



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 03:40 PM UTC

PDB ID : 7ZM8 / pdb_00007zm8
EMDB ID : EMD-14792
Title : CryoEM structure of mitochondrial complex I from *Chaetomium thermophilum* (inhibited by DDM) - membrane arm
Authors : Laube, E.; Kuehlbrandt, W.
Deposited on : 2022-04-19
Resolution : 2.76 Å (reported)
Based on initial models : 6RFR, 6RFQ

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

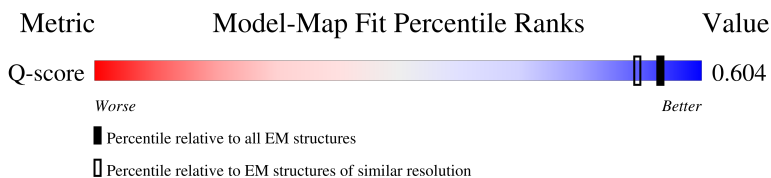
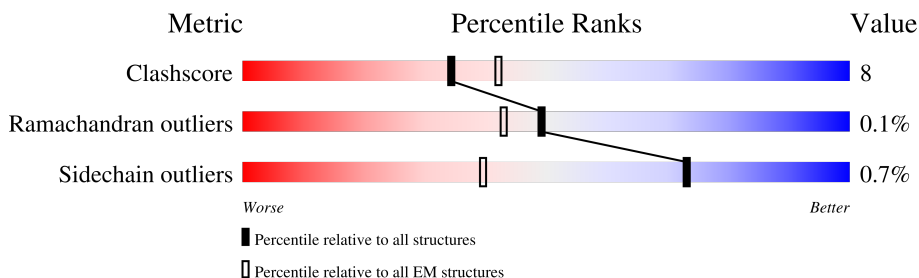
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.76 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.



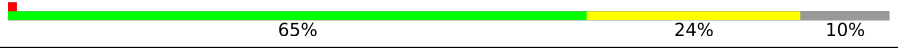
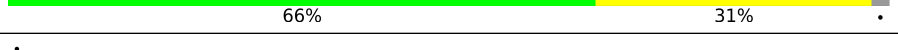
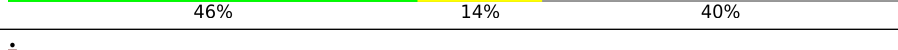
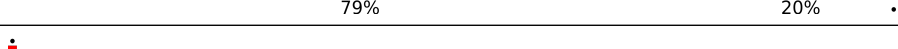
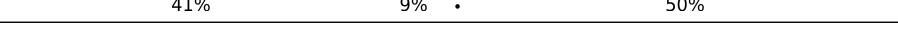
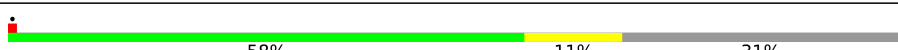
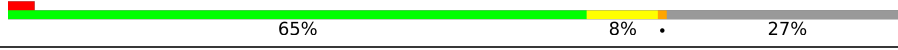
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10642 (2.26 - 3.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	378	8% 79% 21%
2	2	571	79% 18% ..
3	3	146	51% 18% 31%
4	4	542	74% 17% 9%

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Mol	Chain	Length	Quality of chain
5	5	679	
6	6	224	
7	8	86	
8	9	785	
9	D	86	
10	J	199	
11	L	89	
12	Q	141	
13	R	99	
14	S	143	
15	U	186	
16	W	121	
17	X	191	
18	a	815	
19	b	94	
20	c	93	
21	d	105	
22	e	46	
23	g	82	
24	i	93	
25	j	75	
26	n	184	

2 Entry composition [i](#)

There are 32 unique types of molecules in this entry. The entry contains 37030 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	378	Total	C	N	O	S	0	0
			2848	1914	430	494	10		

- Molecule 2 is a protein called NADH dehydrogenase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	558	Total	C	N	O	S	0	0
			4456	2993	672	780	11		

- Molecule 3 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	101	Total	C	N	O	S	0	0
			790	541	115	132	2		

- Molecule 4 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	494	Total	C	N	O	S	0	0
			3904	2650	572	670	12		

- Molecule 5 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	670	Total	C	N	O	S	0	0
			5276	3552	793	906	25		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	445	ARG	-	insertion	UNP G1DJA3
5	446	LEU	-	insertion	UNP G1DJA3
5	447	ALA	-	insertion	UNP G1DJA3

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Chain	Residue	Modelled	Actual	Comment	Reference
5	448	ILE	-	insertion	UNP G1DJA3
5	449	ASP	-	insertion	UNP G1DJA3
5	450	ASN	-	insertion	UNP G1DJA3
5	451	PHE	-	insertion	UNP G1DJA3
5	452	PHE	-	insertion	UNP G1DJA3
5	453	SER	-	insertion	UNP G1DJA3
5	454	ALA	-	insertion	UNP G1DJA3
5	455	GLN	-	insertion	UNP G1DJA3
5	456	ALA	-	insertion	UNP G1DJA3
5	457	ILE	-	insertion	UNP G1DJA3
5	458	LYS	-	insertion	UNP G1DJA3

- Molecule 6 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	189	Total	C	N	O	S	0	0
			1460	985	219	250	6		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	8	77	Total	C	N	O	S	0	0
			654	405	125	118	6		

- Molecule 8 is a protein called Subunit NDUF5 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	9	102	Total	C	N	O	S	0	0
			802	497	146	153	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
9	100	VAL	-	insertion	UNP G0SG48

- Molecule 9 is a protein called Subunit NDUF1 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	85	Total	C	N	O	S	0	0
			678	432	127	115	4		

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	188	Total	C	N	O	S	0	0
			1408	892	263	251	2		

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	87	Total	C	N	O	S	0	0
			673	453	102	115	3		

- Molecule 12 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Q	85	Total	C	N	O	S	0	0
			670	421	109	139	1		

- Molecule 13 is a protein called Complex I-B22.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	R	98	Total	C	N	O	S	0	0
			807	520	149	137	1		

- Molecule 14 is a protein called Complex I-ESSS.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	S	72	Total	C	N	O	0	0
			598	393	96	109		

- Molecule 15 is a protein called NADH-ubiquinone oxidoreductase.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	U	167	Total	C	N	O	S	0	0
			1353	852	252	240	9		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	W	101	Total	C	N	O	S	0	0
			825	527	156	140	2		

- Molecule 17 is a protein called NADH-ubiquinone oxidoreductase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	X	186	Total	C	N	O	S	0	0
			1467	934	266	259	8		

- Molecule 18 is a protein called NADH dehydrogenase (Ubiquinone)-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	a	143	Total	C	N	O	S	0	0
			1167	750	195	217	5		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	166	VAL	ALA	conflict	UNP G0RXU4
a	168	ALA	MET	conflict	UNP G0RXU4
a	?	-	GLU	deletion	UNP G0RXU4
a	?	-	GLY	deletion	UNP G0RXU4
a	?	-	ASP	deletion	UNP G0RXU4
a	?	-	PRO	deletion	UNP G0RXU4
a	?	-	ASP	deletion	UNP G0RXU4
a	?	-	PRO	deletion	UNP G0RXU4

- Molecule 19 is a protein called Subunit NDUFC2 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
19	b	80	Total	C	N	O	S	0	0
			675	440	124	109	2		

- Molecule 20 is a protein called Subunit NDUF3 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
20	c	64	Total	C	N	O	S	0	0
			510	332	90	86	2		

- Molecule 21 is a protein called Subunit NDUF10 of NADH-ubiquinone oxidoreductase

(Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
21	d	100	Total	C	N	O	S	0	0
			827	526	146	151	4		

- Molecule 22 is a protein called Subunit NDUF2 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
22	e	38	Total	C	N	O	S	0	0
			320	217	58	44	1		

- Molecule 23 is a protein called Subunit NDUF3 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
23	g	77	Total	C	N	O	S	0	0
			604	395	104	104	1		

- Molecule 24 is a protein called Subunit NDUF6 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
24	i	81	Total	C	N	O	S	0	0
			686	453	119	112	2		

- Molecule 25 is a protein called Subunit NDUF4 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
25	j	73	Total	C	N	O	S	0	0
			603	391	108	101	3		

- Molecule 26 is a protein called Subunit NDUF5 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
26	n	135	Total	C	N	O	S	0	0
			1068	683	189	195	1		

There are 52 discrepancies between the modelled and reference sequences:

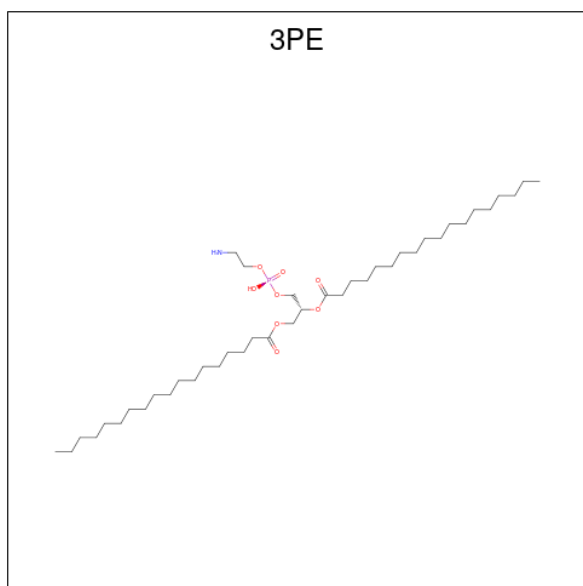
Chain	Residue	Modelled	Actual	Comment	Reference
n	1	MET	-	initiating methionine	UNP G0S086
n	2	LEU	-	insertion	UNP G0S086
n	3	ALA	-	insertion	UNP G0S086
n	4	LEU	-	insertion	UNP G0S086
n	5	ARG	-	insertion	UNP G0S086
n	6	GLN	-	insertion	UNP G0S086
n	7	ARG	-	insertion	UNP G0S086
n	8	ALA	-	insertion	UNP G0S086
n	9	ALA	-	insertion	UNP G0S086
n	10	LEU	-	insertion	UNP G0S086
n	11	LEU	-	insertion	UNP G0S086
n	12	ALA	-	insertion	UNP G0S086
n	13	ARG	-	insertion	UNP G0S086
n	14	ARG	-	insertion	UNP G0S086
n	15	VAL	-	insertion	UNP G0S086
n	16	ARG	-	insertion	UNP G0S086
n	17	PRO	-	insertion	UNP G0S086
n	18	THR	-	insertion	UNP G0S086
n	19	VAL	-	insertion	UNP G0S086
n	20	VAL	-	insertion	UNP G0S086
n	21	VAL	-	insertion	UNP G0S086
n	22	PRO	-	insertion	UNP G0S086
n	23	ARG	-	insertion	UNP G0S086
n	24	ASN	-	insertion	UNP G0S086
n	25	ALA	-	insertion	UNP G0S086
n	26	ARG	-	insertion	UNP G0S086
n	27	THR	-	insertion	UNP G0S086
n	28	TYR	-	insertion	UNP G0S086
n	29	ALA	-	insertion	UNP G0S086
n	30	SER	-	insertion	UNP G0S086
n	31	SER	-	insertion	UNP G0S086
n	32	HIS	-	insertion	UNP G0S086
n	33	ASP	-	insertion	UNP G0S086
n	34	HIS	-	insertion	UNP G0S086
n	35	ASP	-	insertion	UNP G0S086
n	36	HIS	-	insertion	UNP G0S086
n	37	HIS	-	insertion	UNP G0S086
n	38	ASP	-	insertion	UNP G0S086
n	39	HIS	-	insertion	UNP G0S086
n	40	HIS	-	insertion	UNP G0S086
n	41	HIS	-	insertion	UNP G0S086
n	42	ASP	-	insertion	UNP G0S086
n	43	HIS	-	insertion	UNP G0S086

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Chain	Residue	Modelled	Actual	Comment	Reference
n	44	GLY	-	insertion	UNP G0S086
n	45	HIS	-	insertion	UNP G0S086
n	46	ASN	-	insertion	UNP G0S086
n	47	VAL	-	insertion	UNP G0S086
n	48	GLU	-	insertion	UNP G0S086
n	49	GLU	-	insertion	UNP G0S086
n	50	PRO	-	insertion	UNP G0S086
n	51	LEU	-	insertion	UNP G0S086
n	52	GLY	-	insertion	UNP G0S086

- Molecule 27 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



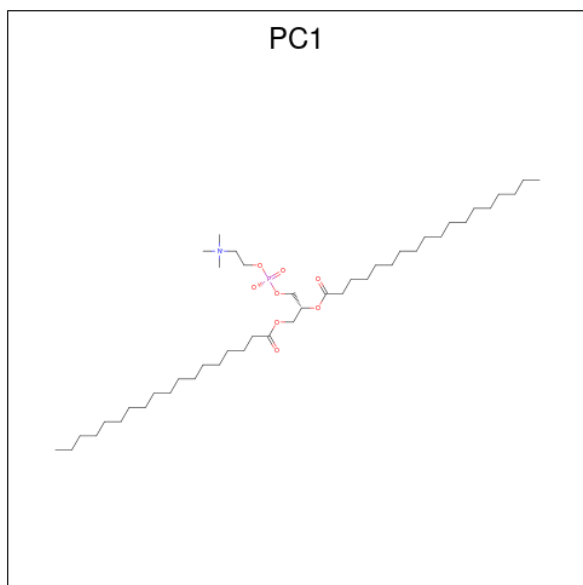
Mol	Chain	Residues	Atoms					AltConf
27	1	1	Total	C	N	O	P	0
			39	29	1	8	1	
27	5	1	Total	C	N	O	P	0
			41	31	1	8	1	
27	5	1	Total	C	N	O	P	0
			42	32	1	8	1	
27	5	1	Total	C	N	O	P	0
			44	34	1	8	1	
27	W	1	Total	C	N	O	P	0
			40	30	1	8	1	
27	W	1	Total	C	N	O	P	0
			36	26	1	8	1	

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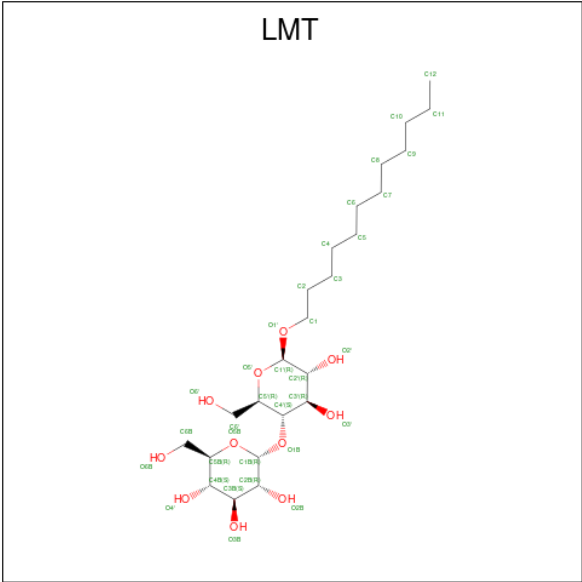
Mol	Chain	Residues	Atoms					AltConf
27	i	1	Total	C	N	O	P	0
			43	33	1	8	1	

- Molecule 28 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



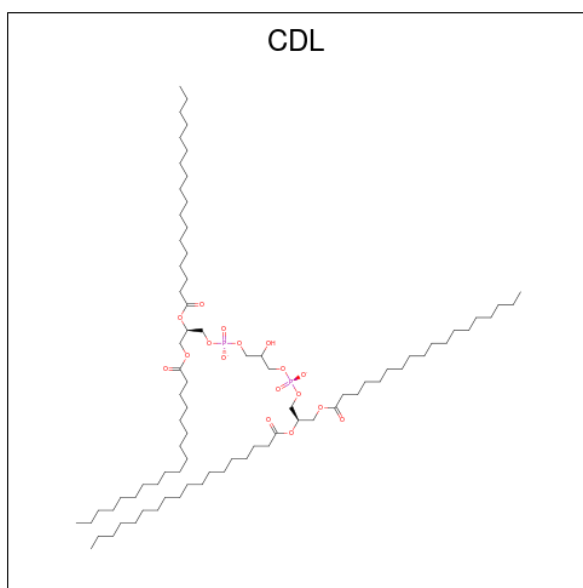
Mol	Chain	Residues	Atoms					AltConf
28	1	1	Total	C	N	O	P	0
			33	23	1	8	1	
28	2	1	Total	C	N	O	P	0
			45	35	1	8	1	
28	5	1	Total	C	N	O	P	0
			40	30	1	8	1	
28	5	1	Total	C	N	O	P	0
			45	35	1	8	1	

- Molecule 29 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



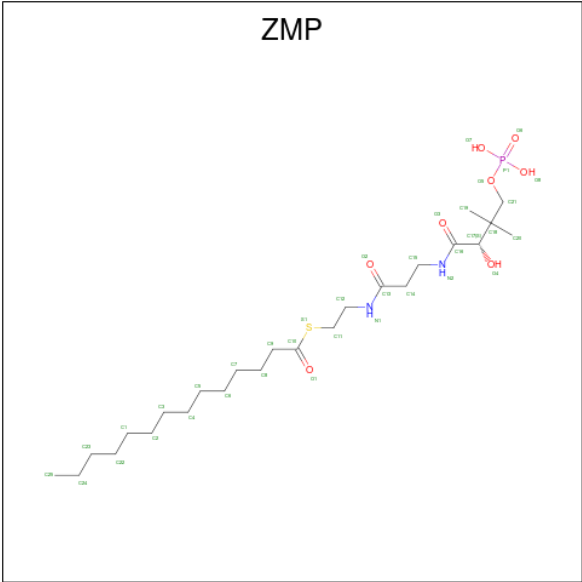
Mol	Chain	Residues	Atoms			AltConf
29	1	1	Total	C	O	0
			35	24	11	
29	1	1	Total	C	O	0
			35	24	11	
29	2	1	Total	C	O	0
			35	24	11	
29	2	1	Total	C	O	0
			35	24	11	
29	2	1	Total	C	O	0
			35	24	11	
29	2	1	Total	C	O	0
			35	24	11	
29	3	1	Total	C	O	0
			35	24	11	
29	3	1	Total	C	O	0
			35	24	11	
29	4	1	Total	C	O	0
			31	20	11	
29	5	1	Total	C	O	0
			35	24	11	
29	J	1	Total	C	O	0
			35	24	11	
29	J	1	Total	C	O	0
			35	24	11	
29	a	1	Total	C	O	0
			35	24	11	
29	g	1	Total	C	O	0
			34	23	11	

- Molecule 30 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
30	2	1	Total	C	O	P	0
			69	50	17	2	
30	D	1	Total	C	O	P	0
			65	46	17	2	
30	S	1	Total	C	O	P	0
			61	42	17	2	
30	X	1	Total	C	O	P	0
			53	34	17	2	
30	X	1	Total	C	O	P	0
			76	57	17	2	

- Molecule 31 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).



Mol	Chain	Residues	Atoms					AltConf	
31	Q	1	Total	C	N	O	P	S	0
			36	25	2	7	1	1	

- Molecule 32 is water.

Mol	Chain	Residues	Atoms		AltConf
32	1	36	Total	O	0
			36	36	
32	2	122	Total	O	0
			122	122	
32	3	6	Total	O	0
			6	6	
32	4	96	Total	O	0
			96	96	
32	5	71	Total	O	0
			71	71	
32	6	21	Total	O	0
			21	21	
32	9	18	Total	O	0
			18	18	
32	D	23	Total	O	0
			23	23	
32	J	3	Total	O	0
			3	3	
32	L	5	Total	O	0
			5	5	
32	Q	3	Total	O	0
			3	3	

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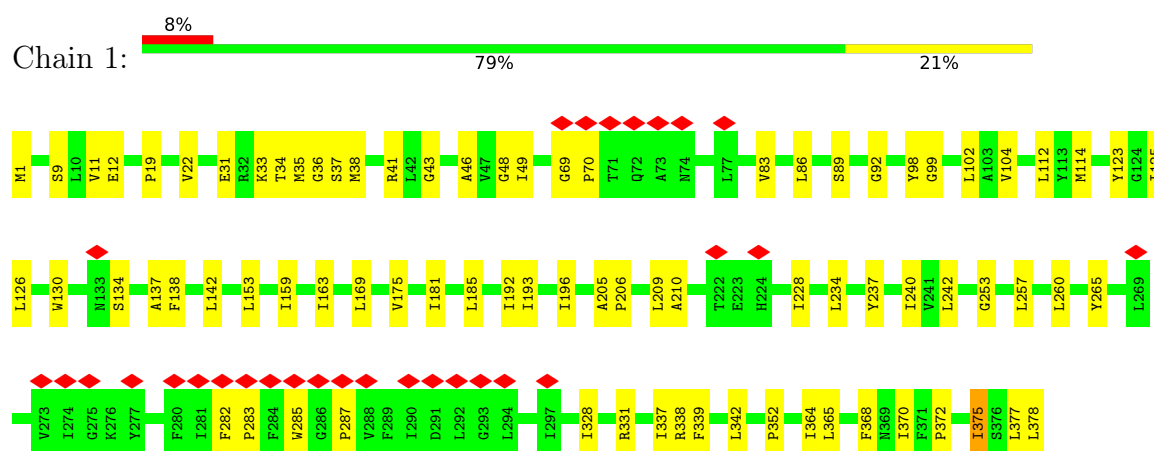
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Mol	Chain	Residues	Atoms		AltConf
32	R	16	Total 16	O 16	0
32	S	7	Total 7	O 7	0
32	U	19	Total 19	O 19	0
32	W	35	Total 35	O 35	0
32	X	37	Total 37	O 37	0
32	a	12	Total 12	O 12	0
32	b	6	Total 6	O 6	0
32	c	1	Total 1	O 1	0
32	d	18	Total 18	O 18	0
32	g	2	Total 2	O 2	0
32	i	5	Total 5	O 5	0
32	j	18	Total 18	O 18	0
32	n	28	Total 28	O 28	0

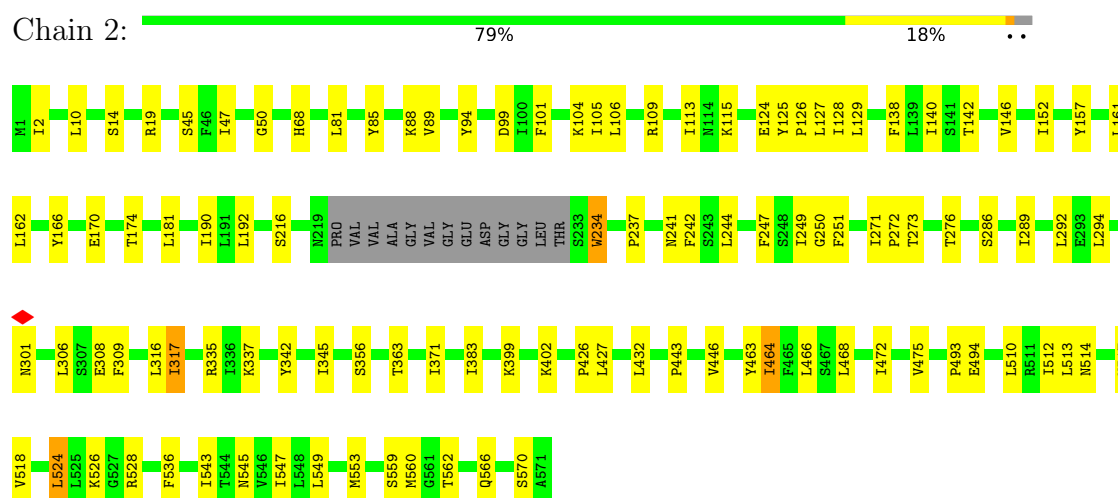
3 Residue-property plots

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: NADH-ubiquinone oxidoreductase chain 1

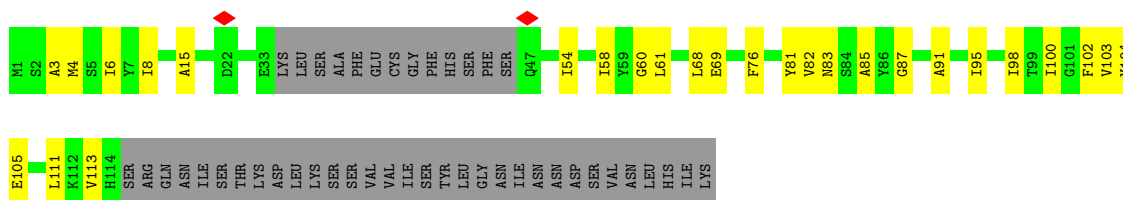


- Molecule 2: NADH dehydrogenase subunit 2

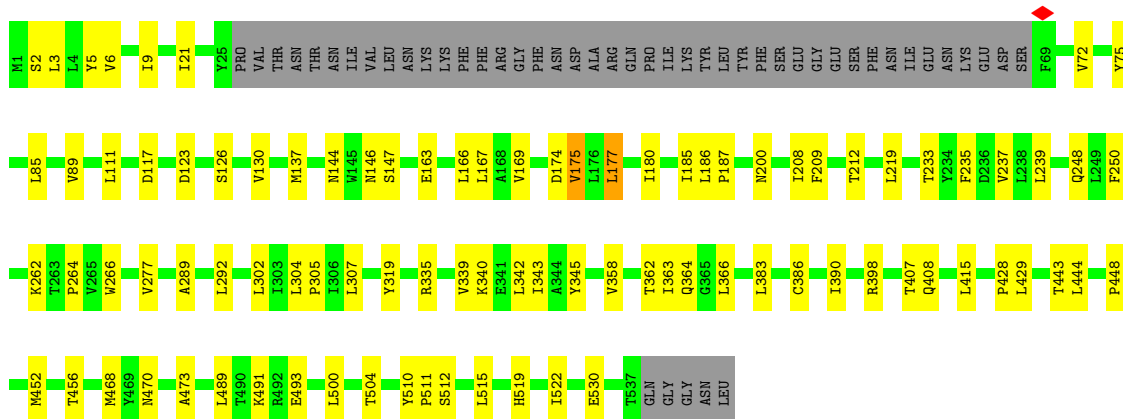


- Molecule 3: NADH-ubiquinone oxidoreductase chain 3

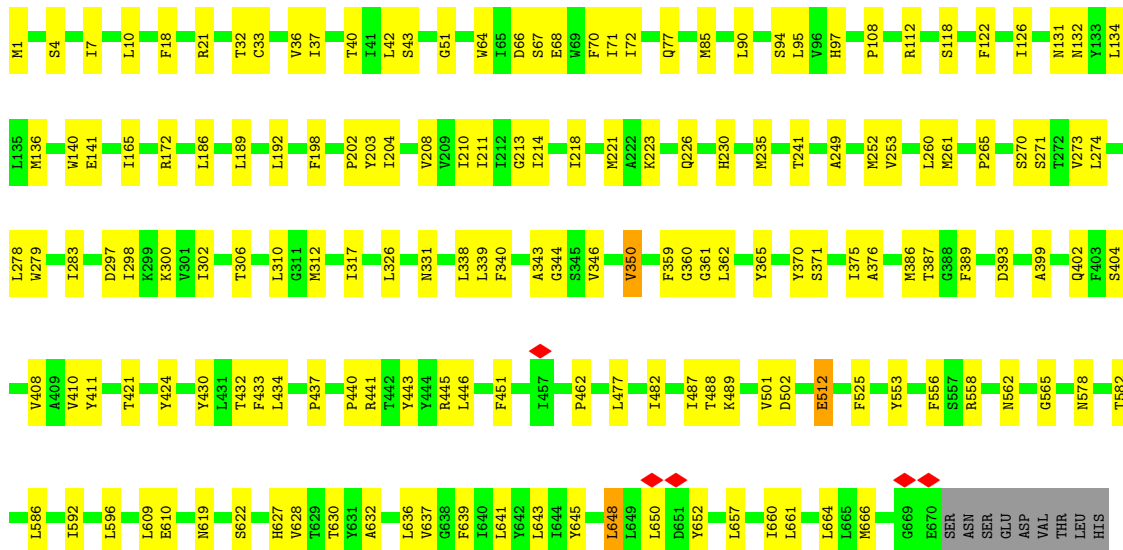




• Molecule 4: NADH-ubiquinone oxidoreductase chain 4



• Molecule 5: NADH-ubiquinone oxidoreductase chain 5



• Molecule 6: NADH-ubiquinone oxidoreductase chain 6



SER
MET
ASP
LEU
GLY
LVS
LVS
GLY
GLY
GLU
GLU
LVS
GLY
GLY

- Molecule 9: Subunit NDUFA1 of NADH-ubiquinone oxidoreductase (Complex I)

Chain D:  80% 17% ..

MET P2 E6 T7 L8 L9 P10 I13 I14 M17 M25 V28 R29 R30 R33 K36 H59 L60 R61 D65 V81 X86

- Molecule 10: NADH-ubiquinone oxidoreductase-like protein

Chain J:  5% 77% 18% 6%

MET ALA PRO ILE GLU GLU HIS HIS Y11 H12 L19 L32 T39 V65 Y69 D70 R73 R80 E81 D84 W85 V86 I90 A95 G96 A97 T98 M99 G100 R105 V109 A113 A126 G127 S128 G129 L130 R131 G132 V133 V134 F134 K135 R136 D137

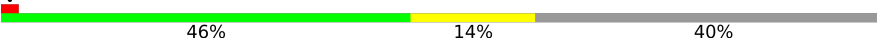
V138 D139 G163 E164 I168 K169 P170 R177 L181 I189 A194 D195 Q198 ALA

- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain L:  66% 31% .

MET R2 I3 T4 L5 F8 L9 I12 L13 G14 F15 N18 N21 N25 L26 I29 N32 L41 S44 D48 D49 I50 I51 G52 Y55 V61 V62 A63 E66 S67 A68 I69 F77 Y78 R79 L80 R81 Y88 LYS

- Molecule 12: Acyl carrier protein

Chain Q:  46% 14% 40%

MET PHE ARG SER ALA VAL LEU ARG SER ALA ALA ALA ALA THR ARG THR THR ILE ILE ARG SER ILE PRO PRO ALA ALA ALA LYS LYS PHE VAL ALA ALA PRO VAL SER ARG VAL THR SER PHE ILE ILE PRO LYS THR ALA TRP GLN VAL ILE ARG CYS TYR ALA SER ASN E57 E63

I68 F75 D76 K77 V78 N79 D80 H89 F90 A91 A92 D93 M106 E109 I114 E115 I116 I124 V127 D128 K129 A130 I131 E132 Y133 Q137 P138 D139 A140 H141

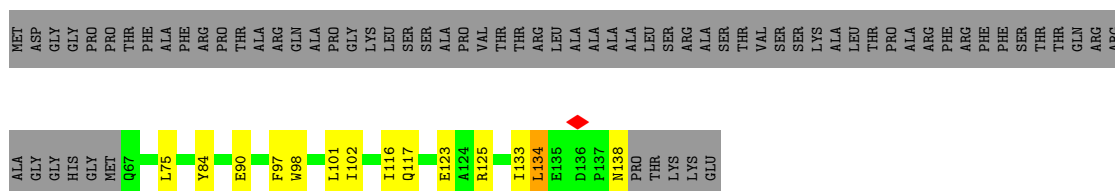
- Molecule 13: Complex I-B22

Chain R:  79% 20% .

MET S2 L8 L15 R29 L33 Y34 L38 F39 D47 L54 L62 V65 X66 H67 P68 P73 P74 T75 E83 L86 P87 Y88 P89 N90 P94 F99

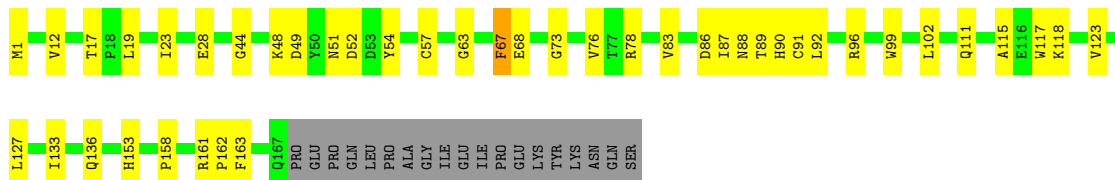
- Molecule 14: Complex I-ESSS

Chain S:  41% 9% 50%



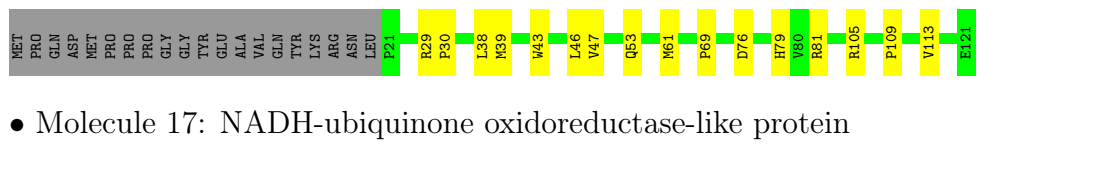
• Molecule 15: NADH-ubiquinone oxidoreductase

Chain U: 67% 23% 10%



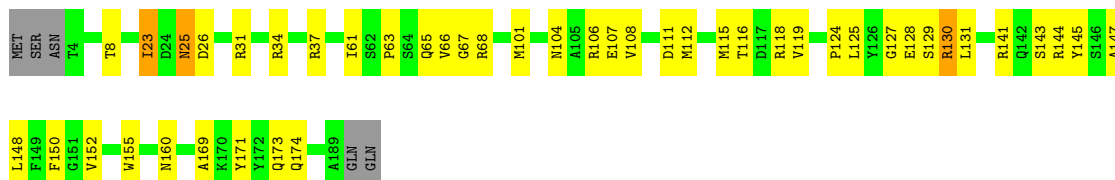
• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain W: 70% 13% 17%



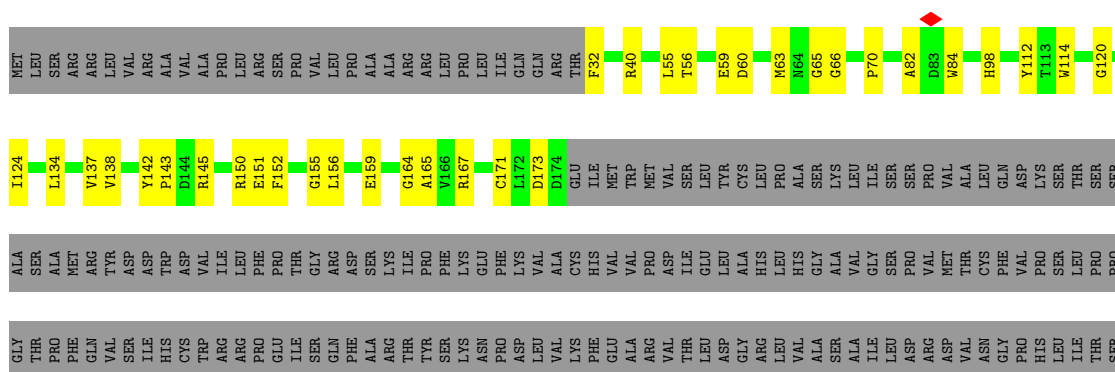
• Molecule 17: NADH-ubiquinone oxidoreductase-like protein

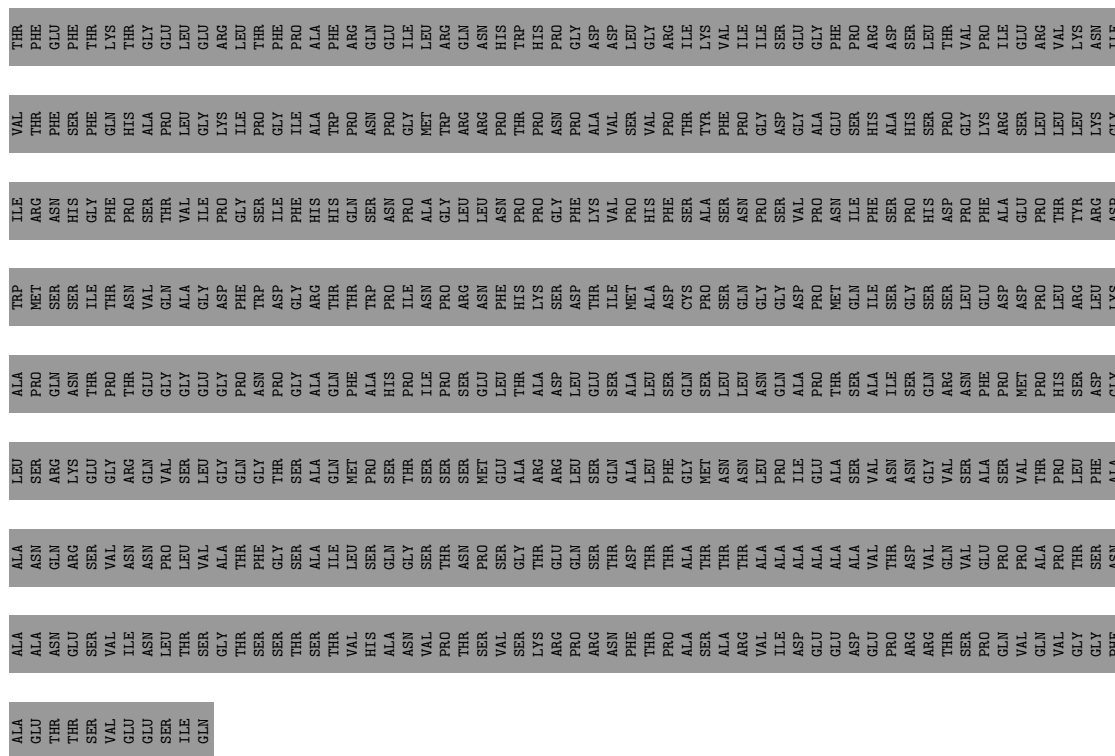
Chain X: 74% 22%



• Molecule 18: NADH dehydrogenase (Ubiquinone)-like protein

Chain a: 13% 82%

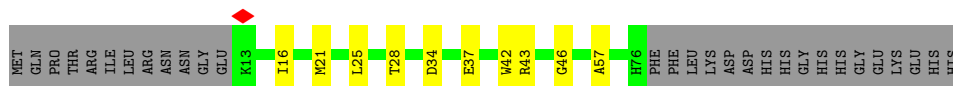




- Molecule 19: Subunit NDUFC2 of NADH-ubiquinone oxidoreductase (Complex I)



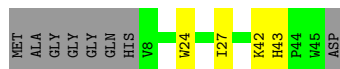
- Molecule 20: Subunit NDUF33 of NADH-ubiquinone oxidoreductase (Complex I)



- Molecule 21: Subunit NDUFB10 of NADH-ubiquinone oxidoreductase (Complex I)



- Molecule 22: Subunit NDUF2 of NADH-ubiquinone oxidoreductase (Complex I)



- Molecule 23: Subunit NDUFA3 of NADH-ubiquinone oxidoreductase (Complex I)

Chain g:  87% 6% • 6%



- Molecule 24: Subunit NDUFB6 of NADH-ubiquinone oxidoreductase (Complex I)

Chain i:  65% 23% 13%



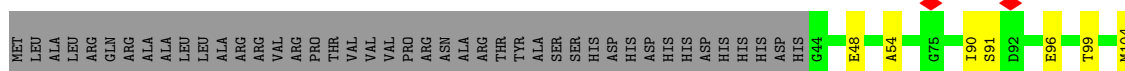
- Molecule 25: Subunit NDUFB4 of NADH-ubiquinone oxidoreductase (Complex I)

Chain j:  81% 16% •



- Molecule 26: Subunit NDUFB5 of NADH-ubiquinone oxidoreductase (Complex I)

Chain n:  65% 8% • 27%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	37767	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.887	Depositor
Minimum map value	-1.296	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.140	Depositor
Recommended contour level	0.12	Depositor
Map size ($\text{\AA}$)	153.4554, 154.48529, 277.04364	wwPDB
Map dimensions	269, 150, 149	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.029902, 1.029902, 1.029902	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZMP, LMT, PC1, CDL, 3PE

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	1	0.68	0/2917	0.99	3/3991 (0.1%)
2	2	0.71	1/4562 (0.0%)	1.02	6/6205 (0.1%)
3	3	0.60	0/811	0.93	0/1105
4	4	0.70	0/4002	1.05	10/5454 (0.2%)
5	5	0.53	0/5418	0.80	4/7376 (0.1%)
6	6	0.71	0/1487	1.01	0/2026
7	8	0.40	0/667	0.61	0/892
8	9	0.74	0/819	1.10	3/1105 (0.3%)
9	D	0.62	0/674	0.96	1/911 (0.1%)
10	J	0.50	0/1435	0.81	2/1940 (0.1%)
11	L	0.65	0/680	1.00	0/921
12	Q	0.39	0/680	0.54	0/922
13	R	0.73	1/832 (0.1%)	1.11	3/1133 (0.3%)
14	S	0.59	0/622	0.83	0/850
15	U	0.81	1/1390 (0.1%)	1.18	6/1885 (0.3%)
16	W	0.71	0/844	1.07	1/1139 (0.1%)
17	X	0.74	0/1506	1.16	8/2036 (0.4%)
18	a	0.34	0/1204	0.59	0/1632
19	b	0.56	0/693	0.92	1/929 (0.1%)
20	c	0.44	1/529 (0.2%)	0.59	1/720 (0.1%)
21	d	0.55	0/845	0.97	3/1137 (0.3%)
22	e	0.74	1/335 (0.3%)	1.04	0/454
23	g	0.72	0/624	0.99	1/857 (0.1%)
24	i	0.40	0/715	0.68	0/971
25	j	0.56	0/617	0.86	0/830
26	n	0.63	0/1100	0.98	2/1491 (0.1%)
All	All	0.63	5/36008 (0.0%)	0.95	55/48912 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	U	90	HIS	C-N	9.33	1.45	1.33
22	e	42	LYS	C-N	-6.91	1.25	1.33
20	c	46	GLY	C-N	5.80	1.41	1.33
2	2	443	PRO	C-O	-5.13	1.20	1.24
13	R	73	PRO	C-O	-5.05	1.20	1.25

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	9	86	ARG	N-CA-C	-7.49	103.72	114.12
1	1	193	ILE	N-CA-C	-6.91	104.25	111.58
4	4	491	LYS	N-CA-C	-6.82	104.21	112.54
17	X	130	ARG	N-CA-C	-6.80	104.73	113.16
19	b	48	TYR	N-CA-C	-6.71	104.05	111.36
21	d	67	HIS	N-CA-C	-6.49	105.18	113.23
10	J	169	LYS	CB-CA-C	6.40	117.31	110.65
26	n	125	ARG	N-CA-C	-6.39	104.74	113.30
4	4	185	ILE	N-CA-C	-6.34	105.42	113.22
4	4	292	LEU	N-CA-C	-6.30	105.56	113.18
15	U	90	HIS	O-C-N	6.04	129.52	122.09
21	d	84	ASN	CA-C-N	-6.01	114.63	123.05
21	d	84	ASN	C-N-CA	-6.01	114.63	123.05
13	R	8	LEU	N-CA-C	-5.94	105.11	112.90
15	U	67	PHE	N-CA-C	-5.94	101.73	110.52
5	5	21	ARG	CB-CA-C	-5.85	101.07	110.79
4	4	266	TRP	N-CA-C	5.84	117.32	111.07
5	5	502	ASP	N-CA-C	-5.82	105.99	112.57
2	2	68	HIS	N-CA-C	-5.75	104.61	111.69
23	g	29	SER	N-CA-C	-5.74	104.95	111.14
1	1	98	TYR	N-CA-C	-5.71	106.12	112.57
10	J	163	GLY	CA-C-O	-5.64	118.33	122.23
13	R	62	LEU	N-CA-C	-5.62	105.54	112.90
2	2	301	ASN	N-CA-C	-5.55	106.55	113.38
2	2	234	TRP	N-CA-C	-5.48	106.55	113.18
15	U	163	PHE	CA-C-N	-5.48	118.00	123.04
15	U	163	PHE	C-N-CA	-5.48	118.00	123.04
1	1	377	LEU	N-CA-C	-5.47	101.04	109.52
2	2	493	PRO	N-CA-C	5.45	119.03	110.80
17	X	25	ASN	N-CA-C	-5.44	106.14	112.89
17	X	23	ILE	N-CA-C	-5.43	106.52	111.67
8	9	10	GLY	CA-C-O	-5.41	113.79	121.52
5	5	462	PRO	N-CA-C	5.38	120.01	112.26
16	W	109	PRO	N-CA-C	5.36	119.51	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	9	39	LYS	N-CA-C	-5.33	106.74	113.18
17	X	116	THR	N-CA-C	-5.32	105.15	111.69
4	4	187	PRO	N-CA-C	5.30	117.16	110.70
26	n	130	LYS	N-CA-C	-5.26	105.72	111.82
2	2	317	ILE	N-CA-C	-5.25	106.01	111.58
2	2	494	GLU	N-CA-C	-5.25	106.83	113.18
4	4	200	ASN	CB-CA-C	5.24	117.66	111.22
5	5	609	LEU	N-CA-C	-5.22	105.65	112.23
13	R	39	PHE	N-CA-C	-5.22	105.19	112.45
17	X	8	THR	CB-CA-C	5.18	119.38	110.79
15	U	57	CYS	CB-CA-C	-5.16	102.78	110.88
20	c	46	GLY	O-C-N	5.13	129.37	122.70
17	X	68	ARG	N-CA-C	5.13	116.87	111.28
9	D	30	HIS	N-CA-C	-5.13	105.32	112.45
17	X	127	GLY	CA-C-N	-5.06	114.94	122.74
17	X	127	GLY	C-N-CA	-5.06	114.94	122.74
4	4	456	THR	N-CA-C	-5.04	107.08	113.18
4	4	177	LEU	N-CA-C	-5.03	105.99	111.82
4	4	289	ALA	CA-C-N	-5.02	117.79	122.66
4	4	289	ALA	C-N-CA	-5.02	117.79	122.66
15	U	67	PHE	CA-C-O	-5.01	115.81	121.72

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	1	2848	0	2891	62	0
2	2	4456	0	4650	77	0
3	3	790	0	807	24	0
4	4	3904	0	4056	69	0
5	5	5276	0	5403	128	0
6	6	1460	0	1567	35	0
7	8	654	0	637	15	0
8	9	802	0	773	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	D	678	0	643	13	0
10	J	1408	0	1411	29	0
11	L	673	0	742	27	0
12	Q	670	0	644	14	0
13	R	807	0	823	14	0
14	S	598	0	548	11	0
15	U	1353	0	1324	29	0
16	W	825	0	846	14	0
17	X	1467	0	1420	30	0
18	a	1167	0	1104	30	0
19	b	675	0	678	7	0
20	c	510	0	458	11	0
21	d	827	0	814	19	0
22	e	320	0	313	1	0
23	g	604	0	614	6	0
24	i	686	0	666	18	0
25	j	603	0	623	18	0
26	n	1068	0	1026	14	0
27	1	39	0	52	1	0
27	5	127	0	175	6	0
27	W	76	0	103	5	0
27	i	43	0	63	4	0
28	1	33	0	40	3	0
28	2	45	0	67	4	0
28	5	85	0	118	9	0
29	1	70	0	92	3	0
29	2	140	0	184	7	0
29	3	70	0	92	4	0
29	4	31	0	35	2	0
29	5	35	0	46	0	0
29	J	70	0	92	3	0
29	a	35	0	46	2	0
29	g	34	0	41	3	0
30	2	69	0	82	2	0
30	D	65	0	74	0	0
30	S	61	0	66	3	0
30	X	129	0	146	3	0
31	Q	36	0	47	2	0
32	1	36	0	0	1	0
32	2	122	0	0	1	0
32	3	6	0	0	0	0
32	4	96	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	5	71	0	0	2	0
32	6	21	0	0	0	0
32	9	18	0	0	0	0
32	D	23	0	0	0	0
32	J	3	0	0	0	0
32	L	5	0	0	0	0
32	Q	3	0	0	0	0
32	R	16	0	0	1	0
32	S	7	0	0	0	0
32	U	19	0	0	0	0
32	W	35	0	0	0	0
32	X	37	0	0	0	0
32	a	12	0	0	0	0
32	b	6	0	0	0	0
32	c	1	0	0	0	0
32	d	18	0	0	0	0
32	g	2	0	0	0	0
32	i	5	0	0	0	0
32	j	18	0	0	2	0
32	n	28	0	0	0	0
All	All	37030	0	37142	597	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 8.

All (597) 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)
4:4:339:VAL:HG13	4:4:468:MET:HE2	1.58	0.86
4:4:408:GLN:HA	28:5:702:PC1:H151	1.59	0.83
1:1:49:ILE:HG12	28:1:402:PC1:H31	1.64	0.79
5:5:221:MET:HG3	5:5:226:GLN:HB2	1.65	0.78
5:5:7:ILE:HG21	24:i:45:VAL:HG21	1.67	0.76
5:5:636:LEU:HD11	11:L:12:ILE:HD12	1.69	0.75
18:a:56:THR:HG22	18:a:59:GLU:HG3	1.68	0.75
12:Q:133:TYR:O	12:Q:137:GLN:HG2	1.88	0.73
5:5:134:LEU:HB2	5:5:192:LEU:HD11	1.71	0.72
2:2:140:ILE:HD11	2:2:286:SER:HA	1.70	0.72
6:6:10:LEU:HD21	8:9:85:ILE:HB	1.72	0.72
29:2:604:LMT:H11	19:b:57:GLN:HE21	1.54	0.72
9:D:6:GLU:HA	9:D:9:ILE:HD12	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:292:LEU:HD11	2:2:363:THR:HG23	1.72	0.71
15:U:111:GLN:HE22	15:U:153:HIS:CD2	2.07	0.71
6:6:12:GLU:HG2	15:U:12:VAL:HG23	1.72	0.70
1:1:370:ILE:HD13	16:W:47:VAL:HG22	1.74	0.70
4:4:428:PRO:HG2	5:5:141:GLU:HG3	1.73	0.70
15:U:51:ASN:HB3	16:W:69:PRO:HG2	1.74	0.69
2:2:543:ILE:HG12	28:2:606:PC1:H3I3	1.73	0.69
4:4:364:GLN:NE2	5:5:68:GLU:O	2.25	0.69
4:4:342:LEU:HD22	4:4:468:MET:HE3	1.74	0.68
7:8:24:LEU:HD11	18:a:159:GLU:HB3	1.76	0.68
7:8:25:ALA:O	18:a:150:ARG:NH1	2.26	0.68
6:6:210:ALA:HA	11:L:69:ILE:HD11	1.76	0.67
4:4:408:GLN:HA	28:5:702:PC1:C15	2.24	0.67
3:3:85:ALA:HB1	30:X:202:CDL:H511	1.76	0.67
1:1:209:LEU:HD23	1:1:338:ARG:HA	1.77	0.67
4:4:237:VAL:HG13	26:n:109:GLU:OE2	1.94	0.66
28:5:702:PC1:H132	28:5:702:PC1:H11	1.75	0.66
2:2:10:LEU:HD13	2:2:127:LEU:HD21	1.77	0.66
5:5:619:ASN:ND2	5:5:666:MET:O	2.28	0.66
2:2:47:ILE:HG12	29:2:604:LMT:H6*1	1.78	0.66
2:2:237:PRO:HG2	2:2:306:LEU:HD11	1.78	0.66
2:2:560:MET:HG3	29:2:604:LMT:H21	1.77	0.66
10:J:80:ARG:NH2	10:J:84:ASP:OD1	2.28	0.66
2:2:146:VAL:HG22	11:L:55:TYR:CD1	2.31	0.66
11:L:18:ASN:ND2	11:L:21:ASN:O	2.29	0.66
5:5:360:GLY:HA3	5:5:437:PRO:HA	1.78	0.66
15:U:19:LEU:HD22	15:U:23:ILE:HD12	1.78	0.66
2:2:308:GLU:O	10:J:131:ARG:NH2	2.30	0.65
2:2:559:SER:HA	2:2:562:THR:HG22	1.78	0.65
5:5:359:PHE:HD2	5:5:432:THR:HG22	1.60	0.65
28:5:702:PC1:H112	24:i:19:GLY:HA2	1.80	0.64
5:5:487:ILE:HG23	5:5:488:THR:HG23	1.80	0.64
15:U:88:ASN:HA	15:U:92:LEU:HD13	1.80	0.64
18:a:63:MET:HE3	25:j:29:PHE:HA	1.80	0.64
1:1:99:GLY:HA3	1:1:102:LEU:HD12	1.81	0.63
10:J:70:ASP:OD1	10:J:73:ARG:NH1	2.32	0.63
5:5:208:VAL:HG22	25:j:63:LEU:HD22	1.80	0.62
6:6:168:PHE:HB3	9:D:81:VAL:HG12	1.79	0.62
1:1:34:THR:HG22	1:1:38:MET:HE2	1.80	0.62
30:S:201:CDL:HB31	26:n:54:ALA:HB2	1.81	0.62
14:S:133:ILE:HG21	21:d:52:VAL:HG22	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:660:ILE:HG22	10:J:99:MET:HE1	1.82	0.62
26:n:96:GLU:HA	26:n:99:THR:HG22	1.80	0.62
5:5:338:LEU:HD13	5:5:477:LEU:HB2	1.82	0.62
5:5:346:VAL:O	5:5:350:VAL:HG22	2.00	0.61
4:4:415:LEU:HD11	5:5:18:PHE:HE1	1.65	0.61
1:1:205:ALA:HB3	1:1:331:ARG:HG3	1.81	0.61
2:2:371:ILE:HD13	29:2:603:LMT:H101	1.81	0.61
5:5:622:SER:HB3	18:a:40:ARG:HH11	1.65	0.61
4:4:277:VAL:HA	4:4:340:LYS:HD3	1.81	0.61
5:5:4:SER:HA	5:5:7:ILE:HG22	1.81	0.61
5:5:112:ARG:HD3	28:5:702:PC1:H2	1.81	0.61
1:1:368:PHE:HE1	27:W:202:3PE:H232	1.65	0.61
12:Q:68:ILE:HD12	12:Q:131:ILE:HD13	1.82	0.61
4:4:147:SER:HA	25:j:4:LEU:HD21	1.83	0.61
15:U:63:GLY:HA3	16:W:105:ARG:HG2	1.83	0.60
18:a:165:ALA:HA	25:j:68:ARG:NH2	2.16	0.60
1:1:125:ILE:HD11	29:1:403:LMT:H4'	1.83	0.60
4:4:500:LEU:O	4:4:504:THR:HG23	2.01	0.60
29:2:604:LMT:H5'	19:b:60:MET:HE1	1.84	0.60
4:4:147:SER:HA	25:j:4:LEU:CD2	2.32	0.60
8:9:6:GLY:H	8:9:10:GLY:HA2	1.66	0.60
9:D:36:LYS:HD3	9:D:61:ARG:HB3	1.82	0.60
5:5:627:HIS:HB2	5:5:630:THR:HG22	1.83	0.60
1:1:12:GLU:HB3	9:D:25:MET:HE3	1.84	0.60
2:2:174:THR:HG23	18:a:32:PHE:HB3	1.84	0.60
4:4:137:MET:HG3	4:4:163:GLU:HG3	1.84	0.59
17:X:63:PRO:HB2	17:X:65:GLN:HE21	1.67	0.59
5:5:1:MET:HG3	5:5:42:LEU:HD22	1.83	0.59
17:X:37:ARG:HG2	17:X:106:ARG:NH2	2.17	0.59
2:2:216:SER:HB2	2:2:237:PRO:HG3	1.85	0.59
17:X:145:TYR:HB3	17:X:148:LEU:HD12	1.84	0.59
14:S:138:ASN:ND2	21:d:2:PRO:O	2.36	0.59
15:U:52:ASP:HB3	23:g:65:PRO:HG2	1.85	0.59
10:J:69:TYR:HB2	10:J:95:ALA:HB2	1.85	0.59
5:5:202:PRO:HG2	21:d:68:LEU:HD21	1.83	0.58
2:2:273:THR:HA	2:2:276:THR:HG22	1.85	0.58
5:5:235:MET:SD	32:5:854:HOH:O	2.57	0.58
13:R:29:ARG:NH1	32:R:102:HOH:O	2.35	0.58
4:4:448:PRO:HD2	32:j:117:HOH:O	2.03	0.58
3:3:83:ASN:HB3	3:3:87:GLY:HA3	1.85	0.58
5:5:253:VAL:HB	5:5:310:LEU:HD11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:9:81:THR:HG23	8:9:84:GLN:H	1.69	0.58
24:i:49:SER:HB3	24:i:53:GLU:OE1	2.03	0.58
2:2:104:LYS:HG3	2:2:513:LEU:HB2	1.85	0.58
4:4:386:CYS:HA	4:4:390:ILE:HD12	1.86	0.58
1:1:181:ILE:HD11	1:1:185:LEU:HD12	1.86	0.58
2:2:464:ILE:HG23	10:J:126:ALA:HB1	1.86	0.58
6:6:31:VAL:O	6:6:35:ILE:HD12	2.04	0.58
2:2:161:LEU:HD13	6:6:213:GLY:HA3	1.86	0.57
19:b:66:GLN:O	19:b:70:GLU:HG2	2.03	0.57
3:3:68:LEU:HD22	11:L:61:VAL:HG22	1.87	0.57
18:a:152:PHE:HB3	18:a:156:LEU:HD13	1.85	0.57
24:i:71:VAL:HG21	24:i:74:ILE:HD12	1.86	0.57
12:Q:124:ILE:HD13	12:Q:129:LYS:HG3	1.86	0.57
13:R:83:GLU:HA	13:R:86:LEU:HG	1.86	0.57
14:S:75:LEU:HD21	30:S:201:CDL:HB62	1.87	0.57
1:1:48:GLY:HA2	28:1:402:PC1:H32	1.87	0.57
2:2:161:LEU:HD21	11:L:69:ILE:HD12	1.86	0.57
4:4:342:LEU:HD22	4:4:468:MET:CE	2.34	0.57
15:U:78:ARG:HE	23:g:80:GLU:HG2	1.70	0.57
4:4:470:ASN:HD22	5:5:165:ILE:HD11	1.70	0.56
5:5:271:SER:HA	5:5:274:LEU:HD12	1.85	0.56
10:J:96:GLY:HA2	10:J:99:MET:SD	2.45	0.56
4:4:175:VAL:HG22	4:4:233:THR:HB	1.87	0.56
5:5:260:LEU:HB2	5:5:317:ILE:HD13	1.87	0.56
2:2:50:GLY:HA3	26:n:130:LYS:HE3	1.87	0.56
5:5:33:CYS:O	5:5:37:ILE:HG12	2.04	0.56
3:3:91:ALA:O	3:3:95:ILE:HG13	2.05	0.56
1:1:86:LEU:HD11	1:1:234:LEU:HD23	1.86	0.56
2:2:2:ILE:HG12	17:X:152:VAL:HA	1.87	0.55
2:2:475:VAL:HG12	29:a:901:LMT:H101	1.88	0.55
5:5:661:LEU:HD21	10:J:65:VAL:HG21	1.87	0.55
13:R:54:LEU:HD22	20:c:16:ILE:HD12	1.88	0.55
1:1:1:MET:HA	9:D:59:HIS:HE1	1.70	0.55
1:1:1:MET:HA	9:D:59:HIS:CE1	2.42	0.55
5:5:652:TYR:HB2	10:J:130:LEU:HB2	1.89	0.55
4:4:489:LEU:HD22	4:4:493:GLU:HB3	1.88	0.55
2:2:514:ASN:HD21	2:2:518:VAL:HB	1.71	0.55
4:4:428:PRO:CG	5:5:141:GLU:HG3	2.37	0.55
11:L:77:PHE:CZ	11:L:81:ARG:HD3	2.42	0.55
1:1:196:ILE:HD12	27:1:401:3PE:H371	1.89	0.55
2:2:138:PHE:O	2:2:142:THR:HG23	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:a:165:ALA:HA	25:j:68:ARG:HH22	1.72	0.55
4:4:6:VAL:HA	4:4:9:ILE:HG12	1.89	0.54
18:a:63:MET:HE3	25:j:30:ARG:H	1.71	0.54
5:5:203:TYR:CE1	10:J:194:ALA:HA	2.41	0.54
17:X:63:PRO:HB2	17:X:65:GLN:NE2	2.21	0.54
20:c:34:ASP:HB3	20:c:37:GLU:HB2	1.90	0.54
1:1:138:PHE:HE1	6:6:90:MET:HE2	1.72	0.54
3:3:4:MET:O	3:3:8:ILE:HG13	2.07	0.54
2:2:181:LEU:HD21	11:L:26:LEU:HD22	1.90	0.54
8:9:7:LEU:HA	11:L:50:ILE:HD13	1.88	0.54
10:J:189:ILE:HD12	25:j:70:ASP:HA	1.89	0.54
17:X:25:ASN:HB3	17:X:144:ARG:HG2	1.89	0.54
17:X:104:ASN:O	17:X:108:VAL:HG23	2.08	0.54
29:3:202:LMT:H1B	29:g:101:LMT:H5B	1.89	0.54
5:5:440:PRO:HD2	5:5:443:TYR:CE2	2.43	0.54
27:W:202:3PE:H251	23:g:43:VAL:HG13	1.90	0.54
5:5:386:MET:HE1	5:5:482:ILE:HG12	1.90	0.54
8:9:81:THR:O	8:9:85:ILE:HG13	2.08	0.54
12:Q:79:ASN:OD1	12:Q:80:ASP:N	2.41	0.54
7:8:73:MET:HE1	18:a:145:ARG:HG3	1.90	0.54
1:1:282:PHE:CG	1:1:283:PRO:HD3	2.43	0.53
12:Q:106:MET:HE1	13:R:15:LEU:HB3	1.90	0.53
2:2:545:ASN:HB3	19:b:11:PHE:CE1	2.44	0.53
4:4:237:VAL:HG13	26:n:109:GLU:CD	2.34	0.53
5:5:556:PHE:HB3	20:c:25:LEU:HD21	1.90	0.53
14:S:123:GLU:HB2	21:d:9:PHE:CZ	2.44	0.53
7:8:47:LEU:HD12	7:8:49:TRP:CH2	2.43	0.53
17:X:106:ARG:NE	17:X:107:GLU:OE2	2.39	0.53
5:5:312:MET:HA	5:5:312:MET:HE2	1.91	0.53
7:8:15:GLU:HB3	7:8:18:ARG:HH11	1.74	0.53
15:U:161:ARG:HG3	15:U:161:ARG:HH11	1.73	0.53
1:1:89:SER:HA	29:1:403:LMT:H31	1.91	0.53
14:S:116:ILE:HG22	14:S:117:GLN:HE21	1.74	0.53
25:j:30:ARG:NH1	32:j:102:HOH:O	2.42	0.53
2:2:105:ILE:HG22	2:2:510:LEU:HD21	1.91	0.53
1:1:36:GLY:HA2	1:1:41:ARG:HG3	1.92	0.52
15:U:115:ALA:HA	15:U:118:LYS:HE2	1.91	0.52
2:2:316:LEU:HD11	2:2:463:TYR:HE2	1.73	0.52
4:4:362:THR:HG22	4:4:364:GLN:H	1.75	0.52
24:i:24:PRO:HB2	24:i:26:ASN:OD1	2.09	0.52
1:1:192:ILE:O	1:1:196:ILE:HG12	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:359:PHE:CD2	5:5:432:THR:HG22	2.43	0.52
2:2:157:TYR:OH	11:L:66:GLU:HB3	2.09	0.52
12:Q:75:PHE:O	12:Q:78:VAL:HG22	2.09	0.52
18:a:164:GLY:O	25:j:68:ARG:NH2	2.42	0.52
5:5:421:THR:HA	5:5:424:TYR:CE2	2.45	0.52
1:1:365:LEU:HA	1:1:370:ILE:HG13	1.92	0.52
2:2:427:LEU:HD22	19:b:21:GLY:HA3	1.91	0.52
4:4:511:PRO:HD2	5:5:64:TRP:O	2.09	0.52
21:d:9:PHE:O	21:d:10:LEU:HD22	2.09	0.52
6:6:42:ASN:ND2	6:6:44:ILE:HB	2.25	0.52
4:4:428:PRO:O	4:4:429:LEU:HB2	2.10	0.51
9:D:33:ASN:O	9:D:36:LYS:HG2	2.10	0.51
12:Q:116:ILE:HD12	12:Q:133:TYR:CE2	2.45	0.51
28:5:703:PC1:H3A1	28:5:703:PC1:H231	1.92	0.51
10:J:100:GLY:HA3	10:J:109:VAL:HA	1.93	0.51
4:4:21:ILE:HD11	4:4:75:TYR:CD1	2.45	0.51
4:4:407:THR:O	28:5:702:PC1:H141	2.10	0.51
2:2:342:TYR:HA	2:2:345:ILE:HD12	1.93	0.51
2:2:513:LEU:HD12	2:2:517:ASN:C	2.36	0.51
3:3:60:GLY:HA3	6:6:84:LEU:HD13	1.91	0.51
4:4:144:ASN:OD1	4:4:147:SER:HB2	2.10	0.51
4:4:340:LYS:HB2	4:4:398:ARG:HD2	1.92	0.51
5:5:441:ARG:HG2	20:c:42:TRP:CZ2	2.46	0.51
5:5:565:GLY:HA3	18:a:114:TRP:CZ2	2.45	0.51
6:6:112:LEU:HD11	10:J:32:LEU:HD23	1.93	0.51
25:j:63:LEU:HD23	25:j:72:ILE:HG23	1.92	0.51
5:5:408:VAL:HG21	18:a:143:PRO:HD2	1.93	0.51
5:5:592:ILE:HA	5:5:596:LEU:HD12	1.93	0.50
2:2:549:LEU:O	2:2:553:MET:HG2	2.10	0.50
5:5:140:TRP:CZ2	5:5:223:LYS:HG3	2.44	0.50
5:5:628:VAL:HG23	11:L:25:MET:HE1	1.93	0.50
7:8:41:ARG:HE	7:8:55:ARG:HH22	1.59	0.50
13:R:94:PRO:HD3	24:i:12:HIS:CD2	2.46	0.50
2:2:566:GLN:O	2:2:570:SER:HB3	2.10	0.50
3:3:61:LEU:CD1	11:L:68:ALA:HB1	2.42	0.50
4:4:174:ASP:HB2	4:4:177:LEU:HB2	1.93	0.50
4:4:407:THR:HG22	4:4:473:ALA:O	2.11	0.50
5:5:361:GLY:O	5:5:433:PHE:HA	2.12	0.50
5:5:189:LEU:HD11	5:5:204:ILE:HD11	1.94	0.50
15:U:86:ASP:HA	15:U:89:THR:HG22	1.92	0.50
2:2:45:SER:HA	29:2:604:LMT:H2B	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:85:TYR:CE1	2:2:115:LYS:HA	2.47	0.50
15:U:17:THR:O	16:W:81:ARG:NH2	2.37	0.50
1:1:35:MET:HE1	1:1:331:ARG:HB3	1.93	0.50
4:4:175:VAL:HG12	4:4:235:PHE:HE1	1.76	0.50
5:5:186:LEU:HG	5:5:192:LEU:HD23	1.93	0.50
24:i:51:GLU:HA	24:i:72:LYS:HG2	1.93	0.50
2:2:105:ILE:HG22	2:2:512:ILE:HD13	1.92	0.50
2:2:383:ILE:HG21	2:2:432:LEU:HB2	1.94	0.50
4:4:2:SER:HB3	4:4:5:TYR:HD1	1.77	0.50
5:5:350:VAL:HG21	5:5:359:PHE:CE1	2.47	0.50
5:5:218:ILE:HA	5:5:221:MET:HE2	1.93	0.49
13:R:47:ASP:OD1	13:R:47:ASP:N	2.44	0.49
2:2:2:ILE:HD11	17:X:152:VAL:HG13	1.94	0.49
2:2:88:LYS:HD2	30:2:601:CDL:HA22	1.95	0.49
5:5:371:SER:O	5:5:375:ILE:HG12	2.12	0.49
15:U:83:VAL:O	15:U:87:ILE:HG12	2.13	0.49
18:a:65:GLY:HA2	25:j:28:TYR:CD2	2.47	0.49
4:4:335:ARG:NH1	5:5:586:LEU:O	2.45	0.49
1:1:22:VAL:HG23	9:D:17:MET:HG3	1.94	0.49
7:8:14:ARG:HA	7:8:17:MET:HE2	1.94	0.49
18:a:151:GLU:OE2	18:a:171:CYS:N	2.44	0.49
24:i:71:VAL:HG23	24:i:74:ILE:HB	1.93	0.49
1:1:138:PHE:CZ	1:1:142:LEU:HD11	2.48	0.49
5:5:77:GLN:HB2	5:5:131:ASN:OD1	2.12	0.49
12:Q:75:PHE:CE2	12:Q:77:LYS:HB2	2.48	0.49
18:a:134:LEU:O	18:a:137:VAL:HG12	2.12	0.49
2:2:157:TYR:CZ	11:L:66:GLU:HB3	2.47	0.49
4:4:219:LEU:HD11	4:4:302:LEU:HD13	1.94	0.49
12:Q:109:GLU:HG3	12:Q:116:ILE:HG12	1.94	0.49
15:U:1:MET:N	16:W:79:HIS:CE1	2.80	0.49
21:d:79:LEU:HB3	25:j:67:ARG:NH2	2.27	0.49
5:5:165:ILE:HG21	28:5:703:PC1:H342	1.92	0.49
1:1:265:TYR:HB3	15:U:158:PRO:HD3	1.95	0.49
5:5:36:VAL:O	5:5:40:THR:OG1	2.30	0.49
2:2:170:GLU:HG2	11:L:80:LEU:HD13	1.95	0.49
5:5:72:ILE:HG23	5:5:132:ASN:ND2	2.27	0.49
5:5:218:ILE:HA	5:5:221:MET:CE	2.42	0.49
5:5:279:TRP:O	5:5:283:ILE:HG12	2.13	0.49
4:4:212:THR:HG23	4:4:262:LYS:HD3	1.95	0.48
7:8:24:LEU:HA	7:8:27:ARG:HG3	1.94	0.48
13:R:88:VAL:HG12	13:R:90:ASN:H	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:134:SER:HB2	1:1:137:ALA:HB3	1.94	0.48
3:3:111:LEU:HB3	3:3:113:VAL:HG23	1.95	0.48
9:D:10:PRO:HA	9:D:13:ILE:HD12	1.94	0.48
14:S:98:TRP:O	14:S:102:ILE:HD12	2.13	0.48
20:c:25:LEU:HA	20:c:28:THR:HG23	1.95	0.48
25:j:62:ASP:HB2	25:j:74:GLU:OE2	2.14	0.48
2:2:317:ILE:HD11	5:5:645:TYR:CE2	2.48	0.48
4:4:166:LEU:O	4:4:169:VAL:HG12	2.13	0.48
5:5:441:ARG:HG2	20:c:42:TRP:CE2	2.48	0.48
10:J:95:ALA:O	10:J:98:THR:OG1	2.29	0.48
30:2:601:CDL:HA32	17:X:61:ILE:HG22	1.95	0.48
5:5:210:ILE:O	5:5:214:ILE:HG12	2.13	0.48
5:5:213:GLY:HA3	5:5:273:VAL:HG11	1.94	0.48
1:1:11:VAL:HG11	9:D:28:VAL:HG11	1.95	0.48
1:1:237:TYR:HA	1:1:240:ILE:HD12	1.96	0.48
5:5:40:THR:OG1	5:5:94:SER:OG	2.30	0.48
17:X:118:ARG:NH1	17:X:124:PRO:O	2.45	0.48
2:2:335:ARG:NH1	32:2:702:HOH:O	2.28	0.48
3:3:100:ILE:O	3:3:103:VAL:HG22	2.14	0.48
12:Q:89:HIS:H	12:Q:93:ASP:HB2	1.78	0.48
13:R:65:TRP:CE2	20:c:21:MET:HE3	2.47	0.48
28:2:606:PC1:H3F2	28:2:606:PC1:H3A1	1.95	0.48
11:L:9:LEU:O	11:L:13:LEU:HG	2.13	0.48
1:1:9:SER:HB2	3:3:6:ILE:HD12	1.94	0.48
1:1:285:TRP:O	1:1:287:PRO:HD3	2.13	0.48
17:X:26:ASP:OD2	17:X:143:SER:HB3	2.14	0.48
4:4:363:ILE:HD13	4:4:522:ILE:HG22	1.96	0.47
10:J:177:ARG:HG2	10:J:181:LEU:HD13	1.96	0.47
14:S:123:GLU:HB2	21:d:9:PHE:CE2	2.49	0.47
17:X:115:MET:O	17:X:119:VAL:HG23	2.14	0.47
7:8:41:ARG:HE	7:8:55:ARG:NH2	2.12	0.47
24:i:42:THR:HA	24:i:45:VAL:HG22	1.94	0.47
5:5:223:LYS:HZ2	5:5:252:MET:HE3	1.79	0.47
17:X:141:ARG:HD2	26:n:133:GLU:HB3	1.96	0.47
2:2:124:GLU:O	2:2:128:ILE:HG13	2.14	0.47
8:9:63:LEU:HG	16:W:113:VAL:HG21	1.96	0.47
18:a:82:ALA:HB3	18:a:84:TRP:CE2	2.49	0.47
5:5:512:GLU:HG2	18:a:150:ARG:HH11	1.78	0.47
14:S:84:TYR:OH	14:S:90:GLU:OE2	2.27	0.47
15:U:96:ARG:HG2	15:U:99:TRP:CZ2	2.49	0.47
21:d:49:GLY:HA2	21:d:81:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:i:63:ARG:O	24:i:68:ARG:NH1	2.31	0.47
3:3:76:PHE:HB2	6:6:193:TYR:CZ	2.49	0.47
4:4:519:HIS:CE1	5:5:67:SER:HA	2.50	0.47
6:6:172:SER:OG	6:6:173:LYS:N	2.48	0.47
17:X:155:TRP:HA	30:X:202:CDL:H782	1.95	0.47
1:1:130:TRP:HE3	6:6:90:MET:HE3	1.79	0.47
5:5:211:ILE:HG12	27:5:706:3PE:H381	1.97	0.47
5:5:297:ASP:HB3	5:5:300:LYS:HB2	1.96	0.47
17:X:112:MET:HG3	17:X:174:GLN:OE1	2.15	0.47
4:4:117:ASP:O	4:4:177:LEU:HD11	2.15	0.47
5:5:632:ALA:HB1	11:L:15:PHE:HD2	1.79	0.47
7:8:53:ASP:OD1	7:8:54:GLU:N	2.48	0.47
10:J:177:ARG:HH21	25:j:74:GLU:HA	1.80	0.47
11:L:63:ALA:O	11:L:66:GLU:HG2	2.14	0.47
21:d:20:PHE:HD2	21:d:93:GLU:HG3	1.79	0.47
5:5:610:GLU:HG3	29:a:901:LMT:H51	1.95	0.47
4:4:111:LEU:H	26:n:104:MET:HE1	1.79	0.47
6:6:5:ILE:HG22	8:9:71:GLU:HG2	1.95	0.47
7:8:42:TYR:OH	24:i:60:GLU:HG3	2.15	0.47
17:X:23:ILE:HG23	17:X:111:ASP:OD2	2.15	0.47
28:2:606:PC1:H361	28:2:606:PC1:H331	1.76	0.46
4:4:235:PHE:O	4:4:239:LEU:HG	2.16	0.46
4:4:364:GLN:HG2	5:5:70:PHE:CE2	2.50	0.46
8:9:89:GLY:H	8:9:97:THR:HG22	1.79	0.46
3:3:69:GLU:HG3	6:6:207:LEU:HD13	1.96	0.46
4:4:304:LEU:N	4:4:305:PRO:CD	2.78	0.46
5:5:558:ARG:O	5:5:562:ASN:ND2	2.40	0.46
17:X:147:ALA:HA	17:X:150:PHE:CE1	2.50	0.46
5:5:32:THR:HG23	5:5:118:SER:OG	2.16	0.46
17:X:124:PRO:HG3	17:X:128:GLU:HG2	1.96	0.46
1:1:104:VAL:HG13	3:3:3:ALA:HB1	1.98	0.46
12:Q:139:ASP:HB3	13:R:75:THR:HG21	1.98	0.46
17:X:125:LEU:HD23	17:X:125:LEU:HA	1.80	0.46
24:i:45:VAL:HG12	27:i:101:3PE:H222	1.97	0.46
2:2:216:SER:CB	2:2:237:PRO:HG3	2.45	0.46
18:a:60:ASP:OD1	18:a:66:GLY:N	2.44	0.46
22:e:24:TRP:H	22:e:27:ILE:HG12	1.80	0.46
1:1:112:LEU:HD23	1:1:169:LEU:HD13	1.97	0.46
2:2:446:VAL:HG12	2:2:547:ILE:HG23	1.97	0.46
29:3:202:LMT:H51	30:X:201:CDL:H712	1.98	0.46
5:5:10:LEU:HB2	5:5:122:PHE:CD1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:140:ILE:HD12	2:2:289:ILE:HB	1.96	0.46
2:2:190:ILE:HG13	2:2:250:GLY:HA3	1.98	0.46
3:3:82:VAL:O	3:3:83:ASN:C	2.59	0.46
4:4:343:ILE:HD12	4:4:383:LEU:HB3	1.98	0.46
5:5:365:TYR:CE2	5:5:446:LEU:HD21	2.50	0.46
8:9:41:ILE:HB	8:9:42:PRO:HD3	1.98	0.46
1:1:31:GLU:HG3	1:1:328:ILE:HG12	1.97	0.46
2:2:125:TYR:N	2:2:126:PRO:HD2	2.31	0.46
4:4:85:LEU:O	4:4:89:VAL:HG23	2.16	0.46
2:2:271:ILE:O	2:2:337:LYS:NZ	2.49	0.46
1:1:46:ALA:HA	28:1:402:PC1:H142	1.99	0.45
5:5:628:VAL:CG2	11:L:25:MET:HE1	2.45	0.45
2:2:468:LEU:O	2:2:472:ILE:HG13	2.15	0.45
5:5:298:ILE:O	5:5:302:ILE:HG13	2.16	0.45
1:1:368:PHE:CE1	27:W:202:3PE:H232	2.48	0.45
4:4:146:ASN:O	25:j:4:LEU:HD21	2.17	0.45
4:4:530:GLU:HG2	21:d:88:LYS:HG3	1.97	0.45
3:3:54:ILE:O	3:3:58:ILE:HG12	2.16	0.45
3:3:95:ILE:O	3:3:98:ILE:HG12	2.16	0.45
5:5:370:TYR:OH	20:c:57:ALA:O	2.29	0.45
21:d:23:VAL:HG13	21:d:30:ARG:HG3	1.97	0.45
1:1:372:PRO:O	3:3:81:TYR:HB2	2.17	0.45
2:2:45:SER:HB2	17:X:101:MET:HB3	1.98	0.45
2:2:242:PHE:CD1	6:6:124:MET:HG3	2.51	0.45
9:D:65:ASP:OD2	15:U:96:ARG:NH2	2.50	0.45
15:U:73:GLY:O	15:U:76:VAL:HG22	2.17	0.45
29:1:404:LMT:H102	29:1:404:LMT:H71	1.68	0.45
2:2:526:LYS:HB2	2:2:528:ARG:HG2	1.97	0.45
12:Q:128:ASP:OD1	12:Q:129:LYS:N	2.49	0.45
27:i:101:3PE:H362	27:i:101:3PE:H392	1.55	0.45
5:5:501:VAL:O	21:d:65:VAL:HB	2.17	0.45
5:5:639:PHE:O	5:5:643:LEU:HD23	2.16	0.45
7:8:44:THR:O	7:8:47:LEU:HD23	2.15	0.45
8:9:11:PRO:HB2	26:n:147:PHE:CZ	2.51	0.45
29:J:202:LMT:H22	29:J:202:LMT:H1'	1.50	0.45
2:2:399:LYS:HA	2:2:402:LYS:NZ	2.32	0.45
5:5:51:GLY:O	32:5:801:HOH:O	2.20	0.45
5:5:211:ILE:HA	27:5:706:3PE:H3A2	1.99	0.45
7:8:28:ASP:OD2	18:a:150:ARG:NH2	2.48	0.45
1:1:378:LEU:HD22	16:W:53:GLN:HE21	1.82	0.45
5:5:261:MET:SD	5:5:326:LEU:HB2	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:402:GLN:O	5:5:404:SER:N	2.49	0.45
2:2:192:LEU:HD22	11:L:8:PHE:CZ	2.52	0.45
4:4:519:HIS:HE1	5:5:67:SER:HA	1.82	0.45
5:5:85:MET:HE3	5:5:85:MET:HB3	1.74	0.45
5:5:136:MET:HE3	5:5:136:MET:HB3	1.69	0.45
11:L:29:ILE:HA	11:L:32:MET:HE3	1.99	0.45
30:S:201:CDL:H521	26:n:54:ALA:HA	1.99	0.45
15:U:99:TRP:HA	15:U:102:LEU:HD12	1.99	0.45
10:J:195:ASP:HB2	21:d:76:GLU:CG	2.47	0.44
15:U:123:VAL:HG13	15:U:127:LEU:HD12	1.98	0.44
1:1:370:ILE:HG21	16:W:47:VAL:HA	1.99	0.44
4:4:137:MET:HE3	4:4:163:GLU:HA	1.99	0.44
5:5:657:LEU:HD11	10:J:69:TYR:CG	2.51	0.44
13:R:29:ARG:O	13:R:33:LEU:HD13	2.17	0.44
17:X:129:SER:HB2	17:X:160:ASN:O	2.17	0.44
2:2:426:PRO:CG	29:2:605:LMT:H5'	2.47	0.44
4:4:515:LEU:HD23	4:4:515:LEU:HA	1.83	0.44
27:5:701:3PE:H321	27:5:701:3PE:H32	1.77	0.44
1:1:375:ILE:HD13	16:W:61:MET:HE3	1.99	0.44
5:5:343:ALA:O	5:5:346:VAL:HG22	2.18	0.44
13:R:34:TYR:CE1	13:R:38:LEU:HD11	2.53	0.44
15:U:161:ARG:HG3	15:U:161:ARG:NH1	2.32	0.44
2:2:166:TYR:CD1	2:2:272:PRO:HG2	2.53	0.44
29:3:202:LMT:H111	23:g:29:SER:HB3	2.00	0.44
4:4:72:VAL:HA	4:4:75:TYR:CD2	2.52	0.44
5:5:399:ALA:HB1	5:5:410:VAL:HG23	2.00	0.44
10:J:138:VAL:HG22	10:J:139:ASP:H	1.82	0.44
10:J:168:ILE:O	10:J:170:PRO:HD3	2.17	0.44
27:i:101:3PE:H321	27:i:101:3PE:H32	1.84	0.44
5:5:361:GLY:O	5:5:362:LEU:HB2	2.17	0.44
1:1:19:PRO:HA	1:1:22:VAL:HG22	2.00	0.44
2:2:129:LEU:HD23	2:2:162:LEU:HD11	2.00	0.44
2:2:234:TRP:CD2	8:9:55:LYS:HG2	2.53	0.44
3:3:54:ILE:HD11	6:6:218:THR:HB	1.98	0.44
4:4:250:PHE:CD1	29:4:601:LMT:H12	2.53	0.44
5:5:226:GLN:O	5:5:230:HIS:HB3	2.17	0.44
8:9:88:LEU:HD11	8:9:101:HIS:CE1	2.53	0.44
2:2:553:MET:HB3	19:b:7:PHE:CE2	2.53	0.44
10:J:80:ARG:HH22	10:J:84:ASP:CG	2.25	0.44
11:L:41:LEU:HD23	11:L:41:LEU:HA	1.88	0.44
18:a:55:LEU:HB3	18:a:60:ASP:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:83:VAL:CG2	3:3:15:ALA:HB1	2.47	0.44
2:2:524:LEU:HD13	2:2:524:LEU:HA	1.82	0.44
5:5:339:LEU:HG	5:5:376:ALA:CB	2.47	0.44
8:9:13:ARG:HG2	11:L:48:ASP:HB3	2.00	0.44
13:R:86:LEU:HD23	13:R:86:LEU:HA	1.84	0.44
5:5:553:TYR:CD1	20:c:25:LEU:HD12	2.53	0.43
10:J:164:GLU:HG2	10:J:170:PRO:HG2	1.99	0.43
1:1:185:LEU:HD23	1:1:185:LEU:HA	1.85	0.43
2:2:244:LEU:HD22	2:2:294:LEU:HD21	2.00	0.43
7:8:31:ALA:O	7:8:35:ILE:HG12	2.17	0.43
13:R:83:GLU:HG2	13:R:86:LEU:HD11	2.00	0.43
15:U:117:TRP:CD2	15:U:162:PRO:HA	2.53	0.43
20:c:42:TRP:CE2	20:c:43:ARG:HG2	2.53	0.43
24:i:67:SER:O	24:i:71:VAL:HG22	2.18	0.43
2:2:94:TYR:CD1	2:2:99:ASP:HB3	2.53	0.43
2:2:249:ILE:HG21	5:5:639:PHE:HD1	1.84	0.43
2:2:514:ASN:ND2	2:2:518:VAL:HB	2.32	0.43
3:3:61:LEU:HD21	6:6:214:ALA:HB3	2.00	0.43
4:4:512:SER:HA	4:4:515:LEU:HB2	2.00	0.43
5:5:37:ILE:HD13	5:5:94:SER:HB3	2.00	0.43
15:U:67:PHE:O	15:U:68:GLU:HB2	2.18	0.43
19:b:49:TRP:O	19:b:53:ILE:HG12	2.18	0.43
5:5:172:ARG:HD3	5:5:172:ARG:HA	1.91	0.43
5:5:389:PHE:O	5:5:393:ASP:HB2	2.18	0.43
6:6:66:LEU:HD23	6:6:69:VAL:HG21	2.00	0.43
10:J:195:ASP:HB2	21:d:76:GLU:HG2	1.99	0.43
1:1:114:MET:HE3	1:1:114:MET:HB2	1.83	0.43
2:2:19:ARG:HE	2:2:19:ARG:HB2	1.37	0.43
17:X:119:VAL:CG2	17:X:125:LEU:HD21	2.48	0.43
1:1:123:TYR:CE1	6:6:51:ILE:HD13	2.54	0.43
4:4:248:GLN:HA	4:4:307:LEU:HD22	2.00	0.43
5:5:140:TRP:CE2	5:5:223:LYS:HG3	2.54	0.43
10:J:19:LEU:HB3	10:J:70:ASP:OD2	2.19	0.43
4:4:72:VAL:HA	4:4:75:TYR:HD2	1.83	0.43
6:6:92:ILE:HG22	6:6:94:ILE:HG13	2.01	0.43
11:L:44:SER:OG	11:L:52:GLY:HA3	2.17	0.43
31:Q:201:ZMP:H9A	31:Q:201:ZMP:H11A	1.84	0.43
15:U:54:TYR:OH	16:W:76:ASP:OD2	2.36	0.43
1:1:352:PRO:HG3	3:3:102:PHE:HE2	1.83	0.43
5:5:249:ALA:HA	5:5:306:THR:HG21	2.00	0.43
6:6:107:ILE:HD13	6:6:107:ILE:HA	1.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:i:59:PRO:HG3	24:i:65:TYR:CD2	2.54	0.43
1:1:364:ILE:HD13	27:W:202:3PE:H382	2.01	0.43
2:2:106:LEU:HD23	2:2:106:LEU:HA	1.89	0.43
4:4:186:LEU:HG	4:4:209:PHE:CD2	2.54	0.43
5:5:553:TYR:HD1	20:c:25:LEU:HD12	1.84	0.43
10:J:86:VAL:O	10:J:90:ILE:HD12	2.19	0.43
17:X:66:VAL:HG22	17:X:67:GLY:H	1.82	0.43
4:4:264:PRO:HD2	32:4:785:HOH:O	2.19	0.42
5:5:648:LEU:HB3	5:5:650:LEU:HG	2.00	0.42
5:5:664:LEU:HD12	10:J:99:MET:HE2	2.01	0.42
6:6:33:SER:O	6:6:37:VAL:HG23	2.19	0.42
15:U:44:GLY:O	15:U:48:LYS:HB2	2.19	0.42
2:2:109:ARG:O	2:2:113:ILE:HG12	2.18	0.42
5:5:445:ARG:HD3	5:5:451:PHE:CG	2.54	0.42
5:5:632:ALA:HB1	11:L:15:PHE:CD2	2.54	0.42
10:J:80:ARG:NH2	10:J:86:VAL:HB	2.34	0.42
15:U:49:ASP:HB3	23:g:72:LEU:HD11	2.01	0.42
15:U:133:ILE:HD12	15:U:136:GLN:NE2	2.34	0.42
17:X:31:ARG:HG2	17:X:34:ARG:HH22	1.83	0.42
1:1:92:GLY:HA3	1:1:242:LEU:HD21	2.01	0.42
5:5:338:LEU:HD13	5:5:477:LEU:CB	2.47	0.42
8:9:87:ASN:HA	8:9:90:LEU:HD22	2.01	0.42
27:W:202:3PE:H351	27:W:202:3PE:H381	1.66	0.42
26:n:115:LYS:O	26:n:119:LEU:HB2	2.19	0.42
1:1:37:SER:OG	9:D:7:THR:HG21	2.19	0.42
6:6:42:ASN:HB3	6:6:45:VAL:HG23	2.00	0.42
14:S:125:ARG:HG3	14:S:134:LEU:HD23	2.00	0.42
2:2:152:ILE:HD12	2:2:152:ILE:HA	1.93	0.42
4:4:2:SER:OG	4:4:3:LEU:N	2.51	0.42
6:6:92:ILE:HG23	11:L:78:TYR:CE1	2.54	0.42
17:X:169:ALA:O	17:X:173:GLN:HG3	2.19	0.42
1:1:83:VAL:HG23	3:3:15:ALA:HB1	2.00	0.42
2:2:316:LEU:HG	2:2:356:SER:HB3	2.02	0.42
26:n:104:MET:HG3	26:n:108:LEU:HD12	2.01	0.42
29:3:202:LMT:H12	29:g:101:LMT:H12	2.00	0.42
31:Q:201:ZMP:H12	31:Q:201:ZMP:H14A	1.61	0.42
17:X:130:ARG:HE	17:X:130:ARG:HB3	1.66	0.42
27:i:101:3PE:H3A1	27:i:101:3PE:H3D2	1.70	0.42
2:2:241:ASN:HB3	2:2:309:PHE:O	2.20	0.42
8:9:91:LEU:HD23	8:9:91:LEU:H	1.85	0.42
18:a:155:GLY:O	18:a:167:ARG:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:159:ILE:O	1:1:163:ILE:HG12	2.19	0.42
1:1:210:ALA:HB3	32:1:502:HOH:O	2.20	0.42
4:4:319:TYR:CE2	4:4:443:THR:HG23	2.55	0.42
17:X:129:SER:OG	17:X:131:LEU:HB2	2.20	0.42
2:2:14:SER:HB3	3:3:104:TYR:HA	2.01	0.42
5:5:68:GLU:OE2	21:d:86:LYS:HA	2.20	0.42
1:1:175:VAL:HG13	1:1:253:GLY:O	2.20	0.41
4:4:452:MET:HE1	29:J:202:LMT:H111	2.01	0.41
27:5:701:3PE:H3A1	27:5:701:3PE:H3D1	1.79	0.41
1:1:126:LEU:HD11	1:1:142:LEU:HD23	2.01	0.41
6:6:195:ASN:H	6:6:195:ASN:HD22	1.66	0.41
26:n:90:ILE:HG13	26:n:91:SER:N	2.35	0.41
5:5:32:THR:HG22	5:5:97:HIS:CD2	2.55	0.41
5:5:122:PHE:O	5:5:126:ILE:HG12	2.21	0.41
5:5:278:LEU:HD11	5:5:410:VAL:HG21	2.02	0.41
27:5:704:3PE:H222	27:5:704:3PE:H252	1.74	0.41
9:D:10:PRO:O	9:D:14:ILE:HG13	2.20	0.41
10:J:11:TYR:HE1	10:J:81:GLU:HA	1.84	0.41
14:S:133:ILE:HD13	21:d:77:ARG:HG2	2.01	0.41
18:a:138:VAL:O	18:a:142:TYR:HB3	2.20	0.41
4:4:177:LEU:HA	4:4:180:ILE:HD12	2.03	0.41
5:5:198:PHE:HB3	5:5:265:PRO:HB2	2.01	0.41
5:5:204:ILE:O	25:j:68:ARG:HG3	2.20	0.41
5:5:270:SER:O	5:5:273:VAL:HG22	2.21	0.41
6:6:35:ILE:O	6:6:39:ILE:HG12	2.20	0.41
16:W:39:MET:HE2	16:W:39:MET:HB3	1.76	0.41
1:1:130:TRP:CZ3	6:6:90:MET:HG2	2.56	0.41
4:4:237:VAL:HG22	26:n:109:GLU:HG2	2.03	0.41
5:5:108:PRO:HG3	24:i:7:ILE:HD13	2.03	0.41
6:6:27:SER:HB2	11:L:3:ILE:HD13	2.03	0.41
18:a:173:ASP:OD1	18:a:173:ASP:N	2.51	0.41
3:3:102:PHE:O	3:3:105:GLU:HG2	2.20	0.41
4:4:510:TYR:HB2	27:5:704:3PE:H272	2.02	0.41
5:5:331:ASN:HB3	5:5:387:THR:HG22	2.03	0.41
5:5:430:TYR:HA	5:5:434:LEU:HB2	2.01	0.41
18:a:70:PRO:HD2	18:a:98:HIS:HA	2.03	0.41
1:1:123:TYR:HE1	6:6:51:ILE:HD13	1.86	0.41
2:2:242:PHE:CE1	6:6:124:MET:HG3	2.54	0.41
5:5:68:GLU:HG3	21:d:46:VAL:HG11	2.03	0.41
5:5:278:LEU:HG	5:5:410:VAL:HG11	2.03	0.41
16:W:29:ARG:HB2	16:W:30:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:W:38:LEU:HD23	16:W:38:LEU:HA	1.87	0.41
17:X:115:MET:HB2	17:X:171:TYR:CD1	2.56	0.41
4:4:126:SER:O	4:4:130:VAL:HG23	2.21	0.41
29:4:601:LMT:H72	29:4:601:LMT:H42	1.94	0.41
6:6:167:LEU:HD11	8:9:57:ALA:HB1	2.02	0.41
18:a:32:PHE:HD1	18:a:32:PHE:HA	1.76	0.41
18:a:70:PRO:O	18:a:98:HIS:HD2	2.04	0.41
21:d:18:PRO:HG3	21:d:41:GLU:HG3	2.03	0.41
23:g:19:ALA:HB1	29:g:101:LMT:H42	2.03	0.41
24:i:26:ASN:ND2	26:n:48:GLU:HB3	2.35	0.41
1:1:69:GLY:HA2	1:1:70:PRO:HD3	1.95	0.41
1:1:153:LEU:HD23	1:1:153:LEU:HA	1.95	0.41
5:5:95:LEU:HD23	5:5:95:LEU:HA	1.84	0.41
5:5:211:ILE:HG21	29:J:202:LMT:H122	2.03	0.41
5:5:582:THR:O	5:5:586:LEU:HD23	2.20	0.41
5:5:637:VAL:O	5:5:641:LEU:HD23	2.21	0.41
28:5:702:PC1:H112	24:i:19:GLY:CA	2.50	0.41
6:6:36:CYS:HA	6:6:39:ILE:HG12	2.02	0.41
11:L:5:LEU:HD12	11:L:5:LEU:HA	1.76	0.41
18:a:120:GLY:O	18:a:124:ILE:HG12	2.20	0.41
2:2:81:LEU:HA	2:2:536:PHE:HE1	1.86	0.41
4:4:343:ILE:HD11	4:4:468:MET:HE1	2.03	0.41
7:8:71:GLN:NE2	7:8:75:GLU:OE2	2.34	0.41
10:J:96:GLY:HA3	10:J:113:ALA:HA	2.03	0.41
13:R:67:HIS:ND1	13:R:68:PRO:HD2	2.36	0.41
15:U:28:GLU:H	15:U:28:GLU:HG2	1.73	0.41
16:W:43:TRP:CZ3	16:W:46:LEU:HD23	2.56	0.41
21:d:38:ILE:HD13	21:d:93:GLU:HG2	2.03	0.41
1:1:206:PRO:HB2	1:1:337:ILE:HD12	2.03	0.40
28:2:606:PC1:H321	28:2:606:PC1:H31	1.48	0.40
4:4:358:VAL:HA	4:4:366:LEU:HD23	2.03	0.40
12:Q:109:GLU:HG2	12:Q:114:ILE:O	2.22	0.40
1:1:130:TRP:CE3	6:6:90:MET:HE3	2.54	0.40
5:5:411:TYR:CE2	5:5:525:PHE:HD2	2.39	0.40
5:5:596:LEU:HD11	25:j:42:TYR:CG	2.57	0.40
14:S:97:PHE:O	14:S:101:LEU:HD13	2.22	0.40
2:2:101:PHE:CE1	17:X:61:ILE:HD11	2.56	0.40
2:2:247:PHE:CZ	2:2:251:PHE:HE2	2.39	0.40
4:4:335:ARG:HD3	5:5:586:LEU:HD12	2.03	0.40
5:5:241:THR:HG21	5:5:344:GLY:HA3	2.03	0.40
6:6:66:LEU:HB3	6:6:69:VAL:CG2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:9:66:ALA:HA	8:9:69:GLU:HG2	2.02	0.40
12:Q:127:VAL:O	12:Q:131:ILE:HG12	2.21	0.40
15:U:87:ILE:O	15:U:91:CYS:N	2.54	0.40
1:1:33:LYS:HA	1:1:43:GLY:HA3	2.03	0.40
1:1:339:PHE:O	1:1:342:LEU:HG	2.21	0.40
4:4:167:LEU:HD23	4:4:167:LEU:HA	1.90	0.40
5:5:43:SER:OG	5:5:90:LEU:HD13	2.22	0.40
5:5:66:ASP:OD1	5:5:71:ILE:HD13	2.21	0.40
5:5:578:ASN:OD1	18:a:112:TYR:HE2	2.03	0.40
24:i:75:LYS:HA	24:i:78:GLU:HG2	2.03	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 PDB entries followed by that with respect to all EM entries.

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	1	376/378 (100%)	359 (96%)	16 (4%)	1 (0%)	36	56
2	2	554/571 (97%)	540 (98%)	14 (2%)	0	100	100
3	3	97/146 (66%)	95 (98%)	2 (2%)	0	100	100
4	4	490/542 (90%)	473 (96%)	17 (4%)	0	100	100
5	5	668/679 (98%)	637 (95%)	30 (4%)	1 (0%)	48	71
6	6	185/224 (83%)	180 (97%)	5 (3%)	0	100	100
7	8	75/86 (87%)	73 (97%)	2 (3%)	0	100	100
8	9	100/785 (13%)	98 (98%)	2 (2%)	0	100	100
9	D	79/86 (92%)	75 (95%)	4 (5%)	0	100	100
10	J	186/199 (94%)	183 (98%)	3 (2%)	0	100	100
11	L	85/89 (96%)	83 (98%)	2 (2%)	0	100	100
12	Q	83/141 (59%)	82 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	R	96/99 (97%)	92 (96%)	4 (4%)	0	100	100
14	S	70/143 (49%)	68 (97%)	2 (3%)	0	100	100
15	U	165/186 (89%)	163 (99%)	2 (1%)	0	100	100
16	W	99/121 (82%)	99 (100%)	0	0	100	100
17	X	184/191 (96%)	178 (97%)	6 (3%)	0	100	100
18	a	141/815 (17%)	137 (97%)	4 (3%)	0	100	100
19	b	78/94 (83%)	76 (97%)	1 (1%)	1 (1%)	9	18
20	c	62/93 (67%)	60 (97%)	2 (3%)	0	100	100
21	d	98/105 (93%)	93 (95%)	5 (5%)	0	100	100
22	e	36/46 (78%)	35 (97%)	1 (3%)	0	100	100
23	g	75/82 (92%)	72 (96%)	3 (4%)	0	100	100
24	i	79/93 (85%)	73 (92%)	6 (8%)	0	100	100
25	j	71/75 (95%)	69 (97%)	2 (3%)	0	100	100
26	n	133/184 (72%)	127 (96%)	6 (4%)	0	100	100
All	All	4365/6253 (70%)	4220 (97%)	142 (3%)	3 (0%)	49	71

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	b	28	PHE
1	1	228	ILE
5	5	350	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	1	297/326 (91%)	294 (99%)	3 (1%)	68	81
2	2	509/518 (98%)	505 (99%)	4 (1%)	73	84
3	3	83/128 (65%)	83 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	4	431/477 (90%)	426 (99%)	5 (1%)	63	78
5	5	581/596 (98%)	577 (99%)	4 (1%)	76	86
6	6	167/203 (82%)	165 (99%)	2 (1%)	63	78
7	8	68/75 (91%)	68 (100%)	0	100	100
8	9	84/687 (12%)	82 (98%)	2 (2%)	43	65
9	D	68/69 (99%)	67 (98%)	1 (2%)	57	74
10	J	131/146 (90%)	130 (99%)	1 (1%)	73	84
11	L	74/76 (97%)	74 (100%)	0	100	100
12	Q	74/119 (62%)	74 (100%)	0	100	100
13	R	87/89 (98%)	87 (100%)	0	100	100
14	S	58/111 (52%)	57 (98%)	1 (2%)	53	71
15	U	148/167 (89%)	148 (100%)	0	100	100
16	W	84/102 (82%)	84 (100%)	0	100	100
17	X	143/152 (94%)	143 (100%)	0	100	100
18	a	123/697 (18%)	123 (100%)	0	100	100
19	b	66/74 (89%)	65 (98%)	1 (2%)	57	74
20	c	47/80 (59%)	47 (100%)	0	100	100
21	d	87/94 (93%)	87 (100%)	0	100	100
22	e	30/35 (86%)	29 (97%)	1 (3%)	33	57
23	g	65/69 (94%)	65 (100%)	0	100	100
24	i	69/78 (88%)	69 (100%)	0	100	100
25	j	63/64 (98%)	63 (100%)	0	100	100
26	n	108/150 (72%)	106 (98%)	2 (2%)	50	70
All	All	3745/5382 (70%)	3718 (99%)	27 (1%)	73	86

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	257	LEU
1	1	260	LEU
1	1	375	ILE
2	2	89	VAL
2	2	464	ILE
2	2	466	LEU

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Mol	Chain	Res	Type
2	2	524	LEU
4	4	123	ASP
4	4	175	VAL
4	4	208	ILE
4	4	345	TYR
4	4	444	LEU
5	5	340	PHE
5	5	489	LYS
5	5	512	GLU
5	5	648	LEU
6	6	198	VAL
6	6	219	ILE
8	9	19	GLN
8	9	85	ILE
9	D	81	VAL
10	J	39	THR
14	S	134	LEU
19	b	29	ASN
22	e	43	HIS
26	n	119	LEU
26	n	134	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	147	GLN
1	1	341	GLN
2	2	26	ASN
2	2	68	HIS
2	2	80	GLN
2	2	347	HIS
2	2	364	GLN
2	2	377	ASN
2	2	397	ASN
2	2	483	ASN
2	2	514	ASN
3	3	83	ASN
4	4	108	GLN
4	4	144	ASN
4	4	151	ASN
4	4	248	GLN
4	4	276	HIS

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Mol	Chain	Res	Type
4	4	519	HIS
5	5	171	ASN
5	5	436	ASN
5	5	511	HIS
6	6	93	ASN
6	6	182	ASN
6	6	183	ASN
6	6	195	ASN
7	8	56	HIS
8	9	19	GLN
8	9	28	ASN
8	9	101	HIS
9	D	44	GLN
9	D	48	GLN
9	D	77	ASN
10	J	45	ASN
13	R	51	GLN
14	S	117	GLN
15	U	11	HIS
15	U	51	ASN
15	U	126	ASN
15	U	153	HIS
15	U	154	HIS
16	W	72	GLN
16	W	79	HIS
16	W	87	GLN
16	W	120	GLN
17	X	7	GLN
17	X	65	GLN
18	a	81	HIS
18	a	88	GLN
18	a	101	HIS
19	b	57	GLN
19	b	79	GLN
21	d	33	GLN
24	i	30	ASN
25	j	6	HIS
26	n	84	HIS
26	n	110	GLN
26	n	126	HIS
26	n	153	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

31 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$
29	LMT	1	403	-	36,36,36	1.10	2 (5%)	47,47,47	1.07	2 (4%)
29	LMT	2	603	-	36,36,36	0.40	0	47,47,47	0.74	0
28	PC1	5	702	-	39,39,53	0.40	0	45,47,61	0.54	0
29	LMT	a	901	-	36,36,36	0.35	0	47,47,47	0.85	1 (2%)
29	LMT	2	605	-	36,36,36	0.40	0	47,47,47	0.69	0
27	3PE	W	202	-	35,35,50	1.02	4 (11%)	38,40,55	1.20	2 (5%)
27	3PE	1	401	-	38,38,50	0.33	0	41,43,55	0.55	0
28	PC1	2	606	-	44,44,53	1.02	4 (9%)	50,52,61	1.19	3 (6%)
29	LMT	4	601	-	32,32,36	1.19	2 (6%)	43,43,47	0.89	0
29	LMT	2	602	-	36,36,36	0.36	0	47,47,47	0.73	1 (2%)
29	LMT	2	604	-	36,36,36	0.40	0	47,47,47	0.83	1 (2%)
29	LMT	5	705	-	36,36,36	1.11	2 (5%)	47,47,47	1.33	5 (10%)
30	CDL	D	101	-	64,64,99	0.33	0	70,76,111	0.42	0
28	PC1	5	703	-	44,44,53	0.34	0	50,52,61	0.37	0
29	LMT	3	202	-	36,36,36	0.39	0	47,47,47	1.00	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CDL	S	201	-	60,60,99	0.32	0	66,72,111	0.42	0
29	LMT	J	202	-	36,36,36	0.40	0	47,47,47	0.74	1 (2%)
29	LMT	1	404	-	36,36,36	1.13	2 (5%)	47,47,47	0.95	2 (4%)
28	PC1	1	402	-	32,32,53	0.34	0	38,40,61	0.39	0
27	3PE	5	704	-	41,41,50	0.95	4 (9%)	44,46,55	1.17	2 (4%)
27	3PE	W	201	-	39,39,50	0.31	0	42,44,55	0.34	0
29	LMT	g	101	-	35,35,36	1.10	2 (5%)	46,46,47	1.08	3 (6%)
27	3PE	i	101	-	42,42,50	0.94	4 (9%)	45,47,55	1.08	2 (4%)
29	LMT	J	201	-	36,36,36	1.13	2 (5%)	47,47,47	1.18	3 (6%)
30	CDL	2	601	-	68,68,99	0.34	0	74,80,111	0.43	0
30	CDL	X	201	-	52,52,99	0.37	0	58,64,111	0.46	0
31	ZMP	Q	201	12	30,35,36	0.19	0	34,42,45	0.40	0
27	3PE	5	706	-	42,42,50	0.29	0	44,46,55	0.34	0
27	3PE	5	701	-	40,40,50	0.95	4 (10%)	43,45,55	1.20	3 (6%)
29	LMT	3	201	-	36,36,36	0.37	0	47,47,47	0.70	1 (2%)
30	CDL	X	202	-	75,75,99	0.33	0	81,87,111	0.36	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LMT	1	403	-	-	10/21/61/61	0/2/2/2
29	LMT	2	603	-	-	7/21/61/61	0/2/2/2
28	PC1	5	702	-	-	10/43/43/57	-
29	LMT	a	901	-	-	7/21/61/61	0/2/2/2
29	LMT	2	605	-	-	10/21/61/61	0/2/2/2
27	3PE	W	202	-	-	13/39/39/54	-
27	3PE	1	401	-	-	16/42/42/54	-
28	PC1	2	606	-	-	19/48/48/57	-
29	LMT	4	601	-	-	9/17/57/61	0/2/2/2
29	LMT	2	602	-	-	8/21/61/61	0/2/2/2
29	LMT	2	604	-	-	8/21/61/61	0/2/2/2
29	LMT	5	705	-	-	7/21/61/61	0/2/2/2
30	CDL	D	101	-	-	19/75/75/110	-
28	PC1	5	703	-	-	10/48/48/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LMT	3	202	-	-	8/21/61/61	0/2/2/2
30	CDL	S	201	-	-	17/70/70/110	-
29	LMT	J	202	-	-	5/21/61/61	0/2/2/2
29	LMT	1	404	-	-	8/21/61/61	0/2/2/2
28	PC1	1	402	-	-	4/36/36/57	-
27	3PE	5	704	-	-	16/45/45/54	-
27	3PE	W	201	-	-	6/43/43/54	-
29	LMT	g	101	-	-	6/20/60/61	0/2/2/2
27	3PE	i	101	-	-	18/46/46/54	-
29	LMT	J	201	-	-	11/21/61/61	0/2/2/2
30	CDL	2	601	-	-	25/79/79/110	-
30	CDL	X	201	-	-	19/63/63/110	-
31	ZMP	Q	201	12	-	10/40/42/43	-
27	3PE	5	706	-	-	15/45/45/54	-
27	3PE	5	701	-	-	13/44/44/54	-
29	LMT	3	201	-	-	2/21/61/61	0/2/2/2
30	CDL	X	202	-	-	15/86/86/110	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	J	201	LMT	O5'-C1'	3.35	1.50	1.41
29	4	601	LMT	O5'-C1'	3.26	1.50	1.41
29	J	201	LMT	O5B-C1B	3.26	1.50	1.41
29	4	601	LMT	O5B-C1B	3.25	1.50	1.41
29	1	404	LMT	O5B-C1B	3.25	1.50	1.41
29	1	403	LMT	O5B-C1B	3.16	1.50	1.41
29	5	705	LMT	O5B-C1B	3.12	1.49	1.41
29	g	101	LMT	O5B-C1B	3.11	1.49	1.41
29	1	404	LMT	O5'-C1'	3.01	1.49	1.41
29	g	101	LMT	O5'-C1'	2.98	1.49	1.41
29	1	403	LMT	O5'-C1'	2.95	1.49	1.41
29	5	705	LMT	O5'-C1'	2.85	1.49	1.41
27	W	202	3PE	O21-C2	-2.79	1.40	1.46
27	5	701	3PE	O21-C2	-2.73	1.40	1.46
27	i	101	3PE	O21-C2	-2.70	1.40	1.46
27	5	704	3PE	O21-C2	-2.61	1.40	1.46
27	5	701	3PE	O31-C3	-2.37	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	5	704	3PE	O31-C31	2.35	1.40	1.33
28	2	606	PC1	O21-C21	2.34	1.40	1.34
27	5	704	3PE	O21-C21	2.31	1.40	1.34
27	i	101	3PE	O31-C31	2.31	1.40	1.33
27	W	202	3PE	O31-C31	2.30	1.40	1.33
28	2	606	PC1	O31-C31	2.29	1.40	1.33
27	W	202	3PE	O31-C3	-2.17	1.40	1.45
27	i	101	3PE	O21-C21	2.17	1.40	1.34
27	i	101	3PE	O31-C3	-2.15	1.40	1.45
28	2	606	PC1	O31-C3	-2.13	1.40	1.45
27	5	701	3PE	O21-C21	2.12	1.40	1.34
27	5	704	3PE	O31-C3	-2.12	1.40	1.45
27	5	701	3PE	O31-C31	2.09	1.39	1.33
28	2	606	PC1	O21-C2	-2.03	1.41	1.46
27	W	202	3PE	O21-C21	2.03	1.40	1.34

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	2	606	PC1	O21-C21-C22	4.75	121.77	111.48
27	5	704	3PE	O21-C21-C22	4.42	121.04	111.48
27	5	701	3PE	O21-C21-C22	4.10	120.35	111.48
29	J	201	LMT	O1B-C1B-C2B	3.81	117.46	108.09
27	W	202	3PE	O21-C21-C22	3.76	119.62	111.48
27	i	101	3PE	O21-C21-C22	3.64	119.35	111.48
29	5	705	LMT	C3'-C4'-C5'	3.64	118.99	110.93
29	a	901	LMT	C1B-O1B-C4'	-3.48	109.74	117.98
29	5	705	LMT	O5'-C5'-C4'	3.40	116.76	109.72
29	5	705	LMT	C2'-C3'-C4'	3.40	117.40	109.68
27	W	202	3PE	O31-C31-C32	3.04	121.10	111.83
29	g	101	LMT	C1B-O1B-C4'	-2.93	111.02	117.98
29	5	705	LMT	C1B-O5B-C5B	-2.79	108.27	113.72
29	3	202	LMT	O1B-C4'-C3'	2.73	114.17	107.23
27	5	704	3PE	O31-C31-C32	2.65	119.91	111.83
29	1	404	LMT	C1B-O1B-C4'	-2.60	111.82	117.98
29	J	202	LMT	C1B-O1B-C4'	-2.50	112.04	117.98
28	2	606	PC1	O31-C31-C32	2.46	119.34	111.83
27	5	701	3PE	O31-C31-C32	2.40	119.15	111.83
27	5	701	3PE	C3-C2-C1	-2.33	106.35	111.78
29	1	403	LMT	C2'-C3'-C4'	2.31	114.93	109.68
29	1	403	LMT	C1B-O1B-C4'	-2.31	112.50	117.98
29	5	705	LMT	C1B-O1B-C4'	-2.30	112.53	117.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	i	101	3PE	O31-C31-C32	2.23	118.63	111.83
29	J	201	LMT	O2B-C2B-C3B	-2.17	105.27	110.38
29	g	101	LMT	C1'-O5'-C5'	-2.14	109.54	113.72
29	2	602	LMT	C1B-O1B-C4'	-2.13	112.93	117.98
29	g	101	LMT	C2'-C3'-C4'	2.13	114.51	109.68
29	2	604	LMT	C1B-O1B-C4'	-2.08	113.05	117.98
29	J	201	LMT	O5'-C1'-C2'	2.08	114.64	110.37
29	3	202	LMT	O1B-C4'-C5'	-2.07	104.04	109.48
29	1	404	LMT	O5'-C5'-C4'	2.07	114.00	109.72
29	3	201	LMT	C1B-O1B-C4'	-2.06	113.09	117.98
28	2	606	PC1	C11-C12-N	-2.04	109.29	115.82

There are no chirality outliers.

All (351) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	1	401	3PE	C1-O11-P-O14
27	1	401	3PE	C11-O13-P-O11
27	1	401	3PE	C11-O13-P-O12
27	5	701	3PE	O13-C11-C12-N
27	5	704	3PE	C1-O11-P-O13
27	5	704	3PE	C1-O11-P-O14
27	5	704	3PE	C11-O13-P-O11
27	5	704	3PE	C11-O13-P-O12
27	5	704	3PE	O13-C11-C12-N
27	5	704	3PE	O21-C2-C3-O31
27	5	704	3PE	C22-C21-O21-C2
27	5	706	3PE	C11-O13-P-O11
27	5	706	3PE	C11-O13-P-O12
27	W	202	3PE	C1-O11-P-O12
27	W	202	3PE	C1-O11-P-O13
27	W	202	3PE	C1-O11-P-O14
27	i	101	3PE	C1-O11-P-O14
27	i	101	3PE	C11-O13-P-O11
27	i	101	3PE	C11-O13-P-O14
27	i	101	3PE	C12-C11-O13-P
28	1	402	PC1	C11-O13-P-O14
28	2	606	PC1	C11-O13-P-O14
28	2	606	PC1	C11-O13-P-O11
28	2	606	PC1	C1-O11-P-O12
28	2	606	PC1	C1-O11-P-O14
28	2	606	PC1	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
28	2	606	PC1	C22-C21-O21-C2
28	2	606	PC1	O32-C31-O31-C3
28	2	606	PC1	C32-C31-O31-C3
28	5	702	PC1	C11-O13-P-O14
28	5	702	PC1	C11-O13-P-O11
28	5	702	PC1	C22-C21-O21-C2
28	5	703	PC1	C11-O13-P-O12
28	5	703	PC1	C11-O13-P-O11
29	1	404	LMT	O5'-C1'-O1'-C1
29	2	604	LMT	O5'-C1'-O1'-C1
29	4	601	LMT	C2-C1-O1'-C1'
29	J	201	LMT	C2B-C1B-O1B-C4'
29	J	202	LMT	C2-C1-O1'-C1'
29	a	901	LMT	O5'-C1'-O1'-C1
29	g	101	LMT	O5'-C1'-O1'-C1
30	2	601	CDL	O1-C1-CB2-OB2
30	2	601	CDL	CA2-C1-CB2-OB2
30	2	601	CDL	CA2-OA2-PA1-OA4
30	2	601	CDL	CA2-OA2-PA1-OA5
30	2	601	CDL	CA3-OA5-PA1-OA3
30	2	601	CDL	CB3-OB5-PB2-OB4
30	2	601	CDL	C51-CB5-OB6-CB4
30	D	101	CDL	CA2-OA2-PA1-OA3
30	D	101	CDL	CA2-OA2-PA1-OA5
30	D	101	CDL	CA3-OA5-PA1-OA2
30	S	201	CDL	CB2-OB2-PB2-OB3
30	S	201	CDL	CB3-OB5-PB2-OB2
30	S	201	CDL	CB3-OB5-PB2-OB4
30	X	201	CDL	CB2-OB2-PB2-OB3
30	X	202	CDL	OA7-CA5-OA6-CA4
30	X	202	CDL	C11-CA5-OA6-CA4
31	Q	201	ZMP	O3-C16-C17-C18
31	Q	201	ZMP	N2-C16-C17-C18
31	Q	201	ZMP	N2-C16-C17-O4
31	Q	201	ZMP	O1-C10-S1-C11
31	Q	201	ZMP	C9-C10-S1-C11
29	4	601	LMT	O5B-C1B-O1B-C4'
27	5	701	3PE	O32-C31-O31-C3
27	W	201	3PE	O32-C31-O31-C3
29	2	605	LMT	O5B-C1B-O1B-C4'
29	5	705	LMT	O5B-C1B-O1B-C4'
29	g	101	LMT	O5B-C1B-O1B-C4'

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Mol	Chain	Res	Type	Atoms
27	5	701	3PE	C32-C31-O31-C3
27	1	401	3PE	O32-C31-O31-C3
27	i	101	3PE	O32-C31-O31-C3
27	1	401	3PE	O22-C21-O21-C2
28	1	402	PC1	O22-C21-O21-C2
28	2	606	PC1	O22-C21-O21-C2
28	5	702	PC1	O22-C21-O21-C2
30	2	601	CDL	OB7-CB5-OB6-CB4
27	W	201	3PE	C32-C31-O31-C3
27	i	101	3PE	C32-C31-O31-C3
28	1	402	PC1	C22-C21-O21-C2
31	Q	201	ZMP	C14-C13-N1-C12
27	1	401	3PE	C32-C31-O31-C3
27	5	704	3PE	O22-C21-O21-C2
30	S	201	CDL	OA9-CA7-OA8-CA6
29	4	601	LMT	C4'-C5'-C6'-O6'
30	S	201	CDL	O1-C1-CB2-OB2
30	X	201	CDL	O1-C1-CA2-OA2
29	5	705	LMT	O5'-C5'-C6'-O6'
29	1	404	LMT	C4'-C5'-C6'-O6'
27	1	401	3PE	C22-C21-O21-C2
30	S	201	CDL	C11-CA5-OA6-CA4
30	X	201	CDL	C51-CB5-OB6-CB4
29	J	201	LMT	O5'-C5'-C6'-O6'
29	1	403	LMT	O5B-C5B-C6B-O6B
29	2	605	LMT	O5'-C5'-C6'-O6'
29	2	602	LMT	O5'-C1'-O1'-C1
29	4	601	LMT	O5'-C1'-O1'-C1
29	1	403	LMT	O5'-C5'-C6'-O6'
31	Q	201	ZMP	O2-C13-N1-C12
29	4	601	LMT	O5'-C5'-C6'-O6'
29	g	101	LMT	O5'-C5'-C6'-O6'
30	X	201	CDL	OB7-CB5-OB6-CB4
30	S	201	CDL	CA2-C1-CB2-OB2
28	5	702	PC1	C11-C12-N-C13
28	5	702	PC1	C11-C12-N-C14
29	1	403	LMT	C4B-C5B-C6B-O6B
29	1	403	LMT	C4'-C5'-C6'-O6'
29	J	201	LMT	C4'-C5'-C6'-O6'
29	g	101	LMT	C4'-C5'-C6'-O6'
29	4	601	LMT	C2'-C1'-O1'-C1
29	g	101	LMT	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
29	1	404	LMT	O5'-C5'-C6'-O6'
30	X	201	CDL	C11-CA5-OA6-CA4
29	2	605	LMT	C4'-C5'-C6'-O6'
30	S	201	CDL	C31-CA7-OA8-CA6
30	S	201	CDL	OA7-CA5-OA6-CA4
29	1	404	LMT	O5B-C5B-C6B-O6B
27	5	704	3PE	C31-C32-C33-C34
27	i	101	3PE	C31-C32-C33-C34
27	1	401	3PE	C21-C22-C23-C24
29	2	603	LMT	O5'-C1'-O1'-C1
27	5	704	3PE	C22-C23-C24-C25
29	3	202	LMT	C5'-C4'-O1B-C1B
29	3	202	LMT	O5B-C1B-O1B-C4'
30	X	201	CDL	OA7-CA5-OA6-CA4
29	4	601	LMT	C4B-C5B-C6B-O6B
29	2	603	LMT	C2'-C1'-O1'-C1
29	2	604	LMT	C2'-C1'-O1'-C1
29	2	605	LMT	C2'-C1'-O1'-C1
29	a	901	LMT	C2'-C1'-O1'-C1
29	5	705	LMT	C4'-C5'-C6'-O6'
28	2	606	PC1	C1-C2-O21-C21
29	2	605	LMT	O5'-C1'-O1'-C1
30	D	101	CDL	C51-CB5-OB6-CB4
28	5	702	PC1	C11-C12-N-C15
29	J	201	LMT	C3-C4-C5-C6
29	3	202	LMT	C3'-C4'-O1B-C1B
29	1	403	LMT	C3-C4-C5-C6
30	X	201	CDL	C72-C73-C74-C75
29	J	201	LMT	C5-C6-C7-C8
30	S	201	CDL	C13-C14-C15-C16
29	2	604	LMT	O5'-C5'-C6'-O6'
30	D	101	CDL	CB5-C51-C52-C53
30	X	202	CDL	CB7-C71-C72-C73
31	Q	201	ZMP	C3-C4-C5-C6
30	D	101	CDL	OB7-CB5-OB6-CB4
28	2	606	PC1	C24-C25-C26-C27
27	W	201	3PE	C22-C21-O21-C2
29	1	404	LMT	C1-C2-C3-C4
27	W	202	3PE	C33-C34-C35-C36
29	a	901	LMT	O5'-C5'-C6'-O6'
27	5	706	3PE	C32-C31-O31-C3
29	2	605	LMT	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
27	5	706	3PE	C22-C21-O21-C2
29	3	202	LMT	C5-C6-C7-C8
30	D	101	CDL	CA5-C11-C12-C13
29	4	601	LMT	C3-C4-C5-C6
29	2	603	LMT	O5'-C5'-C6'-O6'
29	g	101	LMT	C1-C2-C3-C4
29	2	605	LMT	O5B-C5B-C6B-O6B
30	X	202	CDL	C75-C76-C77-C78
31	Q	201	ZMP	O3-C16-C17-O4
29	5	705	LMT	O1'-C1-C2-C3
28	2	606	PC1	O11-C1-C2-C3
30	D	101	CDL	OB5-CB3-CB4-CB6
29	2	602	LMT	O5B-C5B-C6B-O6B
28	2	606	PC1	C21-C22-C23-C24
29	a	901	LMT	C6-C7-C8-C9
30	2	601	CDL	C31-CA7-OA8-CA6
27	5	704	3PE	C1-C2-C3-O31
30	2	601	CDL	CB3-CB4-CB6-OB8
29	3	201	LMT	O5B-C5B-C6B-O6B
30	2	601	CDL	C75-C76-C77-C78
27	W	202	3PE	C34-C35-C36-C37
29	1	403	LMT	C2-C3-C4-C5
27	1	401	3PE	C23-C24-C25-C26
27	5	704	3PE	C21-C22-C23-C24
30	S	201	CDL	CA6-CA4-OA6-CA5
29	2	602	LMT	C6-C7-C8-C9
27	1	401	3PE	O11-C1-C2-O21
27	5	706	3PE	O32-C31-O31-C3
30	2	601	CDL	OB6-CB4-CB6-OB8
31	Q	201	ZMP	C22-C1-C2-C3
29	4	601	LMT	O5B-C5B-C6B-O6B
27	W	201	3PE	O22-C21-O21-C2
28	2	606	PC1	C23-C24-C25-C26
28	2	606	PC1	C3D-C3E-C3F-C3G
30	X	202	CDL	C72-C71-CB7-OB8
30	2	601	CDL	C51-C52-C53-C54
30	X	202	CDL	C11-C12-C13-C14
29	1	403	LMT	C2-C1-O1'-C1'
29	2	602	LMT	C2-C1-O1'-C1'
29	J	201	LMT	C2-C1-O1'-C1'
30	D	101	CDL	CA4-CA3-OA5-PA1
27	i	101	3PE	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
30	D	101	CDL	C52-C51-CB5-OB6
30	2	601	CDL	OA9-CA7-OA8-CA6
28	5	702	PC1	C21-C22-C23-C24
29	2	604	LMT	C5-C6-C7-C8
29	J	201	LMT	C11-C10-C9-C8
29	J	202	LMT	C11-C10-C9-C8
28	5	702	PC1	C1-C2-C3-O31
27	i	101	3PE	C33-C34-C35-C36
27	5	706	3PE	C21-C22-C23-C24
27	1	401	3PE	C22-C23-C24-C25
30	2	601	CDL	OB5-CB3-CB4-OB6
30	D	101	CDL	OB5-CB3-CB4-OB6
30	X	201	CDL	OA5-CA3-CA4-OA6
30	X	202	CDL	OB5-CB3-CB4-OB6
28	5	703	PC1	O21-C2-C3-O31
27	W	202	3PE	C31-C32-C33-C34
29	2	602	LMT	C9-C10-C11-C12
27	5	701	3PE	C31-C32-C33-C34
27	5	701	3PE	C23-C24-C25-C26
28	5	703	PC1	O31-C31-C32-C33
29	J	202	LMT	C6-C7-C8-C9
30	X	202	CDL	CB2-C1-CA2-OA2
29	1	403	LMT	O1'-C1-C2-C3
27	W	202	3PE	O11-C1-C2-C3
28	2	606	PC1	C3B-C3C-C3D-C3E
28	5	703	PC1	C32-C31-O31-C3
27	W	202	3PE	C37-C38-C39-C3A
28	5	703	PC1	C31-C32-C33-C34
27	5	706	3PE	O22-C21-O21-C2
27	i	101	3PE	C21-C22-C23-C24
30	D	101	CDL	C73-C74-C75-C76
30	X	201	CDL	CB6-CB4-OB6-CB5
27	5	706	3PE	C38-C39-C3A-C3B
27	i	101	3PE	C26-C27-C28-C29
27	i	101	3PE	O11-C1-C2-O21
30	S	201	CDL	CA5-C11-C12-C13
27	1	401	3PE	C12-C11-O13-P
27	5	701	3PE	C12-C11-O13-P
27	5	706	3PE	C12-C11-O13-P
27	1	401	3PE	O21-C2-C3-O31
27	5	706	3PE	O21-C2-C3-O31
28	5	702	PC1	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
30	S	201	CDL	OA6-CA4-CA6-OA8
30	X	201	CDL	OA6-CA4-CA6-OA8
27	5	706	3PE	O31-C31-C32-C33
27	5	706	3PE	C34-C35-C36-C37
29	2	602	LMT	C11-C10-C9-C8
28	1	402	PC1	O13-C11-C12-N
28	2	606	PC1	O13-C11-C12-N
29	J	201	LMT	C6-C7-C8-C9
30	X	201	CDL	C31-CA7-OA8-CA6
27	5	701	3PE	C22-C21-O21-C2
30	2	601	CDL	OB5-CB3-CB4-CB6
30	X	201	CDL	OA5-CA3-CA4-CA6
30	X	202	CDL	OB5-CB3-CB4-CB6
29	5	705	LMT	C3-C4-C5-C6
30	S	201	CDL	C76-C77-C78-C79
27	W	202	3PE	O11-C1-C2-O21
28	2	606	PC1	O11-C1-C2-O21
27	W	201	3PE	C22-C23-C24-C25
27	5	706	3PE	C3A-C3B-C3C-C3D
29	J	201	LMT	C4B-C5B-C6B-O6B
27	i	101	3PE	C3A-C3B-C3C-C3D
30	X	201	CDL	CA3-CA4-CA6-OA8
29	J	201	LMT	O1'-C1-C2-C3
30	2	601	CDL	CB7-C71-C72-C73
29	2	603	LMT	C2-C3-C4-C5
28	5	703	PC1	O32-C31-O31-C3
29	5	705	LMT	C2-C3-C4-C5
27	1	401	3PE	C11-O13-P-O14
27	5	701	3PE	C1-O11-P-O14
27	5	701	3PE	C11-O13-P-O14
27	5	704	3PE	C1-O11-P-O12
27	5	704	3PE	C11-O13-P-O14
27	i	101	3PE	O13-C11-C12-N
28	5	703	PC1	C1-O11-P-O14
30	2	601	CDL	CA3-OA5-PA1-OA2
30	2	601	CDL	CA3-OA5-PA1-OA4
30	2	601	CDL	CB2-OB2-PB2-OB3
30	2	601	CDL	CB3-OB5-PB2-OB2
30	2	601	CDL	CB3-OB5-PB2-OB3
30	D	101	CDL	CA3-OA5-PA1-OA3
30	S	201	CDL	CB2-OB2-PB2-OB5
30	S	201	CDL	C1-CB2-OB2-PB2

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Mol	Chain	Res	Type	Atoms
30	X	201	CDL	C1-CA2-OA2-PA1
30	X	201	CDL	CB7-C71-C72-C73
29	2	605	LMT	C6-C7-C8-C9
29	J	201	LMT	O5B-C5B-C6B-O6B
28	2	606	PC1	C39-C3A-C3B-C3C
27	W	202	3PE	C35-C36-C37-C38
27	5	701	3PE	O22-C21-O21-C2
29	1	403	LMT	C1-C2-C3-C4
29	2	602	LMT	C4'-C5'-C6'-O6'
30	X	201	CDL	CA7-C31-C32-C33
30	X	201	CDL	C32-C31-CA7-OA8
29	3	202	LMT	C6-C7-C8-C9
29	1	404	LMT	C4B-C5B-C6B-O6B
29	a	901	LMT	C5-C6-C7-C8
29	2	604	LMT	C2-C1-O1'-C1'
29	3	202	LMT	C2-C1-O1'-C1'
30	2	601	CDL	CB4-CB3-OB5-PB2
29	2	604	LMT	C7-C8-C9-C10
30	X	201	CDL	OA9-CA7-OA8-CA6
27	i	101	3PE	C36-C37-C38-C39
30	X	201	CDL	CB2-C1-CA2-OA2
30	D	101	CDL	OA5-CA3-CA4-OA6
29	a	901	LMT	C3'-C4'-O1B-C1B
30	X	202	CDL	C72-C71-CB7-OB9
27	i	101	3PE	C32-C33-C34-C35
30	D	101	CDL	C52-C51-CB5-OB7
27	W	202	3PE	C23-C24-C25-C26
29	2	602	LMT	C7-C8-C9-C10
30	2	601	CDL	C54-C55-C56-C57
29	2	603	LMT	O5B-C1B-O1B-C4'
29	2	604	LMT	C4-C5-C6-C7
29	2	604	LMT	C1-C2-C3-C4
29	1	404	LMT	C3-C4-C5-C6
27	5	701	3PE	C3B-C3C-C3D-C3E
30	D	101	CDL	OA5-CA3-CA4-CA6
30	S	201	CDL	OA5-CA3-CA4-CA6
30	X	202	CDL	C72-C73-C74-C75
29	5	705	LMT	C3'-C4'-O1B-C1B
30	X	202	CDL	C79-C80-C81-C82
27	i	101	3PE	C27-C28-C29-C2A
27	W	201	3PE	C29-C2A-C2B-C2C
27	5	701	3PE	C3A-C3B-C3C-C3D

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Mol	Chain	Res	Type	Atoms
29	J	202	LMT	C3'-C4'-O1B-C1B
27	1	401	3PE	C3-C2-O21-C21
30	2	601	CDL	C56-C57-C58-C59
30	D	101	CDL	C71-CB7-OB8-CB6
28	5	703	PC1	C1-C2-C3-O31
29	3	201	LMT	C6-C7-C8-C9
29	2	603	LMT	C6-C7-C8-C9
27	W	202	3PE	O21-C21-C22-C23
27	i	101	3PE	C35-C36-C37-C38
29	J	202	LMT	C5'-C4'-O1B-C1B
27	5	706	3PE	C22-C23-C24-C25
29	a	901	LMT	C5'-C4'-O1B-C1B
30	X	202	CDL	C76-C77-C78-C79
27	5	701	3PE	C33-C34-C35-C36
29	2	605	LMT	C2-C1-O1'-C1'
29	3	202	LMT	C2B-C1B-O1B-C4'
30	D	101	CDL	OB9-CB7-OB8-CB6
29	2	605	LMT	C7-C8-C9-C10
29	3	202	LMT	O5'-C1'-O1'-C1
29	2	603	LMT	C2B-C1B-O1B-C4'
28	5	703	PC1	O32-C31-C32-C33
30	X	202	CDL	O1-C1-CA2-OA2
27	5	704	3PE	O31-C31-C32-C33
27	5	706	3PE	C36-C37-C38-C39
27	1	401	3PE	C2-C1-O11-P
30	X	202	CDL	C1-CB2-OB2-PB2
30	D	101	CDL	C17-C18-C19-C20
27	W	202	3PE	O22-C21-C22-C23
27	5	704	3PE	O32-C31-C32-C33
29	1	404	LMT	C9-C10-C11-C12
29	1	403	LMT	C4-C5-C6-C7

There are no ring outliers.

25 monomers are involved in 63 short contacts:

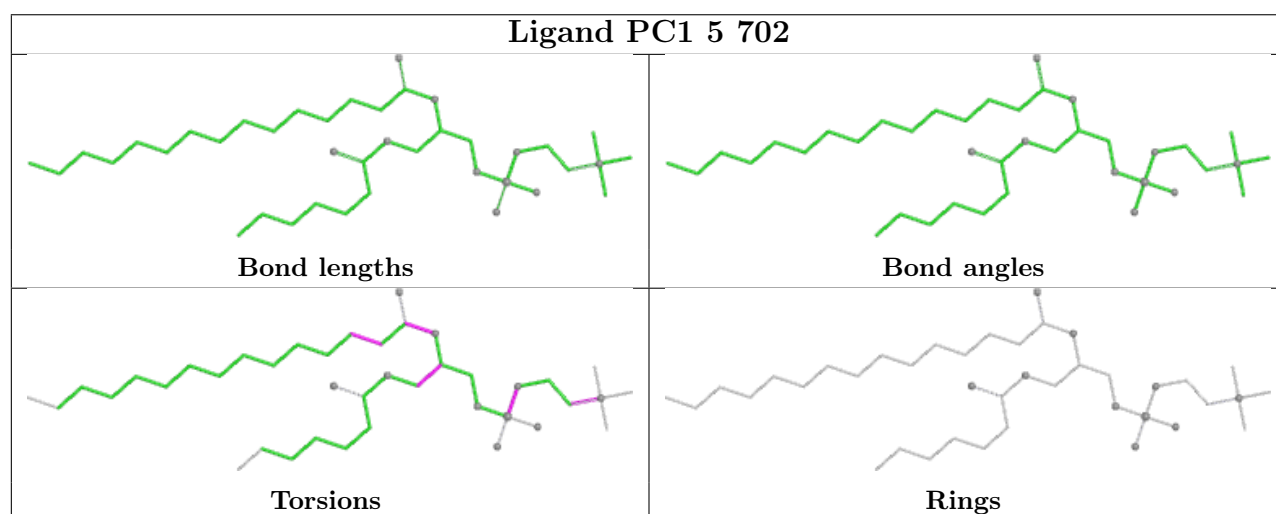
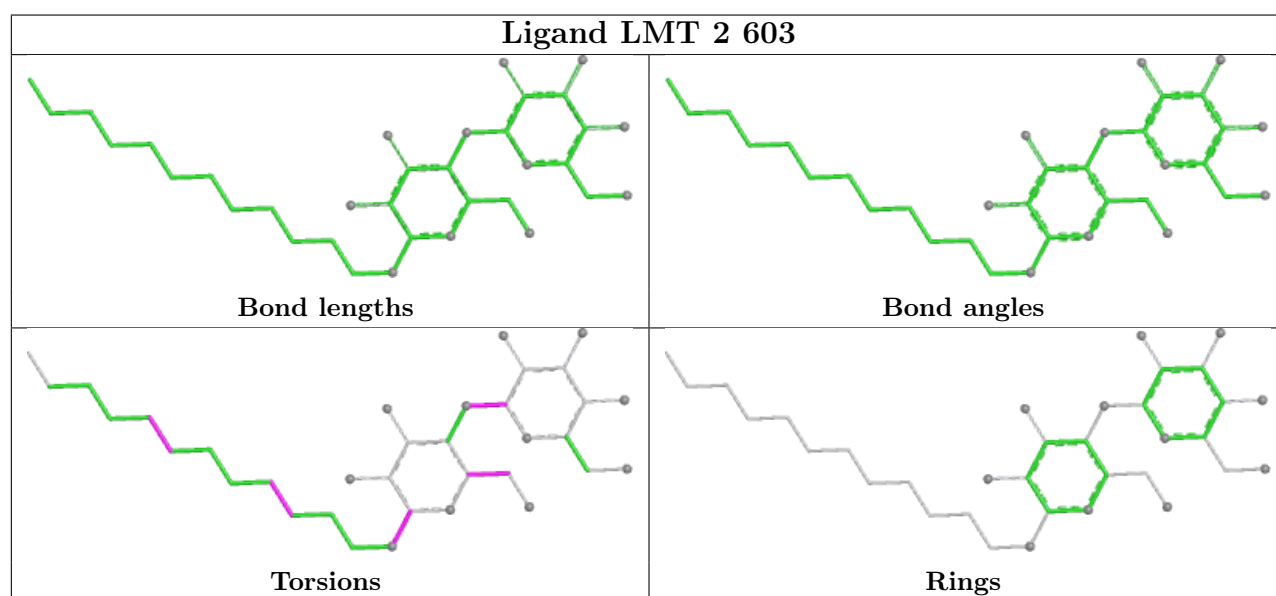
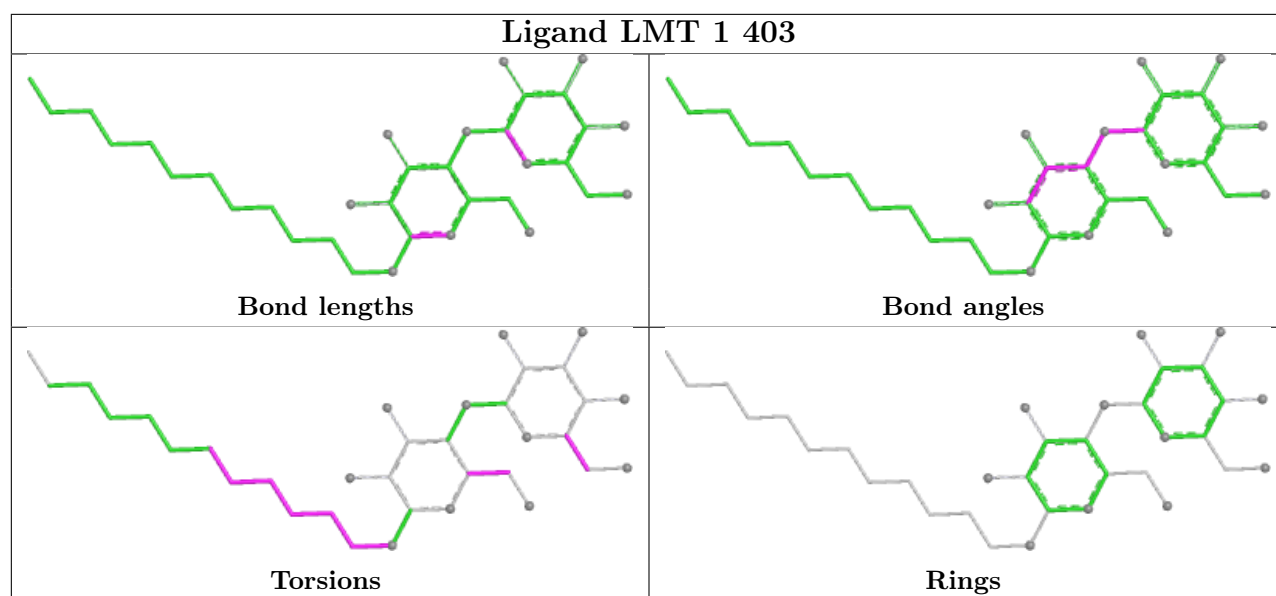
Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	1	403	LMT	2	0
29	2	603	LMT	1	0
28	5	702	PC1	7	0
29	a	901	LMT	2	0
29	2	605	LMT	1	0
27	W	202	3PE	5	0

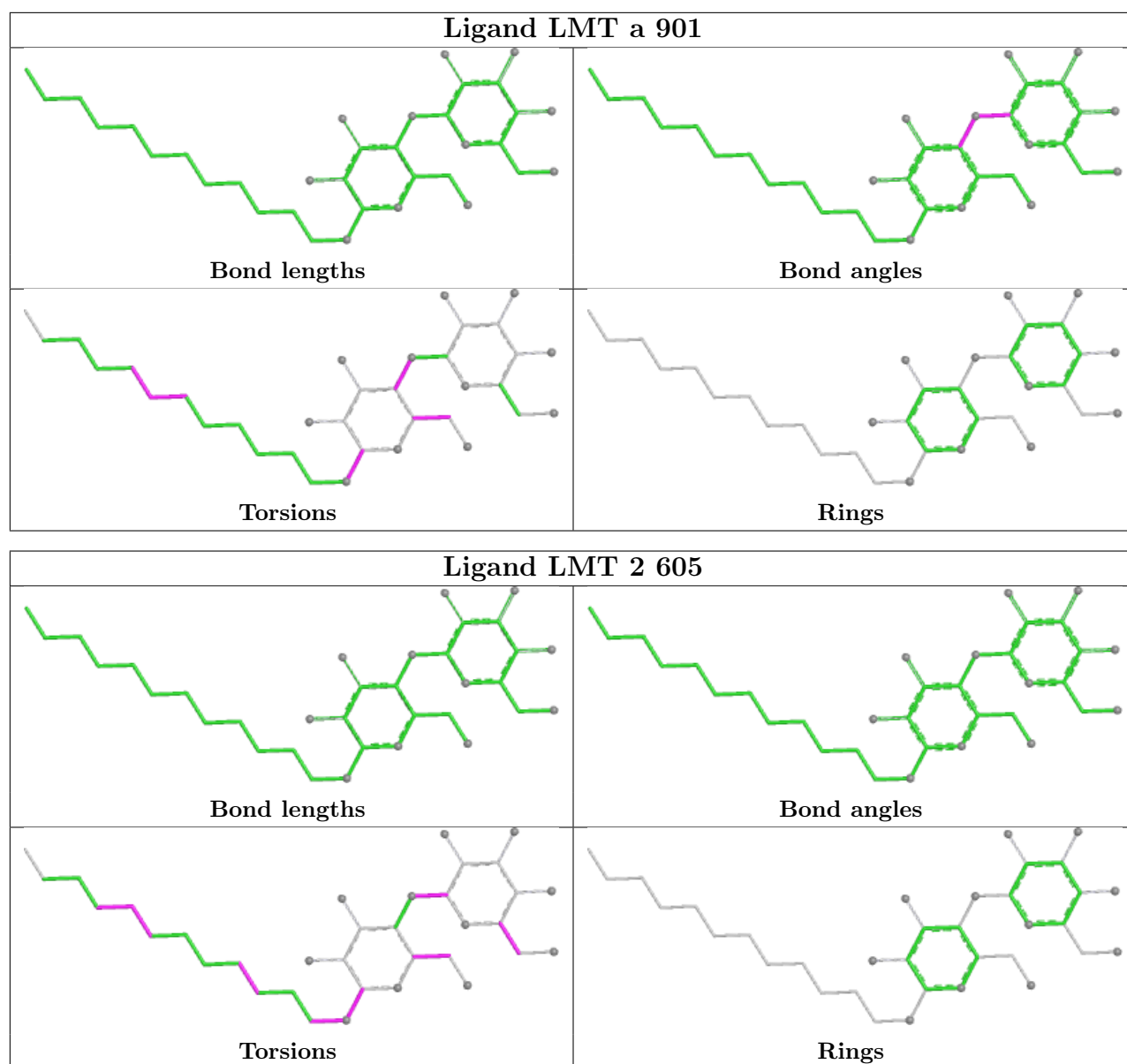
Continued on next page...

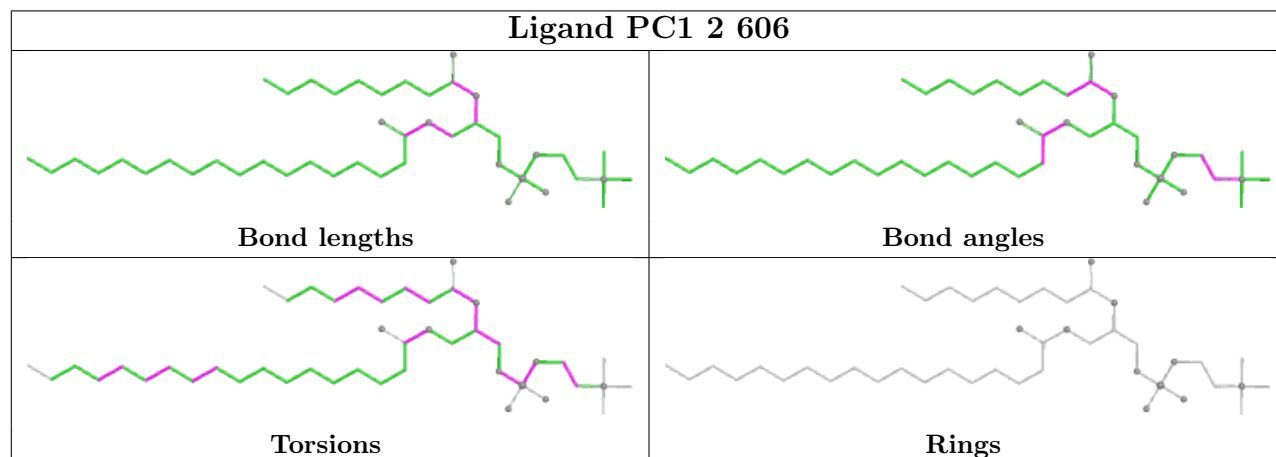
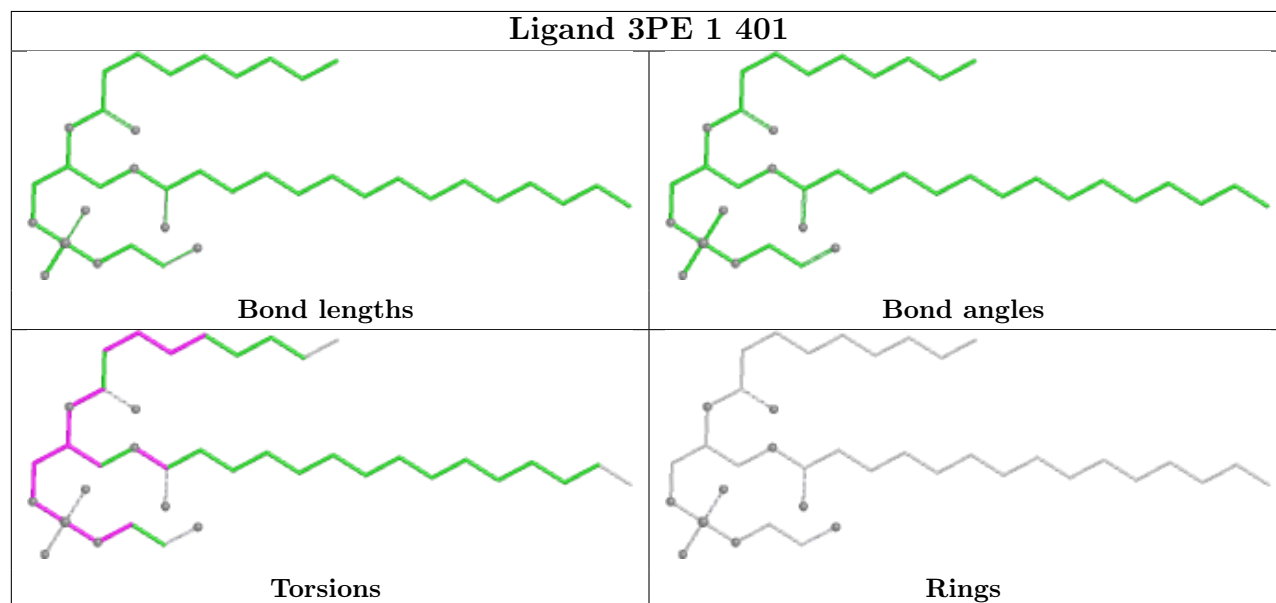
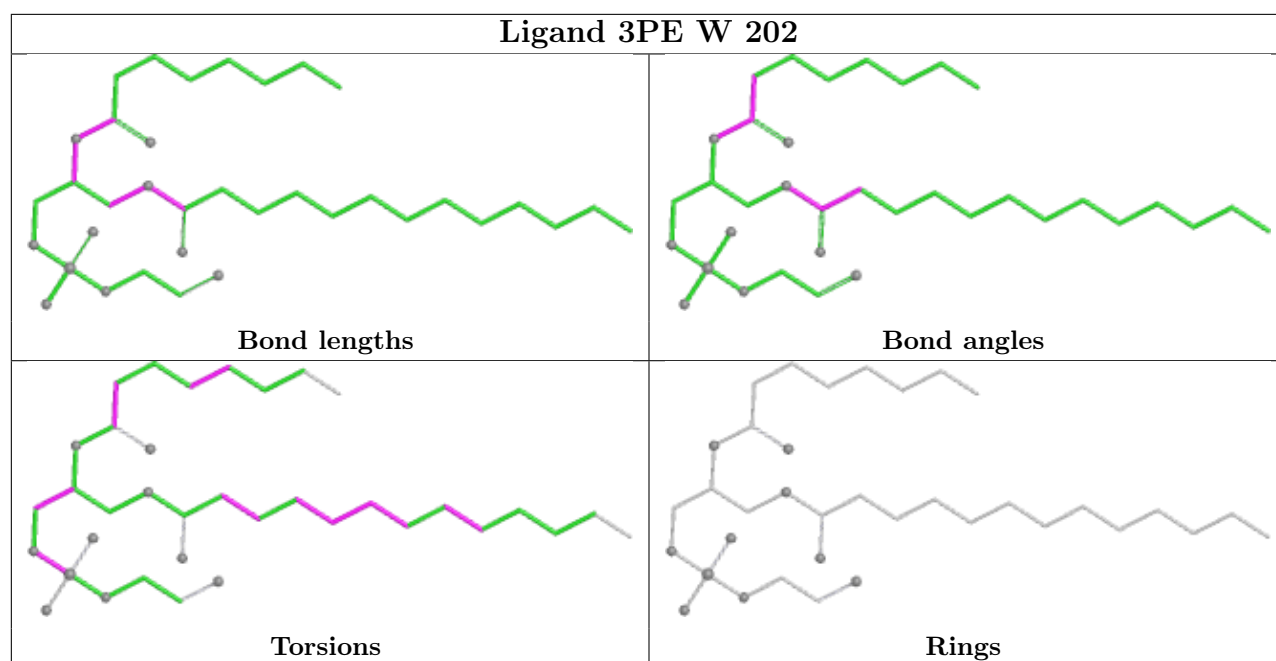
Continued from previous page...

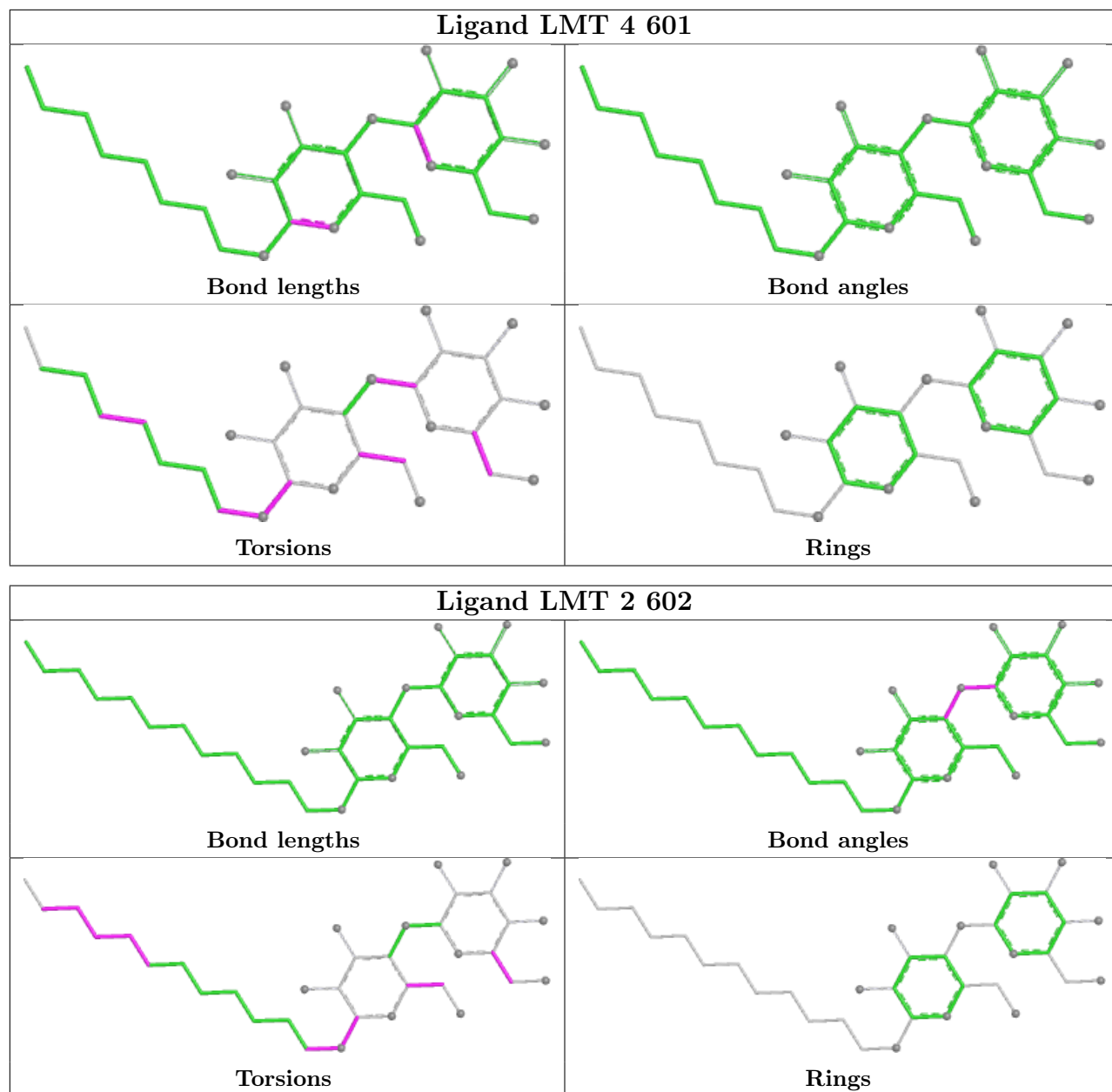
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	1	401	3PE	1	0
28	2	606	PC1	4	0
29	4	601	LMT	2	0
29	2	604	LMT	5	0
28	5	703	PC1	2	0
29	3	202	LMT	4	0
30	S	201	CDL	3	0
29	J	202	LMT	3	0
29	1	404	LMT	1	0
28	1	402	PC1	3	0
27	5	704	3PE	2	0
29	g	101	LMT	3	0
27	i	101	3PE	4	0
30	2	601	CDL	2	0
30	X	201	CDL	1	0
31	Q	201	ZMP	2	0
27	5	706	3PE	2	0
27	5	701	3PE	2	0
30	X	202	CDL	2	0

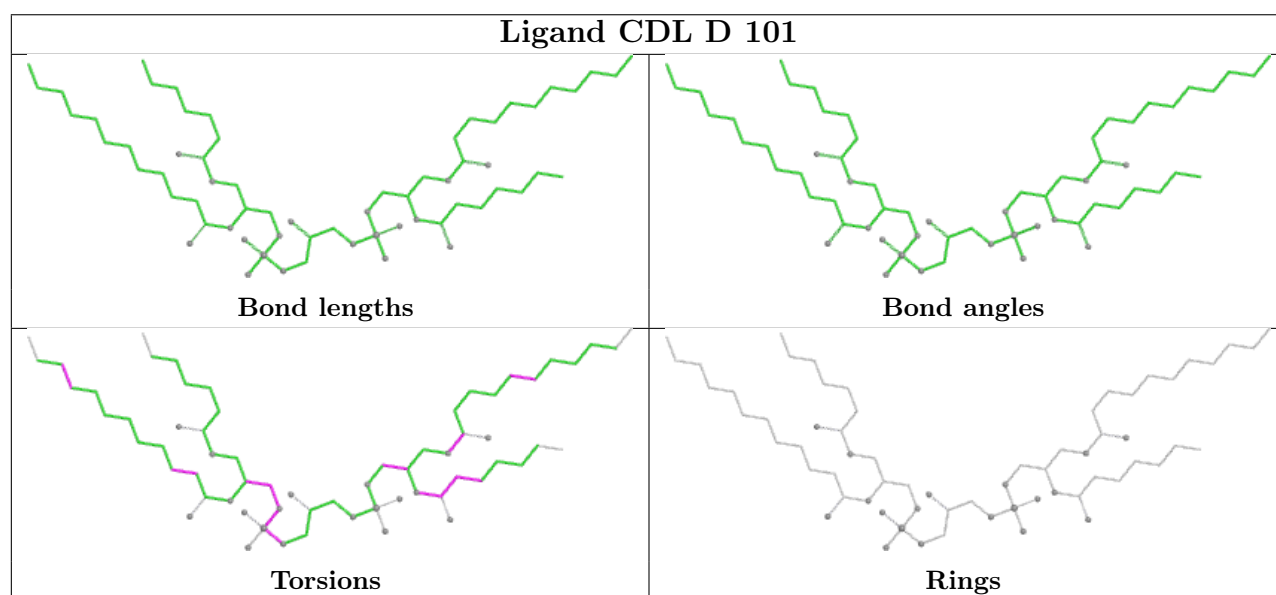
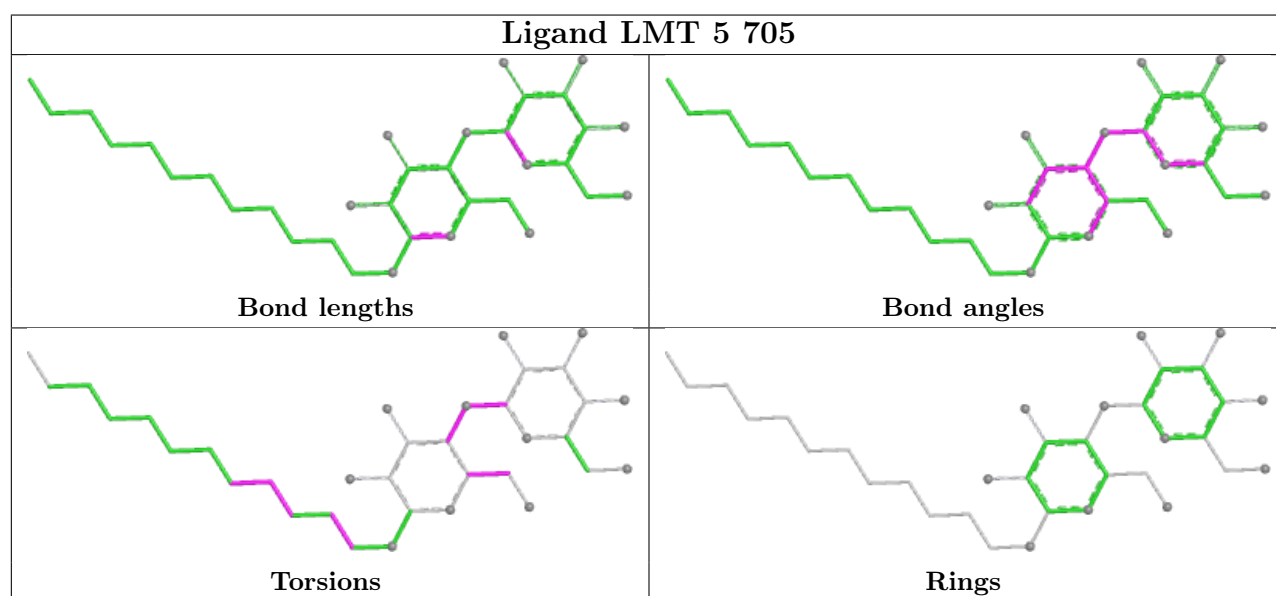
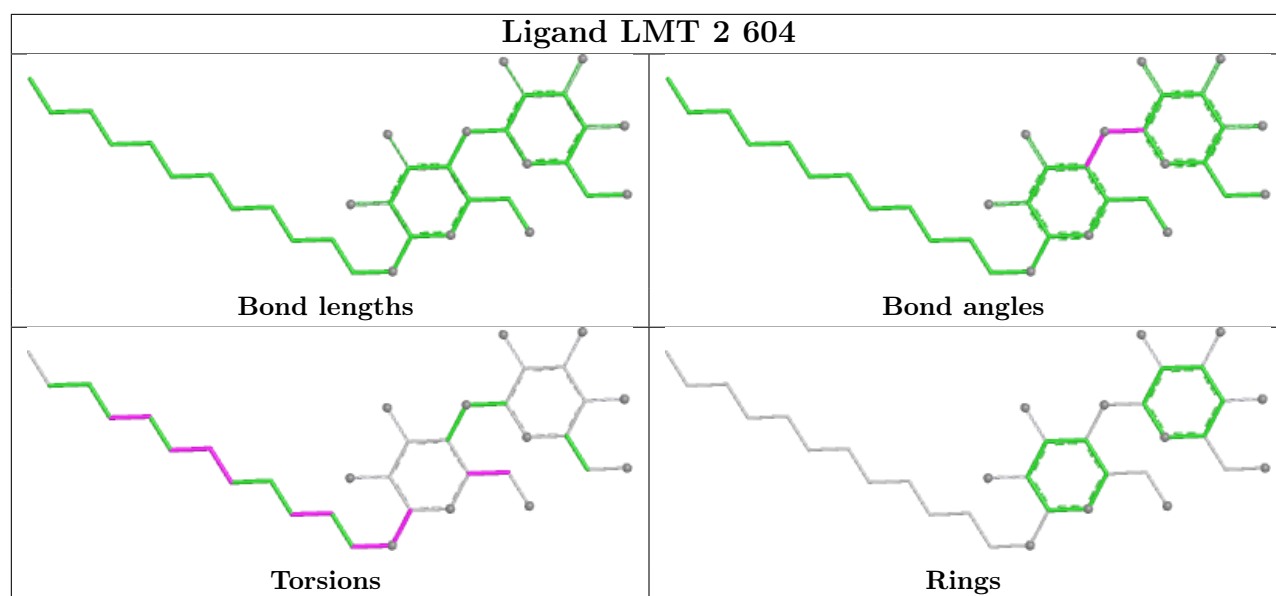
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

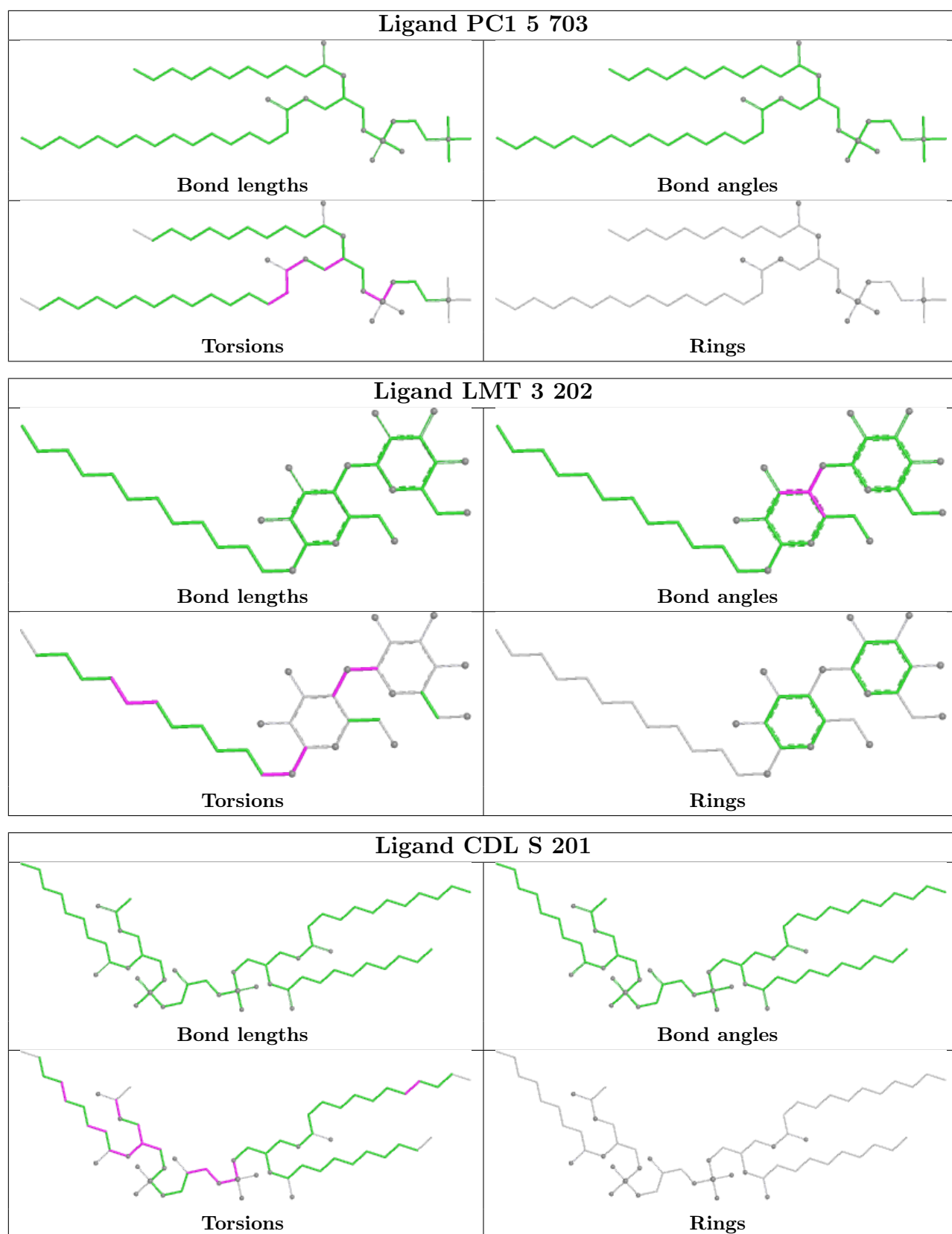


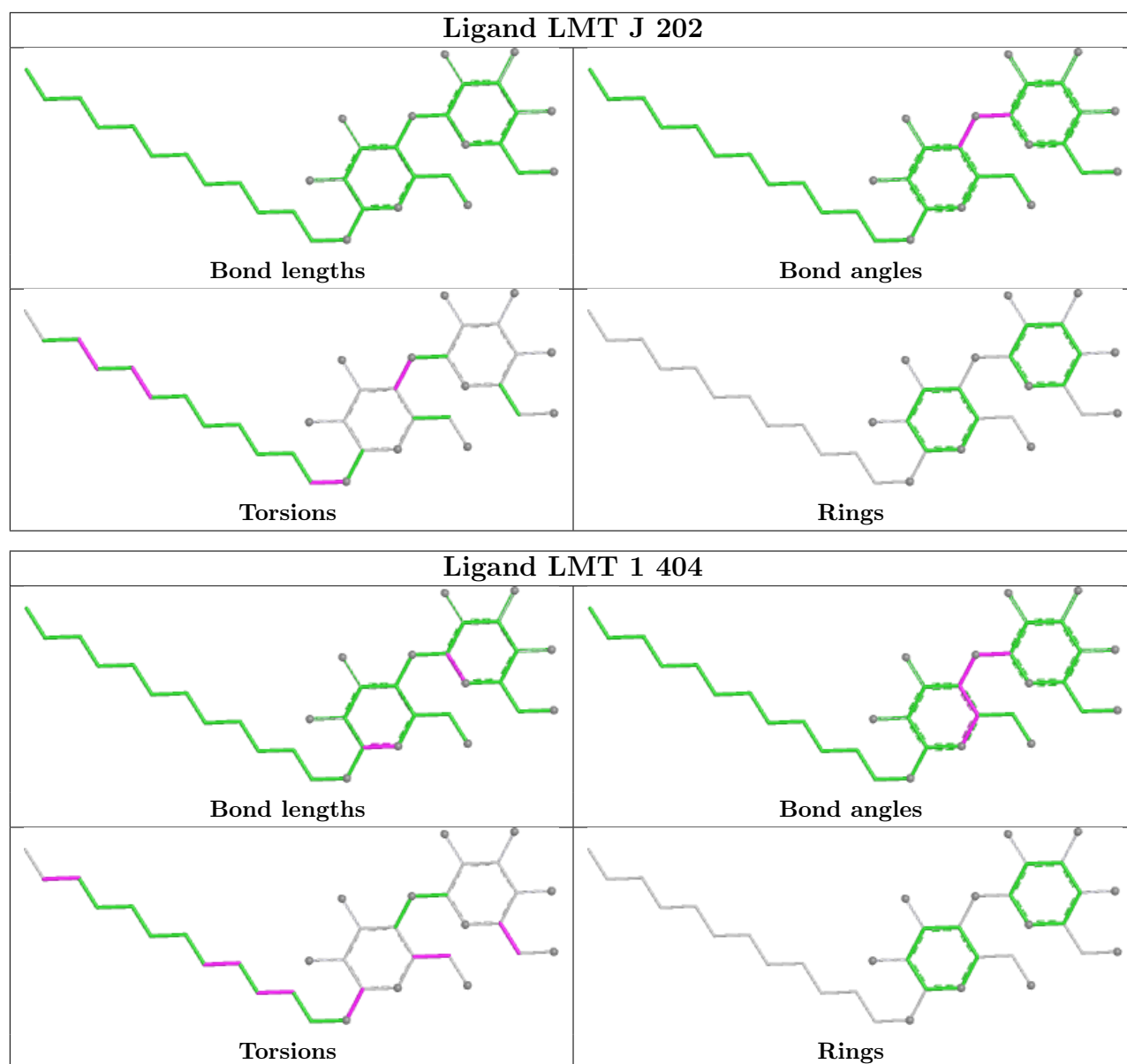


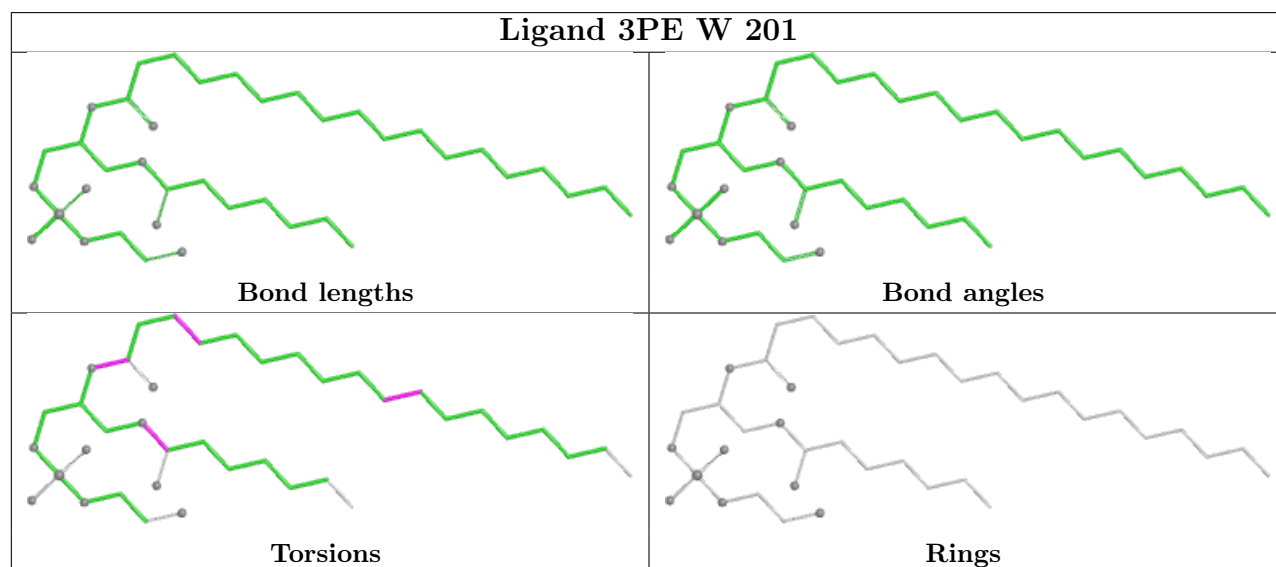
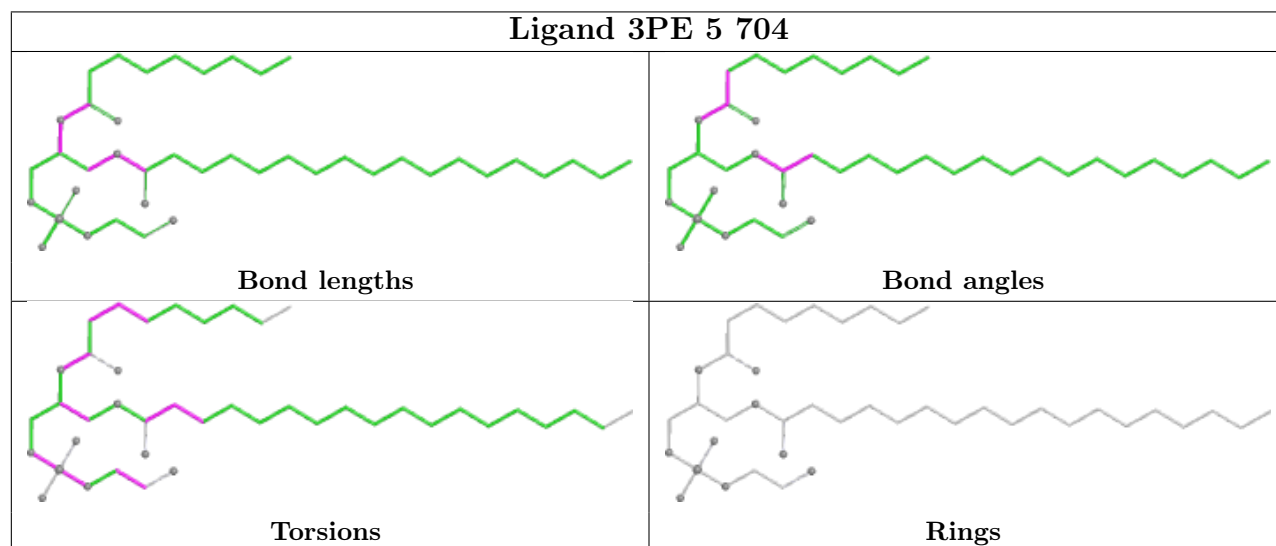
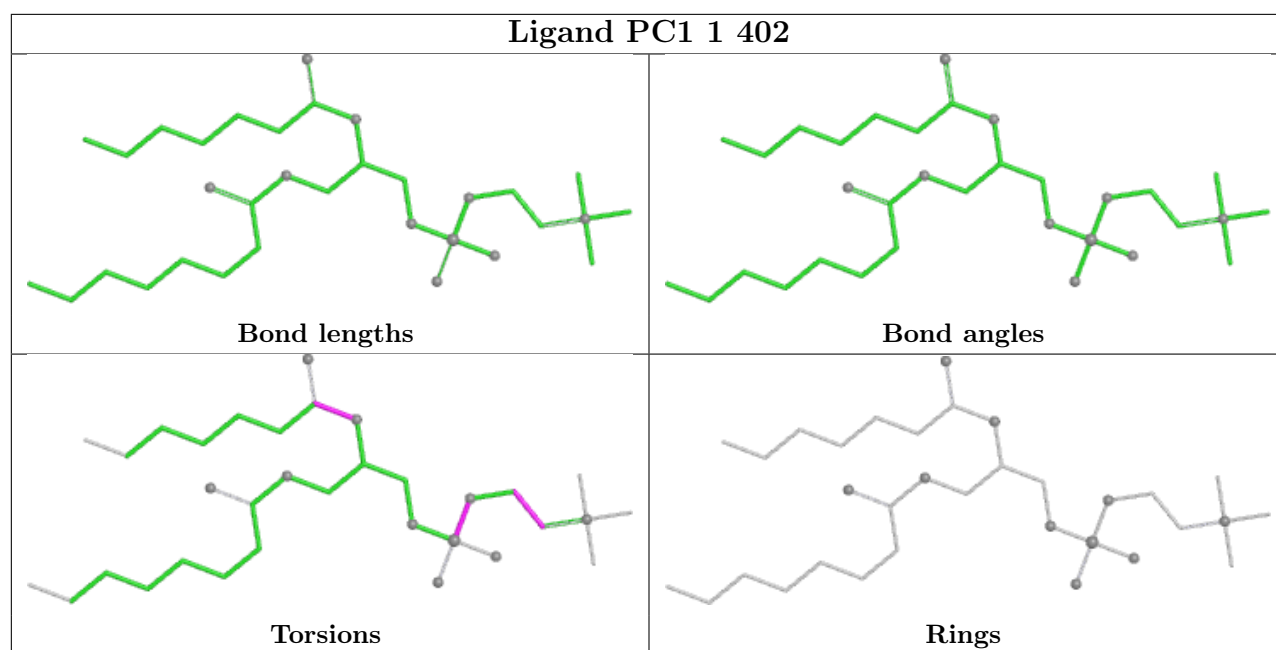


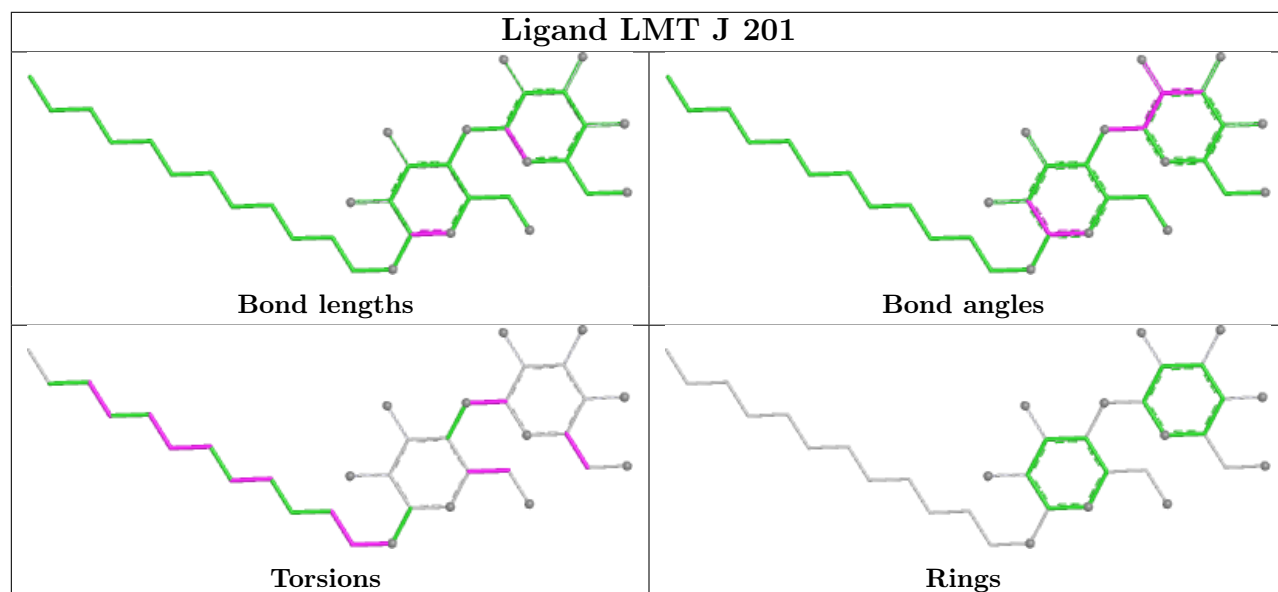
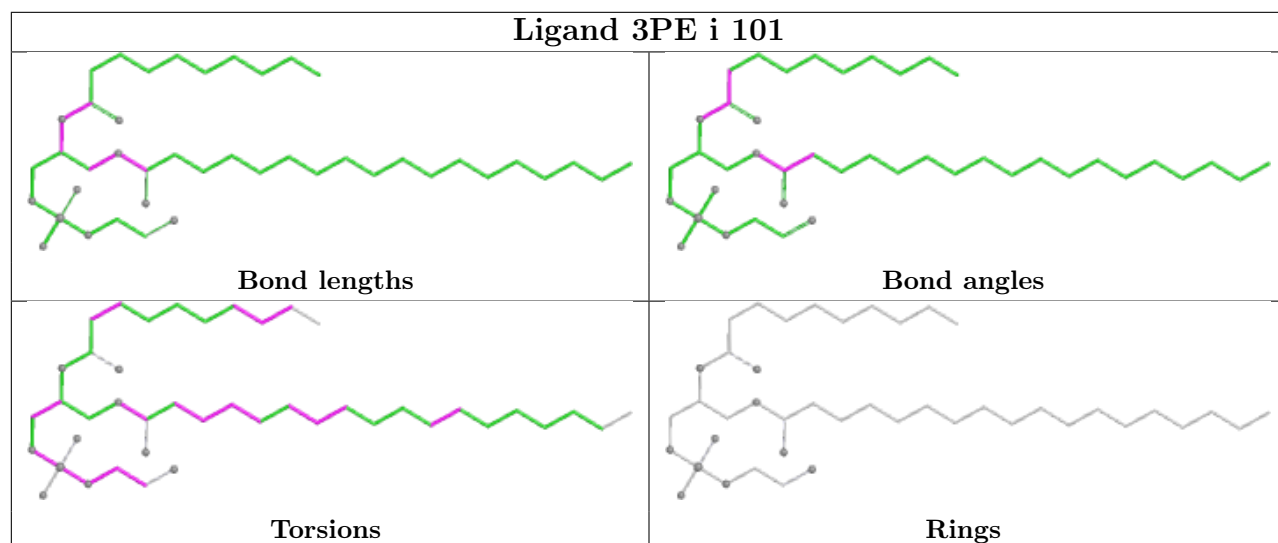
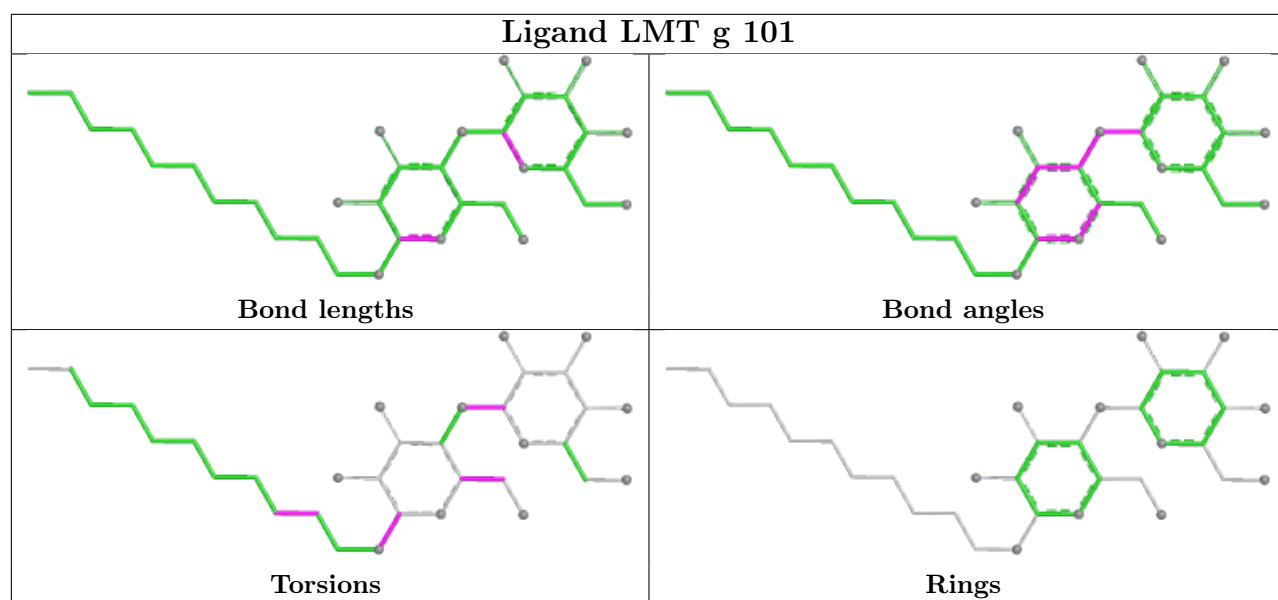


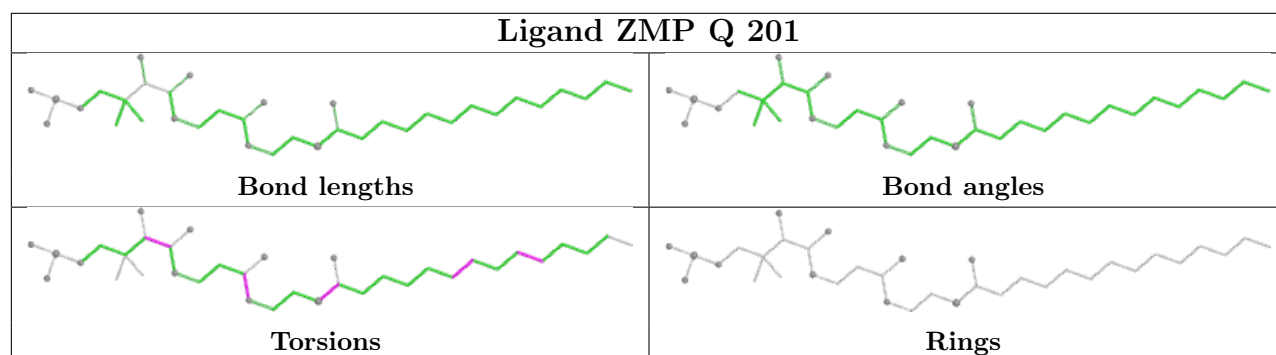
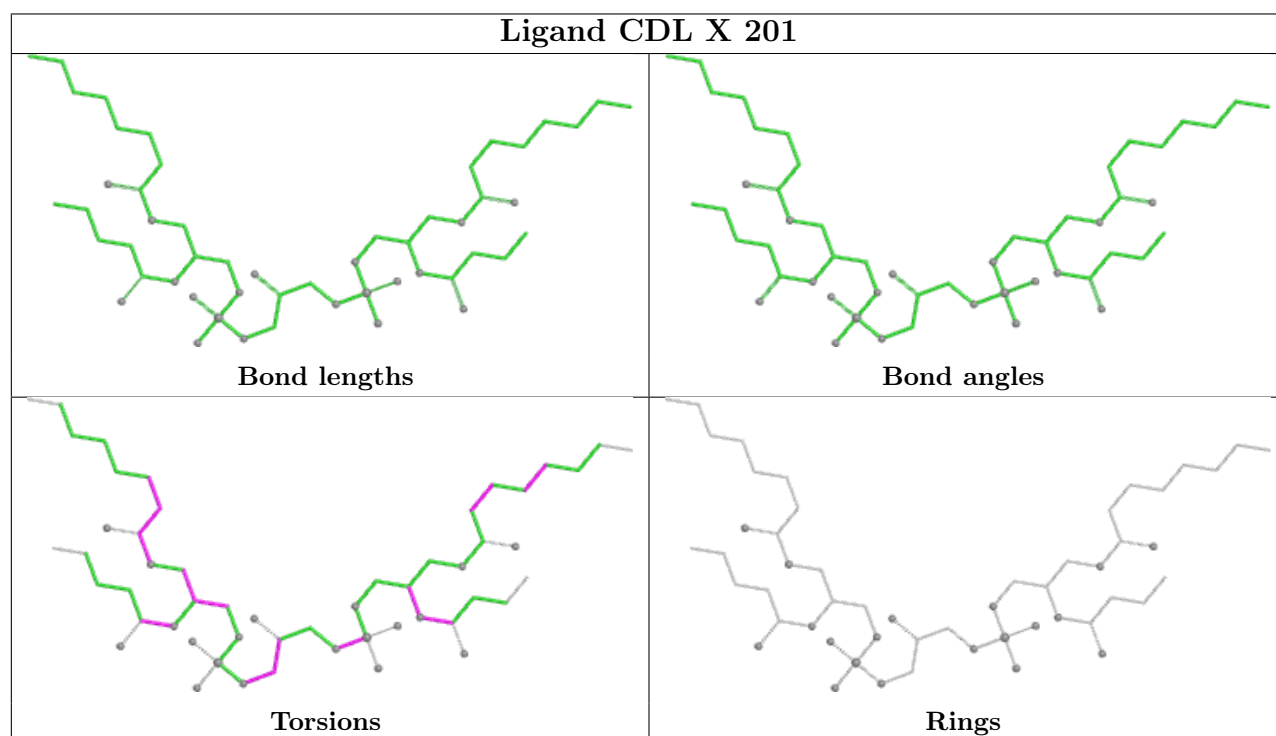
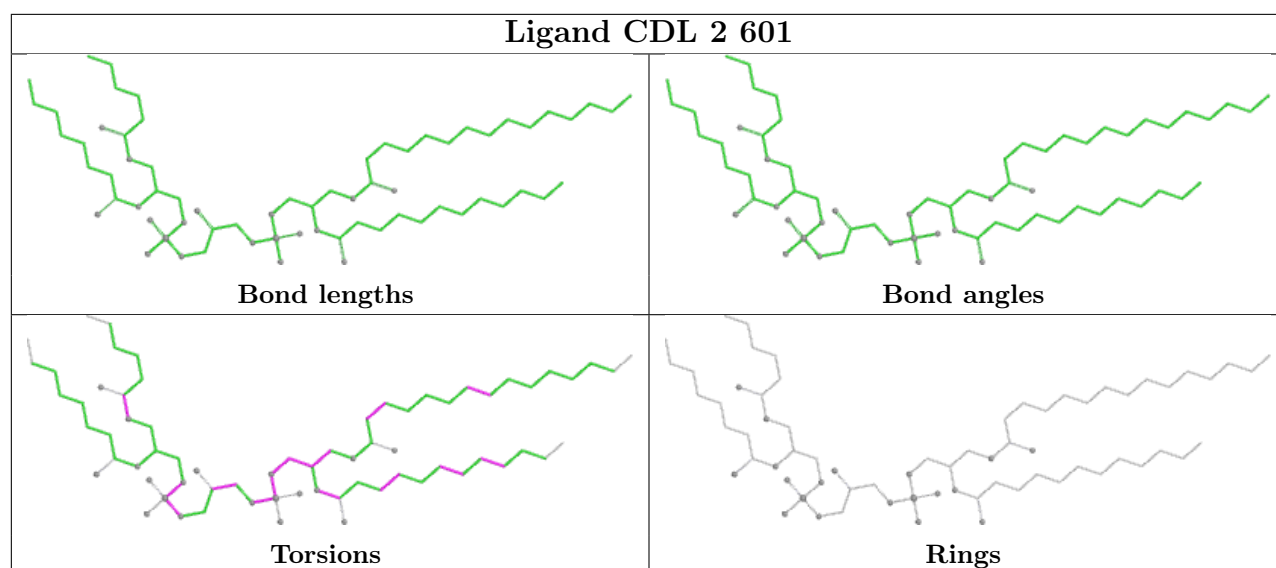


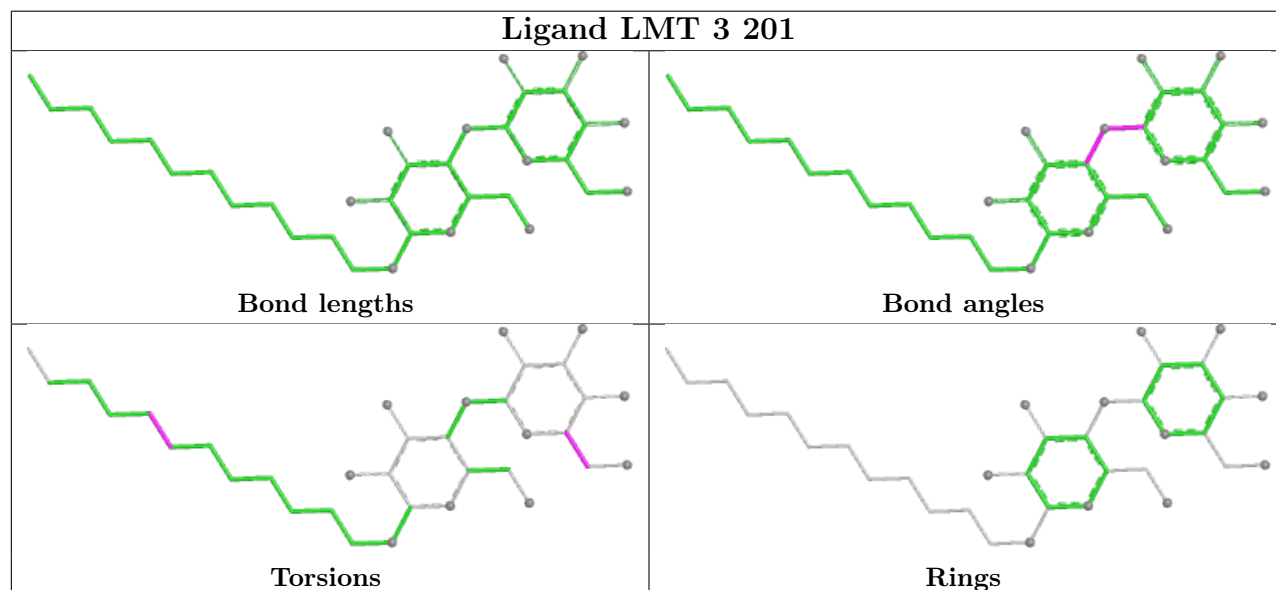
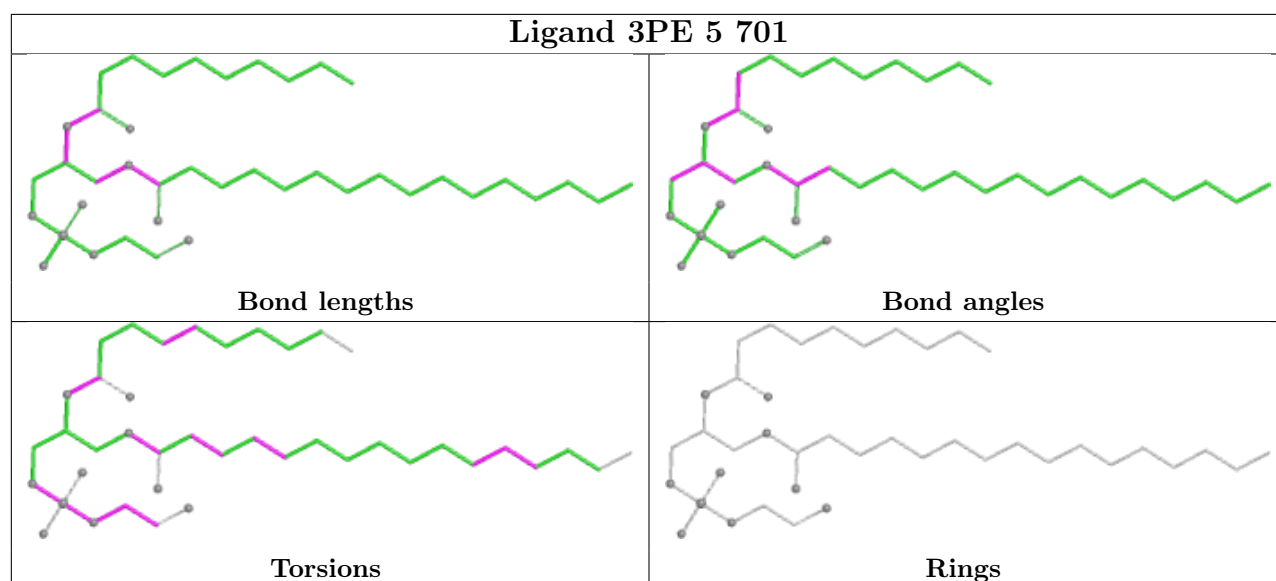
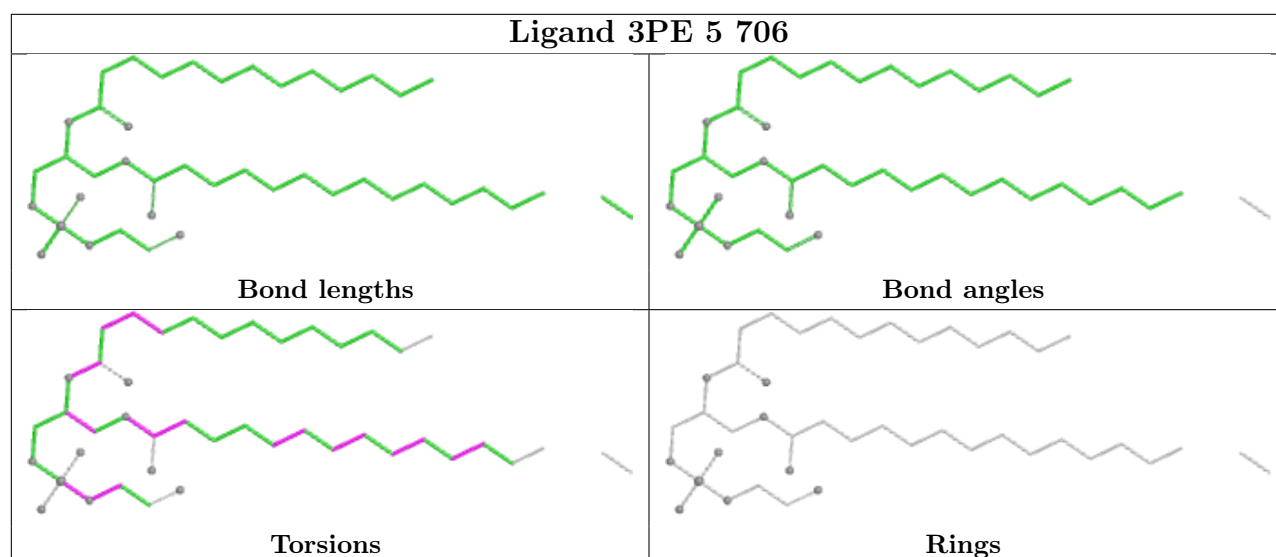


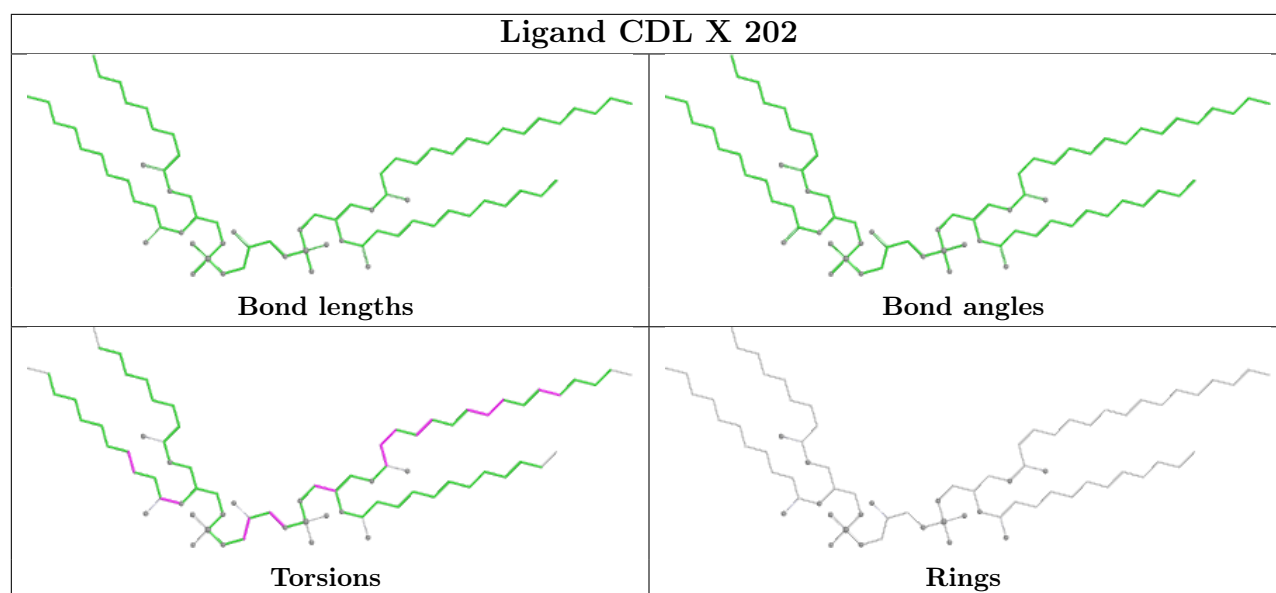












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

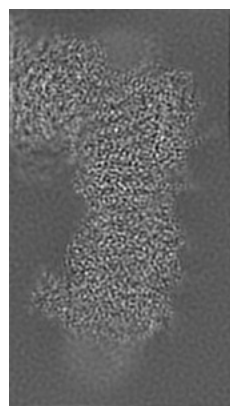
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14792. These allow visual inspection of the internal detail of the map and identification of artifacts.

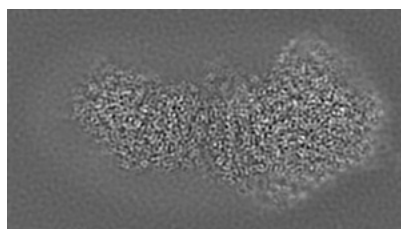
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

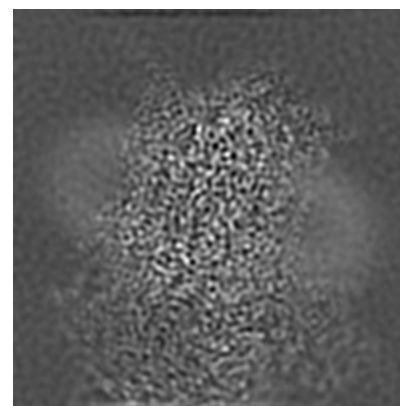
6.1.1 Primary map



X

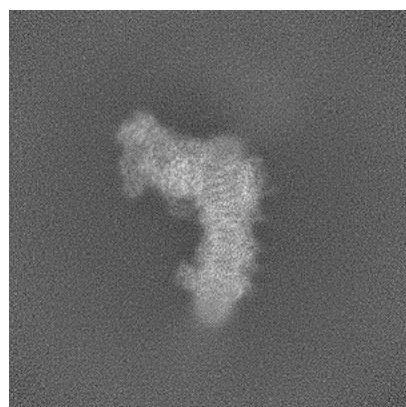


Y

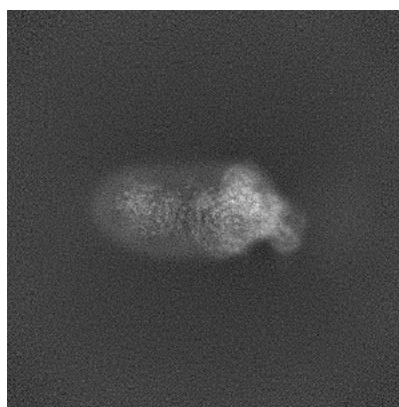


Z

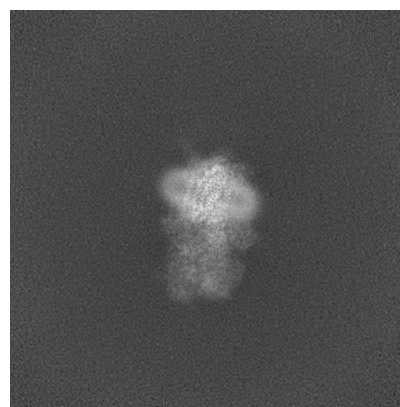
6.1.2 Raw map



X



Y

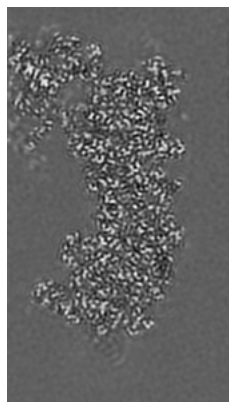


Z

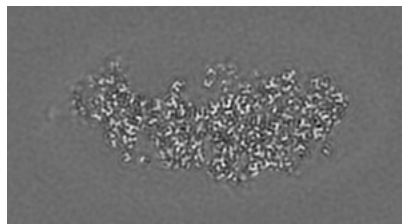
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

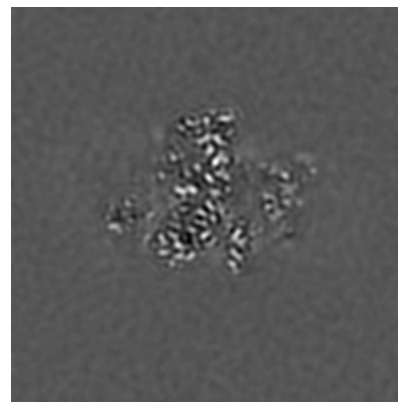
6.2.1 Primary map



X Index: 74

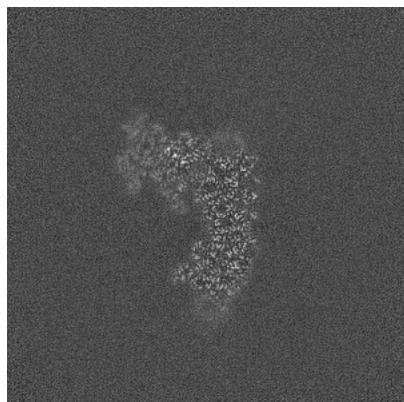


Y Index: 75

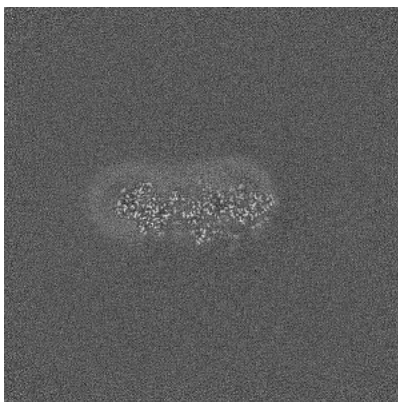


Z Index: 134

6.2.2 Raw map



X Index: 256



Y Index: 256

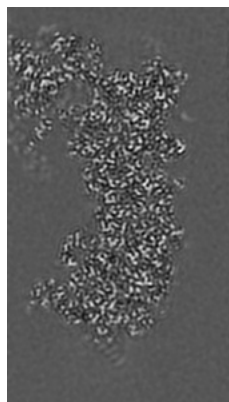


Z Index: 256

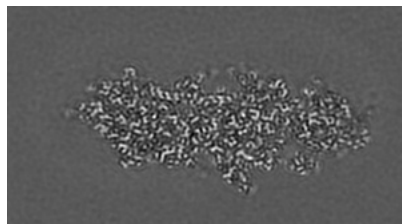
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

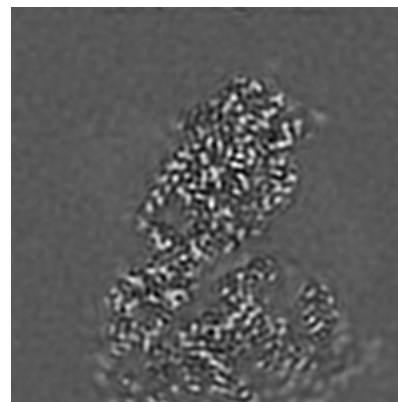
6.3.1 Primary map



X Index: 75

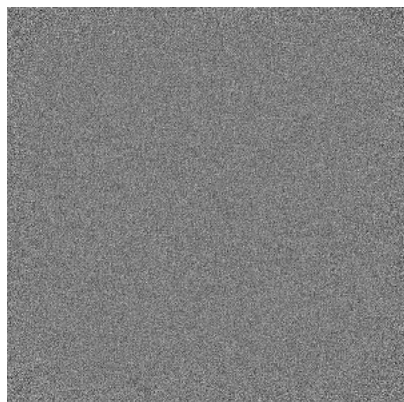


Y Index: 63

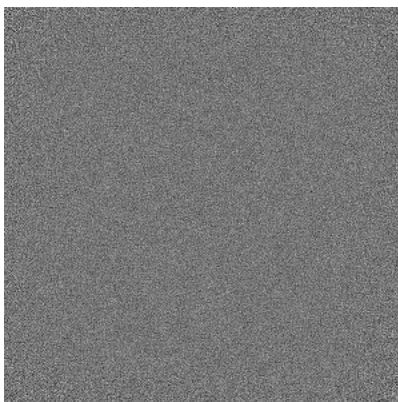


Z Index: 214

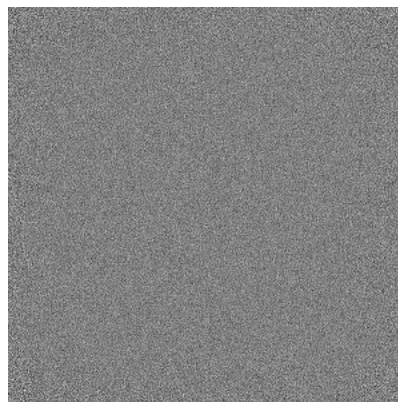
6.3.2 Raw map



X Index: 0



Y Index: 0

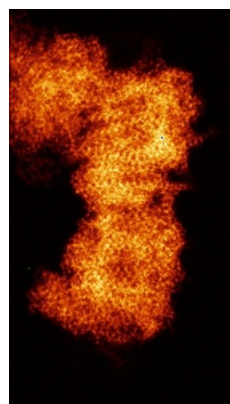


Z Index: 0

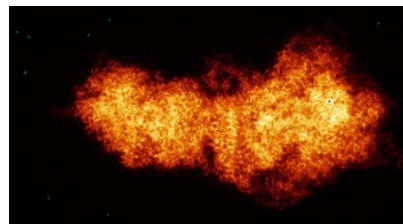
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

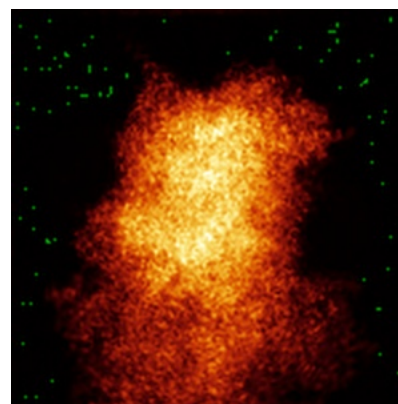
6.4.1 Primary map



X

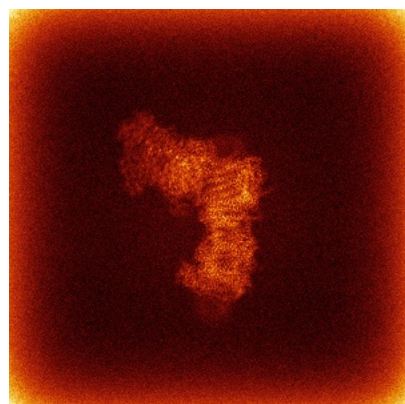


Y

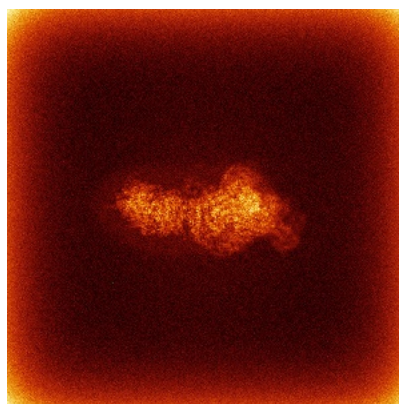


Z

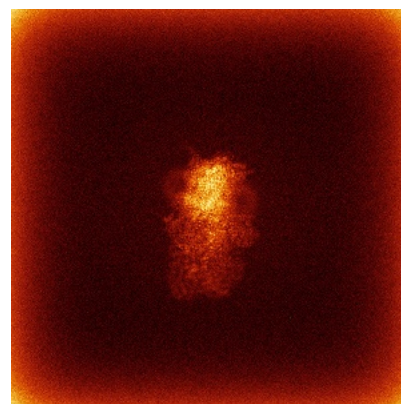
6.4.2 Raw map



X



Y

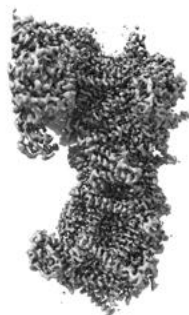


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



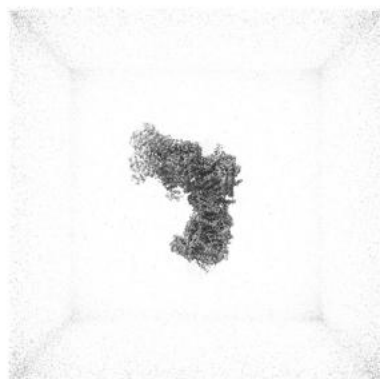
Y



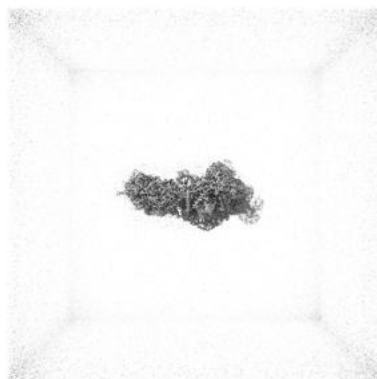
Z

The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

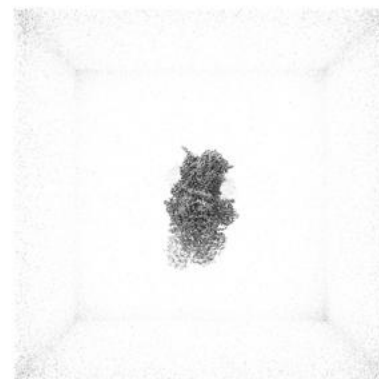
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

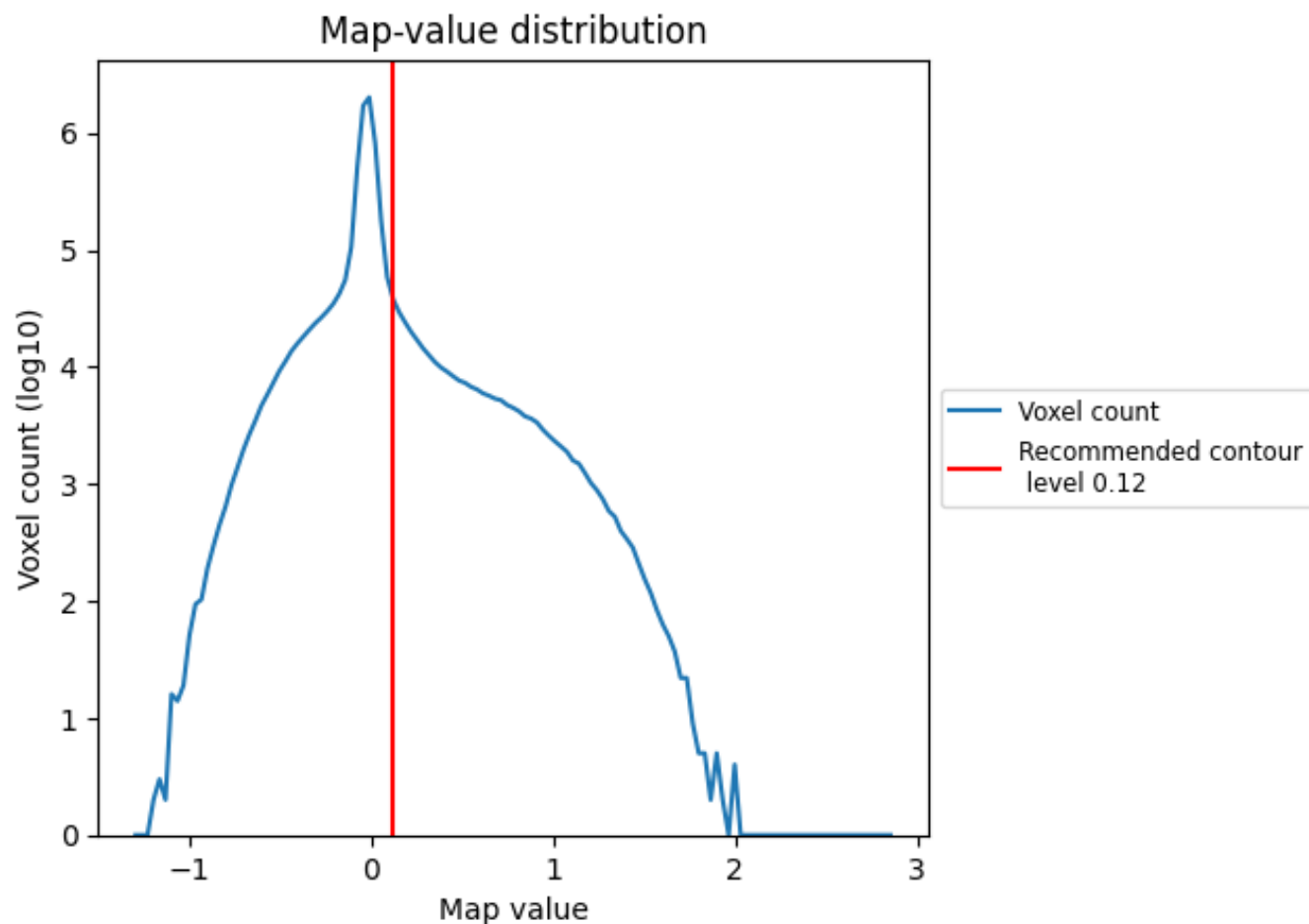
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

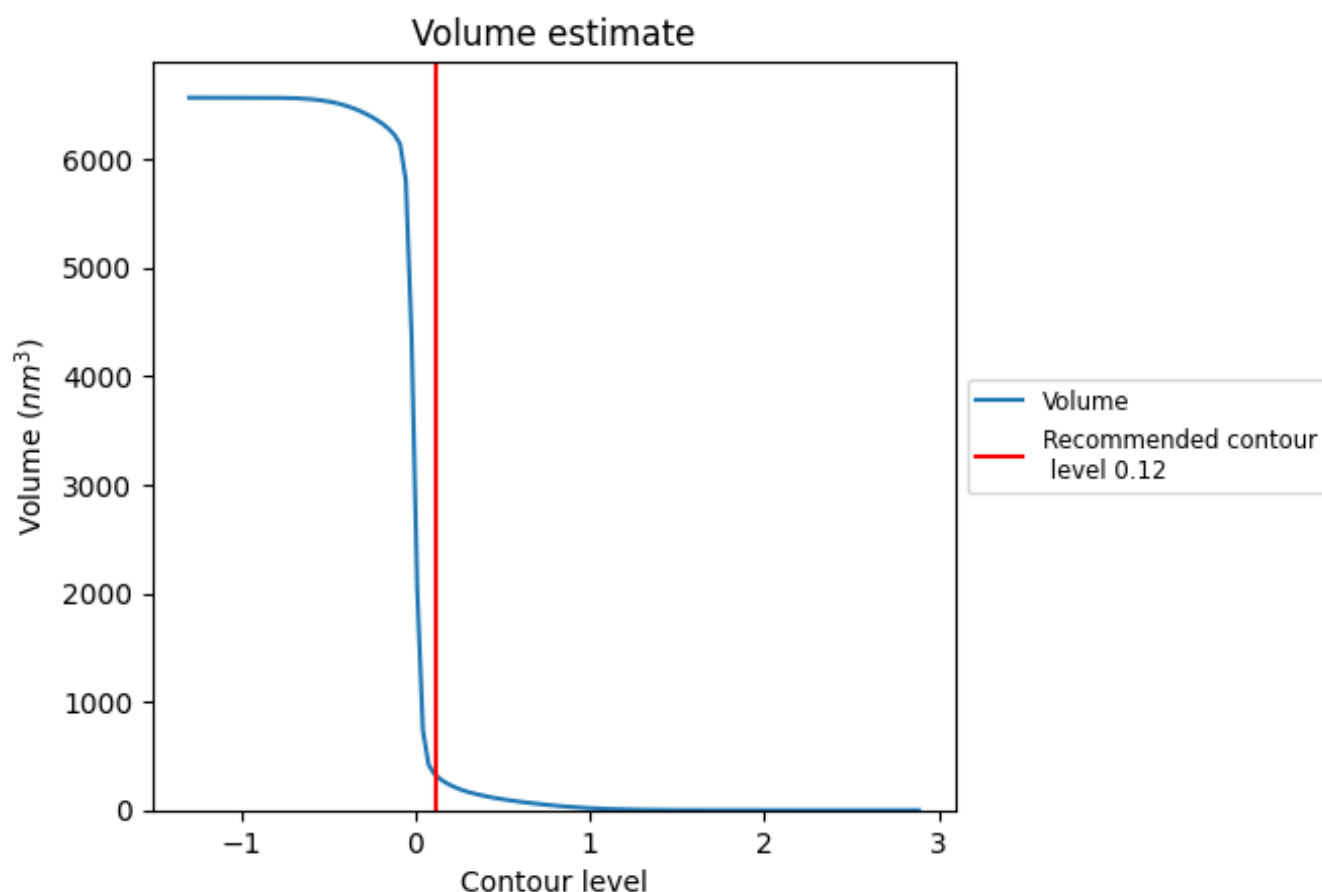
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 319 nm³; this corresponds to an approximate mass of 288 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

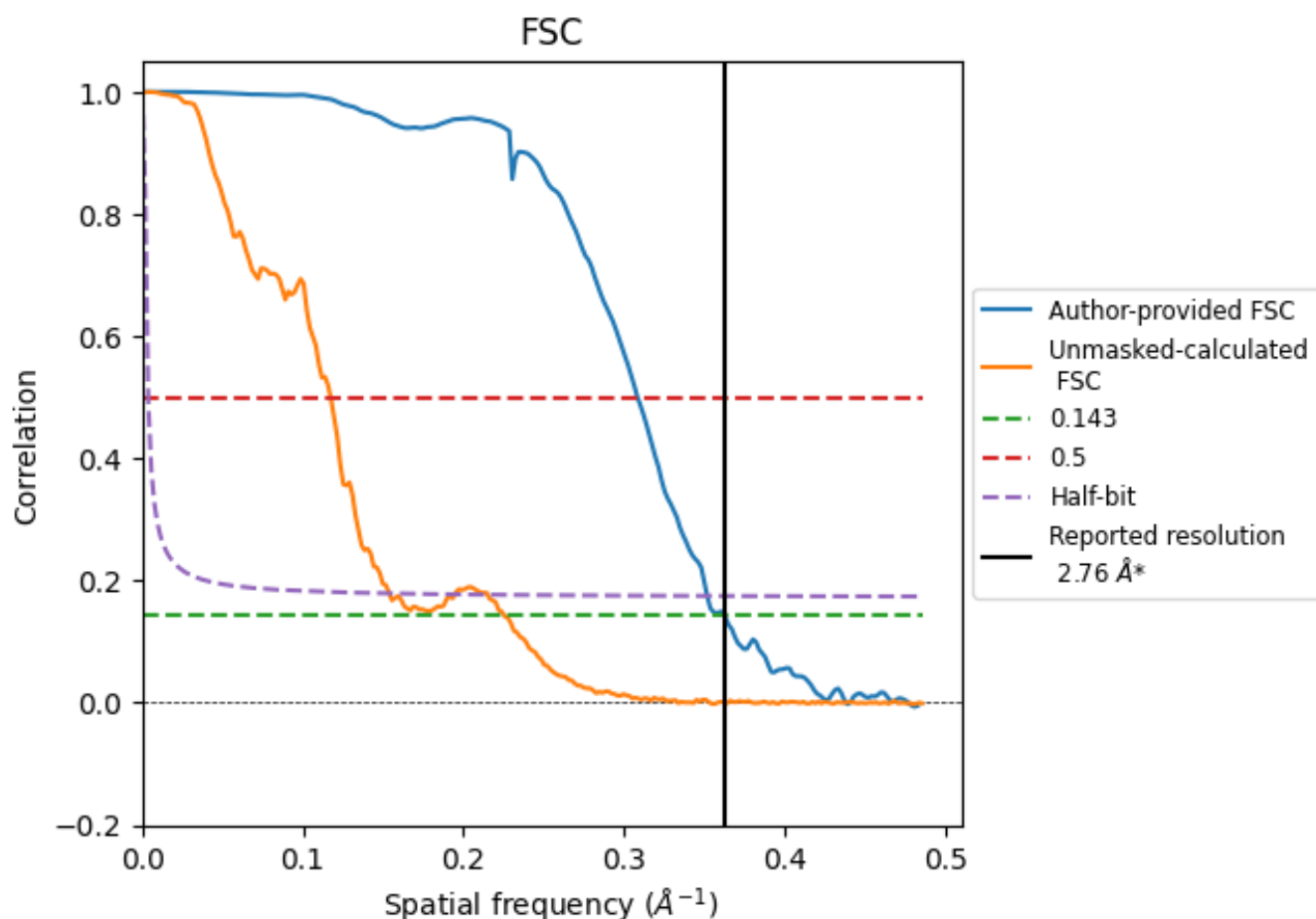
7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.362 Å⁻¹

8.2 Resolution estimates [i](#)

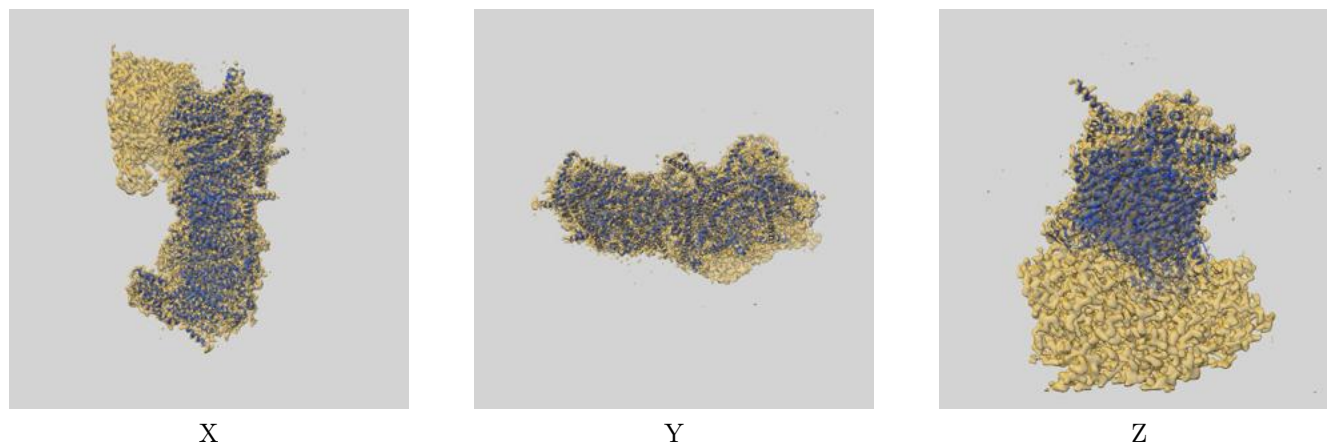
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.76	-	-
Author-provided FSC curve	2.76	3.24	2.84
Unmasked-calculated*	4.44	8.53	6.51

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.44 differs from the reported value 2.76 by more than 10 %

9 Map-model fit [i](#)

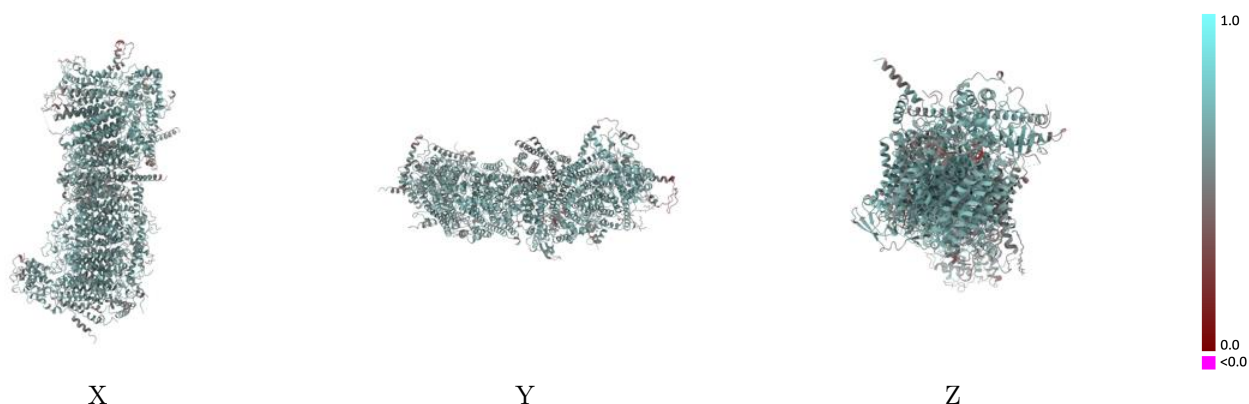
This section contains information regarding the fit between EMDB map EMD-14792 and PDB model 7ZM8. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)

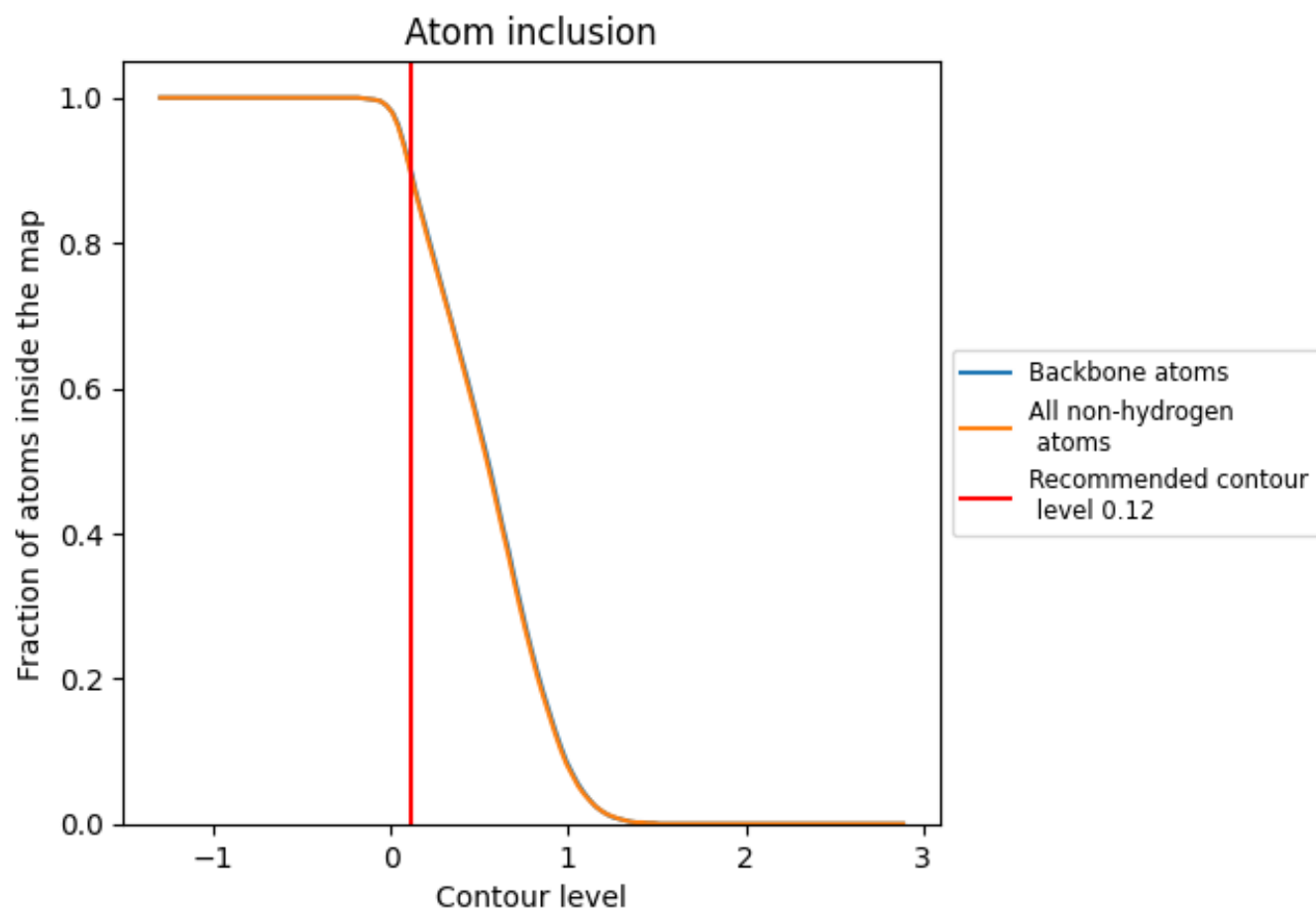


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8900	 0.6040
1	 0.8440	 0.5810
2	 0.9370	 0.6370
3	 0.8260	 0.5680
4	 0.9600	 0.6430
5	 0.9220	 0.6160
6	 0.8880	 0.6040
8	 0.8320	 0.5480
9	 0.8420	 0.5700
D	 0.9250	 0.6300
J	 0.7420	 0.5350
L	 0.9430	 0.6260
Q	 0.8090	 0.5280
R	 0.8560	 0.5780
S	 0.9060	 0.5980
U	 0.9200	 0.6170
W	 0.8590	 0.6000
X	 0.9260	 0.6210
a	 0.8650	 0.5740
b	 0.8710	 0.6010
c	 0.8460	 0.5580
d	 0.9220	 0.6170
e	 0.8060	 0.5490
g	 0.8680	 0.5910
i	 0.8590	 0.5860
j	 0.9400	 0.6250
n	 0.8290	 0.5680

