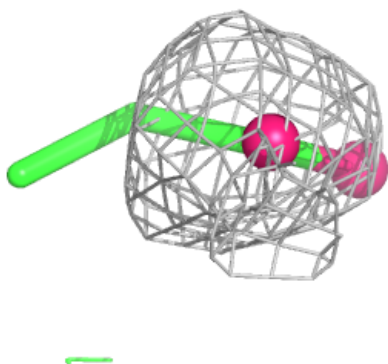
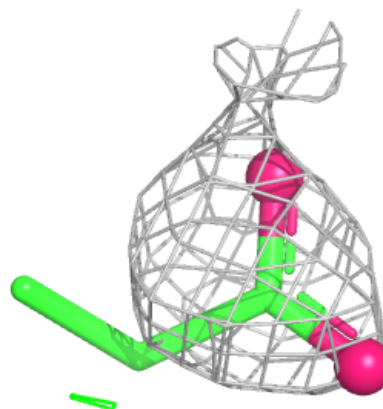
Electron density around ACD A 1001:

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

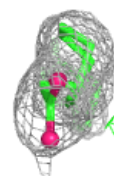
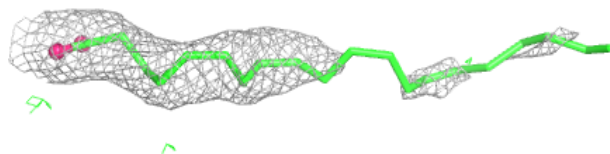
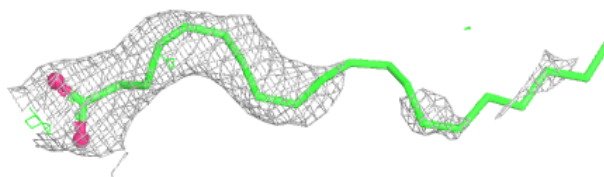


Electron density around ACD A 1008:

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

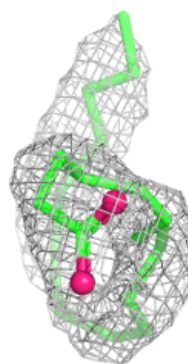
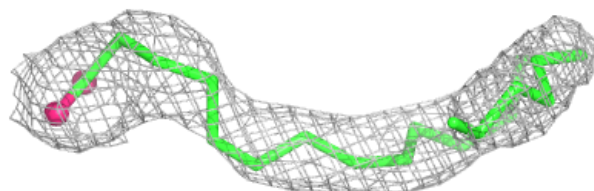
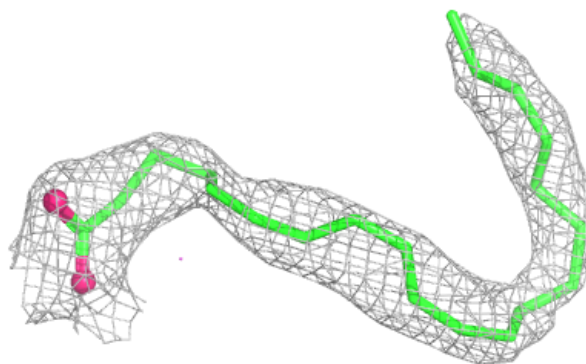
**Electron density around ACD A 1002:**

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



Electron density around ACD A 1003:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.