



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 04:45 am BST

PDB ID : 5J0Z
Title : Crystal structure of GLIC in complex with DHA
Authors : Basak, S.; Schmandt, N.; Chakrapani, S.
Deposited on : 2016-03-28
Resolution : 3.25 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

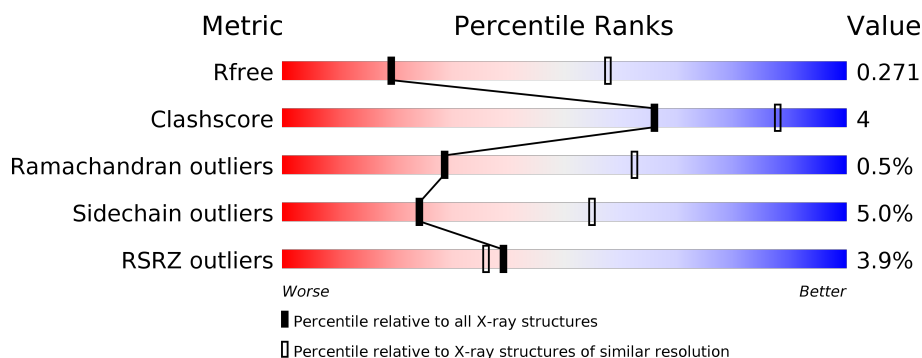
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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 on 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	311	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>15%</div> <div>.</div> </div> </div>
1	B	311	<div> <div>4%</div> <div> <div></div> <div>86%</div> <div>13%</div> <div>.</div> </div> </div>
1	C	311	<div> <div>4%</div> <div> <div></div> <div>85%</div> <div>13%</div> <div>.</div> </div> </div>
1	D	311	<div> <div>6%</div> <div> <div></div> <div>86%</div> <div>13%</div> <div>.</div> </div> </div>
1	E	311	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>15%</div> <div>.</div> </div> </div>

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	SO4	A	405	-	-	-	X
4	SO4	C	401	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12852 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.

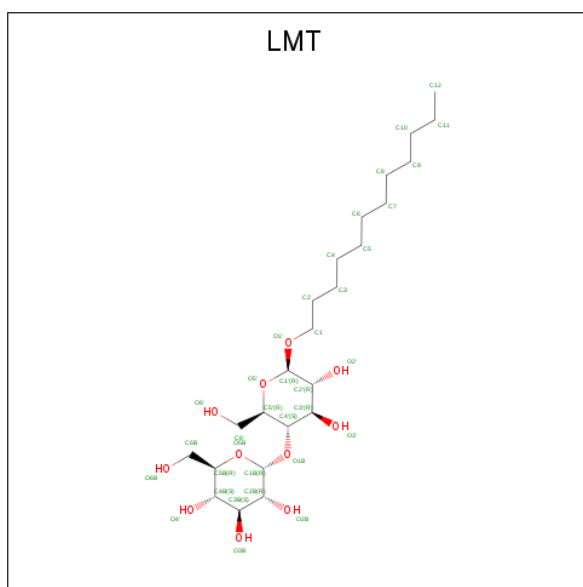
- Molecule 1 is a protein called Proton-gated ion channel.

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			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	D	1	Total	Cl	0	0
			1	1		
2	E	1	Total	Cl	0	0
			1	1		

- Molecule 3 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 12 12	0	0
3	A	1	Total C 8 8	0	0
3	A	1	Total C 7 7	0	0
3	B	1	Total C 8 8	0	0
3	D	1	Total C 8 8	0	0
3	D	1	Total C 8 8	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



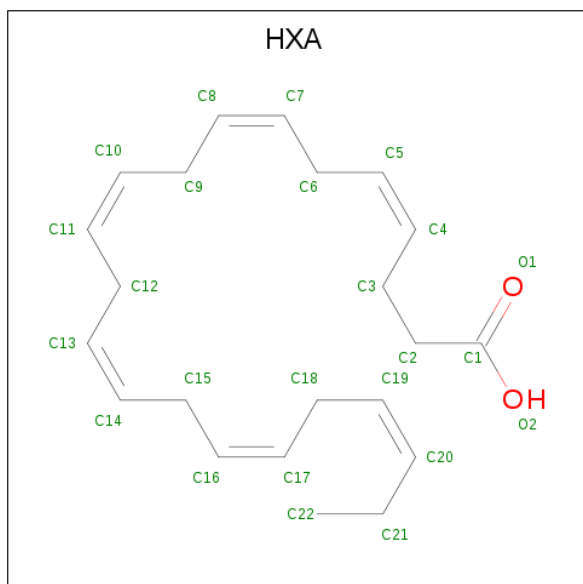
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

- Molecule 6 is DOCOSA-4,7,10,13,16,19-HEXAENOIC ACID (three-letter code: HXA) (formula: $C_{22}H_{32}O_2$).



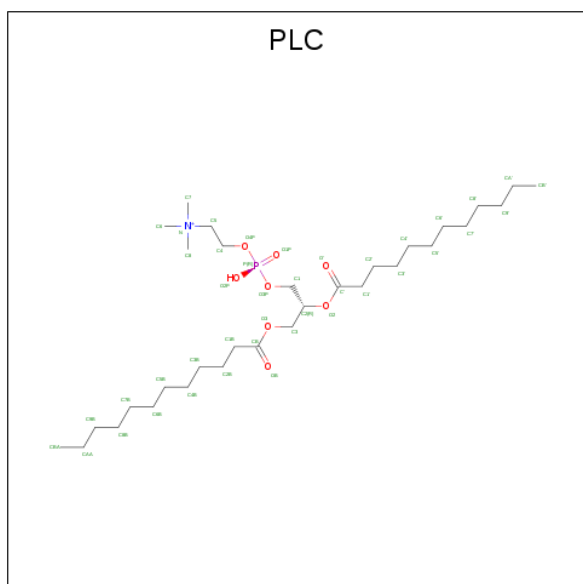
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			15	13	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			15	13	2		
6	C	1	Total	C	O	0	0
			15	13	2		
6	D	1	Total	C	O	0	0
			15	13	2		
6	E	1	Total	C	O	0	0
			15	13	2		

- Molecule 7 is DIUNDECYL PHOSPHATIDYL CHOLINE (three-letter code: PLC) (formula: $C_{32}H_{65}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			35	25	1	8	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	4	Total	O	0	0
			4	4		
8	B	7	Total	O	0	0
			7	7		
8	C	7	Total	O	0	0
			7	7		
8	D	3	Total	O	0	0
			3	3		

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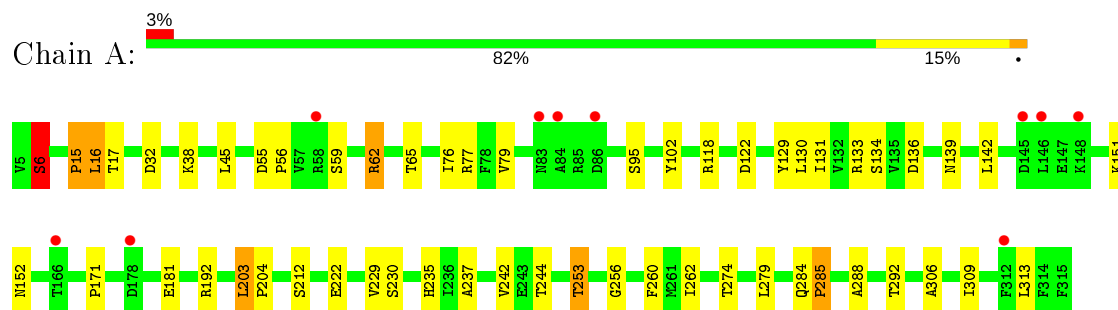
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	E	4	Total	O	0	0
			4	4		

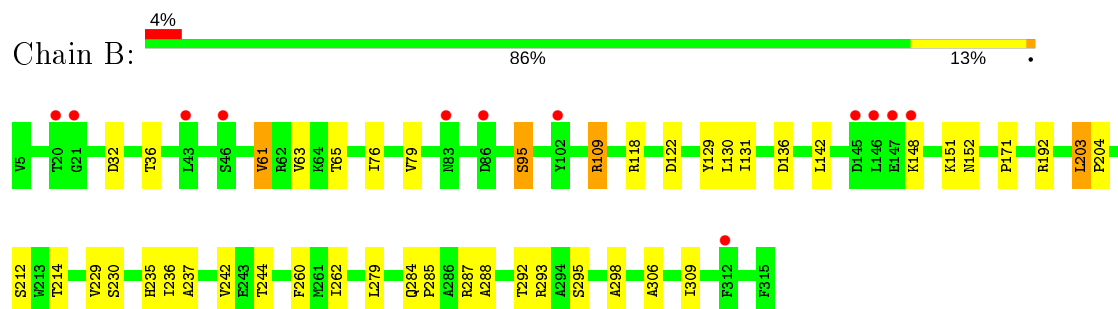
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

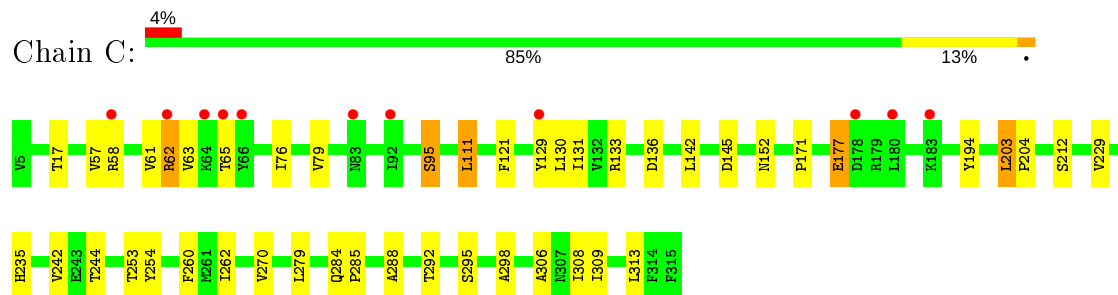
- Molecule 1: Proton-gated ion channel



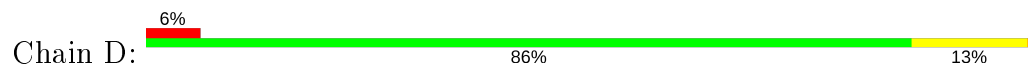
- Molecule 1: Proton-gated ion channel

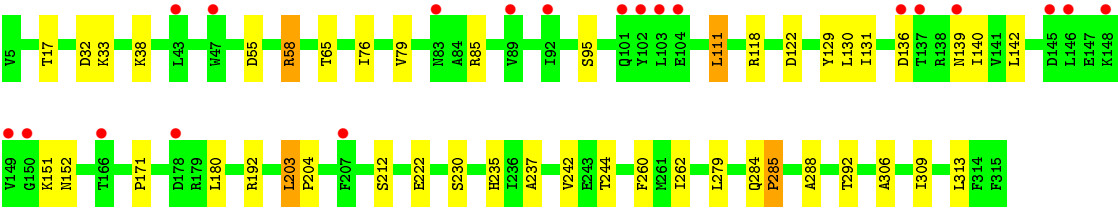


- Molecule 1: Proton-gated ion channel

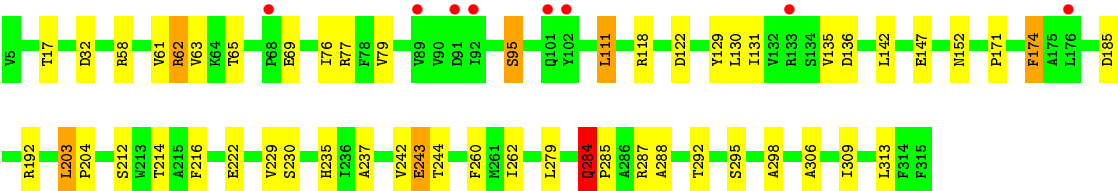
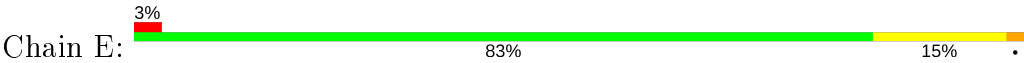


- Molecule 1: Proton-gated ion channel





● 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	181.87Å 133.32Å 159.92Å 90.00° 102.36° 90.00°	Depositor
Resolution (Å)	30.00 – 3.25 61.31 – 3.25	Depositor EDS
% Data completeness (in resolution range)	96.3 (30.00-3.25) 96.5 (61.31-3.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 3.26Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.232 , 0.261 0.244 , 0.271	Depositor DCC
R_{free} test set	2907 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	93.2	Xtriage
Anisotropy	0.385	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 76.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	12852	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% 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: HXA, CL, LMT, PLC, SO4, ACT

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	0.67	1/2593 (0.0%)	0.91	8/3545 (0.2%)
1	B	0.66	0/2593	0.90	7/3545 (0.2%)
1	C	0.67	0/2593	0.89	5/3545 (0.1%)
1	D	0.66	1/2593 (0.0%)	0.91	6/3545 (0.2%)
1	E	0.65	1/2593 (0.0%)	0.94	10/3545 (0.3%)
All	All	0.66	3/12965 (0.0%)	0.91	36/17725 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	222	GLU	CG-CD	5.57	1.60	1.51
1	A	222	GLU	CG-CD	5.38	1.60	1.51
1	E	222	GLU	CG-CD	5.23	1.59	1.51

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	118	ARG	NE-CZ-NH2	9.73	125.16	120.30
1	E	174	PHE	CB-CG-CD1	9.32	127.32	120.80
1	E	174	PHE	CB-CG-CD2	-8.84	114.61	120.80
1	E	284	GLN	CB-CA-C	8.70	127.80	110.40
1	D	118	ARG	NE-CZ-NH1	-8.09	116.25	120.30
1	B	287	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	C	62	ARG	NE-CZ-NH1	7.91	124.25	120.30
1	B	109	ARG	CG-CD-NE	7.76	128.09	111.80
1	E	62	ARG	NE-CZ-NH1	7.57	124.09	120.30
1	A	16	LEU	N-CA-CB	7.42	125.24	110.40
1	A	62	ARG	NE-CZ-NH1	7.33	123.97	120.30
1	D	38	LYS	CD-CE-NZ	6.55	126.76	111.70
1	A	15	PRO	N-CA-C	6.02	127.76	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	284	GLN	CA-CB-CG	6.02	126.63	113.40
1	A	151	LYS	CD-CE-NZ	5.78	125.00	111.70
1	C	133	ARG	NE-CZ-NH1	-5.73	117.43	120.30
1	D	151	LYS	CD-CE-NZ	5.70	124.81	111.70
1	A	222	GLU	OE1-CD-OE2	-5.70	116.46	123.30
1	B	136	ASP	N-CA-CB	-5.68	100.37	110.60
1	B	151	LYS	CD-CE-NZ	5.67	124.74	111.70
1	E	136	ASP	N-CA-CB	-5.62	100.48	110.60
1	A	118	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	C	177	GLU	OE1-CD-OE2	-5.58	116.60	123.30
1	D	111	LEU	CA-CB-CG	5.55	128.07	115.30
1	C	111	LEU	CA-CB-CG	5.48	127.91	115.30
1	A	6	SER	N-CA-CB	5.48	118.72	110.50
1	E	243	GLU	N-CA-CB	5.46	120.42	110.60
1	E	111	LEU	CA-CB-CG	5.45	127.83	115.30
1	B	61	VAL	CB-CA-C	5.39	121.64	111.40
1	D	222	GLU	OE1-CD-OE2	-5.31	116.92	123.30
1	B	118	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	E	222	GLU	OE1-CD-OE2	-5.20	117.06	123.30
1	E	118	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	A	62	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	C	177	GLU	CG-CD-OE2	5.10	128.49	118.30
1	B	293	ARG	NE-CZ-NH1	5.05	122.83	120.30

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	27	0
1	B	2525	0	2545	21	0
1	C	2525	0	2545	20	1
1	D	2525	0	2545	19	0
1	E	2525	0	2545	25	1
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1	0	0	1	0
2	E	1	0	0	0	0
3	A	27	0	51	7	0
3	B	8	0	15	1	0
3	D	16	0	27	2	0
4	A	10	0	0	1	0
4	B	10	0	0	0	0
4	C	5	0	0	0	0
4	E	5	0	0	0	0
5	A	4	0	3	1	0
5	E	4	0	3	1	0
6	A	15	0	16	0	0
6	B	15	0	16	0	0
6	C	15	0	16	0	0
6	D	15	0	16	0	0
6	E	15	0	16	0	0
7	A	35	0	44	0	0
8	A	4	0	0	0	0
8	B	7	0	0	0	0
8	C	7	0	0	0	0
8	D	3	0	0	0	0
8	E	4	0	0	0	0
All	All	12852	0	12948	102	1

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 4.

All (102) 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:D:237:ALA:HB2	3:D:403:LMT:H121	1.55	0.89
1:A:32:ASP:OD2	1:A:192:ARG:NH2	2.09	0.85
1:A:237:ALA:HB2	3:A:404:LMT:H122	1.57	0.84
1:B:32:ASP:OD2	1:B:192:ARG:NH2	2.10	0.84
1:E:32:ASP:OD2	1:E:192:ARG:NH2	2.10	0.83
1:A:15:PRO:O	1:A:139:ASN:O	2.02	0.77
1:A:77:ARG:NH2	5:A:407:ACT:O	2.25	0.67
1:A:136:ASP:OD2	1:E:63:VAL:HB	1.96	0.66
1:C:121:PHE:HE1	1:C:194:TYR:CD2	2.16	0.63
1:D:237:ALA:CB	3:D:403:LMT:H121	2.30	0.59
1:D:55:ASP:OD2	1:D:58:ARG:HG2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:122:ASP:OD1	1:E:192:ARG:NH1	2.36	0.59
1:B:122:ASP:OD1	1:B:192:ARG:NH1	2.35	0.58
1:A:122:ASP:OD1	1:A:192:ARG:NH1	2.35	0.58
1:A:56:PRO:O	1:A:59:SER:OG	2.12	0.57
1:D:122:ASP:OD1	1:D:192:ARG:NH1	2.36	0.57
1:D:85:ARG:HG2	2:D:401:CL:CL	2.44	0.55
1:E:235:HIS:CE1	1:E:262:ILE:HG21	2.43	0.54
1:B:63:VAL:HB	1:C:136:ASP:OD2	2.09	0.53
1:B:235:HIS:CE1	1:B:262:ILE:HG21	2.43	0.53
1:A:306:ALA:HA	1:A:309:ILE:HD12	1.92	0.52
1:C:121:PHE:HE1	1:C:194:TYR:HD2	1.56	0.52
1:E:284:GLN:N	1:E:285:PRO:CD	2.73	0.52
1:E:306:ALA:HA	1:E:309:ILE:HD12	1.92	0.52
1:C:121:PHE:CE1	1:C:194:TYR:CD2	2.96	0.51
1:D:306:ALA:HA	1:D:309:ILE:HD12	1.91	0.51
1:A:237:ALA:HB2	3:A:404:LMT:C12	2.37	0.51
1:C:306:ALA:HA	1:C:309:ILE:HD12	1.92	0.51
1:C:63:VAL:HB	1:D:136:ASP:OD2	2.11	0.51
1:A:55:ASP:O	1:A:59:SER:HB3	2.12	0.50
1:A:235:HIS:CE1	1:A:262:ILE:HG21	2.47	0.50
1:B:306:ALA:HA	1:B:309:ILE:HD12	1.93	0.50
1:C:235:HIS:CE1	1:C:262:ILE:HG21	2.47	0.50
1:D:139:ASN:OD1	1:D:180:LEU:HD22	2.12	0.50
1:E:216:PHE:O	1:E:292:THR:HG22	2.12	0.49
1:B:36:THR:OG1	1:B:109:ARG:NH2	2.45	0.49
1:C:284:GLN:N	1:C:285:PRO:CD	2.76	0.48
1:D:284:GLN:N	1:D:285:PRO:CD	2.76	0.48
1:D:235:HIS:CE1	1:D:262:ILE:HG21	2.48	0.48
1:A:284:GLN:N	1:A:285:PRO:CD	2.77	0.48
1:B:284:GLN:N	1:B:285:PRO:CD	2.77	0.48
1:C:63:VAL:HG22	1:C:95:SER:HA	1.96	0.48
1:E:63:VAL:HG22	1:E:95:SER:HA	1.95	0.47
3:A:403:LMT:H122	1:E:237:ALA:HB2	1.97	0.47
1:A:237:ALA:CB	3:A:404:LMT:H122	2.37	0.47
1:D:139:ASN:OD1	1:D:140:ILE:N	2.47	0.47
1:A:260:PHE:CD1	1:A:260:PHE:C	2.88	0.47
1:A:133:ARG:NH1	1:A:181:GLU:OE1	2.48	0.46
1:A:253:THR:HG23	1:A:256:GLY:HA3	1.98	0.46
1:D:260:PHE:CD1	1:D:260:PHE:C	2.90	0.45
1:E:260:PHE:CD1	1:E:260:PHE:C	2.89	0.45
1:B:230:SER:HB2	1:C:229:VAL:HG11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:THR:HG21	1:C:270:VAL:HG12	1.98	0.45
1:B:260:PHE:CD1	1:B:260:PHE:C	2.90	0.45
1:B:63:VAL:HG22	1:B:95:SER:HA	1.97	0.45
1:B:279:LEU:HB2	1:B:288:ALA:HB2	1.99	0.44
1:C:142:LEU:O	1:C:171:PRO:HG3	2.17	0.44
1:C:279:LEU:HB2	1:C:288:ALA:HB2	1.99	0.44
1:C:260:PHE:CD1	1:C:260:PHE:C	2.91	0.44
1:D:279:LEU:HB2	1:D:288:ALA:HB2	2.00	0.44
1:E:279:LEU:HB2	1:E:288:ALA:HB2	1.99	0.44
1:B:76:ILE:CG2	1:B:130:LEU:HD22	2.47	0.44
1:D:142:LEU:O	1:D:171:PRO:HG3	2.17	0.44
3:A:403:LMT:C12	1:E:237:ALA:HB2	2.47	0.44
1:A:76:ILE:CG2	1:A:130:LEU:HD22	2.48	0.44
1:A:142:LEU:O	1:A:171:PRO:HG3	2.17	0.44
1:D:76:ILE:CG2	1:D:130:LEU:HD22	2.48	0.44
1:C:76:ILE:CG2	1:C:130:LEU:HD22	2.48	0.43
1:E:76:ILE:CG2	1:E:130:LEU:HD22	2.48	0.43
1:B:142:LEU:O	1:B:171:PRO:HG3	2.18	0.43
1:E:142:LEU:O	1:E:171:PRO:HG3	2.18	0.43
1:E:77:ARG:NH2	5:E:403:ACT:O	2.50	0.43
1:B:148:LYS:HA	1:C:177:GLU:HG2	2.00	0.43
1:A:279:LEU:HB2	1:A:288:ALA:HB2	2.00	0.43
1:D:230:SER:HB2	1:E:229:VAL:HG11	1.99	0.43
1:A:203:LEU:HB2	1:A:204:PRO:HD3	2.00	0.43
3:A:404:LMT:H111	1:B:236:ILE:HG22	2.00	0.42
1:D:203:LEU:HB2	1:D:204:PRO:HD3	2.00	0.42
1:E:203:LEU:HB2	1:E:204:PRO:HD3	2.01	0.42
1:B:203:LEU:HB2	1:B:204:PRO:HD3	2.01	0.42
1:D:79:VAL:HB	1:D:129:TYR:HB2	2.01	0.42
1:E:79:VAL:HB	1:E:129:TYR:HB2	2.02	0.42
1:C:203:LEU:HB2	1:C:204:PRO:HD3	2.01	0.41
1:C:253:THR:HG22	1:C:254:TYR:N	2.35	0.41
1:A:79:VAL:HB	1:A:129:TYR:HB2	2.01	0.41
1:A:230:SER:HB2	1:B:229:VAL:HG11	2.02	0.41
1:B:79:VAL:HB	1:B:129:TYR:HB2	2.01	0.41
1:A:229:VAL:HG11	1:E:230:SER:HB2	2.01	0.41
1:C:79:VAL:HB	1:C:129:TYR:HB2	2.03	0.41
1:E:216:PHE:O	1:E:292:THR:CG2	2.69	0.41
1:A:134:SER:HB3	1:A:139:ASN:HA	2.03	0.41
1:A:38:LYS:NZ	4:A:405:SO4:O4	2.53	0.41
1:A:45:LEU:HB2	1:A:102:TYR:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:ALA:HB2	3:B:401:LMT:C12	2.51	0.41
1:E:185:ASP:OD1	1:E:185:ASP:C	2.59	0.41
1:E:284:GLN:HG3	1:E:287:ARG:HB3	2.02	0.41
1:A:274:THR:HG21	1:E:214:THR:HB	2.03	0.40
3:A:403:LMT:H122	1:E:237:ALA:CB	2.51	0.40
1:B:295:SER:HA	1:B:298:ALA:HB3	2.03	0.40
1:C:295:SER:HA	1:C:298:ALA:HB3	2.03	0.40
1:E:295:SER:HA	1:E:298:ALA:HB3	2.04	0.40
1:D:32:ASP:OD1	1:D:192:ARG:NH2	2.54	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:ASP:OD1	1:E:147:GLU:OE1[4_745]	2.19	0.01

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	309/311 (99%)	270 (87%)	35 (11%)	4 (1%)	12	41
1	B	309/311 (99%)	274 (89%)	35 (11%)	0	100	100
1	C	309/311 (99%)	274 (89%)	34 (11%)	1 (0%)	41	72
1	D	309/311 (99%)	272 (88%)	35 (11%)	2 (1%)	25	59
1	E	309/311 (99%)	272 (88%)	36 (12%)	1 (0%)	41	72
All	All	1545/1555 (99%)	1362 (88%)	175 (11%)	8 (0%)	29	62

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	SER
1	A	16	LEU
1	C	313	LEU
1	D	313	LEU
1	A	313	LEU
1	E	313	LEU
1	D	285	PRO
1	A	285	PRO

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	280/280 (100%)	267 (95%)	13 (5%)	27	57
1	B	280/280 (100%)	270 (96%)	10 (4%)	35	63
1	C	280/280 (100%)	264 (94%)	16 (6%)	20	51
1	D	280/280 (100%)	267 (95%)	13 (5%)	27	57
1	E	280/280 (100%)	262 (94%)	18 (6%)	17	47
All	All	1400/1400 (100%)	1330 (95%)	70 (5%)	24	55

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	SER
1	A	17	THR
1	A	62	ARG
1	A	65	THR
1	A	95	SER
1	A	131	ILE
1	A	152	ASN
1	A	203	LEU
1	A	212	SER
1	A	242	VAL
1	A	244	THR
1	A	253	THR

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Mol	Chain	Res	Type
1	A	292	THR
1	B	61	VAL
1	B	65	THR
1	B	95	SER
1	B	131	ILE
1	B	152	ASN
1	B	203	LEU
1	B	212	SER
1	B	242	VAL
1	B	244	THR
1	B	292	THR
1	C	17	THR
1	C	57	VAL
1	C	58	ARG
1	C	61	VAL
1	C	62	ARG
1	C	65	THR
1	C	95	SER
1	C	111	LEU
1	C	131	ILE
1	C	152	ASN
1	C	203	LEU
1	C	212	SER
1	C	242	VAL
1	C	244	THR
1	C	292	THR
1	C	308	ILE
1	D	17	THR
1	D	33	LYS
1	D	58	ARG
1	D	65	THR
1	D	95	SER
1	D	111	LEU
1	D	131	ILE
1	D	152	ASN
1	D	203	LEU
1	D	212	SER
1	D	242	VAL
1	D	244	THR
1	D	292	THR
1	E	17	THR
1	E	58	ARG

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Mol	Chain	Res	Type
1	E	61	VAL
1	E	62	ARG
1	E	65	THR
1	E	69	GLU
1	E	95	SER
1	E	111	LEU
1	E	131	ILE
1	E	135	VAL
1	E	152	ASN
1	E	174	PHE
1	E	203	LEU
1	E	212	SER
1	E	242	VAL
1	E	243	GLU
1	E	244	THR
1	E	284	GLN

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

Mol	Chain	Res	Type
1	A	235	HIS
1	B	235	HIS
1	C	235	HIS
1	D	200	ASN
1	D	235	HIS
1	E	235	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 23 ligands modelled in this entry, 3 are monoatomic - leaving 20 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	LMT	A	404	-	6,6,36	0.76	0	5,5,47	0.89	0
3	LMT	D	402	-	7,7,36	0.76	0	6,6,47	0.47	0
4	SO4	B	402	-	4,4,4	0.29	0	6,6,6	0.36	0
7	PLC	A	409	-	34,34,41	1.37	2 (5%)	40,42,49	1.20	4 (10%)
6	HXA	E	404	-	11,14,23	0.32	0	10,14,23	0.85	1 (10%)
6	HXA	C	402	-	11,14,23	0.22	0	10,14,23	1.12	1 (10%)
6	HXA	B	404	-	11,14,23	0.36	0	10,14,23	1.15	1 (10%)
4	SO4	B	403	-	4,4,4	0.31	0	6,6,6	0.28	0
6	HXA	A	408	-	11,14,23	0.39	0	10,14,23	1.05	1 (10%)
3	LMT	D	403	-	7,7,36	0.55	0	6,6,47	0.66	0
5	ACT	A	407	-	1,3,3	1.76	0	0,3,3	0.00	-
3	LMT	B	401	-	7,7,36	0.72	0	6,6,47	0.57	0
3	LMT	A	402	-	11,11,36	0.52	0	10,10,47	0.40	0
4	SO4	A	405	-	4,4,4	0.42	0	6,6,6	0.31	0
6	HXA	D	404	-	11,14,23	0.35	0	10,14,23	1.53	1 (10%)
4	SO4	A	406	-	4,4,4	0.36	0	6,6,6	0.45	0
4	SO4	C	401	-	4,4,4	0.33	0	6,6,6	0.42	0
3	LMT	A	403	-	7,7,36	0.64	0	6,6,47	0.57	0
4	SO4	E	402	-	4,4,4	0.33	0	6,6,6	0.36	0
5	ACT	E	403	-	1,3,3	3.02	1 (100%)	0,3,3	0.00	-

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	LMT	A	404	-	-	0/4/4/61	-
3	LMT	D	402	-	-	0/5/5/61	-
6	HXA	B	404	-	-	3/10/12/21	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	HXA	C	402	-	-	1/10/12/21	-
3	LMT	B	401	-	-	3/5/5/61	-
6	HXA	A	408	-	-	1/10/12/21	-
3	LMT	D	403	-	-	1/5/5/61	-
3	LMT	A	402	-	-	5/9/9/61	-
6	HXA	E	404	-	-	1/10/12/21	-
6	HXA	D	404	-	-	2/10/12/21	-
7	PLC	A	409	-	-	17/38/38/45	-
3	LMT	A	403	-	-	5/5/5/61	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	409	PLC	O3-CB	5.05	1.48	1.33
7	A	409	PLC	O2-C'	4.46	1.46	1.34
5	E	403	ACT	CH3-C	3.02	1.52	1.48

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	404	HXA	C3-C2-C1	-4.60	104.94	112.58
7	A	409	PLC	O3-CB-C1B	3.74	123.64	111.91
6	B	404	HXA	C3-C2-C1	-3.33	107.04	112.58
6	C	402	HXA	C3-C2-C1	-2.91	107.75	112.58
7	A	409	PLC	O2-C'-C1'	2.87	117.68	111.50
6	A	408	HXA	C3-C2-C1	-2.85	107.85	112.58
7	A	409	PLC	O3-C3-C2	2.30	115.14	108.43
6	E	404	HXA	C3-C2-C1	-2.23	108.87	112.58
7	A	409	PLC	C3-O3-CB	2.17	125.16	117.12

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	404	HXA	C4-C5-C6-C7
6	B	404	HXA	C10-C11-C12-C13
7	A	409	PLC	C1-O3P-P-O1P
7	A	409	PLC	C1-O3P-P-O2P
7	A	409	PLC	C1-O3P-P-O4P
7	A	409	PLC	CB-C1B-C2B-C3B

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Mol	Chain	Res	Type	Atoms
3	A	402	LMT	C2-C3-C4-C5
3	A	403	LMT	C11-C10-C9-C8
7	A	409	PLC	O'-C'-O2-C2
7	A	409	PLC	C1'-C2'-C3'-C4'
7	A	409	PLC	C1'-C'-O2-C2
3	D	403	LMT	C11-C10-C9-C8
7	A	409	PLC	C'-C1'-C2'-C3'
3	A	403	LMT	C5-C6-C7-C8
7	A	409	PLC	C3'-C4'-C5'-C6'
3	B	401	LMT	C11-C10-C9-C8
7	A	409	PLC	O3P-C1-C2-C3
3	B	401	LMT	C6-C7-C8-C9
7	A	409	PLC	O3P-C1-C2-O2
7	A	409	PLC	C4'-C5'-C6'-C7'
6	C	402	HXA	C10-C11-C12-C13
6	D	404	HXA	C10-C11-C12-C13
6	A	408	HXA	C10-C11-C12-C13
6	E	404	HXA	C10-C11-C12-C13
3	A	403	LMT	C7-C8-C9-C10
7	A	409	PLC	C5-C4-O4P-P
3	A	402	LMT	C6-C7-C8-C9
7	A	409	PLC	O4P-C4-C5-N
3	A	402	LMT	C11-C10-C9-C8
3	A	403	LMT	C9-C10-C11-C12
3	B	401	LMT	C5-C6-C7-C8
3	A	402	LMT	C4-C5-C6-C7
6	B	404	HXA	C11-C10-C9-C8
6	D	404	HXA	C4-C5-C6-C7
7	A	409	PLC	C2B-C3B-C4B-C5B
3	A	403	LMT	C6-C7-C8-C9
3	A	402	LMT	C1-C2-C3-C4
7	A	409	PLC	C2B-C1B-CB-O3
7	A	409	PLC	C2B-C1B-CB-OB

There are no ring outliers.

7 monomers are involved in 13 short contacts:

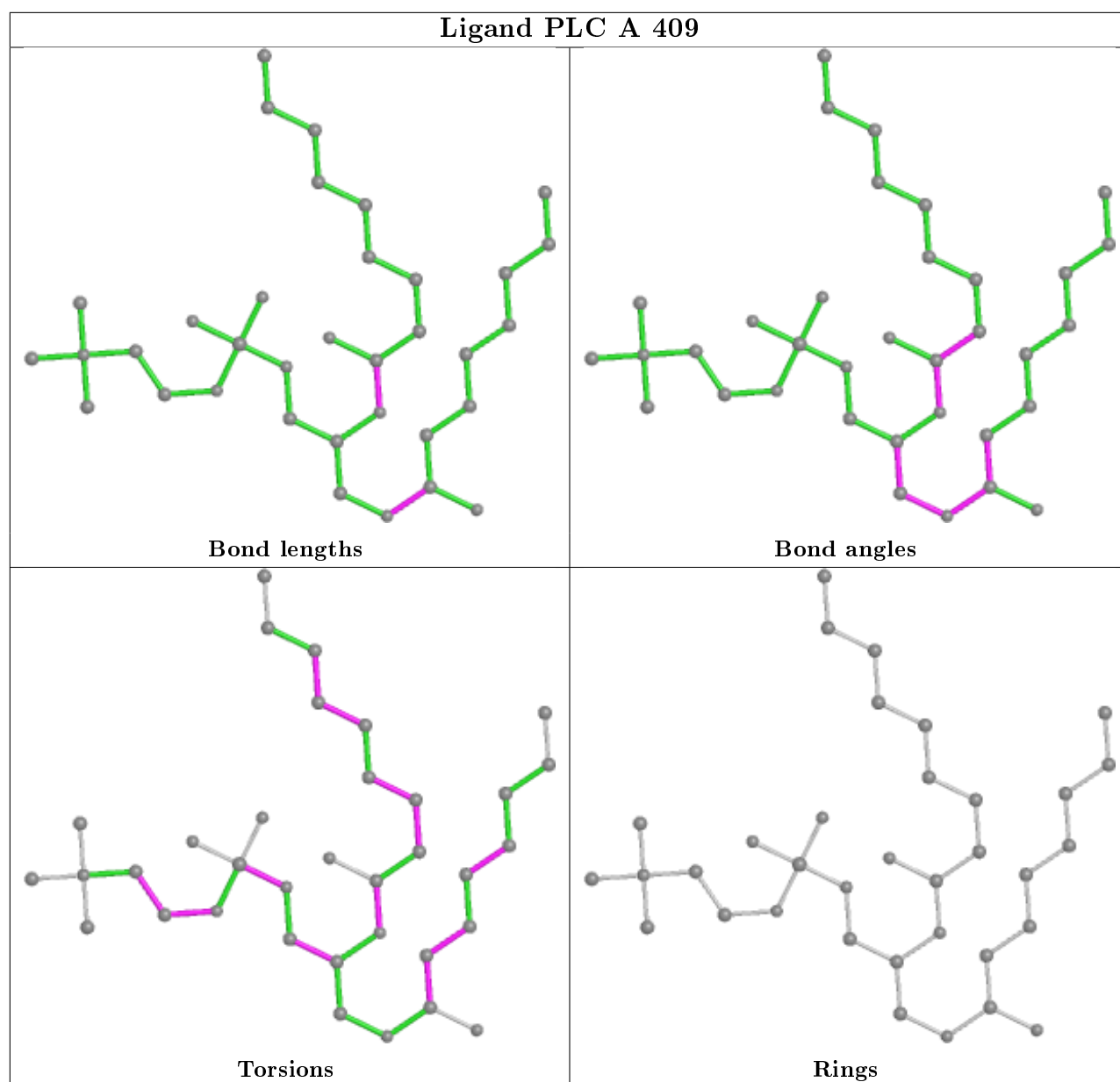
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	404	LMT	4	0
3	D	403	LMT	2	0
5	A	407	ACT	1	0
3	B	401	LMT	1	0

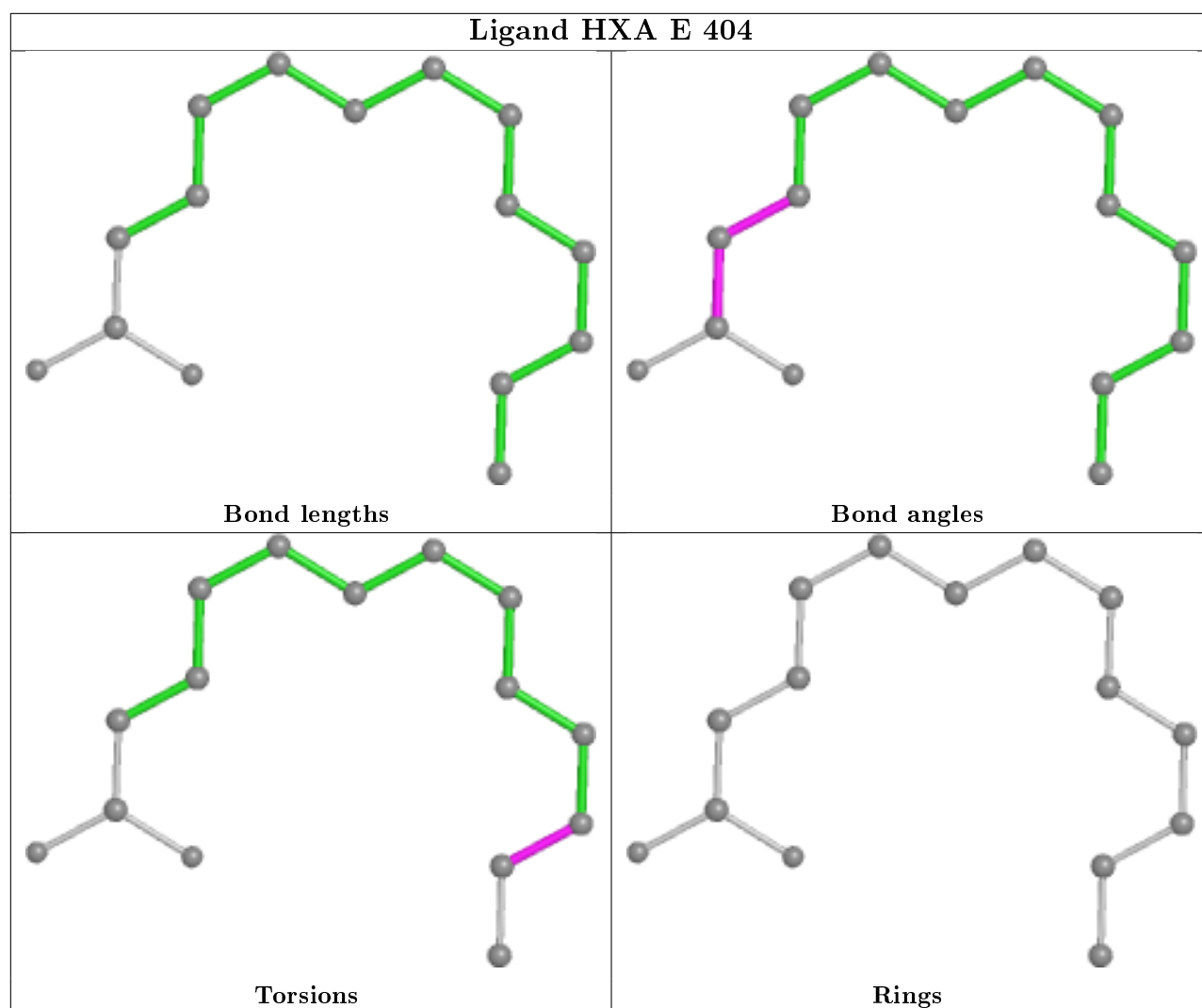
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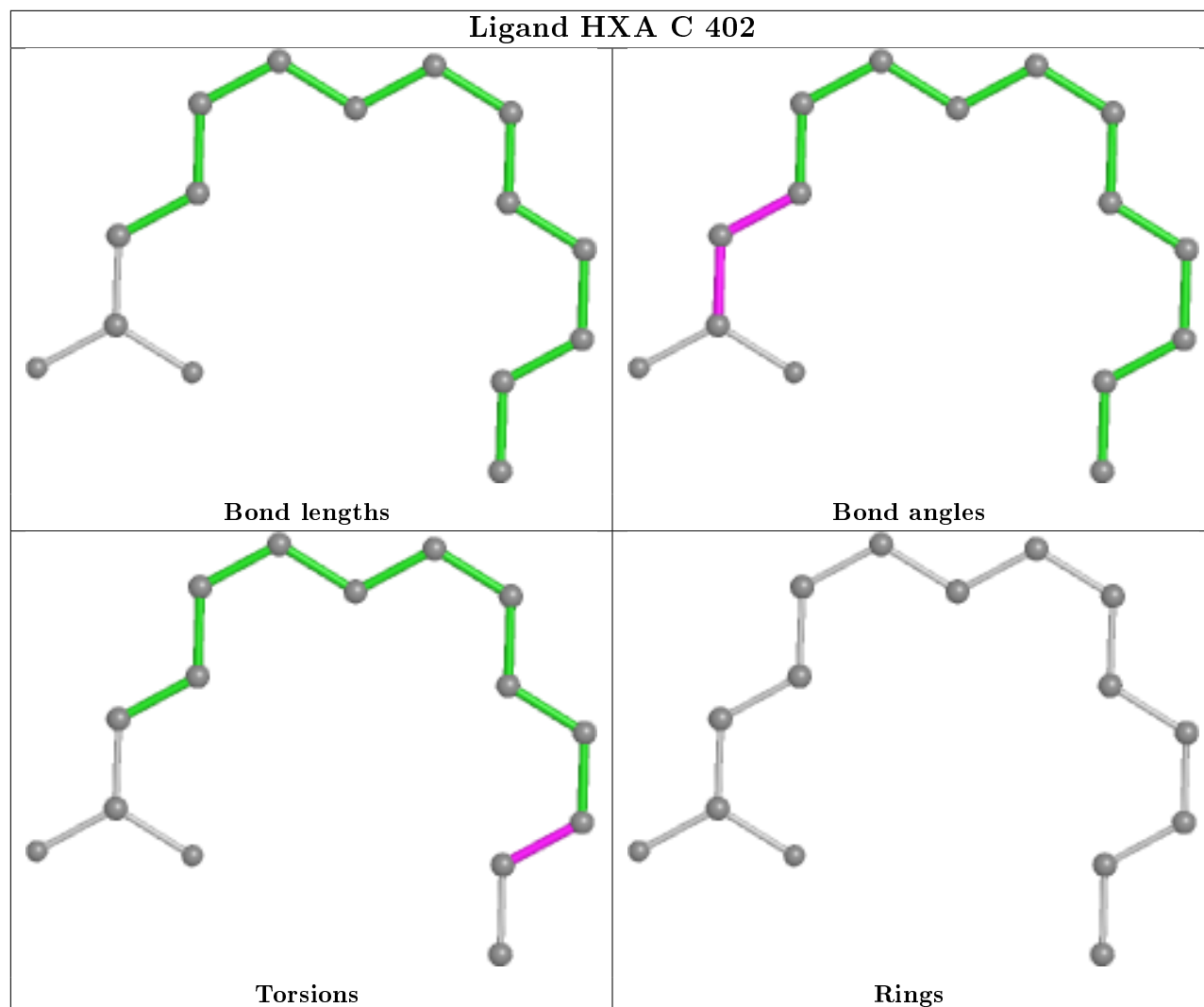
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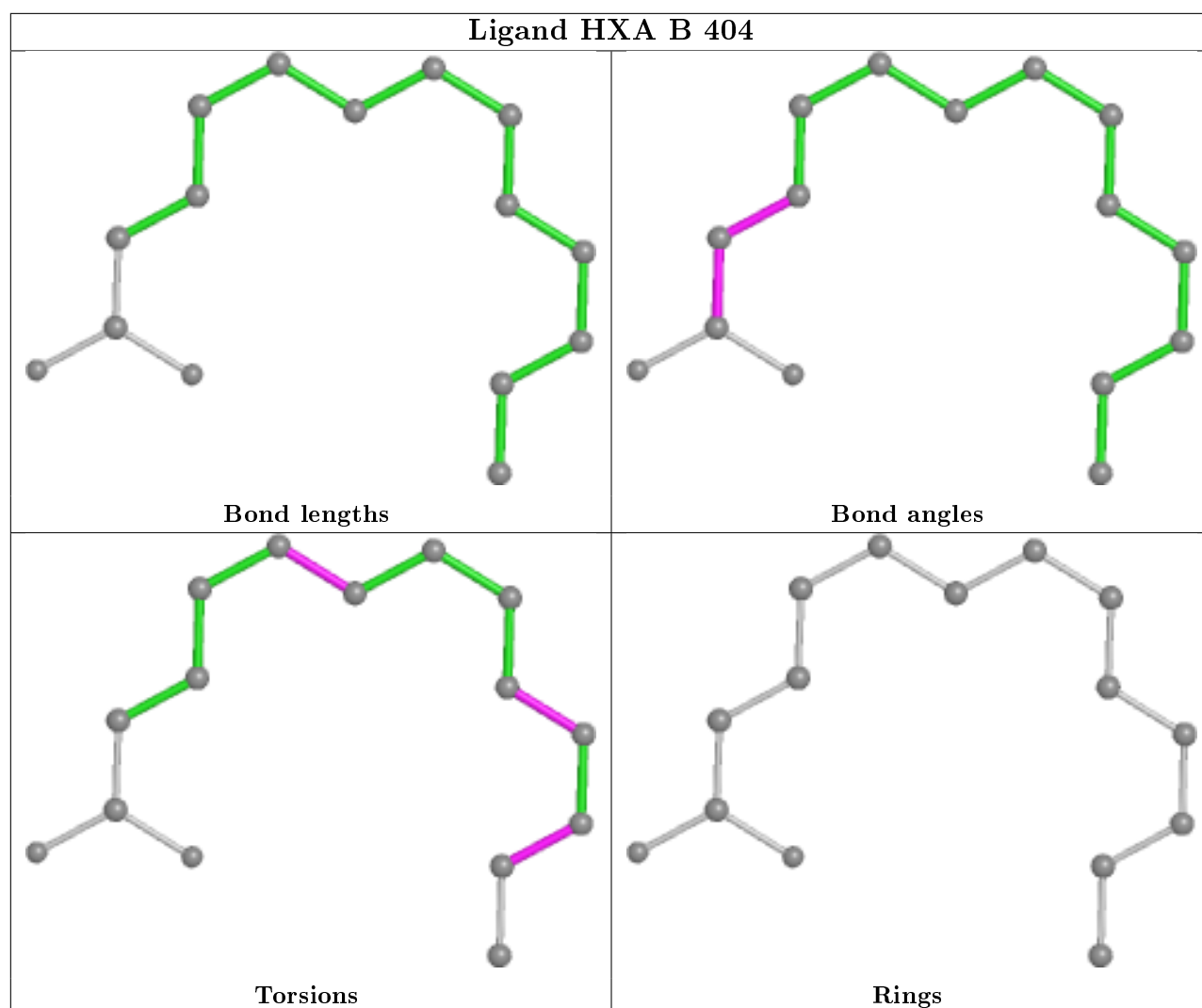
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	405	SO4	1	0
3	A	403	LMT	3	0
5	E	403	ACT	1	0

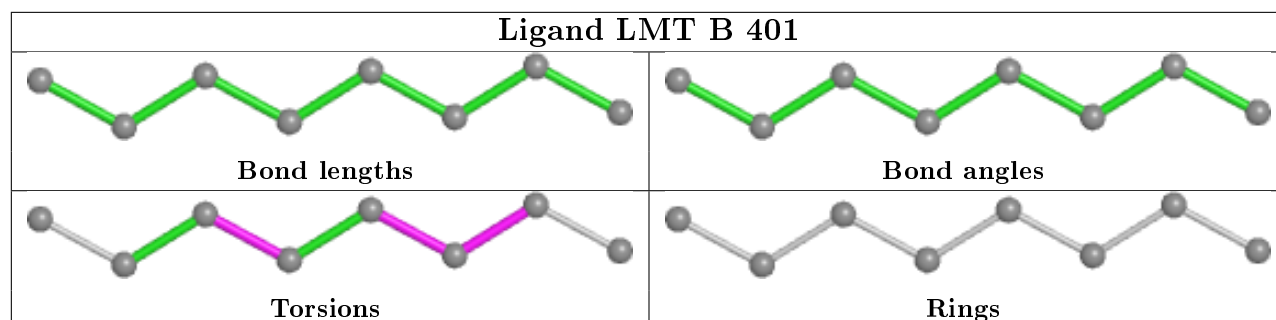
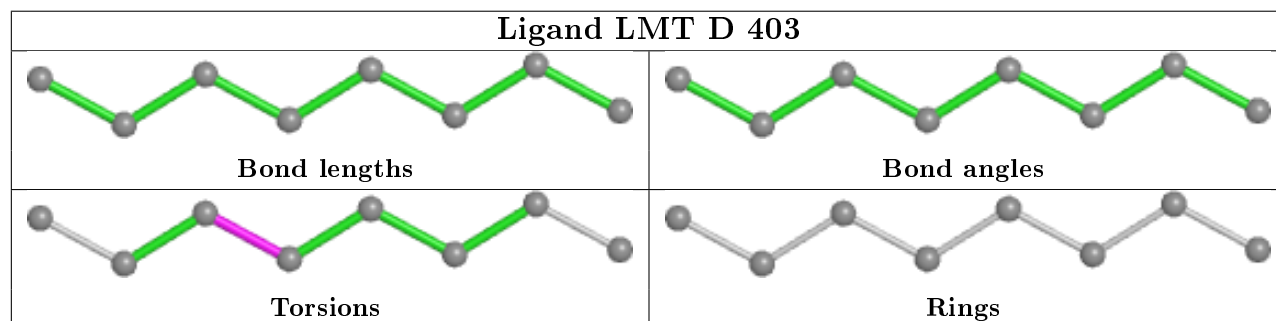
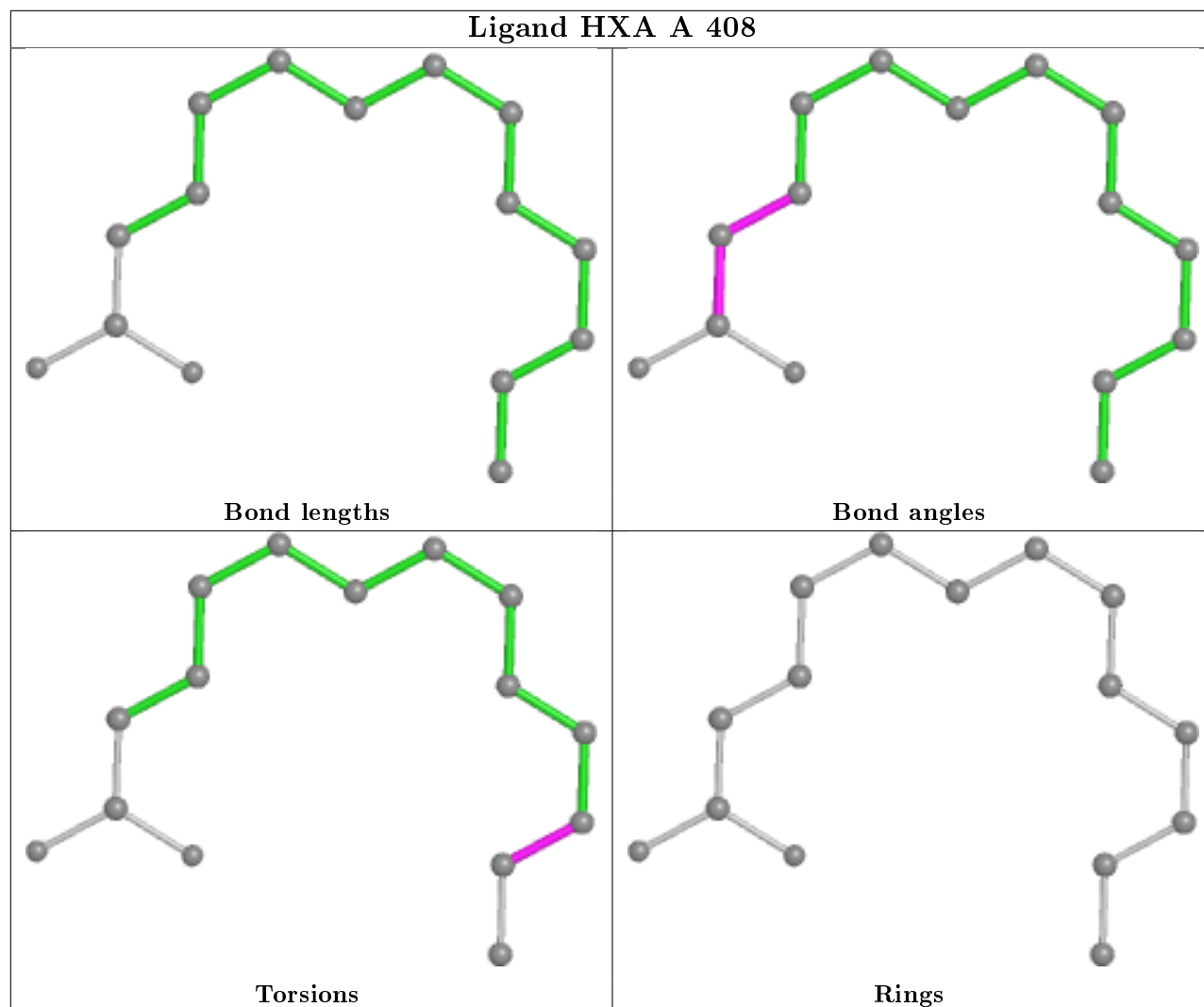
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

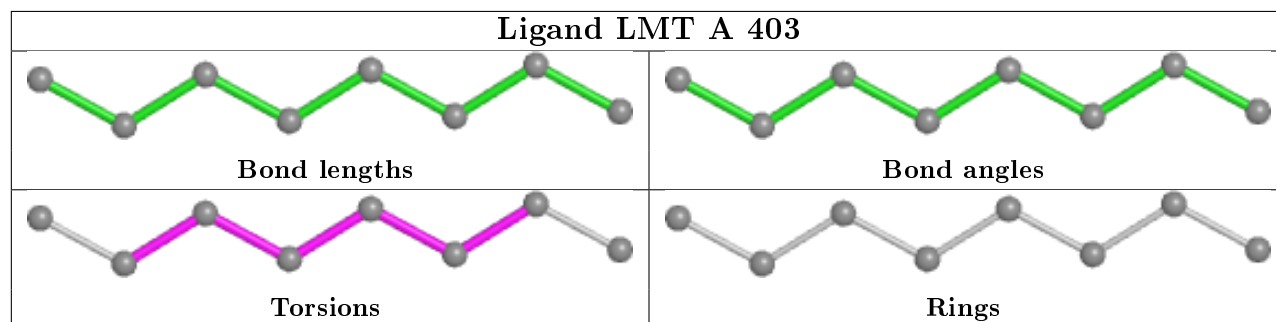
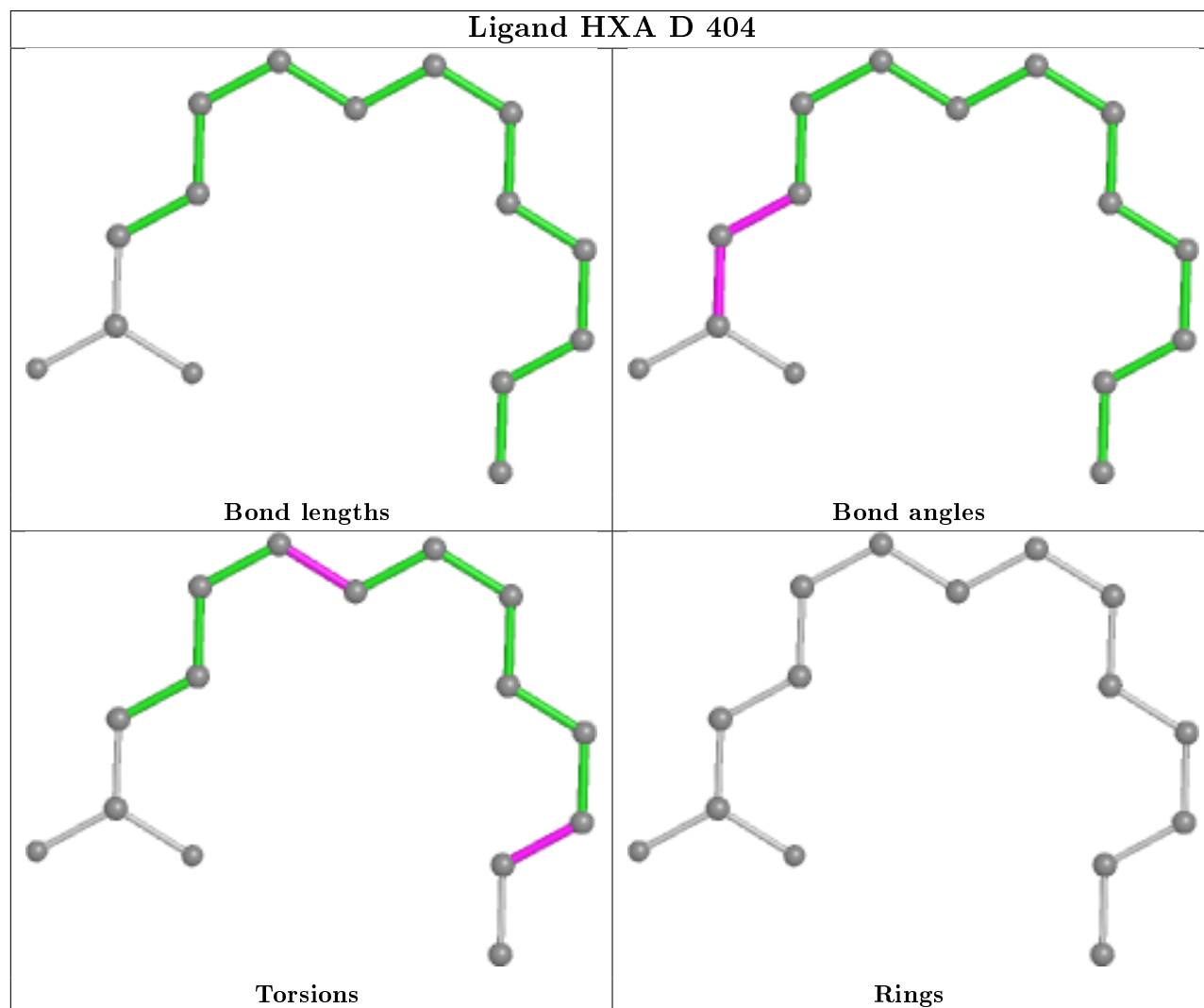
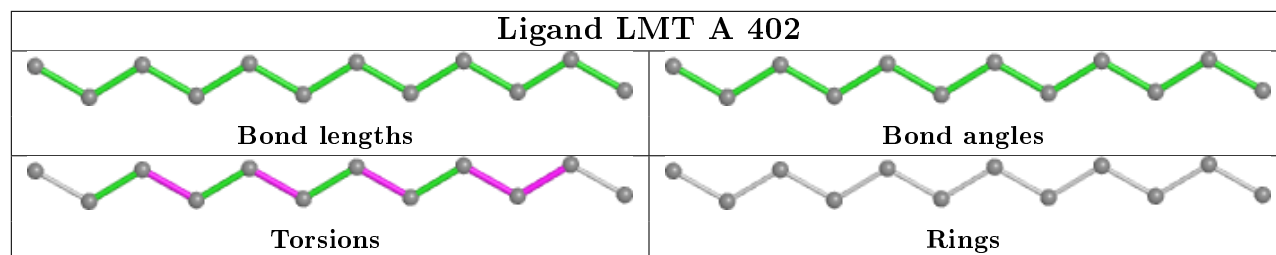












5.7 Other polymers

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	311/311 (100%)	-0.07	10 (3%)	47	45	61, 96, 154, 209	0
1	B	311/311 (100%)	0.08	12 (3%)	39	36	66, 98, 139, 169	0
1	C	311/311 (100%)	-0.01	11 (3%)	44	40	63, 97, 144, 191	0
1	D	311/311 (100%)	0.04	20 (6%)	19	18	57, 101, 154, 191	0
1	E	311/311 (100%)	-0.11	8 (2%)	56	52	62, 96, 147, 175	0
All	All	1555/1555 (100%)	-0.02	61 (3%)	39	36	57, 98, 148, 209	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	83	ASN	5.5
1	D	102	TYR	4.4
1	B	146	LEU	4.0
1	A	146	LEU	3.8
1	C	66	TYR	3.8
1	D	149	VAL	3.6
1	E	101	GLN	3.6
1	C	83	ASN	3.5
1	A	83	ASN	3.4
1	D	178	ASP	3.4
1	E	102	TYR	3.3
1	B	312	PHE	3.3
1	D	146	LEU	3.2
1	C	178	ASP	3.0
1	D	43	LEU	3.0
1	C	65	THR	2.9
1	C	64	LYS	2.9
1	B	86	ASP	2.8
1	B	46	SER	2.8
1	C	129	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	148	LYS	2.8
1	D	101	GLN	2.7
1	A	148	LYS	2.7
1	E	91	ASP	2.6
1	E	92	ILE	2.6
1	D	145	ASP	2.6
1	D	166	THR	2.6
1	A	145	ASP	2.5
1	A	86	ASP	2.5
1	C	183	LYS	2.5
1	D	139	ASN	2.4
1	D	207	PHE	2.4
1	D	83	ASN	2.4
1	D	104	GLU	2.4
1	B	145	ASP	2.3
1	D	150	GLY	2.3
1	A	178	ASP	2.3
1	B	147	GLU	2.3
1	D	103	LEU	2.3
1	D	137	THR	2.3
1	A	166	THR	2.3
1	B	102	TYR	2.3
1	D	89	VAL	2.2
1	A	84	ALA	2.2
1	E	133	ARG	2.2
1	C	180	LEU	2.2
1	B	20	THR	2.2
1	B	21	GLY	2.1
1	E	68	PRO	2.1
1	C	58	ARG	2.1
1	E	176	LEU	2.1
1	D	148	LYS	2.1
1	C	92	ILE	2.1
1	D	92	ILE	2.1
1	E	89	VAL	2.1
1	D	136	ASP	2.1
1	A	58	ARG	2.0
1	A	312	PHE	2.0
1	D	47	TRP	2.0
1	C	62	ARG	2.0
1	B	43	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates 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.

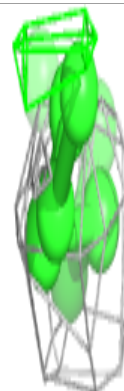
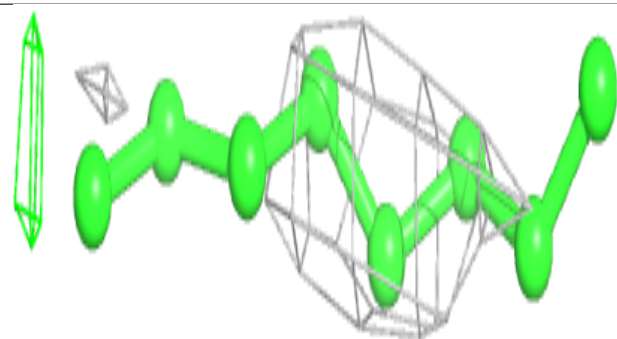
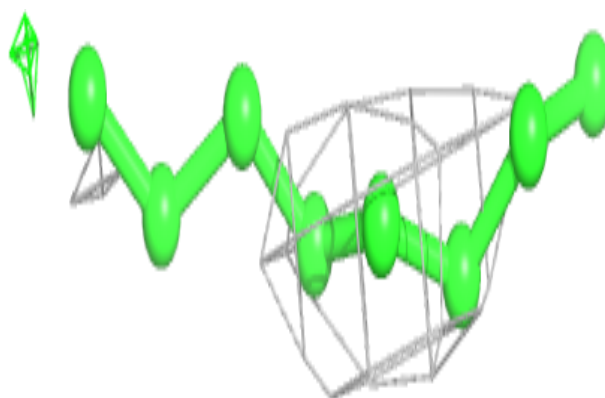
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	A	405	5/5	0.57	0.82	168,170,179,180	0
2	CL	D	401	1/1	0.72	0.25	92,92,92,92	0
4	SO4	C	401	5/5	0.78	0.65	145,166,171,177	0
3	LMT	B	401	8/35	0.79	0.36	83,88,99,103	0
7	PLC	A	409	35/42	0.80	0.29	81,137,179,211	0
6	HXA	C	402	15/24	0.80	0.15	81,132,142,146	0
6	HXA	E	404	15/24	0.81	0.14	99,124,127,131	0
4	SO4	E	402	5/5	0.82	0.52	146,147,156,165	0
2	CL	E	401	1/1	0.82	0.24	103,103,103,103	0
3	LMT	A	404	7/35	0.82	0.38	69,74,93,95	0
6	HXA	D	404	15/24	0.83	0.17	89,117,136,140	0
6	HXA	A	408	15/24	0.86	0.15	81,115,124,124	0
6	HXA	B	404	15/24	0.86	0.23	95,117,145,146	0
3	LMT	D	402	8/35	0.87	0.32	77,82,90,93	0
3	LMT	D	403	8/35	0.87	0.37	84,91,105,105	0
4	SO4	A	406	5/5	0.87	0.58	127,147,162,167	0
2	CL	A	401	1/1	0.87	0.14	83,83,83,83	0
4	SO4	B	403	5/5	0.88	0.91	137,139,150,154	0
4	SO4	B	402	5/5	0.88	0.82	127,142,160,165	0
3	LMT	A	402	12/35	0.89	0.28	49,56,75,77	0
3	LMT	A	403	8/35	0.90	0.37	64,71,76,82	0
5	ACT	E	403	4/4	0.91	0.79	114,132,138,147	0
5	ACT	A	407	4/4	0.95	0.61	100,119,121,123	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.

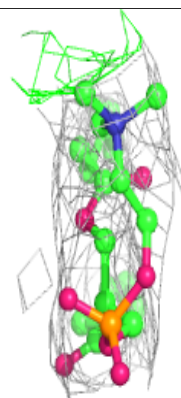
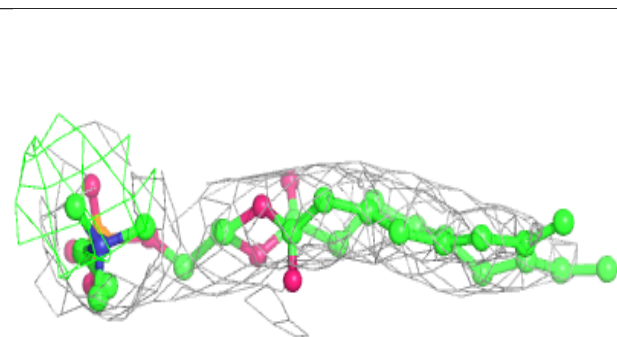
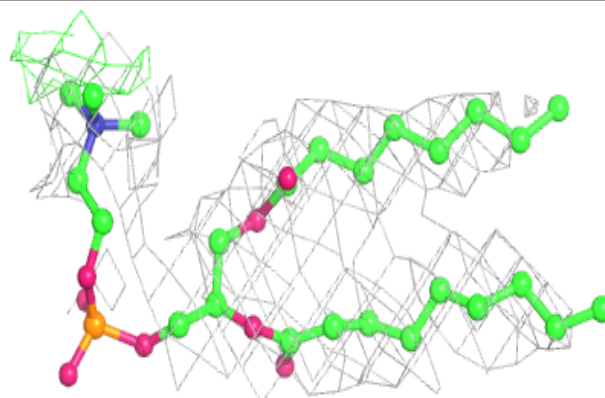
Electron density around LMT B 401:

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



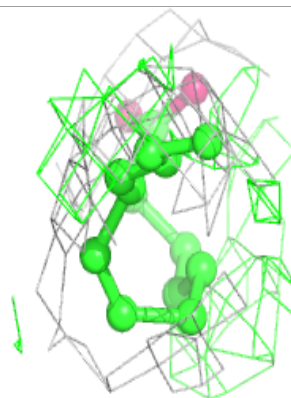
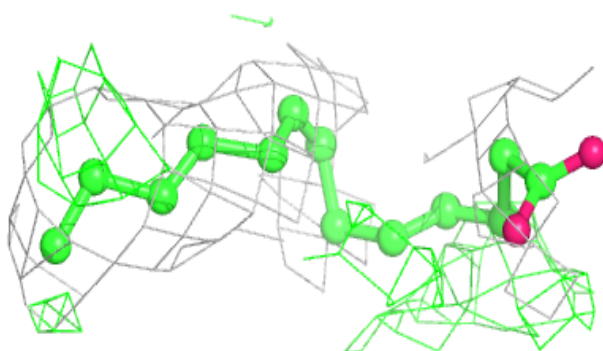
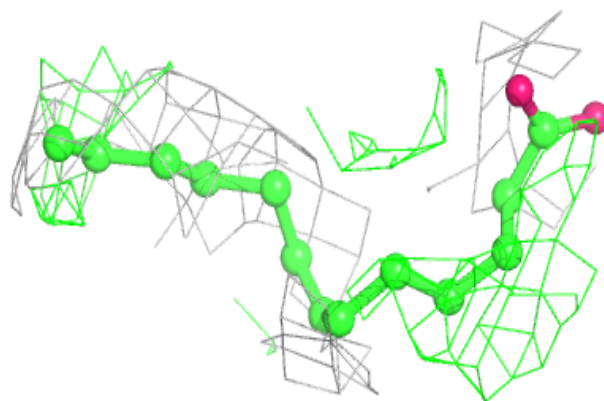
Electron density around PLC A 409:

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

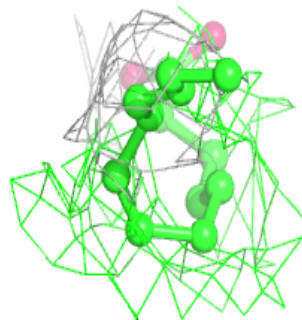
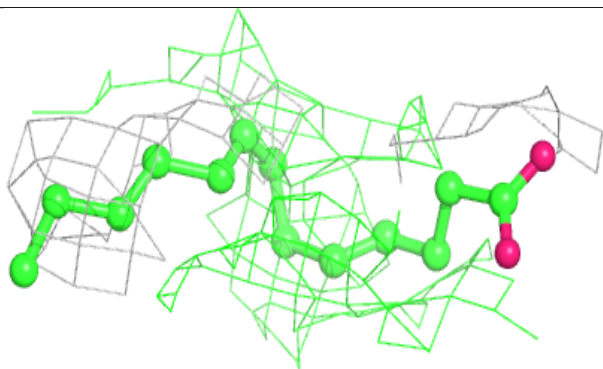
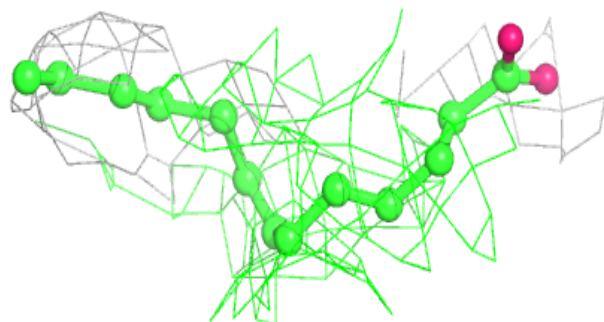


Electron density around HXA C 402:

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

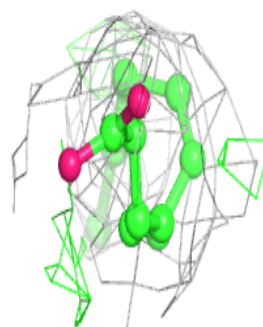
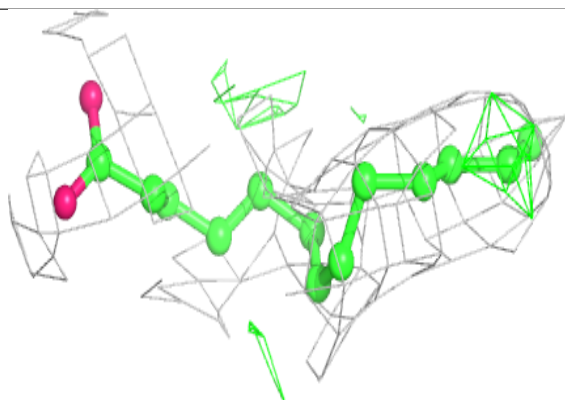
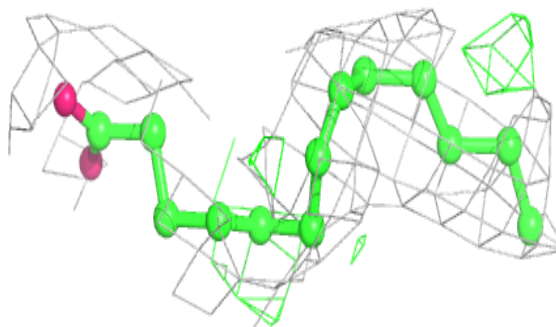
**Electron density around HXA E 404:**

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

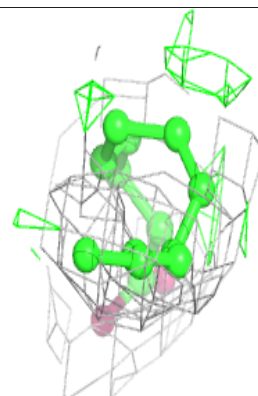
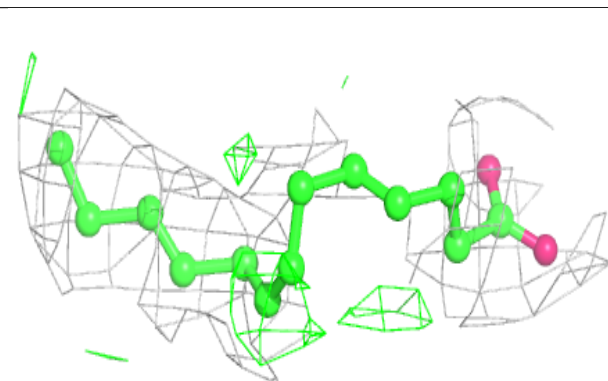
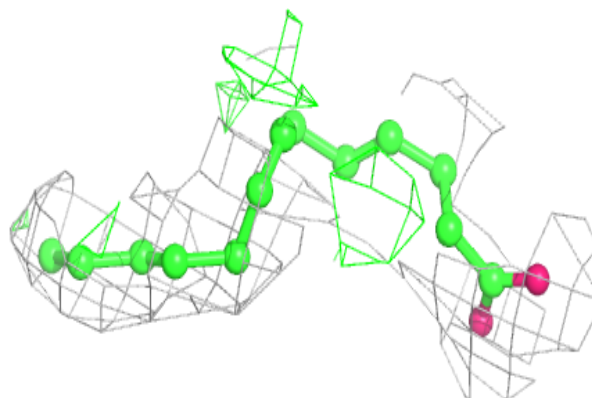


Electron density around HXA D 404:

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

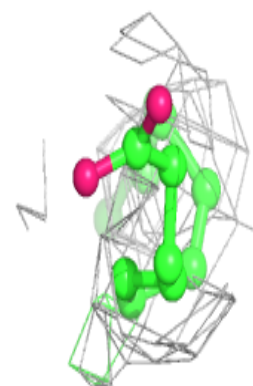
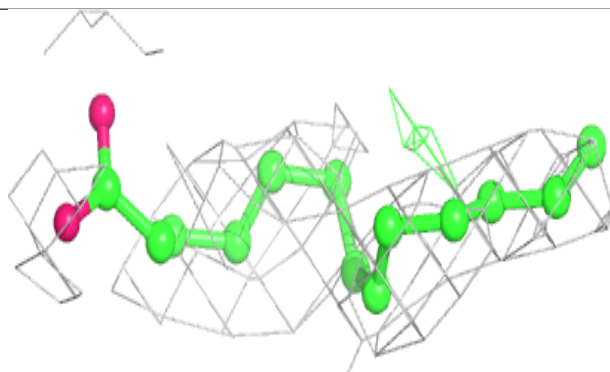
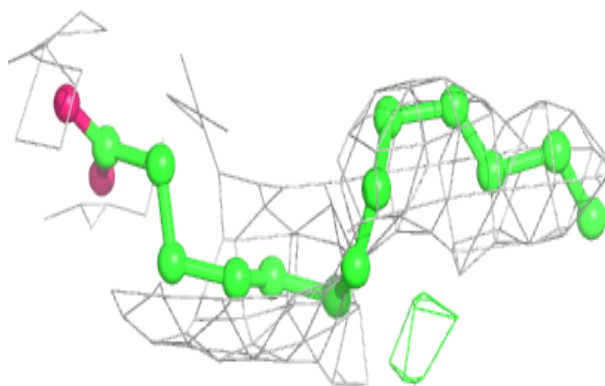
**Electron density around HXA A 408:**

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

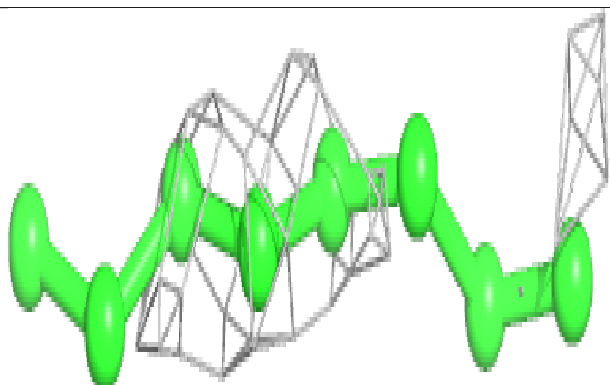
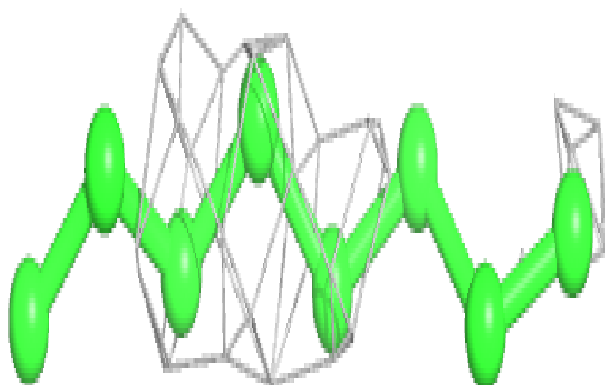


Electron density around HXA B 404:

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

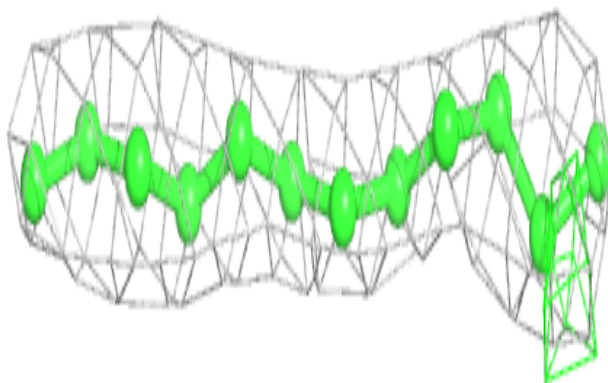
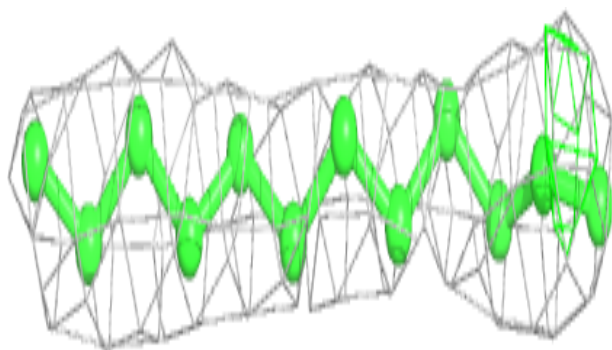
**Electron density around LMT D 403:**

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

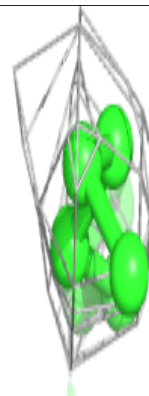
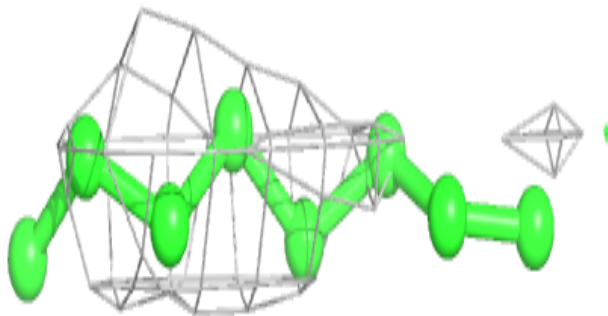
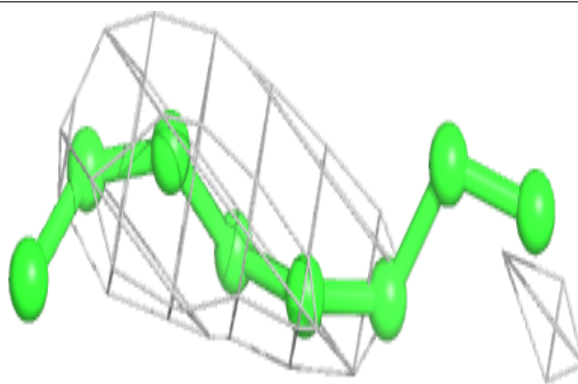


Electron density around LMT A 402:

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

**Electron density around LMT A 403:**

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



6.5 Other polymers

There are no such residues in this entry.