



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 03:54 PM EDT

PDB ID : 3EAM / pdb_00003eam
Title : An open-pore structure of a bacterial pentameric ligand-gated ion channel
Authors : Bocquet, N.; Nury, H.; Baaden, M.; Le Poupon, C.; Changeux, J.P.; Delarue, M.; Corringer, P.J.
Deposited on : 2008-08-26
Resolution : 2.90 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

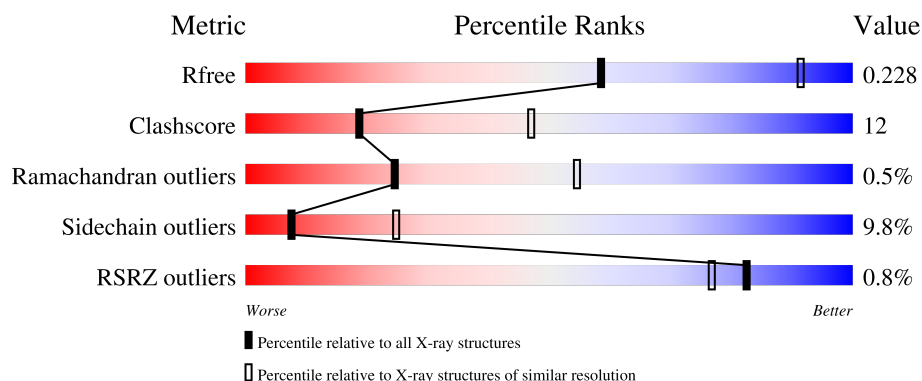
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	% 68% 26% 5% .
1	B	317	% 72% 22% . .
1	C	317	% 67% 27% . . .
1	D	317	% 68% 24% 5% .
1	E	317	% 72% 22% . .

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LMT	A	501	X	-	-	-
2	LMT	B	501	X	-	-	-
2	LMT	C	501	X	-	-	-
2	LMT	C	502	X	-	-	-
2	LMT	E	501	X	-	-	-
2	LMT	E	602	X	-	-	-
3	PC1	A	601	X	-	-	-
3	PC1	A	602	X	-	-	-
3	PC1	A	603	X	-	-	-
3	PC1	B	601	X	-	-	-
3	PC1	B	602	X	-	-	-
3	PC1	C	601	X	-	-	-
3	PC1	C	602	X	-	-	-
3	PC1	C	603	X	-	-	-
3	PC1	D	601	X	-	-	-
3	PC1	D	602	X	-	-	-
3	PC1	E	601	X	-	-	-
3	PC1	E	603	X	-	-	-
3	PC1	E	604	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13505 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.

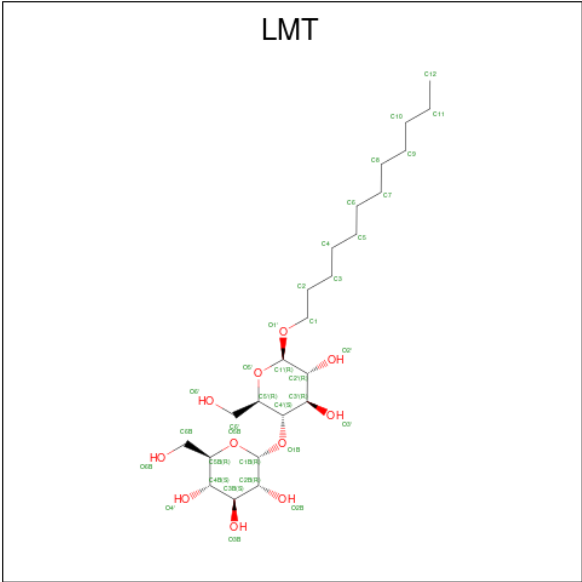
- Molecule 1 is a protein called Glr4197 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	S	0	0	0
			2525	1664	404	453	4			
1	B	311	Total	C	N	O	S	0	0	0
			2525	1664	404	453	4			
1	C	311	Total	C	N	O	S	0	0	0
			2525	1664	404	453	4			
1	D	311	Total	C	N	O	S	0	0	0
			2525	1664	404	453	4			
1	E	311	Total	C	N	O	S	0	0	0
			2525	1664	404	453	4			

There are 5 discrepancies between the modelled and reference sequences:

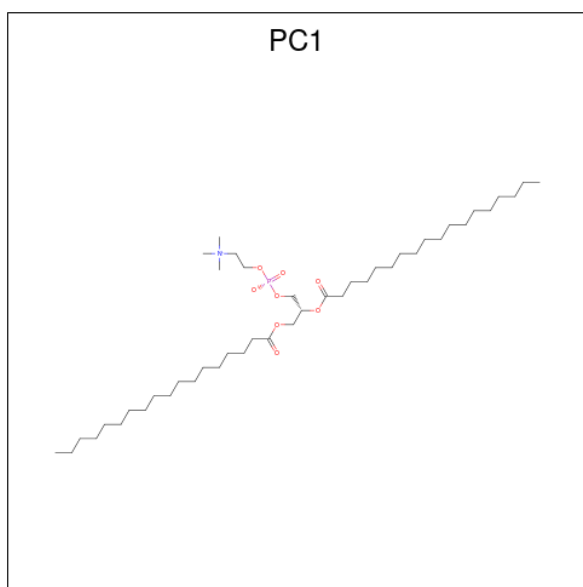
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	GLY	conflict	UNP Q7NDN8
B	1	ALA	GLY	conflict	UNP Q7NDN8
C	1	ALA	GLY	conflict	UNP Q7NDN8
D	1	ALA	GLY	conflict	UNP Q7NDN8
E	1	ALA	GLY	conflict	UNP Q7NDN8

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



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

- Molecule 3 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



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		

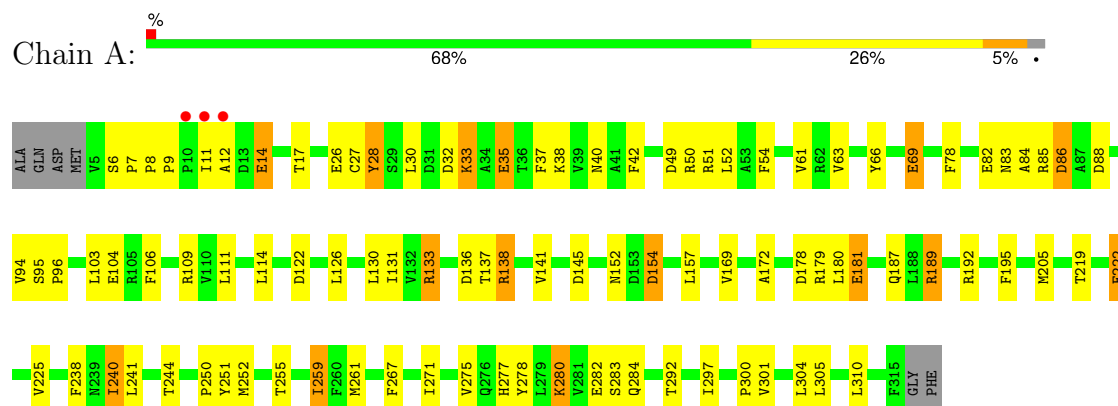
- Molecule 4 is water.

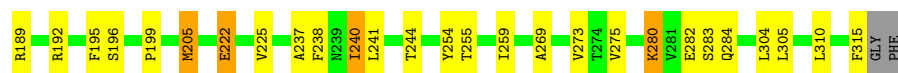
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	20	Total	O	0	0
			20	20		
4	B	24	Total	O	0	0
			24	24		
4	C	21	Total	O	0	0
			21	21		
4	D	24	Total	O	0	0
			24	24		
4	E	22	Total	O	0	0
			22	22		

3 Residue-property plots

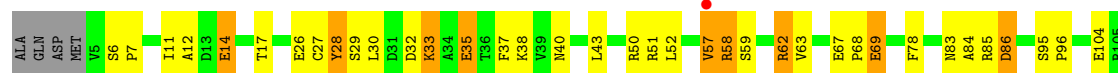
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Glr4197 protein





• Molecule 1: Glr4197 protein



• Molecule 1: Glr4197 protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	183.32Å 133.64Å 160.18Å 90.00° 102.94° 90.00°	Depositor
Resolution (Å)	10.00 – 2.90 10.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (10.00-2.90) 97.4 (10.00-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.89Å)	Xtriage
Refinement program	REFMAC 5.4.0073	Depositor
R, R_{free}	0.199 , 0.231 0.197 , 0.228	Depositor DCC
R_{free} test set	4063 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	59.1	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 63.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13505	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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: PC1, LMT

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	1.26	3/2593 (0.1%)	1.22	10/3545 (0.3%)
1	B	1.23	2/2593 (0.1%)	1.27	10/3545 (0.3%)
1	C	1.29	6/2593 (0.2%)	1.24	12/3545 (0.3%)
1	D	1.22	2/2593 (0.1%)	1.20	10/3545 (0.3%)
1	E	1.22	3/2593 (0.1%)	1.18	8/3545 (0.2%)
All	All	1.24	16/12965 (0.1%)	1.22	50/17725 (0.3%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	73	ILE	CA-CB	-10.79	1.46	1.54
1	A	240	ILE	CA-CB	-6.05	1.47	1.54
1	C	87	ALA	C-O	-5.83	1.17	1.24
1	B	136	ASP	CA-C	5.71	1.60	1.52
1	E	286	ALA	CA-CB	-5.67	1.44	1.53
1	E	11	ILE	CA-CB	5.64	1.60	1.54
1	A	169	VAL	CA-CB	5.52	1.62	1.54
1	A	172	ALA	CA-CB	-5.46	1.46	1.53
1	D	183	LYS	CA-C	5.33	1.58	1.52
1	C	240	ILE	N-CA	-5.26	1.40	1.46
1	C	205	MET	N-CA	-5.23	1.40	1.46
1	B	199	PRO	CA-C	5.20	1.60	1.52
1	D	180	LEU	N-CA	-5.17	1.39	1.46
1	C	269	ALA	CA-CB	-5.15	1.45	1.53
1	E	275	VAL	CA-CB	-5.04	1.48	1.54
1	C	149	VAL	C-O	-5.01	1.18	1.24

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	109	ARG	NE-CZ-NH2	13.40	131.26	119.20
1	B	109	ARG	NE-CZ-NH1	-10.70	110.80	121.50
1	D	179	ARG	NE-CZ-NH2	8.64	126.98	119.20
1	D	179	ARG	NE-CZ-NH1	-8.54	112.96	121.50
1	C	179	ARG	NE-CZ-NH1	-8.51	112.99	121.50
1	B	109	ARG	CD-NE-CZ	8.46	136.25	124.40
1	A	284	GLN	CA-C-N	8.35	128.47	119.28
1	A	284	GLN	C-N-CA	8.35	128.47	119.28
1	C	284	GLN	CA-C-N	8.15	127.80	119.56
1	C	284	GLN	C-N-CA	8.15	127.80	119.56
1	E	284	GLN	CA-C-N	8.11	127.75	119.56
1	E	284	GLN	C-N-CA	8.11	127.75	119.56
1	B	284	GLN	CA-C-N	7.98	127.62	119.56
1	B	284	GLN	C-N-CA	7.98	127.62	119.56
1	C	179	ARG	NE-CZ-NH2	7.74	126.17	119.20
1	D	284	GLN	CA-C-N	7.71	127.76	119.28
1	D	284	GLN	C-N-CA	7.71	127.76	119.28
1	A	222	GLU	CB-CA-C	7.06	121.97	110.88
1	B	95	SER	CB-CA-C	6.77	118.61	108.86
1	E	138	ARG	N-CA-C	6.50	118.03	108.14
1	D	138	ARG	N-CA-C	6.31	118.11	108.07
1	A	282	GLU	N-CA-C	-6.14	105.72	112.72
1	C	179	ARG	CD-NE-CZ	6.10	132.94	124.40
1	C	315	PHE	CA-C-O	6.09	131.16	120.80
1	B	138	ARG	N-CA-C	6.09	117.39	108.14
1	D	179	ARG	CD-NE-CZ	6.03	132.84	124.40
1	C	282	GLU	N-CA-C	-5.99	105.29	112.59
1	A	138	ARG	N-CA-C	5.93	117.51	108.07
1	E	202	ILE	N-CA-C	5.82	116.01	110.42
1	A	88	ASP	CB-CA-C	-5.82	100.15	109.75
1	E	282	GLU	N-CA-C	-5.81	106.10	112.72
1	D	282	GLU	N-CA-C	-5.57	106.37	112.72
1	A	136	ASP	N-CA-C	5.54	117.40	111.36
1	C	179	ARG	CG-CD-NE	-5.50	99.89	112.00
1	A	154	ASP	CB-CA-C	-5.50	99.59	110.27
1	C	178	ASP	N-CA-C	5.42	119.19	112.58
1	A	133	ARG	NE-CZ-NH2	-5.40	114.34	119.20
1	C	154	ASP	CB-CA-C	-5.39	99.18	110.17
1	E	88	ASP	CB-CA-C	-5.38	101.47	110.19
1	D	57	VAL	N-CA-C	5.33	116.00	110.82
1	C	144	VAL	CB-CA-C	-5.27	103.75	110.98
1	B	57	VAL	CB-CA-C	-5.26	102.66	111.29
1	A	301	VAL	N-CA-C	5.23	115.85	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	11	ILE	N-CA-CB	5.14	116.23	110.62
1	D	144	VAL	CB-CA-C	-5.09	104.00	110.98
1	D	179	ARG	CG-CD-NE	-5.09	100.81	112.00
1	C	11	ILE	N-CA-CB	5.05	116.12	110.62
1	E	11	ILE	N-CA-CB	5.04	116.11	110.62
1	B	61	VAL	N-CA-C	5.04	115.83	108.53
1	E	30	LEU	N-CA-C	-5.00	101.94	109.15

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	2525	0	2545	66	0
1	B	2525	0	2545	55	0
1	C	2525	0	2545	72	0
1	D	2525	0	2545	67	0
1	E	2525	0	2545	61	0
2	A	35	0	46	0	0
2	B	35	0	46	9	0
2	C	70	0	92	6	0
2	E	70	0	92	8	0
3	A	113	0	158	2	0
3	B	112	0	157	6	0
3	C	113	0	158	4	0
3	D	108	0	149	7	0
3	E	113	0	158	5	0
4	A	20	0	0	0	0
4	B	24	0	0	1	0
4	C	21	0	0	1	0
4	D	24	0	0	1	0
4	E	22	0	0	1	0
All	All	13505	0	13781	324	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 12.

All (324) 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:C:58:ARG:HG3	1:C:58:ARG:HH11	1.03	1.12
2:B:501:LMT:H6E	1:C:33:LYS:HE2	1.20	1.09
1:A:78:PHE:HE2	1:A:85:ARG:HD3	1.22	1.02
2:B:501:LMT:H6E	1:C:33:LYS:CE	1.94	0.97
1:B:78:PHE:HE2	1:B:85:ARG:HD3	1.31	0.95
1:C:58:ARG:HG3	1:C:58:ARG:NH1	1.71	0.95
1:A:54:PHE:CE2	1:A:96:PRO:HA	2.05	0.91
1:D:78:PHE:HE2	1:D:85:ARG:HD3	1.35	0.89
1:C:78:PHE:HE2	1:C:85:ARG:HD3	1.36	0.88
1:C:58:ARG:HH11	1:C:58:ARG:CG	1.86	0.88
1:E:187:GLN:OE1	1:E:189:ARG:NH2	2.07	0.87
1:D:6:SER:HB2	1:D:7:PRO:HD2	1.58	0.85
1:E:6:SER:HB2	1:E:7:PRO:HD2	1.56	0.85
1:E:78:PHE:HE2	1:E:85:ARG:HD3	1.39	0.85
1:E:133:ARG:NH1	1:E:176:LEU:O	2.10	0.84
1:A:63:VAL:HG21	1:B:136:ASP:OD1	1.77	0.84
1:E:55:ASP:O	1:E:59:SER:HB2	1.77	0.84
1:C:78:PHE:CE2	1:C:85:ARG:HD3	2.13	0.83
1:C:280:LYS:NZ	1:C:280:LYS:HB2	1.94	0.82
1:A:6:SER:HB2	1:A:7:PRO:HD2	1.62	0.82
1:D:62:ARG:HB3	1:D:62:ARG:HH11	1.43	0.82
2:B:501:LMT:H4B	2:B:501:LMT:O3'	1.79	0.81
1:C:133:ARG:NH1	1:C:176:LEU:O	2.13	0.81
1:A:187:GLN:OE1	1:A:189:ARG:NH2	2.12	0.80
1:B:78:PHE:CE2	1:B:85:ARG:HD3	2.17	0.80
2:B:501:LMT:H3B	2:B:501:LMT:H4'	1.63	0.80
1:A:78:PHE:CE2	1:A:85:ARG:HD3	2.14	0.79
1:D:280:LYS:HB2	1:D:280:LYS:NZ	1.98	0.78
1:B:69:GLU:H	1:B:69:GLU:CD	1.91	0.78
1:C:6:SER:HB2	1:C:7:PRO:HD2	1.65	0.77
1:D:133:ARG:NH1	1:D:176:LEU:O	2.17	0.77
1:E:78:PHE:CE2	1:E:85:ARG:HD3	2.20	0.77
1:B:6:SER:HB2	1:B:7:PRO:HD2	1.67	0.76
1:A:280:LYS:HB2	1:A:280:LYS:NZ	2.01	0.75
1:D:69:GLU:CD	1:D:69:GLU:H	1.96	0.74
1:C:187:GLN:OE1	1:C:189:ARG:NH2	2.22	0.73
1:A:131:ILE:HD11	1:A:181:GLU:HG2	1.70	0.73
1:D:187:GLN:OE1	1:D:189:ARG:NH2	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:SER:HB2	1:C:96:PRO:HD3	1.72	0.72
1:C:95:SER:HB2	1:C:96:PRO:CD	2.21	0.71
1:E:280:LYS:HB2	1:E:280:LYS:NZ	2.06	0.70
1:B:133:ARG:NH1	1:B:176:LEU:O	2.25	0.70
3:D:601:PC1:O32	3:D:601:PC1:H2	1.91	0.70
1:A:275:VAL:HG22	3:A:601:PC1:H222	1.75	0.69
1:C:63:VAL:HG12	1:C:64:LYS:H	1.59	0.68
1:B:254:TYR:OH	3:B:602:PC1:H361	1.92	0.68
2:B:501:LMT:H4'	2:B:501:LMT:C3B	2.23	0.68
1:C:280:LYS:HB2	1:C:280:LYS:HZ2	1.58	0.68
1:E:95:SER:HB2	1:E:96:PRO:CD	2.23	0.68
1:C:28:TYR:N	1:C:28:TYR:CD1	2.59	0.67
1:E:95:SER:HB2	1:E:96:PRO:HD3	1.75	0.67
1:B:248:LYS:HE3	4:B:622:HOH:O	1.93	0.67
1:D:78:PHE:CE2	1:D:85:ARG:HD3	2.25	0.67
1:A:137:THR:O	1:A:138:ARG:HB3	1.95	0.66
1:A:280:LYS:HB2	1:A:280:LYS:HZ3	1.61	0.66
1:D:27:CYS:HB3	1:D:157:LEU:HD13	1.78	0.65
1:E:55:ASP:O	1:E:59:SER:CB	2.45	0.65
1:E:55:ASP:HB3	1:E:58:ARG:HG3	1.77	0.65
1:E:69:GLU:CD	1:E:69:GLU:H	2.05	0.64
1:D:6:SER:HB2	1:D:7:PRO:CD	2.28	0.63
1:A:304:LEU:HB2	3:B:601:PC1:H2I2	1.80	0.63
1:A:69:GLU:CD	1:A:69:GLU:H	2.07	0.63
1:A:95:SER:HB2	1:A:96:PRO:CD	2.29	0.63
1:D:131:ILE:HD11	1:D:181:GLU:HG2	1.79	0.63
1:A:32:ASP:OD1	1:A:192:ARG:NH2	2.32	0.63
1:B:131:ILE:HD12	1:B:183:LYS:HB2	1.81	0.63
1:E:240:ILE:O	1:E:244:THR:HG23	1.99	0.62
1:D:240:ILE:O	1:D:244:THR:HG23	1.99	0.62
1:D:95:SER:HB2	1:D:96:PRO:CD	2.30	0.62
1:A:54:PHE:CD2	1:A:96:PRO:HA	2.34	0.61
1:A:195:PHE:CZ	1:B:252:MET:CE	2.83	0.61
1:B:187:GLN:OE1	1:B:189:ARG:NH2	2.33	0.61
1:D:95:SER:HB2	1:D:96:PRO:HD3	1.81	0.61
1:A:95:SER:HB2	1:A:96:PRO:HD3	1.83	0.61
1:C:195:PHE:CZ	1:D:252:MET:CE	2.84	0.60
1:C:55:ASP:CG	1:C:58:ARG:HB2	2.27	0.60
1:D:280:LYS:HB2	1:D:280:LYS:HZ3	1.65	0.60
1:D:14:GLU:O	1:D:138:ARG:NH2	2.26	0.60
3:D:602:PC1:O12	3:D:602:PC1:H32	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:6:SER:HB2	1:E:7:PRO:CD	2.32	0.59
1:A:6:SER:HB2	1:A:7:PRO:CD	2.31	0.59
1:D:28:TYR:CE2	1:D:38:LYS:HD2	2.38	0.59
1:D:137:THR:O	1:D:138:ARG:HB3	2.02	0.59
1:A:33:LYS:HE2	2:E:602:LMT:H6D	1.85	0.59
1:A:14:GLU:O	1:A:138:ARG:NH2	2.27	0.59
1:D:85:ARG:NE	1:D:104:GLU:OE2	2.31	0.59
1:A:252:MET:CE	1:E:195:PHE:CZ	2.86	0.58
1:C:32:ASP:OD1	1:C:192:ARG:NH2	2.37	0.58
3:D:602:PC1:H152	3:D:602:PC1:H12	1.85	0.58
1:C:137:THR:O	1:C:138:ARG:HB3	2.03	0.57
1:C:131:ILE:HD11	1:C:181:GLU:HG2	1.86	0.57
1:E:28:TYR:CD1	1:E:28:TYR:N	2.73	0.57
1:A:35:GLU:HG2	1:A:114:LEU:HG	1.86	0.57
1:A:85:ARG:NE	1:A:104:GLU:OE2	2.32	0.57
1:C:6:SER:HB2	1:C:7:PRO:CD	2.34	0.56
1:E:280:LYS:HB2	1:E:280:LYS:HZ2	1.69	0.56
1:C:69:GLU:CD	1:C:69:GLU:H	2.14	0.56
1:A:252:MET:HE1	1:E:195:PHE:CZ	2.40	0.56
1:B:280:LYS:HB2	1:B:280:LYS:NZ	2.20	0.56
1:C:43:LEU:HB3	1:C:104:GLU:HG2	1.86	0.56
1:B:240:ILE:O	1:B:244:THR:HG23	2.06	0.56
1:E:26:GLU:HA	1:E:26:GLU:OE1	2.05	0.56
1:E:254:TYR:OH	3:E:603:PC1:H352	2.06	0.56
1:B:131:ILE:HD11	1:B:181:GLU:HG2	1.86	0.56
1:A:54:PHE:CE2	1:A:96:PRO:CA	2.85	0.56
1:C:195:PHE:CZ	1:D:252:MET:HE1	2.41	0.55
1:A:241:LEU:HD22	1:B:240:ILE:HG12	1.88	0.55
1:A:122:ASP:OD2	1:A:192:ARG:NH1	2.39	0.54
2:B:501:LMT:C6'	1:C:33:LYS:CE	2.78	0.54
1:A:297:ILE:O	1:A:300:PRO:HD2	2.07	0.54
1:C:82:GLU:OE1	1:C:109:ARG:NH1	2.39	0.54
1:C:195:PHE:HZ	1:D:252:MET:CE	2.21	0.54
1:B:7:PRO:HG3	1:B:135:VAL:HG21	1.88	0.54
1:B:32:ASP:OD1	1:B:192:ARG:NH2	2.40	0.54
1:C:86:ASP:O	1:C:106:PHE:HA	2.08	0.54
1:E:32:ASP:OD1	1:E:192:ARG:NH2	2.39	0.54
1:A:28:TYR:CE2	1:A:38:LYS:HD2	2.43	0.54
2:B:501:LMT:C6'	1:C:33:LYS:NZ	2.71	0.54
1:A:145:ASP:OD1	1:A:145:ASP:C	2.49	0.53
1:C:7:PRO:HG3	1:C:135:VAL:HG21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:58:ARG:HD3	1:E:58:ARG:C	2.33	0.53
1:A:66:TYR:CE1	1:A:94:VAL:HG21	2.43	0.53
1:A:30:LEU:C	1:A:30:LEU:HD23	2.34	0.53
1:A:252:MET:CE	1:E:195:PHE:HZ	2.21	0.53
1:B:26:GLU:HB2	1:B:40:ASN:HB3	1.91	0.53
1:D:237:ALA:HB2	2:E:501:LMT:H91	1.91	0.53
1:B:26:GLU:OE1	1:B:26:GLU:HA	2.09	0.53
1:D:294:ALA:CB	3:D:603:PC1:O22	2.57	0.53
1:A:28:TYR:N	1:A:28:TYR:CD1	2.76	0.52
1:A:32:ASP:CG	1:A:192:ARG:NH2	2.68	0.52
1:E:237:ALA:HA	2:E:602:LMT:H92	1.92	0.52
1:B:275:VAL:HG22	3:B:601:PC1:H221	1.91	0.52
1:C:30:LEU:HD13	1:C:160:TRP:CE2	2.44	0.52
1:A:240:ILE:O	1:A:244:THR:HG23	2.09	0.52
1:C:28:TYR:N	1:C:28:TYR:HD1	2.07	0.52
1:D:43:LEU:HB3	1:D:104:GLU:HG2	1.92	0.52
1:D:86:ASP:O	1:D:106:PHE:HA	2.10	0.51
1:E:131:ILE:HD11	1:E:181:GLU:HG2	1.91	0.51
1:C:122:ASP:OD2	1:C:192:ARG:NH1	2.43	0.51
2:C:501:LMT:H2B	2:C:501:LMT:C3'	2.39	0.51
1:C:240:ILE:O	1:C:244:THR:HG23	2.10	0.51
1:E:30:LEU:HD23	1:E:30:LEU:C	2.36	0.51
1:E:30:LEU:HD13	1:E:160:TRP:CE2	2.46	0.51
1:E:122:ASP:OD2	1:E:192:ARG:NH1	2.43	0.51
1:E:26:GLU:HB2	1:E:40:ASN:HB3	1.92	0.51
1:D:145:ASP:OD1	1:D:145:ASP:C	2.54	0.50
1:A:195:PHE:HZ	1:B:252:MET:CE	2.22	0.50
1:E:30:LEU:HD22	4:E:618:HOH:O	2.12	0.50
1:C:50:ARG:C	1:C:52:LEU:H	2.20	0.50
1:C:117:ARG:NH2	4:C:411:HOH:O	2.45	0.50
2:C:501:LMT:H5B	2:E:501:LMT:O3B	2.11	0.50
1:B:85:ARG:NE	1:B:104:GLU:OE2	2.42	0.50
1:C:35:GLU:HG2	1:C:114:LEU:HG	1.94	0.50
2:C:501:LMT:H1B	1:D:33:LYS:HE2	1.95	0.49
1:A:83:ASN:O	1:A:84:ALA:C	2.55	0.49
1:B:6:SER:HB2	1:B:7:PRO:CD	2.38	0.49
1:E:58:ARG:HD3	1:E:59:SER:N	2.27	0.49
2:E:501:LMT:H12	2:E:501:LMT:H2'	1.54	0.49
1:E:205:MET:HE3	1:E:205:MET:HB2	1.69	0.49
1:E:258:ILE:HD13	3:E:603:PC1:H381	1.94	0.49
1:B:145:ASP:OD1	1:B:145:ASP:C	2.55	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:PHE:HE2	1:C:85:ARG:CD	2.15	0.48
1:A:195:PHE:CZ	1:B:252:MET:HE1	2.47	0.48
1:C:195:PHE:CE1	1:D:252:MET:HE1	2.49	0.48
1:D:32:ASP:OD1	1:D:192:ARG:NH2	2.46	0.48
1:D:131:ILE:HD12	1:D:183:LYS:HB2	1.94	0.48
1:D:217:TRP:CE2	1:D:296:ARG:HD3	2.49	0.48
1:E:27:CYS:HB3	1:E:157:LEU:HD13	1.96	0.48
1:A:267:PHE:O	1:A:271:ILE:HG12	2.14	0.48
1:D:280:LYS:HB2	1:D:280:LYS:HZ2	1.75	0.48
1:D:178:ASP:O	1:D:179:ARG:HG2	2.14	0.47
1:E:65:THR:CG2	1:E:66:TYR:N	2.76	0.47
1:E:255:THR:O	1:E:259:ILE:HG12	2.14	0.47
1:B:48:LYS:HE3	1:B:50:ARG:HH12	1.79	0.47
1:B:54:PHE:CE1	1:B:96:PRO:HA	2.50	0.47
1:C:11:ILE:HG12	1:C:50:ARG:HH21	1.79	0.47
1:B:122:ASP:OD1	1:B:192:ARG:HD2	2.15	0.47
1:C:63:VAL:HG12	1:C:64:LYS:N	2.29	0.47
1:A:255:THR:O	1:A:259:ILE:HG12	2.15	0.47
2:C:501:LMT:H5B	2:E:501:LMT:C3B	2.44	0.47
1:A:27:CYS:HB3	1:A:157:LEU:HD13	1.97	0.47
1:A:195:PHE:CZ	1:B:252:MET:HE2	2.49	0.47
1:D:195:PHE:CD1	1:D:195:PHE:C	2.93	0.47
1:B:28:TYR:N	1:B:28:TYR:CD1	2.83	0.47
1:B:205:MET:HE2	1:B:238:PHE:HB3	1.97	0.47
1:C:280:LYS:HB2	1:C:280:LYS:HZ3	1.78	0.47
1:D:255:THR:O	1:D:259:ILE:HG12	2.15	0.47
1:C:27:CYS:HB3	1:C:157:LEU:HD13	1.97	0.47
1:E:50:ARG:C	1:E:52:LEU:H	2.23	0.47
2:B:501:LMT:H6E	1:C:33:LYS:NZ	2.30	0.46
1:C:196:SER:O	1:C:199:PRO:HD2	2.16	0.46
3:C:602:PC1:H132	3:C:602:PC1:H111	1.75	0.46
1:E:133:ARG:CZ	1:E:179:ARG:HB2	2.45	0.46
1:E:67:GLU:O	1:E:68:PRO:C	2.56	0.46
1:E:86:ASP:O	1:E:106:PHE:HA	2.16	0.46
1:D:30:LEU:C	1:D:30:LEU:HD23	2.41	0.46
1:E:95:SER:CB	1:E:96:PRO:CD	2.93	0.46
1:C:37:PHE:CD1	1:C:126:LEU:HD13	2.50	0.46
3:D:602:PC1:H111	3:D:602:PC1:H153	1.59	0.46
1:C:28:TYR:CE2	1:C:38:LYS:HD2	2.50	0.46
1:D:267:PHE:O	1:D:271:ILE:HG12	2.15	0.46
1:B:30:LEU:HD13	1:B:160:TRP:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:PHE:CE1	1:D:252:MET:CE	2.99	0.45
3:C:603:PC1:H221	3:C:603:PC1:O31	2.16	0.45
1:D:198:ILE:HB	1:D:199:PRO:HD3	1.98	0.45
1:D:28:TYR:N	1:D:28:TYR:CD1	2.84	0.45
1:D:58:ARG:H	1:D:58:ARG:HG2	1.64	0.45
3:E:603:PC1:H152	3:E:603:PC1:H12	1.97	0.45
1:C:122:ASP:CG	1:C:192:ARG:HH11	2.25	0.45
3:B:602:PC1:H152	3:B:602:PC1:H111	1.73	0.45
1:D:63:VAL:HG11	1:E:136:ASP:CG	2.42	0.45
1:E:254:TYR:CZ	1:E:258:ILE:HD11	2.51	0.45
1:A:50:ARG:C	1:A:52:LEU:H	2.24	0.45
1:B:43:LEU:HB3	1:B:104:GLU:HG2	1.99	0.45
1:A:304:LEU:HB2	3:B:601:PC1:C2I	2.46	0.45
1:C:30:LEU:HD23	1:C:30:LEU:C	2.42	0.45
1:B:86:ASP:O	1:B:106:PHE:HA	2.16	0.45
1:C:134:SER:HB3	1:C:139:ASN:HA	1.99	0.45
1:E:85:ARG:NE	1:E:104:GLU:OE2	2.48	0.44
1:E:114:LEU:HB2	1:E:116:PHE:CE2	2.51	0.44
1:A:8:PRO:HB3	1:A:49:ASP:OD1	2.18	0.44
1:B:118:ARG:O	1:B:121:PHE:N	2.48	0.44
1:D:147:GLU:OE2	1:D:147:GLU:HA	2.17	0.44
1:E:58:ARG:C	1:E:58:ARG:CD	2.90	0.44
1:D:222:GLU:H	1:D:222:GLU:CD	2.25	0.44
1:C:50:ARG:C	1:C:52:LEU:N	2.73	0.44
1:D:26:GLU:HB2	1:D:40:ASN:HB3	1.99	0.44
3:E:603:PC1:H322	3:E:603:PC1:H252	1.99	0.44
1:B:32:ASP:CG	1:B:192:ARG:NH2	2.76	0.44
1:C:254:TYR:OH	3:C:602:PC1:H351	2.17	0.44
1:D:32:ASP:CG	1:D:192:ARG:NH2	2.76	0.44
1:E:255:THR:O	1:E:256:GLY:C	2.60	0.44
1:A:63:VAL:CG2	1:B:136:ASP:OD1	2.59	0.44
1:A:310:LEU:HD23	1:A:310:LEU:HA	1.86	0.44
1:C:237:ALA:HA	2:C:501:LMT:H92	1.99	0.44
1:B:195:PHE:CD1	1:B:195:PHE:C	2.95	0.44
1:C:85:ARG:NE	1:C:104:GLU:OE2	2.44	0.44
1:E:64:LYS:HE3	1:E:64:LYS:HB2	1.79	0.44
3:E:601:PC1:O22	3:E:601:PC1:H11	2.18	0.44
1:A:252:MET:HE1	1:E:195:PHE:CE1	2.53	0.43
1:B:35:GLU:HG2	1:B:114:LEU:HG	1.99	0.43
1:D:85:ARG:HD2	1:D:106:PHE:HB2	2.00	0.43
1:E:32:ASP:CG	1:E:192:ARG:NH2	2.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:50:ARG:C	1:E:52:LEU:N	2.75	0.43
1:B:255:THR:O	1:B:259:ILE:HG12	2.18	0.43
1:A:50:ARG:C	1:A:52:LEU:N	2.77	0.43
1:B:160:TRP:CE3	1:B:190:ILE:HD12	2.54	0.43
1:D:122:ASP:OD2	1:D:192:ARG:NH1	2.50	0.43
1:C:122:ASP:OD1	1:C:192:ARG:HD2	2.17	0.43
1:D:38:LYS:HE3	4:D:622:HOH:O	2.18	0.43
2:E:602:LMT:H2B	2:E:602:LMT:H4'	1.45	0.43
1:A:26:GLU:HB2	1:A:40:ASN:HB3	2.00	0.43
1:A:86:ASP:O	1:A:106:PHE:HA	2.18	0.43
1:A:122:ASP:CG	1:A:192:ARG:HH11	2.27	0.43
1:D:85:ARG:HG2	1:D:85:ARG:HH11	1.84	0.43
3:B:601:PC1:H321	3:B:603:PC1:H331	2.01	0.43
1:D:7:PRO:HG3	1:D:135:VAL:HG21	2.01	0.43
1:E:78:PHE:CE1	1:E:130:LEU:HD21	2.54	0.43
1:C:43:LEU:HB3	1:C:104:GLU:CG	2.49	0.43
1:A:95:SER:CB	1:A:96:PRO:CD	2.95	0.42
1:B:137:THR:O	1:B:138:ARG:HB3	2.19	0.42
1:C:26:GLU:HB2	1:C:40:ASN:HB3	2.00	0.42
1:C:55:ASP:O	1:C:59:SER:OG	2.14	0.42
1:D:261:MET:O	1:D:264:LEU:HB2	2.18	0.42
1:B:30:LEU:C	1:B:30:LEU:HD23	2.44	0.42
1:B:49:ASP:OD1	1:B:49:ASP:C	2.59	0.42
1:D:95:SER:CB	1:D:96:PRO:CD	2.97	0.42
1:A:250:PRO:HD2	1:A:251:TYR:CD1	2.54	0.42
1:B:94:VAL:HG22	1:B:100:VAL:HG22	2.01	0.42
1:C:32:ASP:CG	1:C:192:ARG:NH2	2.77	0.42
1:C:178:ASP:O	1:C:179:ARG:HG2	2.19	0.42
1:C:205:MET:HE2	1:C:238:PHE:HB3	2.02	0.42
1:C:222:GLU:CD	1:C:222:GLU:H	2.27	0.42
1:D:241:LEU:HD22	1:E:240:ILE:HG12	2.00	0.42
1:E:122:ASP:CG	1:E:192:ARG:HH11	2.27	0.42
1:A:37:PHE:CD1	1:A:126:LEU:HD13	2.55	0.42
1:A:195:PHE:CE1	1:B:252:MET:CE	3.02	0.42
1:C:195:PHE:CD1	1:C:195:PHE:C	2.96	0.42
2:C:501:LMT:C6B	2:E:501:LMT:O3B	2.68	0.42
1:E:83:ASN:O	1:E:84:ALA:C	2.61	0.42
3:A:602:PC1:H112	3:A:602:PC1:H132	1.67	0.42
1:C:67:GLU:O	1:C:68:PRO:C	2.63	0.42
1:C:275:VAL:HG22	3:C:601:PC1:H221	2.01	0.42
1:D:29:SER:O	1:D:37:PHE:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:205:MET:HE2	1:E:238:PHE:HB3	2.01	0.42
1:B:23:TYR:HB3	1:B:42:PHE:HB2	2.02	0.42
1:A:82:GLU:OE1	1:A:109:ARG:NH1	2.53	0.42
3:D:602:PC1:H32	3:D:602:PC1:P	2.59	0.42
1:C:241:LEU:HD22	1:D:240:ILE:HG12	2.01	0.42
1:D:67:GLU:O	1:D:68:PRO:C	2.61	0.42
3:D:602:PC1:H252	3:D:602:PC1:H331	2.02	0.42
1:A:277:HIS:O	1:A:278:TYR:C	2.61	0.41
1:E:62:ARG:HE	1:E:62:ARG:HB3	1.54	0.41
1:B:48:LYS:HE3	1:B:50:ARG:NH1	2.35	0.41
1:C:8:PRO:HA	1:C:9:PRO:HD3	1.89	0.41
1:C:145:ASP:C	1:C:145:ASP:OD1	2.62	0.41
1:B:222:GLU:CD	1:B:222:GLU:H	2.28	0.41
1:D:83:ASN:O	1:D:84:ALA:C	2.62	0.41
1:D:120:PRO:HD3	1:D:255:THR:OG1	2.19	0.41
1:A:133:ARG:CZ	1:A:179:ARG:HB2	2.51	0.41
1:A:205:MET:HE2	1:A:238:PHE:HB3	2.03	0.41
1:D:145:ASP:OD1	1:D:147:GLU:CB	2.69	0.41
1:D:193:GLN:OE1	1:E:250:PRO:HG3	2.21	0.41
1:E:59:SER:C	1:E:61:VAL:H	2.29	0.41
1:D:50:ARG:C	1:D:52:LEU:H	2.29	0.41
1:B:55:ASP:HB3	1:B:58:ARG:HB2	2.03	0.41
1:D:205:MET:HB2	1:D:205:MET:HE3	1.76	0.41
1:B:122:ASP:OD2	1:B:192:ARG:NH1	2.54	0.41
1:D:299:PHE:HB2	1:D:300:PRO:HD3	2.03	0.41
2:B:501:LMT:H4B	2:B:501:LMT:H4'	2.02	0.40
1:C:310:LEU:HD23	1:C:310:LEU:HA	1.92	0.40
1:D:35:GLU:HG2	1:D:114:LEU:HG	2.03	0.40
1:A:252:MET:CA	1:A:252:MET:HE2	2.50	0.40
1:B:205:MET:HE3	1:B:205:MET:HB2	1.77	0.40
1:D:220:SER:HB3	1:D:223:ALA:HB3	2.01	0.40
1:A:8:PRO:HA	1:A:9:PRO:HD3	1.89	0.40
1:A:261:MET:HE2	1:A:261:MET:HB3	2.00	0.40
1:B:25:ILE:O	1:B:155:VAL:HG22	2.21	0.40
1:B:255:THR:O	1:B:259:ILE:CG1	2.69	0.40
1:E:259:ILE:HG12	1:E:259:ILE:H	1.77	0.40
1:A:42:PHE:HB3	1:A:103:LEU:HD11	2.04	0.40
1:B:131:ILE:CD1	1:B:181:GLU:HG2	2.51	0.40
1:C:120:PRO:HD3	1:C:255:THR:OG1	2.22	0.40
1:E:78:PHE:CE1	1:E:130:LEU:CD2	3.05	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%)	292 (94%)	15 (5%)	2 (1%)	21	51
1	B	309/317 (98%)	289 (94%)	19 (6%)	1 (0%)	36	65
1	C	309/317 (98%)	287 (93%)	20 (6%)	2 (1%)	21	51
1	D	309/317 (98%)	291 (94%)	16 (5%)	2 (1%)	21	51
1	E	309/317 (98%)	291 (94%)	17 (6%)	1 (0%)	36	65
All	All	1545/1585 (98%)	1450 (94%)	87 (6%)	8 (0%)	24	54

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ALA
1	A	51	ARG
1	B	12	ALA
1	C	12	ALA
1	D	12	ALA
1	D	51	ARG
1	E	12	ALA
1	C	51	ARG

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%)	254 (91%)	26 (9%)	8	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	280/284 (99%)	255 (91%)	25 (9%)	9	28
1	C	280/284 (99%)	250 (89%)	30 (11%)	6	22
1	D	280/284 (99%)	252 (90%)	28 (10%)	7	24
1	E	280/284 (99%)	252 (90%)	28 (10%)	7	24
All	All	1400/1420 (99%)	1263 (90%)	137 (10%)	7	25

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ILE
1	A	14	GLU
1	A	17	THR
1	A	28	TYR
1	A	33	LYS
1	A	35	GLU
1	A	61	VAL
1	A	69	GLU
1	A	86	ASP
1	A	111	LEU
1	A	130	LEU
1	A	141	VAL
1	A	152	ASN
1	A	154	ASP
1	A	178	ASP
1	A	180	LEU
1	A	181	GLU
1	A	189	ARG
1	A	219	THR
1	A	222	GLU
1	A	225	VAL
1	A	259	ILE
1	A	280	LYS
1	A	283	SER
1	A	292	THR
1	A	305	LEU
1	B	11	ILE
1	B	14	GLU
1	B	17	THR
1	B	28	TYR
1	B	33	LYS
1	B	35	GLU

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Mol	Chain	Res	Type
1	B	61	VAL
1	B	62	ARG
1	B	69	GLU
1	B	86	ASP
1	B	109	ARG
1	B	111	LEU
1	B	141	VAL
1	B	152	ASN
1	B	178	ASP
1	B	180	LEU
1	B	181	GLU
1	B	222	GLU
1	B	225	VAL
1	B	259	ILE
1	B	273	VAL
1	B	280	LYS
1	B	283	SER
1	B	304	LEU
1	B	305	LEU
1	C	11	ILE
1	C	14	GLU
1	C	17	THR
1	C	28	TYR
1	C	57	VAL
1	C	58	ARG
1	C	61	VAL
1	C	62	ARG
1	C	64	LYS
1	C	69	GLU
1	C	86	ASP
1	C	111	LEU
1	C	130	LEU
1	C	137	THR
1	C	140	ILE
1	C	141	VAL
1	C	152	ASN
1	C	154	ASP
1	C	178	ASP
1	C	179	ARG
1	C	180	LEU
1	C	181	GLU
1	C	222	GLU

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Mol	Chain	Res	Type
1	C	225	VAL
1	C	259	ILE
1	C	273	VAL
1	C	280	LYS
1	C	283	SER
1	C	304	LEU
1	C	305	LEU
1	D	11	ILE
1	D	14	GLU
1	D	17	THR
1	D	28	TYR
1	D	33	LYS
1	D	35	GLU
1	D	57	VAL
1	D	58	ARG
1	D	59	SER
1	D	62	ARG
1	D	69	GLU
1	D	86	ASP
1	D	111	LEU
1	D	140	ILE
1	D	141	VAL
1	D	152	ASN
1	D	154	ASP
1	D	178	ASP
1	D	179	ARG
1	D	180	LEU
1	D	181	GLU
1	D	189	ARG
1	D	225	VAL
1	D	259	ILE
1	D	273	VAL
1	D	280	LYS
1	D	304	LEU
1	D	305	LEU
1	E	11	ILE
1	E	14	GLU
1	E	17	THR
1	E	28	TYR
1	E	35	GLU
1	E	58	ARG
1	E	64	LYS

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Mol	Chain	Res	Type
1	E	65	THR
1	E	69	GLU
1	E	86	ASP
1	E	111	LEU
1	E	130	LEU
1	E	141	VAL
1	E	151	LYS
1	E	152	ASN
1	E	154	ASP
1	E	163	GLU
1	E	178	ASP
1	E	180	LEU
1	E	181	GLU
1	E	189	ARG
1	E	222	GLU
1	E	225	VAL
1	E	259	ILE
1	E	273	VAL
1	E	280	LYS
1	E	283	SER
1	E	304	LEU

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

Mol	Chain	Res	Type
1	B	245	ASN
1	C	307	ASN
1	D	83	ASN
1	D	307	ASN
1	E	245	ASN
1	E	307	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 ⓘ

21 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
3	PC1	E	603	-	38,38,53	1.39	3 (7%)	44,46,61	1.09	3 (6%)
3	PC1	E	604	-	26,26,53	1.79	3 (11%)	28,28,61	2.32	8 (28%)
2	LMT	E	501	-	36,36,36	0.88	2 (5%)	47,47,47	1.38	6 (12%)
2	LMT	A	501	-	36,36,36	0.87	1 (2%)	47,47,47	1.54	8 (17%)
3	PC1	C	601	-	46,46,53	1.54	4 (8%)	52,54,61	1.49	6 (11%)
3	PC1	A	603	-	26,26,53	2.16	3 (11%)	28,28,61	2.41	7 (25%)
3	PC1	A	602	-	38,38,53	1.54	3 (7%)	44,46,61	1.40	4 (9%)
3	PC1	B	603	-	25,25,53	2.04	2 (8%)	26,26,61	2.20	6 (23%)
2	LMT	B	501	-	36,36,36	0.93	1 (2%)	47,47,47	1.64	9 (19%)
3	PC1	D	603	-	20,20,53	1.61	2 (10%)	20,20,61	1.13	4 (20%)
3	PC1	D	602	-	38,38,53	1.47	3 (7%)	44,46,61	1.11	2 (4%)
3	PC1	B	602	-	38,38,53	1.47	3 (7%)	44,46,61	1.25	4 (9%)
3	PC1	C	603	-	26,26,53	2.14	4 (15%)	28,28,61	2.27	7 (25%)
3	PC1	E	601	-	46,46,53	1.45	3 (6%)	52,54,61	1.71	6 (11%)
2	LMT	C	501	-	36,36,36	0.93	1 (2%)	47,47,47	1.30	7 (14%)
3	PC1	D	601	-	46,46,53	1.44	3 (6%)	52,54,61	1.34	7 (13%)
3	PC1	C	602	-	38,38,53	1.45	3 (7%)	44,46,61	1.27	3 (6%)
2	LMT	E	602	-	36,36,36	0.88	0	47,47,47	1.32	7 (14%)
2	LMT	C	502	-	36,36,36	1.32	4 (11%)	47,47,47	2.47	18 (38%)
3	PC1	A	601	-	46,46,53	1.49	4 (8%)	52,54,61	1.56	6 (11%)
3	PC1	B	601	-	46,46,53	1.46	3 (6%)	52,54,61	1.34	5 (9%)

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	PC1	E	603	-	1/1/5/5	23/42/42/57	-
3	PC1	E	604	-	1/1/3/5	9/27/27/57	-
2	LMT	E	501	-	6/6/10/10	9/21/61/61	0/2/2/2
2	LMT	A	501	-	6/6/10/10	10/21/61/61	0/2/2/2
3	PC1	C	601	-	1/1/5/5	21/50/50/57	-
3	PC1	A	603	-	1/1/3/5	14/27/27/57	-
3	PC1	A	602	-	1/1/5/5	27/42/42/57	-
3	PC1	B	603	-	-	13/25/25/57	-
2	LMT	B	501	-	6/6/10/10	10/21/61/61	0/2/2/2
3	PC1	D	603	-	-	7/17/17/57	-
3	PC1	D	602	-	1/1/5/5	26/42/42/57	-
3	PC1	B	602	-	1/1/5/5	28/42/42/57	-
3	PC1	C	603	-	1/1/3/5	10/27/27/57	-
3	PC1	E	601	-	1/1/5/5	26/50/50/57	-
2	LMT	C	501	-	6/6/10/10	14/21/61/61	0/2/2/2
3	PC1	D	601	-	1/1/5/5	19/50/50/57	-
3	PC1	C	602	-	1/1/5/5	25/42/42/57	-
2	LMT	E	602	-	6/6/10/10	8/21/61/61	0/2/2/2
2	LMT	C	502	-	6/6/10/10	11/21/61/61	0/2/2/2
3	PC1	A	601	-	1/1/5/5	17/50/50/57	-
3	PC1	B	601	-	1/1/5/5	22/50/50/57	-

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	603	PC1	O31-C31	6.79	1.53	1.33
3	B	603	PC1	O31-C31	6.60	1.52	1.33
3	C	603	PC1	O21-C21	6.48	1.52	1.34
3	A	603	PC1	O21-C21	6.33	1.52	1.34
3	C	601	PC1	O31-C31	6.30	1.51	1.33
3	E	604	PC1	O21-C21	6.14	1.51	1.34
3	A	603	PC1	O31-C31	6.13	1.51	1.33
3	B	601	PC1	O31-C31	6.11	1.51	1.33
3	A	602	PC1	O21-C21	6.09	1.51	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	601	PC1	O31-C31	5.91	1.50	1.33
3	D	602	PC1	O21-C21	5.86	1.50	1.34
3	B	603	PC1	O21-C21	5.84	1.50	1.33
3	A	601	PC1	O31-C31	5.79	1.50	1.33
3	E	601	PC1	O31-C31	5.64	1.49	1.33
3	C	602	PC1	O31-C31	5.30	1.48	1.33
3	E	604	PC1	O31-C31	5.27	1.48	1.33
3	E	603	PC1	O21-C21	5.19	1.48	1.34
3	C	602	PC1	O21-C21	5.03	1.48	1.34
3	B	602	PC1	O21-C21	4.97	1.48	1.34
3	B	602	PC1	O31-C31	4.95	1.47	1.33
3	A	602	PC1	O31-C31	4.89	1.47	1.33
3	D	602	PC1	O31-C31	4.88	1.47	1.33
3	D	603	PC1	O31-C31	4.83	1.48	1.33
3	D	603	PC1	O21-C21	4.80	1.46	1.30
3	E	603	PC1	O31-C31	4.78	1.47	1.33
3	B	601	PC1	O21-C21	4.69	1.47	1.34
3	D	601	PC1	O21-C21	4.68	1.47	1.34
3	C	601	PC1	O21-C21	4.66	1.47	1.34
3	A	601	PC1	O21-C21	4.58	1.47	1.34
3	E	601	PC1	O21-C21	4.52	1.47	1.34
3	A	603	PC1	C3-C2	4.26	1.60	1.50
3	C	603	PC1	C3-C2	4.21	1.60	1.50
2	C	502	LMT	O1'-C1'	4.01	1.46	1.40
3	E	601	PC1	P-O14	3.82	1.64	1.50
3	B	602	PC1	P-O14	3.68	1.63	1.50
3	A	601	PC1	P-O14	3.67	1.63	1.50
3	B	601	PC1	P-O14	3.64	1.63	1.50
3	D	601	PC1	P-O14	3.49	1.62	1.50
3	C	602	PC1	P-O14	3.43	1.62	1.50
3	A	602	PC1	P-O14	3.37	1.62	1.50
3	C	601	PC1	P-O14	3.34	1.62	1.50
3	D	602	PC1	P-O14	3.28	1.62	1.50
2	C	502	LMT	C3'-C2'	3.10	1.60	1.52
3	E	603	PC1	P-O14	3.09	1.61	1.50
3	E	604	PC1	C3-C2	3.01	1.57	1.50
2	C	502	LMT	O5'-C1'	2.67	1.48	1.41
3	C	601	PC1	C3-C2	2.53	1.58	1.50
2	C	502	LMT	C4B-C5B	2.45	1.58	1.53
2	C	501	LMT	O1'-C1'	2.31	1.44	1.40
2	E	501	LMT	O1'-C1'	2.15	1.43	1.40
2	E	501	LMT	O5B-C1B	2.12	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	LMT	O5B-C1B	2.10	1.47	1.41
2	B	501	LMT	O1'-C1'	2.10	1.43	1.40
3	C	603	PC1	O31-C3	2.07	1.49	1.45
3	A	601	PC1	C3-C2	2.06	1.57	1.50

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	502	LMT	C1B-O1B-C4'	-7.76	99.59	117.98
3	E	601	PC1	O21-C21-C22	7.47	127.64	111.48
3	E	604	PC1	O21-C21-C22	6.73	126.03	111.48
3	C	603	PC1	O21-C21-C22	6.63	125.82	111.48
3	A	601	PC1	O21-C21-C22	6.49	125.51	111.48
3	E	604	PC1	C2-O21-C21	6.26	126.81	117.78
3	C	601	PC1	O21-C21-C22	6.07	124.62	111.48
3	A	603	PC1	O21-C21-C22	5.94	124.33	111.48
3	A	603	PC1	O21-C2-C3	5.41	118.65	106.21
3	A	601	PC1	O31-C31-C32	5.34	128.13	111.83
3	A	603	PC1	C2-O21-C21	5.31	125.44	117.78
3	B	603	PC1	O21-C21-C22	5.23	127.80	111.83
3	B	601	PC1	O21-C21-C22	5.17	122.67	111.48
3	E	601	PC1	O31-C31-C32	5.15	127.53	111.83
3	C	603	PC1	O21-C2-C3	4.98	117.67	106.21
3	A	603	PC1	C3-O31-C31	4.92	135.10	117.12
3	B	603	PC1	C3-O31-C31	4.90	132.22	116.90
2	C	502	LMT	C1B-O5B-C5B	-4.90	104.15	113.72
2	C	502	LMT	C6'-C5'-C4'	-4.62	100.38	113.38
3	B	603	PC1	O21-C21-O22	-4.58	112.18	123.63
3	D	601	PC1	O21-C21-C22	4.57	121.37	111.48
2	C	502	LMT	O1B-C1B-C2B	4.57	119.32	108.09
3	A	602	PC1	O21-C21-C22	4.53	121.28	111.48
3	C	601	PC1	O31-C31-C32	4.44	125.38	111.83
3	A	602	PC1	O31-C31-C32	4.39	125.23	111.83
3	B	601	PC1	O31-C31-C32	4.37	125.17	111.83
3	D	601	PC1	O31-C31-C32	4.37	125.16	111.83
2	B	501	LMT	O5B-C5B-C4B	4.35	117.54	109.70
3	C	603	PC1	O31-C3-C2	4.35	120.74	108.35
3	C	602	PC1	O21-C21-C22	4.32	120.83	111.48
3	E	604	PC1	O21-C2-C3	4.29	116.07	106.21
2	B	501	LMT	O5'-C5'-C4'	4.27	118.55	109.72
3	B	602	PC1	O31-C31-C32	4.22	124.72	111.83
2	A	501	LMT	O1B-C4'-C3'	4.20	117.92	107.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	502	LMT	C1'-C2'-C3'	4.20	118.85	110.01
2	A	501	LMT	C1B-O5B-C5B	4.13	121.78	113.72
2	C	502	LMT	O5B-C5B-C4B	3.92	116.76	109.70
3	E	603	PC1	O21-C21-C22	3.89	119.90	111.48
3	C	603	PC1	C2-O21-C21	3.89	123.39	117.78
2	E	501	LMT	O5'-C5'-C6'	3.88	116.07	106.44
2	C	502	LMT	O5'-C5'-C6'	3.87	116.02	106.44
3	B	602	PC1	O21-C21-C22	3.83	119.78	111.48
2	A	501	LMT	O5B-C1B-C2B	3.79	118.16	110.37
3	E	604	PC1	O31-C31-C32	3.74	123.25	111.83
3	D	602	PC1	O21-C21-C22	3.74	119.57	111.48
3	A	601	PC1	O31-C31-O32	-3.66	114.48	123.63
3	E	601	PC1	O31-C31-O32	-3.64	114.53	123.63
3	C	603	PC1	C3-O31-C31	3.62	130.35	117.12
3	B	603	PC1	O31-C3-C2	3.61	119.17	108.61
3	A	603	PC1	O31-C3-C2	3.54	118.44	108.35
3	C	601	PC1	O21-C21-O22	-3.52	115.47	123.70
3	E	603	PC1	O31-C31-C32	3.51	122.52	111.83
2	C	502	LMT	O1B-C4'-C3'	3.50	116.13	107.23
3	C	601	PC1	C3-O31-C31	3.50	129.90	117.12
3	C	603	PC1	O31-C31-C32	3.47	122.42	111.83
3	A	602	PC1	C2-O21-C21	3.45	126.05	117.80
3	C	602	PC1	O31-C31-C32	3.42	122.26	111.83
2	B	501	LMT	C3B-C4B-C5B	3.41	116.41	110.23
3	B	603	PC1	O21-C2-C3	3.38	118.50	108.61
2	C	502	LMT	C3'-C4'-C5'	3.37	118.40	110.93
3	A	603	PC1	O31-C31-C32	3.34	122.03	111.83
3	E	601	PC1	O21-C21-O22	-3.33	115.91	123.70
3	D	602	PC1	O31-C31-C32	3.26	121.77	111.83
2	C	502	LMT	C1'-O5'-C5'	3.23	120.03	113.72
2	E	602	LMT	O1B-C4'-C3'	3.20	115.37	107.23
2	C	502	LMT	C2'-C3'-C4'	3.20	116.94	109.68
2	E	501	LMT	C1B-O1B-C4'	-3.18	110.44	117.98
3	A	602	PC1	O31-C31-O32	-3.16	115.73	123.63
2	C	502	LMT	O1'-C1'-C2'	3.10	112.98	108.27
2	C	501	LMT	O3'-C3'-C4'	3.08	117.84	109.94
2	B	501	LMT	C3'-C4'-C5'	3.08	117.76	110.93
2	C	501	LMT	C3'-C4'-C5'	3.07	117.74	110.93
2	A	501	LMT	C1B-C2B-C3B	3.07	116.46	110.01
2	A	501	LMT	O5B-C5B-C4B	3.04	115.17	109.70
2	C	502	LMT	O3'-C3'-C4'	-2.91	102.48	109.94
3	B	603	PC1	O31-C31-C32	2.90	120.68	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	PC1	O31-C31-O32	-2.86	116.47	123.63
3	A	601	PC1	O31-C3-C2	2.82	116.52	108.40
3	D	601	PC1	C3-C2-C1	-2.77	105.32	111.78
2	C	502	LMT	C3B-C4B-C5B	2.77	115.25	110.23
2	B	501	LMT	C1B-O5B-C5B	2.73	119.04	113.72
2	C	502	LMT	C1B-C2B-C3B	-2.68	104.37	110.01
2	B	501	LMT	O3'-C3'-C4'	2.68	116.80	109.94
2	C	501	LMT	O1'-C1'-C2'	2.64	112.28	108.27
2	E	501	LMT	O1B-C4'-C3'	2.57	113.75	107.23
2	E	602	LMT	O5'-C5'-C6'	2.56	112.77	106.44
3	A	601	PC1	O21-C21-O22	-2.55	117.75	123.70
3	E	604	PC1	O21-C21-O22	-2.54	117.76	123.70
3	E	603	PC1	O31-C31-O32	-2.54	117.29	123.63
3	E	604	PC1	O31-C31-O32	-2.52	117.33	123.63
3	D	603	PC1	O21-C21-O22	-2.51	116.88	123.33
3	D	601	PC1	C3-O31-C31	2.50	126.25	117.12
2	C	501	LMT	O5B-C1B-C2B	2.48	115.47	110.37
3	E	604	PC1	O31-C3-C2	2.48	115.41	108.35
3	D	603	PC1	O21-C21-C22	2.48	121.82	114.00
2	C	502	LMT	O1B-C1B-O5B	2.46	117.18	110.69
2	B	501	LMT	O5B-C1B-C2B	2.46	115.42	110.37
2	E	501	LMT	C3B-C4B-C5B	2.46	114.69	110.23
3	D	601	PC1	O21-C21-O22	-2.42	118.05	123.70
3	B	601	PC1	O21-C21-O22	-2.41	118.07	123.70
2	E	501	LMT	C1-O1'-C1'	-2.41	109.57	113.68
2	C	501	LMT	O2B-C2B-C3B	2.40	116.04	110.38
2	C	502	LMT	O5'-C1'-O1'	2.38	115.67	110.04
3	C	603	PC1	O22-C21-C22	-2.38	114.47	123.78
2	B	501	LMT	O1B-C4'-C3'	2.37	113.25	107.23
3	B	602	PC1	O21-C21-O22	-2.36	118.18	123.70
2	C	502	LMT	O4'-C4B-C5B	2.34	115.08	109.32
2	E	602	LMT	C1'-O5'-C5'	2.31	118.23	113.72
3	E	601	PC1	C2-O21-C21	-2.29	112.32	117.80
3	E	601	PC1	C3-O31-C31	2.26	125.40	117.12
2	E	602	LMT	C3B-C4B-C5B	2.25	114.32	110.23
2	E	602	LMT	C1B-O5B-C5B	2.23	118.07	113.72
3	B	601	PC1	O21-C2-C3	2.19	116.21	108.34
2	E	602	LMT	O3'-C3'-C4'	2.18	115.53	109.94
2	A	501	LMT	O5'-C5'-C6'	2.18	111.84	106.44
3	D	603	PC1	C3-O31-C31	2.16	123.00	116.07
2	B	501	LMT	O5B-C5B-C6B	2.14	111.75	106.44
3	A	603	PC1	O21-C21-O22	-2.14	118.70	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	501	LMT	C1B-O5B-C5B	2.14	117.89	113.72
2	A	501	LMT	O5'-C5'-C4'	2.13	114.13	109.72
3	B	601	PC1	O31-C31-O32	-2.13	118.29	123.63
3	E	604	PC1	C3-O31-C31	2.13	124.90	117.12
3	D	601	PC1	O21-C2-C3	2.13	115.98	108.34
2	C	501	LMT	O5'-C5'-C4'	2.12	114.11	109.72
3	C	601	PC1	O32-C31-C32	-2.12	115.51	123.78
2	E	602	LMT	O5B-C5B-C6B	2.11	111.67	106.44
3	C	602	PC1	C3-O31-C31	2.11	124.82	117.12
2	C	501	LMT	C1'-O5'-C5'	2.10	117.82	113.72
3	C	601	PC1	O31-C3-C2	2.09	114.42	108.40
3	D	603	PC1	O31-C31-C32	2.08	120.00	112.14
3	A	601	PC1	C3-O31-C31	2.07	124.68	117.12
2	A	501	LMT	O5B-C5B-C6B	2.07	111.56	106.44
3	D	601	PC1	O32-C31-C32	-2.02	115.90	123.78

All (49) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	501	LMT	C3'
2	A	501	LMT	C5'
2	A	501	LMT	C1B
2	A	501	LMT	C5B
2	A	501	LMT	C3B
2	A	501	LMT	C4'
2	B	501	LMT	C3'
2	B	501	LMT	C5'
2	B	501	LMT	C1B
2	B	501	LMT	C5B
2	B	501	LMT	C3B
2	B	501	LMT	C4'
2	C	502	LMT	C3'
2	C	502	LMT	C5'
2	C	502	LMT	C1B
2	C	502	LMT	C5B
2	C	502	LMT	C3B
2	C	502	LMT	C4'
2	C	501	LMT	C3'
2	C	501	LMT	C5'
2	C	501	LMT	C1B
2	C	501	LMT	C5B
2	C	501	LMT	C3B

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Mol	Chain	Res	Type	Atom
2	C	501	LMT	C4'
2	E	501	LMT	C3'
2	E	501	LMT	C5'
2	E	501	LMT	C1B
2	E	501	LMT	C5B
2	E	501	LMT	C3B
2	E	501	LMT	C4'
2	E	602	LMT	C3'
2	E	602	LMT	C5'
2	E	602	LMT	C1B
2	E	602	LMT	C5B
2	E	602	LMT	C3B
2	E	602	LMT	C4'
3	A	602	PC1	C2
3	A	603	PC1	C2
3	A	601	PC1	C2
3	B	601	PC1	C2
3	B	602	PC1	C2
3	C	601	PC1	C2
3	C	602	PC1	C2
3	C	603	PC1	C2
3	D	601	PC1	C2
3	D	602	PC1	C2
3	E	601	PC1	C2
3	E	603	PC1	C2
3	E	604	PC1	C2

All (349) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	LMT	O5'-C1'-O1'-C1
2	A	501	LMT	C2-C1-O1'-C1'
2	B	501	LMT	O5'-C1'-O1'-C1
2	C	502	LMT	C2'-C1'-O1'-C1
2	C	502	LMT	O5'-C1'-O1'-C1
2	C	501	LMT	C2B-C1B-O1B-C4'
2	C	501	LMT	C2-C1-O1'-C1'
2	E	602	LMT	C2B-C1B-O1B-C4'
2	E	602	LMT	O5'-C1'-O1'-C1
3	A	602	PC1	C11-O13-P-O12
3	A	602	PC1	C11-O13-P-O11
3	A	602	PC1	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
3	A	602	PC1	C1-O11-P-O14
3	A	602	PC1	C1-O11-P-O13
3	A	602	PC1	C22-C21-O21-C2
3	A	603	PC1	C3-C2-O21-C21
3	A	603	PC1	O22-C21-O21-C2
3	A	601	PC1	O22-C21-O21-C2
3	A	601	PC1	C22-C21-O21-C2
3	B	601	PC1	C2-C3-O31-C31
3	B	602	PC1	C11-O13-P-O14
3	B	602	PC1	C1-O11-P-O12
3	B	602	PC1	C1-O11-P-O14
3	B	602	PC1	C1-O11-P-O13
3	B	602	PC1	O13-C11-C12-N
3	B	602	PC1	C22-C21-O21-C2
3	C	601	PC1	C11-O13-P-O11
3	C	601	PC1	C1-O11-P-O12
3	C	601	PC1	C1-O11-P-O14
3	C	601	PC1	C1-O11-P-O13
3	C	602	PC1	C11-O13-P-O12
3	C	602	PC1	C11-O13-P-O14
3	C	602	PC1	C11-O13-P-O11
3	C	602	PC1	O13-C11-C12-N
3	C	602	PC1	C2-C1-O11-P
3	C	603	PC1	C3-C2-O21-C21
3	C	603	PC1	O22-C21-O21-C2
3	C	603	PC1	C22-C21-O21-C2
3	D	601	PC1	C2-C3-O31-C31
3	D	602	PC1	C11-O13-P-O14
3	D	602	PC1	C11-O13-P-O11
3	D	602	PC1	C1-O11-P-O12
3	D	602	PC1	C2-C1-O11-P
3	E	603	PC1	C1-O11-P-O12
3	E	603	PC1	O13-C11-C12-N
3	E	603	PC1	C2-C1-O11-P
3	E	604	PC1	C3-C2-O21-C21
3	E	604	PC1	O22-C21-O21-C2
3	E	604	PC1	C22-C21-O21-C2
2	A	501	LMT	C3'-C4'-O1B-C1B
2	C	501	LMT	O5B-C1B-O1B-C4'
2	B	501	LMT	C2B-C1B-O1B-C4'
2	E	501	LMT	O5B-C1B-O1B-C4'
3	A	601	PC1	C2-C3-O31-C31

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Mol	Chain	Res	Type	Atoms
3	E	601	PC1	O32-C31-O31-C3
2	A	501	LMT	O5B-C1B-O1B-C4'
3	A	602	PC1	O22-C21-O21-C2
3	B	601	PC1	O22-C21-O21-C2
3	B	602	PC1	O22-C21-O21-C2
2	C	502	LMT	C4'-C5'-C6'-O6'
3	A	603	PC1	C22-C21-O21-C2
3	D	602	PC1	C32-C31-O31-C3
3	E	601	PC1	C32-C31-O31-C3
2	B	501	LMT	O5B-C5B-C6B-O6B
2	C	502	LMT	O5'-C5'-C6'-O6'
3	B	603	PC1	C32-C31-O31-C3
2	E	602	LMT	O5B-C5B-C6B-O6B
2	E	602	LMT	O5'-C5'-C6'-O6'
3	B	601	PC1	C22-C21-O21-C2
2	A	501	LMT	O5'-C5'-C6'-O6'
2	C	501	LMT	O5'-C5'-C6'-O6'
2	A	501	LMT	C4'-C5'-C6'-O6'
3	B	603	PC1	O32-C31-O31-C3
3	B	603	PC1	O22-C21-O21-C2
3	D	602	PC1	O32-C31-O31-C3
2	C	501	LMT	C4'-C5'-C6'-O6'
3	B	601	PC1	C32-C31-O31-C3
3	B	602	PC1	C32-C31-O31-C3
3	B	603	PC1	C22-C21-O21-C2
3	E	603	PC1	C32-C31-O31-C3
3	E	603	PC1	O32-C31-O31-C3
3	C	602	PC1	C32-C31-O31-C3
2	E	501	LMT	O5B-C5B-C6B-O6B
3	B	601	PC1	C11-C12-N-C14
2	B	501	LMT	C4B-C5B-C6B-O6B
2	A	501	LMT	C2'-C1'-O1'-C1
2	B	501	LMT	C2'-C1'-O1'-C1
2	E	602	LMT	C4B-C5B-C6B-O6B
2	C	502	LMT	O1'-C1-C2-C3
3	B	602	PC1	C31-C32-C33-C34
3	E	601	PC1	C31-C32-C33-C34
2	E	501	LMT	O1'-C1-C2-C3
3	B	603	PC1	C21-C22-C23-C24
3	D	601	PC1	C21-C22-C23-C24
2	C	501	LMT	O1'-C1-C2-C3
3	A	602	PC1	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
3	C	601	PC1	C21-C22-C23-C24
3	D	602	PC1	C31-C32-C33-C34
3	E	604	PC1	C31-C32-C33-C34
3	B	602	PC1	O32-C31-O31-C3
3	B	601	PC1	O32-C31-O31-C3
3	C	602	PC1	O32-C31-O31-C3
3	C	602	PC1	C21-C22-C23-C24
3	B	601	PC1	C21-C22-C23-C24
3	B	603	PC1	C32-C33-C34-C35
3	C	601	PC1	C32-C31-O31-C3
3	A	602	PC1	C11-C12-N-C13
3	B	601	PC1	C11-C12-N-C13
3	E	603	PC1	C11-C12-N-C15
3	D	601	PC1	C22-C21-O21-C2
3	D	601	PC1	O22-C21-O21-C2
2	C	501	LMT	C2'-C1'-O1'-C1
2	E	602	LMT	C2'-C1'-O1'-C1
3	A	601	PC1	C32-C31-O31-C3
2	E	501	LMT	C4B-C5B-C6B-O6B
3	C	601	PC1	C22-C21-O21-C2
3	B	601	PC1	C11-C12-N-C15
3	B	602	PC1	C21-C22-C23-C24
3	C	603	PC1	C22-C23-C24-C25
3	C	602	PC1	C24-C25-C26-C27
3	C	601	PC1	O32-C31-O31-C3
3	C	601	PC1	O22-C21-O21-C2
3	A	602	PC1	C23-C24-C25-C26
3	C	602	PC1	C22-C21-O21-C2
3	E	601	PC1	C22-C21-O21-C2
3	A	601	PC1	C22-C23-C24-C25
3	A	601	PC1	O32-C31-O31-C3
2	C	501	LMT	C1-C2-C3-C4
3	B	601	PC1	C2B-C2C-C2D-C2E
3	D	601	PC1	C28-C29-C2A-C2B
3	C	602	PC1	C31-C32-C33-C34
3	D	603	PC1	C32-C31-O31-C3
2	E	501	LMT	C2-C3-C4-C5
3	C	602	PC1	C27-C28-C29-C2A
3	E	603	PC1	C25-C26-C27-C28
3	C	602	PC1	C33-C34-C35-C36
3	A	602	PC1	C35-C36-C37-C38
3	E	604	PC1	C28-C29-C2A-C2B

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Mol	Chain	Res	Type	Atoms
2	C	502	LMT	C1-C2-C3-C4
3	D	602	PC1	C11-C12-N-C15
3	E	603	PC1	C11-C12-N-C13
3	C	601	PC1	C27-C28-C29-C2A
3	E	604	PC1	C32-C33-C34-C35
3	C	603	PC1	C28-C29-C2A-C2B
3	E	601	PC1	C28-C29-C2A-C2B
3	C	602	PC1	O22-C21-O21-C2
3	B	601	PC1	C2D-C2E-C2F-C2G
2	A	501	LMT	C2B-C1B-O1B-C4'
2	E	501	LMT	C3-C4-C5-C6
3	A	601	PC1	C2D-C2E-C2F-C2G
3	D	603	PC1	C23-C24-C25-C26
2	C	502	LMT	C2-C3-C4-C5
3	E	603	PC1	C37-C38-C39-C3A
3	A	603	PC1	C23-C24-C25-C26
3	E	603	PC1	C35-C36-C37-C38
3	E	604	PC1	C25-C26-C27-C28
3	E	603	PC1	C11-C12-N-C14
2	A	501	LMT	C4B-C5B-C6B-O6B
3	B	603	PC1	C27-C28-C29-C2A
3	C	602	PC1	C32-C33-C34-C35
3	E	601	PC1	O22-C21-O21-C2
3	C	603	PC1	C24-C25-C26-C27
3	A	603	PC1	C31-C32-C33-C34
3	A	602	PC1	O21-C2-C3-O31
3	A	602	PC1	C22-C23-C24-C25
3	D	603	PC1	C27-C28-C29-C2A
3	D	601	PC1	C32-C31-O31-C3
3	C	602	PC1	C22-C23-C24-C25
3	B	602	PC1	C2-C1-O11-P
3	B	601	PC1	C28-C29-C2A-C2B
3	B	601	PC1	C36-C37-C38-C39
3	D	602	PC1	C32-C33-C34-C35
3	A	602	PC1	C11-C12-N-C15
3	B	602	PC1	C11-C12-N-C15
2	C	501	LMT	O5'-C1'-O1'-C1
3	B	603	PC1	C29-C2A-C2B-C2C
3	E	601	PC1	C25-C26-C27-C28
3	E	601	PC1	C26-C27-C28-C29
3	D	601	PC1	O32-C31-O31-C3
3	D	603	PC1	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
3	E	603	PC1	C22-C21-O21-C2
2	E	602	LMT	C4'-C5'-C6'-O6'
2	E	501	LMT	C2'-C1'-O1'-C1
3	A	603	PC1	C21-C22-C23-C24
3	A	601	PC1	C1-C2-C3-O31
3	B	601	PC1	C1-C2-C3-O31
3	B	601	PC1	C2E-C2F-C2G-C2H
3	E	601	PC1	C32-C33-C34-C35
3	C	603	PC1	C23-C24-C25-C26
3	B	602	PC1	C34-C35-C36-C37
2	C	502	LMT	C6-C7-C8-C9
3	B	602	PC1	C11-C12-N-C13
3	D	602	PC1	C11-C12-N-C14
3	A	601	PC1	C24-C25-C26-C27
3	A	603	PC1	C27-C28-C29-C2A
3	B	602	PC1	C36-C37-C38-C39
3	D	602	PC1	C23-C24-C25-C26
2	C	501	LMT	C5-C6-C7-C8
3	A	603	PC1	C29-C2A-C2B-C2C
3	D	602	PC1	C27-C28-C29-C2A
3	E	603	PC1	C26-C27-C28-C29
3	E	603	PC1	C24-C25-C26-C27
3	B	603	PC1	O21-C2-C3-O31
3	A	601	PC1	C2E-C2F-C2G-C2H
3	E	601	PC1	C27-C28-C29-C2A
3	E	601	PC1	C2B-C2C-C2D-C2E
3	A	601	PC1	C28-C29-C2A-C2B
2	B	501	LMT	O1'-C1-C2-C3
3	E	601	PC1	C2E-C2F-C2G-C2H
3	B	603	PC1	C28-C29-C2A-C2B
3	C	602	PC1	C28-C29-C2A-C2B
2	C	502	LMT	C2B-C1B-O1B-C4'
3	C	603	PC1	C32-C33-C34-C35
2	B	501	LMT	C2-C1-O1'-C1'
3	A	602	PC1	O11-C1-C2-C3
3	A	601	PC1	C2F-C2G-C2H-C2I
3	A	602	PC1	C11-C12-N-C14
3	E	601	PC1	C2-C3-O31-C31
3	E	601	PC1	C2F-C2G-C2H-C2I
3	A	603	PC1	C25-C26-C27-C28
3	A	603	PC1	C1-C2-C3-O31
2	B	501	LMT	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
3	A	602	PC1	C28-C29-C2A-C2B
3	C	602	PC1	C25-C26-C27-C28
3	A	602	PC1	C1-C2-C3-O31
3	C	601	PC1	C1-C2-C3-O31
2	C	502	LMT	C11-C10-C9-C8
3	C	602	PC1	C37-C38-C39-C3A
3	A	602	PC1	C24-C25-C26-C27
3	A	603	PC1	C33-C34-C35-C36
3	A	603	PC1	O21-C2-C3-O31
3	A	602	PC1	O11-C1-C2-O21
3	B	601	PC1	C29-C2A-C2B-C2C
3	C	603	PC1	C2B-C2C-C2D-C2E
3	C	601	PC1	O21-C2-C3-O31
3	D	601	PC1	O21-C2-C3-O31
3	E	603	PC1	O22-C21-O21-C2
3	E	604	PC1	C33-C34-C35-C36
3	D	603	PC1	O32-C31-O31-C3
3	B	602	PC1	C24-C25-C26-C27
3	C	601	PC1	C22-C23-C24-C25
3	E	601	PC1	C21-C22-C23-C24
2	A	501	LMT	C2-C3-C4-C5
3	D	602	PC1	C24-C25-C26-C27
3	C	602	PC1	C35-C36-C37-C38
3	C	601	PC1	C2F-C2G-C2H-C2I
3	D	603	PC1	C28-C29-C2A-C2B
3	A	602	PC1	C33-C34-C35-C36
3	B	602	PC1	C22-C23-C24-C25
3	C	601	PC1	C34-C35-C36-C37
3	E	601	PC1	C2D-C2E-C2F-C2G
2	C	501	LMT	C11-C10-C9-C8
3	B	602	PC1	C28-C29-C2A-C2B
3	D	602	PC1	C28-C29-C2A-C2B
3	D	601	PC1	C1-C2-C3-O31
3	E	601	PC1	C22-C23-C24-C25
3	E	603	PC1	O21-C21-C22-C23
3	A	601	PC1	O21-C2-C3-O31
3	B	601	PC1	O21-C2-C3-O31
3	B	602	PC1	O21-C2-C3-O31
3	E	603	PC1	C28-C29-C2A-C2B
3	B	602	PC1	C26-C27-C28-C29
3	D	601	PC1	C2B-C2C-C2D-C2E
3	E	604	PC1	C2A-C2B-C2C-C2D

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Mol	Chain	Res	Type	Atoms
3	E	603	PC1	C23-C24-C25-C26
3	A	601	PC1	O13-C11-C12-N
3	B	601	PC1	O13-C11-C12-N
3	D	601	PC1	O13-C11-C12-N
3	E	601	PC1	O13-C11-C12-N
2	E	501	LMT	C1-C2-C3-C4
3	D	602	PC1	C22-C23-C24-C25
3	B	603	PC1	C2A-C2B-C2C-C2D
3	D	602	PC1	C21-C22-C23-C24
3	A	601	PC1	C27-C28-C29-C2A
3	B	603	PC1	C23-C24-C25-C26
3	E	603	PC1	C21-C22-C23-C24
3	B	602	PC1	C11-C12-N-C14
3	D	602	PC1	C11-C12-N-C13
3	C	601	PC1	C28-C29-C2A-C2B
3	E	603	PC1	C36-C37-C38-C39
3	E	601	PC1	C24-C25-C26-C27
3	B	602	PC1	C35-C36-C37-C38
3	C	601	PC1	C23-C24-C25-C26
3	B	601	PC1	C1-O11-P-O14
3	C	601	PC1	C11-O13-P-O14
3	D	601	PC1	C11-C12-N-C15
3	D	602	PC1	C11-O13-P-O12
3	D	602	PC1	C1-O11-P-O14
3	D	602	PC1	C1-O11-P-O13
3	E	601	PC1	C1-O11-P-O14
3	E	603	PC1	C1-O11-P-O14
3	E	603	PC1	C1-O11-P-O13
3	C	602	PC1	C34-C35-C36-C37
3	D	601	PC1	C2A-C2B-C2C-C2D
3	D	603	PC1	C33-C34-C35-C36
3	D	601	PC1	C36-C37-C38-C39
3	C	602	PC1	C36-C37-C38-C39
3	E	601	PC1	O21-C2-C3-O31
3	B	602	PC1	C1-C2-C3-O31
2	C	502	LMT	C5-C6-C7-C8
3	D	602	PC1	C25-C26-C27-C28
3	B	601	PC1	C2C-C2D-C2E-C2F
3	D	602	PC1	C35-C36-C37-C38
3	D	601	PC1	C24-C25-C26-C27
3	C	601	PC1	C26-C27-C28-C29
3	B	601	PC1	C27-C28-C29-C2A

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Mol	Chain	Res	Type	Atoms
3	E	601	PC1	C29-C2A-C2B-C2C
3	B	602	PC1	C33-C34-C35-C36
3	B	602	PC1	C37-C38-C39-C3A
2	B	501	LMT	C4-C5-C6-C7
3	A	601	PC1	C35-C36-C37-C38
3	B	601	PC1	C26-C27-C28-C29
2	C	501	LMT	C6-C7-C8-C9
3	D	602	PC1	C26-C27-C28-C29
3	A	602	PC1	C36-C37-C38-C39
2	E	602	LMT	C2-C1-O1'-C1'
3	A	602	PC1	C25-C26-C27-C28
3	A	602	PC1	C27-C28-C29-C2A
3	D	601	PC1	C32-C33-C34-C35
3	D	601	PC1	C38-C39-C3A-C3B
3	E	601	PC1	C23-C24-C25-C26
3	C	602	PC1	C23-C24-C25-C26
3	B	603	PC1	C26-C27-C28-C29
3	A	602	PC1	O13-C11-C12-N
3	D	602	PC1	O13-C11-C12-N
3	B	602	PC1	O21-C21-C22-C23
3	D	601	PC1	C11-C12-N-C13
2	C	501	LMT	C9-C10-C11-C12
3	D	602	PC1	O21-C21-C22-C23
2	E	501	LMT	C2B-C1B-O1B-C4'
3	C	603	PC1	C26-C27-C28-C29
3	D	601	PC1	C11-C12-N-C14
3	C	602	PC1	C26-C27-C28-C29
3	E	603	PC1	O22-C21-C22-C23
3	A	603	PC1	C32-C33-C34-C35
3	D	602	PC1	O22-C21-O21-C2
3	A	601	PC1	C36-C37-C38-C39
3	B	602	PC1	O22-C21-C22-C23
2	C	501	LMT	C7-C8-C9-C10
3	C	601	PC1	C2B-C2C-C2D-C2E
3	A	602	PC1	O21-C21-C22-C23
3	E	601	PC1	O31-C31-C32-C33
3	E	601	PC1	C38-C39-C3A-C3B
3	C	601	PC1	C2D-C2E-C2F-C2G
3	C	602	PC1	O21-C21-C22-C23
3	A	603	PC1	C22-C23-C24-C25
2	B	501	LMT	C5-C6-C7-C8
3	A	602	PC1	O32-C31-O31-C3

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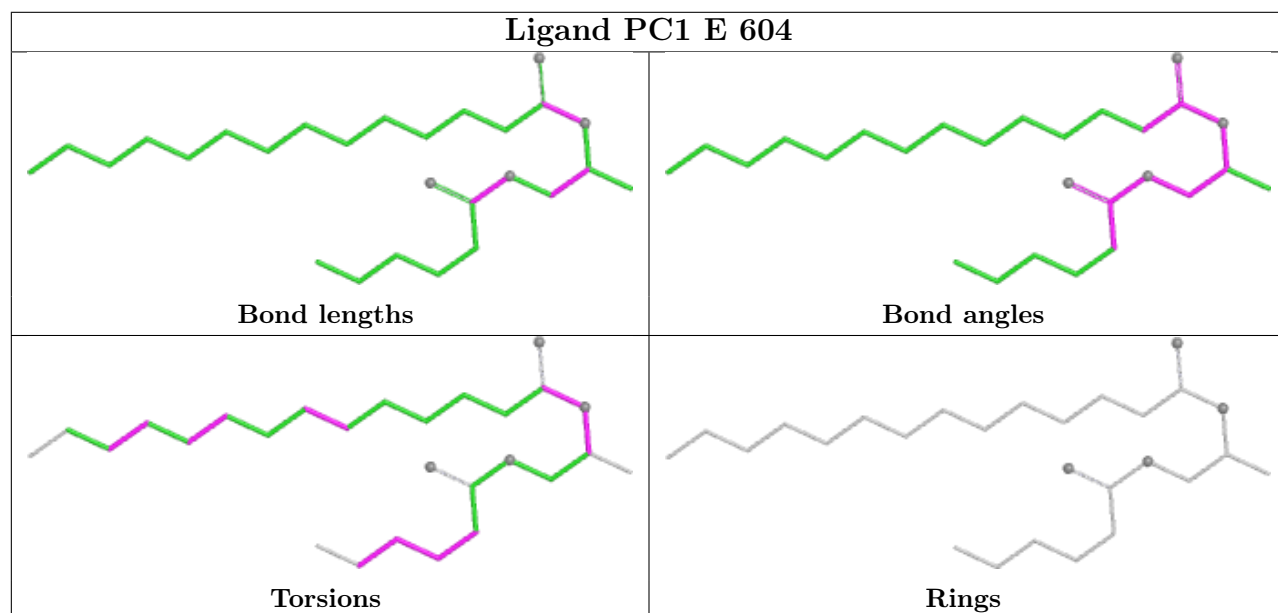
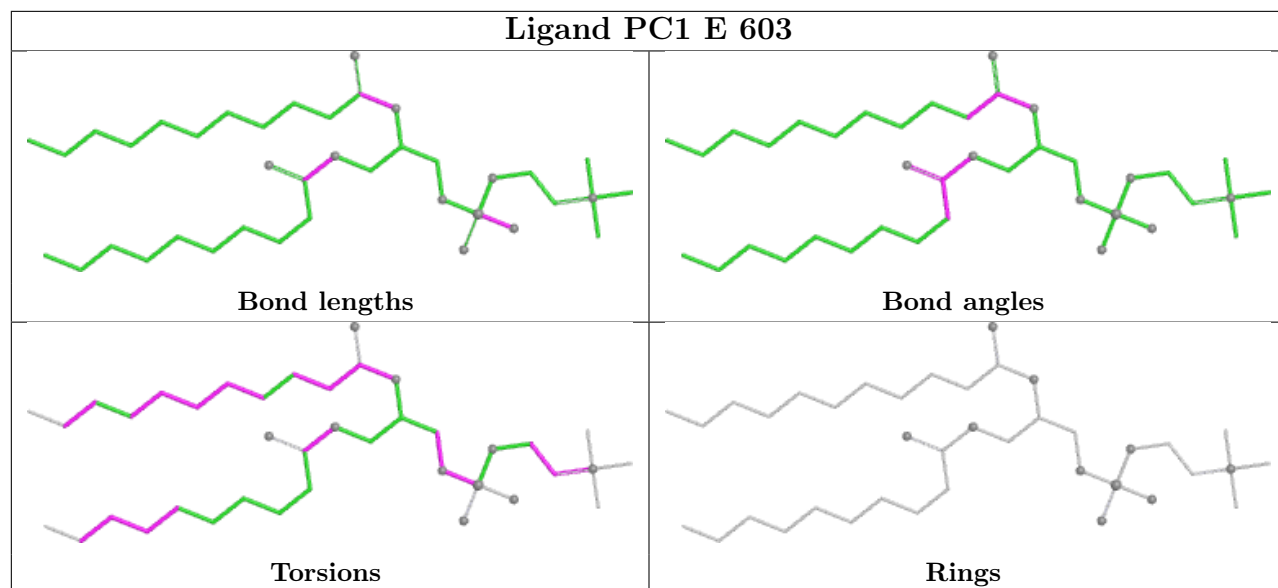
Mol	Chain	Res	Type	Atoms
3	E	601	PC1	O32-C31-C32-C33

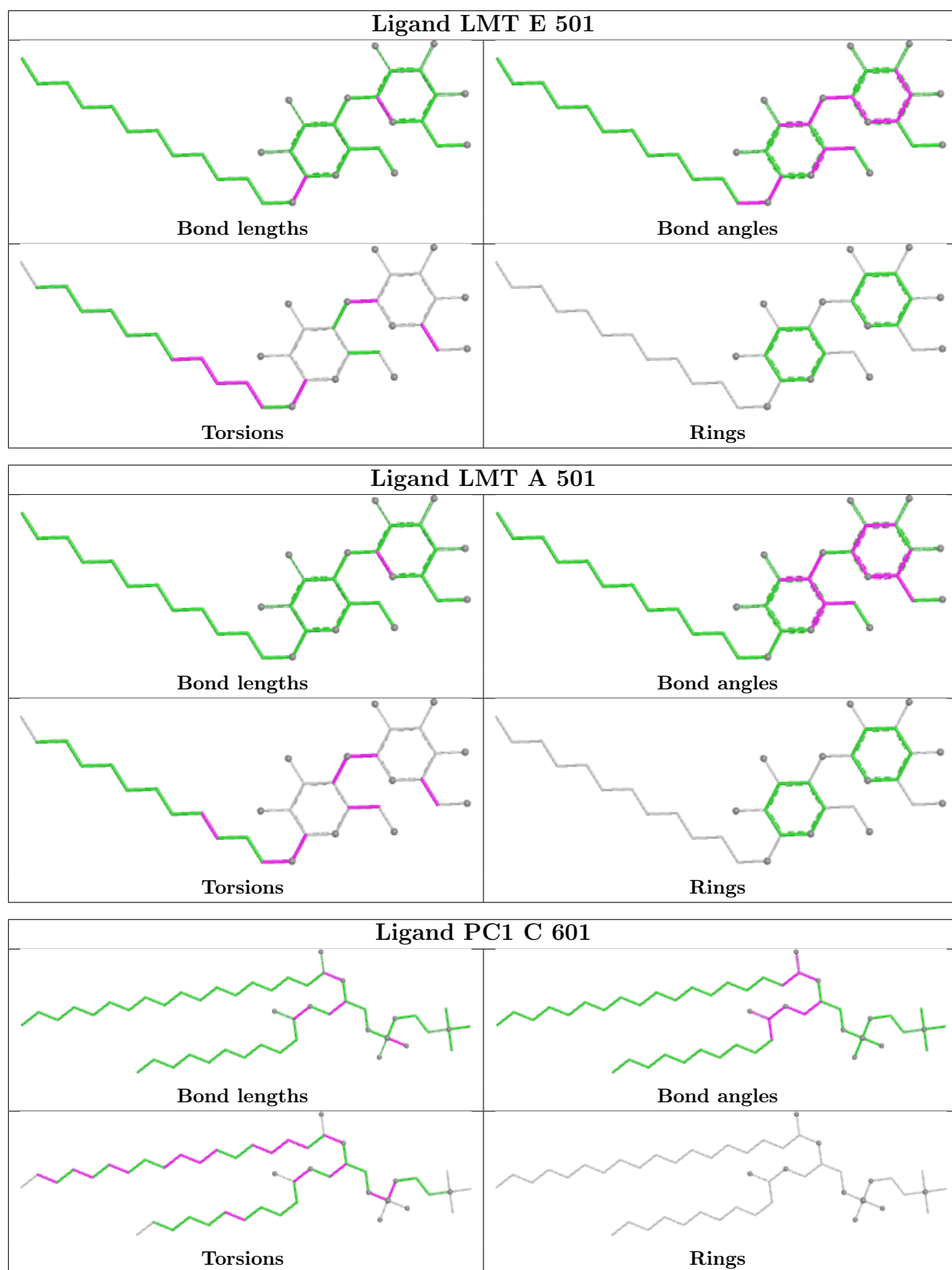
There are no ring outliers.

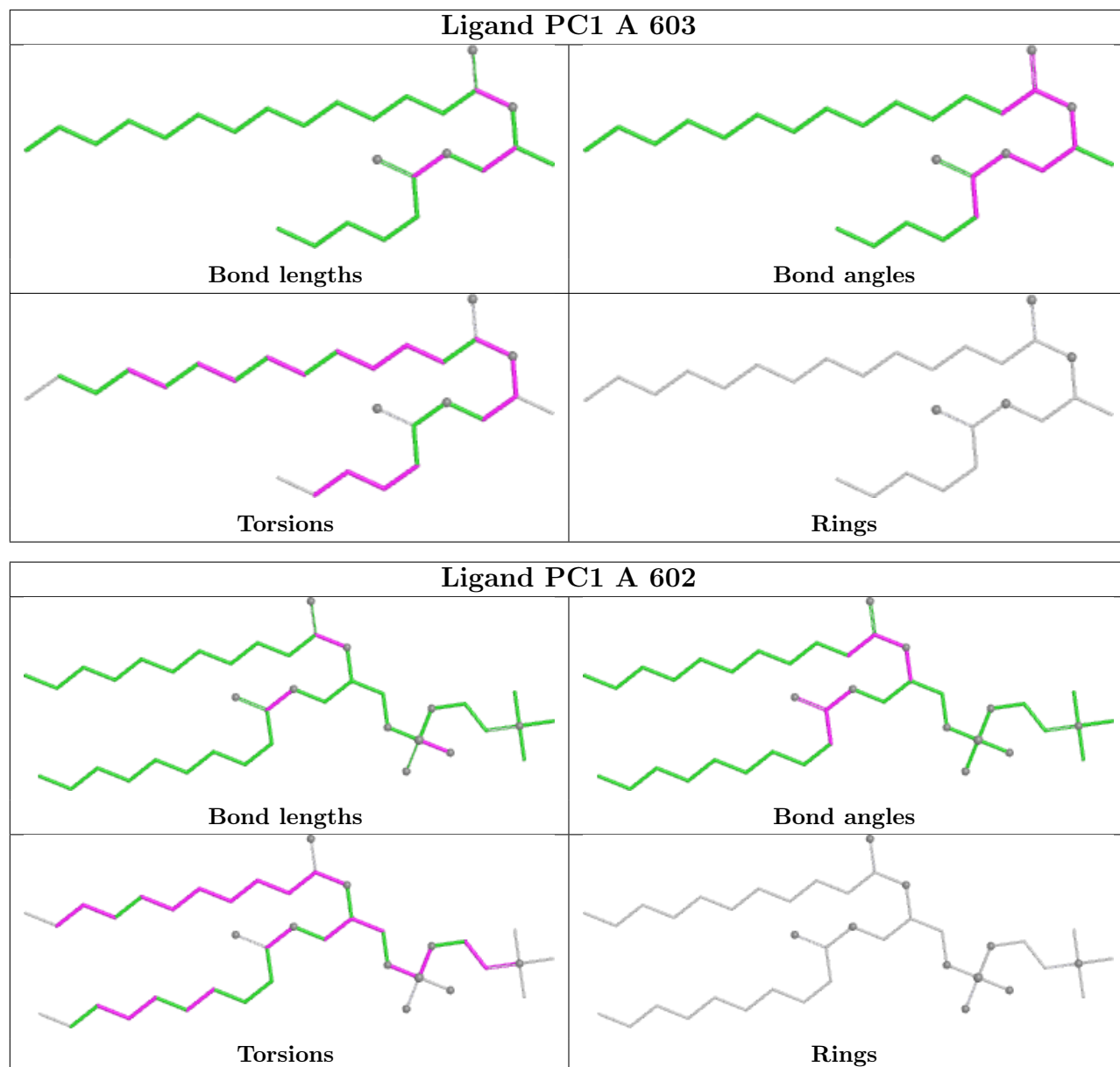
17 monomers are involved in 44 short contacts:

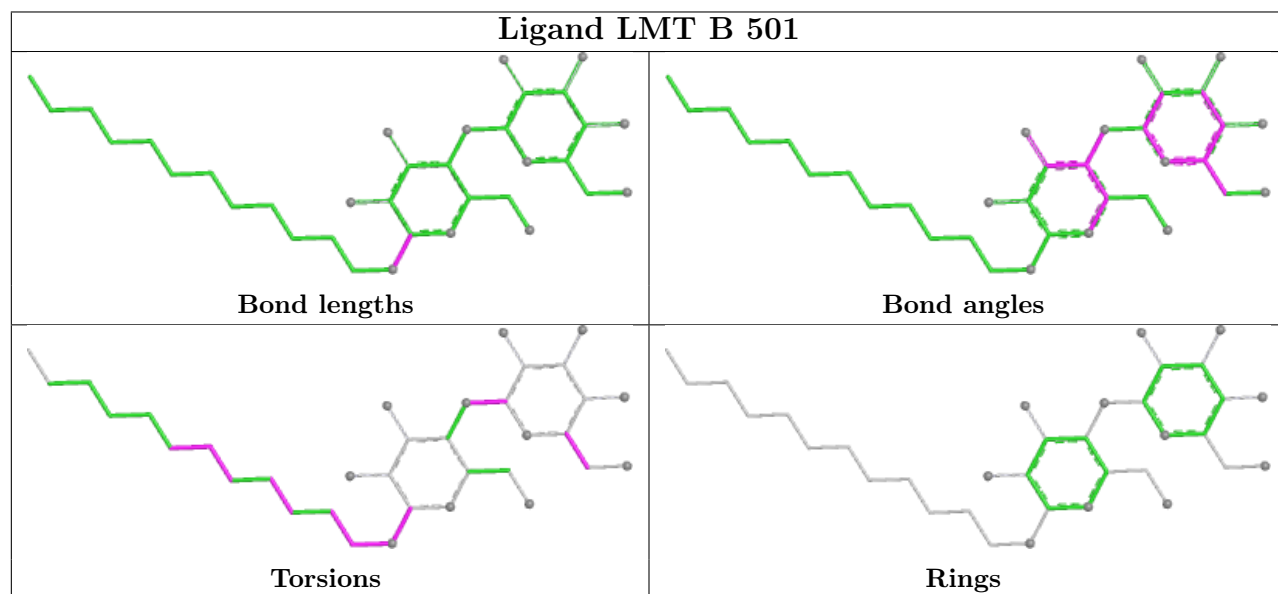
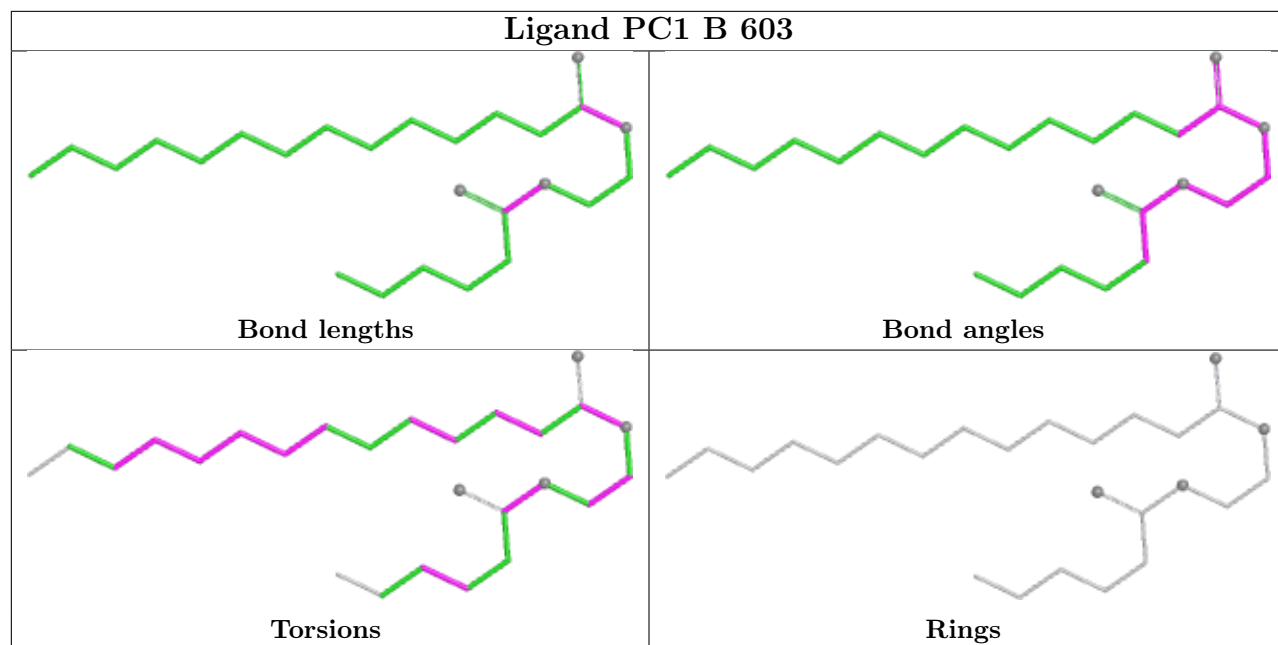
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	603	PC1	4	0
2	E	501	LMT	5	0
3	C	601	PC1	1	0
3	A	602	PC1	1	0
3	B	603	PC1	1	0
2	B	501	LMT	9	0
3	D	603	PC1	1	0
3	D	602	PC1	5	0
3	B	602	PC1	2	0
3	C	603	PC1	1	0
3	E	601	PC1	1	0
2	C	501	LMT	6	0
3	D	601	PC1	1	0
3	C	602	PC1	2	0
2	E	602	LMT	3	0
3	A	601	PC1	1	0
3	B	601	PC1	4	0

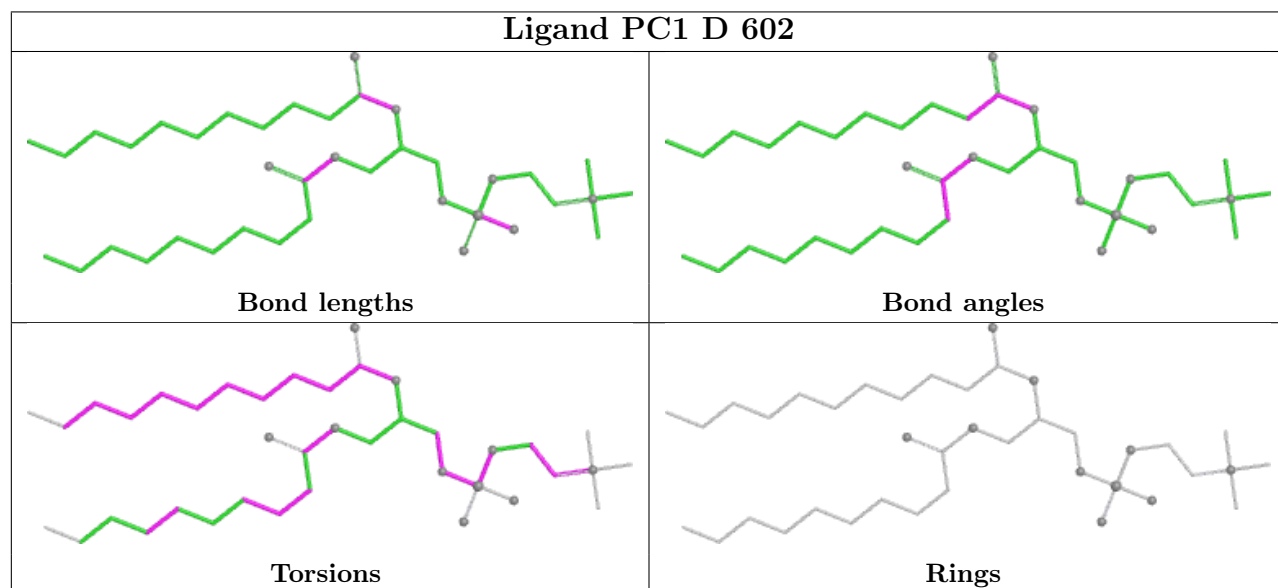
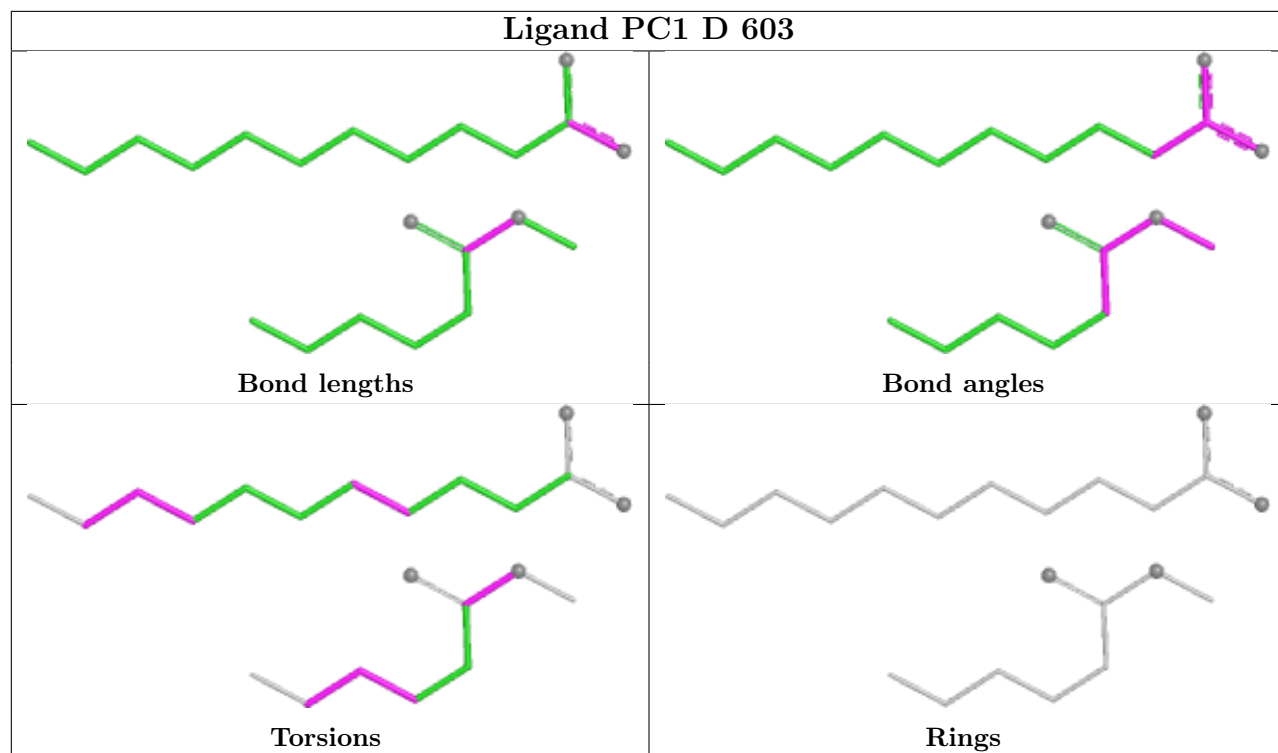
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

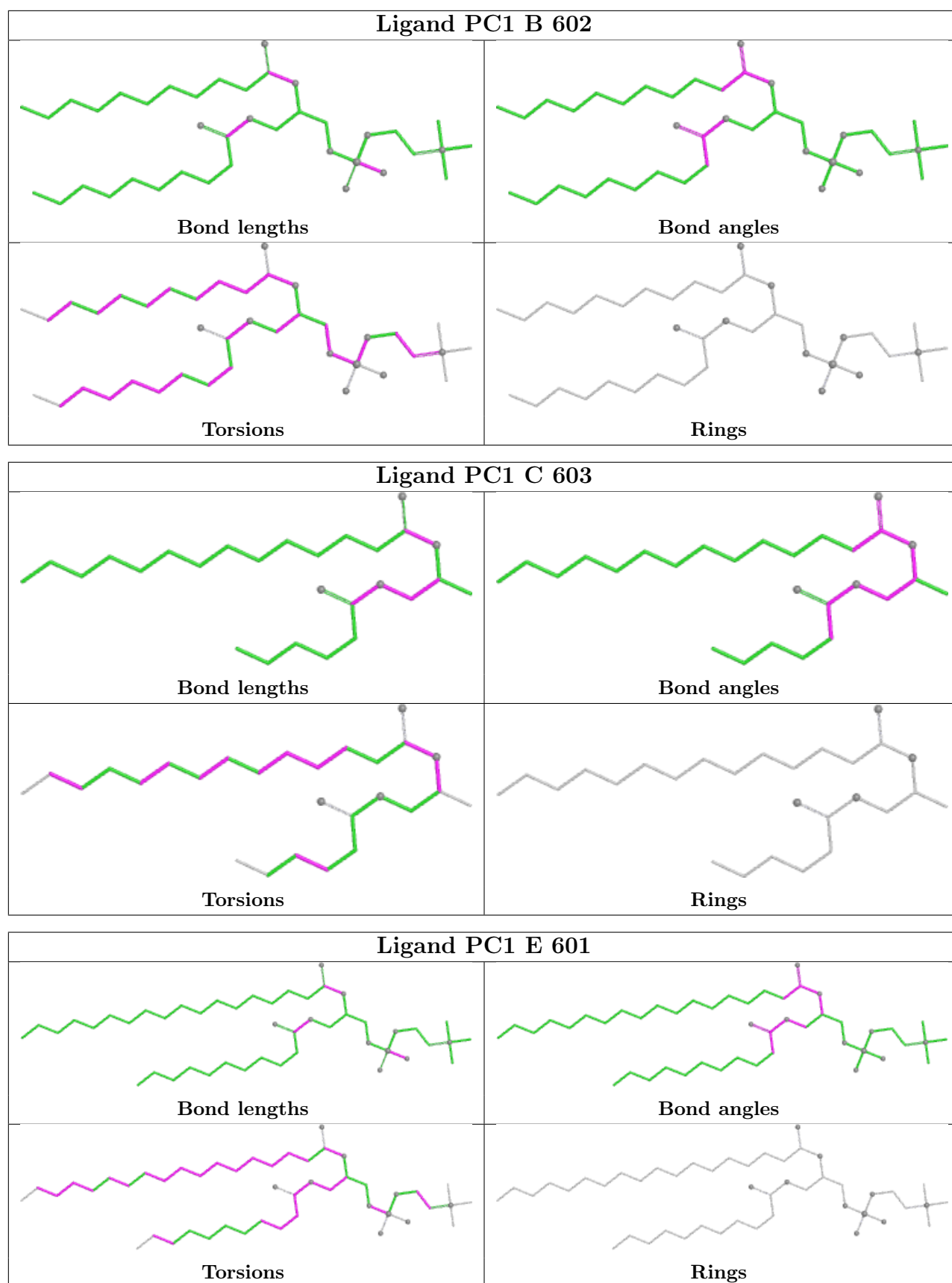


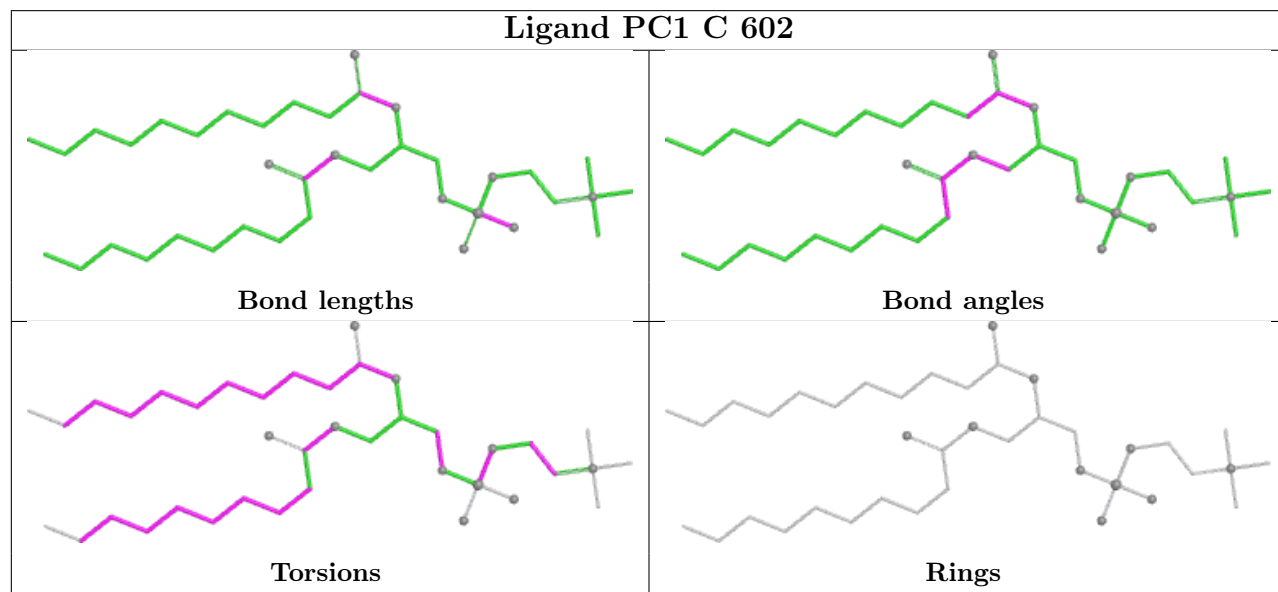
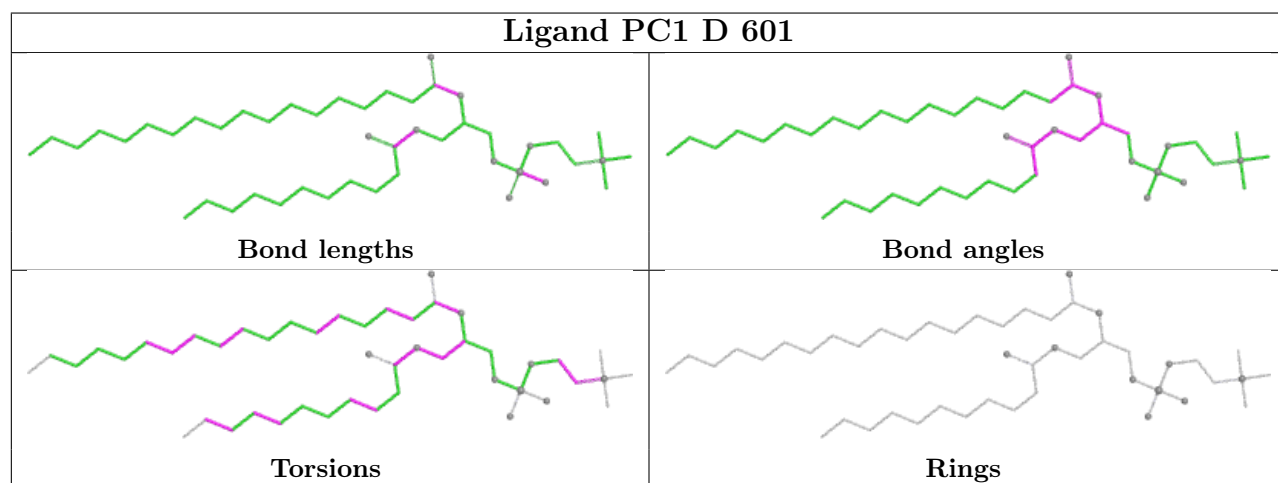
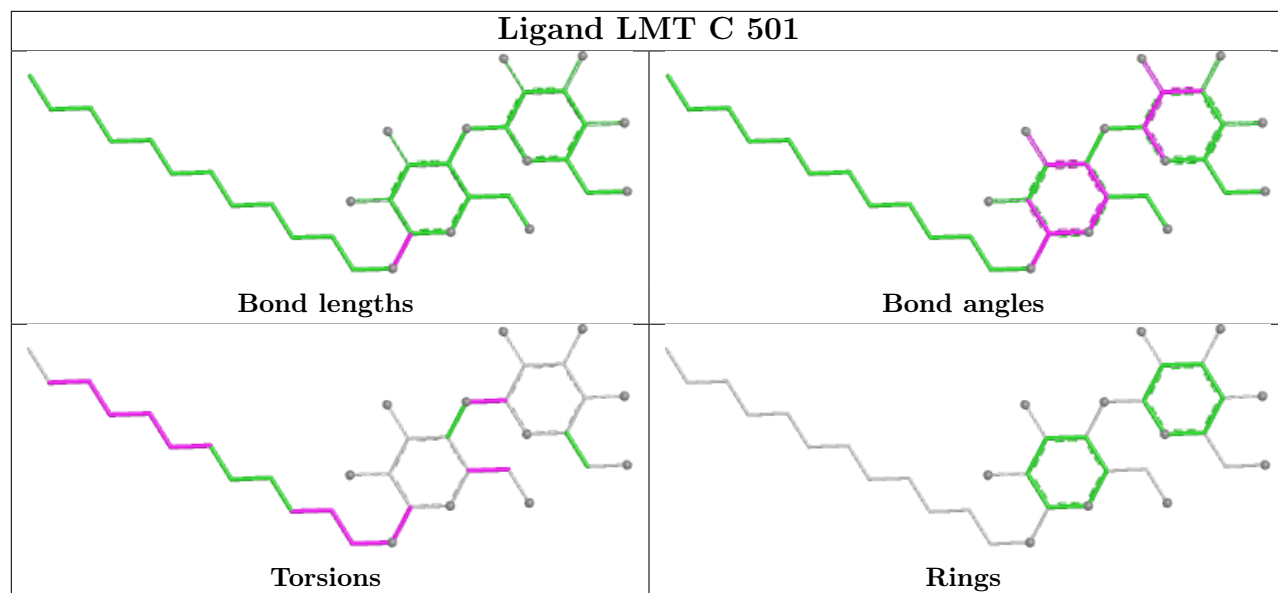


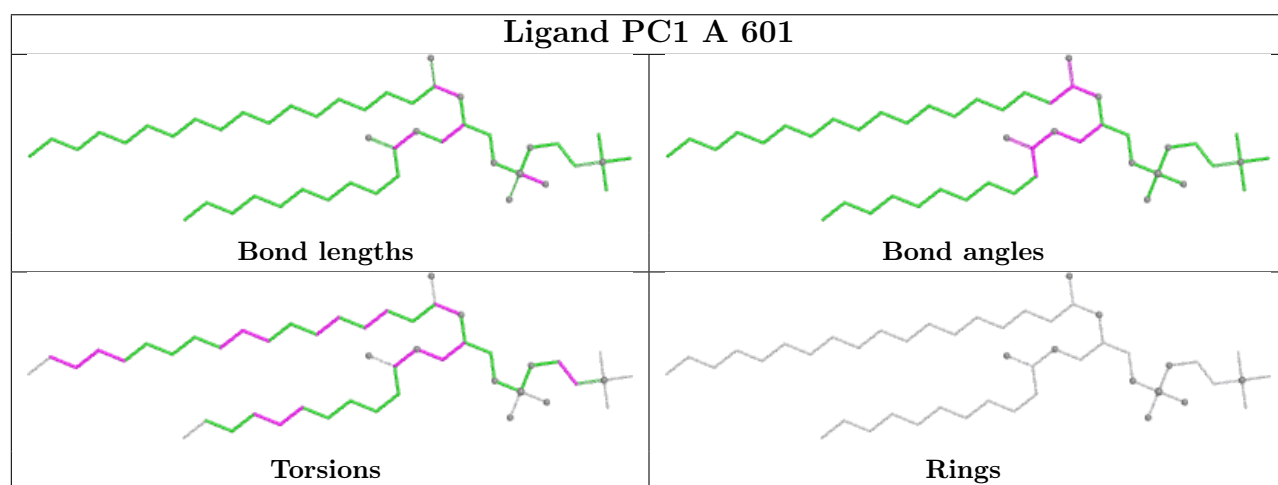
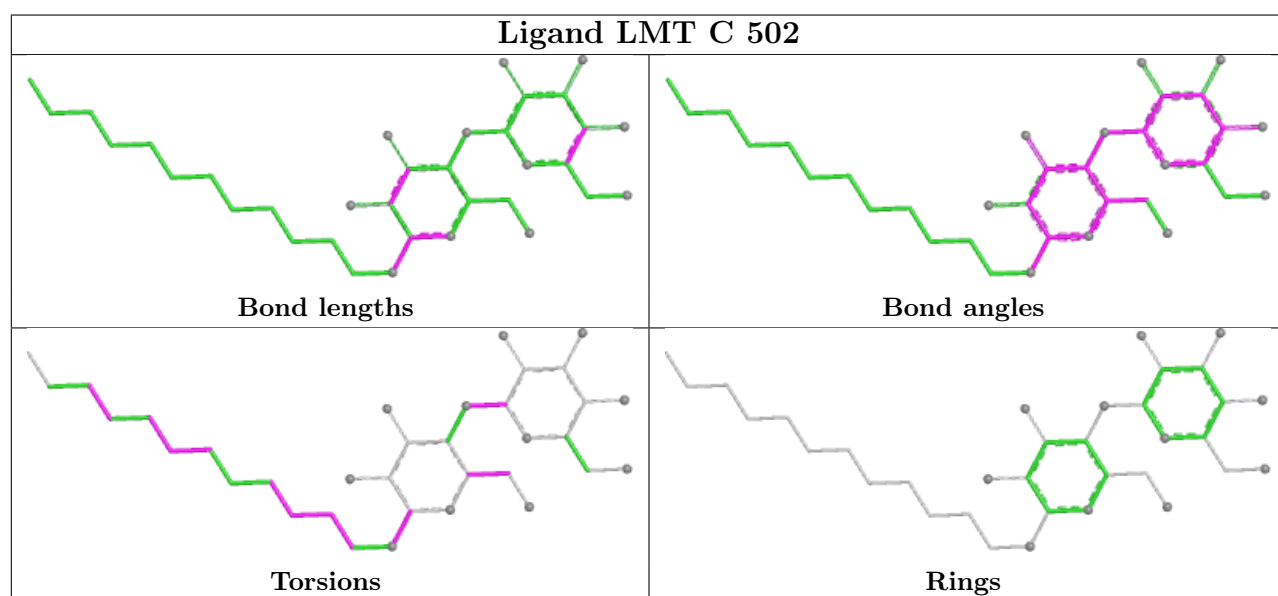
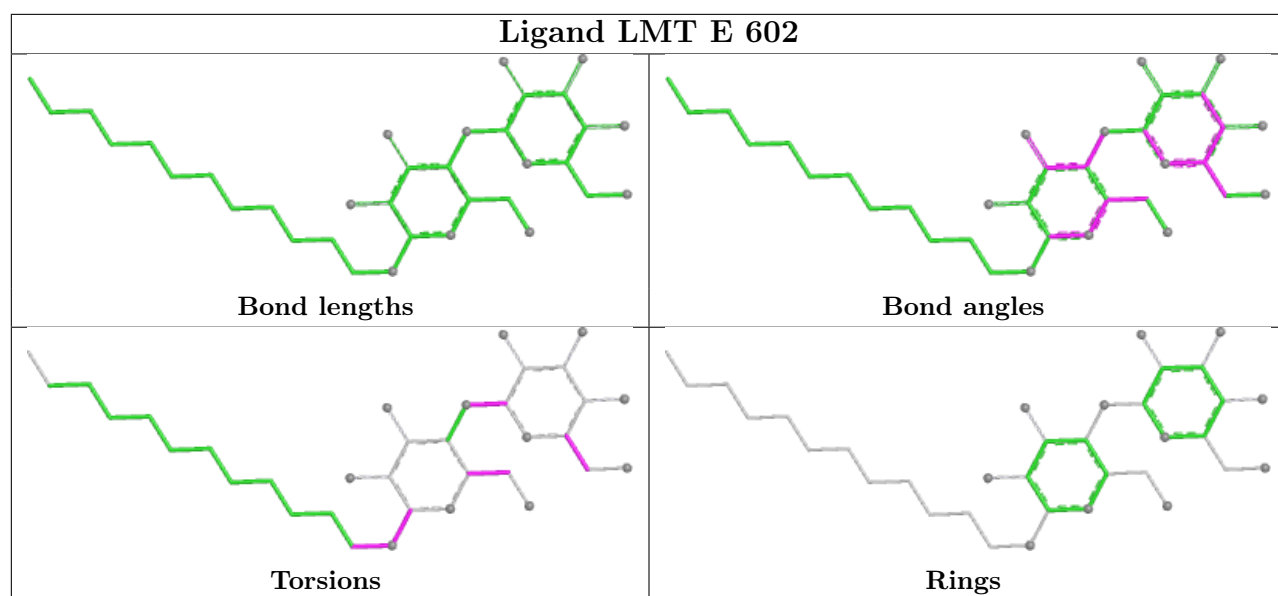


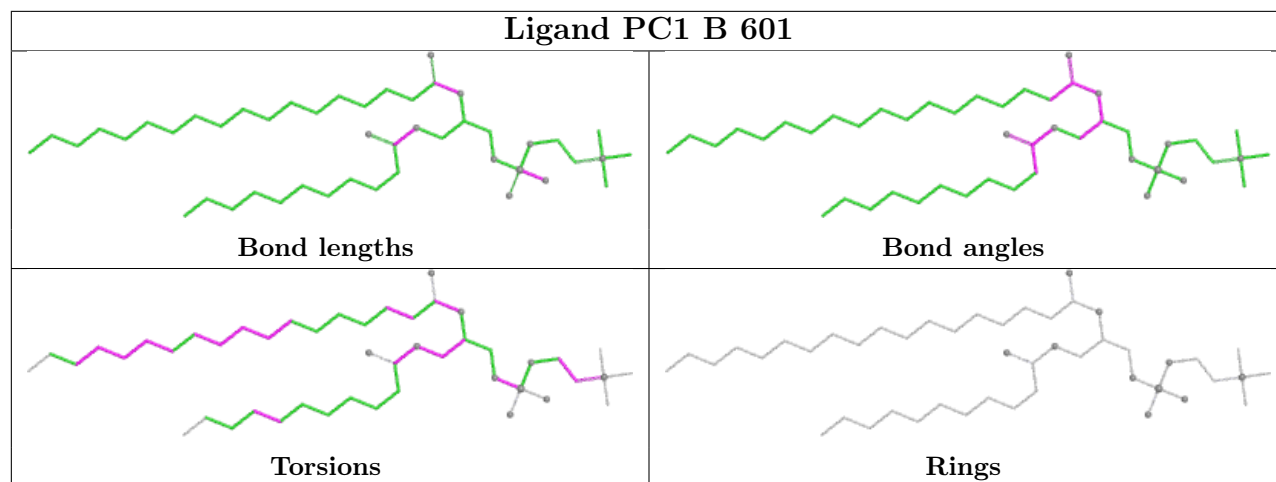












5.7 Other polymers [i](#)

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	311/317 (98%)	-0.72	3 (0%) 79 73	31, 48, 83, 109	0
1	B	311/317 (98%)	-0.70	3 (0%) 79 73	31, 48, 77, 88	0
1	C	311/317 (98%)	-0.74	2 (0%) 85 81	31, 48, 80, 100	0
1	D	311/317 (98%)	-0.78	2 (0%) 85 81	31, 48, 83, 108	0
1	E	311/317 (98%)	-0.76	3 (0%) 79 73	31, 48, 80, 95	0
All	All	1555/1585 (98%)	-0.74	13 (0%) 82 77	31, 48, 81, 109	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	57	VAL	3.1
1	C	11	ILE	2.6
1	A	11	ILE	2.6
1	E	12	ALA	2.5
1	C	12	ALA	2.5
1	A	10	PRO	2.4
1	A	12	ALA	2.4
1	D	245	ASN	2.3
1	E	245	ASN	2.3
1	B	136	ASP	2.2
1	B	12	ALA	2.1
1	B	5	VAL	2.0
1	E	11	ILE	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

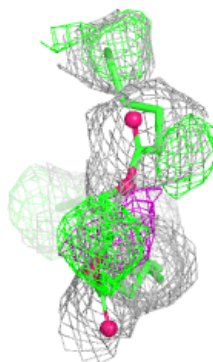
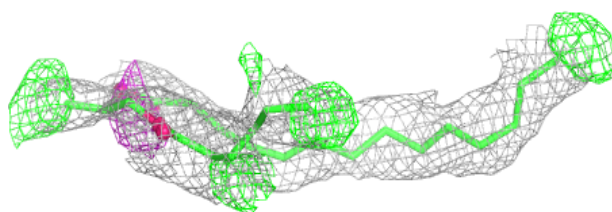
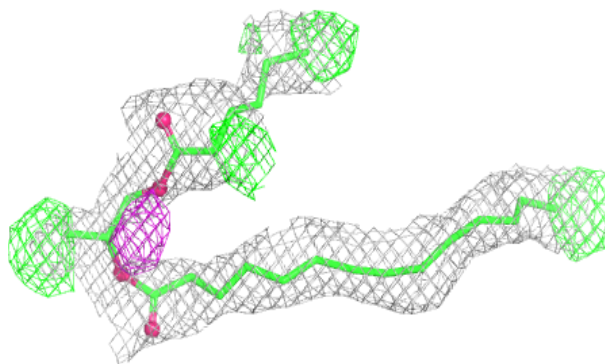
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PC1	A	603	27/54	0.55	0.17	62,90,102,104	0
3	PC1	C	603	27/54	0.74	0.14	61,77,91,93	0
3	PC1	D	603	22/54	0.75	0.14	61,75,89,91	0
3	PC1	A	601	47/54	0.76	0.12	67,85,115,115	0
3	PC1	A	602	39/54	0.77	0.14	75,94,137,137	0
3	PC1	D	601	47/54	0.77	0.13	66,84,115,115	0
3	PC1	B	601	47/54	0.77	0.14	65,89,126,127	0
3	PC1	E	604	27/54	0.77	0.13	64,73,92,93	0
3	PC1	B	603	26/54	0.78	0.13	52,72,85,87	0
3	PC1	C	601	47/54	0.79	0.13	66,96,137,137	0
3	PC1	E	601	47/54	0.80	0.13	50,81,114,115	0
3	PC1	D	602	39/54	0.84	0.13	64,84,125,125	0
3	PC1	C	602	39/54	0.84	0.13	70,97,132,132	0
3	PC1	E	603	39/54	0.85	0.12	61,102,134,134	0
3	PC1	B	602	39/54	0.88	0.13	60,97,131,131	0
2	LMT	B	501	35/35	0.90	0.10	38,120,134,135	0
2	LMT	C	502	35/35	0.90	0.08	28,76,85,91	0
2	LMT	E	602	35/35	0.90	0.12	42,127,153,154	0
2	LMT	A	501	35/35	0.91	0.10	27,120,139,140	0
2	LMT	C	501	35/35	0.92	0.11	29,118,140,140	0
2	LMT	E	501	35/35	0.92	0.10	25,107,130,132	0

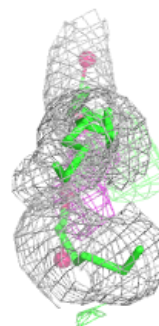
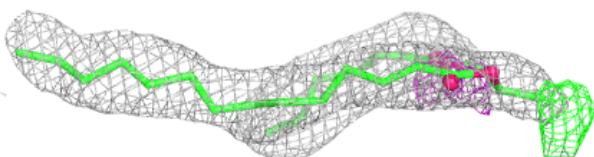
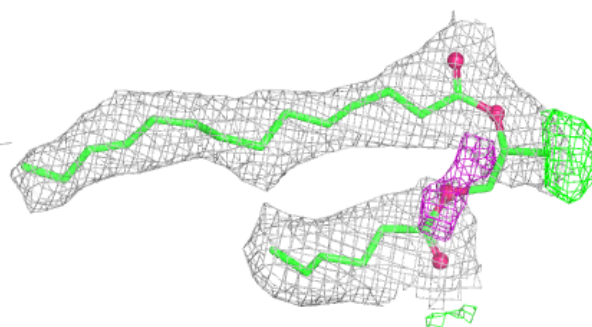
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PC1 A 603:

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

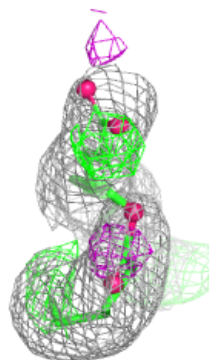
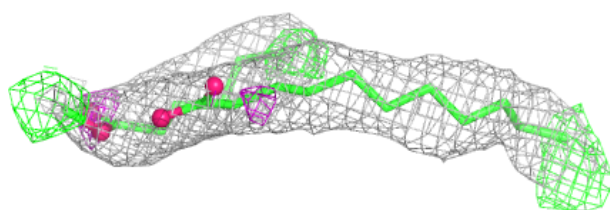
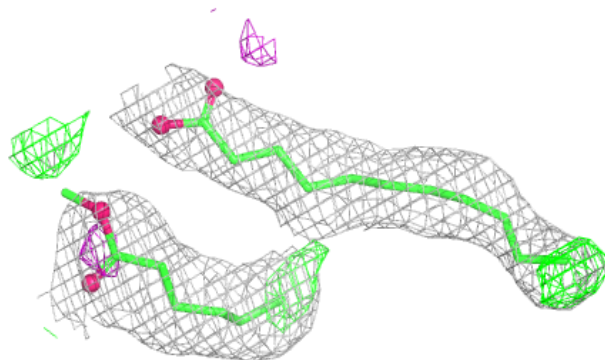
**Electron density around PC1 C 603:**

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

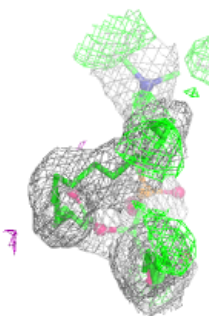
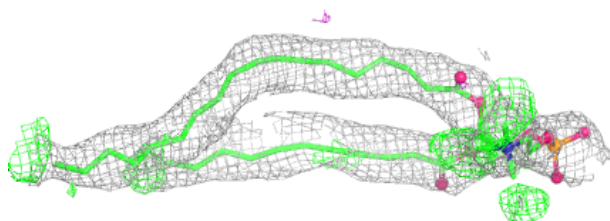
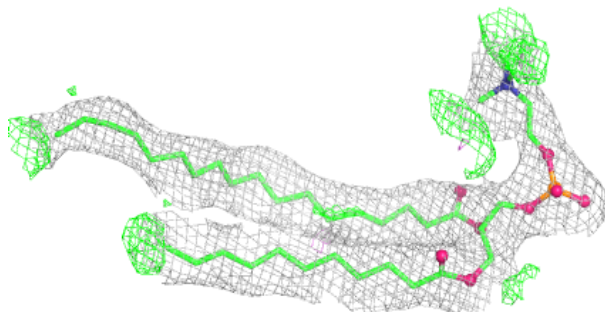


Electron density around PC1 D 603:

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

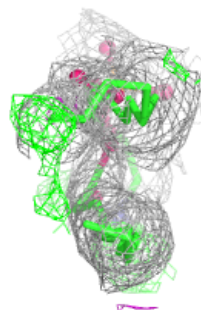
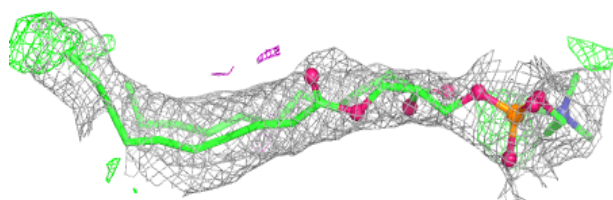
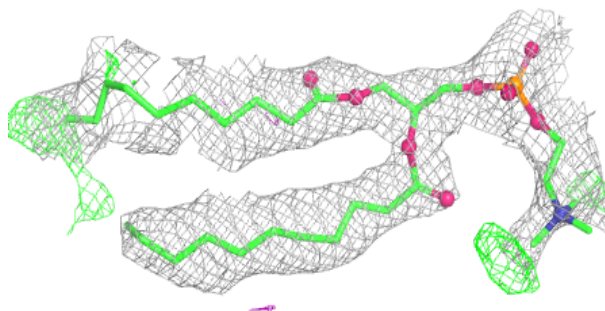
**Electron density around PC1 A 601:**

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

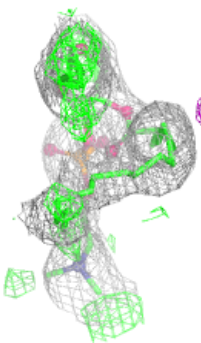
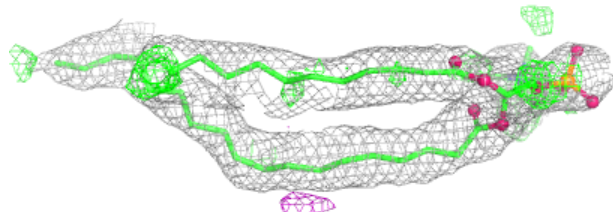
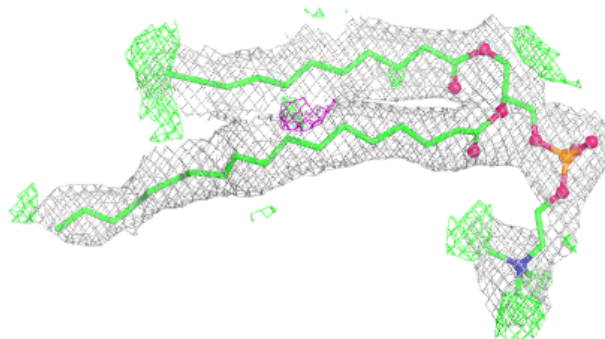


Electron density around PC1 A 602:

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

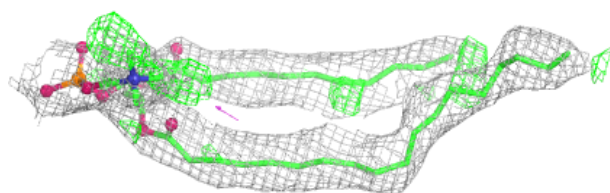
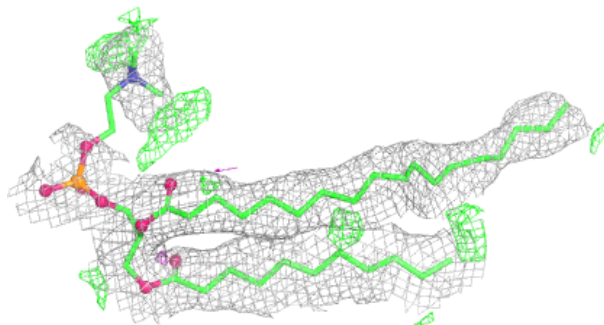
**Electron density around PC1 D 601:**

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

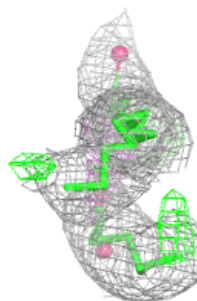
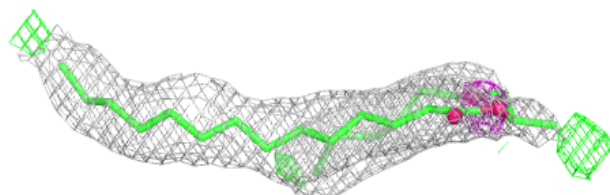
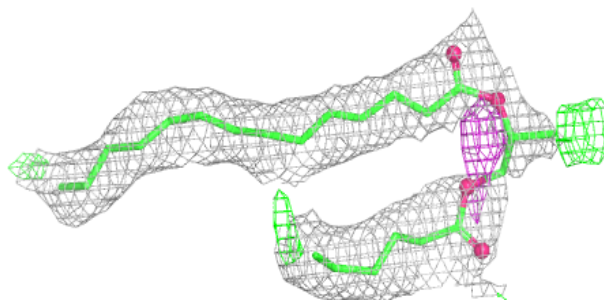


Electron density around PC1 B 601:

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

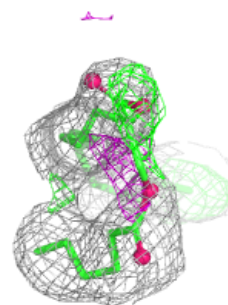
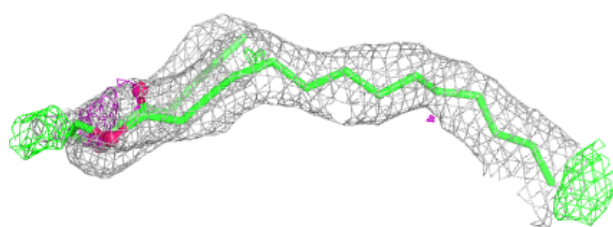
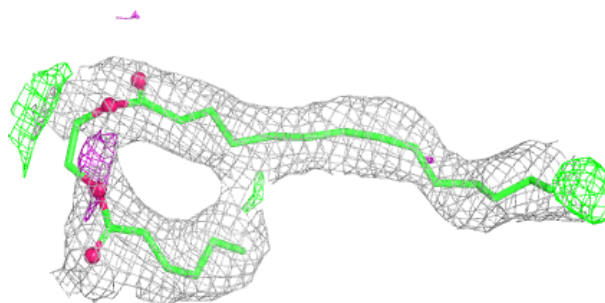
**Electron density around PC1 E 604:**

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

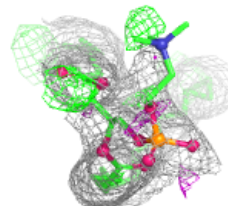
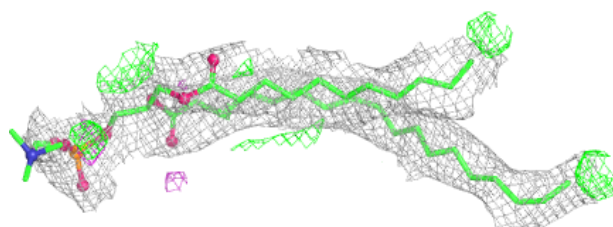
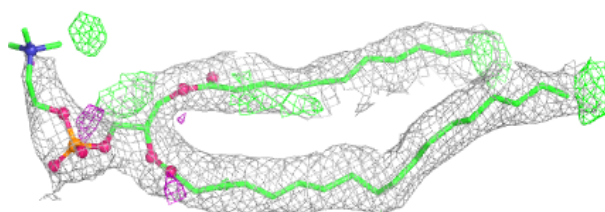


Electron density around PC1 B 603:

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

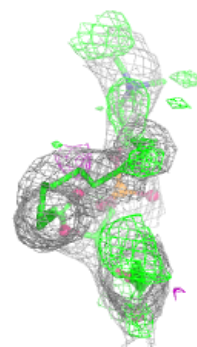
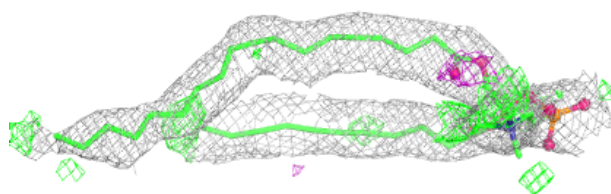
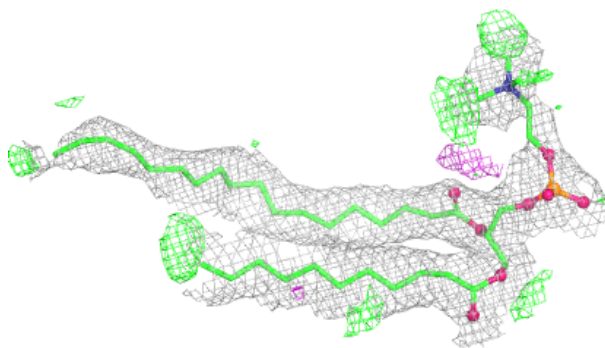
**Electron density around PC1 C 601:**

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

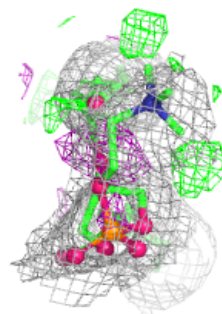
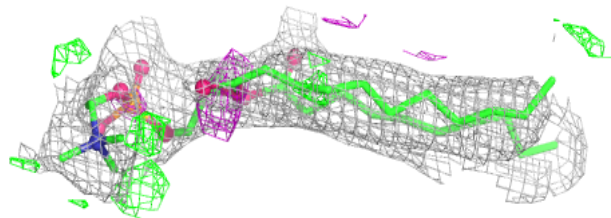
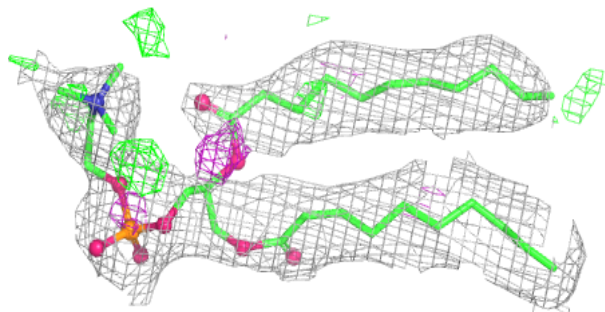


Electron density around PC1 E 601:

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

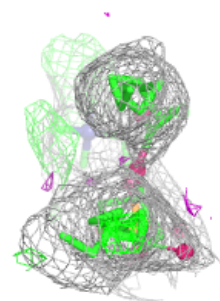
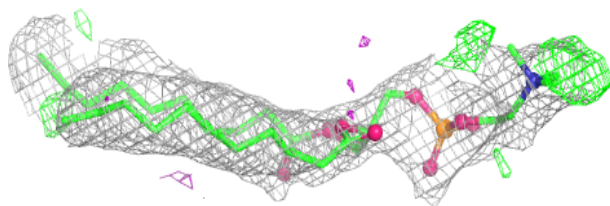
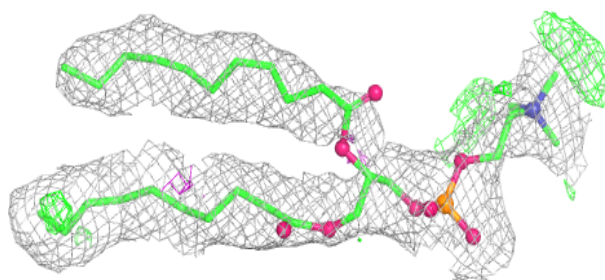
**Electron density around PC1 D 602:**

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

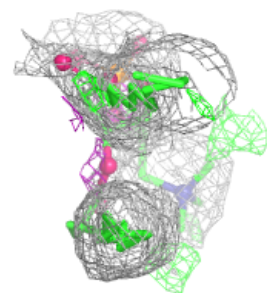
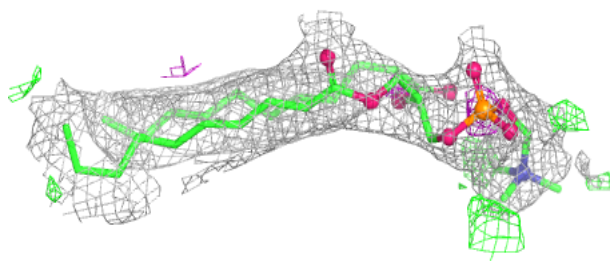
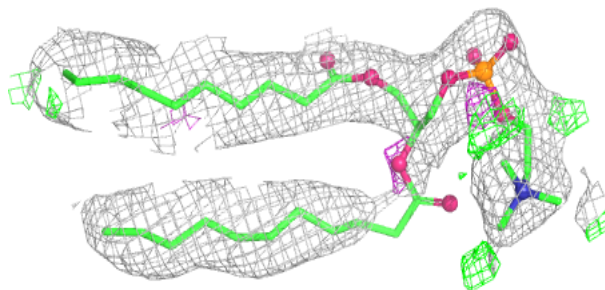


Electron density around PC1 C 602:

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

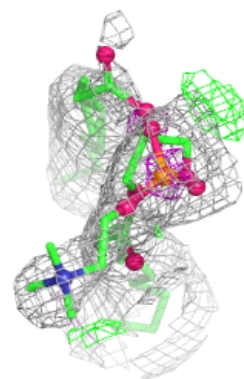
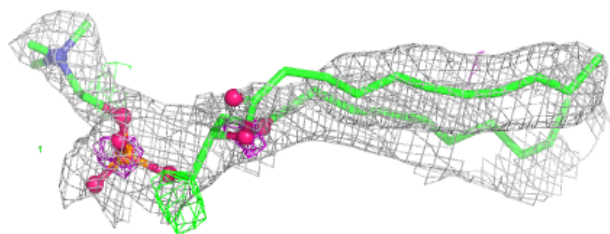
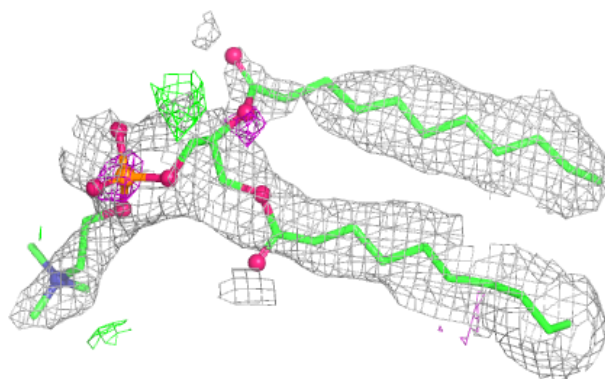
**Electron density around PC1 E 603:**

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

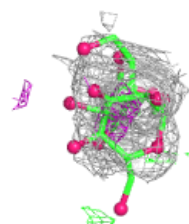
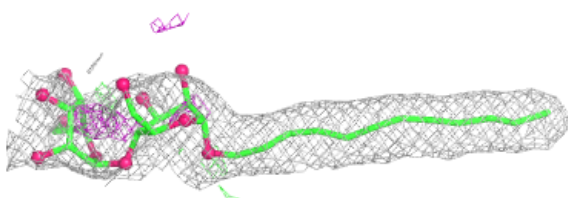
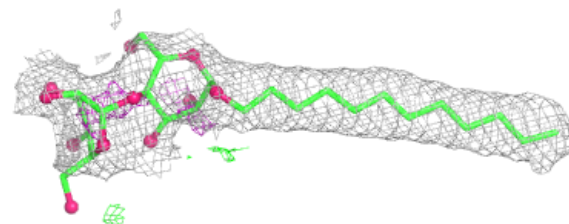


Electron density around PC1 B 602:

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

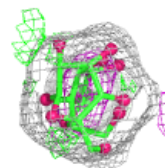
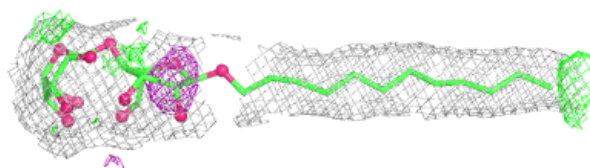
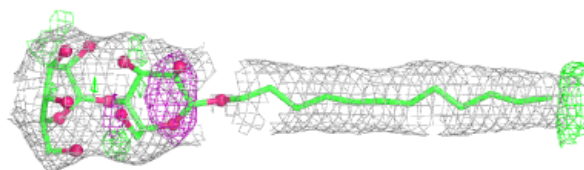
**Electron density around LMT B 501:**

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

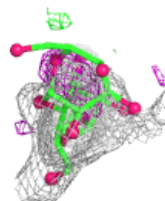
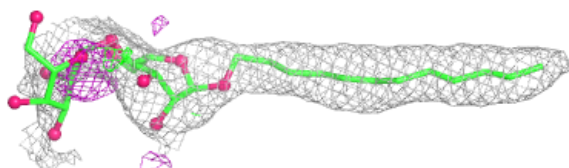
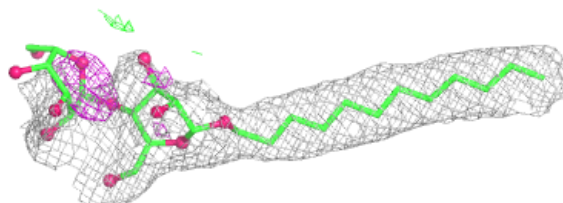


Electron density around LMT C 502:

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

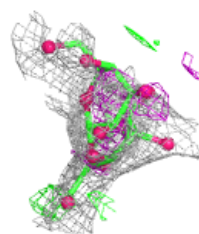
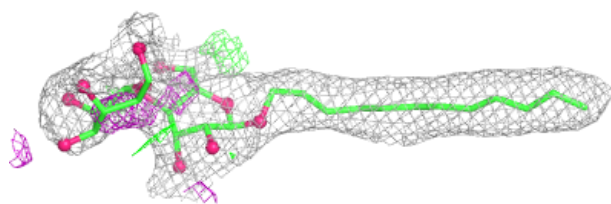
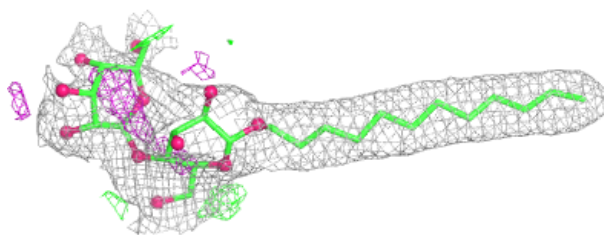
**Electron density around LMT E 602:**

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

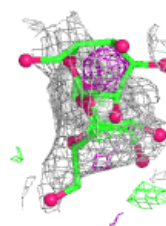
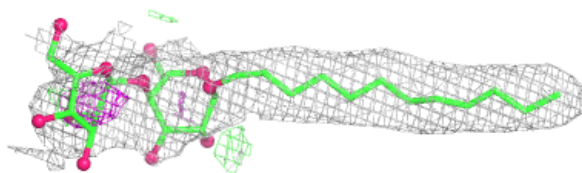


Electron density around LMT A 501:

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

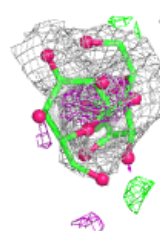
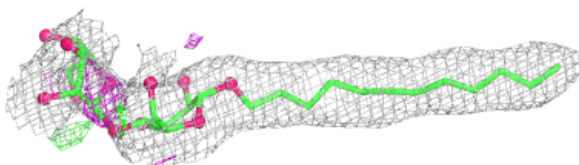
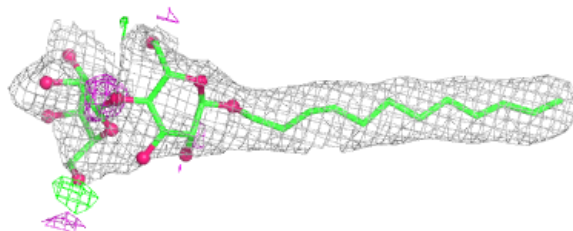
**Electron density around LMT C 501:**

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



Electron density around LMT E 501:

$2mF_o-DF_c$ (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.