



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:01 AM UTC

PDB ID : 5IUX / pdb_00005iux
Title : GLIC-V135C bimane labelled X-ray structure
Authors : Fourati, Z.; Menny, A.; Delarue, M.
Deposited on : 2016-03-18
Resolution : 2.60 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

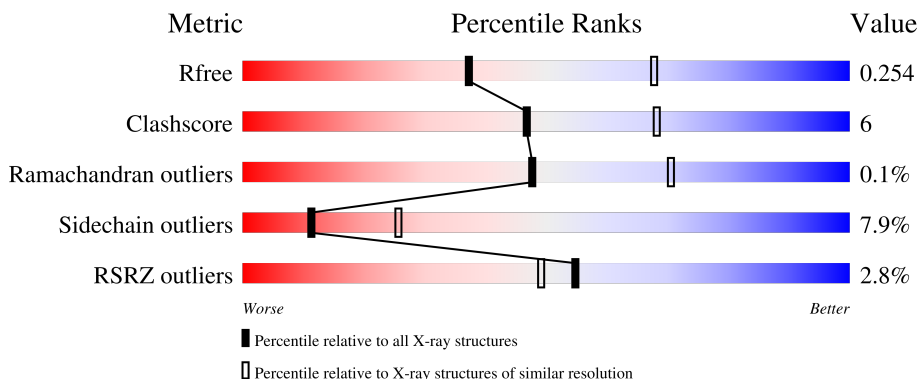
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	317	4% 82% 14% ..
1	B	317	2% 80% 17% ..
1	C	317	2% 74% 23% ...
1	D	317	3% 80% 16% ..
1	E	317	3% 78% 19% ..

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
4	ACT	A	505	-	-	X	-
4	ACT	A	509	-	-	X	-
4	ACT	A	510	-	-	X	-
4	ACT	B	607	-	-	X	-
4	ACT	C	608	-	-	X	-
4	ACT	D	608	-	-	X	-
4	ACT	E	401	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 13699 atoms, of which 52 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.

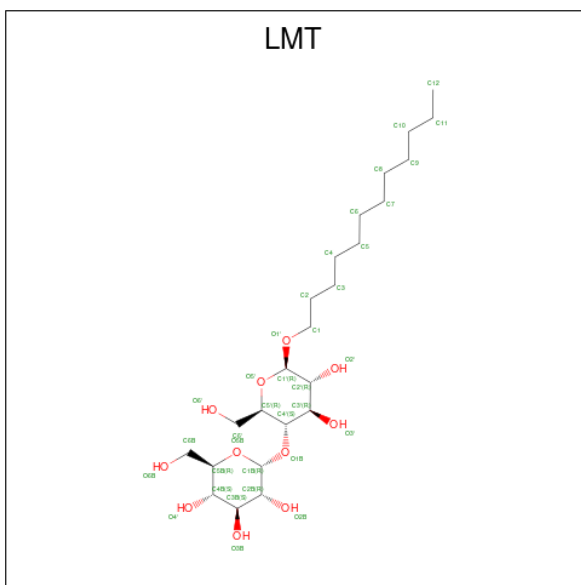
- Molecule 1 is a protein called Proton-gated ion channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	S	0	0	0
			2524	1662	404	454	4			
1	B	311	Total	C	N	O	S	0	1	0
			2533	1668	406	455	4			
1	C	311	Total	C	N	O	S	0	1	0
			2533	1668	406	455	4			
1	D	311	Total	C	N	O	S	0	1	0
			2533	1668	406	455	4			
1	E	311	Total	C	N	O	S	0	1	0
			2533	1668	406	455	4			

There are 10 discrepancies between the modelled and reference sequences:

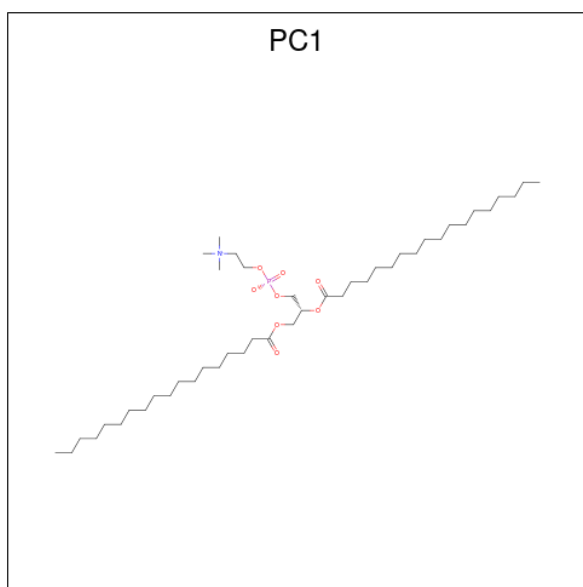
Chain	Residue	Modelled	Actual	Comment	Reference
A	27	SER	CYS	conflict	UNP Q7NDN8
A	135	CYS	VAL	engineered mutation	UNP Q7NDN8
B	27	SER	CYS	conflict	UNP Q7NDN8
B	135	CYS	VAL	engineered mutation	UNP Q7NDN8
C	27	SER	CYS	conflict	UNP Q7NDN8
C	135	CYS	VAL	engineered mutation	UNP Q7NDN8
D	27	SER	CYS	conflict	UNP Q7NDN8
D	135	CYS	VAL	engineered mutation	UNP Q7NDN8
E	27	SER	CYS	conflict	UNP Q7NDN8
E	135	CYS	VAL	engineered mutation	UNP Q7NDN8

- Molecule 2 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 35	C 24	O 11	0	0
2	A	1	Total 35	C 24	O 11	0	0
2	B	1	Total 35	C 24	O 11	0	0
2	C	1	Total 35	C 24	O 11	0	0
2	E	1	Total 35	C 24	O 11	0	0
2	E	1	Total 35	C 24	O 11	0	0

- Molecule 3 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			39	29	1	8	1		
3	A	1	Total	C	O			0	0
			27	23	4				
3	A	1	Total	C	N	O	P	0	0
			47	37	1	8	1		
3	B	1	Total	C	N	O	P	0	0
			47	37	1	8	1		
3	B	1	Total	C	N	O	P	0	0
			39	29	1	8	1		
3	B	1	Total	C	O			0	0
			26	22	4				
3	C	1	Total	C	N	O	P	0	0
			47	37	1	8	1		
3	C	1	Total	C	N	O	P	0	0
			39	29	1	8	1		
3	C	1	Total	C	O			0	0
			27	23	4				
3	D	1	Total	C	N	O	P	0	0
			47	37	1	8	1		
3	D	1	Total	C	N	O	P	0	0
			39	29	1	8	1		
3	D	1	Total	C	O			0	0
			22	18	4				
3	E	1	Total	C	N	O	P	0	0
			47	37	1	8	1		
3	E	1	Total	C	N	O	P	0	0
			39	29	1	8	1		

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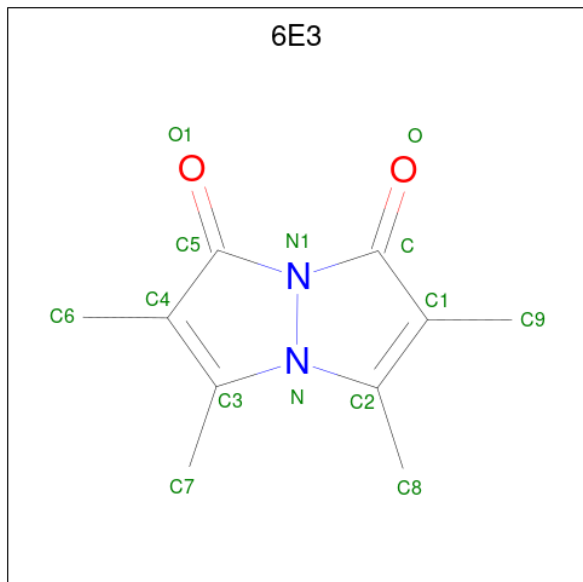
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	C	O	0	0
			27	23	4		

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			7	2	3	2		
4	A	1	Total	C	H	O	0	0
			7	2	3	2		
4	A	1	Total	C	H	O	0	0
			7	2	3	2		
4	B	1	Total	C	H	O	0	0
			7	2	3	2		
4	C	1	Total	C	H	O	0	0
			7	2	3	2		
4	C	1	Total	C	H	O	0	0
			7	2	3	2		
4	D	1	Total	C	H	O	0	0
			7	2	3	2		
4	D	1	Total	C	H	O	0	0
			7	2	3	2		
4	E	1	Total	C	H	O	0	0
			7	2	3	2		
4	E	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 5 is 2,3,5,6-tetramethyl-1H,7H-pyrazolo[1,2-a]pyrazole-1,7-dione (CCD ID: 6E3) (formula: C₁₀H₁₂N₂O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	0	0
			25	10	11	2	2		
5	D	1	Total	C	H	N	O	0	0
			25	10	11	2	2		

- Molecule 6 is BROMIDE ION (CCD ID: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Br	0	0
			1	1		
6	B	1	Total	Br	0	0
			1	1		
6	C	1	Total	Br	0	0
			1	1		
6	D	1	Total	Br	0	0
			1	1		
6	E	1	Total	Br	0	0
			1	1		

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

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total 1	Na 1	0	0
7	D	1	Total 1	Na 1	0	0
7	E	1	Total 1	Na 1	0	0

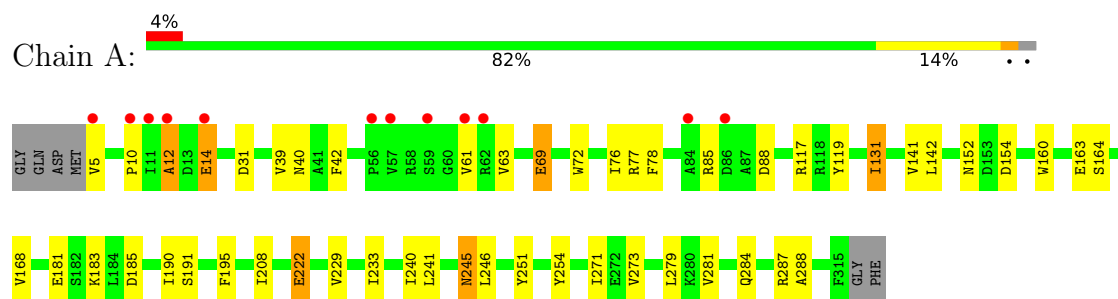
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	26	Total 26	O 26	0	0
8	B	33	Total 33	O 33	0	0
8	C	28	Total 28	O 28	0	0
8	D	29	Total 29	O 29	0	0
8	E	29	Total 29	O 29	0	0

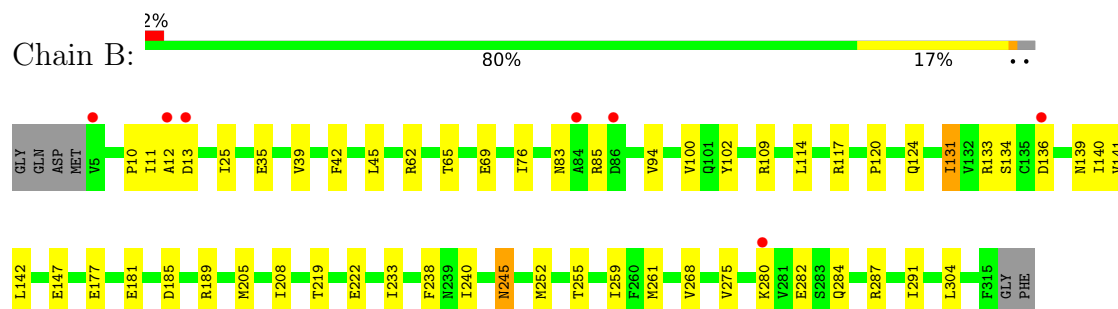
3 Residue-property plots [i](#)

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.

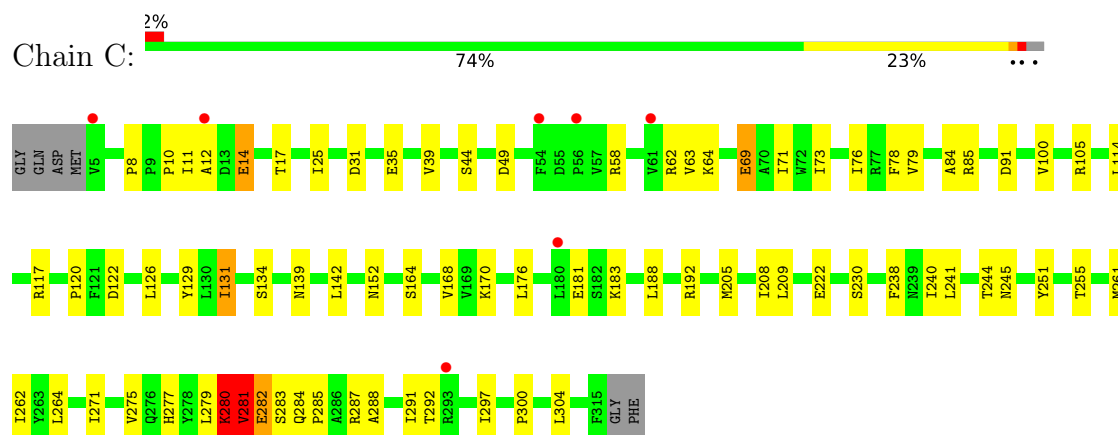
- Molecule 1: Proton-gated ion channel



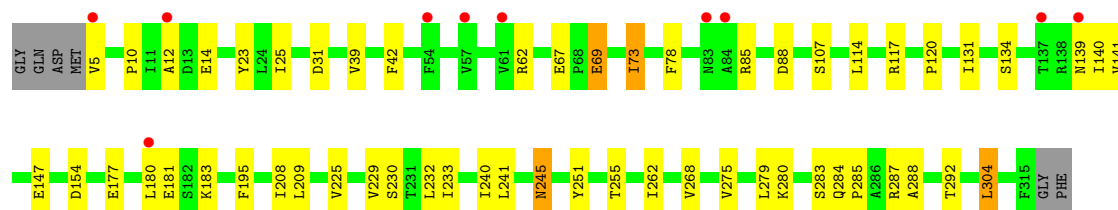
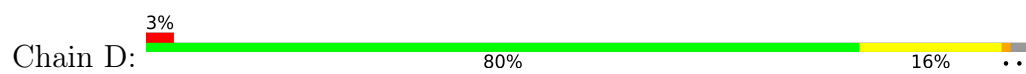
- Molecule 1: Proton-gated ion channel



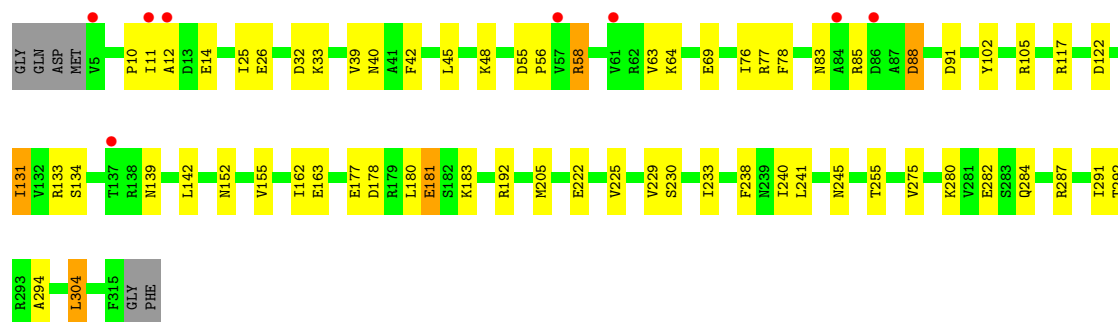
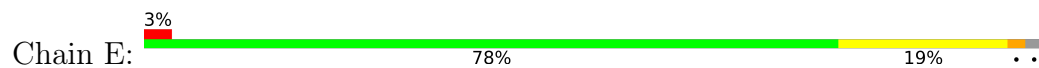
- Molecule 1: Proton-gated ion channel



- Molecule 1: Proton-gated ion channel



• Molecule 1: Proton-gated ion channel



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	182.03Å 134.07Å 159.94Å 90.00° 102.51° 90.00°	Depositor
Resolution (Å)	12.00 – 2.60 12.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (12.00-2.60) 98.7 (12.00-2.60)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.59Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.203 , 0.237 0.217 , 0.254	Depositor DCC
R_{free} test set	5709 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	67.0	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 72.0	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	13699	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, 6E3, NA, PC1, LMT, BR

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	0.84	0/2592	1.26	11/3543 (0.3%)
1	B	0.82	0/2601	1.25	3/3554 (0.1%)
1	C	0.84	1/2601 (0.0%)	1.28	12/3554 (0.3%)
1	D	0.83	0/2601	1.28	9/3554 (0.3%)
1	E	0.79	0/2601	1.25	9/3554 (0.3%)
All	All	0.82	1/12996 (0.0%)	1.26	44/17759 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	281	VAL	N-CA	5.23	1.52	1.46

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	280[A]	LYS	N-CA-C	-7.42	98.83	109.96
1	C	280[B]	LYS	N-CA-C	-7.42	98.83	109.96
1	C	152	ASN	CA-CB-CG	7.27	119.87	112.60
1	E	245	ASN	CA-CB-CG	7.26	119.86	112.60
1	D	31	ASP	CA-CB-CG	7.24	119.83	112.60
1	A	245	ASN	CA-CB-CG	7.17	119.77	112.60
1	D	73	ILE	CB-CA-C	7.05	116.97	110.13
1	E	152	ASN	CA-CB-CG	6.83	119.43	112.60
1	A	152	ASN	CA-CB-CG	6.66	119.25	112.60
1	D	177	GLU	CA-C-N	6.48	131.34	122.07
1	D	177	GLU	C-N-CA	6.48	131.34	122.07
1	B	245	ASN	CA-CB-CG	6.45	119.05	112.60
1	D	245	ASN	CA-CB-CG	6.38	118.98	112.60
1	A	31	ASP	CA-CB-CG	6.30	118.91	112.60
1	E	91	ASP	CA-CB-CG	6.17	118.77	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	154	ASP	CA-CB-CG	6.09	118.69	112.60
1	A	12	ALA	N-CA-C	-5.99	100.49	109.96
1	D	25	ILE	N-CA-C	-5.80	106.16	111.67
1	C	91	ASP	CA-CB-CG	5.78	118.38	112.60
1	C	245	ASN	CA-CB-CG	5.56	118.16	112.60
1	C	282	GLU	N-CA-C	-5.55	106.28	113.16
1	E	56	PRO	CA-C-N	5.53	127.61	120.70
1	E	56	PRO	C-N-CA	5.53	127.61	120.70
1	B	25	ILE	N-CA-C	-5.45	106.49	111.67
1	A	42	PHE	CA-CB-CG	5.33	119.13	113.80
1	E	88	ASP	CA-CB-CG	5.32	117.92	112.60
1	E	25	ILE	N-CA-C	-5.32	107.23	111.81
1	C	84	ALA	CA-C-N	5.28	129.17	121.31
1	C	84	ALA	C-N-CA	5.28	129.17	121.31
1	A	168	VAL	CA-C-N	5.25	129.24	120.62
1	A	168	VAL	C-N-CA	5.25	129.24	120.62
1	A	154	ASP	CA-CB-CG	5.23	117.83	112.60
1	B	185	ASP	CA-CB-CG	5.16	117.76	112.60
1	C	25	ILE	N-CA-C	-5.15	107.73	111.90
1	A	271	ILE	N-CA-CB	5.12	116.19	110.51
1	A	185	ASP	CA-CB-CG	5.12	117.72	112.60
1	E	83	ASN	CA-C-N	5.11	128.93	121.31
1	E	83	ASN	C-N-CA	5.11	128.93	121.31
1	C	168	VAL	CA-C-N	5.08	127.43	120.46
1	C	168	VAL	C-N-CA	5.08	127.43	120.46
1	A	14	GLU	N-CA-C	5.07	115.43	109.60
1	D	225	VAL	CA-C-N	5.05	127.00	120.44
1	D	225	VAL	C-N-CA	5.05	127.00	120.44
1	C	31	ASP	CA-CB-CG	5.04	117.64	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2524	0	2540	26	0
1	B	2533	0	2553	36	0
1	C	2533	0	2553	35	0
1	D	2533	0	2552	24	0
1	E	2533	0	2553	29	0
2	A	70	0	92	6	0
2	B	35	0	46	3	0
2	C	35	0	46	0	0
2	E	70	0	92	3	0
3	A	113	0	158	3	0
3	B	112	0	157	6	0
3	C	113	0	158	4	0
3	D	108	0	149	5	0
3	E	113	0	158	5	0
4	A	12	9	9	14	0
4	B	4	3	3	3	0
4	C	8	6	6	3	0
4	D	8	6	6	2	0
4	E	8	6	6	2	0
5	A	14	11	0	1	0
5	D	14	11	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	1	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	E	1	0	0	0	0
8	A	26	0	0	2	0
8	B	33	0	0	3	0
8	C	28	0	0	0	0
8	D	29	0	0	1	0
8	E	29	0	0	0	0
All	All	13647	52	13837	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 6.

All (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:131:ILE:HG21	4:A:505:ACT:H1	1.27	1.14
1:D:131:ILE:HG21	4:D:608:ACT:H2	1.35	1.07
1:A:85:ARG:NH2	4:A:509:ACT:H3	1.88	0.88
3:A:504:PC1:H32	8:A:602:HOH:O	1.82	0.80
1:B:133:ARG:HH12	1:B:177:GLU:HB2	1.53	0.73
1:B:10:PRO:HB2	1:B:12:ALA:O	1.89	0.71
4:A:510:ACT:CH3	1:B:131:ILE:HG21	2.20	0.70
1:E:78:PHE:HE2	1:E:85:ARG:HD3	1.54	0.69
1:C:280[A]:LYS:O	1:C:281:VAL:HB	1.93	0.69
1:B:219:THR:HA	1:B:280[A]:LYS:NZ	2.08	0.69
4:A:510:ACT:H3	1:B:131:ILE:HG12	1.76	0.67
3:D:602:PC1:H232	3:D:602:PC1:H31	1.76	0.66
1:A:85:ARG:HH22	4:A:509:ACT:H3	1.58	0.66
1:D:78:PHE:HE2	1:D:85:ARG:HD3	1.62	0.65
1:C:280[B]:LYS:O	1:C:281:VAL:HB	1.97	0.64
1:B:42:PHE:HZ	4:C:608:ACT:O	1.81	0.64
1:B:76:ILE:HD12	1:B:142:LEU:HD21	1.78	0.64
1:C:78:PHE:HE2	1:C:85:ARG:HD3	1.62	0.64
1:C:78:PHE:CE2	1:C:85:ARG:HD3	2.33	0.64
1:B:219:THR:HA	1:B:280[A]:LYS:HZ1	1.64	0.63
1:D:10:PRO:HB2	1:D:12:ALA:O	2.00	0.61
1:A:131:ILE:CG2	4:A:505:ACT:H1	2.18	0.61
1:A:10:PRO:HB2	1:A:12:ALA:O	2.02	0.60
4:A:505:ACT:O	1:E:42:PHE:CZ	2.56	0.58
1:A:85:ARG:HH22	4:A:509:ACT:CH3	2.16	0.58
4:A:505:ACT:H3	1:E:105:ARG:NH1	2.18	0.58
1:B:85:ARG:HH22	4:B:607:ACT:H1	1.67	0.58
1:E:122:ASP:OD1	1:E:192:ARG:HD2	2.04	0.57
1:E:76:ILE:HD12	1:E:142:LEU:HD21	1.87	0.56
1:E:131:ILE:HG21	4:E:401:ACT:H2	1.85	0.56
1:C:10:PRO:HB2	1:C:12:ALA:O	2.05	0.56
1:D:120:PRO:HD3	1:D:255:THR:OG1	2.06	0.56
1:A:77:ARG:HH21	4:A:505:ACT:C	2.20	0.55
1:B:245:ASN:HB3	8:B:703:HOH:O	2.06	0.55
1:A:279:LEU:HB2	1:A:288:ALA:HB2	1.90	0.54
1:A:85:ARG:HH21	4:A:509:ACT:H3	1.70	0.54
1:E:275:VAL:HG22	3:E:404:PC1:H221	1.89	0.54
1:C:205:MET:HE2	1:C:238:PHE:HB3	1.90	0.54
1:C:277:HIS:O	1:C:280[B]:LYS:O	2.25	0.53
3:B:601:PC1:H31	8:B:708:HOH:O	2.09	0.53
1:D:245:ASN:HB3	8:D:711:HOH:O	2.09	0.53
1:A:160:TRP:CE3	1:A:190:ILE:HD12	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:78:PHE:CE2	1:E:85:ARG:HD3	2.39	0.53
1:D:268:VAL:HG11	3:D:603:PC1:H281	1.91	0.52
1:E:26:GLU:HB2	1:E:40:ASN:HB3	1.92	0.52
1:B:42:PHE:CZ	4:C:608:ACT:O	2.60	0.51
1:C:134:SER:HB3	1:C:139:ASN:HA	1.92	0.51
1:A:78:PHE:HE2	1:A:85:ARG:HD3	1.76	0.51
1:E:134:SER:HB3	1:E:139:ASN:HA	1.91	0.51
1:B:76:ILE:H	4:B:607:ACT:H2	1.76	0.51
1:C:277:HIS:O	1:C:280[A]:LYS:O	2.28	0.51
1:B:268:VAL:HG11	3:B:604:PC1:H281	1.93	0.50
1:A:222:GLU:H	1:A:222:GLU:CD	2.20	0.50
2:A:501:LMT:H6E	2:B:602:LMT:H6'2	1.94	0.50
1:A:117:ARG:HG3	1:A:251:TYR:CD2	2.46	0.50
1:C:297:ILE:O	1:C:300:PRO:HD2	2.12	0.50
1:E:155:VAL:HG12	1:E:162:ILE:HD13	1.94	0.49
1:D:23:TYR:HB3	1:D:42:PHE:HB2	1.95	0.49
2:A:506:LMT:H51	2:B:602:LMT:H82	1.93	0.49
1:C:35:GLU:HG2	1:C:114:LEU:HG	1.93	0.49
1:D:78:PHE:CE2	1:D:85:ARG:HD3	2.44	0.49
1:A:119:TYR:CE2	1:A:246:LEU:HD21	2.48	0.49
1:B:94:VAL:HG22	1:B:100:VAL:HG22	1.94	0.49
1:E:291:ILE:HG23	3:E:406:PC1:H232	1.94	0.49
1:A:195:PHE:HZ	1:B:252:MET:HE2	1.77	0.48
1:A:241:LEU:HD22	1:B:240:ILE:HG12	1.96	0.48
1:A:229:VAL:HG11	1:E:230:SER:HB2	1.95	0.48
1:A:245:ASN:HB3	8:A:605:HOH:O	2.12	0.48
1:D:195:PHE:C	1:D:195:PHE:CD1	2.91	0.48
1:D:241:LEU:HD22	1:E:240:ILE:HG12	1.95	0.48
1:D:209:LEU:HD13	1:D:262:ILE:HG23	1.95	0.48
1:E:133:ARG:HH12	1:E:177:GLU:HB2	1.78	0.47
1:B:275:VAL:HG22	3:B:601:PC1:H221	1.97	0.47
1:E:55:ASP:HB3	1:E:58:ARG:HG3	1.94	0.47
1:E:77:ARG:HH21	4:E:401:ACT:C	2.28	0.47
1:C:261:MET:HA	1:C:264:LEU:HD12	1.96	0.47
1:D:275:VAL:HG22	3:D:601:PC1:H221	1.96	0.47
1:C:275:VAL:HG22	3:C:601:PC1:H221	1.95	0.47
1:D:39:VAL:O	1:D:107:SER:HA	2.15	0.47
1:D:304:LEU:HD23	3:E:404:PC1:H2I1	1.96	0.47
1:B:35:GLU:HA	1:B:114:LEU:HD12	1.96	0.47
1:B:35:GLU:HA	1:B:114:LEU:CD1	2.45	0.47
1:D:139:ASN:HD22	1:D:180:LEU:HD13	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:602:PC1:H152	3:D:602:PC1:H11	1.97	0.46
1:B:85:ARG:NH2	4:B:607:ACT:H1	2.30	0.46
1:C:280[A]:LYS:O	1:C:281:VAL:CB	2.63	0.45
1:D:283:SER:C	1:D:285:PRO:HD3	2.42	0.45
1:D:117:ARG:HG3	1:D:251:TYR:CD2	2.51	0.45
1:B:205:MET:HE2	1:B:238:PHE:HB3	1.98	0.45
1:B:255:THR:HG22	1:B:259:ILE:CD1	2.46	0.45
4:A:510:ACT:H2	1:B:131:ILE:HG21	1.97	0.45
1:C:241:LEU:HD22	1:D:240:ILE:HG12	1.98	0.45
1:D:69:GLU:H	1:D:69:GLU:CD	2.23	0.45
1:A:63:VAL:HG21	1:B:136:ASP:HB3	1.99	0.45
1:C:8:PRO:HB3	1:C:49:ASP:OD1	2.17	0.45
1:D:230:SER:HB2	1:E:229:VAL:HG11	1.99	0.45
1:C:279:LEU:HB2	1:C:288:ALA:HB2	1.97	0.45
1:A:254:TYR:HE1	3:A:502:PC1:H332	1.82	0.45
1:C:76:ILE:HD12	1:C:142:LEU:HD21	1.98	0.44
1:C:120:PRO:HD3	1:C:255:THR:OG1	2.17	0.44
1:C:131:ILE:HG21	4:C:608:ACT:H1	1.98	0.44
3:C:603:PC1:H32	3:C:603:PC1:H322	1.75	0.44
1:B:85:ARG:HG2	6:B:605:BR:BR	2.73	0.44
4:A:510:ACT:H2	1:B:131:ILE:CG2	2.48	0.44
1:B:120:PRO:HD3	1:B:255:THR:OG1	2.18	0.44
1:C:12:ALA:HB3	1:C:14:GLU:HG3	1.98	0.44
1:E:10:PRO:HB2	1:E:12:ALA:O	2.18	0.44
1:E:12:ALA:HB3	1:E:14:GLU:HG3	1.99	0.44
1:C:283:SER:C	1:C:285:PRO:HD3	2.42	0.44
1:A:240:ILE:HG12	1:E:241:LEU:HD22	2.00	0.44
4:A:510:ACT:CH3	1:B:131:ILE:CG2	2.93	0.44
1:B:134:SER:HB3	1:B:139:ASN:HA	2.00	0.44
3:B:603:PC1:H321	3:B:603:PC1:H241	1.99	0.44
1:B:291:ILE:HG12	3:B:604:PC1:H31	2.00	0.43
2:A:501:LMT:H82	2:A:506:LMT:H52	1.99	0.43
1:C:280[B]:LYS:O	1:C:281:VAL:CB	2.66	0.43
1:B:45:LEU:HB2	1:B:102:TYR:HB3	2.01	0.43
1:B:134:SER:HA	1:B:140:ILE:HD12	2.01	0.43
1:E:275:VAL:HG13	3:E:404:PC1:H32	2.01	0.43
1:A:76:ILE:HD12	1:A:142:LEU:HD21	2.00	0.43
1:C:69:GLU:H	1:C:69:GLU:CD	2.27	0.43
1:C:208:ILE:HG22	1:D:232:LEU:HD21	2.01	0.42
1:C:291:ILE:HG23	3:C:604:PC1:H251	2.00	0.42
1:C:117:ARG:HG3	1:C:251:TYR:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:131:ILE:HD11	1:E:181:GLU:HG2	2.00	0.42
1:B:261:MET:HE2	1:B:261:MET:HB3	1.94	0.42
3:D:602:PC1:H31	3:D:602:PC1:H322	1.88	0.42
1:E:294:ALA:HB3	3:E:406:PC1:H231	2.01	0.42
1:B:219:THR:HA	1:B:280[A]:LYS:HZ3	1.84	0.42
1:E:33:LYS:HD3	2:E:403:LMT:H6'2	2.02	0.42
3:A:504:PC1:H2I1	1:E:304:LEU:HD23	2.02	0.42
2:A:506:LMT:H122	2:B:602:LMT:H12	2.01	0.42
1:C:240:ILE:O	1:C:244:THR:HG23	2.19	0.42
1:A:69:GLU:H	1:A:69:GLU:CD	2.28	0.42
2:A:506:LMT:H41	2:E:403:LMT:H102	2.01	0.42
1:C:105:ARG:HD2	4:D:608:ACT:OXT	2.20	0.42
1:D:279:LEU:HB2	1:D:288:ALA:HB2	2.00	0.42
1:E:205:MET:HE2	1:E:238:PHE:HB3	2.02	0.42
1:B:255:THR:HG22	1:B:259:ILE:HD11	2.02	0.42
1:C:126:LEU:HB2	1:C:188:LEU:HB3	2.02	0.41
1:C:209:LEU:HD13	1:C:262:ILE:HG23	2.02	0.41
1:C:271:ILE:O	1:C:275:VAL:HG23	2.20	0.41
1:D:134:SER:HB3	1:D:139:ASN:HA	2.02	0.41
1:A:72:TRP:HE1	5:A:507:6E3:C8	2.33	0.41
3:B:601:PC1:C3	8:B:708:HOH:O	2.67	0.41
1:C:79:VAL:HB	1:C:129:TYR:HB2	2.02	0.41
1:A:163:GLU:OE2	1:A:191:SER:HB3	2.21	0.41
1:E:32:ASP:CG	1:E:192:ARG:HH22	2.28	0.41
1:B:114:LEU:HA	1:B:124:GLN:OE1	2.21	0.40
3:C:603:PC1:H361	3:C:603:PC1:H281	2.03	0.40
1:A:195:PHE:CD2	1:A:195:PHE:C	2.99	0.40
1:E:45:LEU:HB2	1:E:102:TYR:HB3	2.03	0.40
2:A:506:LMT:H61	2:E:403:LMT:H82	2.04	0.40
1:C:122:ASP:OD1	1:C:192:ARG:HD2	2.22	0.40
1:C:230:SER:HB2	1:D:229:VAL:HG11	2.02	0.40

There are no symmetry-related clashes.

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	309/317 (98%)	297 (96%)	12 (4%)	0	100	100
1	B	310/317 (98%)	297 (96%)	13 (4%)	0	100	100
1	C	310/317 (98%)	292 (94%)	17 (6%)	1 (0%)	36	58
1	D	310/317 (98%)	303 (98%)	7 (2%)	0	100	100
1	E	310/317 (98%)	298 (96%)	12 (4%)	0	100	100
All	All	1549/1585 (98%)	1487 (96%)	61 (4%)	1 (0%)	48	70

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	281	VAL

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	280/284 (99%)	261 (93%)	19 (7%)	14	32
1	B	281/284 (99%)	260 (92%)	21 (8%)	12	28
1	C	281/284 (99%)	254 (90%)	27 (10%)	8	17
1	D	281/284 (99%)	260 (92%)	21 (8%)	12	28
1	E	281/284 (99%)	255 (91%)	26 (9%)	8	18
All	All	1404/1420 (99%)	1290 (92%)	114 (8%)	11	24

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	14	GLU
1	A	39	VAL
1	A	40	ASN

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Mol	Chain	Res	Type
1	A	61	VAL
1	A	69	GLU
1	A	88	ASP
1	A	131	ILE
1	A	141	VAL
1	A	164	SER
1	A	181	GLU
1	A	183	LYS
1	A	208	ILE
1	A	222	GLU
1	A	233	ILE
1	A	273	VAL
1	A	281	VAL
1	A	284	GLN
1	A	287	ARG
1	B	11	ILE
1	B	13	ASP
1	B	39	VAL
1	B	62	ARG
1	B	65	THR
1	B	69	GLU
1	B	83	ASN
1	B	109	ARG
1	B	117	ARG
1	B	131	ILE
1	B	141	VAL
1	B	147	GLU
1	B	181	GLU
1	B	189	ARG
1	B	208	ILE
1	B	222	GLU
1	B	233	ILE
1	B	282	GLU
1	B	284	GLN
1	B	287	ARG
1	B	304	LEU
1	C	11	ILE
1	C	14	GLU
1	C	17	THR
1	C	39	VAL
1	C	44	SER
1	C	58	ARG

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Mol	Chain	Res	Type
1	C	62	ARG
1	C	63	VAL
1	C	64	LYS
1	C	69	GLU
1	C	71	ILE
1	C	73	ILE
1	C	100	VAL
1	C	131	ILE
1	C	164	SER
1	C	170	LYS
1	C	176	LEU
1	C	181	GLU
1	C	183	LYS
1	C	222	GLU
1	C	280[A]	LYS
1	C	280[B]	LYS
1	C	282	GLU
1	C	284	GLN
1	C	287	ARG
1	C	292	THR
1	C	304	LEU
1	D	5	VAL
1	D	14	GLU
1	D	62	ARG
1	D	67	GLU
1	D	69	GLU
1	D	73	ILE
1	D	88	ASP
1	D	114	LEU
1	D	140	ILE
1	D	141	VAL
1	D	147	GLU
1	D	181	GLU
1	D	183	LYS
1	D	208	ILE
1	D	233	ILE
1	D	280[A]	LYS
1	D	280[B]	LYS
1	D	284	GLN
1	D	287	ARG
1	D	292	THR
1	D	304	LEU

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Mol	Chain	Res	Type
1	E	11	ILE
1	E	39	VAL
1	E	48	LYS
1	E	58	ARG
1	E	63	VAL
1	E	64	LYS
1	E	69	GLU
1	E	88	ASP
1	E	117	ARG
1	E	131	ILE
1	E	163	GLU
1	E	178	ASP
1	E	180	LEU
1	E	181	GLU
1	E	183	LYS
1	E	222	GLU
1	E	225	VAL
1	E	233	ILE
1	E	255	THR
1	E	280[A]	LYS
1	E	280[B]	LYS
1	E	282	GLU
1	E	284	GLN
1	E	287	ARG
1	E	292	THR
1	E	304	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	245	ASN
1	B	239	ASN
1	B	245	ASN
1	B	284	GLN
1	C	239	ASN
1	D	245	ASN
1	D	307	ASN
1	E	239	ASN
1	E	245	ASN

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 ⓘ

Of 42 ligands modelled in this entry, 9 are monoatomic - leaving 33 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	ACT	A	505	-	3,3,3	0.78	0	3,3,3	1.37	0
4	ACT	D	608	-	3,3,3	0.90	0	3,3,3	1.43	0
5	6E3	A	507	1	15,15,15	0.46	0	24,24,24	0.94	1 (4%)
2	LMT	C	602	-	36,36,36	1.41	6 (16%)	47,47,47	1.51	8 (17%)
3	PC1	E	406	-	26,26,53	1.01	1 (3%)	28,28,61	0.76	0
3	PC1	D	602	-	38,38,53	1.35	5 (13%)	44,46,61	1.33	4 (9%)
3	PC1	C	604	-	26,26,53	1.12	2 (7%)	28,28,61	0.81	0
3	PC1	D	603	-	20,20,53	0.82	0	20,20,61	0.94	0
4	ACT	C	607	-	3,3,3	1.18	0	3,3,3	0.86	0
2	LMT	A	506	-	36,36,36	1.43	8 (22%)	47,47,47	1.29	4 (8%)
2	LMT	E	402	-	36,36,36	1.51	7 (19%)	47,47,47	1.40	9 (19%)
4	ACT	A	510	-	3,3,3	0.92	0	3,3,3	1.61	1 (33%)
3	PC1	E	405	-	38,38,53	1.34	5 (13%)	44,46,61	1.10	1 (2%)
4	ACT	B	607	-	3,3,3	0.94	0	3,3,3	1.18	0
4	ACT	E	409	-	3,3,3	1.08	0	3,3,3	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	LMT	B	602	-	36,36,36	1.38	6 (16%)	47,47,47	1.46	8 (17%)
3	PC1	C	603	-	38,38,53	1.35	5 (13%)	44,46,61	1.13	3 (6%)
2	LMT	E	403	-	36,36,36	1.42	7 (19%)	47,47,47	1.16	4 (8%)
3	PC1	B	603	-	38,38,53	1.33	6 (15%)	44,46,61	1.19	2 (4%)
2	LMT	A	501	-	36,36,36	1.16	6 (16%)	47,47,47	1.52	10 (21%)
3	PC1	C	601	-	46,46,53	1.34	8 (17%)	52,54,61	1.16	2 (3%)
5	6E3	D	604	1	15,15,15	0.44	0	24,24,24	1.16	3 (12%)
3	PC1	A	502	-	38,38,53	1.41	7 (18%)	44,46,61	1.19	2 (4%)
3	PC1	B	604	-	25,25,53	0.88	1 (4%)	26,26,61	1.07	2 (7%)
4	ACT	E	401	-	3,3,3	1.20	0	3,3,3	0.71	0
3	PC1	D	601	-	46,46,53	1.36	7 (15%)	52,54,61	1.30	5 (9%)
4	ACT	A	509	-	3,3,3	1.10	0	3,3,3	1.11	0
3	PC1	A	503	-	26,26,53	1.14	3 (11%)	28,28,61	0.86	1 (3%)
4	ACT	D	607	-	3,3,3	1.21	0	3,3,3	0.73	0
3	PC1	A	504	-	46,46,53	1.29	4 (8%)	52,54,61	1.13	3 (5%)
4	ACT	C	608	-	3,3,3	0.93	0	3,3,3	1.26	0
3	PC1	E	404	-	46,46,53	1.30	6 (13%)	52,54,61	1.01	2 (3%)
3	PC1	B	601	-	46,46,53	1.23	4 (8%)	52,54,61	1.01	1 (1%)

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
5	6E3	A	507	1	-	-	0/2/2/2
2	LMT	C	602	-	-	5/21/61/61	0/2/2/2
3	PC1	E	406	-	-	13/27/27/57	-
3	PC1	D	602	-	-	24/42/42/57	-
3	PC1	C	604	-	-	7/27/27/57	-
3	PC1	D	603	-	-	3/17/17/57	-
2	LMT	A	506	-	-	4/21/61/61	0/2/2/2
2	LMT	E	402	-	-	11/21/61/61	0/2/2/2
3	PC1	E	405	-	-	11/42/42/57	-
2	LMT	B	602	-	-	11/21/61/61	0/2/2/2
3	PC1	C	603	-	-	23/42/42/57	-
2	LMT	E	403	-	-	7/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PC1	B	603	-	-	14/42/42/57	-
2	LMT	A	501	-	-	9/21/61/61	0/2/2/2
3	PC1	C	601	-	-	14/50/50/57	-
5	6E3	D	604	1	-	-	0/2/2/2
3	PC1	A	502	-	-	14/42/42/57	-
3	PC1	B	604	-	-	15/25/25/57	-
3	PC1	D	601	-	-	15/50/50/57	-
3	PC1	A	503	-	-	8/27/27/57	-
3	PC1	A	504	-	-	13/50/50/57	-
3	PC1	E	404	-	-	17/50/50/57	-
3	PC1	B	601	-	-	18/50/50/57	-

All (104) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	504	PC1	P-O13	5.08	1.79	1.59
3	E	404	PC1	P-O13	5.07	1.79	1.59
3	D	602	PC1	P-O13	4.86	1.78	1.59
3	E	405	PC1	P-O13	4.83	1.78	1.59
3	D	601	PC1	P-O13	4.78	1.78	1.59
3	C	603	PC1	P-O13	4.74	1.77	1.59
3	B	601	PC1	P-O13	4.68	1.77	1.59
3	A	502	PC1	P-O13	4.66	1.77	1.59
3	C	601	PC1	P-O13	4.59	1.77	1.59
3	B	603	PC1	P-O13	4.37	1.76	1.59
2	E	402	LMT	C3'-C4'	3.87	1.62	1.52
3	A	503	PC1	C3-C2	3.57	1.58	1.50
2	E	403	LMT	C4B-C5B	3.56	1.60	1.53
3	C	604	PC1	C3-C2	3.42	1.58	1.50
2	E	403	LMT	C3'-C4'	3.42	1.61	1.52
3	E	406	PC1	C3-C2	3.34	1.58	1.50
2	A	506	LMT	C4B-C5B	3.33	1.60	1.53
2	A	506	LMT	C3'-C4'	3.31	1.61	1.52
2	B	602	LMT	C3'-C2'	3.23	1.60	1.52
2	B	602	LMT	C4B-C5B	3.06	1.59	1.53
3	D	601	PC1	C3-C2	3.04	1.60	1.50
2	C	602	LMT	C1'-C2'	3.03	1.61	1.52
2	E	402	LMT	C4'-C5'	2.99	1.61	1.52
2	C	602	LMT	C4B-C5B	2.98	1.59	1.53
2	B	602	LMT	C4B-C3B	2.98	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	506	LMT	C3'-C2'	2.97	1.60	1.52
2	A	506	LMT	C4B-C3B	2.96	1.60	1.52
2	E	402	LMT	C4B-C5B	2.89	1.59	1.53
3	D	601	PC1	C12-C11	2.89	1.60	1.51
3	E	404	PC1	C12-C11	2.87	1.60	1.51
2	E	402	LMT	C1B-C2B	2.86	1.60	1.52
3	A	504	PC1	C12-C11	2.76	1.59	1.51
3	C	601	PC1	C1-C2	2.76	1.59	1.50
2	C	602	LMT	C4B-C3B	2.75	1.59	1.52
3	C	601	PC1	C3-C2	2.71	1.59	1.50
3	B	601	PC1	C12-C11	2.69	1.59	1.51
2	E	402	LMT	C4B-C3B	2.69	1.59	1.52
3	D	601	PC1	C1-C2	2.67	1.59	1.50
3	B	603	PC1	C12-C11	2.67	1.59	1.51
3	A	504	PC1	C12-N	2.66	1.59	1.51
3	C	603	PC1	C12-C11	2.64	1.59	1.51
3	A	502	PC1	C12-C11	2.63	1.59	1.51
3	E	405	PC1	C12-C11	2.62	1.59	1.51
2	E	403	LMT	C4'-C5'	2.61	1.60	1.52
2	B	602	LMT	C1'-C2'	2.59	1.60	1.52
3	E	404	PC1	C12-N	2.59	1.59	1.51
3	B	601	PC1	C12-N	2.56	1.59	1.51
3	C	601	PC1	C12-C11	2.55	1.59	1.51
3	D	602	PC1	O21-C21	2.54	1.41	1.34
3	D	601	PC1	C12-N	2.53	1.59	1.51
3	D	601	PC1	P-O11	2.49	1.69	1.59
3	C	601	PC1	P-O11	2.49	1.69	1.59
2	B	602	LMT	C3'-C4'	2.49	1.59	1.52
3	A	502	PC1	C1-C2	2.48	1.58	1.50
2	C	602	LMT	C3B-C2B	2.47	1.58	1.52
2	E	402	LMT	C3B-C2B	2.47	1.58	1.52
3	A	504	PC1	P-O11	2.46	1.69	1.59
3	A	502	PC1	P-O11	2.46	1.69	1.59
3	D	602	PC1	C12-C11	2.46	1.58	1.51
2	A	506	LMT	C1'-C2'	2.45	1.59	1.52
2	E	403	LMT	C3B-C2B	2.45	1.58	1.52
3	B	604	PC1	O31-C31	2.44	1.40	1.33
2	E	403	LMT	C1B-C2B	2.43	1.59	1.52
2	A	501	LMT	C3'-C2'	2.41	1.58	1.52
3	E	405	PC1	C12-N	2.41	1.58	1.51
2	E	403	LMT	C4B-C3B	2.39	1.58	1.52
3	C	604	PC1	O31-C31	2.38	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	PC1	C12-N	2.37	1.58	1.51
3	B	603	PC1	C1-C2	2.36	1.58	1.50
3	D	602	PC1	P-O11	2.35	1.68	1.59
3	B	603	PC1	P-O11	2.35	1.68	1.59
2	A	506	LMT	C3B-C2B	2.33	1.58	1.52
2	A	501	LMT	C4B-C3B	2.30	1.58	1.52
3	B	603	PC1	O21-C21	2.29	1.40	1.34
3	C	603	PC1	P-O11	2.27	1.68	1.59
2	A	501	LMT	C1'-C2'	2.25	1.59	1.52
3	E	405	PC1	O21-C21	2.25	1.40	1.34
2	A	506	LMT	C1B-C2B	2.25	1.59	1.52
3	D	601	PC1	O31-C31	2.24	1.39	1.33
3	E	404	PC1	C3-C2	2.24	1.57	1.50
3	A	502	PC1	O21-C21	2.20	1.40	1.34
3	C	603	PC1	C12-N	2.20	1.58	1.51
2	A	501	LMT	C4B-C5B	2.20	1.57	1.53
3	E	404	PC1	P-O11	2.20	1.68	1.59
3	C	601	PC1	O21-C21	2.16	1.40	1.34
3	B	601	PC1	P-O11	2.16	1.67	1.59
2	C	602	LMT	O5'-C1'	2.15	1.47	1.41
2	E	402	LMT	C3'-C2'	2.15	1.57	1.52
3	A	502	PC1	C3-C2	2.15	1.57	1.50
2	A	506	LMT	C4'-C5'	2.14	1.58	1.52
2	C	602	LMT	C1B-C2B	2.13	1.58	1.52
2	A	501	LMT	C3'-C4'	2.13	1.58	1.52
3	C	601	PC1	O31-C31	2.13	1.39	1.33
3	A	503	PC1	O31-C31	2.12	1.39	1.33
3	A	503	PC1	O21-C21	2.11	1.40	1.34
3	E	404	PC1	C1-C2	2.10	1.57	1.50
2	E	403	LMT	C3'-C2'	2.08	1.57	1.52
3	C	603	PC1	C1-C2	2.06	1.57	1.50
3	C	601	PC1	C12-N	2.06	1.57	1.51
2	B	602	LMT	C3B-C2B	2.02	1.57	1.52
2	A	501	LMT	C3B-C2B	2.02	1.57	1.52
3	B	603	PC1	C12-N	2.01	1.57	1.51
3	D	602	PC1	C12-N	2.01	1.57	1.51
3	E	405	PC1	P-O11	2.01	1.67	1.59

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	601	PC1	O12-P-O14	4.80	134.76	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	603	PC1	O12-P-O14	4.79	134.72	112.44
3	A	502	PC1	O12-P-O14	4.79	134.71	112.44
3	D	602	PC1	O12-P-O14	4.76	134.58	112.44
3	E	405	PC1	O12-P-O14	4.68	134.21	112.44
3	C	603	PC1	O12-P-O14	4.67	134.18	112.44
3	D	601	PC1	O12-P-O14	4.48	133.29	112.44
3	B	601	PC1	O12-P-O14	4.40	132.89	112.44
3	E	404	PC1	O12-P-O14	4.39	132.88	112.44
3	A	504	PC1	O12-P-O14	4.30	132.45	112.44
2	E	402	LMT	C1B-O5B-C5B	4.18	121.88	113.72
2	E	402	LMT	C1-O1'-C1'	4.11	120.70	113.68
3	C	601	PC1	C2-O21-C21	4.09	127.59	117.80
2	C	602	LMT	C1'-O5'-C5'	4.05	121.62	113.72
2	C	602	LMT	O1B-C4'-C3'	3.95	117.27	107.23
3	D	601	PC1	C2-O21-C21	3.68	126.61	117.80
5	D	604	6E3	C2-N-C3	-3.60	125.19	138.94
2	C	602	LMT	C2'-C3'-C4'	-3.58	101.56	109.68
2	B	602	LMT	C1'-C2'-C3'	3.48	117.32	110.01
3	B	603	PC1	C2-O21-C21	3.41	125.95	117.80
3	A	502	PC1	C2-O21-C21	3.36	125.85	117.80
2	A	506	LMT	C2'-C3'-C4'	3.32	117.22	109.68
3	D	602	PC1	C2-O21-C21	3.23	125.53	117.80
3	A	504	PC1	C2-O21-C21	3.19	125.44	117.80
5	A	507	6E3	C2-N-C3	-3.16	126.86	138.94
2	A	506	LMT	C1B-O5B-C5B	3.15	119.87	113.72
2	A	506	LMT	C1'-C2'-C3'	3.06	116.44	110.01
3	D	601	PC1	O31-C31-O32	-3.05	115.99	123.63
2	A	501	LMT	C3B-C4B-C5B	-3.03	104.75	110.23
2	B	602	LMT	C1B-O5B-C5B	3.02	119.62	113.72
2	A	501	LMT	O5B-C1B-C2B	2.98	116.50	110.37
3	B	604	PC1	C3-O31-C31	2.98	126.23	116.90
2	E	403	LMT	O1'-C1'-C2'	-2.98	103.74	108.27
2	A	501	LMT	C1B-O1B-C4'	-2.96	110.95	117.98
2	A	501	LMT	O5'-C5'-C4'	-2.96	103.61	109.72
2	B	602	LMT	C2'-C3'-C4'	2.87	116.18	109.68
2	A	501	LMT	O2'-C2'-C3'	-2.86	103.63	110.38
3	D	602	PC1	O31-C31-O32	-2.76	116.73	123.63
2	A	501	LMT	C1'-C2'-C3'	2.73	115.75	110.01
3	D	601	PC1	C3-O31-C31	2.70	126.99	117.12
2	C	602	LMT	C1B-O1B-C4'	-2.64	111.72	117.98
2	B	602	LMT	O3'-C3'-C4'	-2.60	103.27	109.94
2	A	506	LMT	O2'-C2'-C3'	-2.55	104.35	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	602	LMT	O2B-C2B-C3B	-2.55	104.36	110.38
2	A	501	LMT	C1B-O5B-C5B	2.42	118.45	113.72
2	A	501	LMT	O1'-C1'-C2'	-2.41	104.61	108.27
3	A	504	PC1	O21-C2-C1	2.35	116.79	108.34
3	E	404	PC1	C2-O21-C21	2.35	123.43	117.80
2	C	602	LMT	C1B-O5B-C5B	2.34	118.29	113.72
2	C	602	LMT	O3B-C3B-C4B	-2.28	105.01	110.38
2	B	602	LMT	O1'-C1'-C2'	-2.28	104.81	108.27
3	B	604	PC1	O31-C31-O32	-2.27	117.94	123.63
3	A	503	PC1	C2-O21-C21	2.25	121.03	117.78
2	A	501	LMT	C4B-C3B-C2B	-2.23	106.92	110.83
2	A	501	LMT	O3'-C3'-C4'	-2.22	104.24	109.94
2	E	402	LMT	O5B-C1B-C2B	2.21	114.91	110.37
3	D	602	PC1	C3-O31-C31	2.21	125.18	117.12
2	E	403	LMT	C3'-C4'-C5'	-2.19	106.07	110.93
3	D	601	PC1	O31-C31-C32	2.18	118.48	111.83
2	E	403	LMT	O2B-C2B-C3B	-2.17	105.25	110.38
2	E	402	LMT	O2B-C2B-C1B	2.17	115.25	110.08
3	C	603	PC1	O31-C31-O32	-2.14	118.29	123.63
2	E	402	LMT	O2'-C2'-C3'	-2.12	105.37	110.38
5	D	604	6E3	C-N1-C5	-2.11	124.09	135.40
2	B	602	LMT	O2'-C2'-C3'	-2.10	105.42	110.38
2	E	402	LMT	O5B-C5B-C4B	2.10	113.48	109.70
5	D	604	6E3	C9-C1-C2	-2.09	123.86	127.32
2	E	402	LMT	O2B-C2B-C3B	-2.09	105.46	110.38
2	E	402	LMT	O1B-C4'-C3'	2.07	112.50	107.23
2	C	602	LMT	C1-O1'-C1'	2.07	117.22	113.68
2	E	402	LMT	C1B-O1B-C4'	2.04	122.81	117.98
2	E	403	LMT	O2'-C2'-C3'	-2.04	105.57	110.38
2	C	602	LMT	O5'-C1'-C2'	2.02	114.53	110.37
2	B	602	LMT	O5B-C5B-C4B	2.02	113.34	109.70
4	A	510	ACT	OXT-C-O	2.01	129.50	122.03
3	C	603	PC1	C3-O31-C31	2.01	124.45	117.12

There are no chirality outliers.

All (256) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	LMT	C2-C1-O1'-C1'
2	C	602	LMT	O5'-C1'-O1'-C1
3	A	502	PC1	C11-O13-P-O12
3	A	502	PC1	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
3	A	502	PC1	C22-C21-O21-C2
3	A	503	PC1	C22-C21-O21-C2
3	A	504	PC1	C1-O11-P-O12
3	A	504	PC1	O21-C2-C3-O31
3	A	504	PC1	C22-C21-O21-C2
3	B	601	PC1	C1-O11-P-O13
3	B	601	PC1	C22-C21-O21-C2
3	B	603	PC1	O13-C11-C12-N
3	B	603	PC1	O22-C21-O21-C2
3	B	603	PC1	C22-C21-O21-C2
3	B	604	PC1	O32-C31-O31-C3
3	B	604	PC1	C32-C31-O31-C3
3	C	601	PC1	C11-O13-P-O11
3	C	603	PC1	C11-O13-P-O12
3	C	603	PC1	C1-O11-P-O12
3	C	603	PC1	O21-C2-C3-O31
3	C	603	PC1	C22-C21-O21-C2
3	C	603	PC1	O32-C31-O31-C3
3	C	603	PC1	C32-C31-O31-C3
3	C	604	PC1	C22-C21-O21-C2
3	D	601	PC1	C1-O11-P-O12
3	D	601	PC1	C1-O11-P-O14
3	D	601	PC1	C1-O11-P-O13
3	D	601	PC1	O13-C11-C12-N
3	D	601	PC1	O22-C21-O21-C2
3	D	601	PC1	O32-C31-O31-C3
3	D	601	PC1	C32-C31-O31-C3
3	D	602	PC1	C11-O13-P-O14
3	D	602	PC1	C11-O13-P-O11
3	D	602	PC1	C1-O11-P-O14
3	D	602	PC1	C1-O11-P-O13
3	D	602	PC1	O13-C11-C12-N
3	D	602	PC1	O32-C31-O31-C3
3	D	602	PC1	C32-C31-O31-C3
3	E	404	PC1	C11-O13-P-O12
3	E	404	PC1	O13-C11-C12-N
3	E	405	PC1	C11-O13-P-O14
3	E	405	PC1	C11-O13-P-O11
3	E	405	PC1	O13-C11-C12-N
3	E	406	PC1	C22-C21-O21-C2
2	B	602	LMT	O5B-C1B-O1B-C4'
3	A	502	PC1	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
3	A	504	PC1	O22-C21-O21-C2
3	B	601	PC1	O22-C21-O21-C2
3	C	603	PC1	O22-C21-O21-C2
3	C	604	PC1	O22-C21-O21-C2
3	E	405	PC1	O22-C21-O21-C2
3	E	406	PC1	O22-C21-O21-C2
3	D	601	PC1	C22-C21-O21-C2
3	A	503	PC1	O22-C21-O21-C2
3	E	405	PC1	C22-C21-O21-C2
3	B	604	PC1	O21-C2-C3-O31
2	A	501	LMT	C4B-C5B-C6B-O6B
3	B	604	PC1	C22-C21-O21-C2
2	C	602	LMT	C2'-C1'-O1'-C1
2	A	501	LMT	O5B-C5B-C6B-O6B
3	B	604	PC1	O22-C21-O21-C2
3	B	601	PC1	O21-C2-C3-O31
2	A	506	LMT	O5'-C5'-C6'-O6'
2	C	602	LMT	O1'-C1-C2-C3
3	B	603	PC1	C31-C32-C33-C34
3	D	601	PC1	C21-C22-C23-C24
3	D	601	PC1	C31-C32-C33-C34
3	D	602	PC1	C21-C22-C23-C24
3	E	406	PC1	C31-C32-C33-C34
2	A	506	LMT	O5'-C1'-O1'-C1
2	B	602	LMT	O5'-C1'-O1'-C1
3	C	601	PC1	O22-C21-O21-C2
3	D	602	PC1	O22-C21-O21-C2
2	E	402	LMT	C3'-C4'-O1B-C1B
2	E	403	LMT	C5'-C4'-O1B-C1B
2	A	501	LMT	O5B-C1B-O1B-C4'
3	C	601	PC1	C22-C21-O21-C2
3	D	602	PC1	C22-C21-O21-C2
3	E	404	PC1	O22-C21-O21-C2
2	A	506	LMT	C2'-C1'-O1'-C1
2	B	602	LMT	C2'-C1'-O1'-C1
3	C	603	PC1	C21-C22-C23-C24
3	E	404	PC1	C22-C21-O21-C2
2	E	402	LMT	C5'-C4'-O1B-C1B
3	A	502	PC1	C25-C26-C27-C28
3	D	601	PC1	C28-C29-C2A-C2B
3	A	502	PC1	C35-C36-C37-C38
3	B	603	PC1	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
3	B	603	PC1	C33-C34-C35-C36
3	E	406	PC1	C2A-C2B-C2C-C2D
3	E	406	PC1	C32-C33-C34-C35
3	D	602	PC1	C27-C28-C29-C2A
3	A	502	PC1	C36-C37-C38-C39
2	B	602	LMT	C1-C2-C3-C4
3	A	504	PC1	C28-C29-C2A-C2B
3	E	405	PC1	C1-C2-C3-O31
3	A	502	PC1	C24-C25-C26-C27
3	A	504	PC1	C22-C23-C24-C25
3	B	604	PC1	C22-C23-C24-C25
3	C	603	PC1	C24-C25-C26-C27
3	C	604	PC1	C28-C29-C2A-C2B
2	E	402	LMT	O5'-C5'-C6'-O6'
2	E	403	LMT	C1-C2-C3-C4
2	E	402	LMT	C5-C6-C7-C8
3	B	603	PC1	C21-C22-C23-C24
3	C	603	PC1	C31-C32-C33-C34
2	B	602	LMT	O5B-C5B-C6B-O6B
3	B	603	PC1	C34-C35-C36-C37
3	E	404	PC1	C26-C27-C28-C29
2	E	403	LMT	O5'-C1'-O1'-C1
3	B	601	PC1	C2C-C2D-C2E-C2F
3	C	601	PC1	C27-C28-C29-C2A
3	B	601	PC1	C2E-C2F-C2G-C2H
3	A	503	PC1	C22-C23-C24-C25
3	B	601	PC1	C21-C22-C23-C24
3	C	601	PC1	C28-C29-C2A-C2B
2	E	402	LMT	C3-C4-C5-C6
3	B	604	PC1	C25-C26-C27-C28
3	B	601	PC1	C28-C29-C2A-C2B
3	E	406	PC1	C28-C29-C2A-C2B
2	A	506	LMT	C4'-C5'-C6'-O6'
2	E	403	LMT	C3'-C4'-O1B-C1B
3	D	602	PC1	C36-C37-C38-C39
2	E	402	LMT	O1'-C1-C2-C3
3	A	503	PC1	C28-C29-C2A-C2B
3	B	601	PC1	C2B-C2C-C2D-C2E
2	E	402	LMT	C2-C3-C4-C5
3	A	503	PC1	C32-C33-C34-C35
3	C	603	PC1	C32-C33-C34-C35
3	C	601	PC1	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
3	A	504	PC1	C1-C2-O21-C21
2	A	501	LMT	O1'-C1-C2-C3
3	B	603	PC1	C28-C29-C2A-C2B
3	E	404	PC1	C28-C29-C2A-C2B
3	E	404	PC1	C27-C28-C29-C2A
3	D	603	PC1	C21-C22-C23-C24
3	C	604	PC1	C24-C25-C26-C27
3	D	601	PC1	C2D-C2E-C2F-C2G
3	B	604	PC1	C23-C24-C25-C26
2	B	602	LMT	C2-C1-O1'-C1'
2	E	402	LMT	C2-C1-O1'-C1'
3	C	601	PC1	C2-C1-O11-P
3	C	603	PC1	C34-C35-C36-C37
3	D	602	PC1	C32-C33-C34-C35
3	A	504	PC1	O11-C1-C2-C3
3	B	601	PC1	O11-C1-C2-C3
3	E	406	PC1	C24-C25-C26-C27
3	E	404	PC1	C24-C25-C26-C27
3	C	601	PC1	C2F-C2G-C2H-C2I
3	E	405	PC1	C35-C36-C37-C38
3	B	604	PC1	C29-C2A-C2B-C2C
3	A	504	PC1	C1-C2-C3-O31
3	B	601	PC1	C1-C2-C3-O31
3	C	603	PC1	C1-C2-C3-O31
2	B	602	LMT	C2-C3-C4-C5
3	E	406	PC1	O21-C2-C3-O31
3	D	603	PC1	C32-C33-C34-C35
3	E	405	PC1	C22-C23-C24-C25
3	E	404	PC1	O21-C2-C3-O31
3	C	603	PC1	C28-C29-C2A-C2B
3	E	404	PC1	C2F-C2G-C2H-C2I
2	E	402	LMT	C2'-C1'-O1'-C1
3	D	602	PC1	C31-C32-C33-C34
3	C	604	PC1	C2B-C2C-C2D-C2E
3	C	604	PC1	C23-C24-C25-C26
3	E	404	PC1	C2D-C2E-C2F-C2G
3	E	406	PC1	C33-C34-C35-C36
2	B	602	LMT	O1'-C1-C2-C3
3	D	603	PC1	C28-C29-C2A-C2B
3	C	603	PC1	C22-C23-C24-C25
3	B	601	PC1	O11-C1-C2-O21
3	D	602	PC1	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
2	A	501	LMT	C11-C10-C9-C8
3	D	601	PC1	O21-C2-C3-O31
3	D	602	PC1	O21-C2-C3-O31
3	C	603	PC1	C25-C26-C27-C28
3	E	404	PC1	C29-C2A-C2B-C2C
3	C	604	PC1	C31-C32-C33-C34
3	A	504	PC1	O13-C11-C12-N
3	B	601	PC1	O13-C11-C12-N
3	C	603	PC1	O13-C11-C12-N
2	A	501	LMT	C2B-C1B-O1B-C4'
2	C	602	LMT	C2-C1-O1'-C1'
2	E	403	LMT	C2-C1-O1'-C1'
2	B	602	LMT	C5'-C4'-O1B-C1B
3	B	601	PC1	C2D-C2E-C2F-C2G
3	A	504	PC1	O11-C1-C2-O21
2	C	602	LMT	C11-C10-C9-C8
3	E	405	PC1	O21-C2-C3-O31
3	D	601	PC1	C1-C2-C3-O31
2	E	402	LMT	C1-C2-C3-C4
3	A	503	PC1	C2B-C2C-C2D-C2E
3	B	601	PC1	C1-O11-P-O14
3	B	603	PC1	C11-O13-P-O14
3	C	601	PC1	C11-O13-P-O14
3	C	601	PC1	C1-O11-P-O14
3	C	601	PC1	C1-O11-P-O13
3	C	603	PC1	C11-O13-P-O11
3	C	603	PC1	C1-O11-P-O14
3	C	603	PC1	C1-O11-P-O13
3	D	602	PC1	C11-O13-P-O12
3	D	602	PC1	C1-O11-P-O12
3	E	404	PC1	C11-O13-P-O11
3	E	405	PC1	C11-O13-P-O12
2	B	602	LMT	C9-C10-C11-C12
3	A	502	PC1	C1-C2-O21-C21
3	B	603	PC1	C1-C2-O21-C21
3	D	601	PC1	C3-C2-O21-C21
3	B	604	PC1	C24-C25-C26-C27
3	A	502	PC1	O11-C1-C2-C3
3	A	502	PC1	C23-C24-C25-C26
3	D	602	PC1	C22-C23-C24-C25
3	A	503	PC1	C2A-C2B-C2C-C2D
3	A	503	PC1	C21-C22-C23-C24

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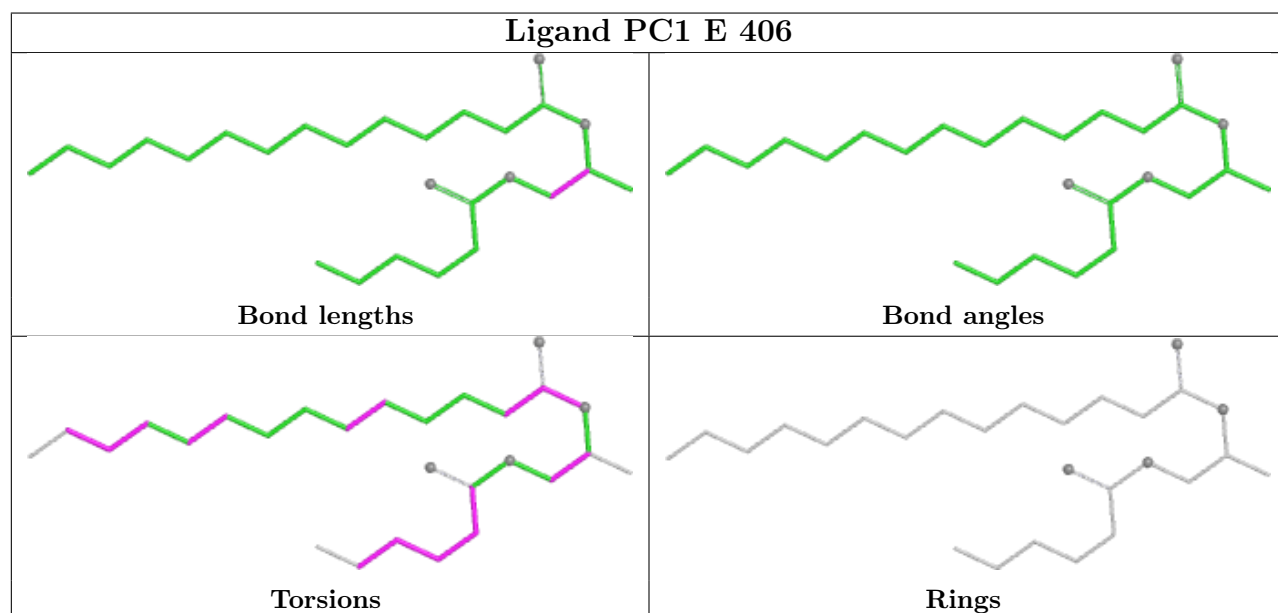
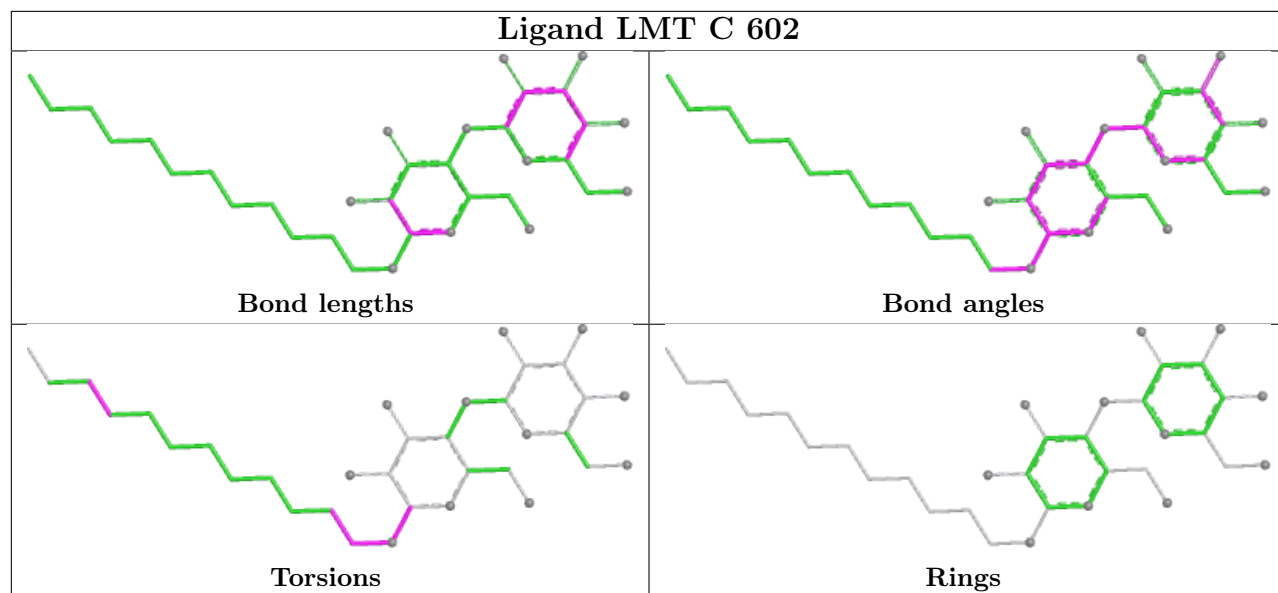
Mol	Chain	Res	Type	Atoms
2	E	403	LMT	C2'-C1'-O1'-C1
2	E	403	LMT	C2-C3-C4-C5
3	C	601	PC1	C1-C2-O21-C21
3	B	604	PC1	C21-C22-C23-C24
2	E	402	LMT	C7-C8-C9-C10
3	E	404	PC1	C1-C2-C3-O31
2	B	602	LMT	C3'-C4'-O1B-C1B
2	A	501	LMT	C5'-C4'-O1B-C1B
3	A	502	PC1	C22-C23-C24-C25
3	C	601	PC1	C2D-C2E-C2F-C2G
3	D	602	PC1	C1-C2-O21-C21
3	E	406	PC1	C2B-C2C-C2D-C2E
3	E	404	PC1	C34-C35-C36-C37
2	A	501	LMT	C3'-C4'-O1B-C1B
3	A	502	PC1	O13-C11-C12-N
3	C	601	PC1	O13-C11-C12-N
3	B	601	PC1	O31-C31-C32-C33
3	B	603	PC1	O31-C31-C32-C33
3	C	603	PC1	C36-C37-C38-C39
3	A	504	PC1	O31-C31-C32-C33
3	B	604	PC1	O31-C31-C32-C33
3	C	603	PC1	O31-C31-C32-C33
3	E	404	PC1	O21-C21-C22-C23
3	D	602	PC1	C35-C36-C37-C38
3	D	602	PC1	C33-C34-C35-C36
3	B	601	PC1	C29-C2A-C2B-C2C
3	E	406	PC1	O31-C31-C32-C33
3	D	602	PC1	C3-C2-O21-C21
3	E	405	PC1	C23-C24-C25-C26
3	B	603	PC1	C2-C1-O11-P
3	E	406	PC1	O32-C31-C32-C33
3	B	604	PC1	O32-C31-C32-C33
3	B	601	PC1	O32-C31-C32-C33
3	E	404	PC1	O22-C21-C22-C23
3	B	604	PC1	O21-C21-C22-C23
3	B	603	PC1	O32-C31-C32-C33
3	D	602	PC1	C28-C29-C2A-C2B
3	C	603	PC1	O32-C31-C32-C33
3	A	502	PC1	O22-C21-C22-C23
3	B	604	PC1	O22-C21-C22-C23
3	E	406	PC1	O21-C21-C22-C23
3	A	504	PC1	O32-C31-C32-C33

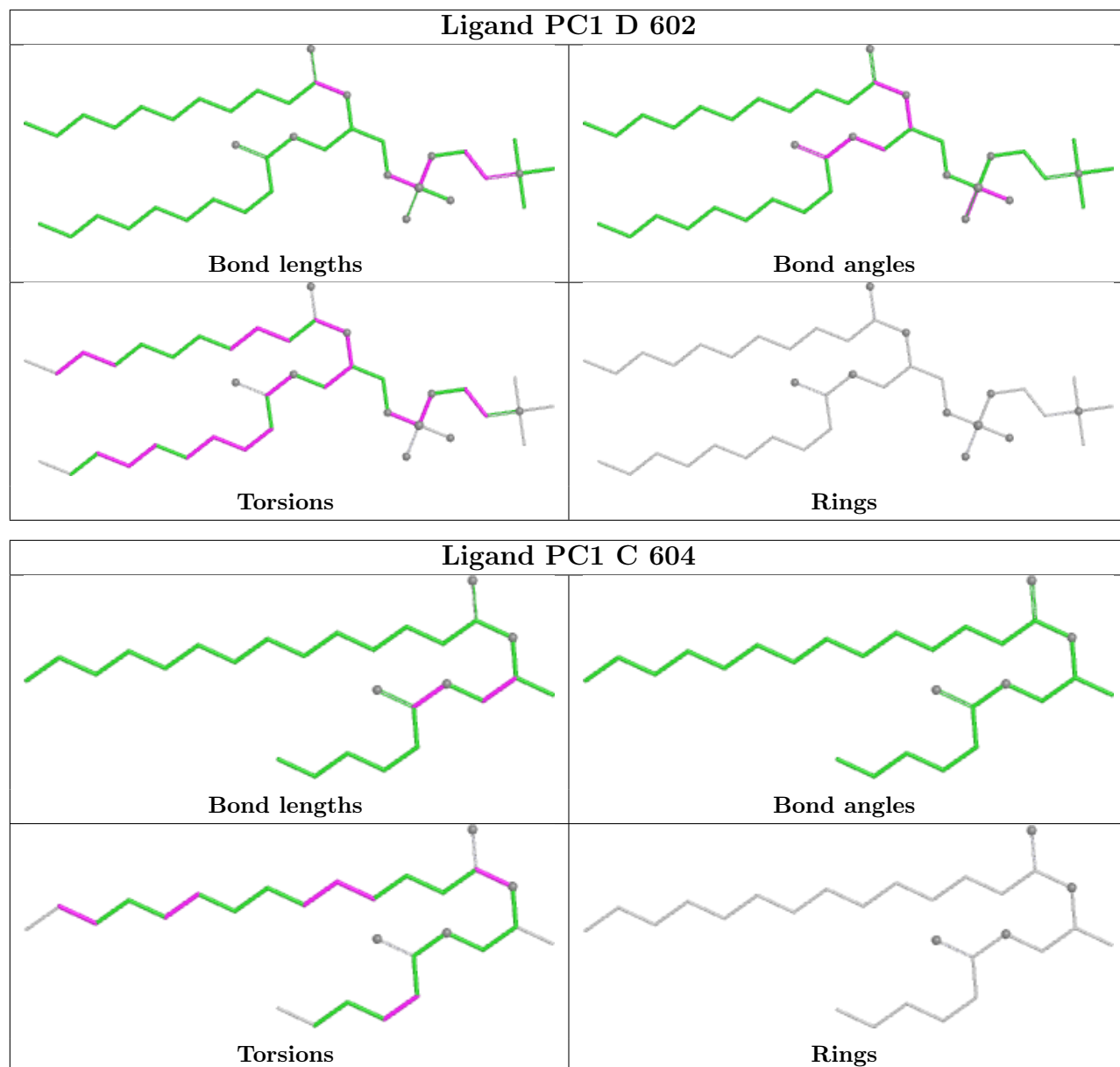
There are no ring outliers.

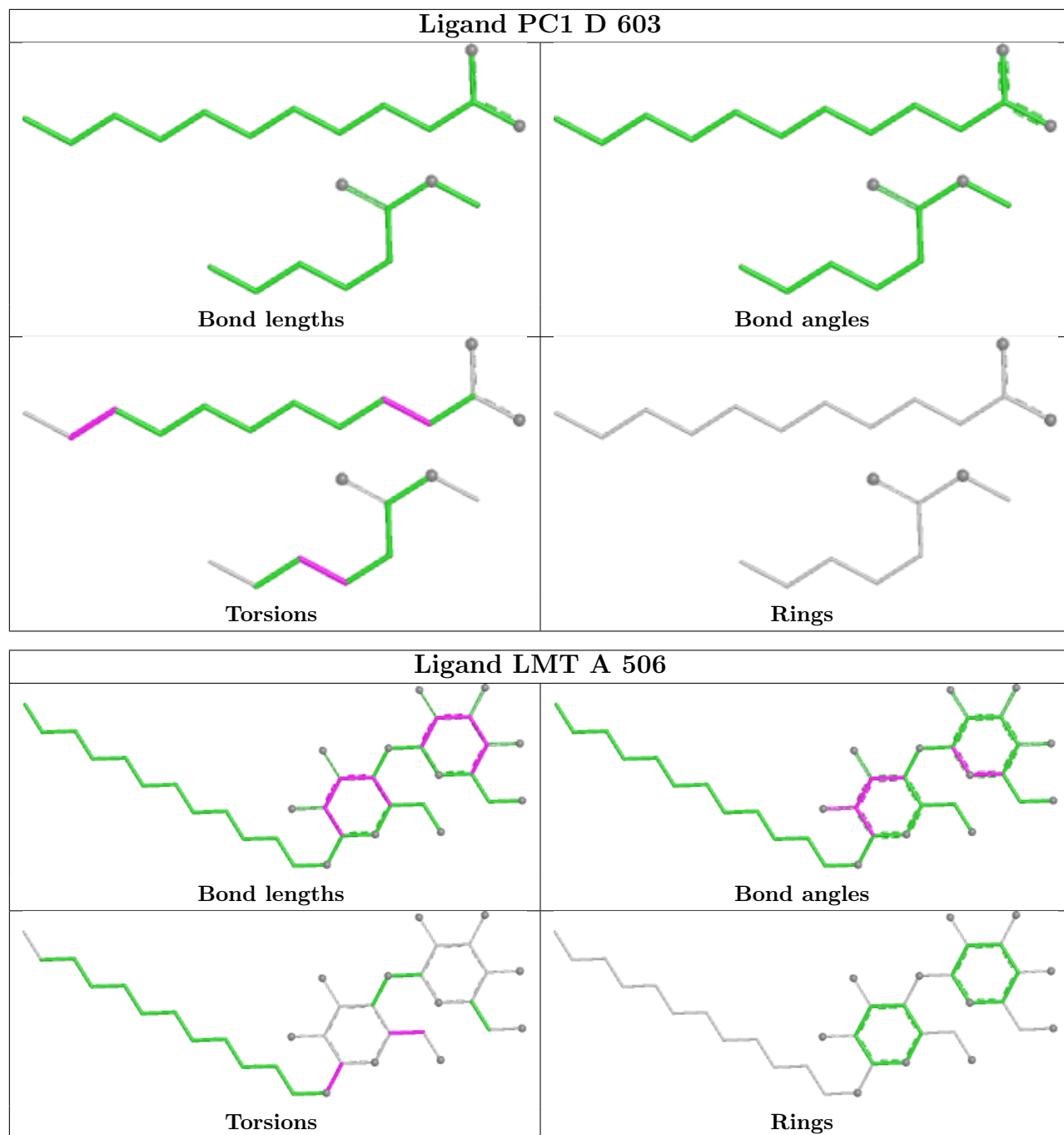
25 monomers are involved in 55 short contacts:

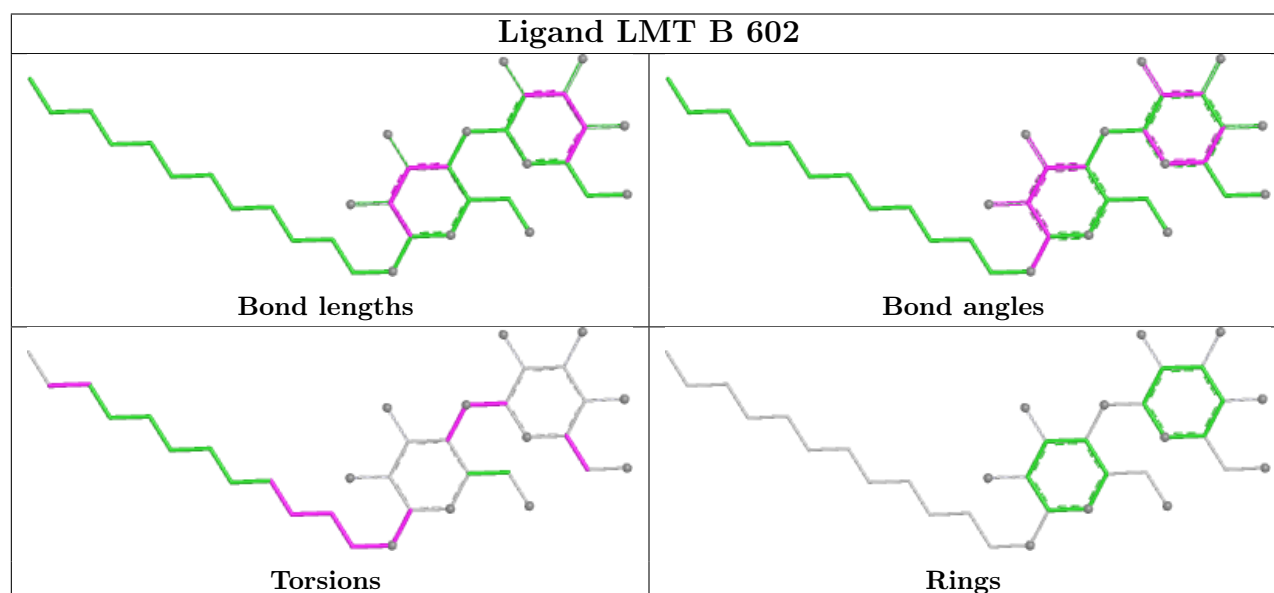
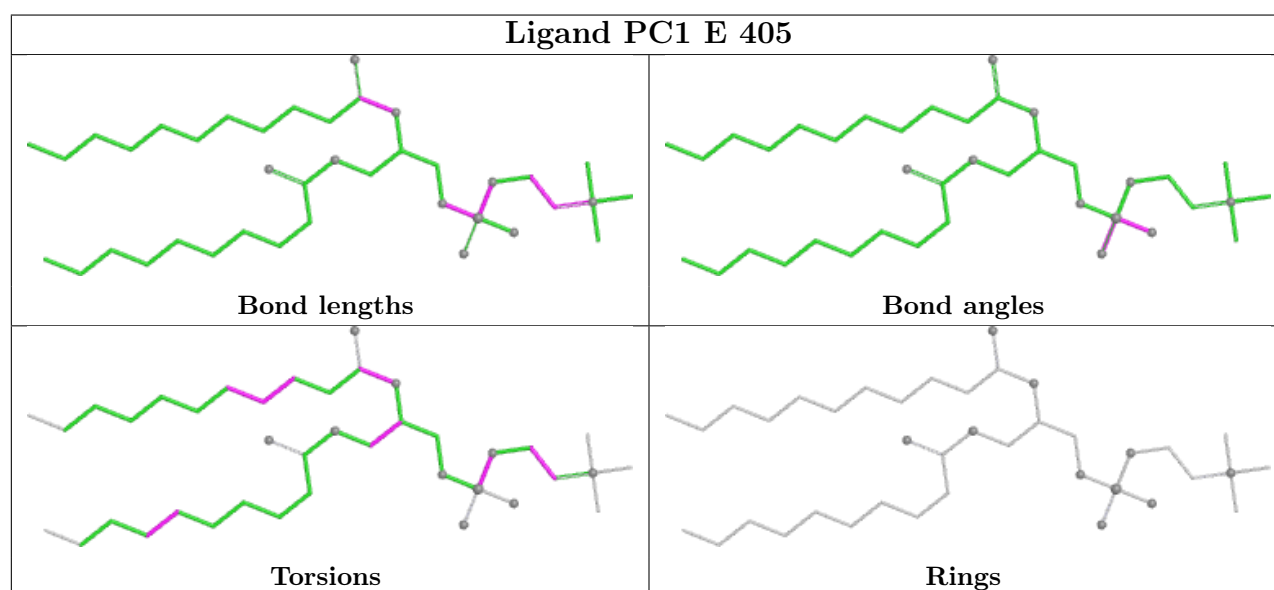
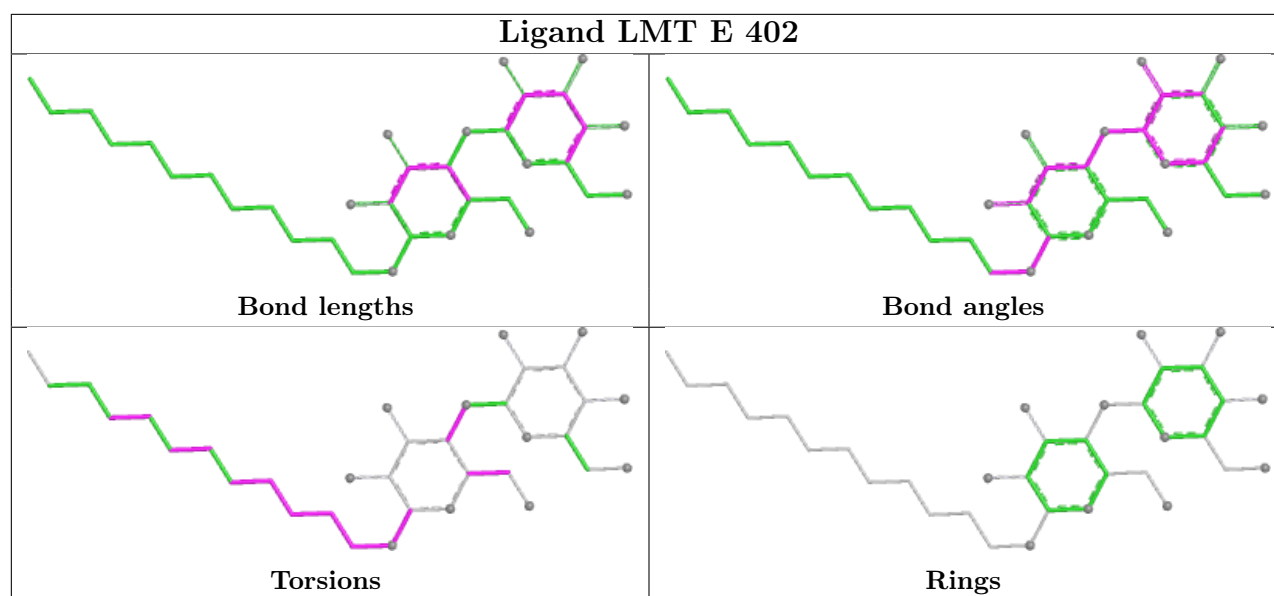
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	505	ACT	5	0
4	D	608	ACT	2	0
5	A	507	6E3	1	0
3	E	406	PC1	2	0
3	D	602	PC1	3	0
3	C	604	PC1	1	0
3	D	603	PC1	1	0
2	A	506	LMT	5	0
4	A	510	ACT	5	0
4	B	607	ACT	3	0
2	B	602	LMT	3	0
3	C	603	PC1	2	0
2	E	403	LMT	3	0
3	B	603	PC1	1	0
2	A	501	LMT	2	0
3	C	601	PC1	1	0
3	A	502	PC1	1	0
3	B	604	PC1	2	0
4	E	401	ACT	2	0
3	D	601	PC1	1	0
4	A	509	ACT	4	0
3	A	504	PC1	2	0
4	C	608	ACT	3	0
3	E	404	PC1	3	0
3	B	601	PC1	3	0

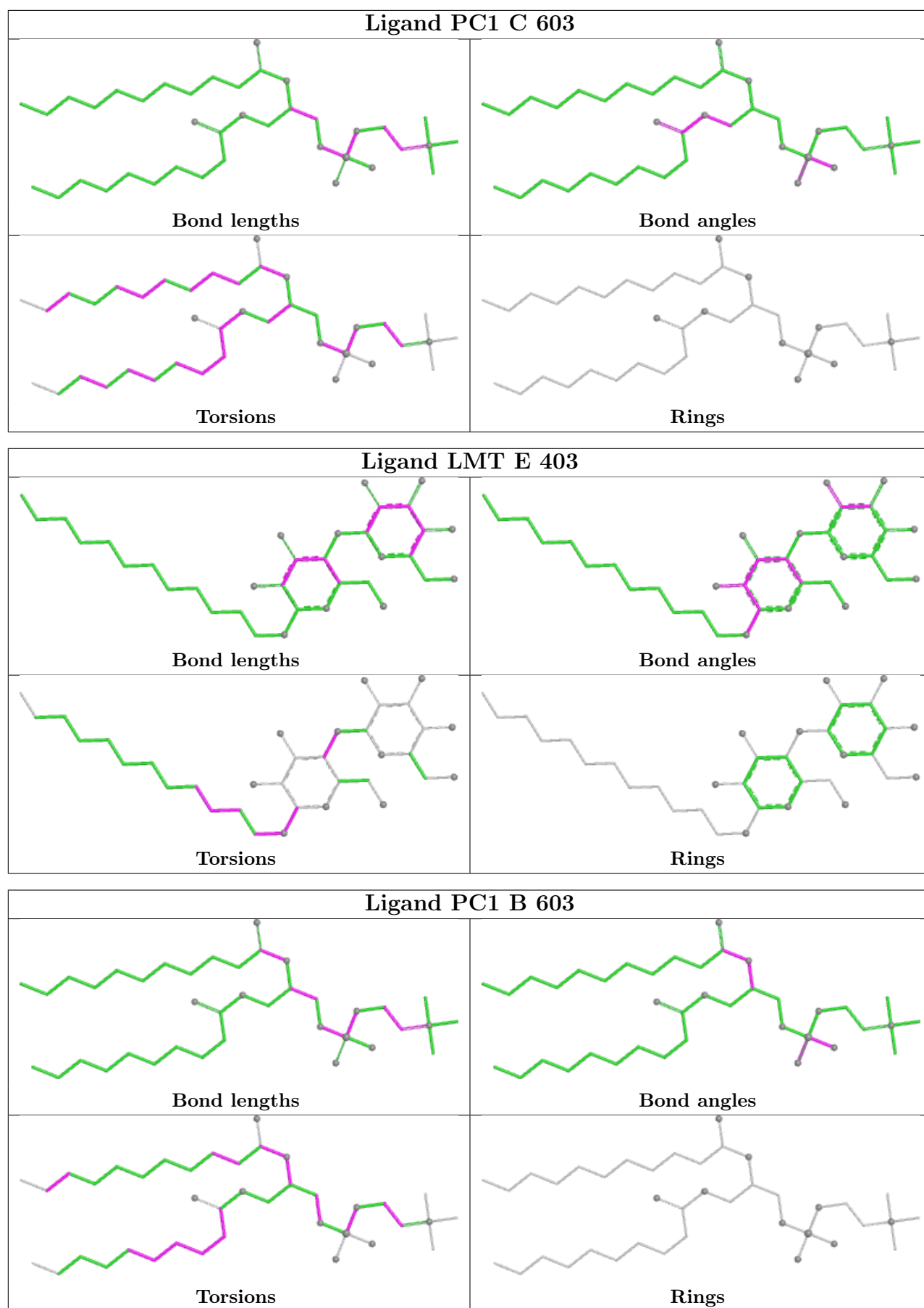
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

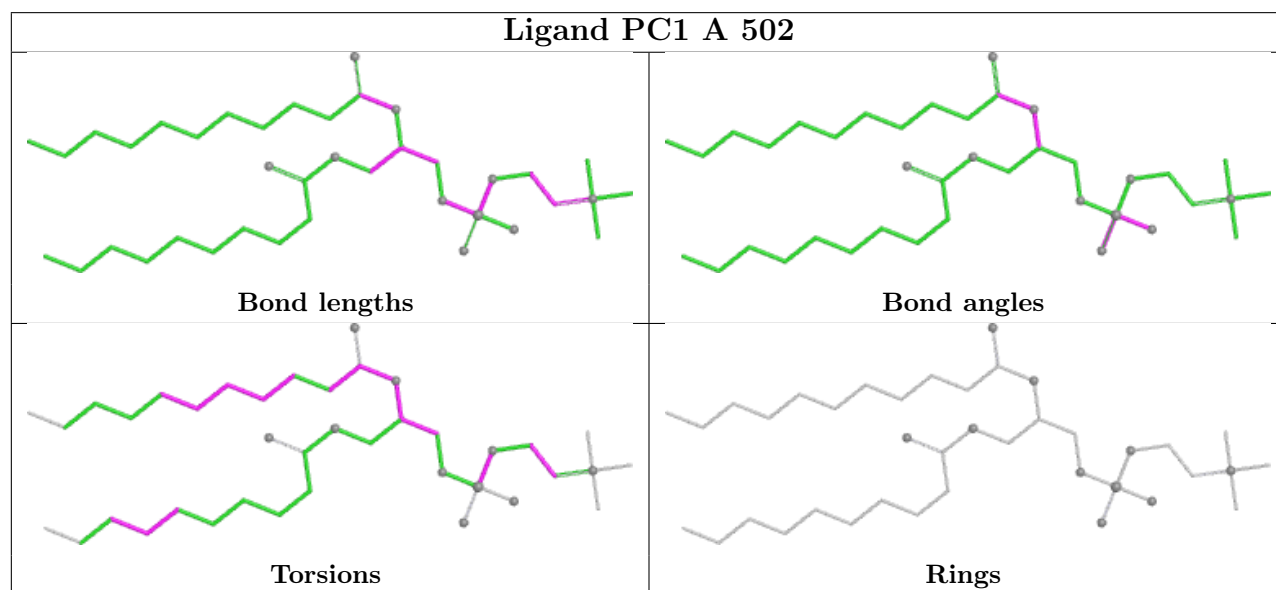
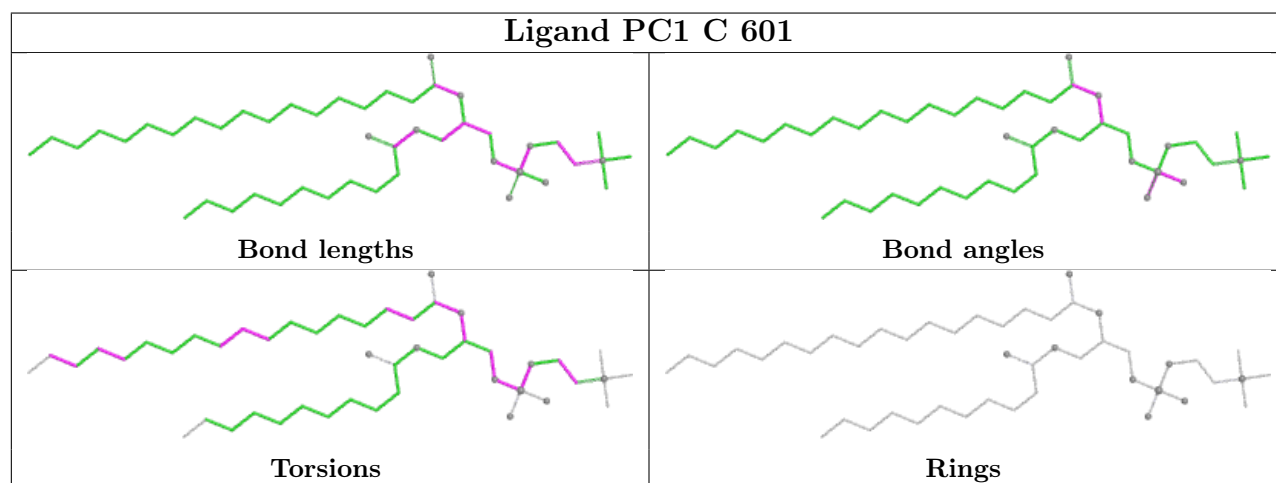
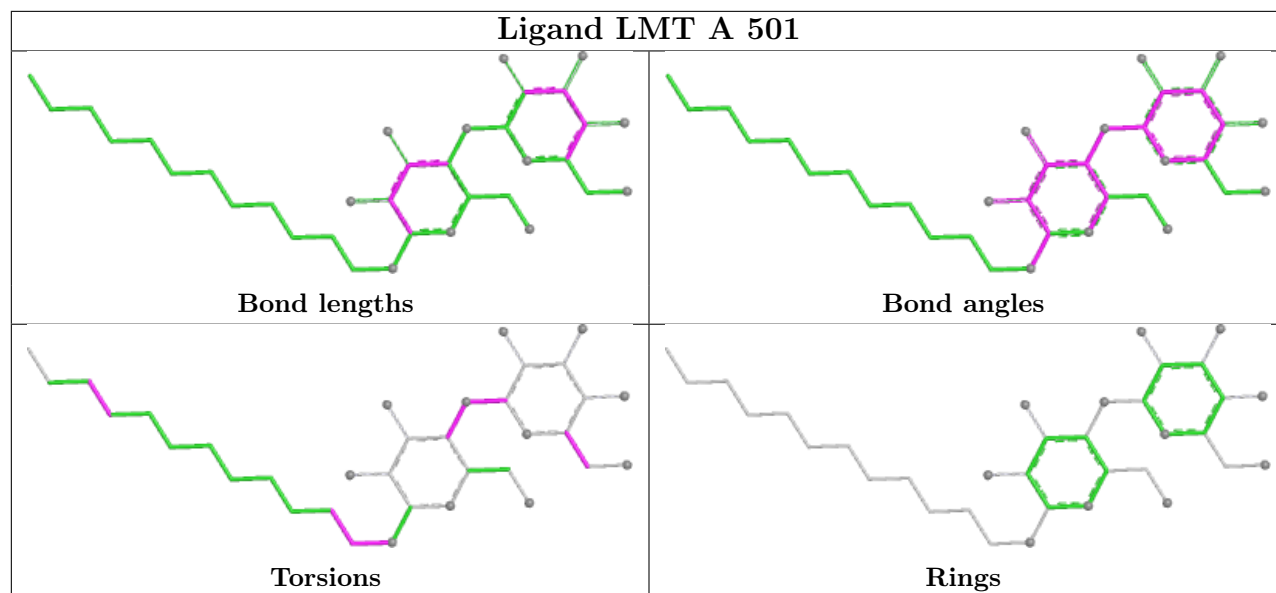


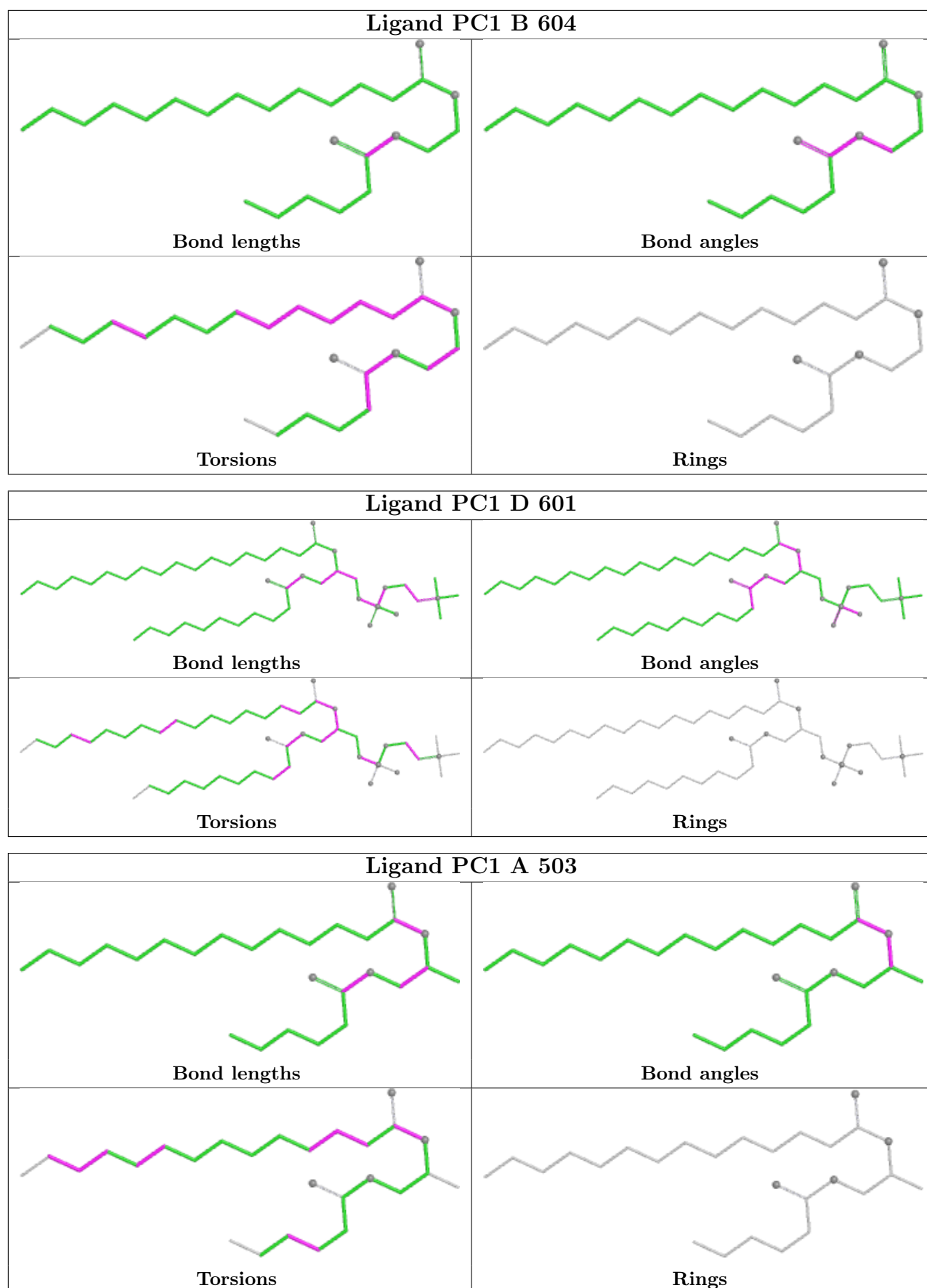


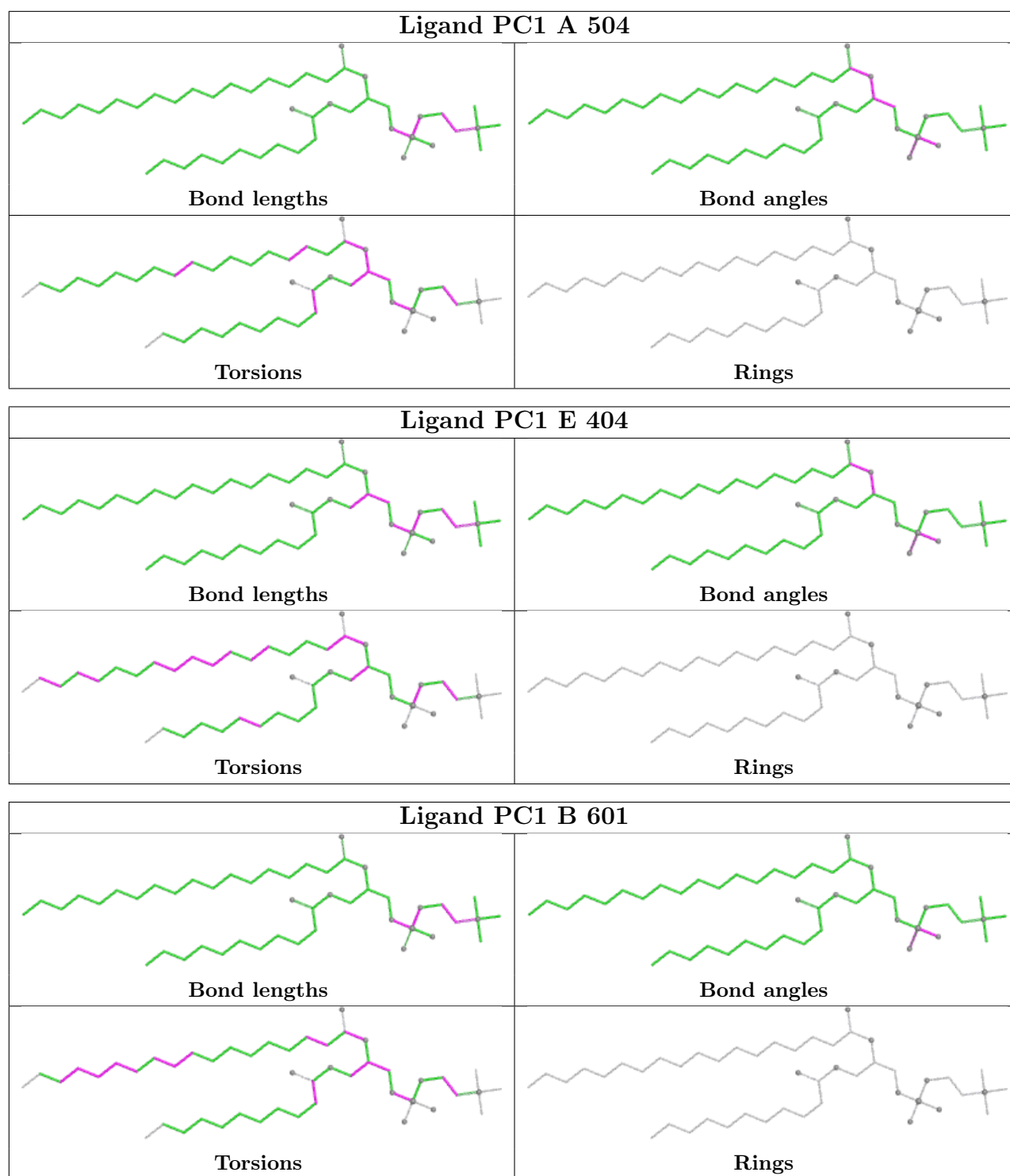












5.7 Other polymers [\(i\)](#)

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	311/317 (98%)	0.00	12 (3%) 43 38	57, 79, 126, 155	0
1	B	311/317 (98%)	-0.02	7 (2%) 61 55	39, 79, 112, 132	1 (0%)
1	C	311/317 (98%)	0.02	7 (2%) 61 55	39, 79, 124, 164	1 (0%)
1	D	311/317 (98%)	0.02	10 (3%) 50 44	40, 81, 122, 155	1 (0%)
1	E	311/317 (98%)	0.00	8 (2%) 57 51	38, 81, 126, 149	1 (0%)
All	All	1555/1585 (98%)	0.00	44 (2%) 55 49	38, 80, 123, 164	4 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	11	ILE	3.9
1	E	5	VAL	3.8
1	A	84	ALA	3.7
1	E	61	VAL	3.7
1	D	12	ALA	3.6
1	C	5	VAL	3.6
1	E	12	ALA	3.5
1	D	57	VAL	3.5
1	B	84	ALA	3.4
1	B	12	ALA	3.4
1	B	280[A]	LYS	3.3
1	A	14	GLU	3.2
1	D	61	VAL	3.2
1	B	5	VAL	3.1
1	A	57	VAL	3.0
1	A	12	ALA	2.9
1	E	84	ALA	2.9
1	A	5	VAL	2.9
1	A	61	VAL	2.9
1	C	54	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	86	ASP	2.7
1	E	86	ASP	2.7
1	E	11	ILE	2.6
1	A	86	ASP	2.5
1	A	10	PRO	2.5
1	A	56	PRO	2.5
1	D	5	VAL	2.5
1	D	84	ALA	2.5
1	C	61	VAL	2.4
1	E	137	THR	2.4
1	D	54	PHE	2.4
1	C	56	PRO	2.3
1	D	139	ASN	2.2
1	D	137	THR	2.2
1	D	83	ASN	2.1
1	B	13	ASP	2.1
1	C	12	ALA	2.1
1	E	57	VAL	2.1
1	C	180	LEU	2.1
1	D	180	LEU	2.1
1	C	293	ARG	2.0
1	A	62	ARG	2.0
1	B	136	ASP	2.0
1	A	59	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

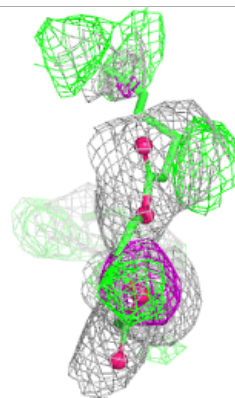
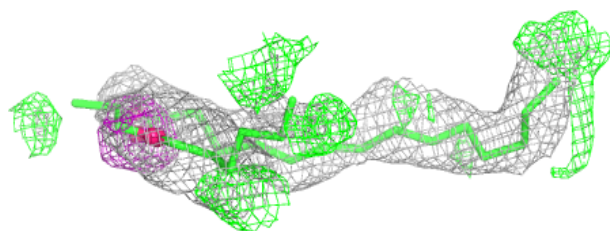
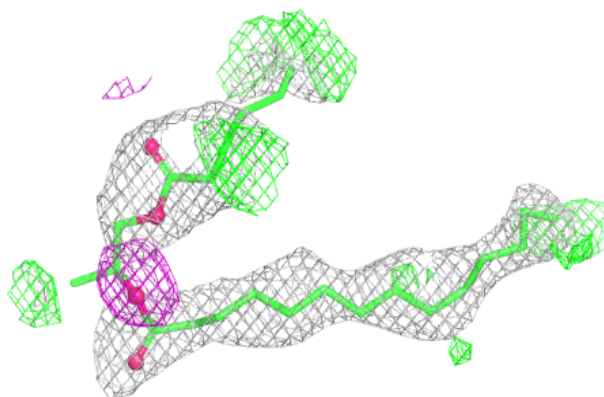
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PC1	A	503	27/54	0.58	0.21	96,123,134,134	0
5	6E3	D	604	14/14	0.60	0.20	137,153,156,156	0
6	BR	B	605	1/1	0.60	0.22	245,245,245,245	0
3	PC1	C	604	27/54	0.61	0.20	94,113,132,133	0
3	PC1	E	406	27/54	0.64	0.20	95,112,134,135	0
4	ACT	D	607	4/4	0.64	0.20	93,93,99,100	0
3	PC1	A	504	47/54	0.65	0.19	98,113,135,137	0
4	ACT	C	608	4/4	0.66	0.20	119,119,121,123	0
3	PC1	C	601	47/54	0.66	0.19	99,118,147,148	0
3	PC1	A	502	39/54	0.68	0.17	82,111,149,150	0
4	ACT	D	608	4/4	0.69	0.22	118,118,122,123	0
4	ACT	A	509	4/4	0.70	0.17	96,96,102,104	0
5	6E3	A	507	14/14	0.70	0.19	136,151,152,152	0
3	PC1	D	603	22/54	0.70	0.20	100,114,133,135	0
3	PC1	D	601	47/54	0.70	0.19	103,116,144,146	0
3	PC1	D	602	39/54	0.72	0.18	89,118,154,155	0
3	PC1	B	603	39/54	0.73	0.17	82,121,151,152	0
3	PC1	C	603	39/54	0.74	0.16	102,126,166,167	0
3	PC1	E	404	47/54	0.74	0.17	96,112,141,142	0
3	PC1	B	604	26/54	0.75	0.17	90,108,125,125	0
3	PC1	B	601	47/54	0.75	0.18	109,117,143,144	0
3	PC1	E	405	39/54	0.76	0.16	96,129,157,157	0
6	BR	C	605	1/1	0.76	0.21	238,238,238,238	0
4	ACT	A	510	4/4	0.81	0.20	125,125,128,130	0
2	LMT	E	403	35/35	0.82	0.19	70,156,174,175	0
4	ACT	E	401	4/4	0.82	0.15	112,112,114,115	0
7	NA	B	606	1/1	0.82	0.11	101,101,101,101	0
7	NA	D	606	1/1	0.82	0.32	117,117,117,117	0
6	BR	E	407	1/1	0.83	0.19	235,235,235,235	0
4	ACT	A	505	4/4	0.84	0.16	107,107,110,111	0
6	BR	D	605	1/1	0.87	0.14	201,201,201,201	0
7	NA	E	408	1/1	0.87	0.20	112,112,112,112	0
4	ACT	C	607	4/4	0.88	0.10	103,104,104,104	0
2	LMT	B	602	35/35	0.88	0.15	64,149,169,171	0
2	LMT	A	501	35/35	0.89	0.14	57,145,160,161	0
2	LMT	C	602	35/35	0.89	0.15	50,146,167,169	0
2	LMT	E	402	35/35	0.89	0.13	52,141,164,164	0
2	LMT	A	506	35/35	0.89	0.15	75,146,162,162	0
6	BR	A	508	1/1	0.90	0.12	195,195,195,195	0
7	NA	C	606	1/1	0.91	0.09	90,90,90,90	0
4	ACT	B	607	4/4	0.91	0.09	93,94,95,95	0
4	ACT	E	409	4/4	0.91	0.08	94,96,99,99	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.

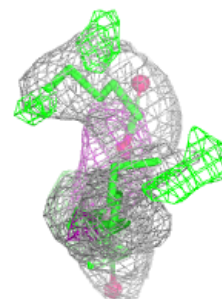
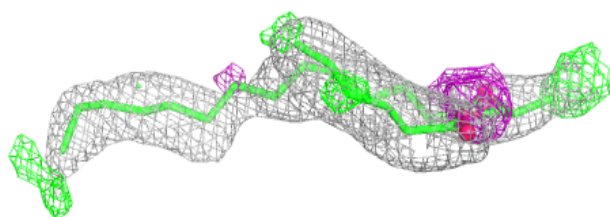
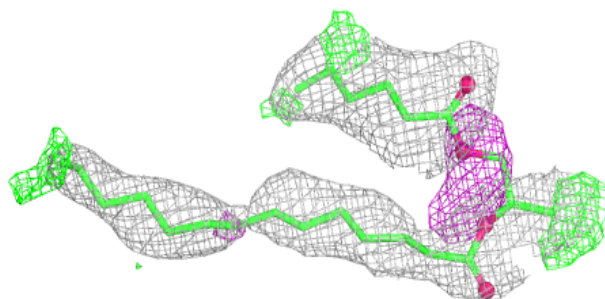
Electron density around PC1 A 503:

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

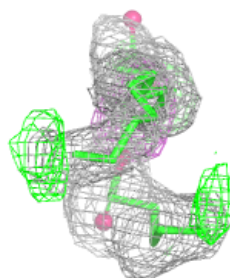
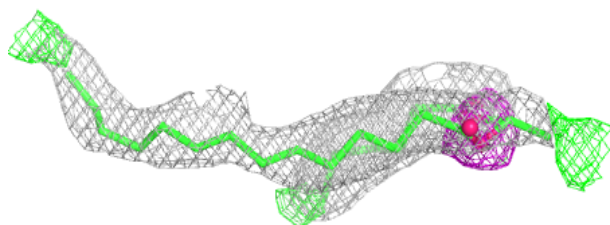
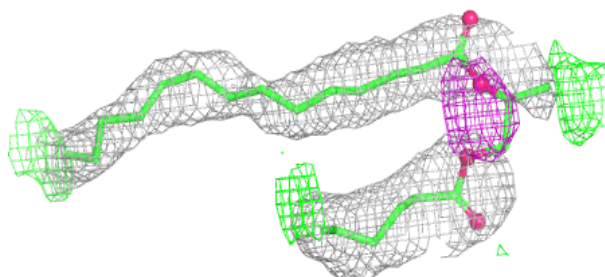


Electron density around PC1 C 604:

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

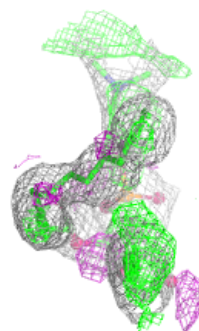
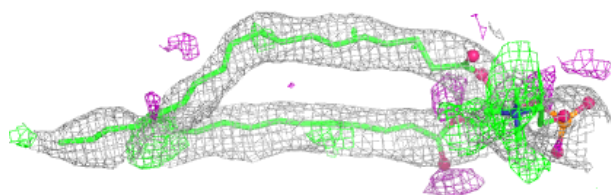
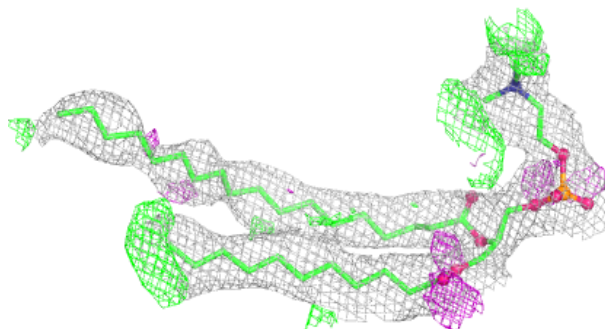
**Electron density around PC1 E 406:**

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

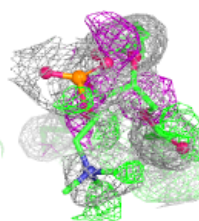
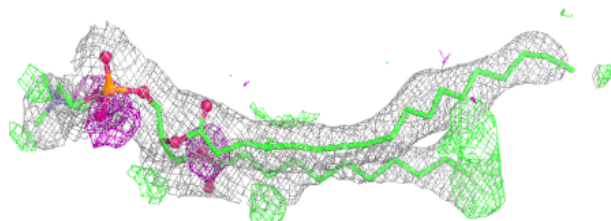
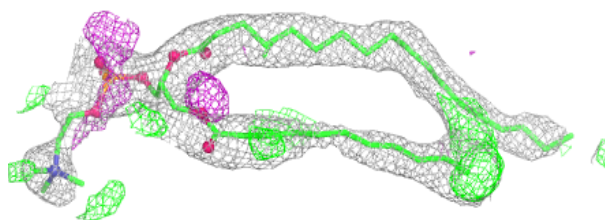


Electron density around PC1 A 504:

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

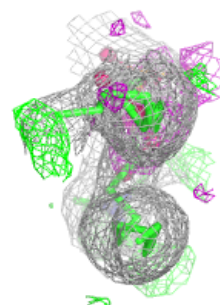
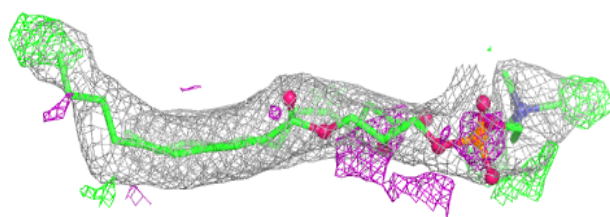
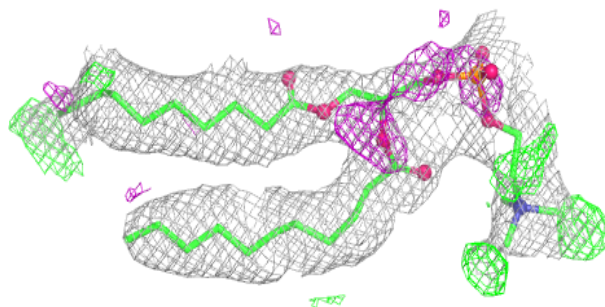
**Electron density around PC1 C 601:**

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

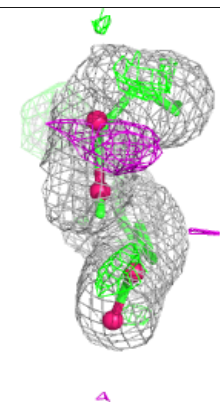
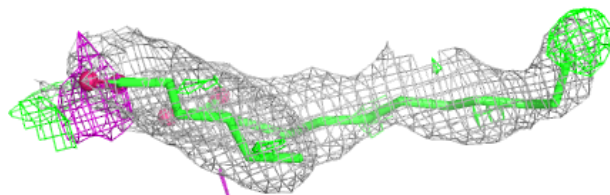
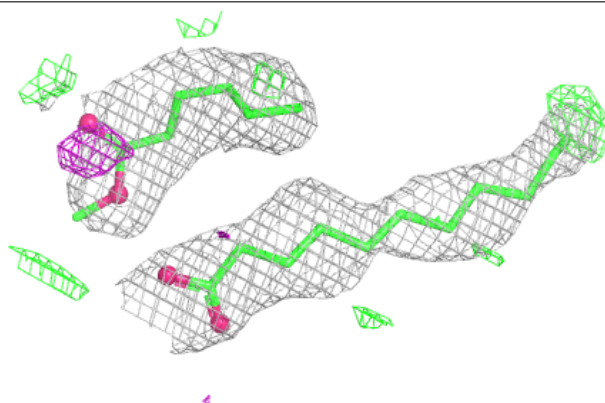


Electron density around PC1 A 502:

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

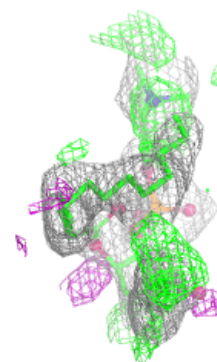
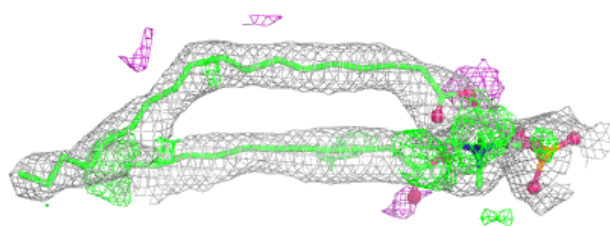
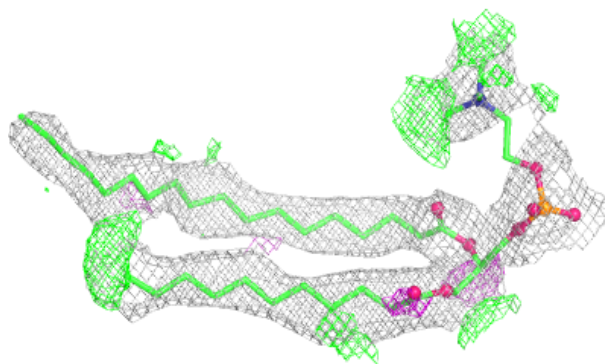
**Electron density around PC1 D 603:**

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

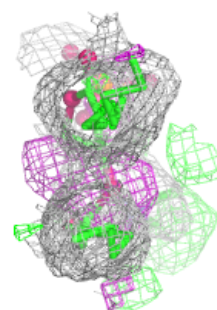
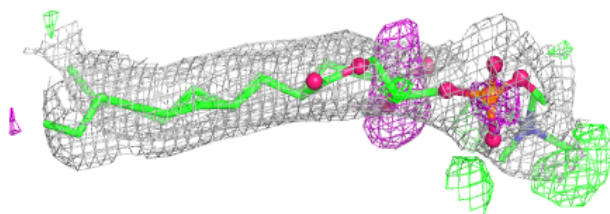
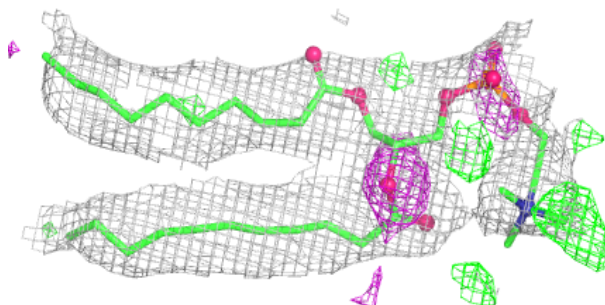


Electron density around PC1 D 601:

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

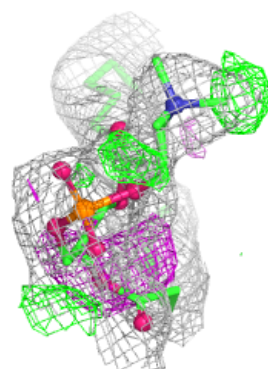
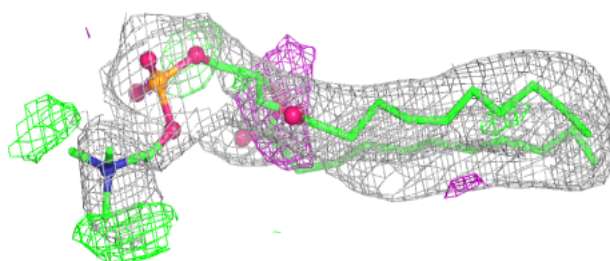
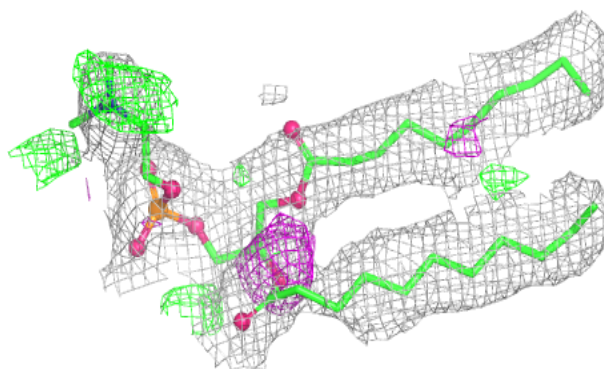
**Electron density around PC1 D 602:**

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

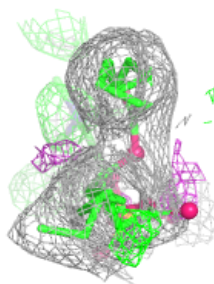
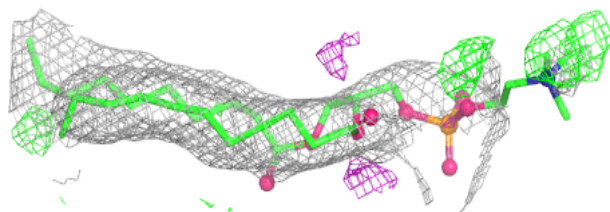
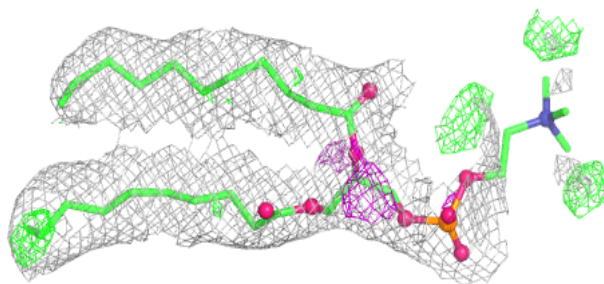


Electron density around PC1 B 603:

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

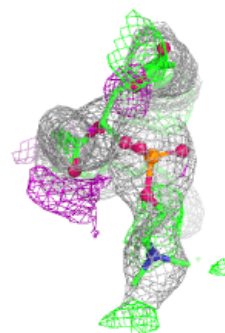
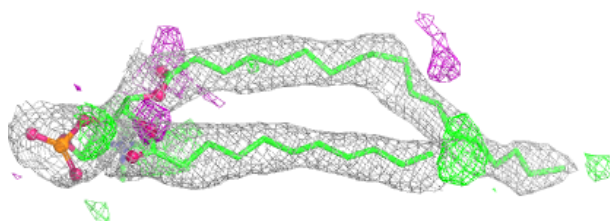
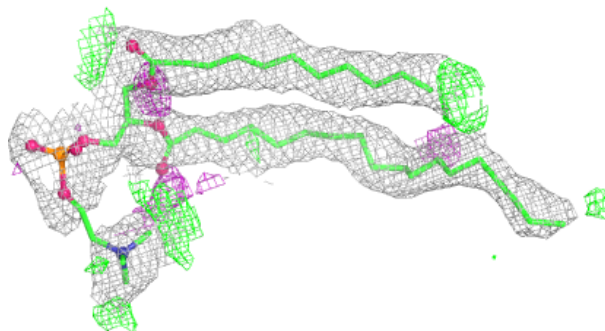
**Electron density around PC1 C 603:**

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

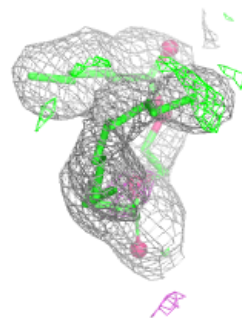
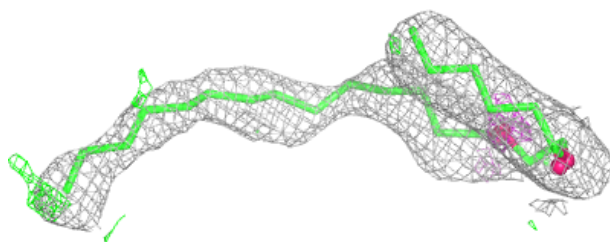
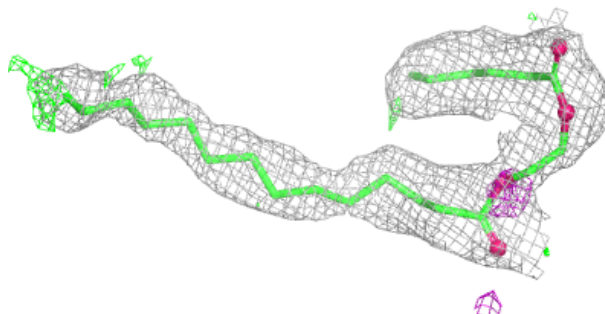


Electron density around PC1 E 404:

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

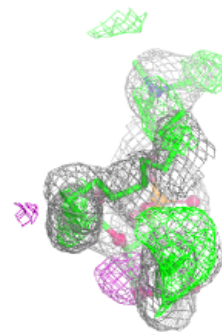
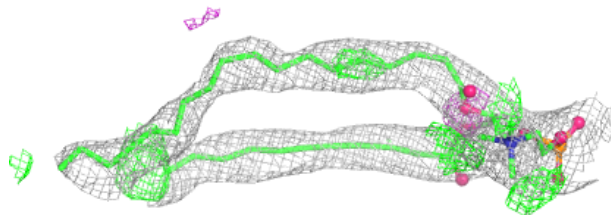
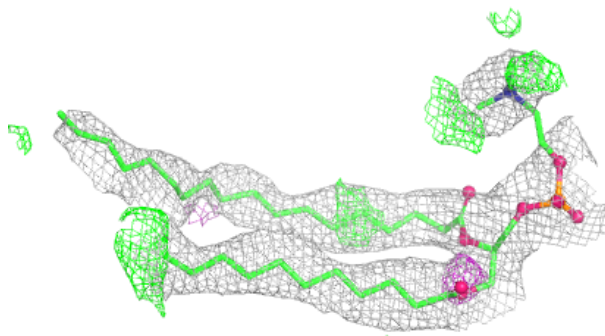
**Electron density around PC1 B 604:**

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

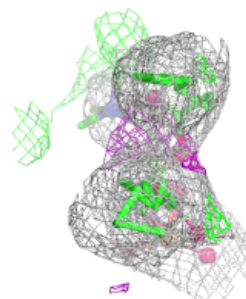
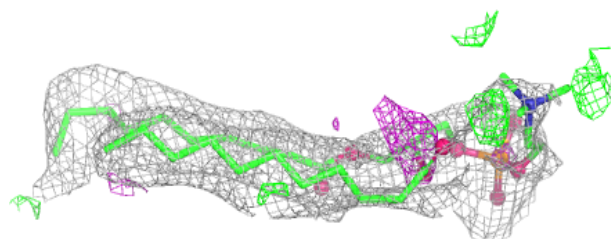
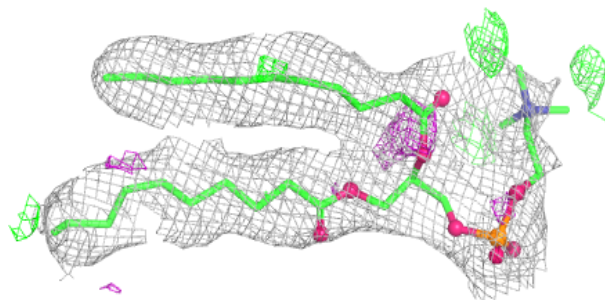


Electron density around PC1 B 601:

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

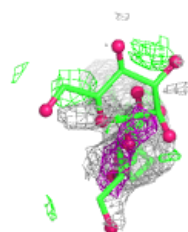
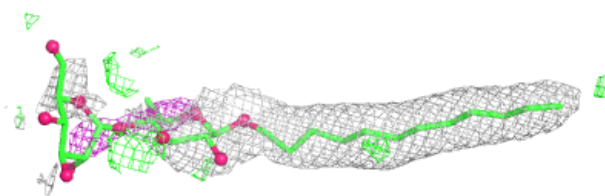
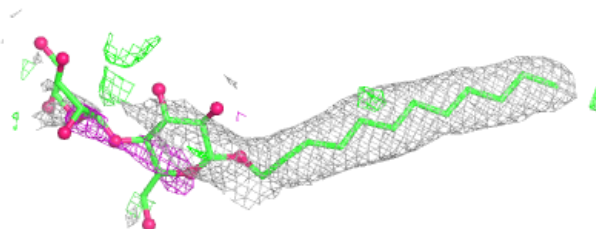
**Electron density around PC1 E 405:**

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

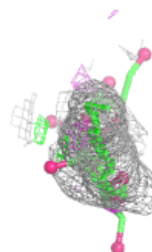
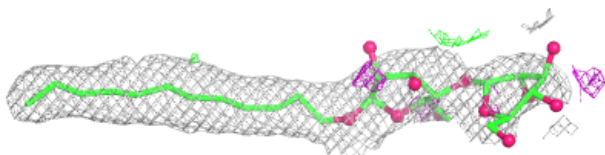
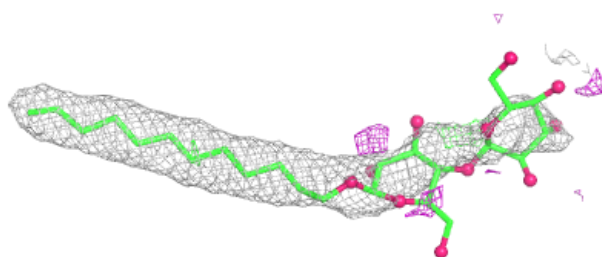


Electron density around LMT E 403:

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

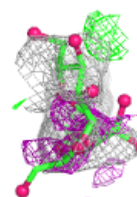
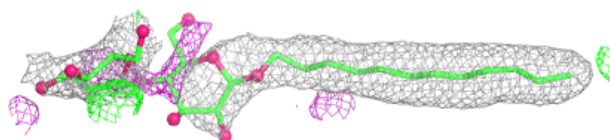
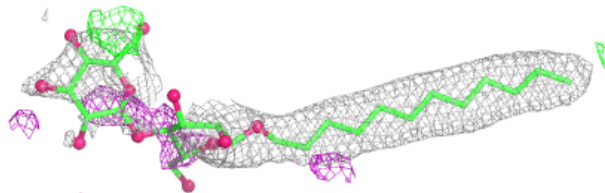
**Electron density around LMT B 602:**

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

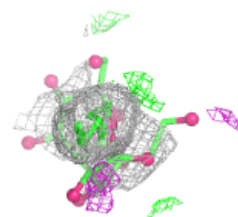
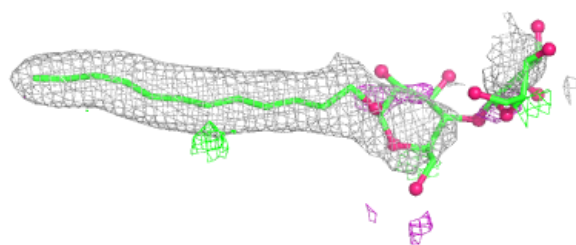
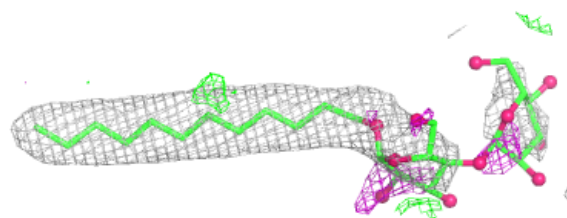


Electron density around LMT A 501:

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

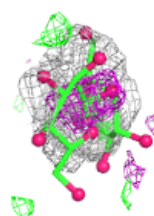
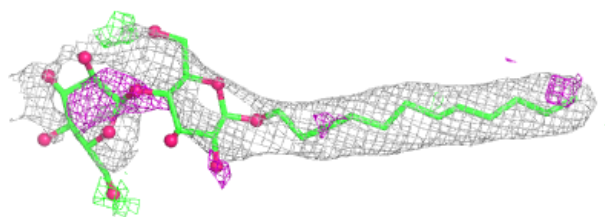
**Electron density around LMT C 602:**

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

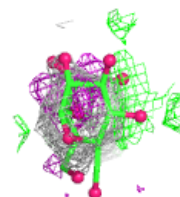
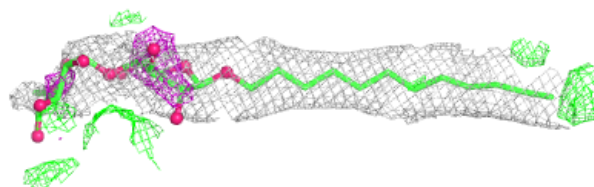
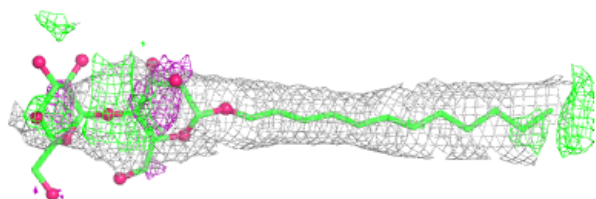


Electron density around LMT E 402:

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

**Electron density around LMT A 506:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.