



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:22 PM UTC

PDB ID : 6J8M / pdb_00006j8m
Title : Low-dose structure of bovine heart cytochrome c oxidase in the fully oxidized state determined using 30 keV X-ray
Authors : Ueno, G.; Shimada, A.; Yamashita, E.; Hasegawa, K.; Kumasaka, T.; Shinzawa-Itoh, K.; Yoshikawa, S.; Tsukihara, T.; Yamamoto, M.
Deposited on : 2019-01-20
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

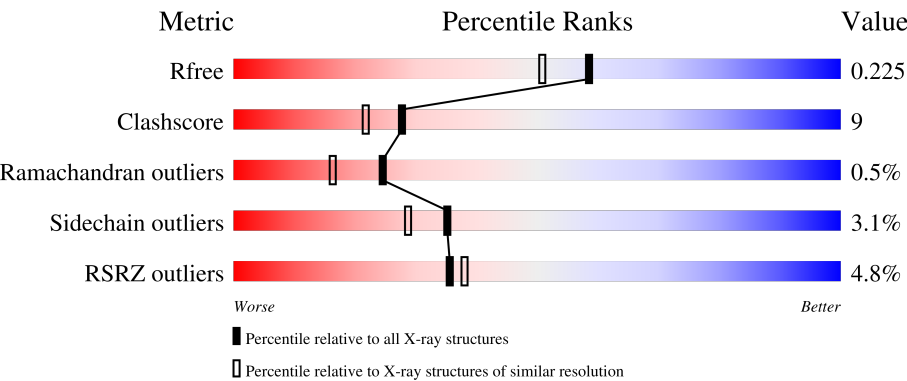
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	514	86%13%.
1	N	514	87%13%.
2	B	227	4%84%14%.
2	O	227	4%76%21%.

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Mol	Chain	Length	Quality of chain
3	C	261	
3	P	261	
4	D	147	
4	Q	147	
5	E	109	
5	R	109	
6	F	98	
6	S	98	
7	G	85	
7	T	85	
8	H	85	
8	U	85	
9	I	73	
9	V	73	
10	J	59	
10	W	59	
11	K	56	
11	X	56	
12	L	47	
12	Y	47	
13	M	46	
13	Z	46	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	PER	A	607[B]	-	-	X	-

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 33893 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	12	0
			4124	2753	638	693	40			
1	N	514	Total	C	N	O	S	0	13	0
			4123	2752	638	693	40			

- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	6	0
			1868	1213	288	348	19			
2	O	227	Total	C	N	O	S	0	5	0
			1870	1215	289	348	18			

- Molecule 3 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	259	Total	C	N	O	S	0	8	0
			2174	1451	345	364	14			
3	P	259	Total	C	N	O	S	0	8	0
			2173	1451	344	363	15			

- Molecule 4 is a protein called Cytochrome c oxidase subunit 4 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	6	0
			1249	814	206	224	5			
4	Q	144	Total	C	N	O	S	0	1	0
			1203	782	197	219	5			

- Molecule 5 is a protein called Cytochrome c oxidase subunit 5A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	105	Total	C	N	O	S	0	1	0
			863	550	148	163	2			
5	R	105	Total	C	N	O	S	0	0	0
			852	544	144	162	2			

- Molecule 6 is a protein called Cytochrome c oxidase subunit 5B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	98	Total	C	N	O	S	0	5	0
			789	489	142	152	6			
6	S	98	Total	C	N	O	S	0	1	0
			755	468	135	147	5			

- Molecule 7 is a protein called Cytochrome c oxidase subunit 6A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
7	G	84	Total 686	C 440	N 130	O 114	P 1	S 1	0	1	0
7	T	84	Total 706	C 454	N 133	O 117	P 1	S 1	0	3	0

- Molecule 8 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	79	Total	C	N	O	S	0	0	0
			662	417	121	119	5			
8	U	79	Total	C	N	O	S	0	0	0
			662	417	121	119	5			

- Molecule 9 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			
9	V	73	Total	C	N	O	S	0	1	0
			609	395	108	101	5			

- Molecule 10 is a protein called Cytochrome c oxidase subunit 7A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	58	Total	C	N	O	S	0	0	0
			460	297	78	82	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	58	Total	C	N	O	S	0	0	0
			460	297	78	82	3			

- Molecule 11 is a protein called Cytochrome c oxidase subunit 7B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	N	O	S	0	1	0
			391	255	66	68	2			
11	X	49	Total	C	N	O	S	0	1	0
			391	255	66	68	2			

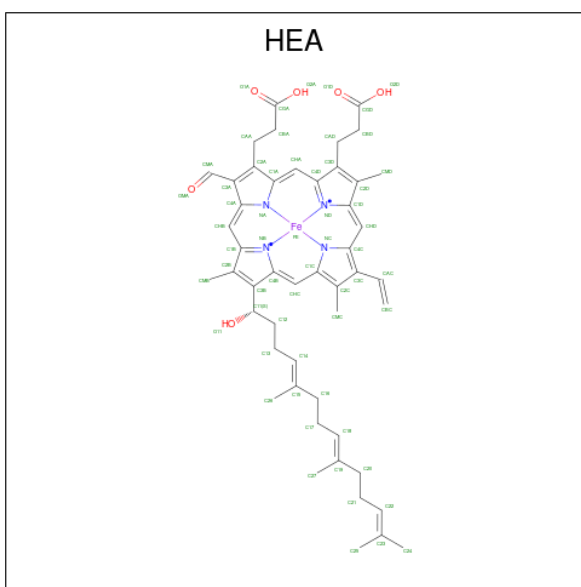
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			380	254	64	60	2			
12	Y	46	Total	C	N	O	S	0	0	0
			380	254	64	60	2			

- Molecule 13 is a protein called Cytochrome c oxidase subunit 8B.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			335	223	53	59			
13	Z	43	Total	C	N	O	0	0	0
			335	223	53	59			

- Molecule 14 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
14	A	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
14	N	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
14	N	1	Total 60	C 49	Fe 1	N 4	O 6	0	0

- Molecule 15 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total	Cu	0	0
			1	1		
15	N	1	Total	Cu	0	0
			1	1		

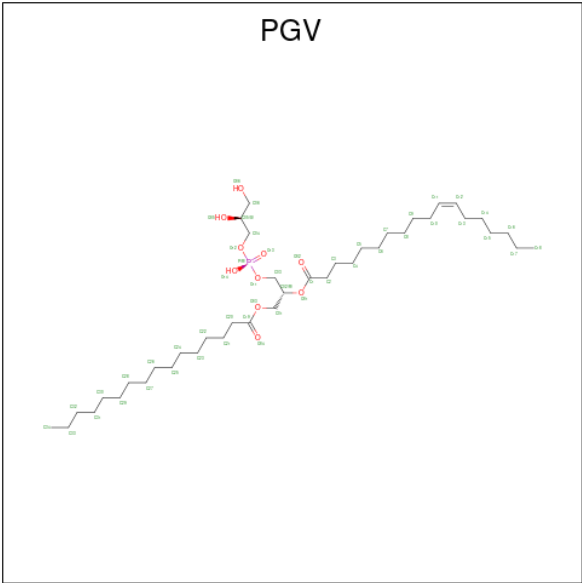
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Mg	0	0
			1	1		
16	N	1	Total	Mg	0	0
			1	1		

- Molecule 17 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Na	0	0
			1	1		
17	C	1	Total	Na	0	0
			1	1		
17	N	1	Total	Na	0	0
			1	1		
17	P	1	Total	Na	0	0
			1	1		

- Molecule 18 is (1R)-2-{{[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



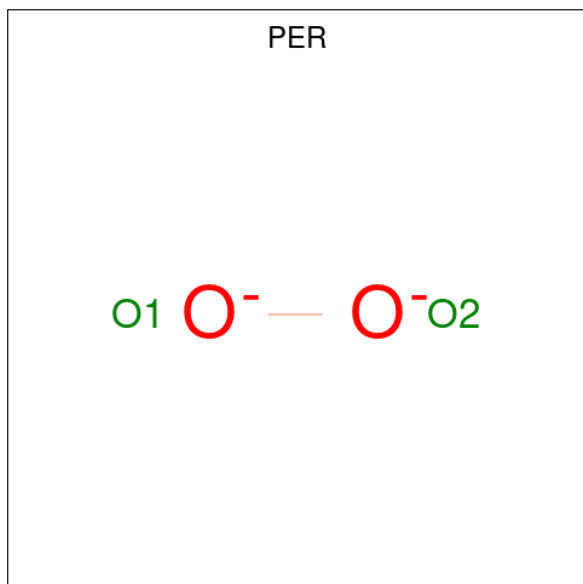
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	A	1	Total	C	O	P	0	0
			51	40	10	1		
18	A	1	Total	C	O	P	0	0
			51	40	10	1		
18	C	1	Total	C	O	P	0	0
			51	40	10	1		
18	C	1	Total	C	O	P	0	0
			51	40	10	1		
18	N	1	Total	C	O	P	0	0
			51	40	10	1		
18	N	1	Total	C	O	P	0	0
			51	40	10	1		
18	P	1	Total	C	O	P	0	0
			51	40	10	1		

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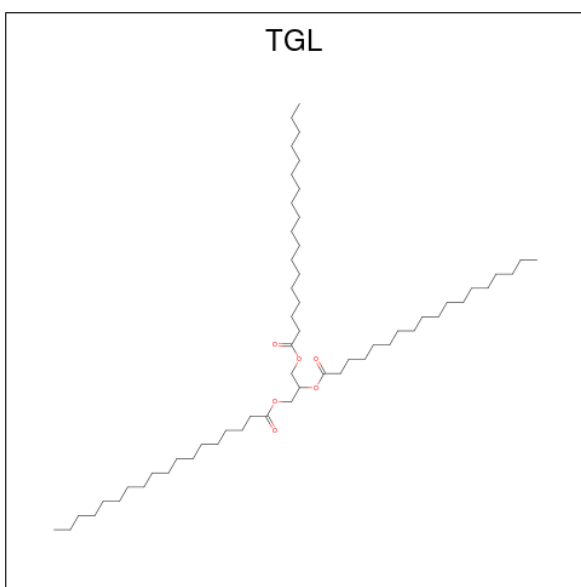
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	P	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 19 is PEROXIDE ION (CCD ID: PER) (formula: O₂).



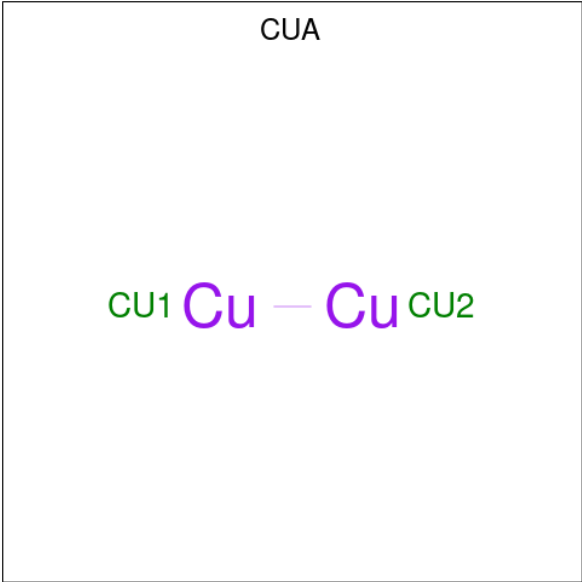
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	1	Total	O	0	1
			4	4		
19	N	1	Total	O	0	1
			4	4		

- Molecule 20 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: C₅₇H₁₁₀O₆).



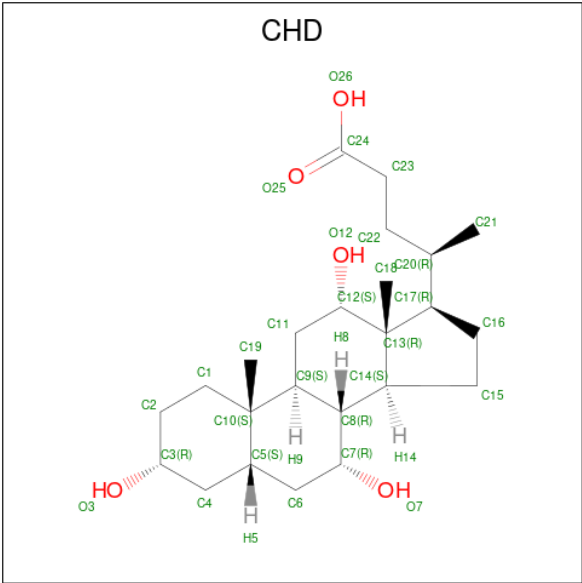
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	B	1	Total	C	O	0	0
			63	57	6		
20	D	1	Total	C	O	0	0
			63	57	6		
20	L	1	Total	C	O	0	0
			63	57	6		
20	N	1	Total	C	O	0	0
			63	57	6		
20	N	1	Total	C	O	0	0
			63	57	6		
20	Q	1	Total	C	O	0	0
			63	57	6		

- Molecule 21 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	B	1	Total	Cu	0	0
			2	2		
21	O	1	Total	Cu	0	0
			2	2		

- Molecule 22 is CHOLIC ACID (CCD ID: CHD) (formula: C₂₄H₄₀O₅).



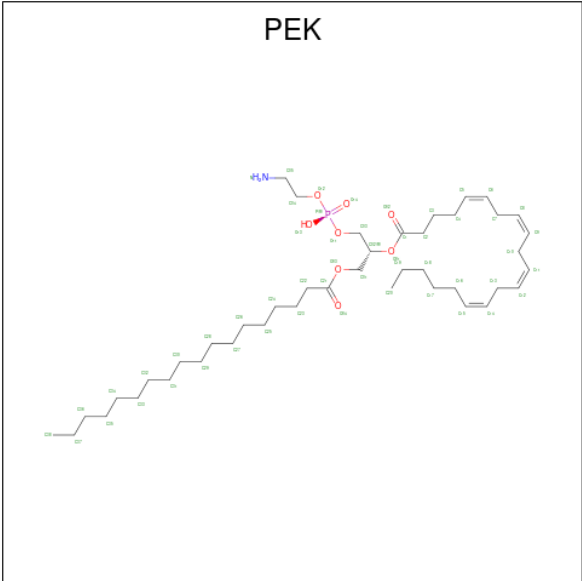
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	B	1	Total	C	O	0
			29	24	5	
22	C	1	Total	C	O	0
			29	24	5	

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	C	1	Total	C	O	0	0
			29	24	5		
22	J	1	Total	C	O	0	0
			29	24	5		
22	N	1	Total	C	O	0	0
			29	24	5		
22	O	1	Total	C	O	0	0
			29	24	5		
22	P	1	Total	C	O	0	0
			29	24	5		
22	W	1	Total	C	O	0	0
			29	24	5		

- Molecule 23 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (CCD ID: PEK) (formula: C₄₃H₇₈NO₈P).



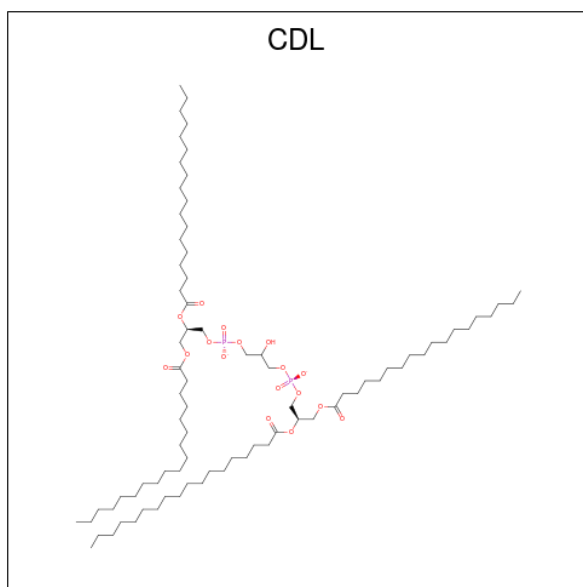
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

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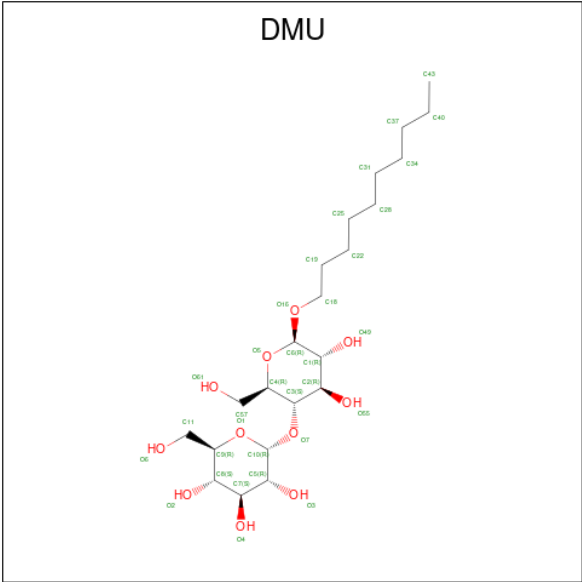
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 24 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



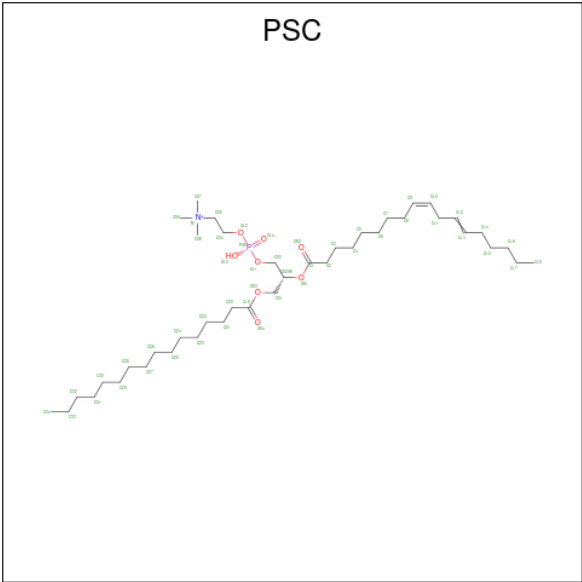
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	C	1	Total	C	O	P		0	0
			100	81	17	2			
24	G	1	Total	C	O	P		0	0
			100	81	17	2			
24	P	1	Total	C	O	P		0	0
			100	81	17	2			
24	T	1	Total	C	O	P		0	0
			100	81	17	2			

- Molecule 25 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: $C_{22}H_{42}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	C	1	Total	C	O	0	0
			33	22	11		
25	M	1	Total	C	O	0	0
			33	22	11		
25	P	1	Total	C	O	0	0
			33	22	11		
25	Z	1	Total	C	O	0	0
			33	22	11		

- Molecule 26 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (CCD ID: PSC) (formula: C₄₂H₈₁NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	E	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
26	R	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 27 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	F	1	Total	Zn	0	0
			1	1		
27	S	1	Total	Zn	0	0
			1	1		

- Molecule 28 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	270	Total	O	0	0
			270	270		
28	B	206	Total	O	0	0
			206	206		
28	C	145	Total	O	0	0
			145	145		
28	D	167	Total	O	0	0
			167	167		
28	E	113	Total	O	0	0
			113	113		
28	F	137	Total	O	0	0
			137	137		
28	G	77	Total	O	0	0
			77	77		
28	H	83	Total	O	0	0
			83	83		
28	I	50	Total	O	0	0
			50	50		
28	J	42	Total	O	0	0
			42	42		
28	K	44	Total	O	0	0
			44	44		
28	L	36	Total	O	0	0
			36	36		
28	M	28	Total	O	0	0
			28	28		
28	N	266	Total	O	0	0
			266	266		

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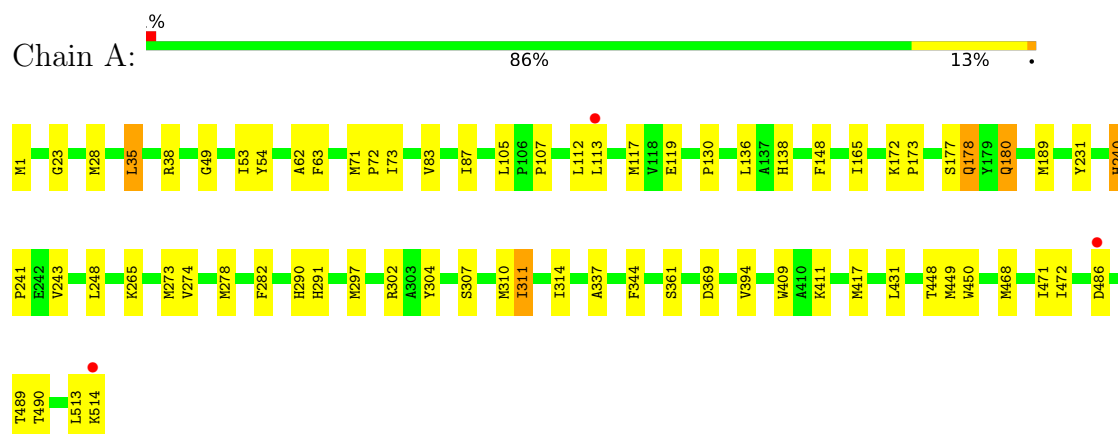
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	O	168	Total 168	O 168	0	0
28	P	138	Total 138	O 138	0	0
28	Q	84	Total 84	O 84	0	0
28	R	91	Total 91	O 91	0	0
28	S	126	Total 126	O 126	0	0
28	T	62	Total 62	O 62	0	0
28	U	68	Total 68	O 68	0	0
28	V	41	Total 41	O 41	0	0
28	W	44	Total 44	O 44	0	0
28	X	28	Total 28	O 28	0	0
28	Y	24	Total 24	O 24	0	0
28	Z	20	Total 20	O 20	0	0

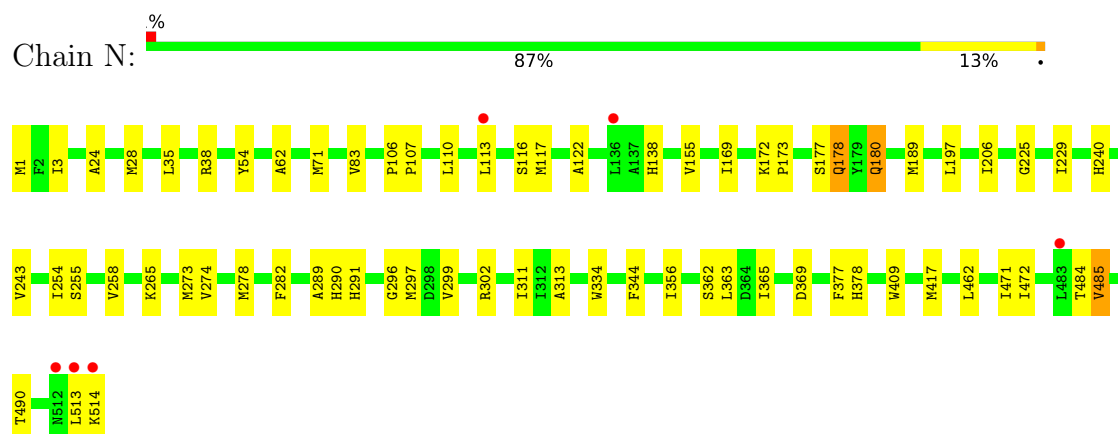
3 Residue-property plots

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 electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

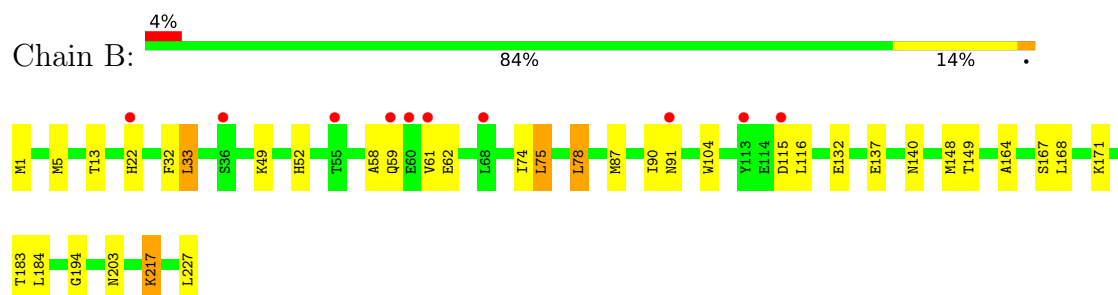
• Molecule 1: Cytochrome c oxidase subunit 1



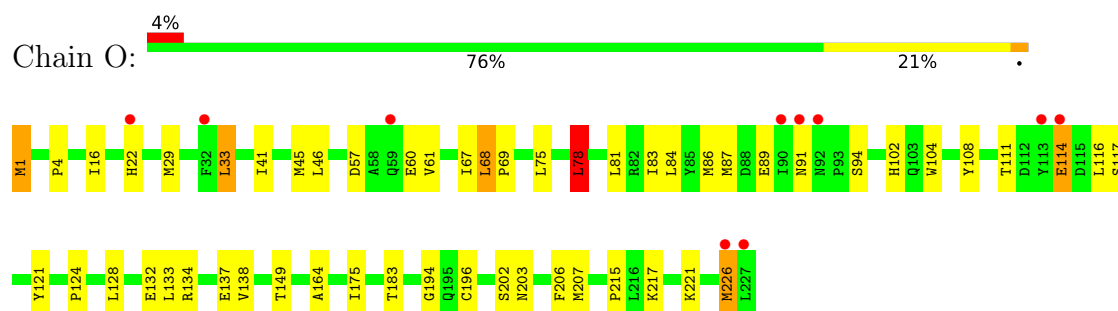
• Molecule 1: Cytochrome c oxidase subunit 1



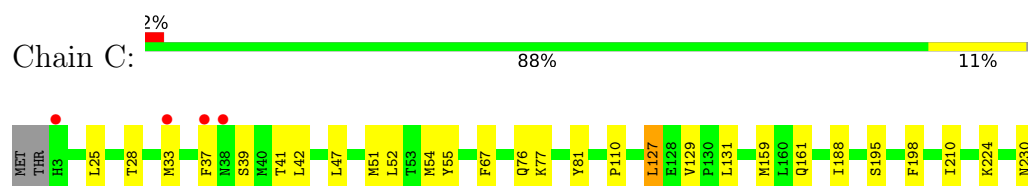
• Molecule 2: Cytochrome c oxidase subunit 2



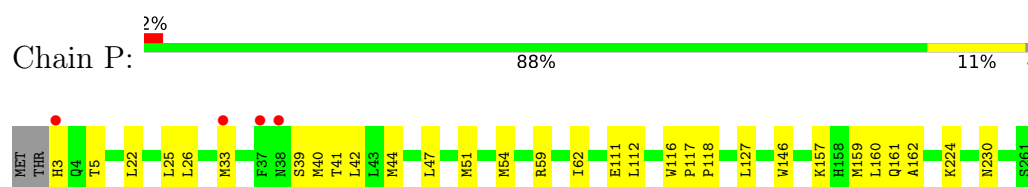
- Molecule 2: Cytochrome c oxidase subunit 2



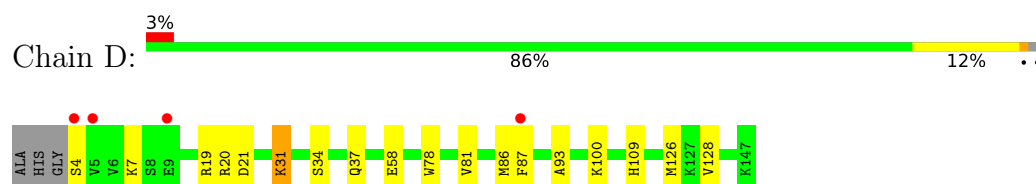
- Molecule 3: Cytochrome c oxidase subunit 3



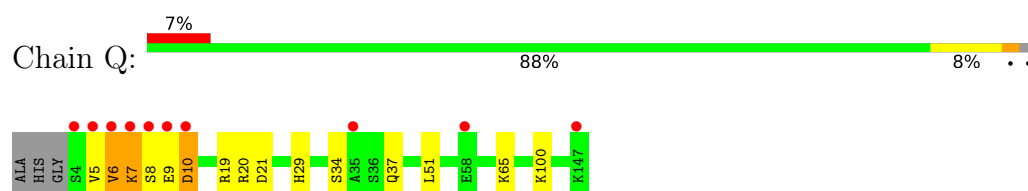
- Molecule 3: Cytochrome c oxidase subunit 3



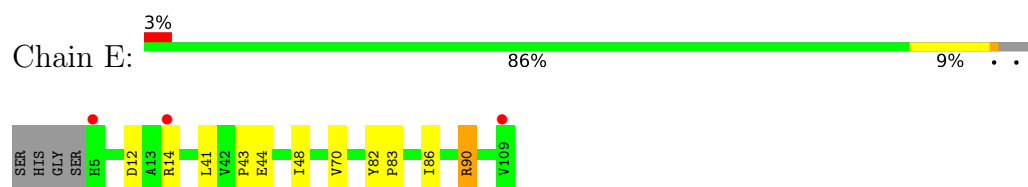
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



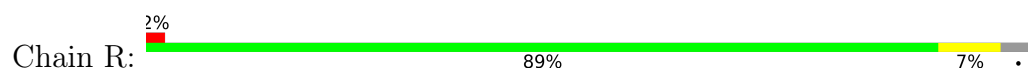
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



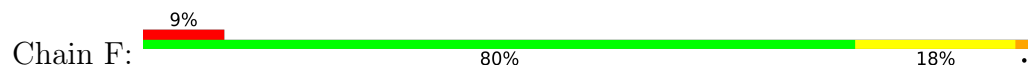
- Molecule 5: Cytochrome c oxidase subunit 5A



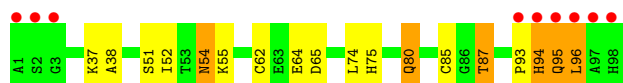
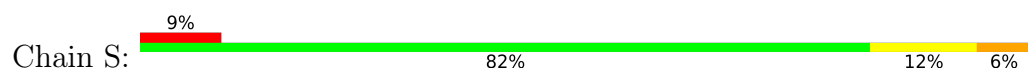
- Molecule 5: Cytochrome c oxidase subunit 5A



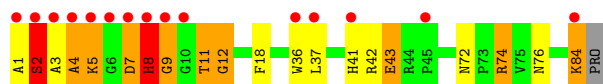
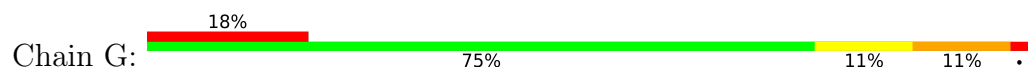
- Molecule 6: Cytochrome c oxidase subunit 5B



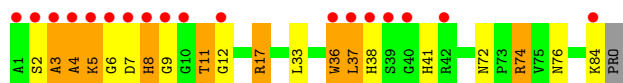
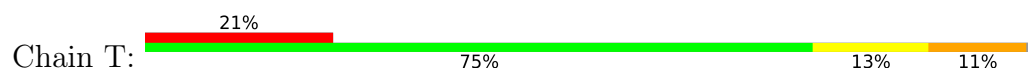
- Molecule 6: Cytochrome c oxidase subunit 5B



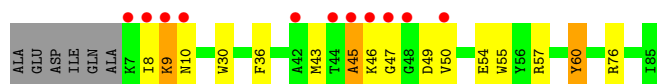
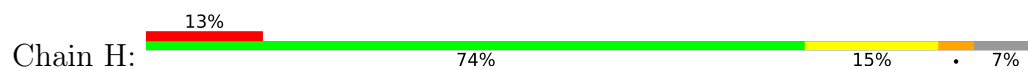
- Molecule 7: Cytochrome c oxidase subunit 6A2



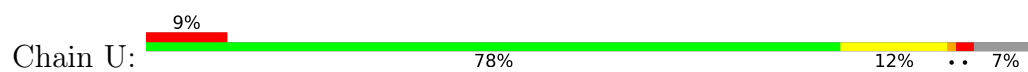
- Molecule 7: Cytochrome c oxidase subunit 6A2



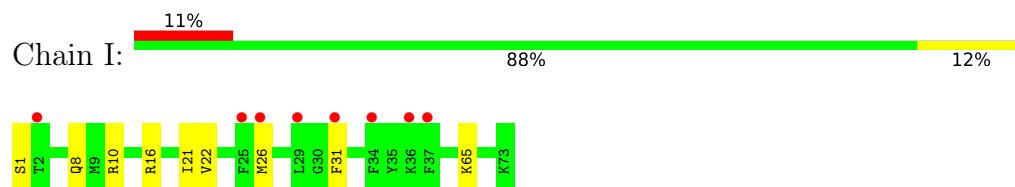
- Molecule 8: Cytochrome c oxidase subunit 6B1



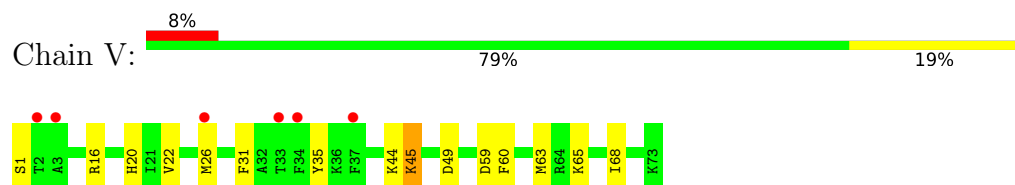
- Molecule 8: Cytochrome c oxidase subunit 6B1



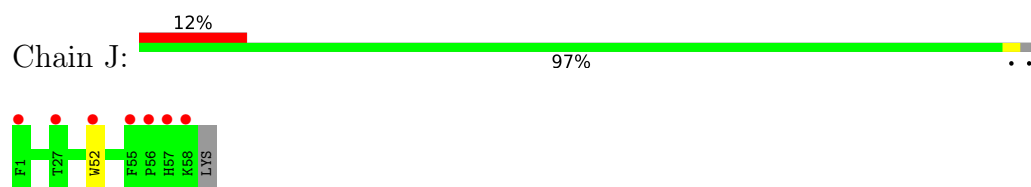
• Molecule 9: Cytochrome c oxidase subunit 6C



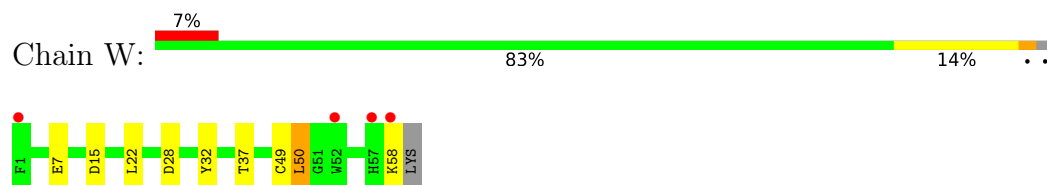
• Molecule 9: Cytochrome c oxidase subunit 6C



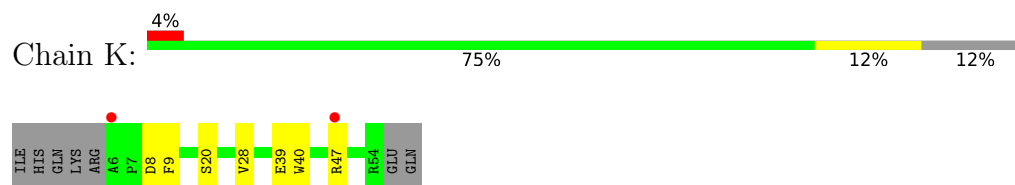
• Molecule 10: Cytochrome c oxidase subunit 7A1



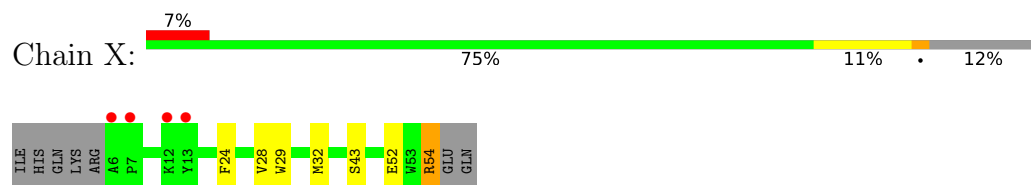
• Molecule 10: Cytochrome c oxidase subunit 7A1



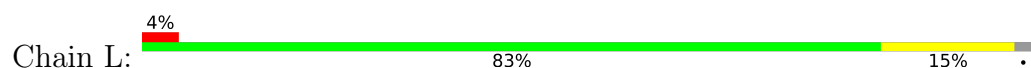
• Molecule 11: Cytochrome c oxidase subunit 7B



• Molecule 11: Cytochrome c oxidase subunit 7B

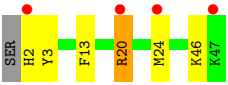
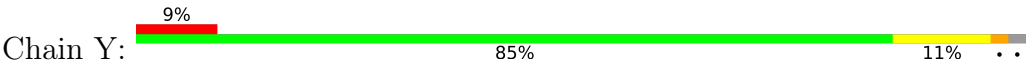


• Molecule 12: Cytochrome c oxidase subunit 7C

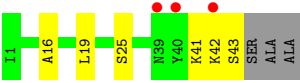
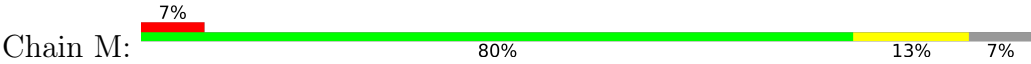




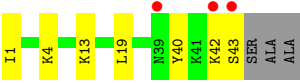
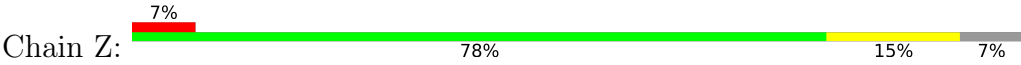
● Molecule 12: Cytochrome c oxidase subunit 7C



● Molecule 13: Cytochrome c oxidase subunit 8B



● Molecule 13: Cytochrome c oxidase subunit 8B



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	182.02Å 203.54Å 177.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.90 40.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.0 (40.00-1.90) 98.0 (40.00-1.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.8.0048	Depositor
R, R_{free}	0.172 , 0.199 0.175 , 0.225	Depositor DCC
R_{free} test set	33115 reflections (2.62%)	wwPDB-VP
Wilson B-factor (Å ²)	29.9	Xtriage
Anisotropy	0.649	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 67.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.008 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	33893	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, HEA, CDL, NA, PER, ZN, TPO, SAC, CU, PSC, PGV, FME, DMU, CUA, PEK, TGL, CHD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.04	3/4253 (0.1%)	1.01	13/5805 (0.2%)
1	N	0.96	3/4252 (0.1%)	0.99	3/5804 (0.1%)
2	B	0.91	0/1906	0.96	0/2595
2	O	0.79	0/1908	0.96	2/2599 (0.1%)
3	C	0.91	1/2261 (0.0%)	0.90	1/3090 (0.0%)
3	P	0.87	0/2260	0.88	0/3088
4	D	0.80	0/1284	0.90	1/1730 (0.1%)
4	Q	0.63	0/1237	0.90	1/1668 (0.1%)
5	E	0.80	0/882	0.83	0/1196
5	R	0.70	0/871	0.89	0/1182
6	F	0.88	0/806	0.99	1/1093 (0.1%)
6	S	0.95	0/772	1.07	1/1048 (0.1%)
7	G	0.94	0/702	0.98	4/953 (0.4%)
7	T	0.86	0/724	1.00	2/984 (0.2%)
8	H	0.80	0/682	0.98	0/921
8	U	0.79	0/682	0.92	1/921 (0.1%)
9	I	0.75	0/605	0.94	0/802
9	V	0.64	0/613	0.98	0/812
10	J	0.73	0/471	0.85	0/636
10	W	0.76	0/471	0.91	0/636
11	K	0.89	0/405	0.91	0/556
11	X	0.68	0/405	0.86	0/556
12	L	0.89	0/393	0.93	0/526
12	Y	0.82	0/393	0.83	0/526
13	M	0.84	0/345	0.90	0/470
13	Z	0.79	0/345	0.90	0/470
All	All	0.88	7/29928 (0.0%)	0.95	30/40667 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
6	F	0	1
6	S	0	1
All	All	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	83	VAL	CA-CB	6.70	1.57	1.54
1	A	130	PRO	CA-C	6.35	1.58	1.52
1	N	173	PRO	CA-C	6.22	1.55	1.51
1	N	106	PRO	CA-C	6.13	1.57	1.52
1	A	83	VAL	CA-CB	5.79	1.57	1.54
3	C	129	VAL	CA-CB	5.36	1.57	1.53
1	A	248	LEU	CA-C	5.24	1.58	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	S	94	HIS	N-CA-C	13.97	127.51	110.19
1	N	240	HIS	N-CA-CB	8.75	118.70	110.39
1	A	240	HIS	N-CA-CB	7.09	118.79	110.42
4	Q	7	LYS	N-CA-C	6.99	120.84	109.59
1	A	35	LEU	CA-CB-CG	-6.61	93.15	116.30
7	T	7	ASP	N-CA-C	6.61	124.88	110.80
7	G	7	ASP	N-CA-C	6.43	124.49	110.80
7	T	8	HIS	N-CA-C	5.96	118.02	110.33
7	G	8	HIS	N-CA-C	5.96	123.49	110.80
1	A	240	HIS	CA-CB-CG	-5.83	107.97	113.80
1	A	240	HIS	CA-C-N	-5.79	112.76	119.47
1	A	240	HIS	C-N-CA	-5.79	112.76	119.47
1	N	71	MET	CG-SD-CE	-5.64	88.48	100.90
6	F	94	HIS	N-CA-C	5.61	122.74	110.80
2	O	78	LEU	CA-C-N	-5.59	113.27	119.19
2	O	78	LEU	C-N-CA	-5.59	113.27	119.19
4	D	20	ARG	NE-CZ-NH2	-5.48	114.27	119.20
7	G	2	SER	N-CA-C	-5.47	106.49	112.72
1	A	119	GLU	CB-CA-C	-5.44	110.29	116.54
3	C	129	VAL	N-CA-CB	5.38	113.89	110.50
8	U	46	LYS	N-CA-C	5.38	122.26	110.80
1	A	448	THR	N-CA-C	5.34	116.78	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	49	GLY	N-CA-C	-5.21	103.76	110.69
7	G	12	GLY	N-CA-C	5.09	128.07	113.30
1	A	314	ILE	CA-C-N	-5.08	113.70	119.28
1	A	314	ILE	C-N-CA	-5.08	113.70	119.28
1	A	105	LEU	CA-C-N	-5.05	115.18	120.38
1	A	105	LEU	C-N-CA	-5.05	115.18	120.38
1	A	310	MET	N-CA-C	5.03	116.98	111.50
1	N	299	VAL	N-CA-C	5.00	115.72	110.62

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	F	93	PRO	Peptide
6	S	93	PRO	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4124	0	4102	64	0
1	N	4123	0	4098	75	0
2	B	1868	0	1864	27	0
2	O	1870	0	1867	41	0
3	C	2174	0	2082	36	0
3	P	2173	0	2083	36	0
4	D	1249	0	1242	27	1
4	Q	1203	0	1191	10	0
5	E	863	0	857	8	0
5	R	852	0	845	3	0
6	F	789	0	769	20	0
6	S	755	0	734	17	0
7	G	686	0	651	32	0
7	T	706	0	664	27	0
8	H	662	0	623	19	0
8	U	662	0	623	16	0
9	I	601	0	613	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	V	609	0	621	12	0
10	J	460	0	459	2	0
10	W	460	0	459	8	0
11	K	391	0	374	7	0
11	X	391	0	374	7	0
12	L	380	0	380	8	0
12	Y	380	0	380	9	0
13	M	335	0	352	9	0
13	Z	335	0	352	3	0
14	A	120	0	108	11	0
14	N	120	0	108	12	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	C	1	0	0	0	0
17	N	1	0	0	0	0
17	P	1	0	0	0	0
18	A	102	0	152	17	0
18	C	102	0	152	3	0
18	N	102	0	152	8	0
18	P	102	0	152	9	0
19	A	4	0	0	3	0
19	N	4	0	0	2	0
20	B	63	0	110	1	0
20	D	63	0	110	11	0
20	L	63	0	110	11	0
20	N	126	0	220	10	0
20	Q	63	0	110	6	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	29	0	39	1	0
22	C	58	0	78	1	0
22	J	29	0	38	0	0
22	N	29	0	39	1	0
22	O	29	0	39	1	0
22	P	29	0	39	1	0
22	W	29	0	39	5	0
23	C	106	0	154	19	0
23	G	53	0	77	7	0
23	P	53	0	77	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	T	106	0	154	8	0
24	C	100	0	156	14	0
24	G	100	0	156	17	0
24	P	100	0	156	10	0
24	T	100	0	156	20	0
25	C	33	0	42	6	0
25	M	33	0	42	0	0
25	P	33	0	42	4	0
25	Z	33	0	42	1	0
26	E	52	0	80	7	0
26	R	52	0	80	6	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	A	270	0	0	11	0
28	B	206	0	0	13	2
28	C	145	0	0	4	0
28	D	167	0	0	10	1
28	E	113	0	0	1	0
28	F	137	0	0	6	0
28	G	77	0	0	3	0
28	H	83	0	0	2	0
28	I	50	0	0	1	0
28	J	42	0	0	0	0
28	K	44	0	0	2	0
28	L	36	0	0	0	0
28	M	28	0	0	0	0
28	N	266	0	0	17	0
28	O	168	0	0	4	0
28	P	138	0	0	9	0
28	Q	84	0	0	0	0
28	R	91	0	0	2	0
28	S	126	0	0	1	0
28	T	62	0	0	2	0
28	U	68	0	0	3	0
28	V	41	0	0	1	0
28	W	44	0	0	2	0
28	X	28	0	0	0	0
28	Y	24	0	0	1	0
28	Z	20	0	0	0	0
All	All	33893	0	31868	570	2

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 9.

All (570) 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:D:4:SER:HB3	28:D:389:HOH:O	1.32	1.26
23:P:302:PEK:H383	24:T:103:CDL:C27	1.65	1.25
6:F:53:THR:HB	28:F:201:HOH:O	1.14	1.24
19:N:607[B]:PER:O2	19:N:607[B]:PER:O1	1.55	1.23
19:N:607[A]:PER:O1	19:N:607[A]:PER:O2	1.55	1.22
19:A:607[B]:PER:O1	19:A:607[B]:PER:O2	1.55	1.21
19:A:607[A]:PER:O2	19:A:607[A]:PER:O1	1.55	1.21
1:A:297[B]:MET:HB3	28:A:833:HOH:O	1.38	1.20
1:A:486:ASP:OD1	4:D:19[A]:ARG:HD2	1.45	1.14
20:L:101:TGL:OC1	20:L:101:TGL:HC41	1.45	1.11
20:D:201:TGL:HG31	28:D:392:HOH:O	1.48	1.11
6:S:85:CYS:SG	6:S:87[A]:THR:HG23	1.91	1.11
23:P:302:PEK:C38	24:T:103:CDL:H273	1.81	1.09
24:T:103:CDL:H111	24:T:103:CDL:HA21	1.33	1.09
8:H:9:LYS:HD3	8:H:10:ASN:H	0.96	1.09
18:P:303:PGV:H172	24:P:305:CDL:H632	1.27	1.06
2:O:124:PRO:HB2	28:O:401:HOH:O	1.51	1.06
8:U:9:LYS:HG3	8:U:10:ASN:H	1.18	1.02
3:P:3:HIS:HB3	28:P:506:HOH:O	1.59	1.02
23:P:302:PEK:H383	24:T:103:CDL:H273	1.06	1.01
2:O:57:ASP:H	26:R:201:PSC:H211	1.25	1.00
1:N:297[B]:MET:SD	1:N:302[B]:ARG:HG2	2.02	1.00
1:N:297[B]:MET:CG	1:N:302[B]:ARG:HG3	1.90	0.99
1:N:258:VAL:N	28:N:701:HOH:O	1.96	0.99
1:N:296:GLY:HA2	8:U:23:GLN:HE21	1.25	0.98
8:H:9:LYS:HD3	8:H:10:ASN:N	1.80	0.96
6:F:85:CYS:SG	6:F:87:THR:HG23	2.06	0.96
5:E:14[B]:ARG:HD2	5:E:14[B]:ARG:O	1.66	0.95
1:N:296:GLY:HA2	8:U:23:GLN:NE2	1.81	0.95
1:N:297[B]:MET:SD	1:N:302[B]:ARG:CG	2.55	0.94
3:P:157:LYS:NZ	23:P:302:PEK:H051	1.82	0.93
26:E:201:PSC:H071	9:I:10:ARG:HH21	1.33	0.92
7:T:72:ASN:H	7:T:76:ASN:HD22	1.17	0.92
28:N:883:HOH:O	2:O:87:MET:SD	2.27	0.92
1:A:486:ASP:OD1	4:D:19[A]:ARG:CD	2.19	0.90
3:P:157:LYS:HZ1	23:P:302:PEK:H051	1.34	0.90
11:X:54:ARG:HH21	11:X:54:ARG:HG3	1.33	0.90
24:G:101:CDL:H352	2:O:78:LEU:HD12	1.51	0.90
12:L:20:ARG:NH2	20:L:101:TGL:HC52	1.86	0.88
1:A:472:ILE:HG21	20:L:101:TGL:HA91	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:19[B]:ARG:HG2	4:D:21:ASP:OD1	1.74	0.87
23:C:303:PEK:C38	24:G:101:CDL:H273	2.05	0.86
1:N:297[B]:MET:HG2	1:N:302[B]:ARG:HG3	1.57	0.85
7:G:5:LYS:HG3	23:G:102:PEK:H351	1.58	0.85
23:C:303:PEK:H222	23:C:303:PEK:H32	1.59	0.84
28:B:596:HOH:O	26:E:201:PSC:H282	1.78	0.84
5:E:14[B]:ARG:HD2	5:E:14[B]:ARG:C	2.01	0.84
8:H:9:LYS:CD	8:H:10:ASN:H	1.88	0.83
2:B:59:GLN:HG2	28:P:496:HOH:O	1.79	0.83
1:N:206:ILE:HD11	28:N:933:HOH:O	1.78	0.83
8:U:9:LYS:CG	8:U:10:ASN:H	1.87	0.83
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.27	0.82
18:A:608:PGV:H342	23:C:302:PEK:H382	1.60	0.82
23:C:303:PEK:H383	24:G:101:CDL:H273	1.62	0.82
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.60	0.82
9:V:65:LYS:O	11:X:54:ARG:NH1	2.12	0.82
1:N:255:SER:O	28:N:701:HOH:O	1.97	0.81
8:H:43:MET:HE1	8:U:43:MET:HE1	1.62	0.81
1:A:113[B]:LEU:CD2	1:A:117[B]:MET:SD	2.69	0.81
3:C:33:MET:HE3	3:C:39:SER:OG	1.81	0.80
4:D:78:TRP:CA	20:D:201:TGL:HB22	2.11	0.80
18:P:303:PGV:C17	24:P:305:CDL:H632	2.12	0.79
7:G:72:ASN:H	7:G:76:ASN:HD22	1.29	0.79
6:S:52:ILE:HA	6:S:94:HIS:HB3	1.65	0.79
1:A:112:LEU:HD13	28:A:801:HOH:O	1.82	0.79
1:N:28:MET:CE	14:N:601:HEA:C27	2.61	0.79
28:A:913:HOH:O	2:B:87:MET:SD	2.39	0.79
24:T:103:CDL:H781	24:T:103:CDL:H561	1.64	0.78
9:V:45:LYS:HD3	9:V:49:ASP:OD2	1.83	0.78
2:O:116:LEU:HD13	2:O:226:MET:HG2	1.66	0.78
6:F:75:HIS:H	6:F:80[B]:GLN:HE22	1.32	0.78
3:C:188[B]:ILE:HD13	3:C:198:PHE:HB2	1.65	0.77
7:T:76:ASN:HD21	23:T:102:PEK:HN2	1.29	0.77
23:C:302:PEK:HN2	7:G:76:ASN:HD21	1.32	0.77
1:N:297[B]:MET:SD	1:N:302[B]:ARG:HG3	2.22	0.77
23:T:101:PEK:H361	24:T:103:CDL:H861	1.67	0.76
6:S:75:HIS:H	6:S:80:GLN:HE22	1.32	0.76
23:C:303:PEK:H052	6:F:1:ALA:H2	1.49	0.76
1:N:28:MET:CE	14:N:601:HEA:H271	2.16	0.76
1:A:513:LEU:O	1:A:514:LYS:HB2	1.86	0.76
1:A:311[B]:ILE:HG22	24:T:103:CDL:H421	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:365:ILE:HD11	28:N:729:HOH:O	1.86	0.75
2:O:116:LEU:CD1	2:O:226:MET:HG2	2.15	0.75
2:O:183:THR:HG23	28:O:541:HOH:O	1.87	0.75
4:D:19[B]:ARG:CG	4:D:21:ASP:OD1	2.34	0.75
23:P:302:PEK:H383	24:T:103:CDL:H272	1.66	0.75
4:D:31:LYS:HD2	28:D:452:HOH:O	1.87	0.74
7:G:5:LYS:HB3	1:N:278[B]:MET:CE	2.18	0.74
1:N:273:MET:HE2	28:N:776:HOH:O	1.87	0.73
12:L:20:ARG:HH21	20:L:101:TGL:HC32	1.52	0.73
18:N:606:PGV:H012	18:N:606:PGV:H222	1.70	0.73
3:P:40[B]:MET:O	3:P:44[B]:MET:HG3	1.88	0.73
11:X:54:ARG:HG3	11:X:54:ARG:NH2	1.96	0.73
1:A:113[B]:LEU:HD21	1:A:117[B]:MET:SD	2.28	0.73
6:F:92[A]:VAL:HG23	6:F:92[A]:VAL:O	1.88	0.72
20:N:611:TGL:HC32	12:Y:20:ARG:HH21	1.55	0.72
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.71	0.72
4:D:34:SER:H	4:D:37:GLN:HE21	1.38	0.72
12:L:14:SER:H	20:L:101:TGL:HC31	1.55	0.71
20:Q:201:TGL:H362	9:V:20:HIS:HE1	1.54	0.71
1:A:28:MET:CE	14:A:601:HEA:C27	2.67	0.71
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.73	0.71
18:A:608:PGV:C34	23:C:302:PEK:H382	2.20	0.71
26:E:201:PSC:C07	9:I:10:ARG:HH21	2.04	0.71
26:R:201:PSC:H011	26:R:201:PSC:O02	1.90	0.71
18:A:606:PGV:H292	13:M:16:ALA:HA	1.73	0.70
24:C:306:CDL:H212	24:C:306:CDL:H632	1.72	0.70
4:D:78:TRP:HA	20:D:201:TGL:HB22	1.72	0.70
23:P:302:PEK:H203	7:T:36[A]:TRP:HE1	1.55	0.70
24:T:103:CDL:H522	24:T:103:CDL:HB61	1.73	0.70
20:L:101:TGL:OC1	20:L:101:TGL:CC4	2.30	0.70
7:G:5:LYS:HB3	1:N:278[B]:MET:HE3	1.75	0.69
11:X:54:ARG:HH21	11:X:54:ARG:CG	2.05	0.69
1:A:113[B]:LEU:HD22	1:A:117[B]:MET:SD	2.32	0.69
1:A:136[B]:LEU:HD11	28:A:963:HOH:O	1.92	0.69
3:P:41:THR:HA	3:P:44[B]:MET:HE2	1.75	0.69
23:C:303:PEK:C05	6:F:1:ALA:H2	2.05	0.68
1:A:28:MET:CE	14:A:601:HEA:H271	2.23	0.68
1:N:254:ILE:O	28:N:701:HOH:O	2.11	0.68
2:B:91:ASN:HB3	2:B:149:THR:HG21	1.76	0.68
1:N:28:MET:HE2	14:N:601:HEA:H273	1.75	0.68
18:N:606:PGV:H041	18:N:606:PGV:H02	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:606:PGV:H181	18:A:606:PGV:H301	1.75	0.68
2:O:57:ASP:N	26:R:201:PSC:H211	2.06	0.67
20:Q:201:TGL:HB51	20:Q:201:TGL:HA22	1.75	0.67
1:A:468:MET:HG3	28:A:942:HOH:O	1.93	0.67
4:Q:34:SER:H	4:Q:37:GLN:NE2	1.91	0.67
2:B:49:LYS:HE2	28:D:441:HOH:O	1.94	0.67
4:D:78:TRP:HB3	20:D:201:TGL:HB22	1.75	0.67
8:U:9:LYS:HG3	8:U:10:ASN:N	2.02	0.67
4:D:78:TRP:CB	20:D:201:TGL:HB22	2.24	0.66
1:A:28:MET:HE1	14:A:601:HEA:C27	2.25	0.66
6:F:54[B]:ASN:ND2	28:F:201:HOH:O	2.07	0.66
1:N:297[B]:MET:HG2	1:N:302[B]:ARG:CG	2.25	0.66
7:G:84:LYS:H	7:G:84:LYS:HZ3	1.44	0.66
8:U:9:LYS:CG	8:U:10:ASN:N	2.59	0.66
20:Q:201:TGL:H362	9:V:20:HIS:CE1	2.30	0.66
2:O:33:LEU:HD13	9:V:31:PHE:CD2	2.31	0.65
24:T:103:CDL:H111	24:T:103:CDL:CA2	2.21	0.65
20:N:611:TGL:HC32	12:Y:20:ARG:NH2	2.11	0.65
1:N:255:SER:C	28:N:701:HOH:O	2.38	0.64
18:A:608:PGV:H183	23:C:302:PEK:H322	1.79	0.64
14:N:601:HEA:HBC1	14:N:601:HEA:HMC1	1.79	0.64
5:E:90:ARG:HD2	28:E:380:HOH:O	1.96	0.64
7:G:5:LYS:NZ	28:G:201:HOH:O	2.16	0.64
6:S:85:CYS:SG	6:S:87[A]:THR:CG2	2.80	0.64
7:T:8:HIS:CG	7:T:9:GLY:H	2.16	0.64
7:T:12:GLY:HA3	28:T:240:HOH:O	1.97	0.64
3:C:33:MET:HB2	25:C:309:DMU:C25	2.28	0.64
3:C:131:LEU:HD21	24:G:101:CDL:HB4	1.79	0.64
6:S:85:CYS:SG	6:S:87[B]:THR:HG22	2.38	0.64
1:N:297[B]:MET:CG	1:N:302[B]:ARG:CG	2.70	0.64
7:G:84:LYS:H	7:G:84:LYS:NZ	1.96	0.64
1:N:513:LEU:O	1:N:514:LYS:HB2	1.98	0.64
23:P:302:PEK:C38	24:T:103:CDL:C27	2.54	0.63
1:N:28:MET:HE2	14:N:601:HEA:C27	2.27	0.63
6:F:92[A]:VAL:HG21	28:F:328:HOH:O	1.99	0.63
7:G:9:GLY:CA	1:N:178:GLN:HE21	2.11	0.62
1:N:417[A]:MET:CE	28:N:889:HOH:O	2.46	0.62
4:Q:19:ARG:CG	4:Q:21:ASP:OD1	2.47	0.62
7:T:72:ASN:H	7:T:76:ASN:ND2	1.95	0.62
4:D:4:SER:HA	28:D:383:HOH:O	1.99	0.62
7:T:2:SER:HB2	23:T:101:PEK:H281	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:C:303:PEK:C05	6:F:1:ALA:N	2.61	0.62
2:O:89:GLU:O	2:O:91:ASN:ND2	2.32	0.62
2:O:91:ASN:HB3	2:O:149:THR:HG21	1.80	0.62
1:N:28:MET:HE1	14:N:601:HEA:C27	2.30	0.62
3:P:3:HIS:HA	28:P:513:HOH:O	1.99	0.61
18:A:606:PGV:H291	13:M:19:LEU:CD2	2.31	0.61
4:D:100:LYS:HE2	28:D:312:HOH:O	1.99	0.61
24:T:103:CDL:H212	24:T:103:CDL:H511	1.82	0.61
18:A:606:PGV:O02	18:A:606:PGV:P	2.58	0.61
24:G:101:CDL:H662	18:P:304:PGV:H171	1.81	0.61
6:S:94:HIS:CD2	6:S:95:GLN:O	2.53	0.61
2:B:22[B]:HIS:HD2	28:B:521:HOH:O	1.82	0.60
2:O:83:ILE:O	2:O:87:MET:HG3	2.00	0.60
12:L:20:ARG:HH22	20:L:101:TGL:HC52	1.66	0.60
1:N:113[A]:LEU:HD12	20:N:611:TGL:H291	1.84	0.60
18:A:606:PGV:H291	13:M:19:LEU:HD23	1.82	0.60
6:F:54[B]:ASN:ND2	28:F:202:HOH:O	2.35	0.60
24:G:101:CDL:H212	1:N:311:ILE:HD12	1.83	0.60
8:U:61:LYS:HE3	28:U:122:HOH:O	2.01	0.60
2:B:217:LYS:HE2	28:B:578:HOH:O	2.02	0.60
6:S:54:ASN:HD22	6:S:54:ASN:C	2.10	0.59
7:G:72:ASN:H	7:G:76:ASN:ND2	2.00	0.59
2:B:164:ALA:O	2:B:194:GLY:HA3	2.01	0.59
20:Q:201:TGL:H352	9:V:16:ARG:HE	1.67	0.59
3:P:59:ARG:HA	24:P:305:CDL:H512	1.84	0.59
3:C:55:TYR:CE1	24:C:306:CDL:H511	2.38	0.59
1:A:177:SER:H	1:A:180:GLN:HE21	1.51	0.59
2:O:1:FME:HE1	2:O:133:LEU:HD22	1.85	0.59
6:F:64:GLU:O	6:F:65:ASP:HB2	2.01	0.58
8:H:43:MET:CE	8:U:43:MET:HE1	2.33	0.58
12:L:20:ARG:HH21	20:L:101:TGL:HC52	1.68	0.58
6:S:64:GLU:O	6:S:65:ASP:HB2	2.02	0.58
18:A:608:PGV:C18	23:C:302:PEK:H322	2.34	0.58
3:C:33:MET:HB2	25:C:309:DMU:C22	2.34	0.58
18:C:305:PGV:H131	24:T:103:CDL:H651	1.85	0.58
1:N:289:ALA:HB1	1:N:297[B]:MET:HE1	1.86	0.58
18:N:606:PGV:H311	13:Z:19:LEU:HD23	1.85	0.58
23:C:303:PEK:H052	6:F:1:ALA:N	2.18	0.57
7:T:5:LYS:NZ	28:T:201:HOH:O	2.23	0.57
7:T:8:HIS:CG	7:T:9:GLY:N	2.72	0.57
1:A:411:LYS:NZ	28:A:701:HOH:O	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:224:LYS:CD	24:C:306:CDL:HB32	2.35	0.57
22:W:101:CHD:O12	22:W:101:CHD:H222	2.05	0.57
1:A:63:PHE:HB3	28:A:854:HOH:O	2.04	0.57
18:P:303:PGV:H182	24:P:305:CDL:H651	1.86	0.57
23:C:303:PEK:H031	28:C:426:HOH:O	2.03	0.57
7:G:3:ALA:O	7:G:4:ALA:CB	2.52	0.57
1:N:514:LYS:HA	6:S:38:ALA:CB	2.33	0.57
3:P:157:LYS:HZ2	23:P:302:PEK:H051	1.66	0.57
1:A:177:SER:H	1:A:180:GLN:NE2	2.03	0.56
2:B:183:THR:HG23	28:B:567:HOH:O	2.05	0.56
7:G:3:ALA:O	7:G:4:ALA:HB2	2.05	0.56
8:U:7:LYS:O	8:U:8:ILE:HB	2.05	0.56
1:A:28:MET:HE2	14:A:601:HEA:C27	2.36	0.56
3:C:33:MET:CE	3:C:42:LEU:H	2.19	0.56
24:G:101:CDL:H851	23:G:102:PEK:H361	1.87	0.56
2:O:84:LEU:HA	2:O:87:MET:HE2	1.86	0.56
1:N:169[A]:ILE:HD11	1:N:189:MET:SD	2.45	0.56
2:B:33:LEU:HD13	9:I:31:PHE:CD2	2.41	0.56
18:P:304:PGV:H032	28:P:488:HOH:O	2.04	0.56
7:T:2:SER:CB	23:T:101:PEK:H281	2.36	0.56
24:G:101:CDL:H212	1:N:311:ILE:CD1	2.36	0.56
7:T:37:LEU:HD23	24:T:103:CDL:H361	1.86	0.56
4:Q:19:ARG:HG3	4:Q:21:ASP:OD1	2.06	0.55
1:A:172:LYS:HZ2	1:A:178:GLN:HE22	1.55	0.55
24:C:306:CDL:H192	28:C:541:HOH:O	2.06	0.55
11:X:24:PHE:O	11:X:28[B]:VAL:HG23	2.05	0.55
18:A:606:PGV:O02	18:A:606:PGV:O14	2.24	0.55
2:B:61:VAL:HG11	28:B:596:HOH:O	2.07	0.55
3:C:51[A]:MET:SD	3:C:54[A]:MET:CE	2.95	0.55
11:K:39:GLU:HB3	28:K:123:HOH:O	2.05	0.55
9:V:45:LYS:HD2	28:V:113:HOH:O	2.07	0.55
2:B:140:ASN:HB3	28:B:504:HOH:O	2.06	0.55
3:P:157:LYS:O	3:P:161:GLN:HG3	2.07	0.55
6:S:51:SER:O	6:S:94:HIS:HB3	2.07	0.55
7:T:3:ALA:O	7:T:4:ALA:HB2	2.06	0.55
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.89	0.54
3:P:33:MET:HE3	3:P:39:SER:OG	2.08	0.54
26:R:201:PSC:O02	26:R:201:PSC:H222	2.07	0.54
10:W:37:THR:OG1	22:W:101:CHD:H5	2.07	0.54
7:G:12:GLY:HA3	28:G:249:HOH:O	2.07	0.54
1:N:35:LEU:HD11	1:N:462:LEU:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:C:303:PEK:H32	23:C:303:PEK:C22	2.33	0.54
6:F:30:PRO:O	6:F:96:LEU:HD11	2.08	0.54
8:H:55:TRP:H	8:U:46:LYS:HZ1	1.56	0.53
24:G:101:CDL:H222	24:G:101:CDL:H511	1.90	0.53
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.89	0.53
1:A:71:MET:HB2	1:A:72:PRO:HD3	1.90	0.53
1:A:273:MET:HE2	28:A:808:HOH:O	2.07	0.53
3:P:3:HIS:HD2	28:P:513:HOH:O	1.92	0.53
1:A:28:MET:HE2	14:A:601:HEA:H273	1.90	0.53
1:A:112:LEU:HD11	28:A:938:HOH:O	2.08	0.53
3:C:33:MET:HE1	3:C:41:THR:HB	1.90	0.53
18:N:606:PGV:H012	18:N:606:PGV:C22	2.37	0.53
3:P:224:LYS:HE3	24:P:305:CDL:HB32	1.90	0.53
1:A:28:MET:HE1	14:A:601:HEA:H271	1.89	0.53
6:F:92[A]:VAL:O	6:F:92[A]:VAL:CG2	2.56	0.53
7:G:3:ALA:CB	23:G:102:PEK:H362	2.39	0.53
3:P:51[A]:MET:HE3	28:P:529:HOH:O	2.08	0.53
5:E:12:ASP:OD2	5:E:44:GLU:HG3	2.08	0.52
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.90	0.52
2:O:1:FME:HE1	2:O:133:LEU:CD2	2.38	0.52
2:O:128:LEU:HD11	2:O:134:ARG:HA	1.92	0.52
12:Y:2:HIS:CD2	12:Y:3:TYR:H	2.26	0.52
1:N:62:ALA:HB2	14:N:601:HEA:HBD1	1.90	0.52
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.45	0.52
4:D:58:GLU:HG3	28:D:301:HOH:O	2.09	0.52
24:G:101:CDL:H351	2:O:81:LEU:HD12	1.91	0.52
26:E:201:PSC:H02	26:E:201:PSC:H212	1.91	0.52
8:U:43:MET:HE3	8:U:49:ASP:N	2.24	0.52
8:H:54:GLU:OE2	8:H:57:ARG:NH2	2.40	0.52
1:N:334:TRP:HZ3	20:Q:201:TGL:HA51	1.75	0.52
24:T:103:CDL:H231	24:T:103:CDL:H531	1.90	0.52
12:Y:2:HIS:CG	12:Y:3:TYR:H	2.27	0.52
4:D:34:SER:H	4:D:37:GLN:NE2	2.07	0.51
7:G:5:LYS:HB3	1:N:278[B]:MET:HE1	1.90	0.51
1:A:409:TRP:HB3	1:A:471:ILE:HG12	1.91	0.51
2:O:164:ALA:O	2:O:194:GLY:HA3	2.10	0.51
8:H:50:VAL:HG23	28:H:147:HOH:O	2.11	0.51
7:G:2:SER:OG	23:G:102:PEK:H291	2.11	0.51
20:D:201:TGL:H342	9:I:16:ARG:HE	1.76	0.51
7:G:42:ARG:NH1	7:G:42:ARG:HA	2.26	0.51
24:G:101:CDL:C85	23:G:102:PEK:H361	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:41:ILE:HG21	26:R:201:PSC:H332	1.93	0.51
24:P:305:CDL:H182	24:P:305:CDL:H622	1.92	0.51
12:Y:20:ARG:NH2	12:Y:24:MET:HG3	2.26	0.51
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.46	0.50
3:C:33:MET:HE2	3:C:42:LEU:H	1.76	0.50
3:P:54:MET:HE1	18:P:303:PGV:H131	1.93	0.50
25:C:309:DMU:H4	10:J:52:TRP:CZ2	2.46	0.50
12:L:2:HIS:CG	12:L:3:TYR:H	2.29	0.50
12:Y:2:HIS:CG	28:Y:122:HOH:O	2.64	0.50
5:E:86:ILE:O	5:E:90:ARG:HG2	2.12	0.50
3:P:5:THR:HG22	6:S:96:LEU:CD1	2.41	0.50
23:C:303:PEK:H051	6:F:1:ALA:N	2.27	0.50
2:B:52:HIS:HE1	26:E:201:PSC:H201	1.77	0.50
8:H:43:MET:HE3	8:H:49:ASP:N	2.27	0.50
1:N:116:SER:HB3	28:N:757:HOH:O	2.12	0.50
7:G:5:LYS:HB2	23:G:102:PEK:H332	1.93	0.50
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.94	0.50
1:N:472:ILE:HG21	20:N:611:TGL:HA91	1.93	0.50
9:I:8:GLN:OE1	9:I:10:ARG:O	2.30	0.50
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.94	0.50
1:N:514:LYS:HD3	28:S:270:HOH:O	2.12	0.50
24:G:101:CDL:H381	24:G:101:CDL:H142	1.94	0.49
3:P:62:ILE:HD12	24:P:305:CDL:H511	1.93	0.49
3:P:5:THR:HG22	6:S:96:LEU:HD11	1.94	0.49
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.94	0.49
3:C:33:MET:HB2	25:C:309:DMU:H13	1.94	0.49
7:G:8:HIS:O	7:G:9:GLY:C	2.55	0.49
24:G:101:CDL:H191	1:N:311:ILE:HD11	1.95	0.49
20:N:611:TGL:H152	12:Y:24:MET:SD	2.53	0.49
7:T:72:ASN:N	7:T:76:ASN:HD22	1.98	0.49
2:B:75:LEU:HB3	28:B:509:HOH:O	2.12	0.49
28:B:525:HOH:O	24:T:103:CDL:H331	2.13	0.49
1:A:172:LYS:NZ	1:A:178:GLN:HE22	2.11	0.49
1:N:177:SER:H	1:N:180:GLN:NE2	2.10	0.48
1:N:334:TRP:CZ3	20:Q:201:TGL:HA51	2.48	0.48
7:T:41:HIS:HB3	7:T:74:ARG:NH1	2.28	0.48
4:D:100:LYS:CE	28:D:312:HOH:O	2.59	0.48
6:F:87:THR:HG21	28:F:310:HOH:O	2.12	0.48
20:L:101:TGL:HC22	20:L:101:TGL:HC82	1.93	0.48
3:C:51[B]:MET:HE3	24:C:306:CDL:H391	1.95	0.48
3:C:224:LYS:HD2	24:C:306:CDL:HB32	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:417[A]:MET:HE2	28:N:889:HOH:O	2.11	0.48
8:U:12:GLN:HB2	28:U:153:HOH:O	2.13	0.48
1:A:265:LYS:HB2	1:A:490:THR:HG21	1.96	0.48
1:A:311[B]:ILE:CG2	24:T:103:CDL:H421	2.38	0.48
3:C:52:LEU:HD23	24:C:306:CDL:H362	1.95	0.48
1:N:3:ILE:HG21	22:W:101:CHD:H232	1.95	0.48
24:G:101:CDL:H222	24:G:101:CDL:C51	2.44	0.48
4:D:78:TRP:HA	20:D:201:TGL:CB2	2.42	0.48
28:N:860:HOH:O	4:Q:100:LYS:HE2	2.13	0.48
22:O:301:CHD:H212	22:O:301:CHD:H12	1.96	0.48
4:D:58:GLU:CG	28:D:301:HOH:O	2.62	0.47
20:D:201:TGL:H242	20:D:201:TGL:HA91	1.96	0.47
3:C:67:PHE:HE2	24:C:306:CDL:H1	1.78	0.47
1:A:165:ILE:HG23	1:A:189[B]:MET:HE1	1.96	0.47
1:A:302[B]:ARG:HH22	2:B:87:MET:HE1	1.80	0.47
22:B:303:CHD:H12	22:B:303:CHD:H212	1.95	0.47
23:C:303:PEK:H222	23:C:303:PEK:C3	2.38	0.47
3:P:112:LEU:HD13	3:P:118:PRO:HG3	1.97	0.47
25:P:307:DMU:H23	10:W:50:LEU:HG	1.96	0.47
8:H:60:TYR:CD1	8:H:60:TYR:C	2.91	0.47
2:O:203[B]:ASN:HD22	2:O:206:PHE:HD2	1.62	0.47
7:T:41:HIS:HB3	7:T:74:ARG:HH12	1.79	0.47
1:A:62:ALA:HB2	14:A:601:HEA:HBD1	1.95	0.47
3:C:224:LYS:HE3	24:C:306:CDL:CB3	2.45	0.47
2:O:16:ILE:HD12	2:O:87:MET:HG2	1.96	0.47
6:S:95:GLN:NE2	6:S:95:GLN:HA	2.24	0.47
7:T:38:HIS:HE1	24:T:103:CDL:H122	1.79	0.47
18:A:608:PGV:H72	3:C:54[B]:MET:HE2	1.94	0.47
3:C:76:GLN:NE2	28:C:401:HOH:O	2.40	0.47
4:D:81:VAL:HG11	20:D:201:TGL:HB52	1.97	0.47
3:P:3:HIS:CD2	28:P:513:HOH:O	2.67	0.47
6:S:62:CYS:HB3	6:S:85:CYS:HB3	1.96	0.47
1:N:274:VAL:HG12	1:N:278[A]:MET:HE2	1.97	0.47
18:N:609:PGV:H262	18:P:303:PGV:H292	1.97	0.47
28:B:532:HOH:O	23:P:302:PEK:H301	2.13	0.47
23:C:303:PEK:H381	24:G:101:CDL:H273	1.94	0.47
1:N:172:LYS:NZ	1:N:178:GLN:HE22	2.13	0.47
24:P:305:CDL:H672	28:P:529:HOH:O	2.14	0.47
18:A:608:PGV:H183	23:C:302:PEK:C32	2.44	0.47
3:C:127:LEU:HD21	22:N:610:CHD:H3	1.96	0.47
7:G:11:TPO:HA	7:G:11:TPO:O3P	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:P:307:DMU:H11	10:W:49:CYS:HB3	1.96	0.47
10:W:15:ASP:OD2	28:W:201:HOH:O	2.20	0.47
1:N:225:GLY:HA3	3:P:112:LEU:HD21	1.97	0.46
1:A:307:SER:O	1:A:311[A]:ILE:HG12	2.14	0.46
24:G:101:CDL:H662	18:P:304:PGV:C17	2.46	0.46
14:N:601:HEA:HBC1	14:N:601:HEA:CMC	2.45	0.46
3:C:188[B]:ILE:CD1	3:C:195:SER:HA	2.45	0.46
4:D:109:HIS:HD2	28:D:365:HOH:O	1.98	0.46
1:N:35:LEU:HB3	25:Z:101:DMU:H24	1.97	0.46
20:N:608:TGL:H142	20:N:608:TGL:HA92	1.97	0.46
2:B:13:THR:OG1	2:B:167:SER:HB2	2.16	0.46
8:H:36:PHE:CD1	8:H:57:ARG:HB2	2.51	0.46
2:O:29:MET:HG3	9:V:35:TYR:CG	2.51	0.46
3:P:51[B]:MET:SD	24:P:305:CDL:H641	2.55	0.46
1:A:87:ILE:O	1:A:173:PRO:HD3	2.15	0.46
5:R:108:LYS:HB3	28:R:385:HOH:O	2.15	0.46
10:W:7:GLU:HG3	28:W:230:HOH:O	2.14	0.46
1:A:282:PHE:HA	7:T:4:ALA:CB	2.44	0.46
2:B:90:ILE:HG13	28:B:561:HOH:O	2.15	0.46
3:C:161[B]:GLN:HG3	28:C:524:HOH:O	2.15	0.46
11:K:47:ARG:HH11	11:K:47:ARG:HG2	1.81	0.46
3:P:160:LEU:HD13	22:P:306:CHD:H181	1.97	0.46
10:W:32:TYR:OH	22:W:101:CHD:H221	2.15	0.46
24:T:103:CDL:H791	24:T:103:CDL:H821	1.40	0.45
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.98	0.45
20:N:608:TGL:H242	20:N:608:TGL:H272	1.49	0.45
2:O:116:LEU:HD11	2:O:226:MET:HG2	1.94	0.45
1:A:297[B]:MET:CB	28:A:833:HOH:O	2.21	0.45
28:B:443:HOH:O	7:T:17:ARG:HD2	2.17	0.45
18:N:606:PGV:H02	18:N:606:PGV:C04	2.43	0.45
4:D:19[B]:ARG:HE	4:D:21:ASP:CG	2.25	0.45
26:R:201:PSC:H21	28:R:382:HOH:O	2.16	0.45
8:U:43:MET:HE3	8:U:49:ASP:H	1.81	0.45
1:A:337:ALA:HB2	1:A:394:VAL:HG23	1.98	0.45
20:L:101:TGL:H221	20:L:101:TGL:HA92	1.60	0.45
2:O:68:LEU:HB3	2:O:69:PRO:HD3	1.99	0.45
4:Q:10:ASP:OD1	4:Q:10:ASP:C	2.60	0.45
7:G:4:ALA:CB	1:N:282:PHE:HA	2.47	0.45
3:C:51[A]:MET:SD	3:C:54[A]:MET:HE1	2.57	0.45
7:G:8:HIS:O	7:G:8:HIS:CD2	2.69	0.45
7:G:41:HIS:HB3	7:G:74:ARG:NH1	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:22:VAL:O	9:I:26:MET:HG2	2.17	0.45
10:W:32:TYR:CE2	22:W:101:CHD:H181	2.52	0.45
24:C:306:CDL:H812	24:C:306:CDL:H842	1.66	0.45
8:H:9:LYS:HA	8:H:9:LYS:NZ	2.32	0.45
22:C:307:CHD:H162	22:C:307:CHD:H231	1.98	0.45
1:A:431:LEU:HD21	1:A:450:TRP:HB2	1.98	0.44
3:C:37:PHE:CG	25:C:309:DMU:H8	2.52	0.44
9:I:65:LYS:NZ	28:I:101:HOH:O	2.50	0.44
2:O:217:LYS:HD2	28:O:567:HOH:O	2.17	0.44
1:A:513:LEU:HD23	1:A:513:LEU:HA	1.56	0.44
2:O:111:THR:HA	2:O:114:GLU:O	2.18	0.44
28:B:443:HOH:O	7:T:17:ARG:CD	2.65	0.44
1:N:485:VAL:HG12	13:Z:1:ILE:HG13	1.99	0.44
18:N:606:PGV:H05	28:N:939:HOH:O	2.17	0.44
2:O:22[B]:HIS:CE1	9:V:44:LYS:HE2	2.53	0.44
2:O:104:TRP:CG	2:O:203[B]:ASN:HB2	2.53	0.44
25:C:309:DMU:H15	25:C:309:DMU:H9	1.83	0.44
2:O:29:MET:HE3	2:O:33:LEU:CD2	2.47	0.44
3:P:47:LEU:O	3:P:51[A]:MET:HG2	2.17	0.44
2:B:227:LEU:HD21	28:B:546:HOH:O	2.18	0.44
3:C:224:LYS:HE3	24:C:306:CDL:HB31	2.00	0.44
20:N:611:TGL:OC1	20:N:611:TGL:HC41	2.18	0.44
3:P:146:TRP:CD2	3:P:162:ALA:HB2	2.53	0.44
7:T:3:ALA:O	7:T:4:ALA:CB	2.66	0.44
7:G:5:LYS:CG	23:G:102:PEK:H351	2.39	0.44
2:O:67:ILE:HD11	28:O:545:HOH:O	2.18	0.44
4:D:87[B]:PHE:HZ	11:K:20:SER:HG	1.64	0.43
2:O:202:SER:C	2:O:203[A]:ASN:HD22	2.26	0.43
5:E:41:LEU:HD22	26:E:201:PSC:H072	2.00	0.43
11:K:8:ASP:HB2	28:K:120:HOH:O	2.17	0.43
1:N:513:LEU:HD23	1:N:513:LEU:HA	1.83	0.43
7:T:5:LYS:HB2	23:T:101:PEK:H322	1.99	0.43
1:A:240:HIS:O	1:A:241:PRO:C	2.58	0.43
4:D:19[B]:ARG:NE	4:D:21:ASP:OD1	2.51	0.43
1:N:409:TRP:HB3	1:N:471:ILE:HG12	1.99	0.43
1:A:514:LYS:HA	6:F:38:ALA:CB	2.46	0.43
2:B:148[B]:MET:HE3	2:B:148[B]:MET:HB2	1.77	0.43
26:E:201:PSC:H201	26:E:201:PSC:H231	1.76	0.43
13:Z:40:TYR:C	13:Z:42:LYS:H	2.25	0.43
7:G:2:SER:H	1:N:197:LEU:HD21	1.82	0.43
1:N:289:ALA:HB1	1:N:297[A]:MET:HE1	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:58:ALA:O	2:B:61:VAL:HG12	2.18	0.43
3:C:210:ILE:HG21	18:C:304:PGV:H281	2.01	0.43
3:P:116:TRP:HA	3:P:117:PRO:C	2.44	0.43
7:T:2:SER:O	23:T:101:PEK:H301	2.19	0.43
1:A:302[B]:ARG:HE	1:A:361:SER:HB2	1.83	0.43
1:A:302[B]:ARG:HH12	2:B:87:MET:CE	2.32	0.43
18:A:606:PGV:H012	11:K:9:PHE:HB2	2.01	0.43
3:C:47:LEU:O	3:C:51[A]:MET:HG2	2.18	0.43
4:D:78:TRP:N	20:D:201:TGL:CB2	2.82	0.43
7:G:7:ASP:HB3	7:G:8:HIS:H	1.54	0.43
7:G:42:ARG:HG3	7:G:43:GLU:H	1.84	0.43
8:H:55:TRP:H	8:U:46:LYS:NZ	2.15	0.43
3:C:67:PHE:CE2	24:C:306:CDL:H1	2.54	0.43
7:T:2:SER:HB2	23:T:101:PEK:C28	2.47	0.43
1:A:53:ILE:HD11	12:L:40:VAL:HG13	2.01	0.43
1:A:282:PHE:HZ	24:T:103:CDL:H761	1.83	0.43
2:B:168:LEU:HD13	2:B:184:LEU:HG	2.01	0.43
1:N:113[B]:LEU:HD11	1:N:117[B]:MET:SD	2.59	0.43
4:Q:29:HIS:CE1	4:Q:65:LYS:HG3	2.54	0.43
20:B:301:TGL:HA91	20:B:301:TGL:HA32	2.00	0.42
3:C:33:MET:HG2	3:C:39:SER:O	2.19	0.42
7:T:11:TPO:O3P	7:T:11:TPO:HA	2.19	0.42
9:V:59:ASP:O	9:V:63[B]:MET:HG3	2.19	0.42
20:L:101:TGL:H321	20:L:101:TGL:H352	2.00	0.42
1:N:122:ALA:HB3	28:N:712:HOH:O	2.18	0.42
3:C:110:PRO:HB3	8:H:30:TRP:CE3	2.55	0.42
12:L:26:THR:HG23	13:M:25:SER:CB	2.49	0.42
1:N:297[B]:MET:HG2	1:N:302[B]:ARG:CD	2.48	0.42
1:N:313:ALA:HB2	1:N:356:ILE:HD11	2.00	0.42
5:R:90:ARG:HB3	5:R:91:PRO:HD3	2.01	0.42
1:A:290:HIS:CD2	1:A:291:HIS:CD2	3.06	0.42
4:D:126:MET:HG3	4:D:128:VAL:HG23	2.00	0.42
2:O:102:HIS:O	2:O:104:TRP:HA	2.20	0.42
8:H:45:ALA:C	8:H:47:GLY:H	2.27	0.42
20:N:611:TGL:HC31	12:Y:13:PHE:HA	2.01	0.42
18:C:304:PGV:H132	24:C:306:CDL:H652	2.01	0.42
7:G:4:ALA:HB1	1:N:282:PHE:HA	2.02	0.42
1:N:243:VAL:HB	14:N:602:HEA:CAC	2.50	0.42
7:T:2:SER:HB2	23:T:101:PEK:C29	2.49	0.42
3:C:37:PHE:CD1	10:J:52:TRP:HZ3	2.38	0.42
3:P:111:GLU:HG3	28:U:147:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:PHE:HB3	3:C:28:THR:HB	2.01	0.42
6:F:87:THR:HG21	28:F:226:HOH:O	2.19	0.42
8:H:76:ARG:HD2	28:H:104:HOH:O	2.19	0.42
1:A:417:MET:CE	14:A:601:HEA:H263	2.50	0.42
3:P:33:MET:HE1	3:P:41:THR:HB	2.01	0.42
10:W:22:LEU:HA	10:W:28:ASP:HB3	2.02	0.42
4:D:86[A]:MET:HG2	20:D:201:TGL:H312	2.02	0.42
5:E:43:PRO:HB2	5:E:48:ILE:HD11	2.02	0.41
14:N:601:HEA:HHC	14:N:601:HEA:H122	2.01	0.41
2:O:108:TYR:O	2:O:117:SER:HA	2.20	0.41
3:P:33:MET:HG2	3:P:39:SER:O	2.19	0.41
3:P:127[A]:LEU:N	3:P:127[A]:LEU:HD22	2.35	0.41
3:P:146:TRP:CZ2	7:T:17:ARG:HG3	2.55	0.41
1:A:243:VAL:HB	14:A:602:HEA:CAC	2.50	0.41
4:D:93:ALA:HB3	11:K:28[B]:VAL:HG12	2.01	0.41
2:O:41:ILE:O	2:O:45:MET:HG2	2.20	0.41
6:S:64:GLU:O	6:S:65:ASP:CB	2.67	0.41
18:A:606:PGV:C29	13:M:16:ALA:HA	2.45	0.41
1:N:54:TYR:HB2	28:N:821:HOH:O	2.20	0.41
1:N:377:PHE:CE1	1:N:378:HIS:CE1	3.07	0.41
3:P:33:MET:HE2	3:P:42:LEU:H	1.85	0.41
11:X:29:TRP:CE3	11:X:32:MET:HE1	2.55	0.41
8:H:45:ALA:O	8:H:47:GLY:N	2.53	0.41
1:N:229:ILE:HD11	2:O:175:ILE:HD13	2.02	0.41
4:Q:19:ARG:HG2	4:Q:21:ASP:OD1	2.18	0.41
1:A:274:VAL:HG12	1:A:278:MET:HE2	2.03	0.41
3:C:257:TYR:O	3:C:261:SER:HB3	2.20	0.41
3:P:40[B]:MET:HE3	3:P:40[B]:MET:HB3	1.75	0.41
6:S:55:LYS:HA	6:S:74:LEU:O	2.21	0.41
1:A:344:PHE:CD1	1:A:344:PHE:C	2.99	0.41
2:B:58:ALA:O	2:B:62:GLU:HG3	2.21	0.41
24:C:306:CDL:H162	24:C:306:CDL:H352	2.03	0.41
7:G:9:GLY:HA3	1:N:178:GLN:HE21	1.84	0.41
1:A:449[A]:MET:HB2	11:K:40:TRP:O	2.20	0.41
1:A:449[A]:MET:SD	2:B:5:MET:HG2	2.61	0.41
1:N:110:LEU:HD21	25:P:307:DMU:H24	2.02	0.41
1:N:344:PHE:CD1	1:N:344:PHE:C	2.98	0.41
1:A:54:TYR:HB2	28:A:792:HOH:O	2.21	0.41
18:A:606:PGV:H291	13:M:19:LEU:HD22	2.03	0.41
2:B:32[B]:PHE:CD1	9:I:31:PHE:CZ	3.09	0.41
2:B:74:ILE:HG22	2:B:78:LEU:HD22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:77:LYS:HE2	3:C:81:TYR:OH	2.20	0.41
3:C:188[B]:ILE:HD12	3:C:195:SER:HA	2.03	0.41
7:G:1:ALA:HB2	18:P:304:PGV:H312	2.02	0.41
7:G:12:GLY:CA	28:G:249:HOH:O	2.68	0.41
7:G:18[B]:PHE:CD1	7:G:18[B]:PHE:C	2.99	0.41
8:H:36:PHE:CE1	8:H:57:ARG:HB2	2.56	0.41
1:N:155:VAL:HG21	18:N:609:PGV:H142	2.03	0.41
1:N:514:LYS:NZ	28:N:706:HOH:O	2.54	0.41
20:N:608:TGL:HB92	20:N:608:TGL:C28	2.51	0.41
2:O:215:PRO:HD3	9:V:60:PHE:CD1	2.55	0.41
3:P:22:LEU:O	3:P:26:LEU:HG	2.20	0.41
4:Q:6:VAL:HB	4:Q:10:ASP:OD2	2.21	0.41
5:R:12:ASP:OD2	5:R:44:GLU:HG3	2.21	0.41
9:V:22:VAL:O	9:V:26:MET:HG2	2.21	0.41
1:A:231:TYR:CD1	1:A:231:TYR:C	2.99	0.41
23:C:303:PEK:H371	23:C:303:PEK:H342	1.87	0.41
24:G:101:CDL:H541	24:G:101:CDL:H771	2.03	0.41
1:N:24:ALA:HB2	14:N:601:HEA:H253	2.02	0.41
12:Y:2:HIS:CG	12:Y:3:TYR:N	2.89	0.41
13:M:41:LYS:O	13:M:43:SER:N	2.52	0.40
1:N:290:HIS:CD2	1:N:291:HIS:CD2	3.08	0.40
2:O:121:TYR:O	2:O:138:VAL:HA	2.21	0.40
3:P:33:MET:HB2	25:P:307:DMU:H9	2.03	0.40
3:P:59:ARG:CA	24:P:305:CDL:H512	2.51	0.40
1:A:23:GLY:HA3	1:A:73:ILE:HG13	2.03	0.40
1:A:489:THR:HA	6:F:71:TRP:O	2.21	0.40
18:A:606:PGV:C29	13:M:19:LEU:HD23	2.49	0.40
1:N:177:SER:H	1:N:180:GLN:HE21	1.68	0.40
28:N:908:HOH:O	4:Q:20:ARG:HG3	2.20	0.40
1:A:304:TYR:CD2	1:A:304:TYR:C	2.98	0.40
1:A:513:LEU:O	1:A:514:LYS:CB	2.62	0.40
14:A:602:HEA:ND	19:A:607[B]:PER:O1	2.54	0.40
8:H:43:MET:HE1	8:U:43:MET:CE	2.40	0.40
2:O:4:PRO:HB2	11:X:43:SER:HA	2.03	0.40
1:A:417:MET:HE1	14:A:601:HEA:H263	2.03	0.40
18:A:606:PGV:H302	13:M:19:LEU:HD23	2.03	0.40
14:N:602:HEA:HBC1	14:N:602:HEA:HMC3	2.03	0.40
23:P:302:PEK:H012	28:P:496:HOH:O	2.20	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:31:LYS:CE	28:B:402:HOH:O[2_585]	2.12	0.08
28:B:482:HOH:O	28:D:361:HOH:O[2_584]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	524/514 (102%)	510 (97%)	14 (3%)	0	100	100
1	N	524/514 (102%)	511 (98%)	13 (2%)	0	100	100
2	B	230/227 (101%)	223 (97%)	7 (3%)	0	100	100
2	O	230/227 (101%)	221 (96%)	9 (4%)	0	100	100
3	C	265/261 (102%)	261 (98%)	4 (2%)	0	100	100
3	P	265/261 (102%)	260 (98%)	5 (2%)	0	100	100
4	D	148/147 (101%)	144 (97%)	4 (3%)	0	100	100
4	Q	143/147 (97%)	138 (96%)	5 (4%)	0	100	100
5	E	104/109 (95%)	104 (100%)	0	0	100	100
5	R	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
6	F	101/98 (103%)	94 (93%)	3 (3%)	4 (4%)	2	0
6	S	97/98 (99%)	91 (94%)	6 (6%)	0	100	100
7	G	82/85 (96%)	71 (87%)	8 (10%)	3 (4%)	2	0
7	T	84/85 (99%)	73 (87%)	8 (10%)	3 (4%)	2	0
8	H	77/85 (91%)	73 (95%)	1 (1%)	3 (4%)	2	0
8	U	77/85 (91%)	69 (90%)	5 (6%)	3 (4%)	2	0
9	I	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
9	V	72/73 (99%)	70 (97%)	2 (3%)	0	100	100
10	J	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
10	W	56/59 (95%)	55 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	48/56 (86%)	47 (98%)	1 (2%)	0	100	100
11	X	48/56 (86%)	46 (96%)	2 (4%)	0	100	100
12	L	44/47 (94%)	41 (93%)	3 (7%)	0	100	100
12	Y	44/47 (94%)	41 (93%)	2 (4%)	1 (2%)	5	1
13	M	41/46 (89%)	39 (95%)	1 (2%)	1 (2%)	4	1
13	Z	41/46 (89%)	39 (95%)	2 (5%)	0	100	100
All	All	3575/3614 (99%)	3448 (96%)	109 (3%)	18 (0%)	24	16

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	94	HIS
7	G	4	ALA
7	T	4	ALA
8	U	8	ILE
8	U	45	ALA
8	U	46	LYS
6	F	95	GLN
8	H	46	LYS
12	Y	46	LYS
7	G	9	GLY
8	H	8	ILE
13	M	42	LYS
7	T	3	ALA
7	T	6	GLY
6	F	97	ALA
8	H	45	ALA
6	F	2	SER
7	G	8	HIS

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	438/426 (103%)	430 (98%)	8 (2%)	51	50
1	N	438/426 (103%)	429 (98%)	9 (2%)	47	44
2	B	215/210 (102%)	208 (97%)	7 (3%)	33	26
2	O	215/210 (102%)	204 (95%)	11 (5%)	21	13
3	C	232/226 (103%)	229 (99%)	3 (1%)	61	61
3	P	232/226 (103%)	230 (99%)	2 (1%)	70	73
4	D	134/129 (104%)	132 (98%)	2 (2%)	57	56
4	Q	129/129 (100%)	122 (95%)	7 (5%)	20	12
5	E	93/95 (98%)	91 (98%)	2 (2%)	45	42
5	R	92/95 (97%)	89 (97%)	3 (3%)	33	26
6	F	86/81 (106%)	84 (98%)	2 (2%)	44	40
6	S	82/81 (101%)	75 (92%)	7 (8%)	10	4
7	G	68/68 (100%)	61 (90%)	7 (10%)	7	2
7	T	70/68 (103%)	62 (89%)	8 (11%)	5	2
8	H	71/75 (95%)	69 (97%)	2 (3%)	38	32
8	U	71/75 (95%)	67 (94%)	4 (6%)	19	11
9	I	57/57 (100%)	56 (98%)	1 (2%)	51	50
9	V	58/57 (102%)	56 (97%)	2 (3%)	32	25
10	J	49/50 (98%)	49 (100%)	0	100	100
10	W	49/50 (98%)	47 (96%)	2 (4%)	27	19
11	K	40/46 (87%)	40 (100%)	0	100	100
11	X	40/46 (87%)	38 (95%)	2 (5%)	22	14
12	L	39/40 (98%)	38 (97%)	1 (3%)	40	35
12	Y	39/40 (98%)	38 (97%)	1 (3%)	40	35
13	M	37/38 (97%)	37 (100%)	0	100	100
13	Z	37/38 (97%)	34 (92%)	3 (8%)	11	5
All	All	3111/3082 (101%)	3015 (97%)	96 (3%)	35	29

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LEU
1	A	38	ARG
1	A	138	HIS

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Mol	Chain	Res	Type
1	A	178	GLN
1	A	180	GLN
1	A	311[A]	ILE
1	A	311[B]	ILE
1	A	369	ASP
2	B	33	LEU
2	B	75	LEU
2	B	78	LEU
2	B	115	ASP
2	B	116	LEU
2	B	171	LYS
2	B	217	LYS
3	C	127	LEU
3	C	159	MET
3	C	230	ASN
4	D	7	LYS
4	D	31	LYS
5	E	70	VAL
5	E	90	ARG
6	F	48	LEU
6	F	95	GLN
7	G	2	SER
7	G	5	LYS
7	G	36	TRP
7	G	37	LEU
7	G	43	GLU
7	G	74	ARG
7	G	84	LYS
8	H	9	LYS
8	H	60	TYR
9	I	21	ILE
12	L	47	LYS
1	N	38	ARG
1	N	138	HIS
1	N	178	GLN
1	N	180	GLN
1	N	362	SER
1	N	363	LEU
1	N	369	ASP
1	N	484	THR
1	N	485	VAL
2	O	33	LEU

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Mol	Chain	Res	Type
2	O	60	GLU
2	O	61	VAL
2	O	68	LEU
2	O	75	LEU
2	O	78	LEU
2	O	86	MET
2	O	94	SER
2	O	114	GLU
2	O	221	LYS
2	O	226	MET
3	P	159	MET
3	P	230	ASN
4	Q	5	VAL
4	Q	6	VAL
4	Q	7	LYS
4	Q	8	SER
4	Q	9	GLU
4	Q	10	ASP
4	Q	51	LEU
5	R	5	HIS
5	R	79	LYS
5	R	80	GLU
6	S	37	LYS
6	S	54	ASN
6	S	80	GLN
6	S	87[A]	THR
6	S	87[B]	THR
6	S	95	GLN
6	S	96	LEU
7	T	5	LYS
7	T	17	ARG
7	T	33	LEU
7	T	36[A]	TRP
7	T	36[B]	TRP
7	T	37	LEU
7	T	74	ARG
7	T	84	LYS
8	U	8	ILE
8	U	9	LYS
8	U	29	CYS
8	U	60	TYR
9	V	45	LYS

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Mol	Chain	Res	Type
9	V	68	ILE
10	W	50	LEU
10	W	58	LYS
11	X	52	GLU
11	X	54	ARG
12	Y	20	ARG
13	Z	4	LYS
13	Z	13	LYS
13	Z	43	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	80	ASN
1	A	98	ASN
1	A	178	GLN
1	A	180	GLN
1	A	422	ASN
1	A	503	HIS
1	A	512	ASN
2	B	59	GLN
2	B	91	ASN
2	B	140	ASN
2	B	181	GLN
3	C	50	ASN
3	C	68	GLN
3	C	76	GLN
4	D	29	HIS
4	D	37	GLN
4	D	101	HIS
4	D	119	GLN
4	D	143	ASN
5	E	78	HIS
5	E	94	ASN
7	G	8	HIS
7	G	34	ASN
7	G	76	ASN
8	H	31	GLN
8	H	37	HIS
1	N	178	GLN
1	N	180	GLN

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Mol	Chain	Res	Type
1	N	422	ASN
1	N	503	HIS
1	N	512	ASN
2	O	59	GLN
2	O	181	GLN
2	O	195	GLN
3	P	50	ASN
3	P	68	GLN
4	Q	29	HIS
4	Q	37	GLN
4	Q	101	HIS
4	Q	109	HIS
4	Q	143	ASN
5	R	5	HIS
5	R	94	ASN
6	S	54	ASN
6	S	80	GLN
6	S	94	HIS
6	S	95	GLN
6	S	98	HIS
7	T	34	ASN
7	T	38	HIS
7	T	76	ASN
8	U	23	GLN
8	U	28	ASN
8	U	32	ASN
8	U	37	HIS
9	V	20	HIS
10	W	29	ASN
10	W	57	HIS
11	X	35	GLN
12	Y	2	HIS
13	Z	39	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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
9	SAC	V	1	9	7,8,9	1.17	1 (14%)	7,9,11	1.81	1 (14%)
7	TPO	T	11	7	8,10,11	1.55	1 (12%)	10,14,16	0.87	0
7	TPO	G	11	7	8,10,11	1.58	1 (12%)	10,14,16	1.16	1 (10%)
9	SAC	I	1	9	7,8,9	1.43	1 (14%)	7,9,11	1.68	2 (28%)
2	FME	B	1	2	8,9,10	1.40	1 (12%)	8,9,11	6.22	3 (37%)
1	FME	N	1	1	8,9,10	0.62	0	8,9,11	1.52	3 (37%)
1	FME	A	1	1	8,9,10	0.62	0	8,9,11	1.30	1 (12%)
2	FME	O	1	2	8,9,10	0.76	0	8,9,11	1.45	1 (12%)

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
9	SAC	V	1	9	-	2/7/8/10	-
7	TPO	T	11	7	-	7/9/11/13	-
7	TPO	G	11	7	-	5/9/11/13	-
9	SAC	I	1	9	-	4/7/8/10	-
2	FME	B	1	2	-	1/7/9/11	-
1	FME	N	1	1	-	1/7/9/11	-
1	FME	A	1	1	-	3/7/9/11	-
2	FME	O	1	2	-	0/7/9/11	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	1	SAC	CA-N	3.68	1.51	1.46
2	B	1	FME	O1-CN	-3.19	1.09	1.22
7	T	11	TPO	P-O1P	3.01	1.59	1.50
7	G	11	TPO	P-O1P	2.99	1.59	1.50
9	V	1	SAC	CA-N	2.83	1.50	1.46

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-17.25	96.30	122.82
9	V	1	SAC	C-CA-N	3.98	117.19	109.50
9	I	1	SAC	C-CA-N	3.26	115.78	109.50
1	A	1	FME	C-CA-N	2.46	114.25	109.50
2	O	1	FME	CG-CB-CA	-2.32	105.79	112.87
1	N	1	FME	CB-CA-N	2.27	114.65	110.52
1	N	1	FME	O-C-CA	-2.17	119.20	124.77
2	B	1	FME	O-C-CA	-2.13	119.30	124.77
7	G	11	TPO	O-C-CA	-2.11	119.36	124.77
1	N	1	FME	C-CA-N	2.08	113.50	109.50
9	I	1	SAC	O-C-CA	-2.06	119.46	124.77
2	B	1	FME	CG-CB-CA	-2.02	106.70	112.87

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	N-CA-CB-CG
2	B	1	FME	O1-CN-N-CA
7	G	11	TPO	N-CA-CB-CG2
7	G	11	TPO	N-CA-CB-OG1
7	G	11	TPO	C-CA-CB-CG2
7	G	11	TPO	O-C-CA-CB
7	G	11	TPO	CA-CB-OG1-P
9	I	1	SAC	C2A-C1A-N-CA
9	I	1	SAC	OAC-C1A-N-CA
9	I	1	SAC	C-CA-N-C1A
1	N	1	FME	O-C-CA-CB
7	T	11	TPO	N-CA-CB-OG1
7	T	11	TPO	O-C-CA-CB
7	T	11	TPO	CA-CB-OG1-P
7	T	11	TPO	CG2-CB-OG1-P
9	V	1	SAC	C2A-C1A-N-CA
9	V	1	SAC	OAC-C1A-N-CA
1	A	1	FME	CB-CG-SD-CE
1	A	1	FME	C-CA-CB-CG
9	I	1	SAC	C-CA-CB-OG
7	T	11	TPO	N-CA-CB-CG2
7	T	11	TPO	CB-OG1-P-O3P
7	T	11	TPO	C-CA-CB-CG2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	T	11	TPO	1	0
7	G	11	TPO	1	0
2	O	1	FME	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 58 ligands modelled in this entry, 10 are monoatomic - leaving 48 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
23	PEK	P	302	-	52,52,52	1.07	2 (3%)	55,57,57	1.06	4 (7%)
18	PGV	P	303	-	50,50,50	0.91	3 (6%)	53,56,56	0.83	3 (5%)
18	PGV	N	606	-	50,50,50	1.00	2 (4%)	53,56,56	1.38	7 (13%)
22	CHD	C	307	-	32,32,32	0.63	0	51,51,51	2.16	19 (37%)
14	HEA	A	602	19,1	67,67,67	1.95	23 (34%)	81,103,103	1.55	13 (16%)
20	TGL	D	201	-	62,62,62	1.13	4 (6%)	65,65,65	0.85	4 (6%)
26	PSC	E	201	-	51,51,51	1.18	3 (5%)	57,59,59	0.95	2 (3%)
20	TGL	Q	201	-	62,62,62	1.16	3 (4%)	65,65,65	0.89	5 (7%)
20	TGL	N	611	-	62,62,62	1.16	3 (4%)	65,65,65	1.25	5 (7%)
20	TGL	N	608	-	62,62,62	1.10	3 (4%)	65,65,65	1.15	5 (7%)
21	CUA	O	302	2	0,1,1	-	-	-	-	-
23	PEK	T	102	-	52,52,52	0.92	3 (5%)	55,57,57	1.26	6 (10%)
23	PEK	C	303	-	52,52,52	1.06	2 (3%)	55,57,57	1.01	5 (9%)
23	PEK	C	302	-	52,52,52	0.85	2 (3%)	55,57,57	0.90	4 (7%)
14	HEA	A	601	1	67,67,67	2.00	21 (31%)	81,103,103	1.70	18 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CHD	B	303	-	32,32,32	1.06	2 (6%)	51,51,51	1.17	4 (7%)
19	PER	A	607[B]	15	1,1,1	0.90	0	-		
14	HEA	N	602	19,1	67,67,67	1.99	19 (28%)	81,103,103	1.38	14 (17%)
24	CDL	G	101	-	99,99,99	1.48	12 (12%)	105,111,111	1.21	6 (5%)
24	CDL	C	306	-	99,99,99	1.41	12 (12%)	105,111,111	1.26	10 (9%)
18	PGV	A	608	-	50,50,50	0.93	2 (4%)	53,56,56	1.24	4 (7%)
18	PGV	N	609	-	50,50,50	0.93	2 (4%)	53,56,56	1.29	5 (9%)
26	PSC	R	201	-	51,51,51	1.20	3 (5%)	57,59,59	1.03	3 (5%)
25	DMU	P	307	-	34,34,34	0.75	1 (2%)	45,45,45	1.00	3 (6%)
18	PGV	C	304	-	50,50,50	0.84	2 (4%)	53,56,56	0.99	2 (3%)
14	HEA	N	601	1	67,67,67	2.07	22 (32%)	81,103,103	1.58	16 (19%)
22	CHD	C	308	-	32,32,32	1.01	1 (3%)	51,51,51	1.26	6 (11%)
19	PER	N	607[B]	15	1,1,1	0.90	0	-		
21	CUA	B	302	2	0,1,1	-	-	-		
22	CHD	N	610	-	32,32,32	0.91	0	51,51,51	1.12	3 (5%)
19	PER	A	607[A]	15,14	1,1,1	0.90	0	-		
25	DMU	C	309	-	34,34,34	0.61	0	45,45,45	1.22	4 (8%)
22	CHD	J	101	-	32,32,32	0.61	0	51,51,51	1.96	13 (25%)
23	PEK	G	102	-	52,52,52	1.04	2 (3%)	55,57,57	1.10	3 (5%)
22	CHD	O	301	-	32,32,32	0.90	0	51,51,51	1.49	9 (17%)
18	PGV	P	304	-	50,50,50	1.15	2 (4%)	53,56,56	1.05	4 (7%)
24	CDL	P	305	-	99,99,99	1.44	12 (12%)	105,111,111	1.29	8 (7%)
20	TGL	B	301	-	62,62,62	1.13	3 (4%)	65,65,65	1.50	7 (10%)
25	DMU	M	101	-	34,34,34	0.51	0	45,45,45	1.13	3 (6%)
23	PEK	T	101	-	52,52,52	1.07	2 (3%)	55,57,57	0.96	3 (5%)
19	PER	N	607[A]	15,14	1,1,1	0.90	0	-		
25	DMU	Z	101	-	34,34,34	0.50	0	45,45,45	0.85	1 (2%)
22	CHD	P	306	-	32,32,32	0.66	0	51,51,51	1.54	10 (19%)
18	PGV	A	606	-	50,50,50	0.95	2 (4%)	53,56,56	1.38	7 (13%)
20	TGL	L	101	-	62,62,62	1.17	3 (4%)	65,65,65	1.48	9 (13%)
24	CDL	T	103	-	99,99,99	1.42	12 (12%)	105,111,111	1.22	9 (8%)
22	CHD	W	101	-	32,32,32	0.63	0	51,51,51	2.31	19 (37%)
18	PGV	C	305	-	50,50,50	1.09	2 (4%)	53,56,56	0.96	3 (5%)

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
23	PEK	P	302	-	-	26/56/56/56	-
18	PGV	P	303	-	-	13/55/55/55	-
18	PGV	N	606	-	-	34/55/55/55	-
22	CHD	C	307	-	-	7/9/74/74	0/4/4/4
14	HEA	A	602	19,1	-	5/36/76/76	-
20	TGL	D	201	-	-	40/65/65/65	-
26	PSC	E	201	-	-	23/55/55/55	-
20	TGL	Q	201	-	-	33/65/65/65	-
20	TGL	N	611	-	-	30/65/65/65	-
20	TGL	N	608	-	-	37/65/65/65	-
23	PEK	T	102	-	-	20/56/56/56	-
23	PEK	C	303	-	-	32/56/56/56	-
23	PEK	C	302	-	-	14/56/56/56	-
14	HEA	A	601	1	-	8/36/76/76	-
22	CHD	B	303	-	-	2/9/74/74	0/4/4/4
14	HEA	N	602	19,1	-	7/36/76/76	-
24	CDL	G	101	-	-	66/110/110/110	-
24	CDL	C	306	-	-	62/110/110/110	-
18	PGV	A	608	-	-	6/55/55/55	-
18	PGV	N	609	-	-	11/55/55/55	-
26	PSC	R	201	-	-	22/55/55/55	-
25	DMU	P	307	-	-	8/19/59/59	0/2/2/2
18	PGV	C	304	-	-	15/55/55/55	-
14	HEA	N	601	1	-	6/36/76/76	-
22	CHD	C	308	-	-	2/9/74/74	0/4/4/4
22	CHD	N	610	-	-	2/9/74/74	0/4/4/4
25	DMU	C	309	-	-	9/19/59/59	0/2/2/2
22	CHD	J	101	-	-	5/9/74/74	0/4/4/4
23	PEK	G	102	-	-	31/56/56/56	-
22	CHD	O	301	-	-	2/9/74/74	0/4/4/4
18	PGV	P	304	-	-	27/55/55/55	-
24	CDL	P	305	-	-	71/110/110/110	-
20	TGL	B	301	-	-	34/65/65/65	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	DMU	M	101	-	-	5/19/59/59	0/2/2/2
23	PEK	T	101	-	-	20/56/56/56	-
25	DMU	Z	101	-	-	5/19/59/59	0/2/2/2
22	CHD	P	306	-	-	4/9/74/74	0/4/4/4
18	PGV	A	606	-	-	31/55/55/55	-
20	TGL	L	101	-	-	37/65/65/65	-
24	CDL	T	103	-	-	59/110/110/110	-
22	CHD	W	101	-	-	8/9/74/74	0/4/4/4
18	PGV	C	305	-	-	29/55/55/55	-

All (192) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	L	101	TGL	OG2-CB1	5.65	1.50	1.34
20	N	611	TGL	OG2-CB1	5.57	1.50	1.34
14	N	601	HEA	FE-ND	5.41	2.11	1.94
14	N	601	HEA	FE-NC	5.38	2.12	1.95
18	P	304	PGV	O03-C19	5.23	1.48	1.33
20	B	301	TGL	OG1-CA1	5.19	1.48	1.33
14	A	602	HEA	FE-NB	5.11	2.10	1.94
24	G	101	CDL	OB6-CB5	5.10	1.48	1.34
23	C	303	PEK	O03-C21	5.06	1.48	1.33
26	R	201	PSC	O01-C1	5.06	1.48	1.34
14	A	602	HEA	FE-ND	5.04	2.10	1.94
23	P	302	PEK	O01-C1	4.97	1.48	1.34
23	T	101	PEK	O03-C21	4.93	1.47	1.33
20	N	608	TGL	OG1-CA1	4.91	1.47	1.33
14	N	602	HEA	FE-ND	4.91	2.10	1.94
14	N	602	HEA	FE-NA	4.91	2.11	1.95
20	L	101	TGL	OG3-CC1	4.90	1.47	1.33
20	Q	201	TGL	OG3-CC1	4.90	1.47	1.33
24	P	305	CDL	OA8-CA7	4.89	1.47	1.33
24	G	101	CDL	OB8-CB7	4.86	1.47	1.33
23	G	102	PEK	O03-C21	4.86	1.47	1.33
20	Q	201	TGL	OG2-CB1	4.85	1.48	1.34
24	P	305	CDL	OB8-CB7	4.84	1.47	1.33
18	P	304	PGV	O01-C1	4.81	1.47	1.34
20	N	608	TGL	OG2-CB1	4.79	1.47	1.34
20	Q	201	TGL	OG1-CA1	4.77	1.47	1.33
20	N	611	TGL	OG3-CC1	4.77	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	T	101	PEK	O01-C1	4.76	1.47	1.34
23	P	302	PEK	O03-C21	4.76	1.47	1.33
26	E	201	PSC	O01-C1	4.75	1.47	1.34
24	T	103	CDL	OA6-CA5	4.73	1.47	1.34
18	C	305	PGV	O03-C19	4.71	1.47	1.33
18	C	305	PGV	O01-C1	4.70	1.47	1.34
24	T	103	CDL	OA8-CA7	4.70	1.47	1.33
24	G	101	CDL	OA6-CA5	4.69	1.47	1.34
24	C	306	CDL	OB8-CB7	4.62	1.46	1.33
14	A	601	HEA	FE-ND	4.62	2.09	1.94
18	N	606	PGV	O03-C19	4.62	1.46	1.33
24	C	306	CDL	OA8-CA7	4.59	1.46	1.33
14	N	602	HEA	FE-NB	4.57	2.09	1.94
23	G	102	PEK	O01-C1	4.56	1.47	1.34
24	G	101	CDL	OA8-CA7	4.53	1.46	1.33
26	E	201	PSC	O03-C19	4.51	1.46	1.33
20	D	201	TGL	OG1-CA1	4.47	1.46	1.33
20	B	301	TGL	OG3-CC1	4.47	1.46	1.33
20	L	101	TGL	OG1-CA1	4.45	1.46	1.33
18	A	606	PGV	O03-C19	4.43	1.46	1.33
24	P	305	CDL	OA6-CA5	4.41	1.46	1.34
24	T	103	CDL	OB6-CB5	4.38	1.46	1.34
24	P	305	CDL	OB6-CB5	4.37	1.46	1.34
26	R	201	PSC	O03-C19	4.37	1.46	1.33
24	C	306	CDL	OA6-CA5	4.37	1.46	1.34
20	N	608	TGL	OG3-CC1	4.36	1.46	1.33
20	D	201	TGL	OG2-CB1	4.34	1.46	1.34
20	N	611	TGL	OG1-CA1	4.34	1.46	1.33
20	B	301	TGL	OG2-CB1	4.32	1.46	1.34
18	P	303	PGV	O03-C19	4.27	1.45	1.33
18	N	606	PGV	O01-C1	4.26	1.46	1.34
23	C	303	PEK	O01-C1	4.24	1.46	1.34
24	T	103	CDL	OB8-CB7	4.18	1.45	1.33
14	A	601	HEA	FE-NA	4.15	2.08	1.95
20	D	201	TGL	OG3-CC1	4.15	1.45	1.33
14	A	601	HEA	C1C-NC	-4.09	1.31	1.39
26	R	201	PSC	C13-C12	4.03	1.54	1.31
14	A	601	HEA	FE-NB	4.00	2.07	1.94
23	T	102	PEK	O03-C21	3.98	1.45	1.33
14	N	601	HEA	CHC-C4B	3.97	1.46	1.38
24	C	306	CDL	C59-C58	-3.96	1.32	1.51
14	N	601	HEA	C1D-ND	-3.92	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	E	201	PSC	C13-C12	3.88	1.53	1.31
14	A	601	HEA	C1A-C2A	-3.86	1.38	1.45
24	C	306	CDL	OB6-CB5	3.85	1.45	1.34
14	N	601	HEA	C3A-C4A	-3.84	1.39	1.46
18	A	606	PGV	O01-C1	3.83	1.45	1.34
14	N	602	HEA	CHD-C1D	3.80	1.46	1.38
14	A	601	HEA	C1D-ND	-3.79	1.33	1.40
14	N	601	HEA	C1C-NC	-3.74	1.32	1.39
23	C	302	PEK	O01-C1	3.72	1.44	1.34
14	N	602	HEA	CHB-C4A	3.70	1.45	1.38
24	T	103	CDL	C59-C58	-3.65	1.33	1.51
24	G	101	CDL	C19-C18	-3.65	1.33	1.51
18	N	609	PGV	O03-C19	3.65	1.44	1.33
24	P	305	CDL	C79-C78	-3.63	1.33	1.51
24	C	306	CDL	C79-C78	-3.62	1.33	1.51
24	P	305	CDL	C22-C21	-3.62	1.33	1.51
24	P	305	CDL	C59-C58	-3.62	1.33	1.51
24	T	103	CDL	C82-C81	-3.60	1.33	1.51
24	G	101	CDL	C22-C21	-3.60	1.33	1.51
14	N	601	HEA	C4D-ND	-3.60	1.31	1.38
24	G	101	CDL	C62-C61	-3.59	1.33	1.51
24	C	306	CDL	C22-C21	-3.58	1.34	1.51
24	P	305	CDL	C19-C18	-3.58	1.34	1.51
24	T	103	CDL	C79-C78	-3.58	1.34	1.51
24	P	305	CDL	C39-C38	-3.57	1.34	1.51
24	T	103	CDL	C19-C18	-3.55	1.34	1.51
14	A	602	HEA	CHD-C1D	3.55	1.45	1.38
24	T	103	CDL	C22-C21	-3.55	1.34	1.51
24	G	101	CDL	C59-C58	-3.54	1.34	1.51
24	C	306	CDL	C19-C18	-3.54	1.34	1.51
24	P	305	CDL	C82-C81	-3.53	1.34	1.51
24	C	306	CDL	C39-C38	-3.52	1.34	1.51
14	A	602	HEA	CHC-C4B	3.52	1.45	1.38
18	A	608	PGV	O03-C19	3.51	1.43	1.33
24	C	306	CDL	C62-C61	-3.51	1.34	1.51
24	G	101	CDL	C79-C78	-3.51	1.34	1.51
14	A	601	HEA	CHA-C1A	3.50	1.45	1.38
24	G	101	CDL	C42-C41	-3.50	1.34	1.51
24	C	306	CDL	C82-C81	-3.50	1.34	1.51
24	G	101	CDL	C39-C38	-3.50	1.34	1.51
24	T	103	CDL	C42-C41	-3.49	1.34	1.51
24	G	101	CDL	C82-C81	-3.49	1.34	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	T	103	CDL	C62-C61	-3.47	1.34	1.51
24	T	103	CDL	C39-C38	-3.45	1.34	1.51
18	C	304	PGV	O03-C19	3.45	1.43	1.33
14	A	601	HEA	FE-NC	3.45	2.06	1.95
14	N	602	HEA	C4D-C3D	-3.44	1.39	1.45
24	P	305	CDL	C42-C41	-3.43	1.34	1.51
24	P	305	CDL	C62-C61	-3.42	1.34	1.51
24	C	306	CDL	C42-C41	-3.42	1.34	1.51
14	A	601	HEA	C4B-NB	-3.42	1.34	1.40
14	N	602	HEA	C3A-C4A	-3.39	1.40	1.46
14	A	601	HEA	CHB-C4A	3.35	1.44	1.38
18	A	608	PGV	O01-C1	3.34	1.43	1.34
14	N	602	HEA	CHA-C1A	3.33	1.44	1.38
23	C	302	PEK	O03-C21	3.33	1.43	1.33
25	P	307	DMU	O16-C6	3.32	1.45	1.40
14	A	601	HEA	CBD-CGD	3.30	1.58	1.50
14	N	601	HEA	C4B-NB	-3.30	1.34	1.40
14	A	602	HEA	FE-NA	3.29	2.06	1.95
14	N	602	HEA	C4B-NB	-3.28	1.34	1.40
14	N	601	HEA	C4A-NA	-3.28	1.33	1.39
14	N	601	HEA	CHB-C4A	3.27	1.44	1.38
14	A	601	HEA	CHC-C4B	3.27	1.45	1.38
14	A	602	HEA	CHB-C4A	3.23	1.44	1.38
14	N	602	HEA	CHC-C4B	3.20	1.44	1.38
14	A	601	HEA	C3A-C4A	-3.19	1.40	1.46
14	N	601	HEA	FE-NB	3.15	2.04	1.94
14	N	601	HEA	FE-NA	3.14	2.05	1.95
14	A	602	HEA	CHA-C1A	3.14	1.44	1.38
23	T	102	PEK	O01-C1	3.12	1.43	1.34
14	A	602	HEA	CHB-C1B	3.04	1.46	1.39
14	N	602	HEA	CHB-C1B	3.02	1.46	1.39
14	N	601	HEA	C4C-NC	-3.01	1.34	1.39
14	A	602	HEA	C4B-NB	-2.97	1.35	1.40
18	C	304	PGV	O01-C1	2.96	1.42	1.34
14	N	601	HEA	C1A-C2A	-2.94	1.40	1.45
18	N	609	PGV	O01-C1	2.93	1.42	1.34
14	N	602	HEA	C1A-NA	-2.93	1.34	1.39
14	A	602	HEA	C4D-C3D	-2.92	1.40	1.45
14	A	602	HEA	C4A-NA	-2.92	1.34	1.39
14	N	601	HEA	C4D-C3D	-2.91	1.40	1.45
18	P	303	PGV	O01-C1	2.89	1.42	1.34
14	N	601	HEA	CHA-C1A	2.83	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	602	HEA	C1D-C2D	-2.77	1.38	1.44
20	D	201	TGL	OB1-CB1	2.76	1.30	1.22
14	A	601	HEA	C4A-NA	-2.74	1.34	1.39
14	A	602	HEA	CHC-C1C	2.70	1.45	1.39
14	N	601	HEA	CHA-C4D	2.67	1.45	1.39
14	A	601	HEA	C4C-NC	-2.67	1.34	1.39
14	A	602	HEA	FE-NC	2.60	2.03	1.95
14	N	602	HEA	CHC-C1C	2.59	1.45	1.39
14	A	601	HEA	C1B-NB	-2.54	1.33	1.38
14	N	601	HEA	O11-C11	2.51	1.48	1.42
14	N	601	HEA	CHD-C1D	2.50	1.43	1.38
14	A	602	HEA	C1C-NC	-2.47	1.35	1.39
14	A	601	HEA	C4D-C3D	-2.43	1.40	1.45
14	A	602	HEA	C3A-C4A	-2.41	1.41	1.46
22	C	308	CHD	C11-C9	2.40	1.57	1.53
22	B	303	CHD	C11-C12	2.37	1.57	1.53
14	N	602	HEA	C1A-C2A	-2.35	1.41	1.45
14	N	601	HEA	CHC-C1C	2.35	1.44	1.39
14	A	602	HEA	C1A-C2A	-2.34	1.41	1.45
14	A	602	HEA	C1D-C2D	-2.32	1.39	1.44
22	B	303	CHD	C11-C9	2.28	1.57	1.53
14	A	601	HEA	C4B-C3B	-2.26	1.40	1.44
14	N	602	HEA	FE-NC	2.25	2.02	1.95
14	A	602	HEA	C4C-NC	-2.20	1.35	1.39
23	T	102	PEK	O01-C02	-2.18	1.41	1.46
14	A	602	HEA	C4D-ND	-2.16	1.34	1.38
18	P	303	PGV	O01-C02	-2.15	1.41	1.46
14	N	602	HEA	C1D-ND	-2.13	1.36	1.40
14	A	601	HEA	CHA-C4D	2.13	1.44	1.39
14	N	602	HEA	C4A-NA	-2.13	1.35	1.39
14	A	602	HEA	CHA-C4D	2.12	1.44	1.39
14	N	601	HEA	C1D-C2D	-2.08	1.40	1.44
14	N	602	HEA	CHD-C4C	2.08	1.44	1.39
14	A	601	HEA	C1D-C2D	-2.05	1.40	1.44
14	A	602	HEA	CMA-C3A	2.05	1.49	1.45
14	A	601	HEA	CHD-C1D	2.05	1.42	1.38
14	A	602	HEA	C4B-C3B	-2.04	1.41	1.44
14	N	601	HEA	C1B-NB	-2.02	1.34	1.38
14	A	602	HEA	CBD-CGD	2.00	1.55	1.50

All (288) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	301	TGL	OG2-CB1-CB2	7.33	127.34	111.48
22	C	307	CHD	C16-C17-C20	6.46	121.95	112.18
22	C	307	CHD	C14-C13-C12	6.26	113.13	107.42
22	J	101	CHD	C17-C13-C14	-5.97	94.13	100.11
22	W	101	CHD	C17-C13-C12	5.82	122.90	117.67
20	N	611	TGL	OG2-CB1-CB2	5.78	123.98	111.48
18	N	606	PGV	O01-C1-C2	5.68	123.77	111.48
20	L	101	TGL	OG2-CB1-CB2	5.60	123.59	111.48
24	G	101	CDL	OB6-CB5-C51	5.51	123.40	111.48
22	W	101	CHD	C15-C14-C8	5.37	125.72	118.36
24	T	103	CDL	OA6-CA5-C11	5.15	122.62	111.48
18	N	609	PGV	O03-C19-O04	-5.13	110.80	123.63
18	A	606	PGV	O01-C1-C2	5.11	122.54	111.48
18	A	608	PGV	O03-C19-O04	-5.11	110.85	123.63
22	C	307	CHD	C17-C13-C14	-4.98	95.11	100.11
20	N	608	TGL	OG2-CB1-CB2	4.98	122.25	111.48
23	P	302	PEK	O01-C1-C2	4.83	121.92	111.48
22	W	101	CHD	C14-C8-C7	4.83	118.25	111.85
23	G	102	PEK	O01-C1-C2	4.67	121.59	111.48
24	P	305	CDL	OA6-CA5-C11	4.62	121.48	111.48
14	A	602	HEA	OMA-CMA-C3A	-4.61	115.21	125.62
24	G	101	CDL	OA6-CA5-C11	4.58	121.39	111.48
18	N	609	PGV	O03-C19-C20	4.55	125.69	111.83
22	J	101	CHD	C13-C17-C20	4.52	124.96	119.48
24	C	306	CDL	OA6-CA5-C11	4.47	121.16	111.48
14	A	602	HEA	CAD-CBD-CGD	-4.46	101.83	113.67
24	P	305	CDL	OB6-CB5-C51	4.43	121.06	111.48
23	C	303	PEK	O01-C1-C2	4.40	120.99	111.48
22	W	101	CHD	C14-C8-C9	-4.35	103.68	109.75
23	T	102	PEK	O01-C1-O02	-4.25	113.76	123.70
22	J	101	CHD	C6-C5-C4	-4.24	106.39	111.23
18	A	608	PGV	O03-C19-C20	4.19	124.60	111.83
23	T	102	PEK	O03-C21-C22	4.18	124.58	111.83
20	L	101	TGL	OG3-CC1-CC2	4.17	124.55	111.83
22	W	101	CHD	C18-C13-C12	-4.17	104.88	109.06
24	T	103	CDL	OB6-CB5-C51	4.17	120.49	111.48
23	T	101	PEK	O01-C1-C2	4.12	120.40	111.48
26	E	201	PSC	O01-C1-C2	4.12	120.39	111.48
20	B	301	TGL	OG3-CC1-CC2	4.11	124.36	111.83
23	T	102	PEK	C2-C3-C4	4.11	122.33	113.35
14	N	601	HEA	OMA-CMA-C3A	-4.10	116.36	125.62
18	P	304	PGV	O01-C1-C2	4.09	120.33	111.48
14	A	601	HEA	C13-C12-C11	-4.01	107.99	114.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	W	101	CHD	C13-C17-C20	4.00	124.33	119.48
22	W	101	CHD	C6-C5-C10	3.95	116.86	112.66
24	P	305	CDL	OB8-CB7-C71	3.92	123.79	111.83
18	C	305	PGV	O01-C1-C2	3.91	119.95	111.48
18	P	304	PGV	O03-C19-C20	3.90	123.74	111.83
24	P	305	CDL	CB4-OB6-CB5	-3.84	108.61	117.80
25	C	309	DMU	C7-C8-C9	3.83	117.17	110.23
26	R	201	PSC	O01-C1-C2	3.79	119.68	111.48
18	N	606	PGV	O03-C19-C20	3.78	123.36	111.83
24	C	306	CDL	OB6-CB5-C51	3.75	119.58	111.48
14	A	602	HEA	CHA-C1A-NA	3.71	128.50	124.45
22	O	301	CHD	C11-C12-C13	3.69	115.02	111.26
20	N	608	TGL	OG1-CA1-CA2	3.65	122.96	111.83
14	A	601	HEA	O11-C11-C3B	-3.64	104.59	111.26
25	M	101	DMU	O16-C6-C1	3.58	113.71	108.27
22	C	307	CHD	C23-C22-C20	-3.57	107.79	114.46
25	C	309	DMU	O1-C9-C8	3.53	116.05	109.70
14	A	602	HEA	C3C-C4C-NC	3.52	112.76	109.80
23	G	102	PEK	O03-C21-C22	3.52	122.56	111.83
24	C	306	CDL	OB8-CB7-C71	3.51	122.53	111.83
18	C	304	PGV	O03-C19-O04	-3.41	115.11	123.63
22	J	101	CHD	C6-C5-C10	3.38	116.26	112.66
14	N	602	HEA	CAD-CBD-CGD	-3.38	104.70	113.67
20	B	301	TGL	OG3-CC1-OC1	-3.36	115.22	123.63
22	J	101	CHD	C16-C17-C20	3.35	117.25	112.18
22	P	306	CHD	C15-C14-C13	3.34	106.78	103.54
20	N	611	TGL	OG3-CC1-CC2	3.33	121.99	111.83
14	N	602	HEA	OMA-CMA-C3A	-3.30	118.17	125.62
20	B	301	TGL	CB3-CB2-CB1	-3.30	101.61	113.69
25	C	309	DMU	C10-O1-C9	3.29	120.14	113.72
22	W	101	CHD	C11-C12-C13	3.29	114.61	111.26
14	A	601	HEA	C3C-C4C-NC	3.26	112.55	109.80
14	A	602	HEA	C27-C19-C20	3.26	120.89	115.23
22	P	306	CHD	C1-C2-C3	3.25	114.79	110.48
25	P	307	DMU	O16-C6-C1	3.25	113.20	108.27
14	N	601	HEA	O2A-CGA-CBA	3.24	124.24	114.00
20	N	608	TGL	OG3-CC1-CC2	3.23	121.70	111.83
22	B	303	CHD	C19-C10-C1	-3.22	103.19	108.31
18	C	304	PGV	O03-C19-C20	3.22	121.64	111.83
18	C	305	PGV	O03-C19-C20	3.20	121.58	111.83
18	A	606	PGV	O03-C19-C20	3.16	121.46	111.83
14	N	602	HEA	CHA-C1A-NA	3.15	127.89	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	G	101	CDL	OB8-CB7-C71	3.14	121.41	111.83
24	G	101	CDL	OA8-CA7-C31	3.13	121.39	111.83
22	C	307	CHD	C19-C10-C1	-3.11	103.37	108.31
14	A	602	HEA	C13-C12-C11	-3.10	109.43	114.39
26	R	201	PSC	O03-C19-C20	3.10	121.29	111.83
22	O	301	CHD	O12-C12-C11	-3.10	102.81	109.12
14	A	601	HEA	CMC-C2C-C1C	-3.10	120.70	125.42
22	C	308	CHD	C5-C6-C7	3.09	118.08	114.40
14	N	601	HEA	O1A-CGA-CBA	-3.09	113.28	123.09
14	N	602	HEA	O2A-CGA-CBA	3.08	123.74	114.00
18	A	606	PGV	O01-C1-O02	-3.08	116.51	123.70
24	C	306	CDL	CB4-OB6-CB5	-3.08	110.43	117.80
14	A	601	HEA	C2B-C1B-NB	3.07	113.45	109.90
14	A	601	HEA	C1B-C2B-C3B	-3.06	103.25	106.80
22	P	306	CHD	C15-C14-C8	3.06	122.56	118.36
20	B	301	TGL	OG1-CA1-CA2	3.06	121.16	111.83
14	A	601	HEA	CHC-C4B-NB	-3.04	120.60	124.37
25	M	101	DMU	C18-O16-C6	-3.04	108.50	113.68
20	Q	201	TGL	OG3-CC1-CC2	3.03	121.08	111.83
22	C	307	CHD	C11-C9-C10	-3.02	110.64	113.70
14	A	601	HEA	O2D-CGD-O1D	-3.01	115.59	123.33
18	N	606	PGV	O03-C19-O04	-2.99	116.16	123.63
14	N	601	HEA	O2D-CGD-CBD	2.98	123.40	114.00
22	J	101	CHD	C4-C5-C10	2.97	115.82	112.66
22	J	101	CHD	C22-C20-C17	2.97	116.48	110.33
14	N	601	HEA	O11-C11-C3B	-2.96	105.83	111.26
20	L	101	TGL	CG2-OG2-CB1	2.96	124.88	117.80
14	N	601	HEA	C13-C14-C15	-2.96	120.86	127.62
18	A	606	PGV	C02-O01-C1	-2.95	110.72	117.80
20	Q	201	TGL	OG2-CB1-CB2	2.95	117.86	111.48
14	N	601	HEA	C27-C19-C20	2.95	120.34	115.23
22	O	301	CHD	C18-C13-C17	-2.94	106.60	111.20
24	C	306	CDL	OB8-CB7-OB9	-2.93	116.30	123.63
14	A	601	HEA	CMC-C2C-C3C	2.93	133.43	126.55
14	A	601	HEA	C27-C19-C20	2.92	120.30	115.23
23	T	101	PEK	O03-C21-C22	2.92	120.74	111.83
23	G	102	PEK	O03-C21-O04	-2.92	116.33	123.63
14	A	602	HEA	CHA-C1A-C2A	-2.92	120.25	124.86
14	A	601	HEA	O2A-CGA-CBA	2.90	123.15	114.00
24	T	103	CDL	OB8-CB7-C71	2.87	120.57	111.83
22	W	101	CHD	C9-C10-C5	2.86	112.48	108.51
22	J	101	CHD	C1-C10-C5	2.86	111.85	107.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	W	101	CHD	C13-C14-C8	-2.85	111.10	114.72
23	C	303	PEK	O03-C21-C22	2.84	120.48	111.83
20	L	101	TGL	OG1-CA1-CA2	2.82	120.43	111.83
22	C	307	CHD	C1-C10-C5	2.82	111.79	107.75
14	A	601	HEA	CAA-CBA-CGA	-2.81	106.20	113.67
14	A	601	HEA	C25-C23-C22	-2.81	114.23	122.66
20	N	611	TGL	OG3-CC1-OC1	-2.80	116.62	123.63
22	W	101	CHD	C6-C5-C4	-2.80	108.03	111.23
24	P	305	CDL	OA8-CA7-C31	2.80	120.37	111.83
20	D	201	TGL	OG3-CC1-OC1	-2.80	116.63	123.63
14	N	601	HEA	C13-C12-C11	-2.80	109.92	114.39
18	A	608	PGV	O01-C1-C2	2.77	117.47	111.48
22	N	610	CHD	C21-C20-C22	-2.76	106.07	110.34
22	C	308	CHD	C19-C10-C1	-2.76	103.92	108.31
22	J	101	CHD	C9-C10-C5	2.75	112.33	108.51
22	C	307	CHD	C15-C14-C8	2.75	122.13	118.36
14	A	602	HEA	O11-C11-C3B	-2.75	106.22	111.26
22	J	101	CHD	C15-C14-C13	2.74	106.20	103.54
24	P	305	CDL	OB8-CB7-OB9	-2.74	116.78	123.63
23	C	302	PEK	O03-C21-O04	-2.74	116.78	123.63
22	W	101	CHD	C1-C10-C5	2.73	111.66	107.75
14	N	602	HEA	CHB-C1B-NB	2.72	127.35	124.42
14	A	601	HEA	O1A-CGA-CBA	-2.71	114.49	123.09
14	A	601	HEA	OMA-CMA-C3A	-2.70	119.53	125.62
24	T	103	CDL	OA8-CA7-C31	2.70	120.07	111.83
18	N	609	PGV	O01-C1-O02	-2.70	117.40	123.70
24	C	306	CDL	OA8-CA7-C31	2.69	120.05	111.83
22	J	101	CHD	C17-C13-C12	2.69	120.09	117.67
24	T	103	CDL	OB8-CB7-OB9	-2.69	116.90	123.63
22	B	303	CHD	C22-C23-C24	-2.68	105.34	112.49
14	N	601	HEA	C3D-C4D-ND	2.68	112.94	110.35
14	N	602	HEA	C13-C12-C11	-2.67	110.12	114.39
23	P	302	PEK	O03-C21-C22	2.67	119.98	111.83
22	N	610	CHD	C6-C5-C4	-2.67	108.17	111.23
18	N	606	PGV	C3-C2-C1	-2.67	103.92	113.69
22	C	307	CHD	C6-C7-C8	2.67	114.41	111.50
18	A	606	PGV	O03-C19-O04	-2.66	116.98	123.63
20	B	301	TGL	OB1-CB1-CB2	-2.65	113.41	123.78
14	N	601	HEA	CHA-C4D-ND	-2.65	121.57	124.42
14	N	601	HEA	C3C-C4C-NC	2.63	112.01	109.80
18	N	609	PGV	O01-C1-C2	2.63	117.17	111.48
20	L	101	TGL	C25-C24-C23	-2.62	101.15	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	602	HEA	CHC-C1C-C2C	-2.61	119.84	127.43
22	O	301	CHD	C16-C17-C20	-2.56	108.30	112.18
22	C	307	CHD	C6-C5-C4	-2.56	108.30	111.23
22	N	610	CHD	C22-C20-C17	-2.56	105.02	110.33
18	P	304	PGV	C01-O03-C19	2.55	126.46	117.12
22	C	307	CHD	C6-C5-C10	2.54	115.37	112.66
26	E	201	PSC	O03-C19-C20	2.53	119.56	111.83
20	L	101	TGL	OG3-CC1-OC1	-2.53	117.31	123.63
20	Q	201	TGL	OG1-CA1-CA2	2.51	119.50	111.83
23	C	302	PEK	O01-C1-C2	2.51	116.92	111.48
22	W	101	CHD	C22-C20-C17	2.49	115.49	110.33
20	D	201	TGL	OG3-CC1-CC2	2.49	119.41	111.83
14	N	602	HEA	CHB-C1B-C2B	-2.48	121.11	125.03
14	A	602	HEA	C1D-C2D-C3D	-2.48	104.38	106.98
22	O	301	CHD	C11-C9-C10	-2.47	111.20	113.70
18	A	606	PGV	C24-C23-C22	-2.46	101.92	114.37
20	L	101	TGL	OG2-CB1-OB1	-2.45	117.98	123.70
22	W	101	CHD	C17-C13-C14	-2.44	97.66	100.11
22	C	307	CHD	C15-C14-C13	2.43	105.89	103.54
14	A	601	HEA	C4C-C3C-C2C	-2.43	104.29	107.30
22	C	308	CHD	C6-C5-C4	-2.42	108.46	111.23
24	G	101	CDL	OA6-CA5-OA7	-2.42	118.04	123.70
22	P	306	CHD	C16-C17-C13	2.42	105.89	103.54
23	C	303	PEK	C01-O03-C21	2.42	125.97	117.12
14	N	602	HEA	C3C-C4C-NC	2.42	111.83	109.80
24	T	103	CDL	OB8-CB6-CB4	2.40	115.33	108.40
22	P	306	CHD	C10-C9-C8	2.40	114.52	111.84
22	P	306	CHD	C4-C3-C2	2.40	113.55	110.62
24	T	103	CDL	OA6-CA5-OA7	-2.39	118.11	123.70
22	W	101	CHD	C1-C2-C3	2.38	113.64	110.48
18	C	305	PGV	C01-O03-C19	2.38	125.83	117.12
18	P	303	PGV	O03-C19-O04	-2.37	117.71	123.63
25	C	309	DMU	O16-C6-C1	2.36	111.86	108.27
14	N	602	HEA	C20-C19-C18	-2.35	115.90	121.17
14	N	602	HEA	CAA-CBA-CGA	-2.33	107.48	113.67
23	T	102	PEK	O03-C21-O04	-2.33	117.81	123.63
22	W	101	CHD	C10-C9-C8	2.33	114.43	111.84
20	D	201	TGL	OG1-CA1-CA2	2.32	118.91	111.83
22	P	306	CHD	C6-C5-C10	2.32	115.12	112.66
24	G	101	CDL	OB6-CB5-OB7	-2.31	118.29	123.70
22	W	101	CHD	C6-C7-C8	2.31	114.02	111.50
22	P	306	CHD	C5-C4-C3	-2.31	109.23	112.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	303	CHD	C4-C3-C2	2.31	113.43	110.62
22	C	307	CHD	C17-C13-C12	-2.30	115.60	117.67
24	P	305	CDL	C54-C53-C52	-2.29	102.77	114.37
18	P	303	PGV	O03-C19-C20	2.29	118.82	111.83
23	T	102	PEK	O01-C1-C2	2.28	116.42	111.48
18	N	609	PGV	O03-C01-C02	2.27	114.93	108.40
23	C	303	PEK	O03-C21-O04	-2.26	117.97	123.63
22	O	301	CHD	C22-C23-C24	-2.26	106.46	112.49
14	A	602	HEA	C3A-C2A-C1A	-2.25	104.91	107.05
22	C	308	CHD	C11-C12-C13	2.25	113.55	111.26
14	N	601	HEA	CHB-C1B-C2B	-2.25	121.48	125.03
22	C	307	CHD	C22-C23-C24	-2.25	106.50	112.49
24	C	306	CDL	OA6-CA5-OA7	-2.24	118.46	123.70
23	C	302	PEK	C01-O03-C21	2.23	125.27	117.12
25	P	307	DMU	C18-O16-C6	2.23	117.48	113.68
22	B	303	CHD	C17-C13-C12	2.22	119.67	117.67
20	B	301	TGL	CG3-OG3-CC1	2.22	125.24	117.12
25	M	101	DMU	C22-C19-C18	-2.22	103.82	113.47
22	C	307	CHD	C16-C17-C13	2.21	105.69	103.54
14	A	601	HEA	O2D-CGD-CBD	2.21	121.00	114.00
18	A	608	PGV	O01-C1-O02	-2.21	118.54	123.70
22	W	101	CHD	C5-C6-C7	2.20	117.02	114.40
18	N	606	PGV	C02-O01-C1	-2.20	112.53	117.80
24	C	306	CDL	OB6-CB5-OB7	-2.20	118.57	123.70
20	N	611	TGL	OG2-CB1-OB1	-2.19	118.58	123.70
22	C	308	CHD	C18-C13-C12	2.19	111.25	109.06
22	O	301	CHD	C11-C9-C8	2.18	114.12	110.89
22	C	308	CHD	C15-C14-C13	2.18	105.66	103.54
14	N	602	HEA	C27-C19-C20	2.18	119.01	115.23
18	P	303	PGV	O01-C1-O02	-2.18	118.61	123.70
20	L	101	TGL	CA4-CA3-CA2	-2.18	105.13	113.13
22	W	101	CHD	C19-C10-C9	-2.14	108.30	111.18
20	Q	201	TGL	OG1-CA1-OA1	-2.14	118.27	123.63
14	A	601	HEA	C1C-CHC-C4B	2.14	131.28	126.25
14	N	601	HEA	C4C-C3C-C2C	-2.14	104.64	107.30
14	N	601	HEA	C25-C23-C22	-2.14	116.25	122.66
22	C	307	CHD	C5-C6-C7	2.14	116.94	114.40
25	Z	101	DMU	C18-O16-C6	-2.13	110.04	113.68
23	C	303	PEK	O01-C1-O02	-2.13	118.72	123.70
24	C	306	CDL	CB6-OB8-CB7	2.13	124.89	117.12
22	C	307	CHD	C4-C5-C10	2.11	114.91	112.66
22	P	306	CHD	C11-C9-C8	2.11	114.02	110.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	P	305	CDL	OA6-CA5-OA7	-2.11	118.77	123.70
22	C	307	CHD	C11-C9-C8	2.11	114.02	110.89
14	A	602	HEA	CHC-C1C-C2C	-2.11	121.31	127.43
22	J	101	CHD	C18-C13-C17	2.11	114.50	111.20
20	N	608	TGL	OG1-CA1-OA1	-2.10	118.37	123.63
25	P	307	DMU	O16-C18-C19	2.10	116.50	109.37
22	P	306	CHD	C14-C8-C9	-2.09	106.83	109.75
23	T	102	PEK	O13-P-O14	2.09	122.17	112.44
24	C	306	CDL	C83-C82-C81	2.09	124.92	114.37
23	T	101	PEK	C01-O03-C21	2.09	124.74	117.12
22	J	101	CHD	C11-C12-C13	2.09	113.39	111.26
22	O	301	CHD	O26-C24-C23	2.08	120.57	114.00
18	N	606	PGV	O01-C1-O02	-2.08	118.85	123.70
14	A	602	HEA	C26-C15-C16	2.07	118.82	115.23
20	D	201	TGL	CG3-OG3-CC1	2.06	124.66	117.12
24	T	103	CDL	OB6-CB5-OB7	-2.06	118.88	123.70
22	O	301	CHD	C19-C10-C1	-2.06	105.03	108.31
14	N	602	HEA	O11-C11-C3B	-2.06	107.49	111.26
14	N	601	HEA	CHA-C1A-NA	2.05	126.69	124.45
18	N	606	PGV	C01-O03-C19	2.05	124.59	117.12
23	P	302	PEK	O03-C21-O04	-2.04	118.52	123.63
14	N	601	HEA	O2D-CGD-O1D	-2.04	118.08	123.33
22	C	307	CHD	O25-C24-C23	-2.04	116.63	123.09
14	N	602	HEA	O1A-CGA-CBA	-2.03	116.65	123.09
23	C	302	PEK	O13-P-O14	2.03	121.88	112.44
14	A	602	HEA	O2D-CGD-CBD	2.03	120.41	114.00
23	P	302	PEK	C01-O03-C21	2.03	124.52	117.12
20	N	608	TGL	OG3-CC1-OC1	-2.03	118.56	123.63
20	L	101	TGL	C23-C22-C21	-2.03	104.13	114.37
18	P	304	PGV	O03-C19-O04	-2.02	118.57	123.63
20	Q	201	TGL	OG3-CC1-OC1	-2.02	118.57	123.63
26	R	201	PSC	O03-C19-O04	-2.02	118.57	123.63
24	T	103	CDL	CA6-OA8-CA7	2.02	124.50	117.12
18	A	606	PGV	O05-C05-C04	2.00	116.61	109.70
20	N	611	TGL	OG3-CG3-CG2	2.00	114.16	108.40

There are no chirality outliers.

All (908) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	601	HEA	C2A-C3A-CMA-OMA
14	N	601	HEA	C2A-C3A-CMA-OMA

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Mol	Chain	Res	Type	Atoms
18	A	606	PGV	C03-O11-P-O12
18	A	606	PGV	C03-O11-P-O13
18	A	606	PGV	C03-O11-P-O14
18	A	606	PGV	O12-C04-C05-O05
18	C	305	PGV	C03-O11-P-O12
18	C	305	PGV	C03-O11-P-O13
18	C	305	PGV	C04-C05-C06-O06
18	N	606	PGV	C03-O11-P-O12
18	N	606	PGV	C03-O11-P-O13
18	N	606	PGV	C03-O11-P-O14
18	N	606	PGV	C02-C03-O11-P
18	N	606	PGV	C04-C05-C06-O06
18	N	606	PGV	O04-C19-O03-C01
18	N	606	PGV	C20-C19-O03-C01
20	B	301	TGL	OB1-CB1-OG2-CG2
20	L	101	TGL	CB2-CB1-OG2-CG2
20	L	101	TGL	OB1-CB1-OG2-CG2
20	N	611	TGL	CB2-CB1-OG2-CG2
20	N	611	TGL	OB1-CB1-OG2-CG2
22	C	307	CHD	C13-C17-C20-C21
22	W	101	CHD	C13-C17-C20-C21
22	W	101	CHD	C13-C17-C20-C22
22	W	101	CHD	C16-C17-C20-C21
22	W	101	CHD	C16-C17-C20-C22
23	C	303	PEK	C03-O11-P-O12
23	C	303	PEK	C03-O11-P-O13
23	C	303	PEK	C03-O11-P-O14
23	C	303	PEK	C04-O12-P-O11
23	C	303	PEK	C04-O12-P-O13
23	C	303	PEK	C04-O12-P-O14
23	C	303	PEK	C2-C1-O01-C02
23	G	102	PEK	C04-O12-P-O11
23	G	102	PEK	C04-O12-P-O14
23	G	102	PEK	O04-C21-O03-C01
23	G	102	PEK	C22-C21-O03-C01
23	G	102	PEK	C12-C13-C14-C15
23	P	302	PEK	C03-O11-P-O12
23	P	302	PEK	C04-O12-P-O14
23	P	302	PEK	O02-C1-O01-C02
23	P	302	PEK	C2-C1-O01-C02
23	P	302	PEK	C4-C5-C6-C7
23	T	101	PEK	C03-O11-P-O14

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Mol	Chain	Res	Type	Atoms
23	T	101	PEK	O12-C04-C05-N
24	C	306	CDL	C1-CA2-OA2-PA1
24	C	306	CDL	CA2-OA2-PA1-OA4
24	C	306	CDL	CA2-OA2-PA1-OA5
24	C	306	CDL	CA3-OA5-PA1-OA4
24	C	306	CDL	C11-CA5-OA6-CA4
24	C	306	CDL	CB2-OB2-PB2-OB3
24	C	306	CDL	CB2-OB2-PB2-OB4
24	C	306	CDL	CB3-OB5-PB2-OB2
24	C	306	CDL	OB7-CB5-OB6-CB4
24	G	101	CDL	CB2-C1-CA2-OA2
24	G	101	CDL	CA2-OA2-PA1-OA4
24	G	101	CDL	CA2-OA2-PA1-OA5
24	G	101	CDL	CA3-OA5-PA1-OA2
24	G	101	CDL	CA3-OA5-PA1-OA3
24	G	101	CDL	CA3-OA5-PA1-OA4
24	G	101	CDL	OA9-CA7-OA8-CA6
24	G	101	CDL	C31-CA7-OA8-CA6
24	G	101	CDL	CB2-OB2-PB2-OB3
24	G	101	CDL	CB3-OB5-PB2-OB2
24	G	101	CDL	CB3-OB5-PB2-OB3
24	G	101	CDL	CB3-OB5-PB2-OB4
24	G	101	CDL	C51-CB5-OB6-CB4
24	P	305	CDL	O1-C1-CA2-OA2
24	P	305	CDL	C1-CA2-OA2-PA1
24	P	305	CDL	CA3-OA5-PA1-OA4
24	P	305	CDL	OA7-CA5-OA6-CA4
24	P	305	CDL	CB2-OB2-PB2-OB3
24	P	305	CDL	CB2-OB2-PB2-OB4
24	P	305	CDL	CB2-OB2-PB2-OB5
24	P	305	CDL	CB3-OB5-PB2-OB2
24	P	305	CDL	CB3-OB5-PB2-OB3
24	P	305	CDL	CB3-OB5-PB2-OB4
24	P	305	CDL	C51-CB5-OB6-CB4
24	T	103	CDL	CA3-OA5-PA1-OA4
24	T	103	CDL	OA6-CA4-CA6-OA8
24	T	103	CDL	C11-CA5-OA6-CA4
24	T	103	CDL	C1-CB2-OB2-PB2
24	T	103	CDL	CB2-OB2-PB2-OB4
24	T	103	CDL	CB2-OB2-PB2-OB5
24	T	103	CDL	CB3-OB5-PB2-OB2
24	T	103	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
24	T	103	CDL	CB3-OB5-PB2-OB4
24	T	103	CDL	C51-CB5-OB6-CB4
25	C	309	DMU	C1-C6-O16-C18
25	P	307	DMU	O5-C6-O16-C18
26	E	201	PSC	C04-O12-P-O11
26	E	201	PSC	C04-O12-P-O13
26	E	201	PSC	O12-C04-C05-N
26	R	201	PSC	C03-O11-P-O12
26	R	201	PSC	C03-O11-P-O13
26	R	201	PSC	C04-O12-P-O11
26	R	201	PSC	C04-O12-P-O13
26	R	201	PSC	C01-C02-O01-C1
26	R	201	PSC	O12-C04-C05-N
20	B	301	TGL	CC2-CC1-OG3-CG3
18	A	606	PGV	O04-C19-O03-C01
20	B	301	TGL	OC1-CC1-OG3-CG3
20	D	201	TGL	OC1-CC1-OG3-CG3
24	C	306	CDL	OB9-CB7-OB8-CB6
26	R	201	PSC	O04-C19-O03-C01
22	C	307	CHD	C16-C17-C20-C21
22	C	307	CHD	C13-C17-C20-C22
23	C	303	PEK	O02-C1-O01-C02
24	C	306	CDL	OA7-CA5-OA6-CA4
24	G	101	CDL	OA7-CA5-OA6-CA4
24	G	101	CDL	OB7-CB5-OB6-CB4
24	P	305	CDL	OB7-CB5-OB6-CB4
24	T	103	CDL	OA7-CA5-OA6-CA4
24	T	103	CDL	OB7-CB5-OB6-CB4
24	C	306	CDL	CB4-CB6-OB8-CB7
26	R	201	PSC	C20-C19-O03-C01
20	B	301	TGL	CB2-CB1-OG2-CG2
24	C	306	CDL	C51-CB5-OB6-CB4
24	P	305	CDL	C11-CA5-OA6-CA4
22	C	307	CHD	C16-C17-C20-C22
18	A	606	PGV	C20-C19-O03-C01
20	D	201	TGL	CC2-CC1-OG3-CG3
24	C	306	CDL	C71-CB7-OB8-CB6
18	P	304	PGV	C10-C11-C12-C13
23	C	302	PEK	C13-C14-C15-C16
23	C	303	PEK	C10-C11-C12-C13
23	T	102	PEK	C4-C5-C6-C7
22	W	101	CHD	C17-C20-C22-C23

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Mol	Chain	Res	Type	Atoms
18	N	606	PGV	O12-C04-C05-O05
24	G	101	CDL	O1-C1-CA2-OA2
24	G	101	CDL	O1-C1-CB2-OB2
24	G	101	CDL	C71-CB7-OB8-CB6
24	T	103	CDL	C71-CB7-OB8-CB6
24	T	103	CDL	OB9-CB7-OB8-CB6
18	N	606	PGV	C2-C1-O01-C02
24	G	101	CDL	C11-CA5-OA6-CA4
25	C	309	DMU	C19-C22-C25-C28
14	A	601	HEA	C27-C19-C20-C21
18	N	606	PGV	O02-C1-O01-C02
14	A	601	HEA	C15-C16-C17-C18
23	C	303	PEK	C34-C35-C36-C37
24	G	101	CDL	OB9-CB7-OB8-CB6
26	E	201	PSC	O04-C19-O03-C01
25	C	309	DMU	O5-C6-O16-C18
26	E	201	PSC	C20-C19-O03-C01
25	P	307	DMU	O6-C11-C9-O1
18	A	606	PGV	C10-C11-C12-C13
18	N	609	PGV	C10-C11-C12-C13
23	C	303	PEK	C4-C5-C6-C7
23	P	302	PEK	C13-C14-C15-C16
23	T	102	PEK	C13-C14-C15-C16
26	E	201	PSC	C11-C12-C13-C14
25	P	307	DMU	O6-C11-C9-C8
25	C	309	DMU	C3-C4-C57-O61
24	T	103	CDL	C40-C41-C42-C43
18	C	305	PGV	O12-C04-C05-C06
24	G	101	CDL	CA2-C1-CB2-OB2
24	T	103	CDL	CA2-C1-CB2-OB2
20	L	101	TGL	CA2-CA1-OG1-CG1
20	N	611	TGL	CA2-CA1-OG1-CG1
20	Q	201	TGL	CC2-CC1-OG3-CG3
18	P	303	PGV	C28-C29-C30-C31
20	N	608	TGL	C24-C25-C26-C27
24	C	306	CDL	C37-C38-C39-C40
24	C	306	CDL	C81-C82-C83-C84
24	G	101	CDL	C15-C16-C17-C18
24	T	103	CDL	C79-C80-C81-C82
26	E	201	PSC	C20-C21-C22-C23
25	P	307	DMU	C1-C6-O16-C18
24	G	101	CDL	C78-C79-C80-C81

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Mol	Chain	Res	Type	Atoms
22	W	101	CHD	C21-C20-C22-C23
24	T	103	CDL	O1-C1-CB2-OB2
20	N	611	TGL	CA9-C20-C21-C22
22	P	306	CHD	C20-C22-C23-C24
23	P	302	PEK	C21-C22-C23-C24
23	T	102	PEK	C1-C2-C3-C4
20	L	101	TGL	OA1-CA1-OG1-CG1
20	Q	201	TGL	OC1-CC1-OG3-CG3
25	C	309	DMU	O5-C4-C57-O61
25	C	309	DMU	O6-C11-C9-O1
18	C	305	PGV	O01-C02-C03-O11
20	N	608	TGL	CA2-CA1-OG1-CG1
23	C	302	PEK	C4-C5-C6-C7
23	C	303	PEK	C7-C8-C9-C10
20	L	101	TGL	CC1-CC2-CC3-CC4
24	G	101	CDL	C41-C42-C43-C44
25	M	101	DMU	O6-C11-C9-O1
14	N	601	HEA	C19-C20-C21-C22
18	N	606	PGV	C1-C2-C3-C4
23	G	102	PEK	C21-C22-C23-C24
23	T	101	PEK	C1-C2-C3-C4
20	N	611	TGL	OA1-CA1-OG1-CG1
25	M	101	DMU	O6-C11-C9-C8
18	C	305	PGV	C1-C2-C3-C4
24	P	305	CDL	CA5-C11-C12-C13
26	E	201	PSC	C1-C2-C3-C4
18	A	608	PGV	C26-C27-C28-C29
20	N	608	TGL	CB1-CB2-CB3-CB4
23	G	102	PEK	C7-C8-C9-C10
23	T	102	PEK	C10-C11-C12-C13
26	R	201	PSC	C11-C10-C9-C8
14	A	601	HEA	C18-C19-C20-C21
20	N	608	TGL	OA1-CA1-OG1-CG1
24	C	306	CDL	CA5-C11-C12-C13
18	A	606	PGV	O12-C04-C05-C06
18	N	606	PGV	O12-C04-C05-C06
24	P	305	CDL	CB2-C1-CA2-OA2
26	E	201	PSC	C04-C05-N-C06
26	E	201	PSC	C04-C05-N-C07
26	E	201	PSC	C04-C05-N-C08
20	D	201	TGL	C21-C22-C23-C24
18	C	305	PGV	O12-C04-C05-O05

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Mol	Chain	Res	Type	Atoms
18	P	304	PGV	C20-C19-O03-C01
18	A	606	PGV	C04-C05-C06-O06
18	P	304	PGV	C04-C05-C06-O06
23	C	303	PEK	C22-C21-O03-C01
22	J	101	CHD	C13-C17-C20-C21
20	Q	201	TGL	C13-C14-C29-C30
23	C	303	PEK	C33-C34-C35-C36
24	C	306	CDL	C17-C18-C19-C20
18	A	606	PGV	C30-C31-C32-C33
18	C	305	PGV	C30-C31-C32-C33
18	N	606	PGV	C25-C26-C27-C28
18	N	609	PGV	C23-C24-C25-C26
20	B	301	TGL	CC4-CC5-CC6-CC7
20	B	301	TGL	C16-C17-C18-C19
20	D	201	TGL	CC2-CC3-CC4-CC5
20	Q	201	TGL	C10-C11-C12-C13
24	C	306	CDL	C51-C52-C53-C54
24	C	306	CDL	C80-C81-C82-C83
24	G	101	CDL	C61-C62-C63-C64
24	T	103	CDL	C62-C63-C64-C65
26	R	201	PSC	C2-C3-C4-C5
23	C	302	PEK	C7-C8-C9-C10
23	G	102	PEK	C4-C5-C6-C7
26	R	201	PSC	C11-C12-C13-C14
18	A	608	PGV	C27-C28-C29-C30
20	D	201	TGL	C19-C33-C34-C35
20	L	101	TGL	CB5-CB6-CB7-CB8
23	C	302	PEK	C32-C33-C34-C35
24	G	101	CDL	C38-C39-C40-C41
24	P	305	CDL	C57-C58-C59-C60
26	R	201	PSC	C20-C21-C22-C23
20	B	301	TGL	C16-C15-CC9-CC8
20	N	608	TGL	CB7-CB8-CB9-C10
20	N	611	TGL	C21-C20-CA9-CA8
20	N	611	TGL	CB5-CB6-CB7-CB8
20	N	611	TGL	CC3-CC4-CC5-CC6
24	G	101	CDL	C35-C36-C37-C38
24	G	101	CDL	C60-C61-C62-C63
24	T	103	CDL	C31-C32-C33-C34
24	T	103	CDL	C71-C72-C73-C74
26	E	201	PSC	C21-C22-C23-C24
20	N	608	TGL	OB1-CB1-OG2-CG2

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Mol	Chain	Res	Type	Atoms
18	A	606	PGV	O05-C05-C06-O06
18	N	606	PGV	O05-C05-C06-O06
18	C	305	PGV	C3-C4-C5-C6
20	N	611	TGL	C21-C22-C23-C24
24	G	101	CDL	C51-C52-C53-C54
24	P	305	CDL	C62-C63-C64-C65
23	C	303	PEK	C1-C2-C3-C4
24	C	306	CDL	C23-C24-C25-C26
18	C	304	PGV	C13-C14-C15-C16
18	P	303	PGV	C24-C25-C26-C27
18	C	305	PGV	C2-C1-O01-C02
20	N	608	TGL	CB2-CB1-OG2-CG2
20	Q	201	TGL	CB2-CB1-OG2-CG2
23	C	303	PEK	C26-C27-C28-C29
18	P	304	PGV	C22-C23-C24-C25
24	T	103	CDL	C80-C81-C82-C83
20	D	201	TGL	CC1-CC2-CC3-CC4
18	C	305	PGV	C22-C23-C24-C25
20	B	301	TGL	CA5-CA6-CA7-CA8
20	N	611	TGL	C10-C11-C12-C13
24	C	306	CDL	C15-C16-C17-C18
24	G	101	CDL	C71-C72-C73-C74
20	D	201	TGL	C16-C15-CC9-CC8
23	T	101	PEK	C23-C24-C25-C26
23	T	101	PEK	C32-C33-C34-C35
24	C	306	CDL	C14-C15-C16-C17
24	P	305	CDL	CB7-C71-C72-C73
18	P	304	PGV	O04-C19-O03-C01
20	B	301	TGL	C10-C11-C12-C13
25	P	307	DMU	C22-C25-C28-C31
24	G	101	CDL	C21-C22-C23-C24
20	Q	201	TGL	CA2-CA1-OG1-CG1
20	L	101	TGL	C11-C10-CB9-CB8
24	G	101	CDL	C43-C44-C45-C46
24	T	103	CDL	C82-C83-C84-C85
20	D	201	TGL	CB1-CB2-CB3-CB4
18	P	304	PGV	C20-C21-C22-C23
20	D	201	TGL	C13-C14-C29-C30
20	L	101	TGL	CB3-CB4-CB5-CB6
20	L	101	TGL	C18-C19-C33-C34
20	N	608	TGL	CA6-CA7-CA8-CA9
20	N	611	TGL	CB4-CB5-CB6-CB7

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Mol	Chain	Res	Type	Atoms
20	N	611	TGL	C13-C14-C29-C30
23	T	102	PEK	C26-C27-C28-C29
24	G	101	CDL	C74-C75-C76-C77
24	T	103	CDL	C43-C44-C45-C46
23	C	303	PEK	O04-C21-O03-C01
18	C	304	PGV	C7-C8-C9-C10
20	L	101	TGL	C16-C15-CC9-CC8
20	N	608	TGL	C13-C14-C29-C30
20	Q	201	TGL	CA7-CA8-CA9-C20
20	Q	201	TGL	C20-C21-C22-C23
24	C	306	CDL	C11-C12-C13-C14
18	C	305	PGV	C4-C5-C6-C7
18	P	304	PGV	C24-C25-C26-C27
23	G	102	PEK	C33-C34-C35-C36
24	P	305	CDL	C37-C38-C39-C40
20	Q	201	TGL	CB9-C10-C11-C12
23	P	302	PEK	C28-C29-C30-C31
25	M	101	DMU	C19-C22-C25-C28
20	N	608	TGL	CA5-CA6-CA7-CA8
26	E	201	PSC	C6-C7-C8-C9
18	P	303	PGV	C10-C11-C12-C13
23	P	302	PEK	C10-C11-C12-C13
23	T	101	PEK	C10-C11-C12-C13
23	C	302	PEK	C30-C31-C32-C33
23	C	302	PEK	C31-C32-C33-C34
24	G	101	CDL	C22-C23-C24-C25
24	P	305	CDL	C42-C43-C44-C45
20	B	301	TGL	C21-C20-CA9-CA8
20	L	101	TGL	CA3-CA4-CA5-CA6
20	N	608	TGL	C16-C15-CC9-CC8
24	P	305	CDL	C18-C19-C20-C21
20	N	611	TGL	C18-C19-C33-C34
20	Q	201	TGL	CB5-CB6-CB7-CB8
24	T	103	CDL	C53-C54-C55-C56
24	C	306	CDL	C55-C56-C57-C58
18	C	305	PGV	O02-C1-O01-C02
20	Q	201	TGL	CB4-CB5-CB6-CB7
23	C	302	PEK	C26-C27-C28-C29
23	T	102	PEK	C33-C34-C35-C36
25	Z	101	DMU	C28-C31-C34-C37
18	C	304	PGV	C27-C28-C29-C30
18	N	606	PGV	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
20	D	201	TGL	C21-C20-CA9-CA8
20	N	608	TGL	CB6-CB7-CB8-CB9
24	C	306	CDL	C13-C14-C15-C16
24	G	101	CDL	C83-C84-C85-C86
24	P	305	CDL	C55-C56-C57-C58
24	T	103	CDL	C31-CA7-OA8-CA6
20	L	101	TGL	C21-C22-C23-C24
20	N	608	TGL	CC5-CC6-CC7-CC8
22	J	101	CHD	C13-C17-C20-C22
18	A	606	PGV	C13-C14-C15-C16
20	L	101	TGL	C13-C14-C29-C30
20	L	101	TGL	CC3-CC4-CC5-CC6
24	P	305	CDL	C22-C23-C24-C25
20	N	611	TGL	C16-C17-C18-C19
20	N	611	TGL	C19-C33-C34-C35
20	L	101	TGL	C22-C23-C24-C25
24	C	306	CDL	C35-C36-C37-C38
24	T	103	CDL	C63-C64-C65-C66
20	D	201	TGL	C23-C24-C25-C26
20	N	608	TGL	CB4-CB5-CB6-CB7
18	A	606	PGV	C2-C1-O01-C02
23	G	102	PEK	C2-C1-O01-C02
20	Q	201	TGL	OB1-CB1-OG2-CG2
20	D	201	TGL	C10-C11-C12-C13
20	N	608	TGL	C20-C21-C22-C23
18	N	606	PGV	C11-C10-C9-C8
18	P	304	PGV	C12-C13-C14-C15
23	C	302	PEK	C15-C16-C17-C18
24	C	306	CDL	C79-C80-C81-C82
24	P	305	CDL	C21-C22-C23-C24
18	C	304	PGV	C25-C26-C27-C28
20	D	201	TGL	CC5-CC6-CC7-CC8
20	D	201	TGL	CC9-C15-C16-C17
20	D	201	TGL	C14-C29-C30-C31
22	J	101	CHD	C16-C17-C20-C21
18	N	606	PGV	C21-C22-C23-C24
20	B	301	TGL	C17-C18-C19-C33
20	D	201	TGL	CB9-C10-C11-C12
24	G	101	CDL	C79-C80-C81-C82
24	T	103	CDL	C39-C40-C41-C42
26	E	201	PSC	C5-C6-C7-C8
18	P	304	PGV	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
24	G	101	CDL	C40-C41-C42-C43
18	N	606	PGV	C14-C15-C16-C17
20	B	301	TGL	C11-C12-C13-C14
23	P	302	PEK	C29-C30-C31-C32
24	C	306	CDL	C63-C64-C65-C66
24	P	305	CDL	C13-C14-C15-C16
24	P	305	CDL	C83-C84-C85-C86
20	Q	201	TGL	OA1-CA1-OG1-CG1
24	C	306	CDL	C53-C54-C55-C56
18	N	606	PGV	C4-C5-C6-C7
24	C	306	CDL	OB5-CB3-CB4-OB6
20	Q	201	TGL	CC5-CC6-CC7-CC8
24	G	101	CDL	C31-C32-C33-C34
25	C	309	DMU	C18-C19-C22-C25
20	B	301	TGL	CA3-CA4-CA5-CA6
20	L	101	TGL	CC6-CC7-CC8-CC9
20	Q	201	TGL	CC3-CC4-CC5-CC6
24	P	305	CDL	C82-C83-C84-C85
20	N	608	TGL	CB3-CB4-CB5-CB6
20	N	608	TGL	C12-C13-C14-C29
20	Q	201	TGL	CC4-CC5-CC6-CC7
23	T	101	PEK	C31-C32-C33-C34
24	P	305	CDL	C11-C12-C13-C14
24	P	305	CDL	C81-C82-C83-C84
18	A	606	PGV	C12-C13-C14-C15
18	C	305	PGV	C12-C13-C14-C15
23	C	303	PEK	C15-C16-C17-C18
20	B	301	TGL	CA2-CA3-CA4-CA5
20	N	611	TGL	C16-C15-CC9-CC8
20	N	611	TGL	C15-C16-C17-C18
20	L	101	TGL	C17-C18-C19-C33
20	N	608	TGL	CB9-C10-C11-C12
24	T	103	CDL	C76-C77-C78-C79
23	G	102	PEK	C24-C25-C26-C27
18	C	304	PGV	C20-C21-C22-C23
20	B	301	TGL	CA4-CA5-CA6-CA7
24	P	305	CDL	C56-C57-C58-C59
24	C	306	CDL	C78-C79-C80-C81
23	P	302	PEK	C26-C27-C28-C29
24	P	305	CDL	C38-C39-C40-C41
25	Z	101	DMU	C25-C28-C31-C34
18	P	304	PGV	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
24	T	103	CDL	C21-C22-C23-C24
23	T	101	PEK	C13-C14-C15-C16
26	E	201	PSC	C11-C10-C9-C8
18	A	606	PGV	C6-C7-C8-C9
20	L	101	TGL	CA9-C20-C21-C22
23	C	303	PEK	C29-C30-C31-C32
24	G	101	CDL	C56-C57-C58-C59
18	C	305	PGV	O05-C05-C06-O06
24	T	103	CDL	OA9-CA7-OA8-CA6
24	C	306	CDL	C39-C40-C41-C42
20	B	301	TGL	CB4-CB5-CB6-CB7
24	G	101	CDL	C54-C55-C56-C57
24	P	305	CDL	C33-C34-C35-C36
18	P	304	PGV	C11-C10-C9-C8
23	T	102	PEK	C2-C3-C4-C5
20	Q	201	TGL	C21-C20-CA9-CA8
24	C	306	CDL	C61-C62-C63-C64
18	A	606	PGV	C01-C02-C03-O11
18	C	305	PGV	C01-C02-C03-O11
18	N	606	PGV	C01-C02-C03-O11
18	A	606	PGV	O02-C1-O01-C02
23	G	102	PEK	O02-C1-O01-C02
20	B	301	TGL	CA9-C20-C21-C22
20	B	301	TGL	C23-C24-C25-C26
20	N	611	TGL	CB7-CB8-CB9-C10
24	P	305	CDL	C35-C36-C37-C38
24	T	103	CDL	C14-C15-C16-C17
18	N	606	PGV	C19-C20-C21-C22
20	L	101	TGL	C19-C33-C34-C35
24	G	101	CDL	C13-C14-C15-C16
24	G	101	CDL	C58-C59-C60-C61
23	C	303	PEK	C25-C26-C27-C28
18	A	606	PGV	C27-C28-C29-C30
20	N	608	TGL	C21-C20-CA9-CA8
24	P	305	CDL	C72-C73-C74-C75
20	Q	201	TGL	C17-C18-C19-C33
20	B	301	TGL	C13-C14-C29-C30
20	N	608	TGL	CC6-CC7-CC8-CC9
20	L	101	TGL	OG1-CG1-CG2-CG3
20	N	611	TGL	OG1-CG1-CG2-CG3
24	G	101	CDL	CA3-CA4-CA6-OA8
18	N	606	PGV	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
26	R	201	PSC	C6-C7-C8-C9
23	P	302	PEK	C25-C26-C27-C28
24	T	103	CDL	C59-C60-C61-C62
20	N	608	TGL	CC2-CC1-OG3-CG3
23	G	102	PEK	C1-C2-C3-C4
20	N	608	TGL	C19-C33-C34-C35
24	G	101	CDL	C72-C73-C74-C75
20	L	101	TGL	C20-C21-C22-C23
24	G	101	CDL	C32-C33-C34-C35
25	M	101	DMU	C31-C34-C37-C40
23	C	302	PEK	C23-C24-C25-C26
24	G	101	CDL	C1-CB2-OB2-PB2
20	Q	201	TGL	C22-C23-C24-C25
23	T	101	PEK	C22-C23-C24-C25
24	P	305	CDL	C15-C16-C17-C18
24	P	305	CDL	C23-C24-C25-C26
18	P	303	PGV	C30-C31-C32-C33
18	C	304	PGV	C12-C13-C14-C15
20	N	611	TGL	CA5-CA6-CA7-CA8
14	A	602	HEA	C2A-C3A-CMA-OMA
14	N	602	HEA	C2A-C3A-CMA-OMA
24	T	103	CDL	C24-C25-C26-C27
20	L	101	TGL	C11-C12-C13-C14
20	N	608	TGL	C11-C10-CB9-CB8
26	R	201	PSC	C23-C24-C25-C26
23	G	102	PEK	O01-C02-C03-O11
24	G	101	CDL	C37-C38-C39-C40
20	B	301	TGL	C29-C30-C31-C32
18	C	304	PGV	C15-C16-C17-C18
20	D	201	TGL	CA3-CA4-CA5-CA6
18	N	606	PGV	C15-C16-C17-C18
24	C	306	CDL	C24-C25-C26-C27
24	T	103	CDL	C83-C84-C85-C86
20	Q	201	TGL	C16-C15-CC9-CC8
18	P	304	PGV	C31-C32-C33-C34
18	A	606	PGV	C2-C3-C4-C5
18	N	606	PGV	C7-C8-C9-C10
20	D	201	TGL	CA6-CA7-CA8-CA9
24	C	306	CDL	C62-C63-C64-C65
20	N	611	TGL	OG2-CG2-CG3-OG3
23	G	102	PEK	O03-C01-C02-O01
24	P	305	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
23	T	102	PEK	C17-C18-C19-C20
20	B	301	TGL	C15-C16-C17-C18
20	N	608	TGL	C25-C26-C27-C28
24	G	101	CDL	C63-C64-C65-C66
26	E	201	PSC	C23-C24-C25-C26
26	E	201	PSC	C26-C27-C28-C29
20	D	201	TGL	C11-C12-C13-C14
23	G	102	PEK	C23-C24-C25-C26
26	R	201	PSC	C29-C30-C31-C32
18	P	303	PGV	C11-C12-C13-C14
18	P	303	PGV	C11-C10-C9-C8
24	P	305	CDL	C84-C85-C86-C87
24	P	305	CDL	C76-C77-C78-C79
26	R	201	PSC	C31-C32-C33-C34
20	B	301	TGL	CB1-CB2-CB3-CB4
23	T	101	PEK	C21-C22-C23-C24
20	D	201	TGL	CA4-CA5-CA6-CA7
24	T	103	CDL	C74-C75-C76-C77
18	C	305	PGV	C2-C3-C4-C5
20	N	608	TGL	C11-C12-C13-C14
24	P	305	CDL	C36-C37-C38-C39
24	T	103	CDL	C78-C79-C80-C81
18	A	606	PGV	C22-C23-C24-C25
23	C	302	PEK	C24-C25-C26-C27
25	C	309	DMU	C19-C18-O16-C6
24	C	306	CDL	C33-C34-C35-C36
24	C	306	CDL	C60-C61-C62-C63
18	C	304	PGV	C1-C2-C3-C4
20	B	301	TGL	C20-C21-C22-C23
20	N	608	TGL	CA4-CA5-CA6-CA7
20	Q	201	TGL	CB1-CB2-CB3-CB4
24	C	306	CDL	OA5-CA3-CA4-CA6
24	C	306	CDL	OB5-CB3-CB4-CB6
20	L	101	TGL	CC4-CC5-CC6-CC7
24	P	305	CDL	C61-C62-C63-C64
24	G	101	CDL	C44-C45-C46-C47
18	P	303	PGV	C7-C8-C9-C10
20	N	608	TGL	OC1-CC1-OG3-CG3
18	A	608	PGV	C10-C11-C12-C13
20	B	301	TGL	CA2-CA1-OG1-CG1
23	G	102	PEK	C25-C26-C27-C28
24	G	101	CDL	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
20	N	608	TGL	CC9-C15-C16-C17
20	L	101	TGL	CB2-CB3-CB4-CB5
23	G	102	PEK	O03-C01-C02-C03
24	T	103	CDL	CA3-CA4-CA6-OA8
24	G	101	CDL	C57-C58-C59-C60
18	C	304	PGV	C28-C29-C30-C31
18	C	305	PGV	C14-C15-C16-C17
20	B	301	TGL	C18-C19-C33-C34
24	P	305	CDL	C74-C75-C76-C77
24	G	101	CDL	C24-C25-C26-C27
18	C	305	PGV	C24-C25-C26-C27
24	T	103	CDL	C58-C59-C60-C61
20	L	101	TGL	C15-C16-C17-C18
24	T	103	CDL	C15-C16-C17-C18
24	T	103	CDL	C75-C76-C77-C78
18	N	606	PGV	O01-C02-C03-O11
18	P	304	PGV	O01-C02-C03-O11
23	P	302	PEK	O01-C02-C03-O11
18	N	606	PGV	C27-C28-C29-C30
20	N	611	TGL	CA2-CA3-CA4-CA5
20	N	611	TGL	C12-C13-C14-C29
18	A	608	PGV	C11-C10-C9-C8
18	C	304	PGV	C02-C03-O11-P
23	T	101	PEK	C4-C5-C6-C7
18	P	304	PGV	C2-C3-C4-C5
20	B	301	TGL	CA7-CA8-CA9-C20
20	D	201	TGL	C11-C10-CB9-CB8
20	Q	201	TGL	C15-C16-C17-C18
18	P	303	PGV	C22-C23-C24-C25
25	Z	101	DMU	O16-C18-C19-C22
24	P	305	CDL	OA6-CA4-CA6-OA8
23	G	102	PEK	C5-C6-C7-C8
23	G	102	PEK	C11-C10-C9-C8
23	G	102	PEK	C11-C12-C13-C14
23	T	101	PEK	C5-C6-C7-C8
23	T	101	PEK	C9-C10-C11-C12
23	T	101	PEK	C11-C12-C13-C14
23	T	101	PEK	C12-C13-C14-C15
18	N	609	PGV	C31-C32-C33-C34
18	N	609	PGV	C29-C30-C31-C32
24	G	101	CDL	C14-C15-C16-C17
18	P	304	PGV	C2-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
24	P	305	CDL	C32-C33-C34-C35
24	C	306	CDL	C82-C83-C84-C85
18	P	304	PGV	C13-C14-C15-C16
24	P	305	CDL	C20-C21-C22-C23
22	C	307	CHD	C21-C20-C22-C23
23	T	102	PEK	C2-C1-O01-C02
20	D	201	TGL	CB2-CB3-CB4-CB5
24	P	305	CDL	C80-C81-C82-C83
24	T	103	CDL	C16-C17-C18-C19
26	R	201	PSC	C5-C6-C7-C8
24	P	305	CDL	OA5-CA3-CA4-CA6
20	N	611	TGL	C33-C34-C35-C36
18	N	606	PGV	C13-C14-C15-C16
18	N	606	PGV	C23-C24-C25-C26
23	C	302	PEK	C25-C26-C27-C28
25	C	309	DMU	C28-C31-C34-C37
18	N	609	PGV	C19-C20-C21-C22
20	D	201	TGL	CA1-CA2-CA3-CA4
18	P	304	PGV	O02-C1-O01-C02
24	G	101	CDL	C75-C76-C77-C78
23	G	102	PEK	O01-C1-C2-C3
24	P	305	CDL	C34-C35-C36-C37
20	N	611	TGL	CB3-CB4-CB5-CB6
23	C	302	PEK	C22-C23-C24-C25
24	G	101	CDL	C20-C21-C22-C23
24	P	305	CDL	C58-C59-C60-C61
24	C	306	CDL	OA5-CA3-CA4-OA6
26	E	201	PSC	O01-C02-C03-O11
20	L	101	TGL	CA2-CA3-CA4-CA5
24	C	306	CDL	CA3-CA4-CA6-OA8
24	P	305	CDL	CA3-CA4-CA6-OA8
23	P	302	PEK	C05-C04-O12-P
26	E	201	PSC	C05-C04-O12-P
26	R	201	PSC	C05-C04-O12-P
23	P	302	PEK	C31-C32-C33-C34
20	D	201	TGL	OG2-CG2-CG3-OG3
24	T	103	CDL	OB6-CB4-CB6-OB8
20	N	608	TGL	CA7-CA8-CA9-C20
24	T	103	CDL	C19-C20-C21-C22
20	B	301	TGL	OA1-CA1-OG1-CG1
25	Z	101	DMU	C22-C25-C28-C31
25	Z	101	DMU	C19-C22-C25-C28

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Mol	Chain	Res	Type	Atoms
23	P	302	PEK	C33-C34-C35-C36
24	P	305	CDL	C43-C44-C45-C46
18	N	609	PGV	C12-C13-C14-C15
20	L	101	TGL	CC5-CC6-CC7-CC8
20	D	201	TGL	C16-C17-C18-C19
24	C	306	CDL	C32-C33-C34-C35
24	P	305	CDL	C31-C32-C33-C34
18	P	304	PGV	C01-C02-C03-O11
23	G	102	PEK	C01-C02-C03-O11
20	L	101	TGL	C25-C26-C27-C28
18	C	304	PGV	C26-C27-C28-C29
23	G	102	PEK	C28-C29-C30-C31
24	T	103	CDL	C57-C58-C59-C60
18	P	304	PGV	C27-C28-C29-C30
20	B	301	TGL	C24-C25-C26-C27
18	A	606	PGV	O01-C02-C03-O11
24	G	101	CDL	OB5-CB3-CB4-OB6
14	A	601	HEA	C4A-C3A-CMA-OMA
14	N	601	HEA	C4A-C3A-CMA-OMA
14	N	602	HEA	C4A-C3A-CMA-OMA
24	C	306	CDL	C57-C58-C59-C60
18	A	606	PGV	C14-C15-C16-C17
20	L	101	TGL	OG1-CG1-CG2-OG2
20	N	611	TGL	OG1-CG1-CG2-OG2
26	R	201	PSC	O03-C01-C02-O01
18	A	606	PGV	C23-C24-C25-C26
20	Q	201	TGL	CA2-CA3-CA4-CA5
20	B	301	TGL	OG1-CG1-CG2-CG3
20	D	201	TGL	CG1-CG2-CG3-OG3
20	N	611	TGL	CG1-CG2-CG3-OG3
24	G	101	CDL	CB3-CB4-CB6-OB8
18	P	304	PGV	C14-C15-C16-C17
24	C	306	CDL	C22-C23-C24-C25
23	C	303	PEK	C17-C18-C19-C20
23	T	101	PEK	C3-C4-C5-C6
20	D	201	TGL	C17-C18-C19-C33
18	A	606	PGV	C04-O12-P-O11
18	A	606	PGV	C04-O12-P-O13
18	A	606	PGV	C04-O12-P-O14
18	C	305	PGV	C03-O11-P-O14
18	C	305	PGV	C04-O12-P-O14
23	G	102	PEK	C03-O11-P-O12

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Mol	Chain	Res	Type	Atoms
23	G	102	PEK	C03-O11-P-O13
23	G	102	PEK	C03-O11-P-O14
23	G	102	PEK	C04-O12-P-O13
23	P	302	PEK	C03-O11-P-O14
23	P	302	PEK	C04-O12-P-O11
23	P	302	PEK	C04-O12-P-O13
23	T	102	PEK	O12-C04-C05-N
24	C	306	CDL	CA3-OA5-PA1-OA2
24	C	306	CDL	CA3-OA5-PA1-OA3
24	C	306	CDL	CB2-OB2-PB2-OB5
24	C	306	CDL	CB3-OB5-PB2-OB3
24	P	305	CDL	CA3-OA5-PA1-OA2
24	P	305	CDL	CA3-OA5-PA1-OA3
24	T	103	CDL	CA2-OA2-PA1-OA3
24	T	103	CDL	CA3-OA5-PA1-OA2
18	A	606	PGV	C25-C26-C27-C28
24	P	305	CDL	C73-C74-C75-C76
18	A	606	PGV	C02-C03-O11-P
18	P	303	PGV	C02-C03-O11-P
24	G	101	CDL	CA4-CA3-OA5-PA1
20	Q	201	TGL	CC1-CC2-CC3-CC4
23	C	303	PEK	C30-C31-C32-C33
20	D	201	TGL	OG2-CB1-CB2-CB3
20	L	101	TGL	CA5-CA6-CA7-CA8
20	Q	201	TGL	CA4-CA5-CA6-CA7
18	P	304	PGV	C5-C6-C7-C8
20	L	101	TGL	C23-C24-C25-C26
20	L	101	TGL	C24-C25-C26-C27
24	G	101	CDL	C12-C13-C14-C15
24	G	101	CDL	C77-C78-C79-C80
18	C	305	PGV	C6-C7-C8-C9
20	B	301	TGL	CA1-CA2-CA3-CA4
18	N	609	PGV	C30-C31-C32-C33
18	N	606	PGV	C01-C02-O01-C1
18	C	305	PGV	C5-C6-C7-C8
20	Q	201	TGL	C25-C26-C27-C28
20	N	608	TGL	CC4-CC5-CC6-CC7
23	P	302	PEK	C01-C02-C03-O11
24	P	305	CDL	C31-CA7-OA8-CA6
20	N	611	TGL	CC6-CC7-CC8-CC9
25	P	307	DMU	C19-C22-C25-C28
26	R	201	PSC	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
20	N	611	TGL	CA7-CA8-CA9-C20
24	C	306	CDL	C42-C43-C44-C45
24	T	103	CDL	C23-C24-C25-C26
24	P	305	CDL	OA9-CA7-OA8-CA6
24	T	103	CDL	C1-CA2-OA2-PA1
25	P	307	DMU	C28-C31-C34-C37
24	G	101	CDL	OA6-CA4-CA6-OA8
18	N	609	PGV	O03-C19-C20-C21
23	T	102	PEK	C30-C31-C32-C33
14	N	601	HEA	C15-C16-C17-C18
20	L	101	TGL	CG1-CG2-CG3-OG3
24	T	103	CDL	CB3-CB4-CB6-OB8
20	B	301	TGL	CA6-CA7-CA8-CA9
24	P	305	CDL	C78-C79-C80-C81
18	C	305	PGV	C31-C32-C33-C34
18	A	606	PGV	C26-C27-C28-C29
23	G	102	PEK	C22-C23-C24-C25
20	Q	201	TGL	C23-C24-C25-C26
24	C	306	CDL	C12-C13-C14-C15
24	P	305	CDL	C52-C53-C54-C55
18	N	606	PGV	C2-C3-C4-C5
24	T	103	CDL	C11-C12-C13-C14
26	E	201	PSC	C24-C25-C26-C27
24	C	306	CDL	CB5-C51-C52-C53
18	N	606	PGV	C12-C13-C14-C15
23	P	302	PEK	C15-C16-C17-C18
23	T	102	PEK	C15-C16-C17-C18
20	L	101	TGL	OG1-CA1-CA2-CA3
24	P	305	CDL	OA5-CA3-CA4-OA6
20	Q	201	TGL	CB7-CB8-CB9-C10
24	C	306	CDL	C38-C39-C40-C41
24	T	103	CDL	C61-C62-C63-C64
23	P	302	PEK	C22-C23-C24-C25
20	D	201	TGL	CA5-CA6-CA7-CA8
20	Q	201	TGL	CA6-CA7-CA8-CA9
23	P	302	PEK	O03-C01-C02-O01
18	P	304	PGV	C23-C24-C25-C26
23	T	101	PEK	C27-C28-C29-C30
18	A	608	PGV	O03-C19-C20-C21
23	T	102	PEK	O03-C21-C22-C23
20	Q	201	TGL	C12-C13-C14-C29
24	G	101	CDL	C52-C53-C54-C55

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Mol	Chain	Res	Type	Atoms
24	T	103	CDL	C54-C55-C56-C57
24	P	305	CDL	C16-C17-C18-C19
24	P	305	CDL	CA4-CA3-OA5-PA1
24	C	306	CDL	C21-C22-C23-C24
22	O	301	CHD	C22-C23-C24-O25
18	N	609	PGV	C25-C26-C27-C28
23	C	302	PEK	C16-C17-C18-C19
20	N	608	TGL	C23-C24-C25-C26
22	P	306	CHD	C22-C23-C24-O25
20	N	608	TGL	CA3-CA4-CA5-CA6
22	J	101	CHD	C22-C23-C24-O25
22	P	306	CHD	C22-C23-C24-O26
22	O	301	CHD	C22-C23-C24-O26
26	R	201	PSC	C12-C13-C14-C15
22	C	307	CHD	C22-C23-C24-O25
22	J	101	CHD	C22-C23-C24-O26
24	P	305	CDL	C79-C80-C81-C82
23	C	303	PEK	C5-C6-C7-C8
23	C	303	PEK	C6-C7-C8-C9
23	P	302	PEK	C6-C7-C8-C9
23	T	101	PEK	C11-C10-C9-C8
26	E	201	PSC	C10-C11-C12-C13
14	N	601	HEA	CAD-CBD-CGD-O1D
20	L	101	TGL	C21-C20-CA9-CA8
24	G	101	CDL	C34-C35-C36-C37
22	P	306	CHD	C13-C17-C20-C21
23	C	303	PEK	C27-C28-C29-C30
25	P	307	DMU	C3-C4-C57-O61
14	A	602	HEA	CAD-CBD-CGD-O2D
20	D	201	TGL	CA2-CA1-OG1-CG1
20	L	101	TGL	CC2-CC3-CC4-CC5
24	C	306	CDL	C34-C35-C36-C37
14	N	602	HEA	CAD-CBD-CGD-O2D
22	B	303	CHD	C22-C23-C24-O25
23	C	303	PEK	C23-C24-C25-C26
23	C	303	PEK	C31-C32-C33-C34
23	T	102	PEK	C23-C24-C25-C26
24	C	306	CDL	C41-C42-C43-C44
14	N	602	HEA	C26-C15-C16-C17
18	C	305	PGV	C05-C04-O12-P
18	C	305	PGV	C29-C30-C31-C32
20	D	201	TGL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
20	N	608	TGL	OG1-CG1-CG2-CG3
20	D	201	TGL	OA1-CA1-OG1-CG1
22	B	303	CHD	C22-C23-C24-O26
18	P	304	PGV	C6-C7-C8-C9
18	C	304	PGV	C30-C31-C32-C33
14	N	601	HEA	CAD-CBD-CGD-O2D
14	N	602	HEA	CAD-CBD-CGD-O1D
23	C	303	PEK	C13-C14-C15-C16
22	C	307	CHD	C22-C23-C24-O26
26	E	201	PSC	C01-C02-C03-O11
20	L	101	TGL	OG2-CG2-CG3-OG3
18	A	606	PGV	C24-C25-C26-C27
18	N	606	PGV	C20-C21-C22-C23
18	P	304	PGV	C3-C4-C5-C6
20	D	201	TGL	CC4-CC5-CC6-CC7
14	A	602	HEA	CAD-CBD-CGD-O1D
23	T	102	PEK	C16-C17-C18-C19
24	P	305	CDL	C77-C78-C79-C80
24	C	306	CDL	C54-C55-C56-C57
14	A	602	HEA	CAA-CBA-CGA-O1A
20	B	301	TGL	CC9-C15-C16-C17
18	N	609	PGV	C4-C5-C6-C7
18	A	606	PGV	C20-C21-C22-C23
20	D	201	TGL	C24-C25-C26-C27
23	C	303	PEK	C3-C4-C5-C6
26	E	201	PSC	C7-C8-C9-C10
22	C	308	CHD	C22-C23-C24-O26
18	P	303	PGV	C1-C2-C3-C4
24	G	101	CDL	C52-C51-CB5-OB6
22	N	610	CHD	C22-C23-C24-O26
24	C	306	CDL	C59-C60-C61-C62
24	C	306	CDL	C71-C72-C73-C74
22	N	610	CHD	C22-C23-C24-O25
18	C	304	PGV	C05-C04-O12-P
20	Q	201	TGL	C11-C12-C13-C14
24	P	305	CDL	CB3-CB4-CB6-OB8
18	A	608	PGV	C19-C20-C21-C22
20	Q	201	TGL	C11-C10-CB9-CB8
24	P	305	CDL	C40-C41-C42-C43
23	T	102	PEK	C22-C23-C24-C25
22	C	308	CHD	C22-C23-C24-O25
22	W	101	CHD	C22-C23-C24-O26

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Mol	Chain	Res	Type	Atoms
18	P	303	PGV	C23-C24-C25-C26
18	P	304	PGV	C15-C16-C17-C18
24	C	306	CDL	OA6-CA4-CA6-OA8
22	W	101	CHD	C22-C23-C24-O25
24	P	305	CDL	C12-C13-C14-C15
24	T	103	CDL	C60-C61-C62-C63
23	P	302	PEK	C14-C15-C16-C17
23	T	102	PEK	C3-C4-C5-C6
24	G	101	CDL	OB5-CB3-CB4-CB6
20	B	301	TGL	CC5-CC6-CC7-CC8
18	P	304	PGV	O01-C1-C2-C3
20	D	201	TGL	CB5-CB6-CB7-CB8
14	A	601	HEA	C2C-C3C-CAC-CBC
23	T	102	PEK	O02-C1-O01-C02
20	N	608	TGL	C33-C34-C35-C36
20	N	608	TGL	C29-C30-C31-C32
20	D	201	TGL	C20-C21-C22-C23
23	G	102	PEK	O02-C1-C2-C3
23	C	303	PEK	C35-C36-C37-C38
24	T	103	CDL	C20-C21-C22-C23
14	A	602	HEA	CAA-CBA-CGA-O2A
20	B	301	TGL	C12-C13-C14-C29
23	T	102	PEK	O01-C1-C2-C3
18	C	305	PGV	C25-C26-C27-C28
20	D	201	TGL	CA9-C20-C21-C22
14	A	601	HEA	CAD-CBD-CGD-O2D
14	A	601	HEA	CAD-CBD-CGD-O1D
14	N	602	HEA	CAA-CBA-CGA-O1A
18	N	606	PGV	O03-C19-C20-C21
23	T	101	PEK	O03-C21-C22-C23
24	T	103	CDL	C52-C51-CB5-OB6
24	T	103	CDL	C72-C71-CB7-OB8
26	R	201	PSC	O03-C01-C02-C03
14	N	602	HEA	CAA-CBA-CGA-O2A
20	D	201	TGL	OG1-CA1-CA2-CA3
20	Q	201	TGL	C24-C25-C26-C27
20	N	608	TGL	C22-C23-C24-C25
24	P	305	CDL	OB5-CB3-CB4-CB6
23	C	303	PEK	C2-C3-C4-C5
20	D	201	TGL	OG3-CC1-CC2-CC3
18	C	305	PGV	C7-C8-C9-C10
18	P	303	PGV	C05-C04-O12-P

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Mol	Chain	Res	Type	Atoms
23	G	102	PEK	C02-C03-O11-P
23	T	101	PEK	O04-C21-C22-C23
25	M	101	DMU	C34-C37-C40-C43
24	T	103	CDL	C72-C71-CB7-OB9
18	C	304	PGV	C24-C25-C26-C27
23	P	302	PEK	O01-C1-C2-C3
24	C	306	CDL	C12-C11-CA5-OA6
18	C	304	PGV	C11-C12-C13-C14
18	P	304	PGV	O02-C1-C2-C3
24	P	305	CDL	OB9-CB7-OB8-CB6
23	T	102	PEK	O02-C1-C2-C3
23	C	302	PEK	O03-C21-C22-C23
20	D	201	TGL	OC1-CC1-CC2-CC3
18	C	305	PGV	C10-C11-C12-C13
18	N	609	PGV	C26-C27-C28-C29
20	N	608	TGL	OG3-CC1-CC2-CC3
18	N	606	PGV	O04-C19-C20-C21
18	P	303	PGV	C29-C30-C31-C32
24	P	305	CDL	C12-C11-CA5-OA6
20	N	611	TGL	C20-C21-C22-C23
23	C	303	PEK	O01-C1-C2-C3
24	P	305	CDL	C71-CB7-OB8-CB6
24	G	101	CDL	C36-C37-C38-C39
24	T	103	CDL	C52-C51-CB5-OB7

There are no ring outliers.

43 monomers are involved in 219 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	P	302	PEK	11	0
18	P	303	PGV	5	0
18	N	606	PGV	6	0
22	C	307	CHD	1	0
14	A	602	HEA	2	0
20	D	201	TGL	11	0
26	E	201	PSC	7	0
20	Q	201	TGL	6	0
20	N	611	TGL	7	0
20	N	608	TGL	3	0
23	T	102	PEK	1	0
23	C	303	PEK	13	0
23	C	302	PEK	6	0

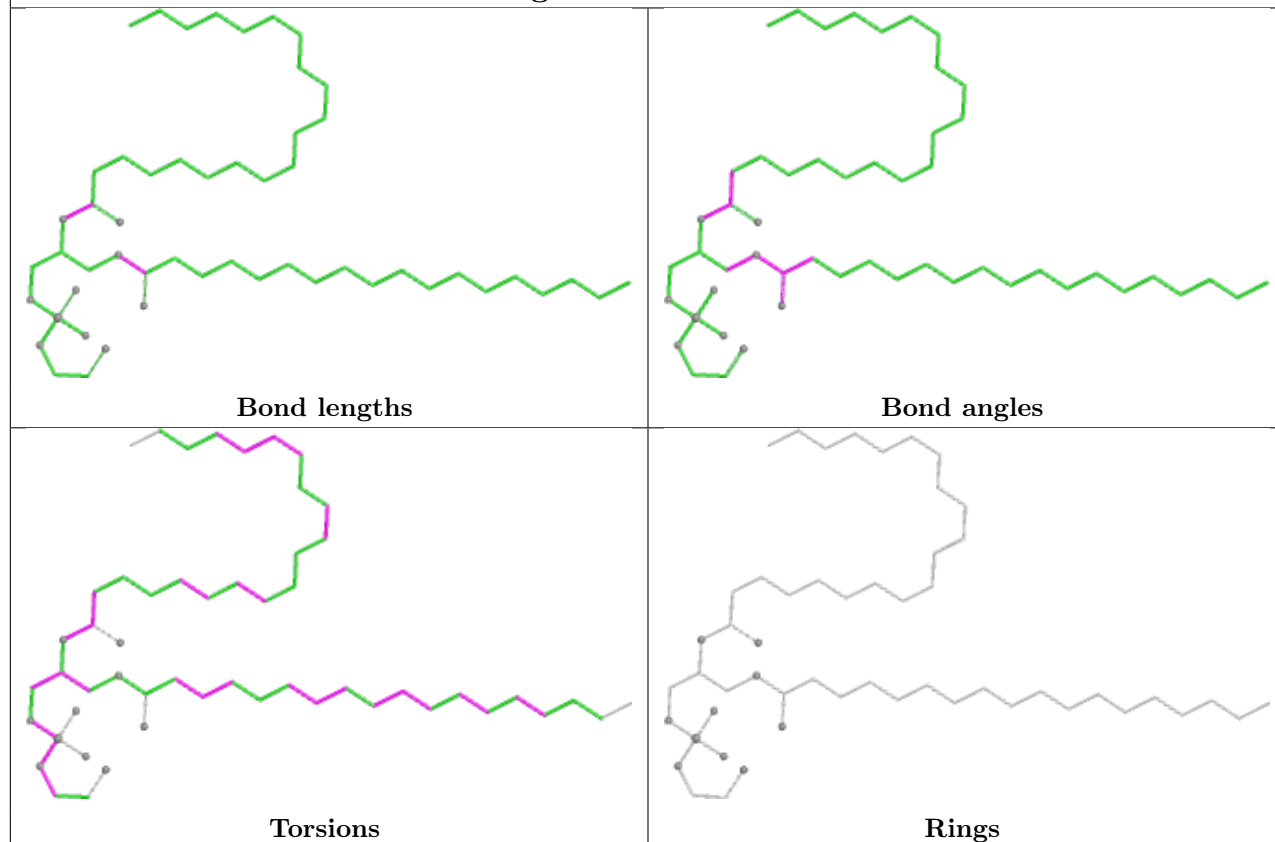
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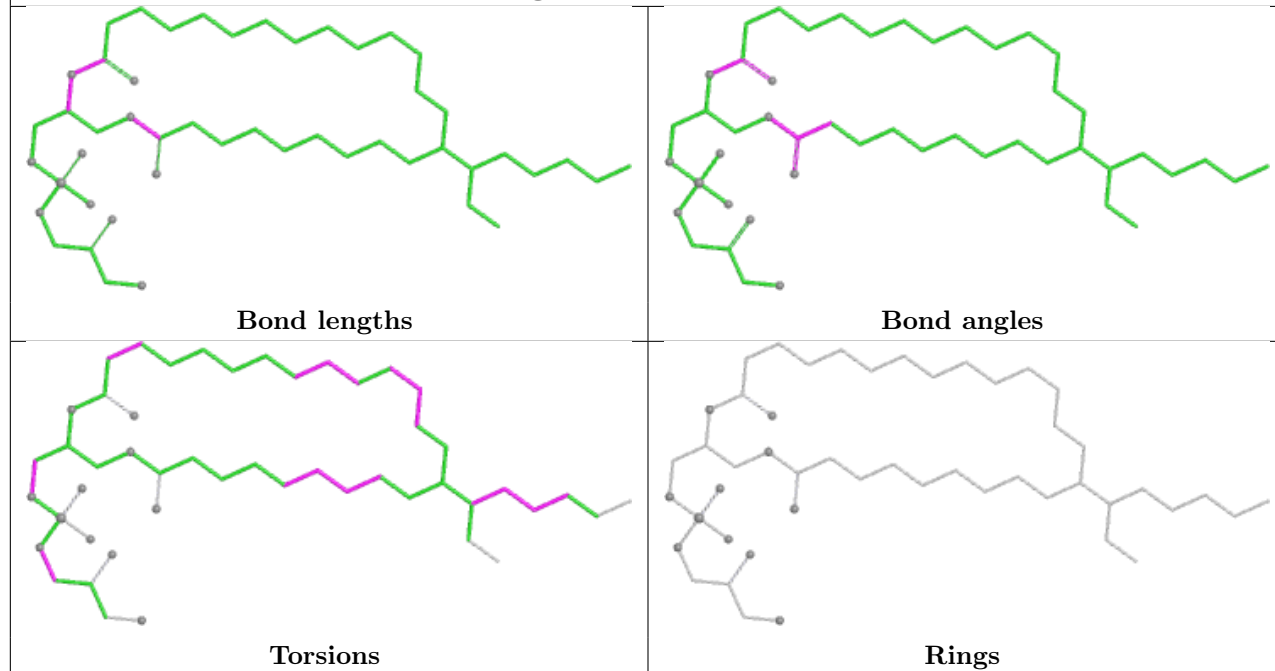
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	601	HEA	9	0
22	B	303	CHD	1	0
19	A	607[B]	PER	2	0
14	N	602	HEA	2	0
24	G	101	CDL	17	0
24	C	306	CDL	14	0
18	A	608	PGV	6	0
18	N	609	PGV	2	0
26	R	201	PSC	6	0
25	P	307	DMU	4	0
18	C	304	PGV	2	0
14	N	601	HEA	10	0
19	N	607[B]	PER	1	0
22	N	610	CHD	1	0
19	A	607[A]	PER	1	0
25	C	309	DMU	6	0
23	G	102	PEK	7	0
22	O	301	CHD	1	0
18	P	304	PGV	4	0
24	P	305	CDL	10	0
20	B	301	TGL	1	0
23	T	101	PEK	7	0
19	N	607[A]	PER	1	0
25	Z	101	DMU	1	0
22	P	306	CHD	1	0
18	A	606	PGV	11	0
20	L	101	TGL	11	0
24	T	103	CDL	20	0
22	W	101	CHD	5	0
18	C	305	PGV	1	0

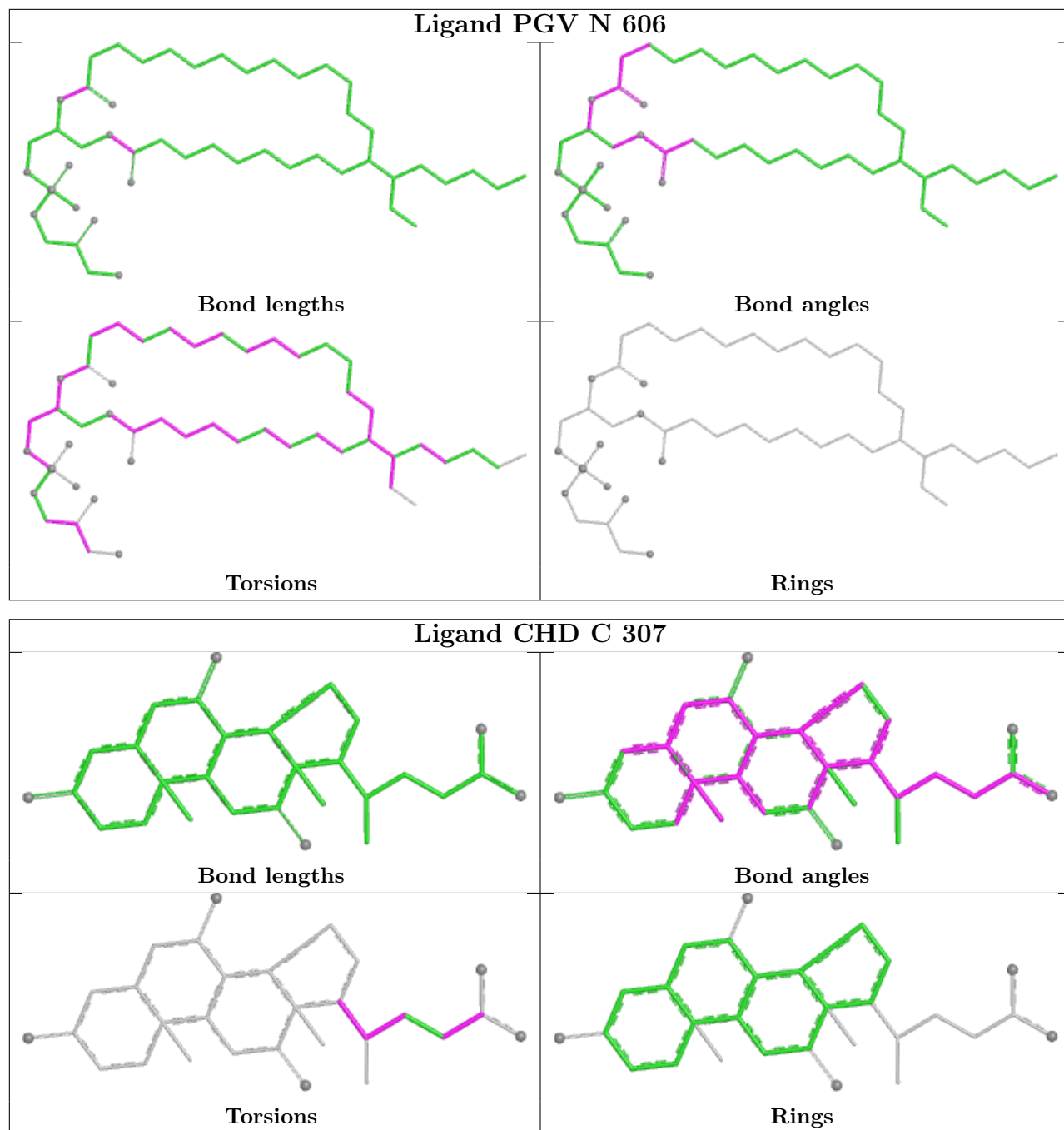
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

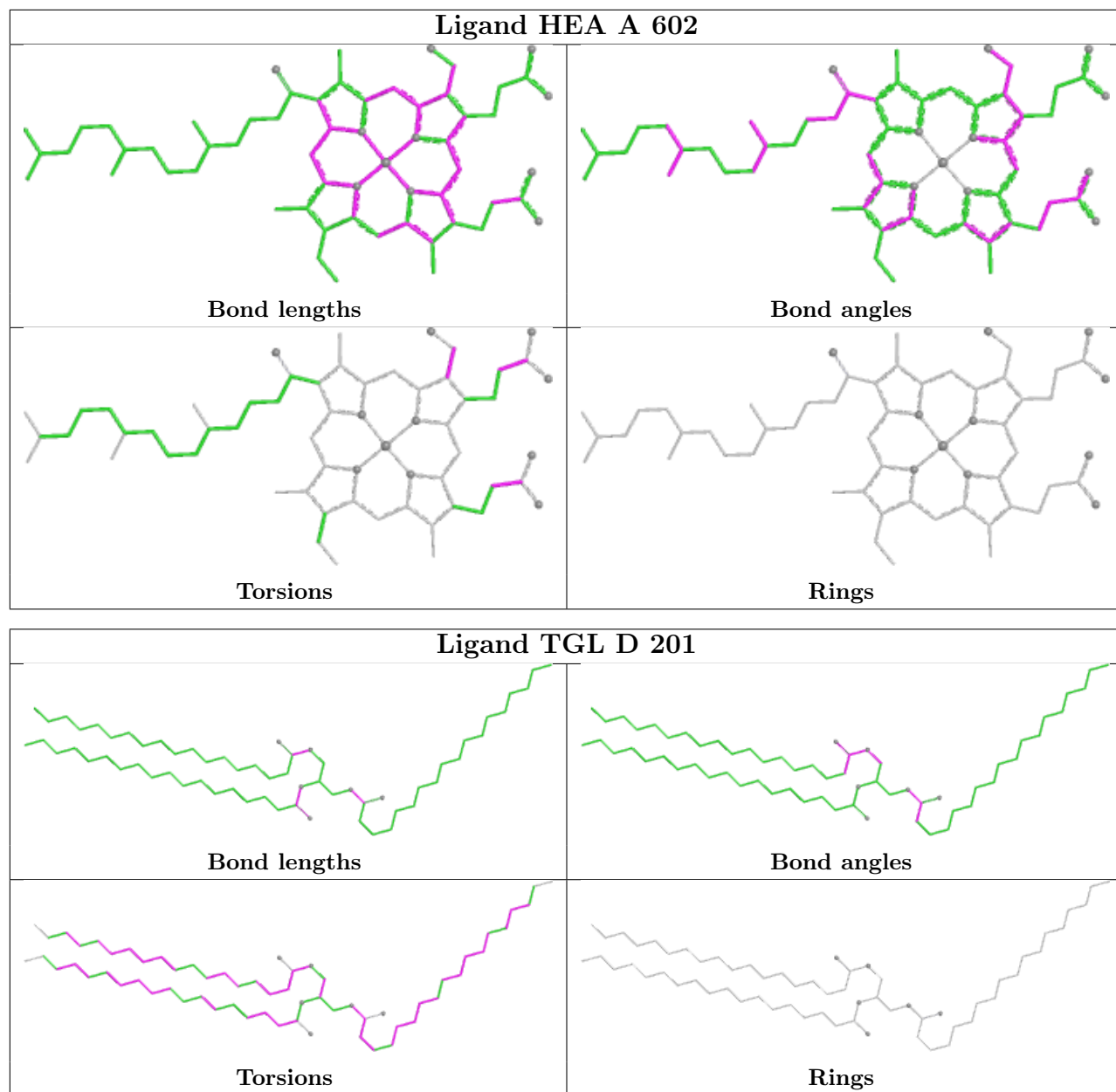
Ligand PEK P 302

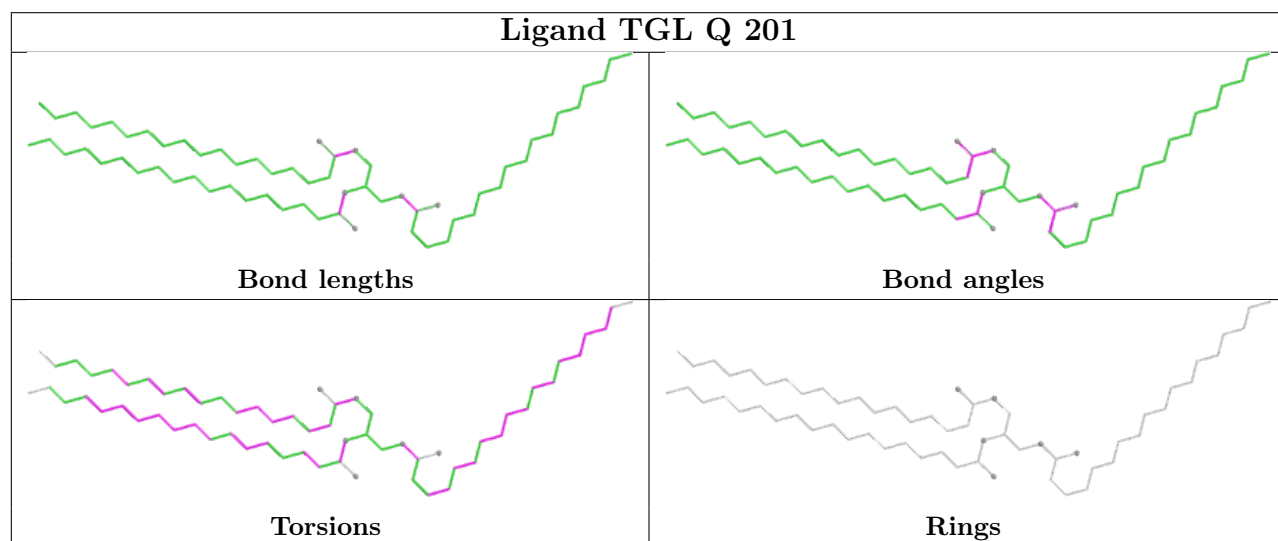
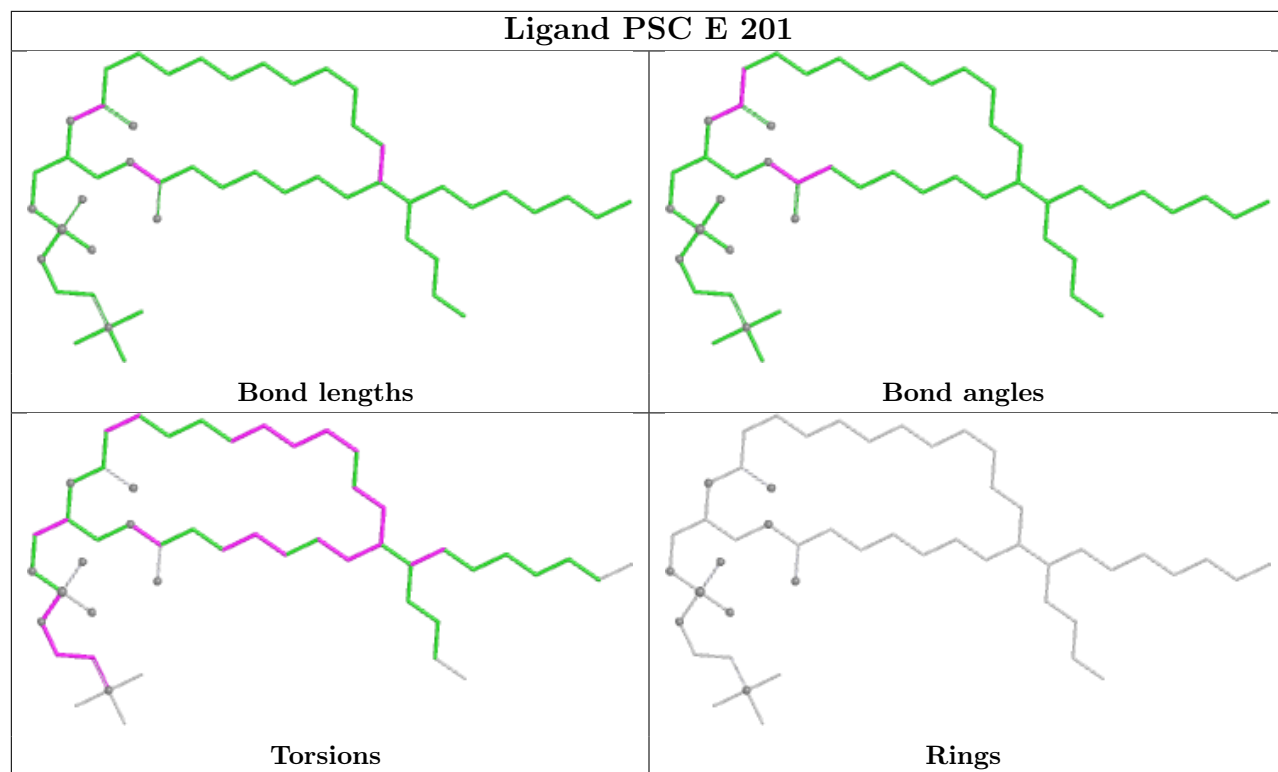


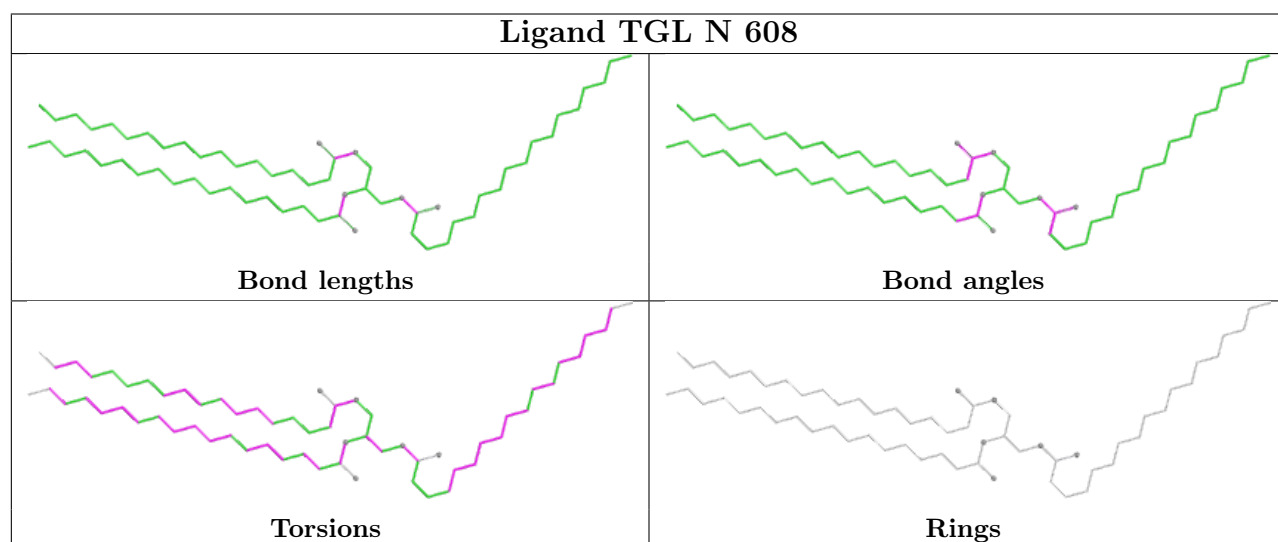
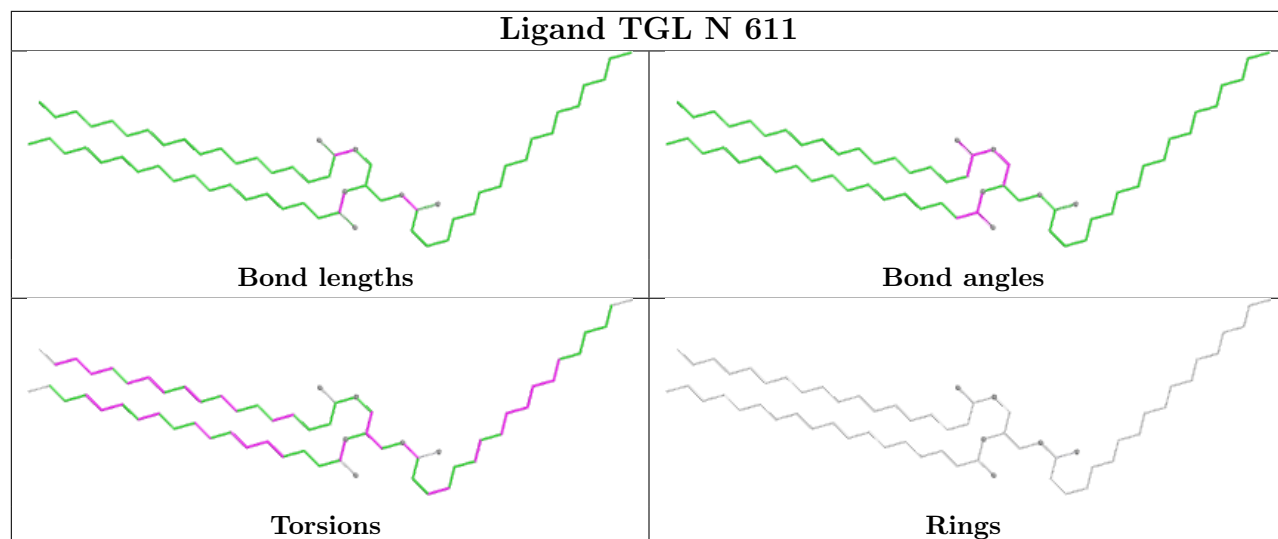
Ligand PGV P 303



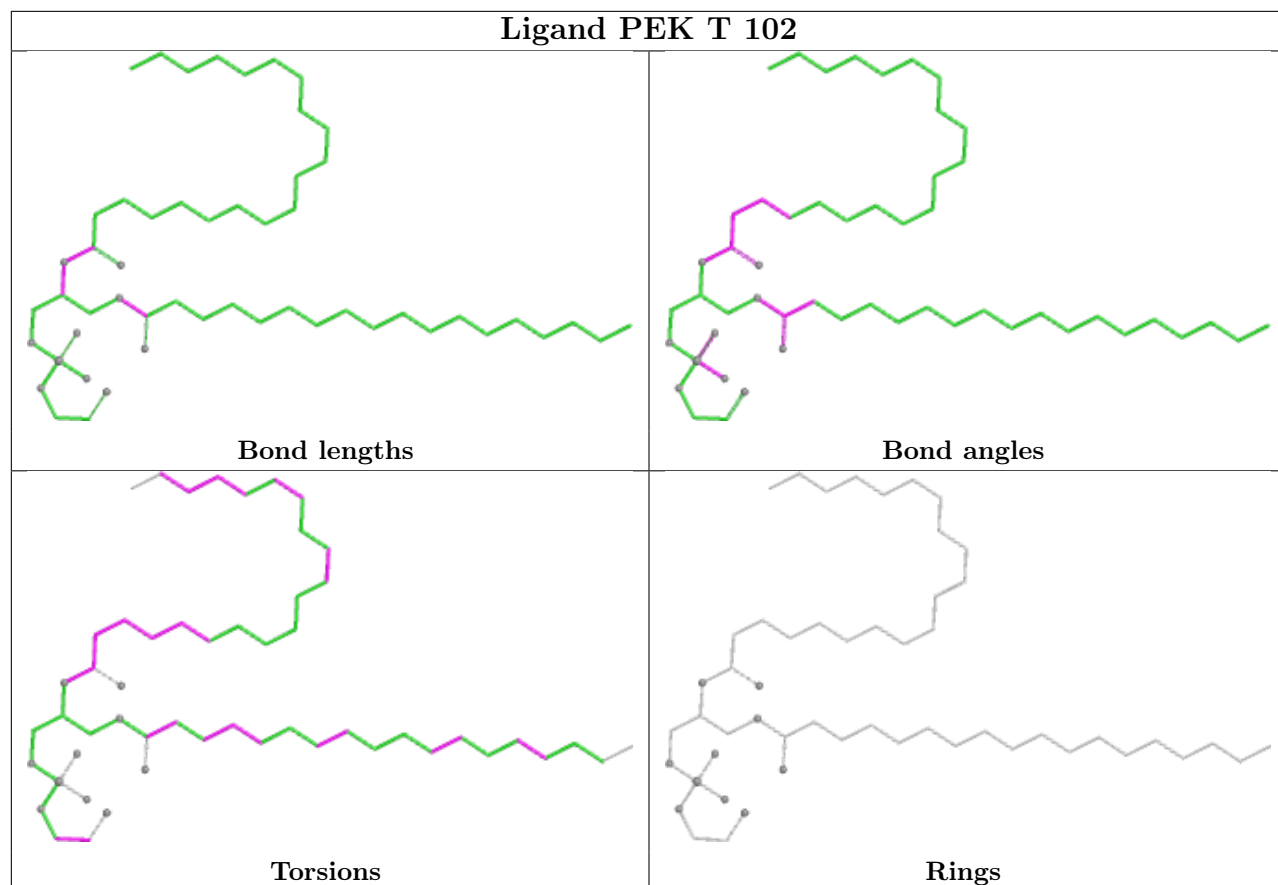




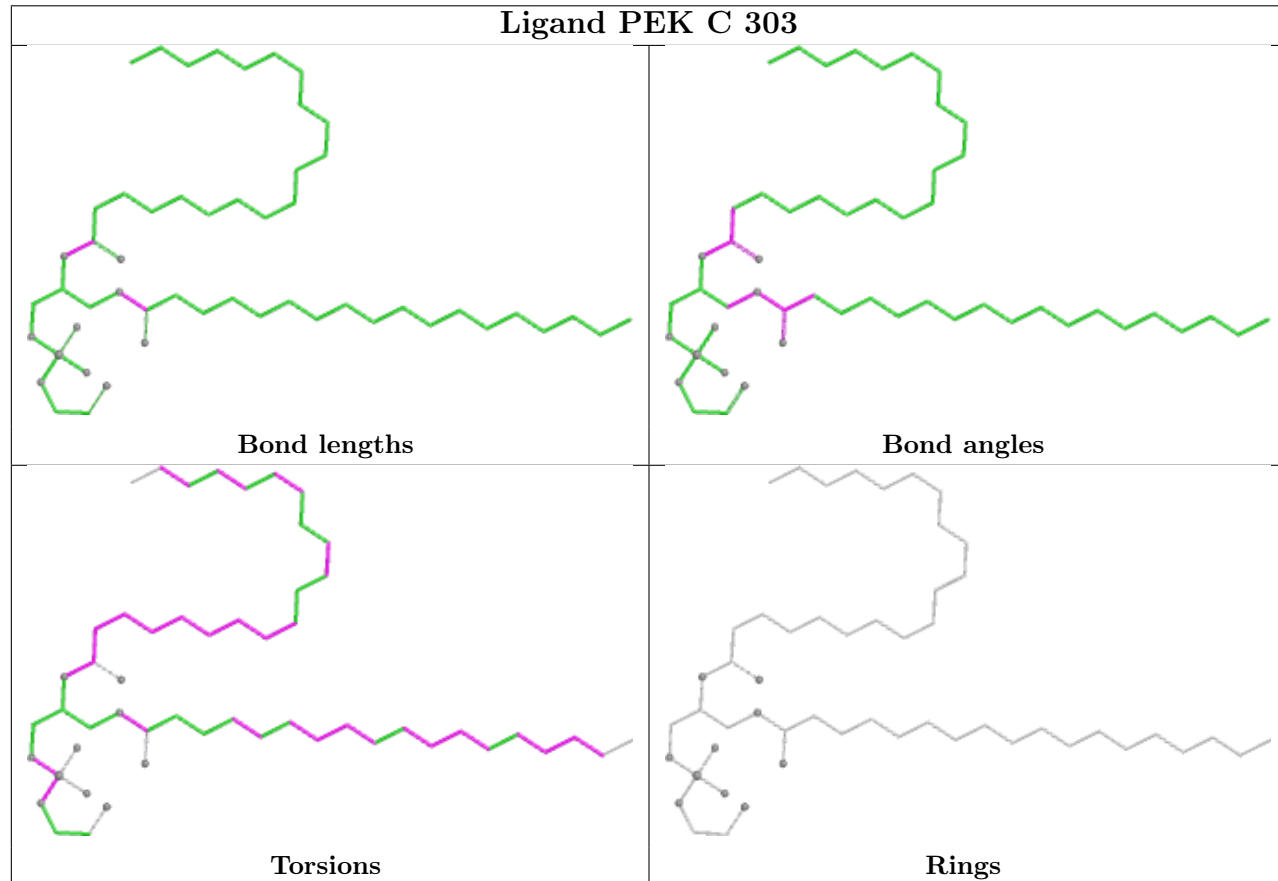




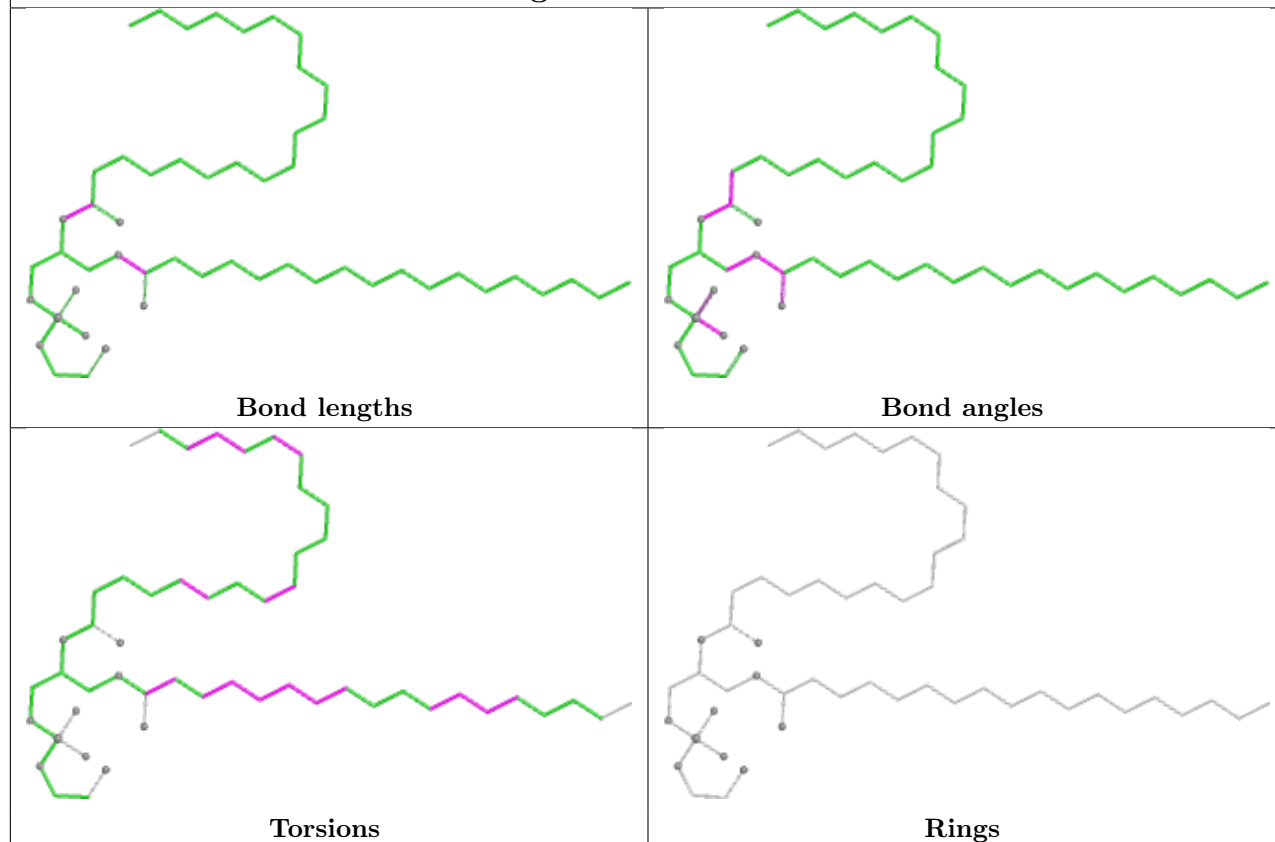
Ligand PEK T 102



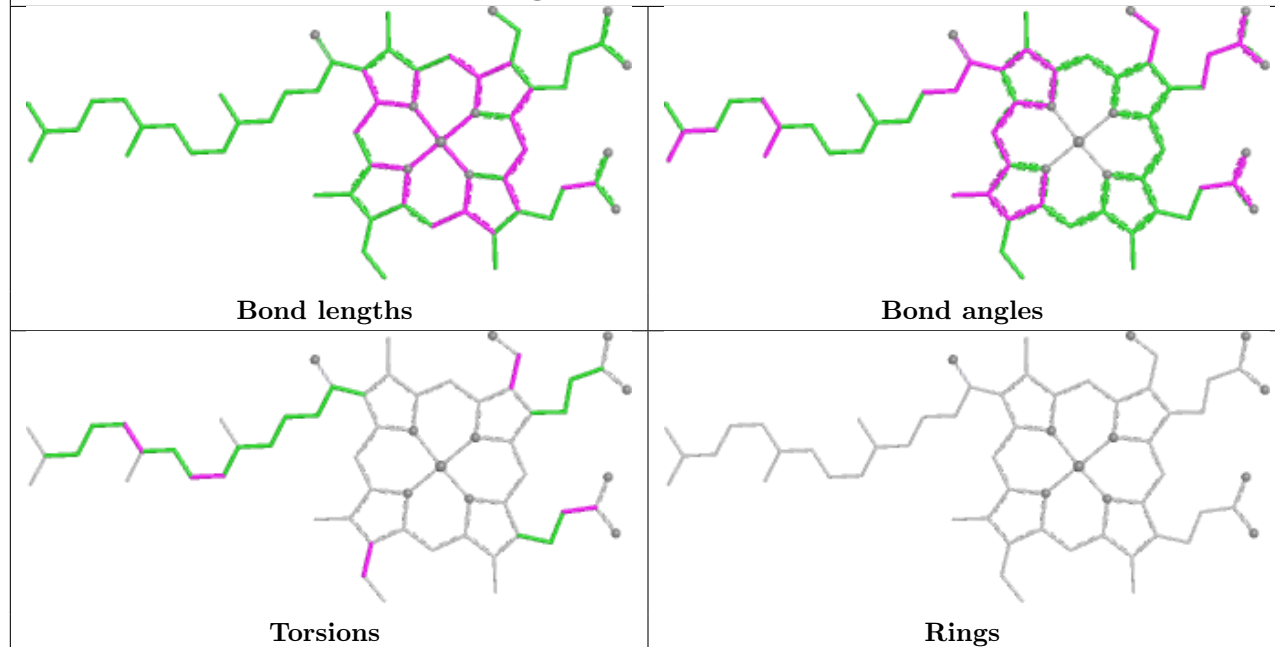
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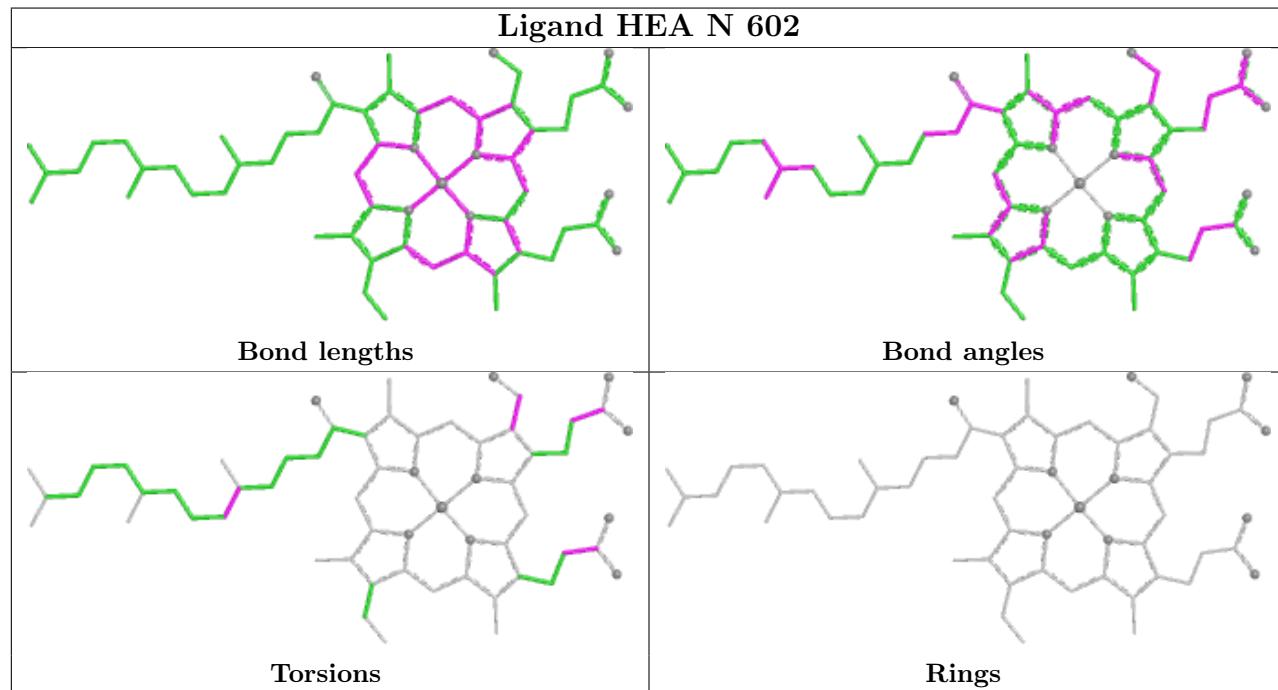
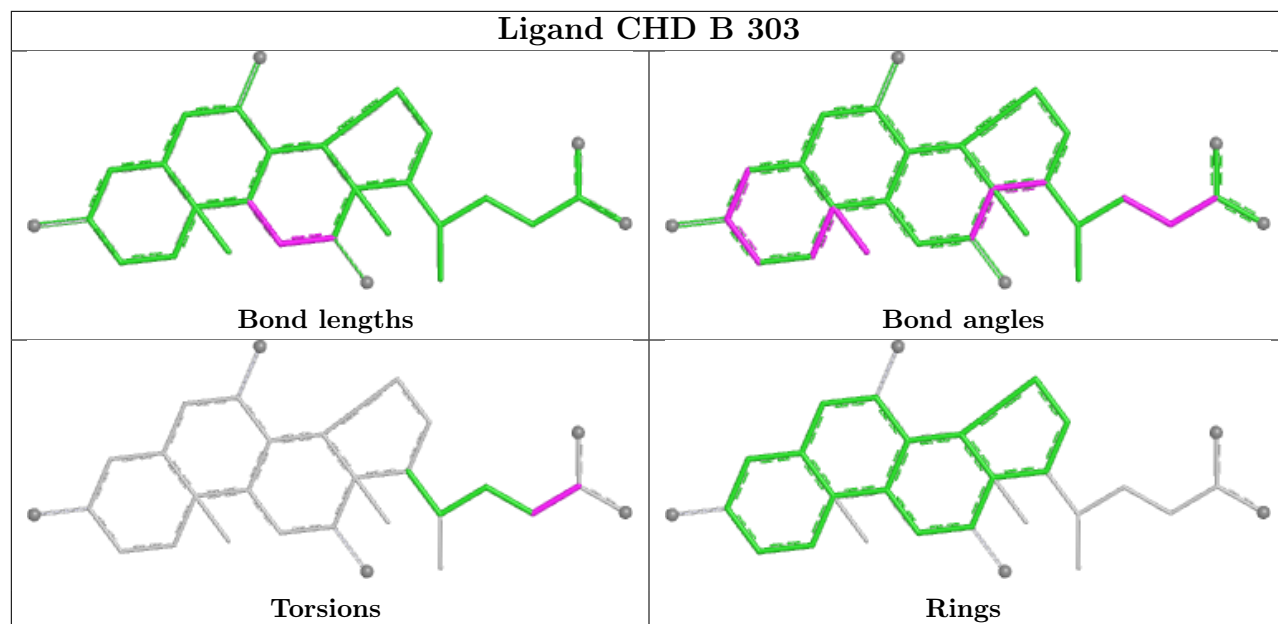


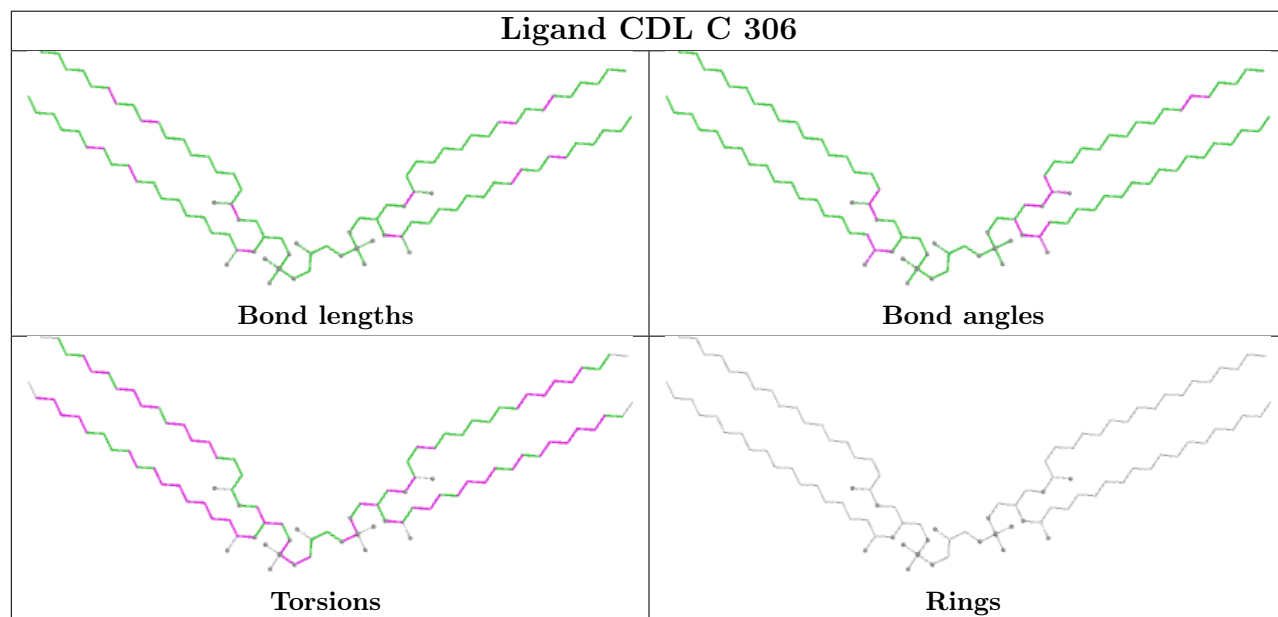
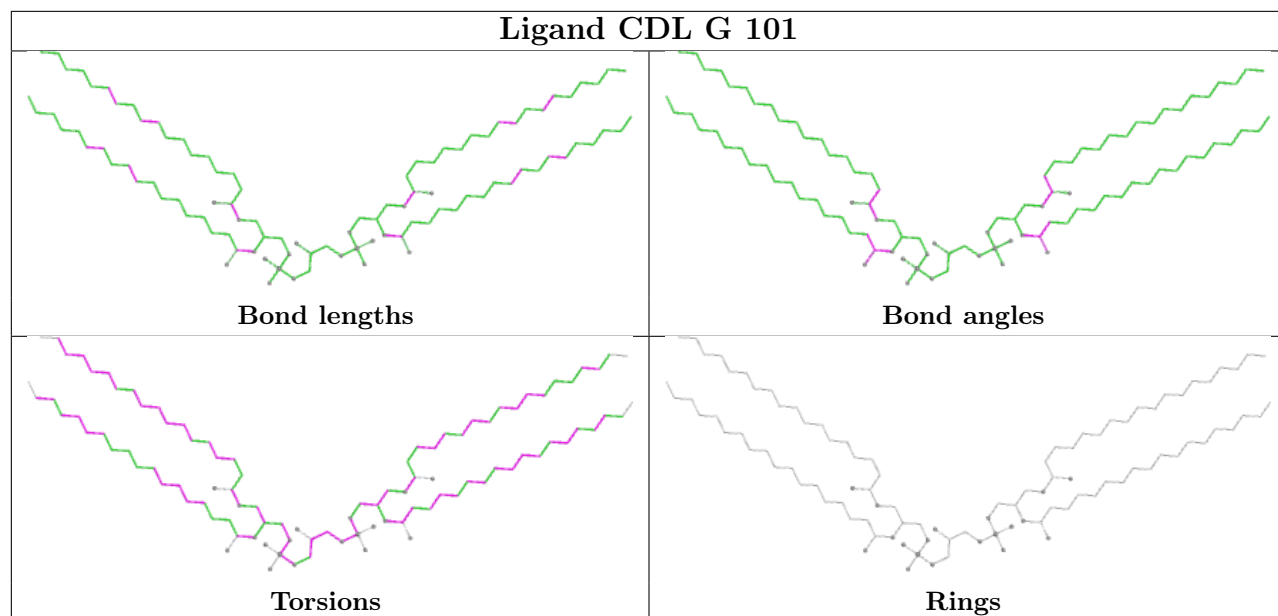
Ligand PEK C 302

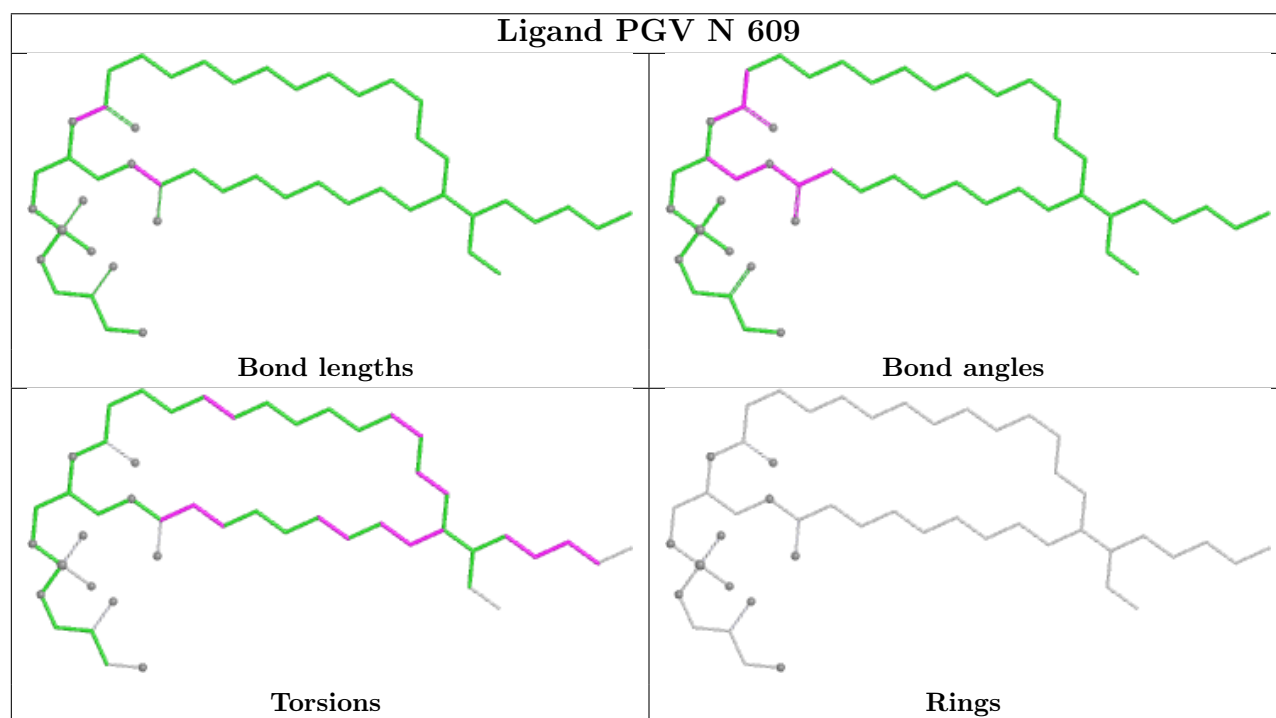
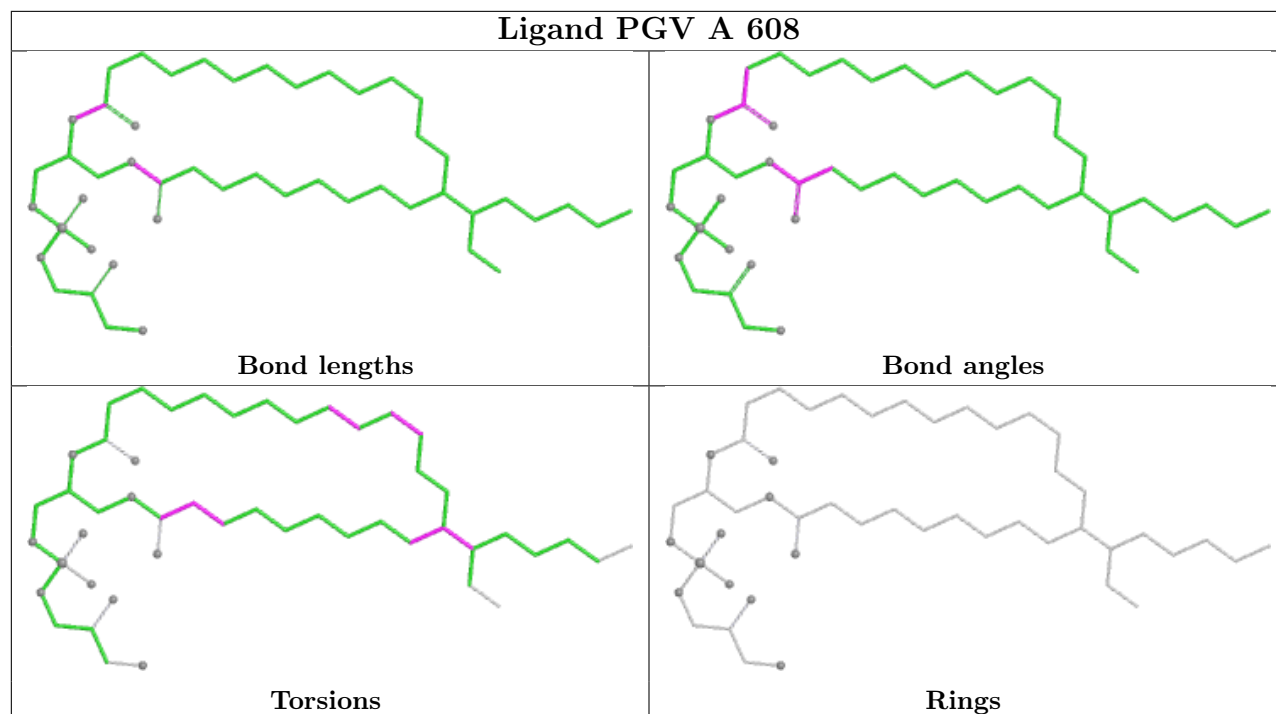


Ligand HEA A 601

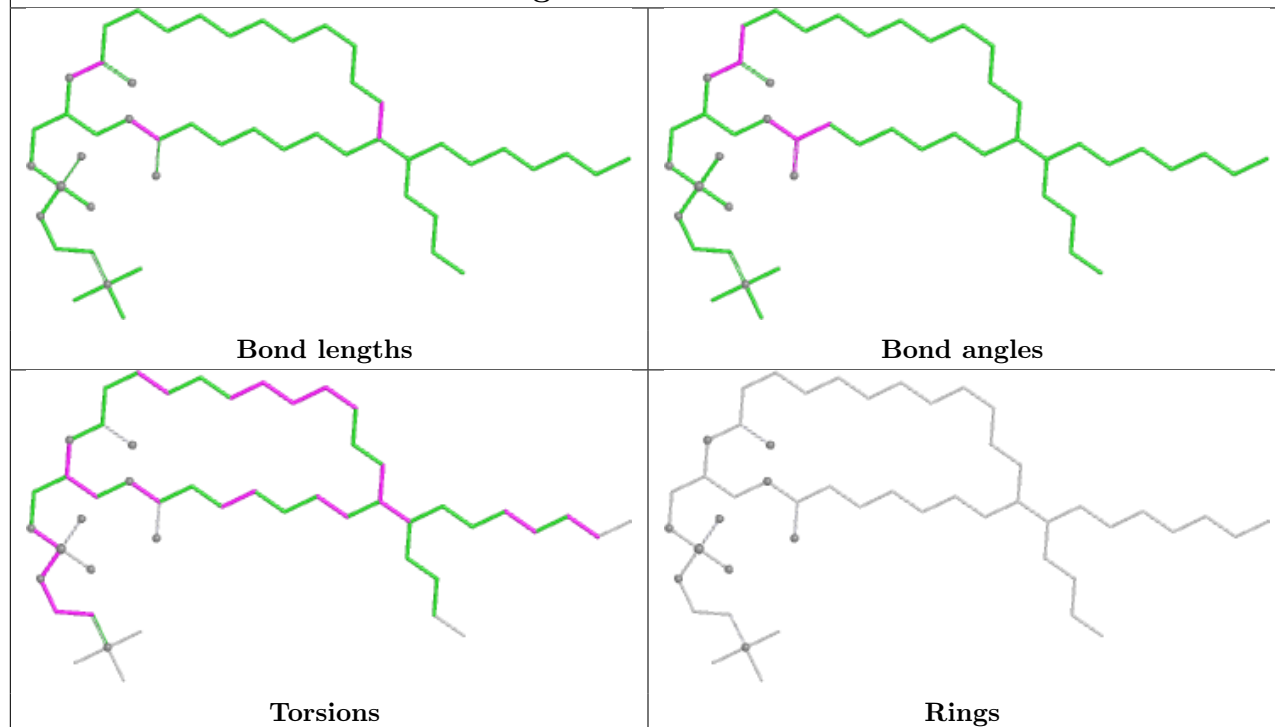




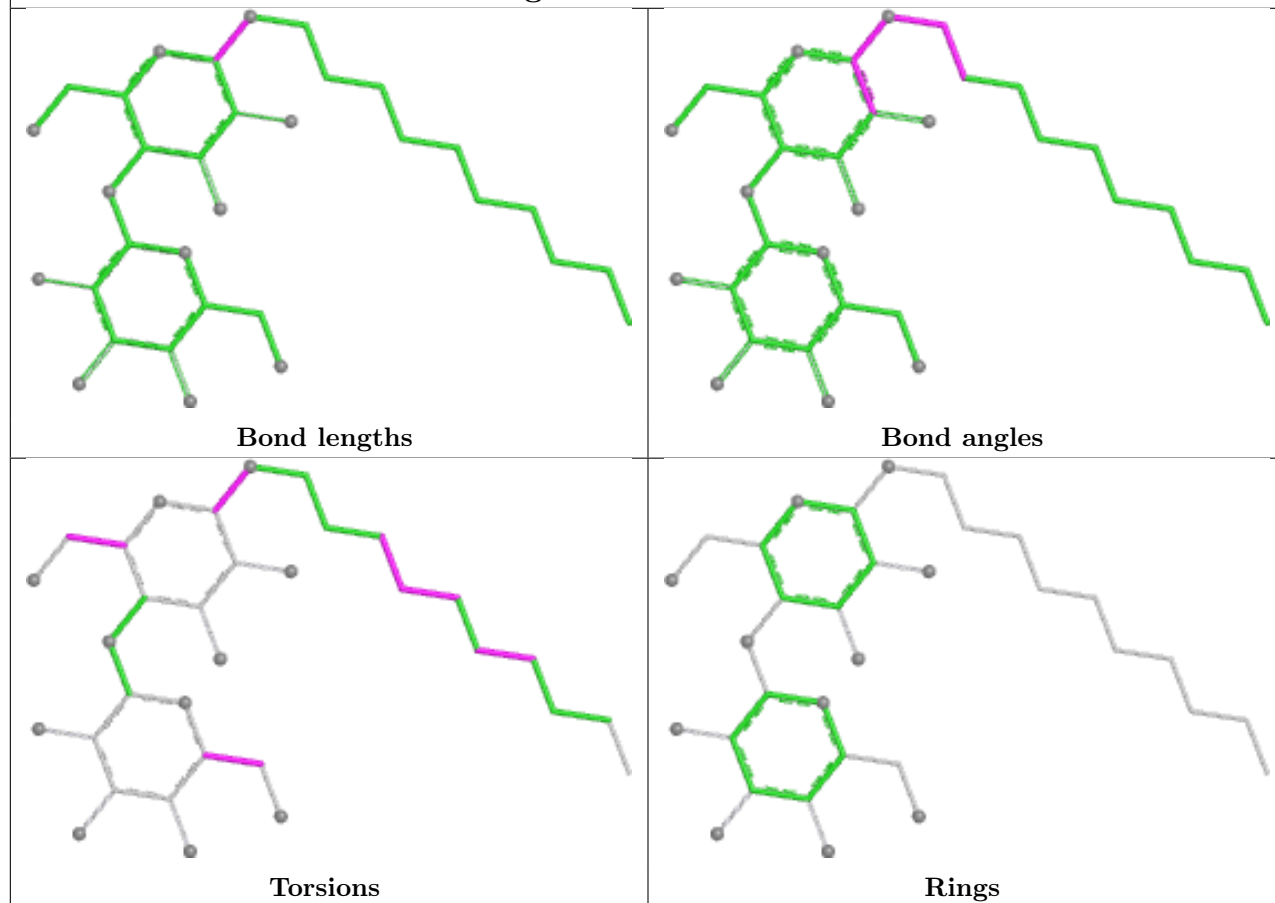


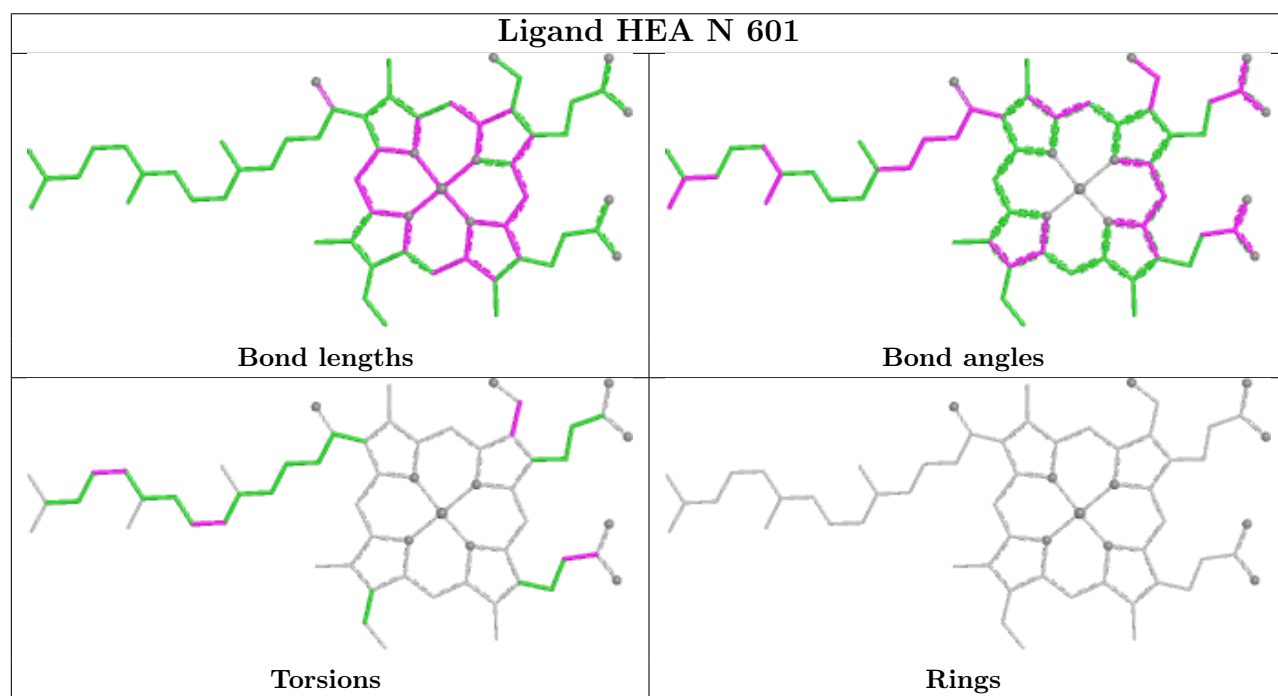
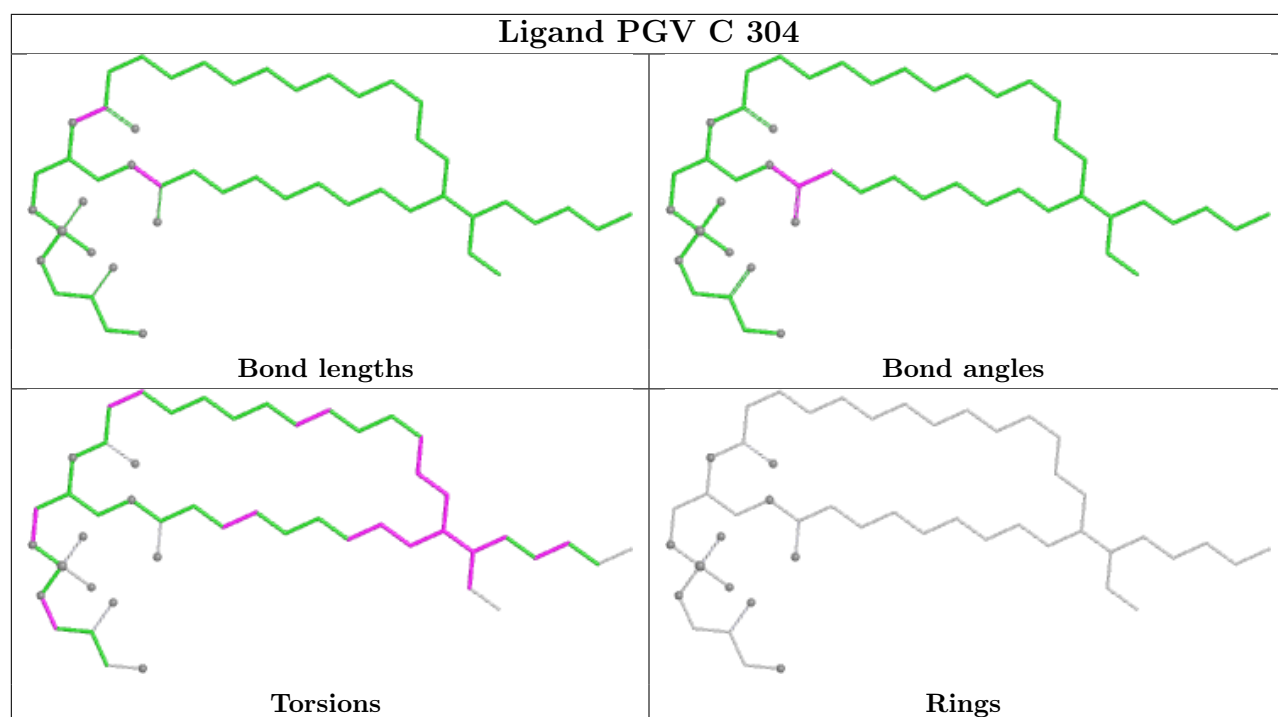


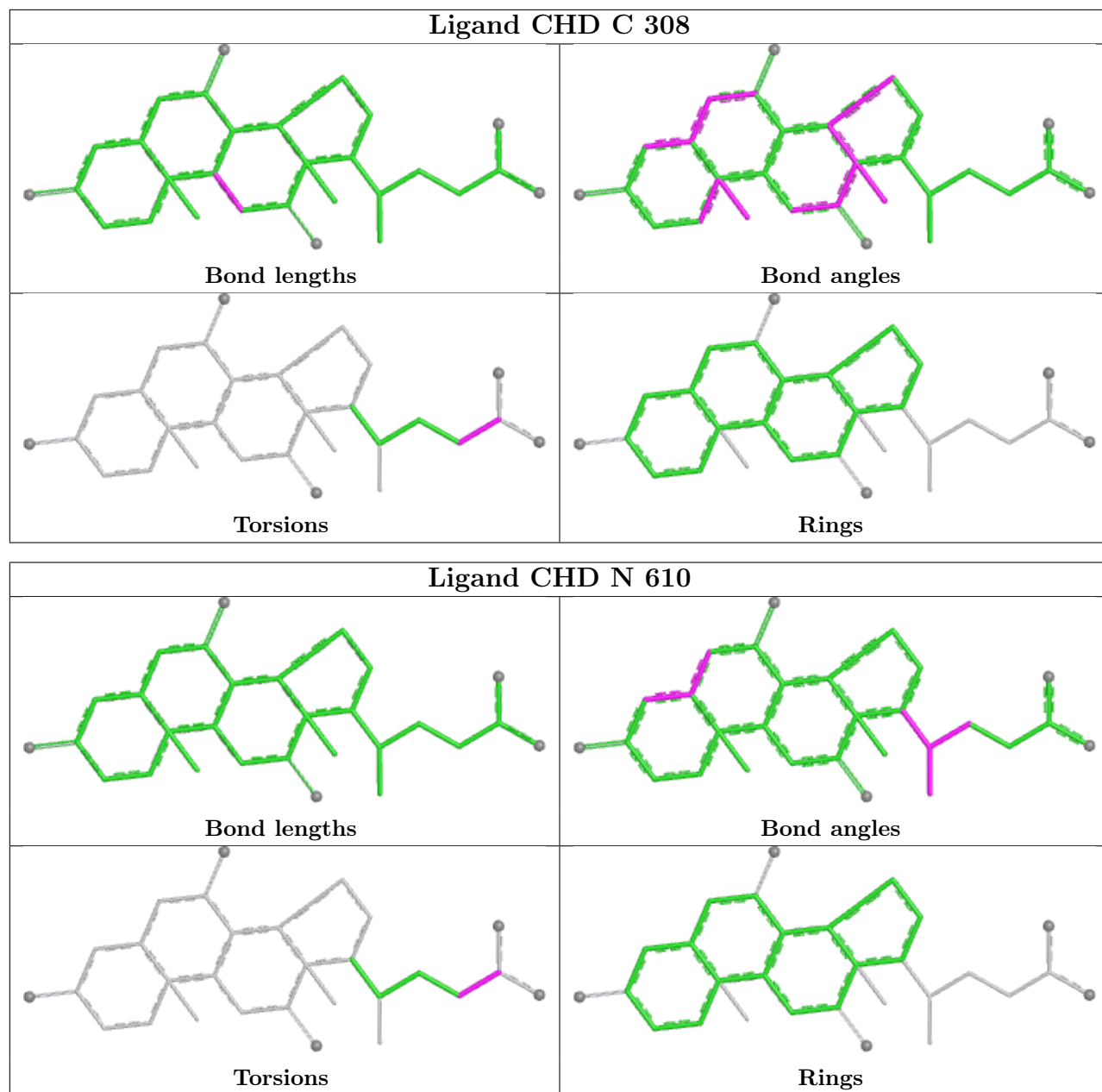
Ligand PSC R 201

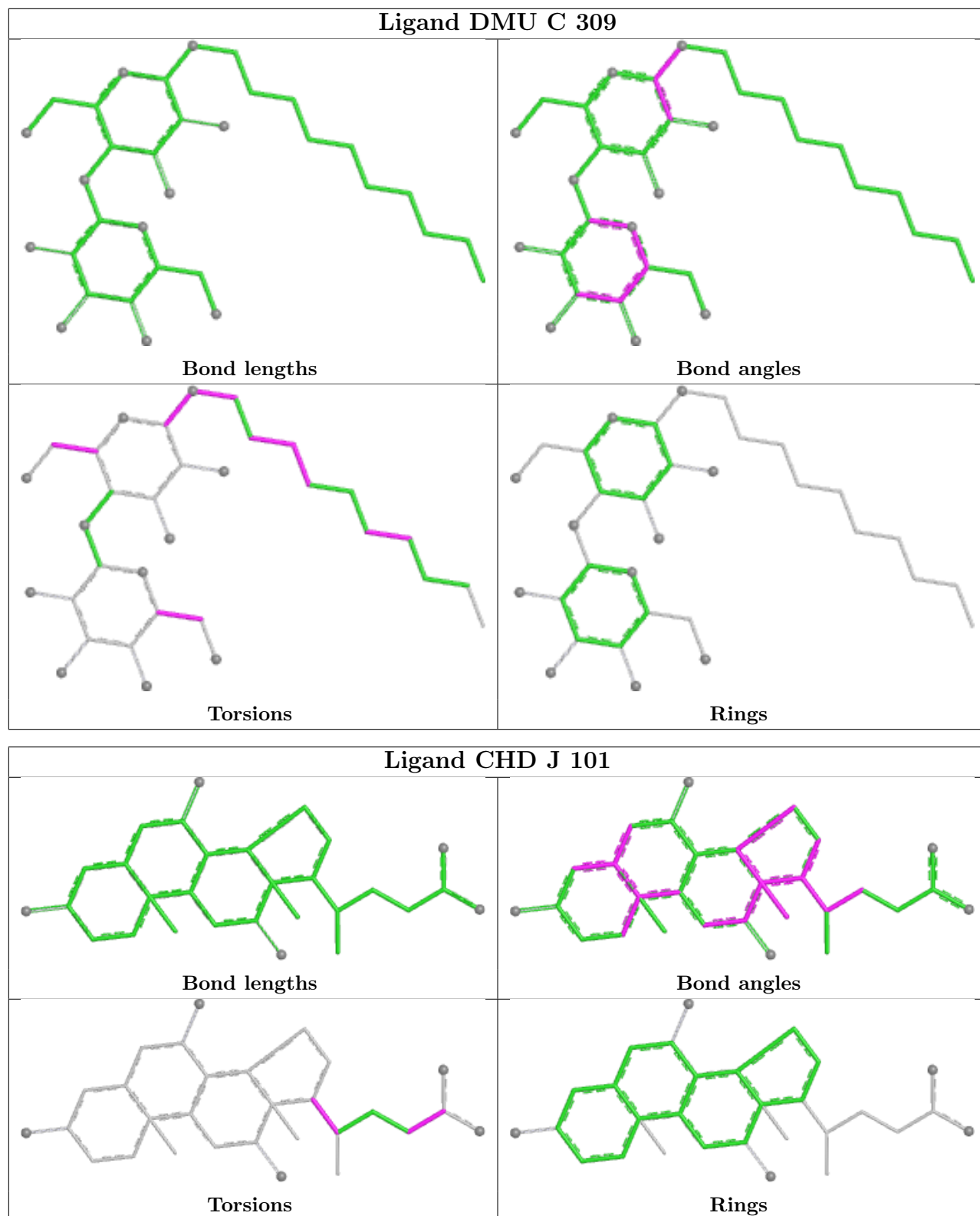


Ligand DMU P 307

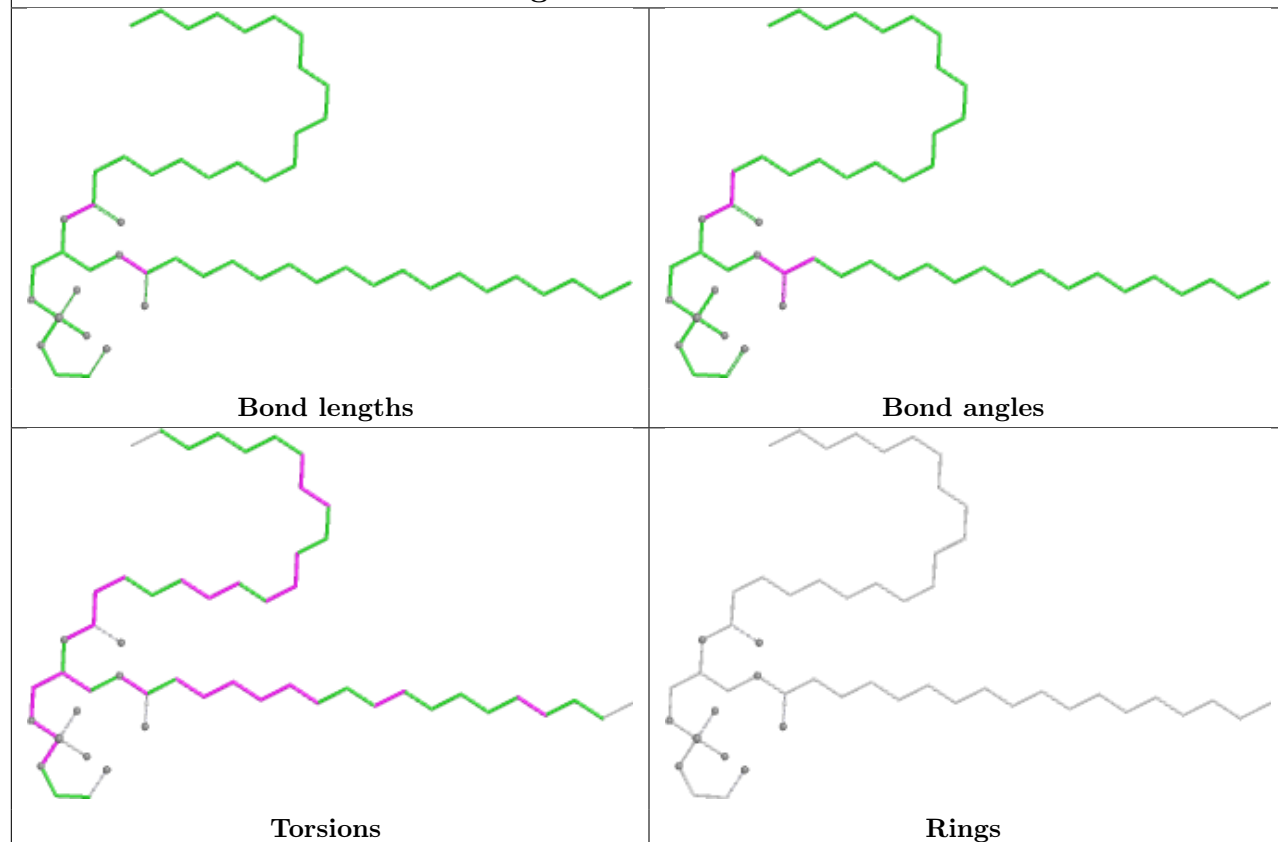




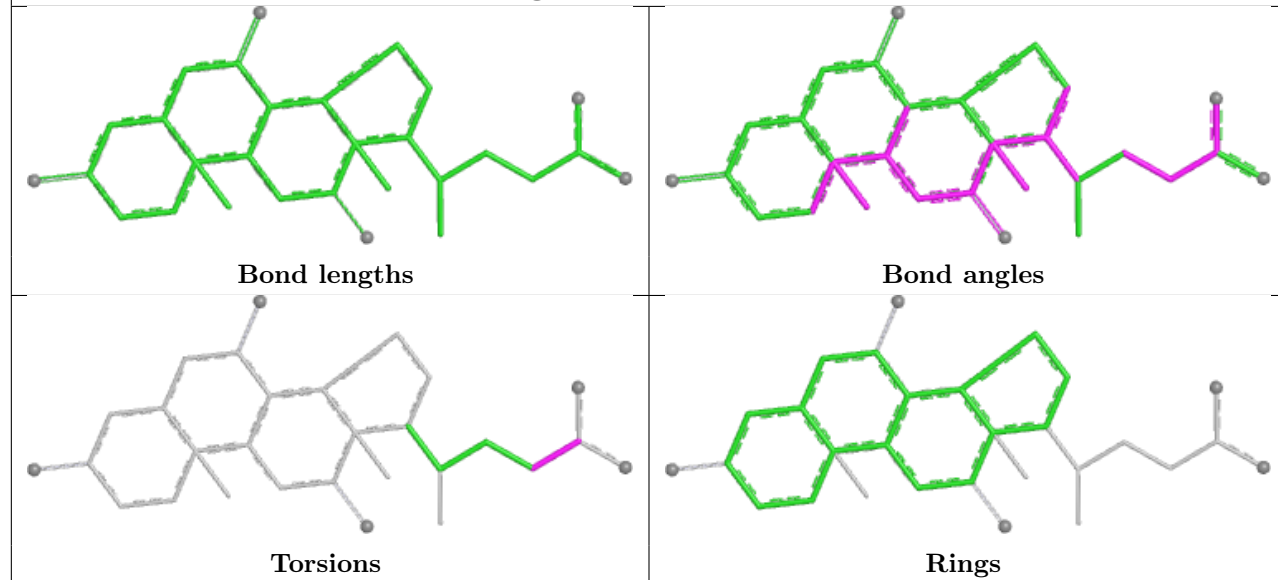


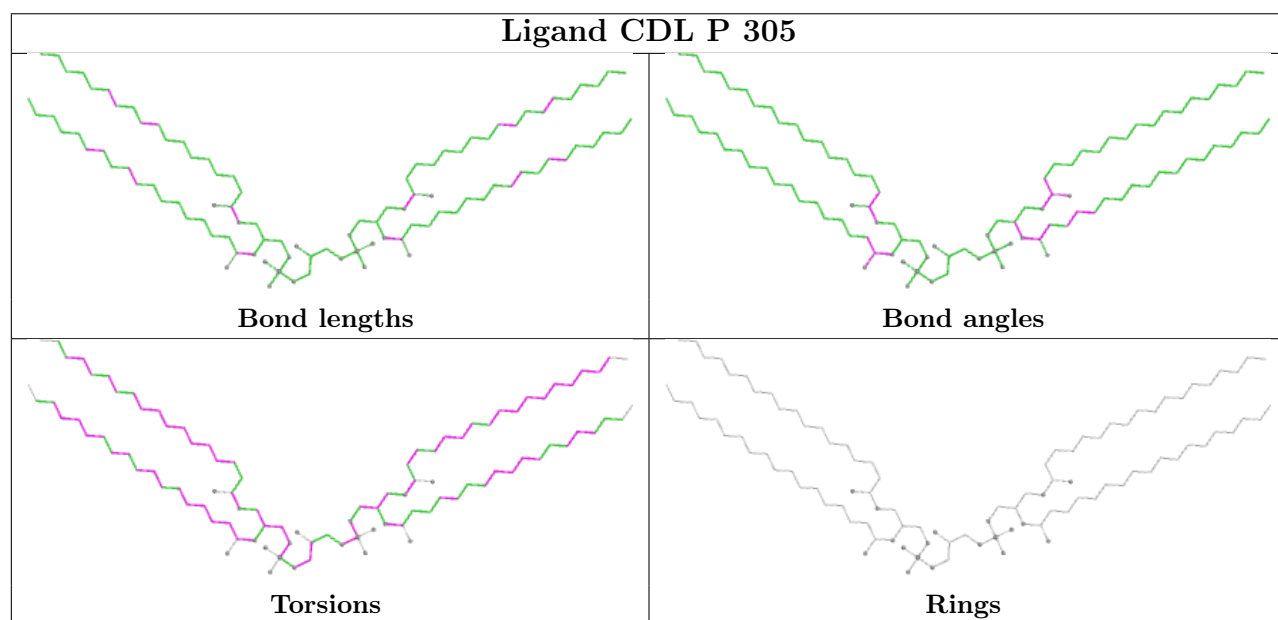
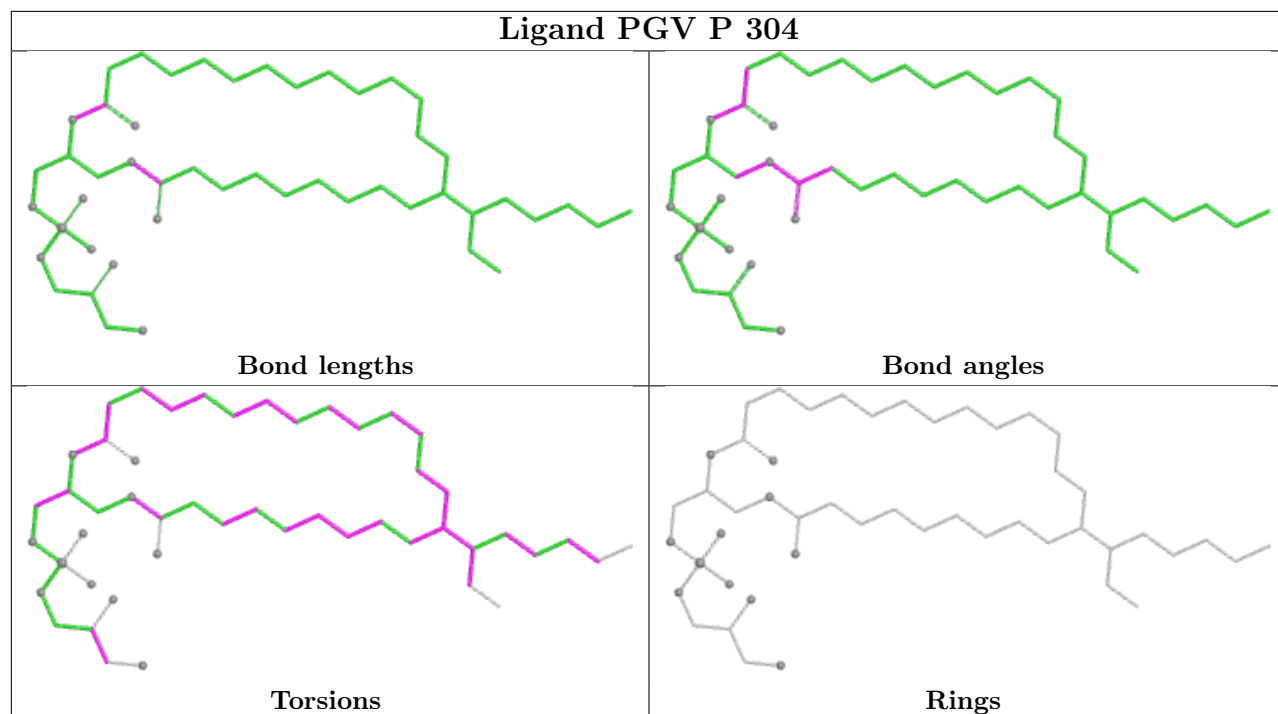


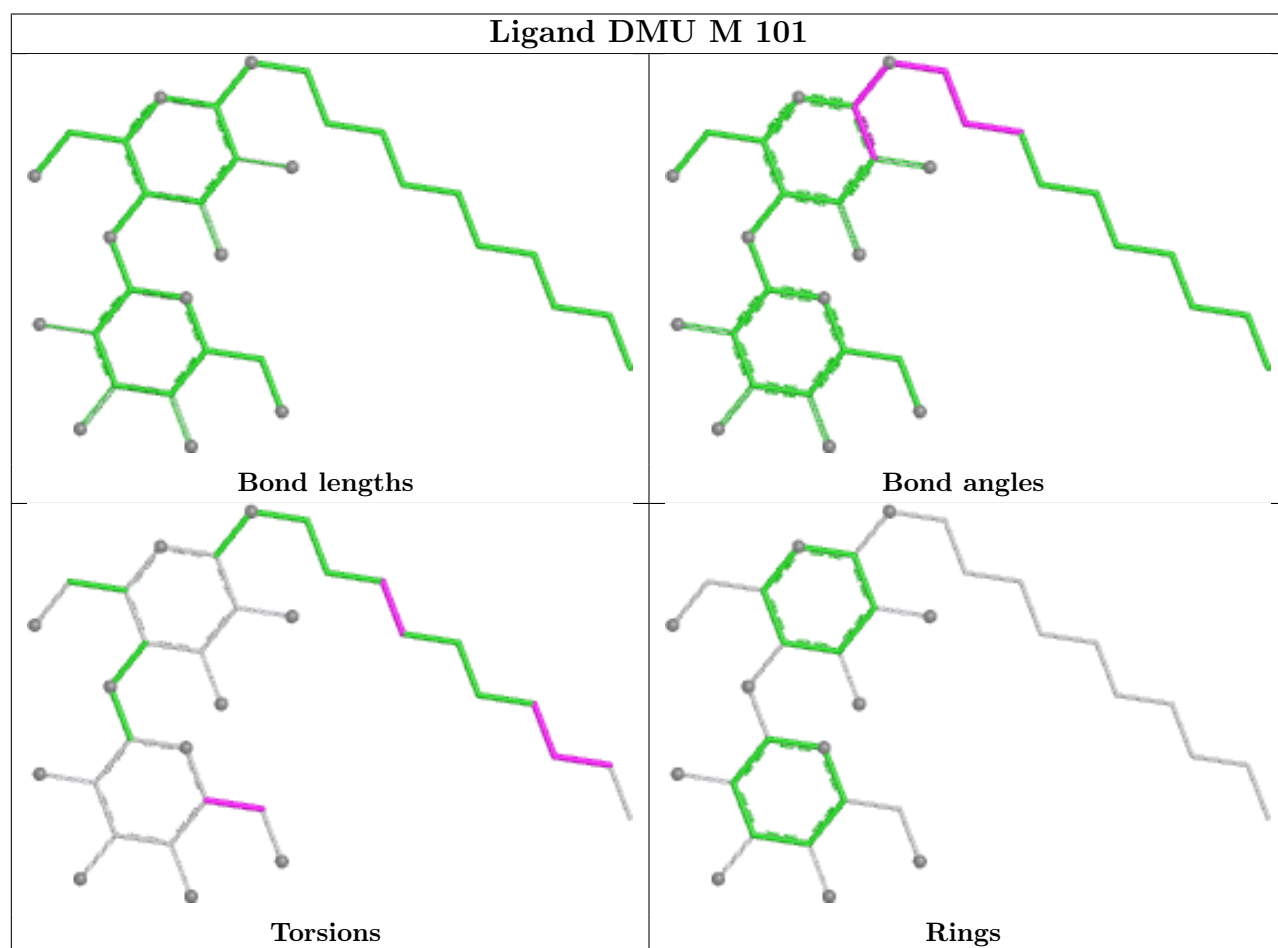
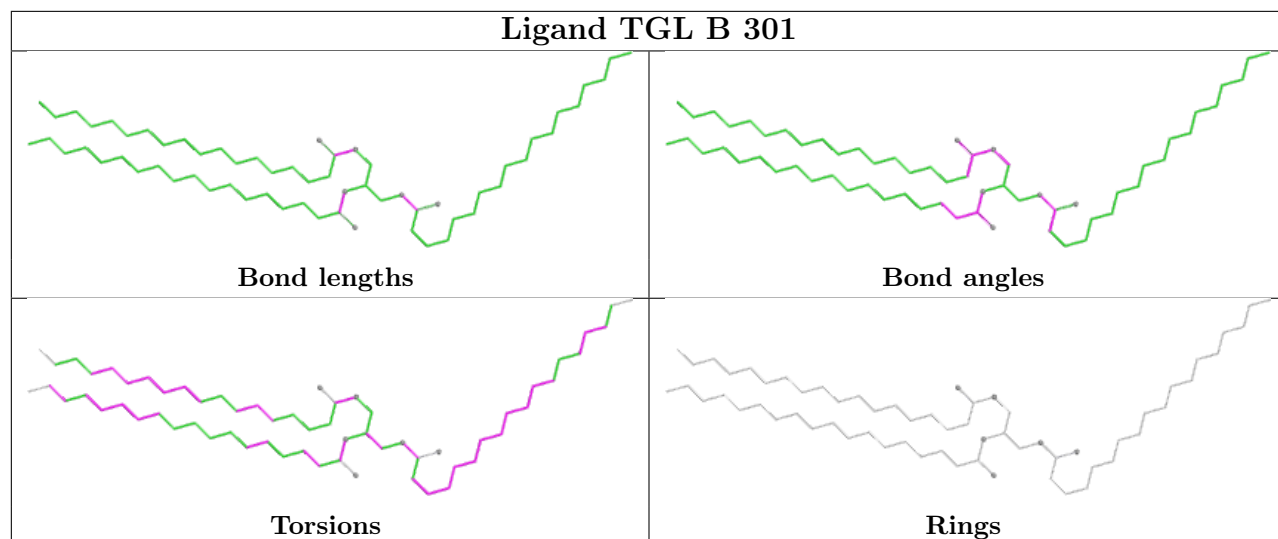
Ligand PEK G 102

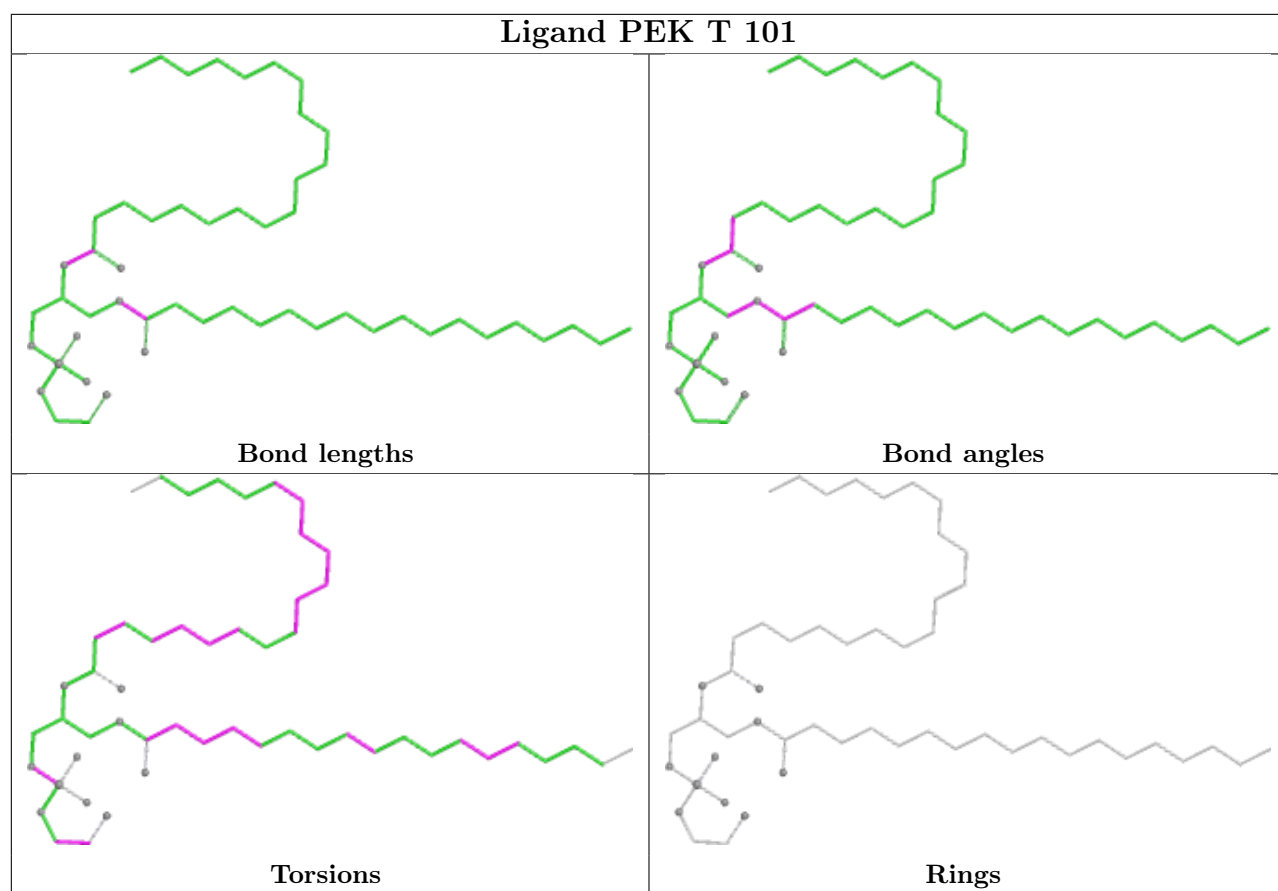


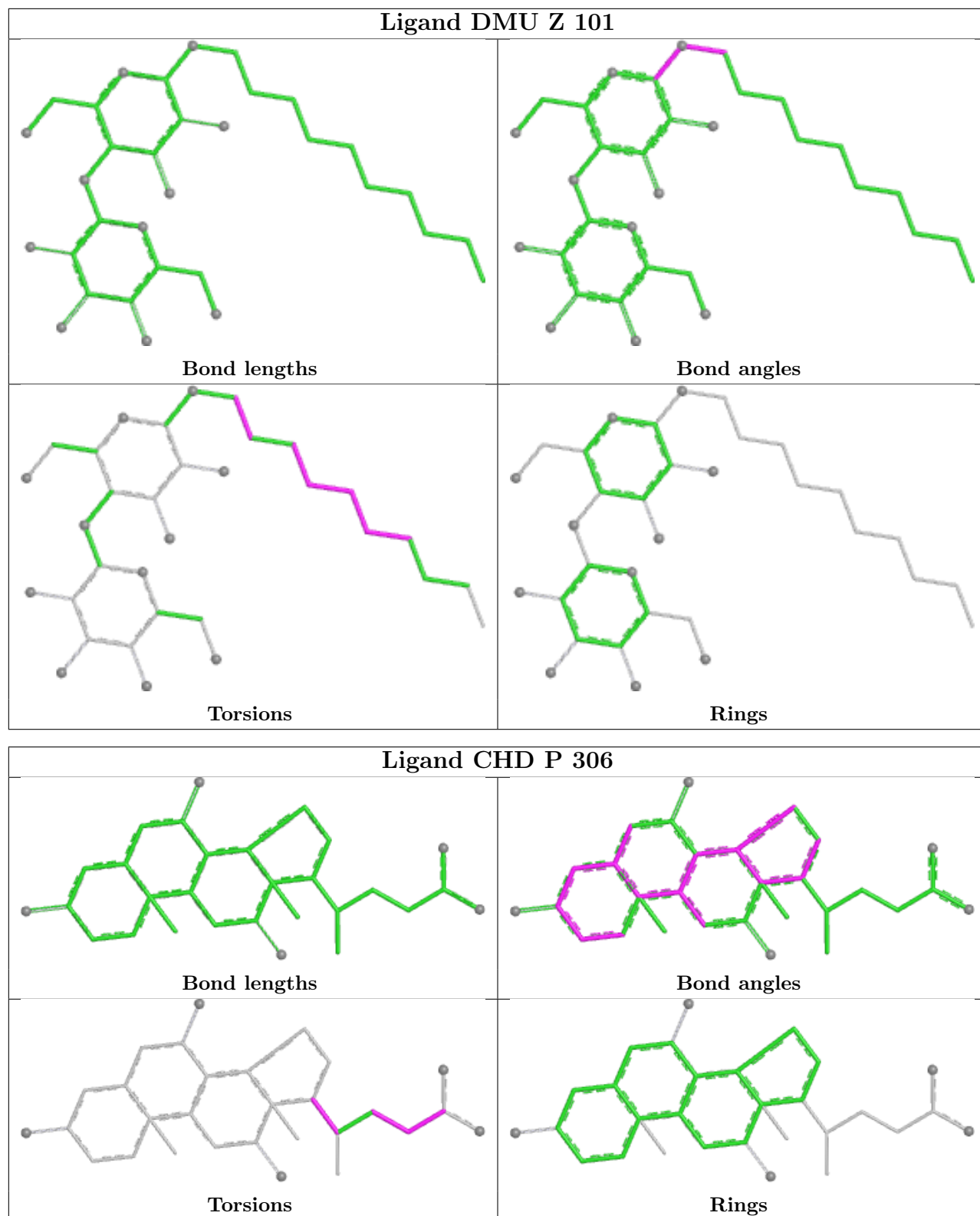
Ligand CHD O 301

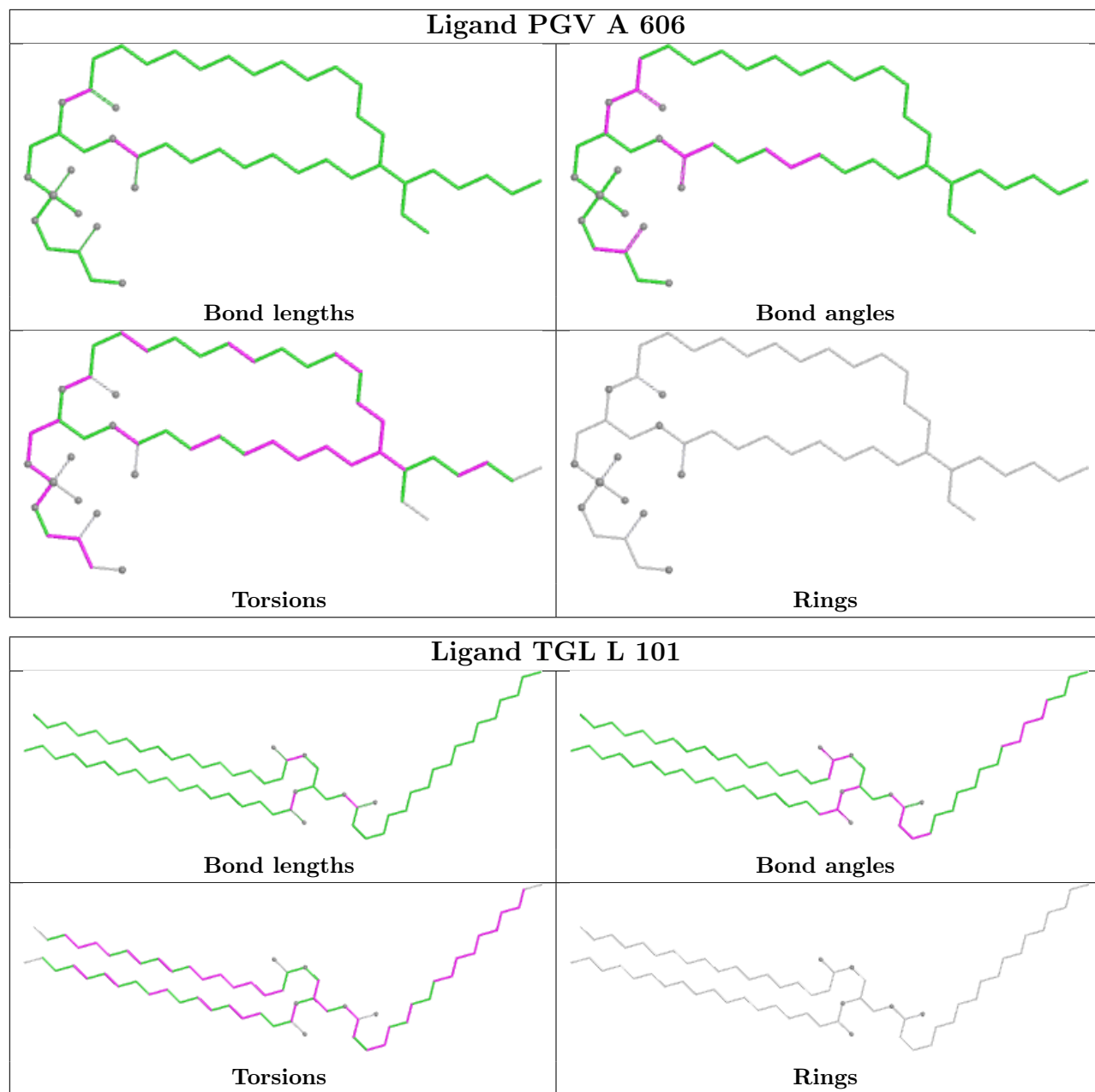


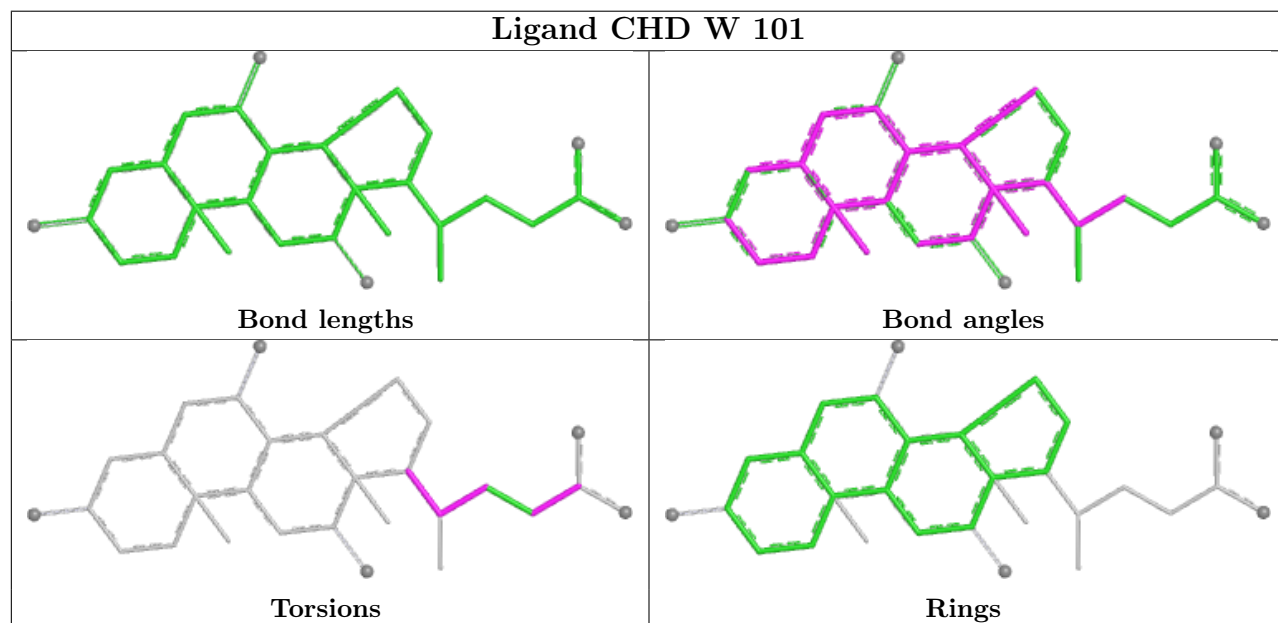
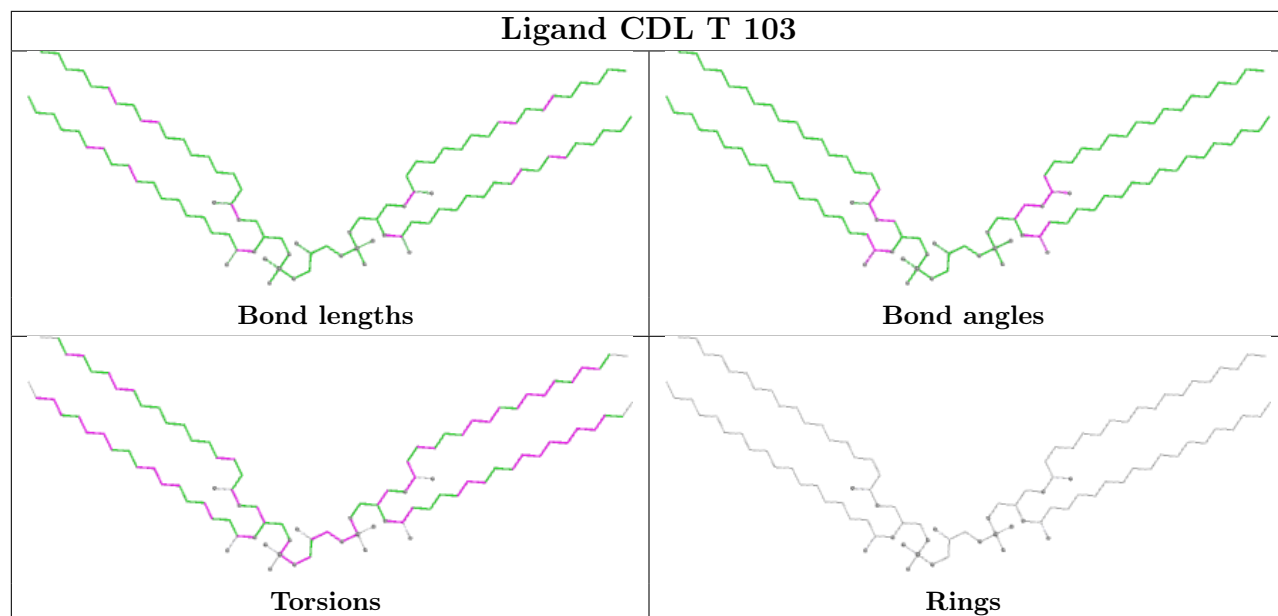


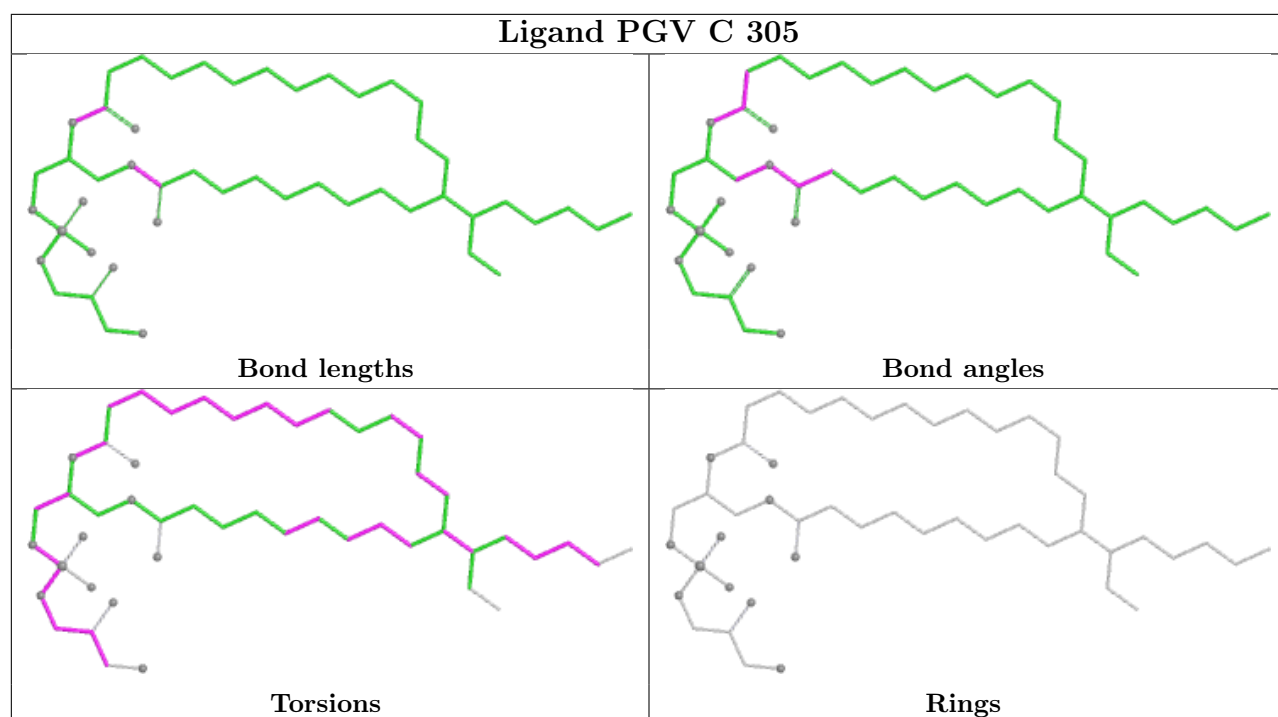












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	513/514 (99%)	-0.49	3 (0%)	85 87	14, 28, 36, 71	12 (2%)
1	N	513/514 (99%)	-0.41	6 (1%)	76 79	14, 31, 40, 70	12 (2%)
2	B	226/227 (99%)	-0.02	10 (4%)	39 41	17, 35, 56, 91	6 (2%)
2	O	226/227 (99%)	0.08	10 (4%)	39 41	18, 40, 63, 84	5 (2%)
3	C	259/261 (99%)	-0.23	4 (1%)	72 75	14, 32, 43, 78	8 (3%)
3	P	259/261 (99%)	-0.22	4 (1%)	72 75	14, 32, 44, 76	8 (3%)
4	D	144/147 (97%)	-0.02	4 (2%)	55 59	16, 36, 57, 76	6 (4%)
4	Q	144/147 (97%)	0.67	10 (6%)	23 24	21, 49, 78, 148	1 (0%)
5	E	105/109 (96%)	-0.15	3 (2%)	53 57	22, 37, 58, 103	1 (0%)
5	R	105/109 (96%)	0.16	2 (1%)	66 70	34, 45, 63, 113	0
6	F	98/98 (100%)	0.39	9 (9%)	14 15	17, 37, 93, 145	5 (5%)
6	S	98/98 (100%)	0.63	9 (9%)	14 15	18, 37, 97, 149	1 (1%)
7	G	83/85 (97%)	1.07	15 (18%)	3 3	16, 41, 104, 128	1 (1%)
7	T	83/85 (97%)	1.04	18 (21%)	2 2	17, 42, 105, 134	3 (3%)
8	H	79/85 (92%)	0.56	11 (13%)	6 6	32, 41, 95, 109	0
8	U	79/85 (92%)	0.55	8 (10%)	12 13	36, 46, 96, 121	0
9	I	72/73 (98%)	0.59	8 (11%)	10 11	35, 47, 74, 86	0
9	V	72/73 (98%)	0.70	6 (8%)	17 18	23, 55, 73, 91	1 (1%)
10	J	58/59 (98%)	0.63	7 (12%)	8 9	32, 43, 65, 107	0
10	W	58/59 (98%)	0.53	4 (6%)	23 24	34, 44, 70, 109	0
11	K	49/56 (87%)	0.27	2 (4%)	41 44	19, 41, 54, 60	1 (2%)
11	X	49/56 (87%)	0.65	4 (8%)	17 18	23, 51, 68, 79	1 (2%)
12	L	46/47 (97%)	0.04	2 (4%)	40 42	30, 34, 54, 88	0
12	Y	46/47 (97%)	0.34	4 (8%)	16 17	33, 41, 61, 107	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	0.22	3 (6%) 22 24	29, 34, 65, 99	0
13	Z	43/46 (93%)	0.48	3 (6%) 22 24	36, 42, 75, 108	0
All	All	3550/3614 (98%)	0.04	169 (4%) 35 38	14, 35, 67, 149	72 (2%)

All (169) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	S	97	ALA	12.9
6	S	1	ALA	11.7
4	Q	5	VAL	10.7
7	T	36[A]	TRP	10.1
4	Q	6	VAL	10.0
6	F	1	ALA	9.6
7	G	36	TRP	9.4
6	S	94	HIS	8.2
6	S	96	LEU	7.0
7	G	2	SER	6.9
6	S	98	HIS	6.9
7	G	6	GLY	6.6
7	T	6	GLY	6.5
7	G	4	ALA	6.3
6	S	95	GLN	6.2
7	T	9	GLY	6.2
7	T	4	ALA	6.0
7	G	5	LYS	6.0
7	T	3	ALA	6.0
7	T	5	LYS	5.9
6	F	2	SER	5.8
7	G	9	GLY	5.8
7	T	2	SER	5.8
8	H	8	ILE	5.8
6	F	97	ALA	5.8
8	U	8	ILE	5.7
7	T	1	ALA	5.6
6	F	96	LEU	5.6
7	G	8	HIS	5.5
7	T	7	ASP	5.5
7	G	3	ALA	5.4
6	S	3	GLY	5.3
9	V	37	PHE	5.3
2	O	113	TYR	5.1

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Mol	Chain	Res	Type	RSRZ
7	G	7	ASP	5.1
7	G	1	ALA	4.9
5	R	109	VAL	4.9
6	S	93	PRO	4.9
6	S	2	SER	4.7
2	B	59	GLN	4.6
2	B	36[A]	SER	4.6
4	D	5	VAL	4.6
7	G	37	LEU	4.5
5	E	109	VAL	4.4
6	F	3	GLY	4.4
8	U	44	THR	4.3
4	Q	7	LYS	4.3
2	O	59	GLN	4.2
7	T	8	HIS	4.1
3	P	3	HIS	4.1
7	T	38	HIS	4.1
1	N	113[A]	LEU	4.0
1	A	514	LYS	4.0
7	G	84	LYS	4.0
6	F	94	HIS	3.9
1	A	113[A]	LEU	3.8
8	H	44	THR	3.7
9	I	25	PHE	3.7
2	O	227	LEU	3.7
10	J	56	PRO	3.7
3	C	3	HIS	3.6
12	L	2	HIS	3.6
9	I	29	LEU	3.6
11	X	6	ALA	3.6
9	I	37	PHE	3.6
4	Q	8	SER	3.5
8	H	7	LYS	3.5
1	N	136[A]	LEU	3.5
7	T	10	GLY	3.5
8	H	46	LYS	3.5
10	W	57	HIS	3.5
4	Q	4	SER	3.5
9	V	3	ALA	3.5
8	U	47	GLY	3.5
12	Y	20	ARG	3.4
3	C	38	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
7	G	41	HIS	3.3
6	F	98	HIS	3.3
8	H	47	GLY	3.3
10	J	1	PHE	3.2
8	U	46	LYS	3.2
7	G	10	GLY	3.2
2	B	113	TYR	3.1
13	Z	43	SER	3.1
11	X	13	TYR	3.1
2	B	60	GLU	3.1
13	M	40	TYR	3.1
13	M	42	LYS	3.0
2	B	91	ASN	3.0
8	H	45	ALA	3.0
10	J	52	TRP	3.0
12	Y	2	HIS	3.0
4	D	87[A]	PHE	3.0
10	J	57	HIS	3.0
3	P	37	PHE	3.0
10	J	58	LYS	3.0
8	U	45	ALA	3.0
11	K	6	ALA	2.9
7	T	42	ARG	2.9
4	D	4	SER	2.9
4	Q	9	GLU	2.8
10	W	52	TRP	2.8
9	V	2	THR	2.8
9	I	2	THR	2.8
7	G	45	PRO	2.8
3	P	33	MET	2.8
1	A	486	ASP	2.8
9	V	26	MET	2.8
12	L	47	LYS	2.7
1	N	513	LEU	2.7
6	F	37[A]	LYS	2.7
5	R	5	HIS	2.7
7	T	37	LEU	2.7
3	C	37	PHE	2.7
11	X	7	PRO	2.7
8	U	48	GLY	2.6
9	I	26	MET	2.6
10	W	58	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
3	C	33	MET	2.6
8	U	42	ALA	2.5
2	O	90	ILE	2.5
3	P	38	ASN	2.5
7	T	12	GLY	2.5
4	Q	35	ALA	2.5
2	B	115	ASP	2.5
8	H	9	LYS	2.4
10	W	1	PHE	2.3
2	O	114	GLU	2.3
10	J	27	THR	2.3
9	V	34	PHE	2.3
12	Y	47	LYS	2.3
4	Q	10	ASP	2.3
2	O	91	ASN	2.3
8	H	10	ASN	2.3
9	V	33	THR	2.3
2	B	61	VAL	2.3
2	O	22[A]	HIS	2.3
1	N	483	LEU	2.3
5	E	14[A]	ARG	2.2
11	K	47	ARG	2.2
9	I	34	PHE	2.2
2	O	92	ASN	2.2
7	T	84	LYS	2.2
4	Q	58	GLU	2.2
8	H	42	ALA	2.2
2	O	32[A]	PHE	2.2
9	I	31	PHE	2.2
2	O	226	MET	2.2
4	Q	147	LYS	2.2
8	U	7	LYS	2.2
11	X	12	LYS	2.2
13	Z	42	LYS	2.2
6	F	95	GLN	2.2
10	J	55	PHE	2.2
1	N	514	LYS	2.2
2	B	22[A]	HIS	2.2
5	E	5	HIS	2.2
13	M	39	ASN	2.2
2	B	55	THR	2.2
7	T	40	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	68	LEU	2.1
1	N	512	ASN	2.1
12	Y	24	MET	2.1
13	Z	39	ASN	2.1
7	T	39	SER	2.0
9	I	36	LYS	2.0
8	H	50	VAL	2.0
4	D	9	GLU	2.0
8	H	48	GLY	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	SAC	V	1	9/10	0.47	0.20	117,122,125,126	0
9	SAC	I	1	9/10	0.49	0.23	85,97,109,115	0
7	TPO	T	11	11/12	0.59	0.29	110,123,134,135	0
7	TPO	G	11	11/12	0.65	0.28	106,116,133,137	0
1	FME	A	1	10/11	0.92	0.13	41,46,68,84	0
1	FME	N	1	10/11	0.94	0.13	43,49,71,73	0
2	FME	B	1	10/11	0.95	0.10	32,34,43,57	0
2	FME	O	1	10/11	0.97	0.08	40,41,51,57	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
23	PEK	G	102	53/53	0.72	0.27	49,105,138,154	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	PEK	T	101	53/53	0.72	0.28	52,96,152,157	0
22	CHD	W	101	29/29	0.73	0.33	96,123,135,140	0
18	PGV	P	304	51/51	0.76	0.23	60,80,108,116	0
24	CDL	G	101	100/100	0.76	0.26	63,90,131,148	0
18	PGV	C	305	51/51	0.77	0.22	53,79,113,119	0
22	CHD	J	101	29/29	0.77	0.21	62,80,116,123	0
24	CDL	T	103	100/100	0.77	0.26	61,90,141,150	0
25	DMU	C	309	33/33	0.77	0.20	45,99,129,131	0
23	PEK	C	303	53/53	0.78	0.24	50,79,121,126	0
26	PSC	E	201	52/52	0.78	0.23	49,98,155,160	0
23	PEK	P	302	53/53	0.79	0.24	51,74,133,139	0
18	PGV	N	606	51/51	0.79	0.24	55,79,121,126	0
20	TGL	Q	201	63/63	0.79	0.27	58,81,112,118	0
24	CDL	P	305	100/100	0.80	0.24	46,83,127,140	0
20	TGL	N	608	63/63	0.80	0.25	53,78,123,143	0
20	TGL	B	301	63/63	0.81	0.22	46,70,96,102	0
25	DMU	P	307	33/33	0.81	0.18	48,98,126,136	0
18	PGV	A	606	51/51	0.81	0.25	41,78,96,100	0
20	TGL	N	611	63/63	0.82	0.26	51,77,104,121	0
20	TGL	D	201	63/63	0.82	0.23	47,70,96,99	0
24	CDL	C	306	100/100	0.82	0.21	50,82,111,115	0
26	PSC	R	201	52/52	0.82	0.25	43,73,150,161	0
20	TGL	L	101	63/63	0.83	0.22	39,68,100,105	0
22	CHD	C	307	29/29	0.87	0.14	55,60,71,81	0
22	CHD	P	306	29/29	0.91	0.12	48,59,64,70	0
25	DMU	Z	101	33/33	0.93	0.10	51,56,65,65	0
22	CHD	C	308	29/29	0.94	0.08	30,33,38,41	0
25	DMU	M	101	33/33	0.94	0.10	41,46,55,61	0
23	PEK	T	102	53/53	0.94	0.13	35,47,81,85	0
17	NA	P	301	1/1	0.95	0.09	47,47,47,47	0
17	NA	C	301	1/1	0.95	0.11	49,49,49,49	0
23	PEK	C	302	53/53	0.95	0.12	31,48,80,85	0
22	CHD	B	303	29/29	0.96	0.07	28,30,34,43	0
22	CHD	N	610	29/29	0.96	0.07	30,33,38,44	0
18	PGV	N	609	51/51	0.96	0.10	29,41,63,69	0
18	PGV	A	608	51/51	0.96	0.10	28,39,64,70	0
18	PGV	C	304	51/51	0.97	0.10	29,36,75,80	0
18	PGV	P	303	51/51	0.97	0.09	28,38,72,76	0
22	CHD	O	301	29/29	0.97	0.06	26,30,34,41	0
14	HEA	A	601	60/60	0.98	0.07	22,26,51,55	0
19	PER	A	607[A]	2/2	0.98	0.07	19,19,19,25	0
19	PER	A	607[B]	2/2	0.98	0.07	15,15,15,15	2

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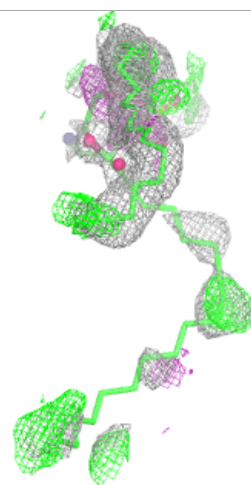
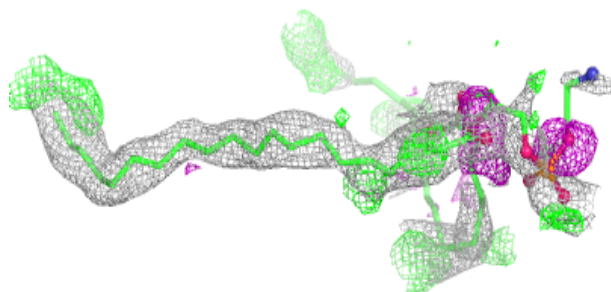
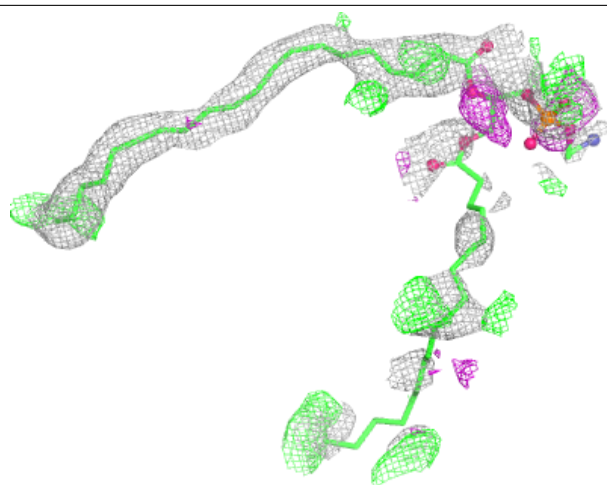
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
19	PER	N	607[A]	2/2	0.98	0.09	21,21,21,25	0
19	PER	N	607[B]	2/2	0.98	0.09	19,19,19,19	2
14	HEA	A	602	60/60	0.98	0.06	23,26,33,34	0
14	HEA	N	601	60/60	0.98	0.08	26,31,52,58	0
14	HEA	N	602	60/60	0.99	0.05	25,28,33,36	0
17	NA	N	605	1/1	0.99	0.03	35,35,35,35	0
16	MG	A	604	1/1	0.99	0.02	29,29,29,29	0
16	MG	N	604	1/1	0.99	0.04	36,36,36,36	0
17	NA	A	605	1/1	0.99	0.02	30,30,30,30	0
15	CU	A	603	1/1	1.00	0.02	27,27,27,27	0
15	CU	N	603	1/1	1.00	0.02	29,29,29,29	0
21	CUA	B	302	2/2	1.00	0.02	29,29,29,30	0
21	CUA	O	302	2/2	1.00	0.02	34,34,34,35	0
27	ZN	F	101	1/1	1.00	0.01	33,33,33,33	0
27	ZN	S	101	1/1	1.00	0.01	34,34,34,34	0

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

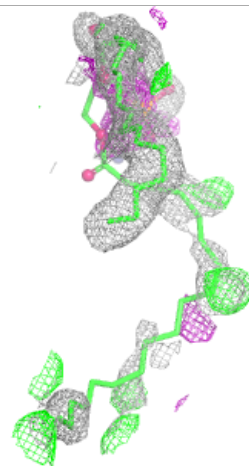
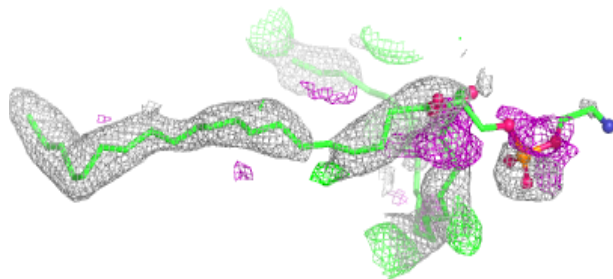
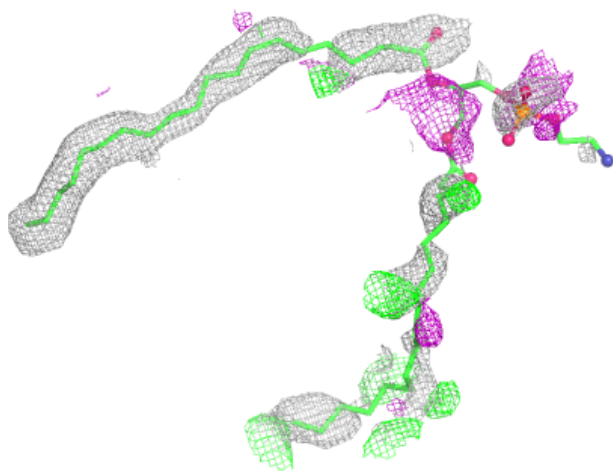
Electron density around PEK G 102:

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



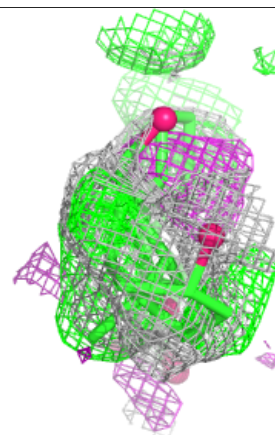
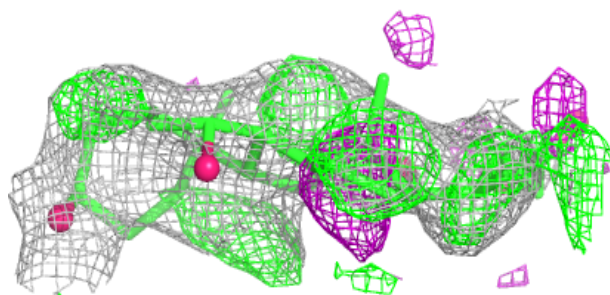
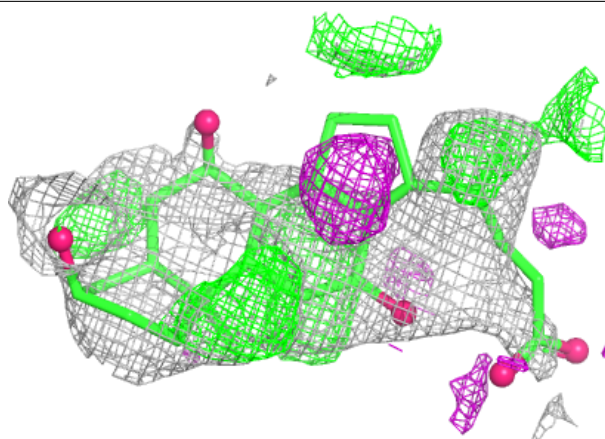
Electron density around PEK T 101:

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

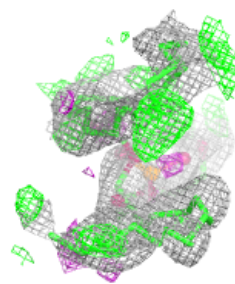
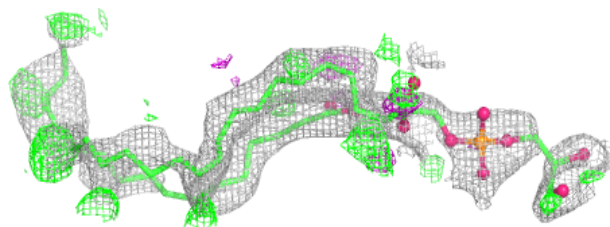
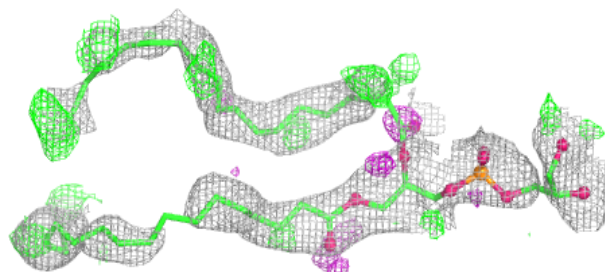


Electron density around CHD W 101:

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

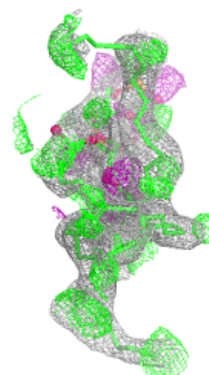
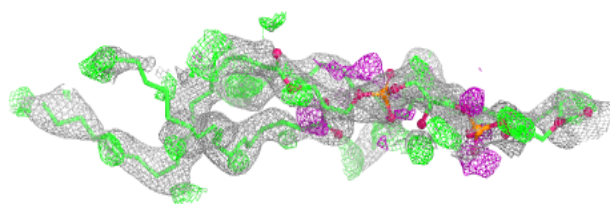
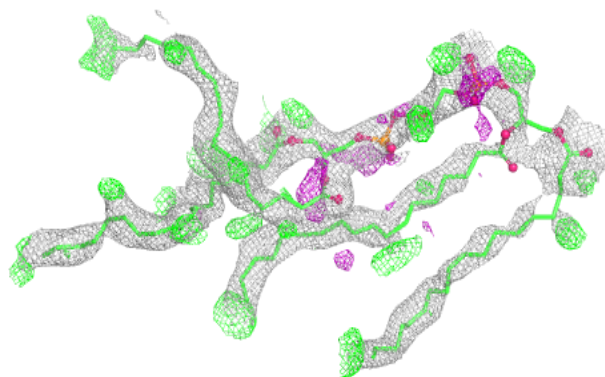
**Electron density around PGV P 304:**

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

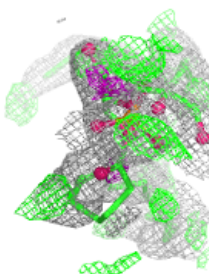
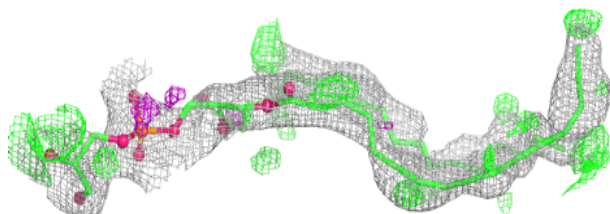
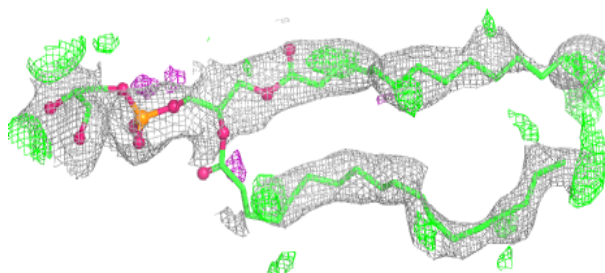


Electron density around CDL G 101:

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

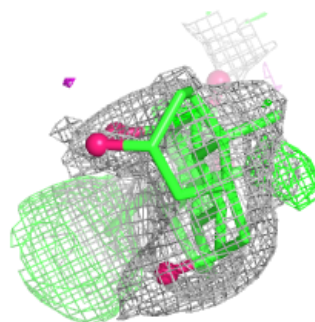
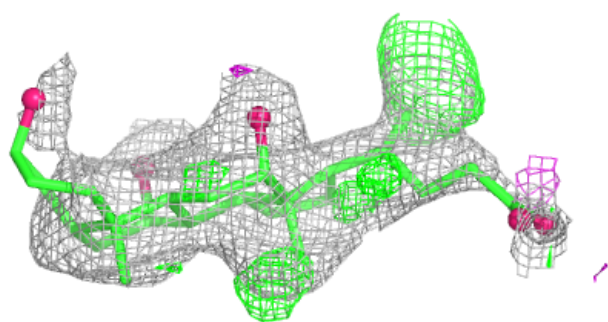
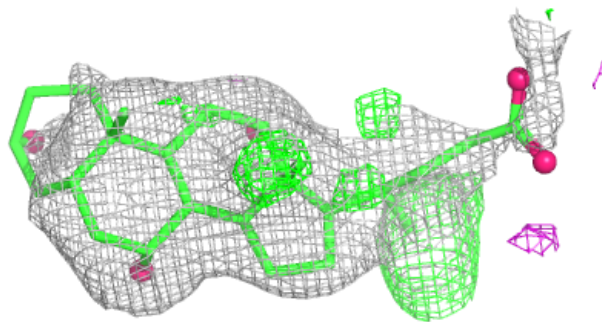
**Electron density around PGV C 305:**

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

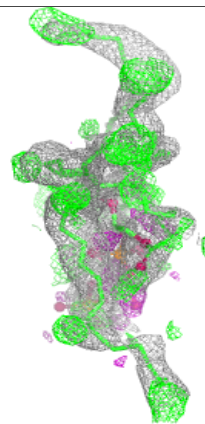
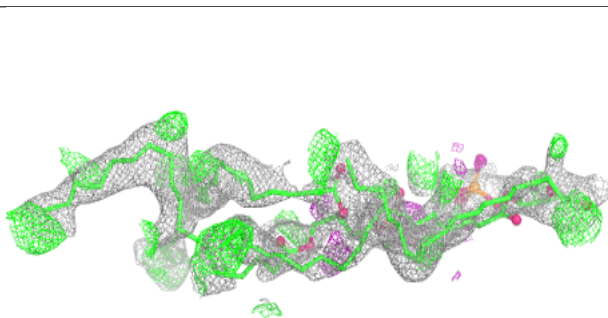
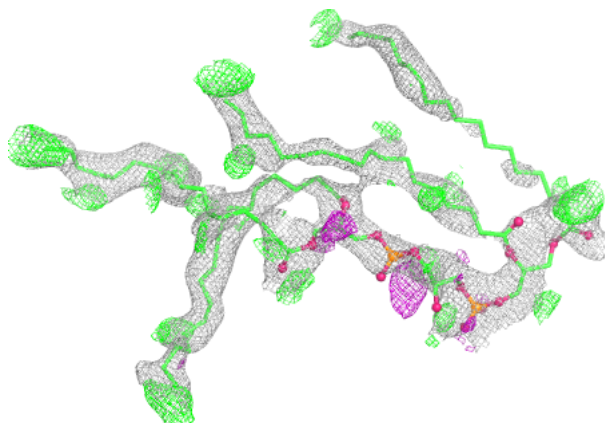


Electron density around CHD J 101:

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

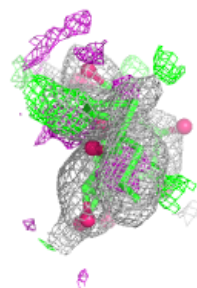
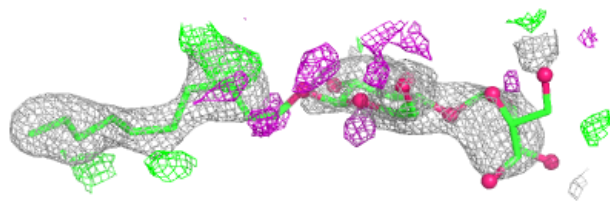
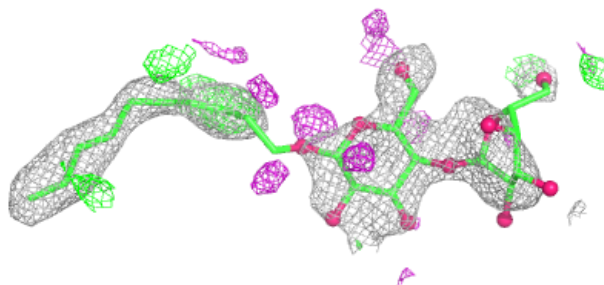
**Electron density around CDL T 103:**

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



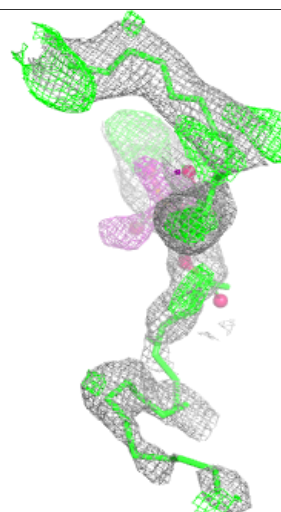
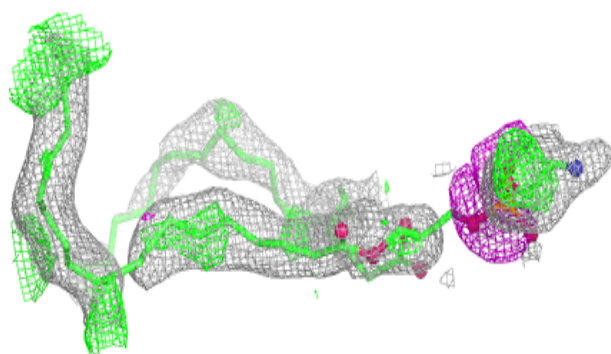
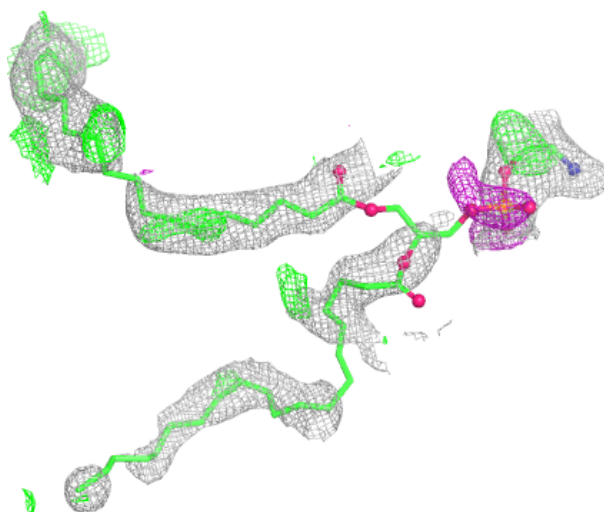
Electron density around DMU C 309:

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



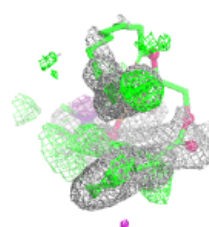
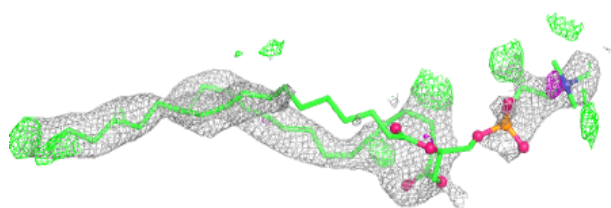
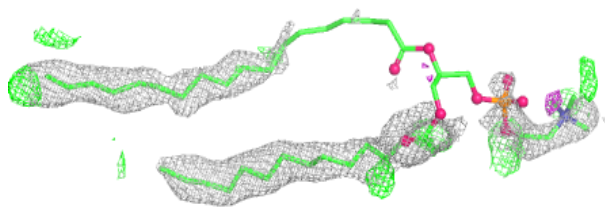
Electron density around PEK C 303:

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

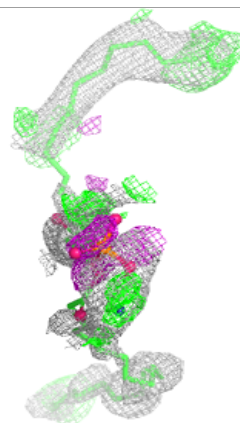
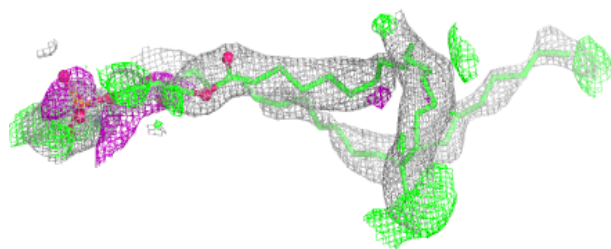
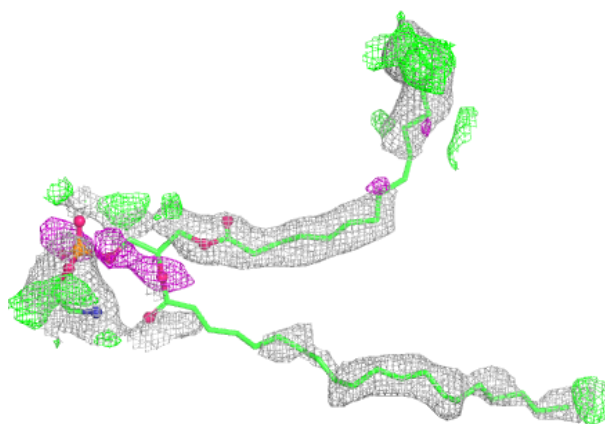


Electron density around PSC E 201:

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

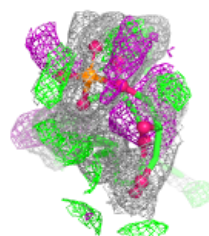
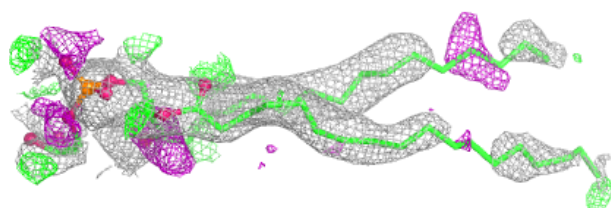
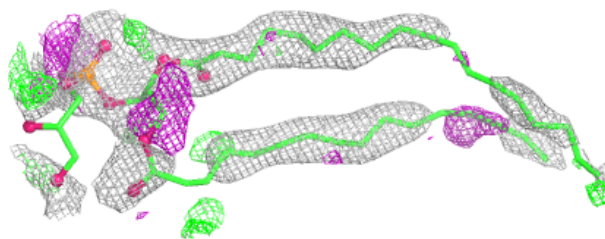
**Electron density around PEK P 302:**

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

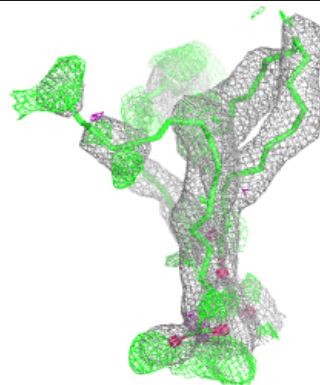
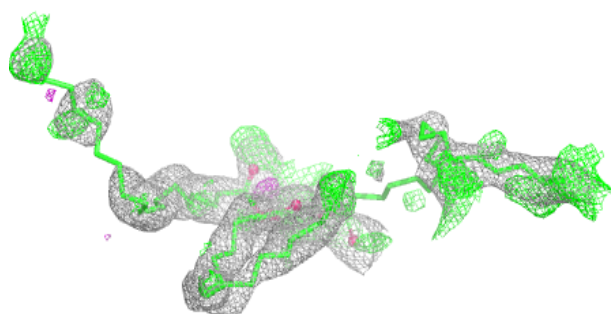
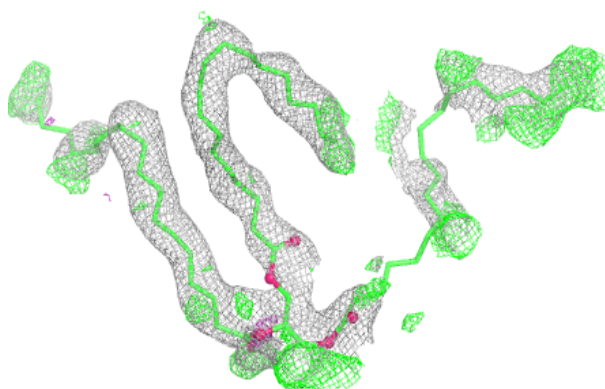


Electron density around PGV N 606:

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

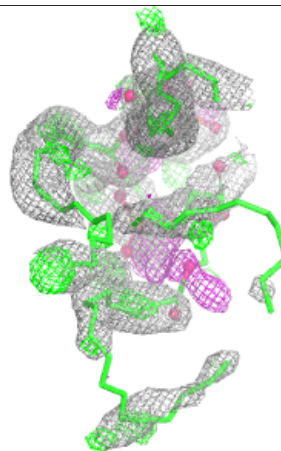
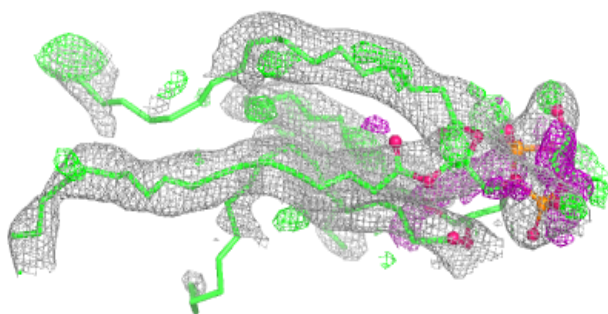
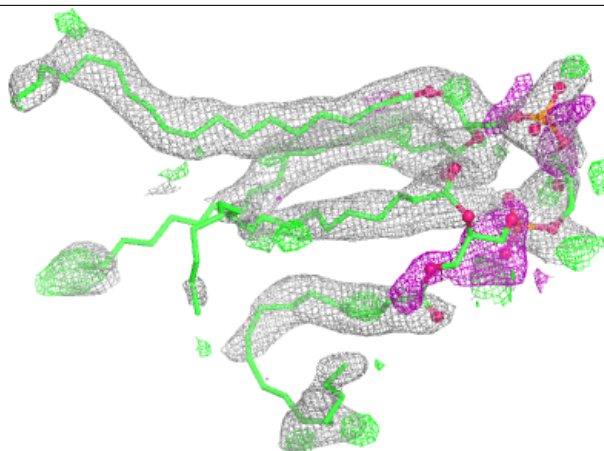
**Electron density around TGL Q 201:**

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

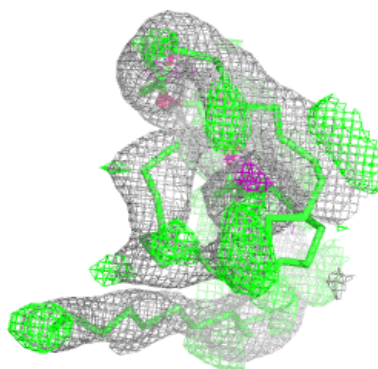
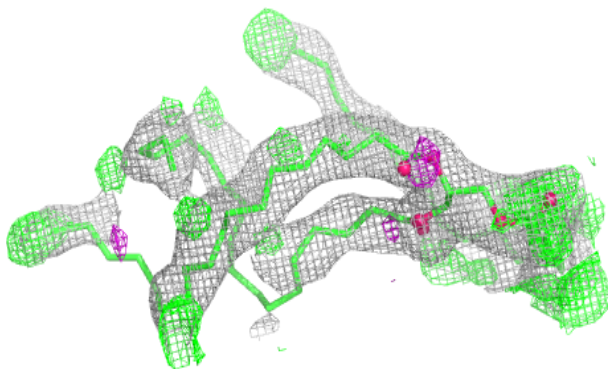
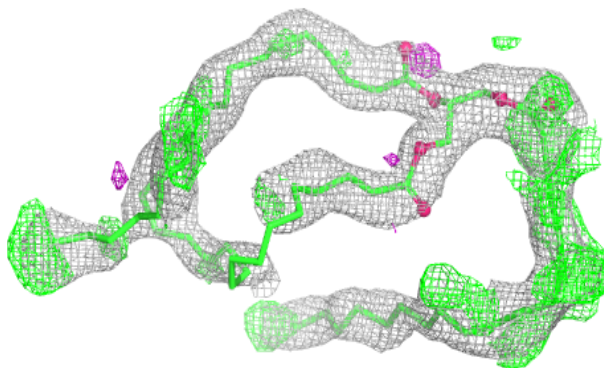


Electron density around CDL P 305:

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

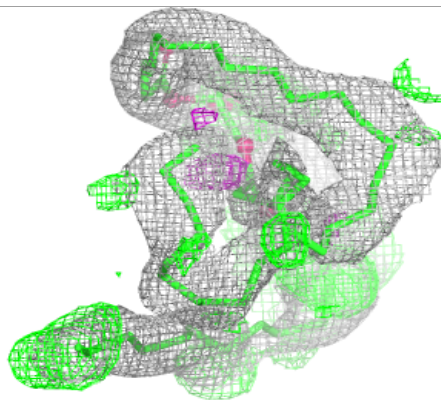
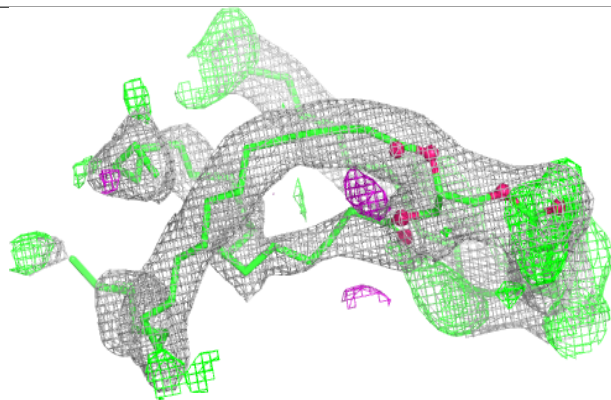
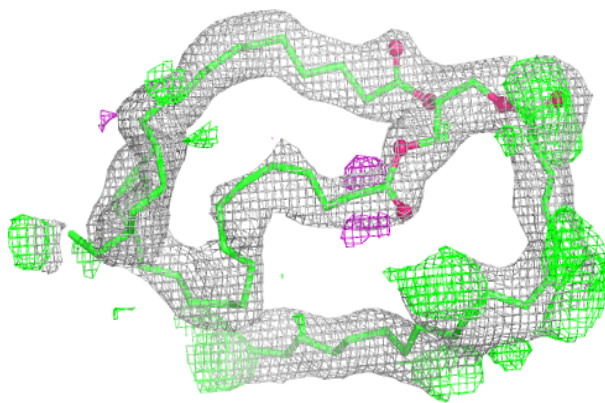
**Electron density around TGL N 608:**

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

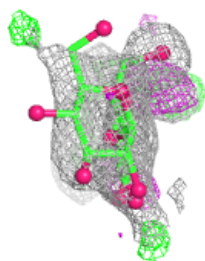
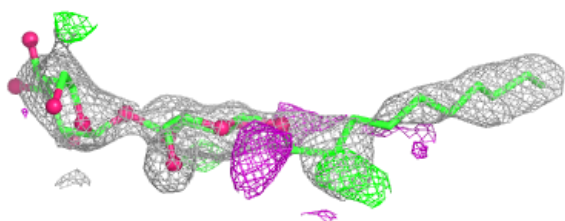
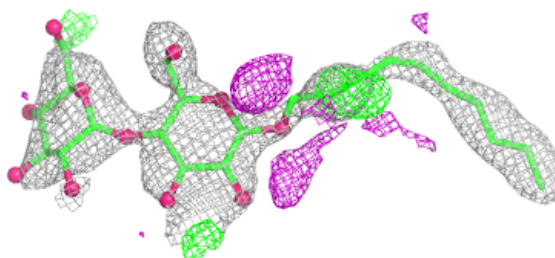


Electron density around TGL B 301:

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

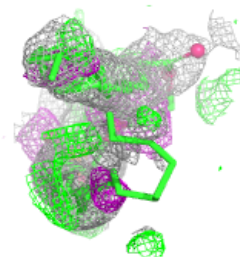
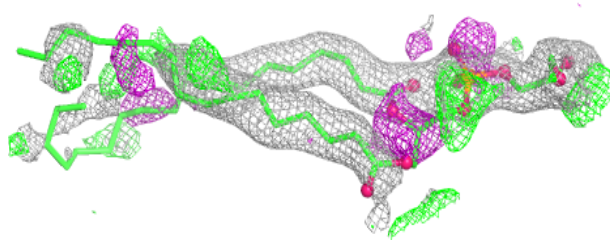
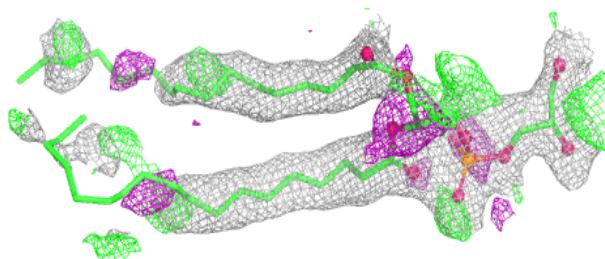
**Electron density around DMU P 307:**

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



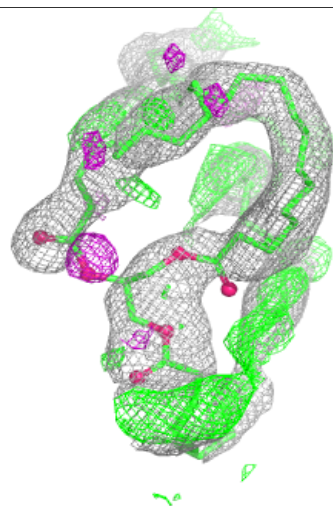
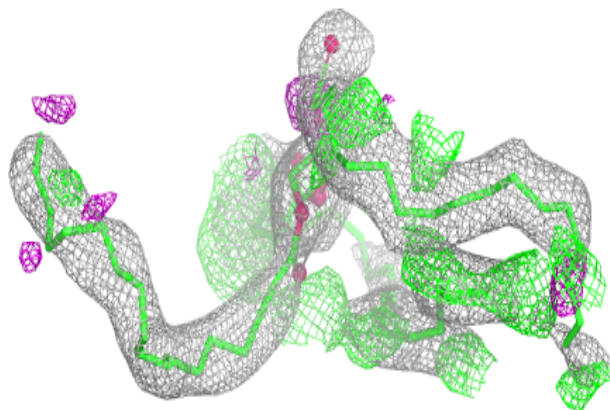
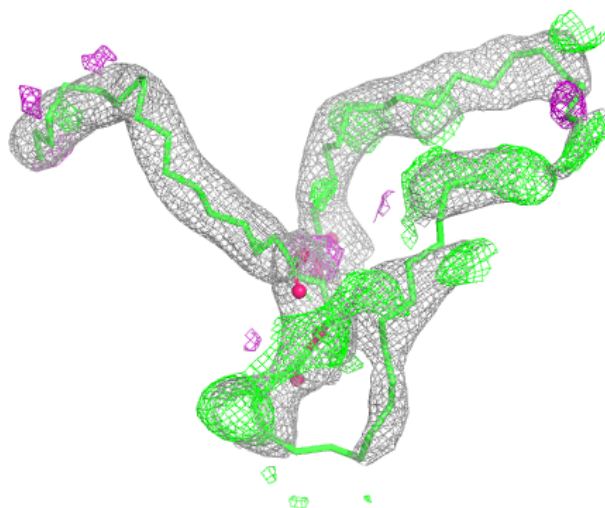
Electron density around PGV A 606:

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



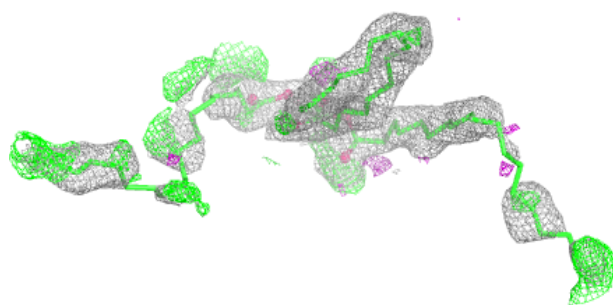
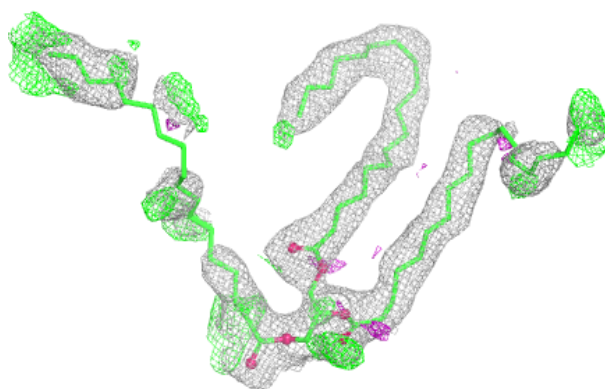
Electron density around TGL N 611:

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

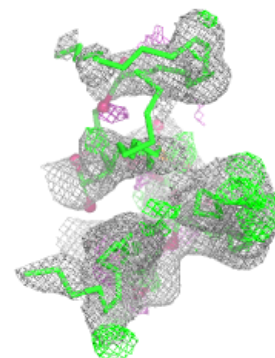
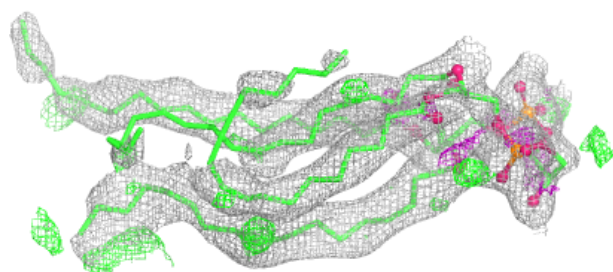
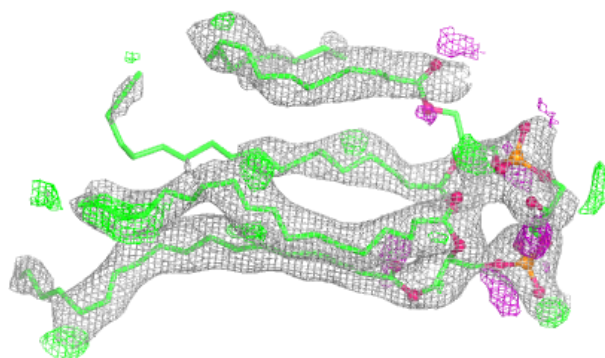


Electron density around TGL D 201:

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

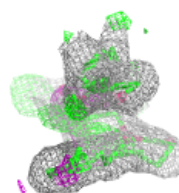
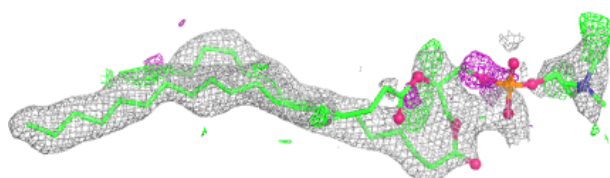
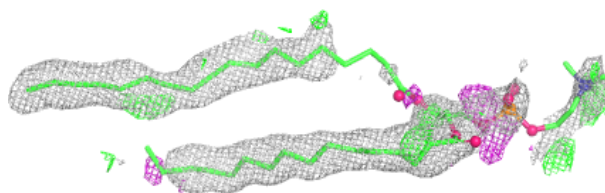
**Electron density around CDL C 306:**

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



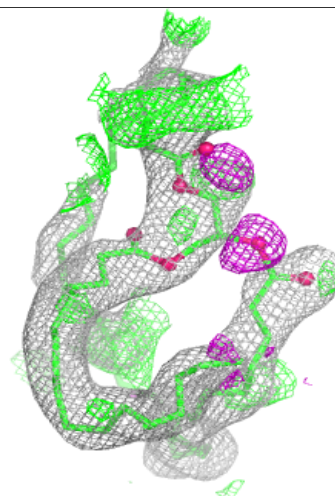
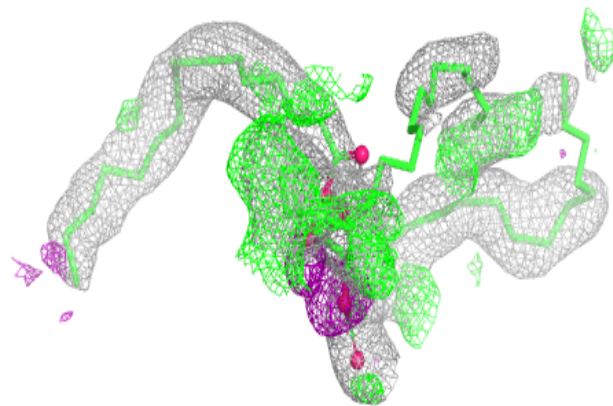
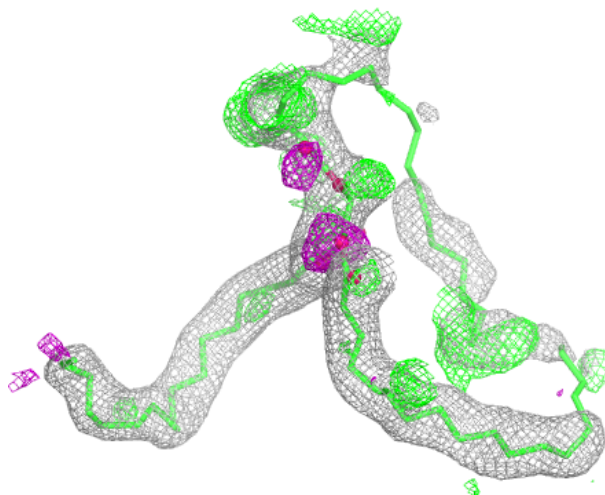
Electron density around PSC R 201:

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



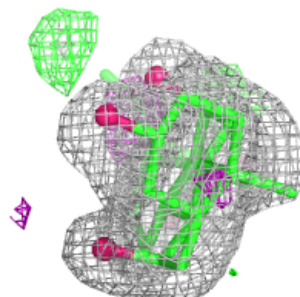
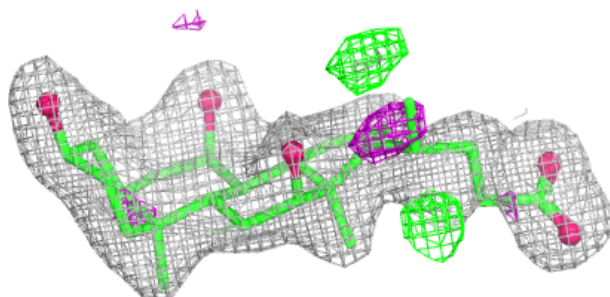
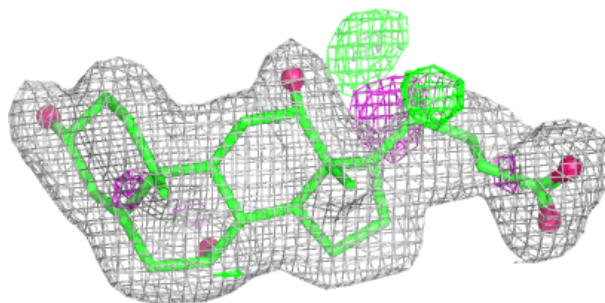
Electron density around TGL L 101:

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

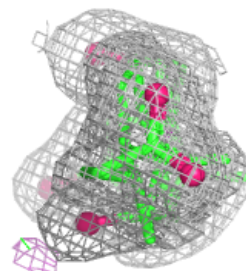
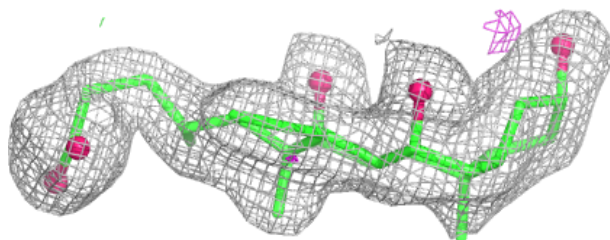
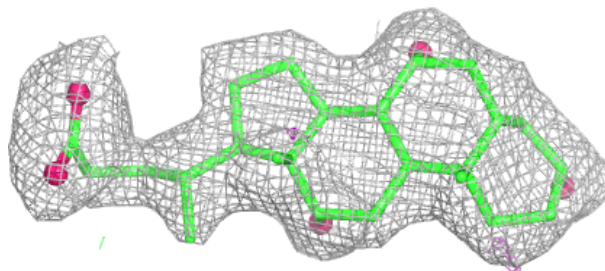


Electron density around CHD C 307:

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

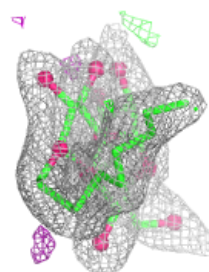
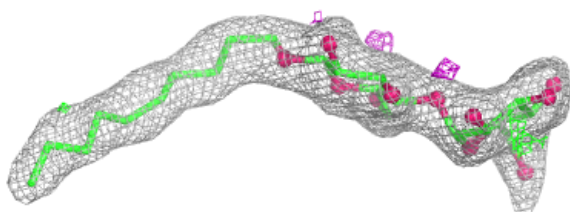
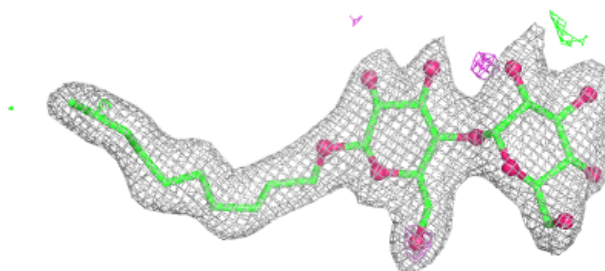
**Electron density around CHD P 306:**

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

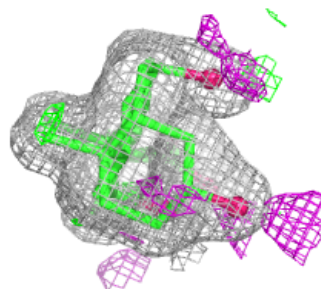
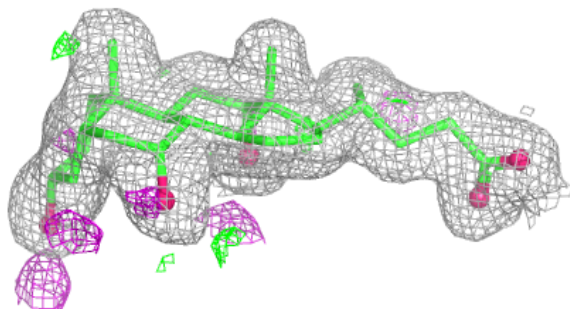
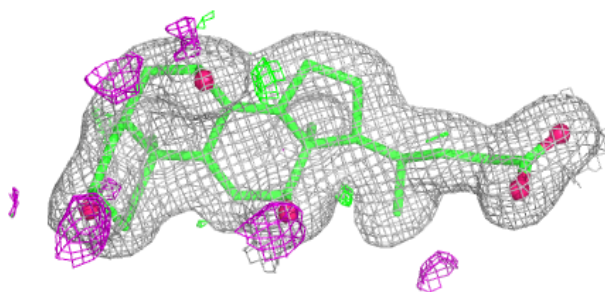


Electron density around DMU Z 101:

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

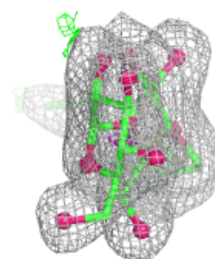
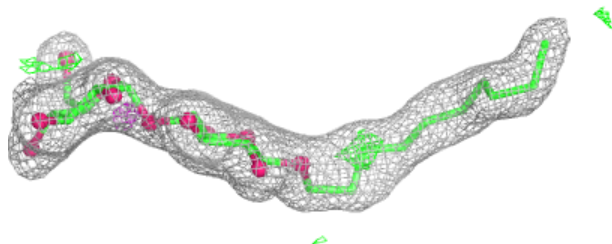
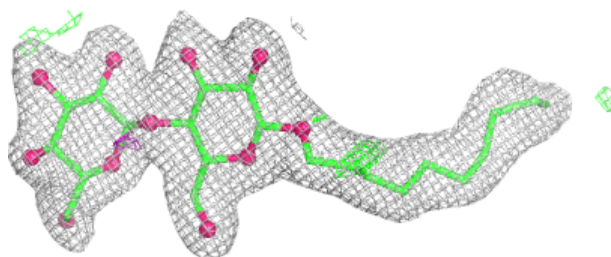
**Electron density around CHD C 308:**

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

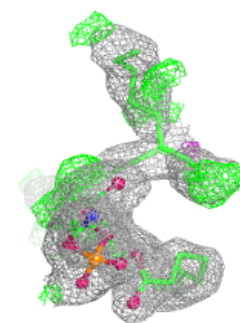
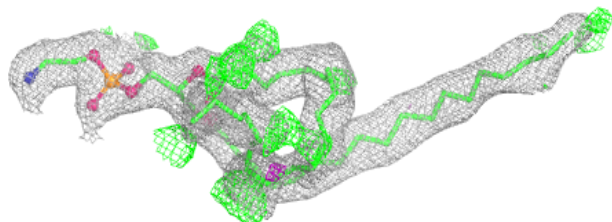
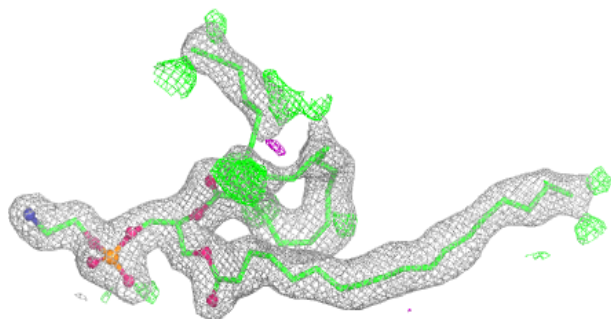


Electron density around DMU M 101:

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

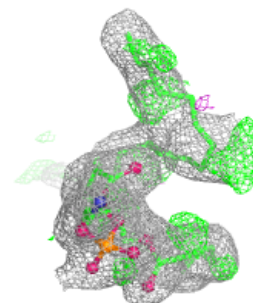
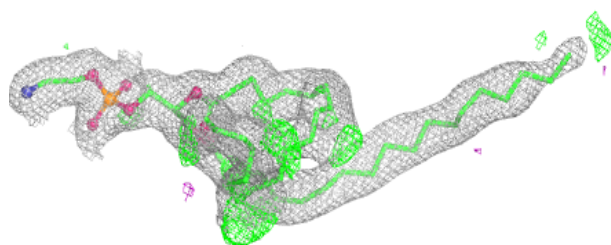
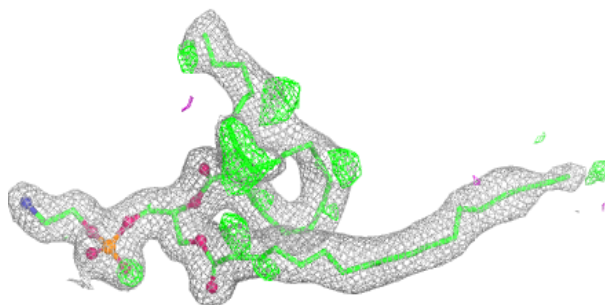
**Electron density around PEK T 102:**

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

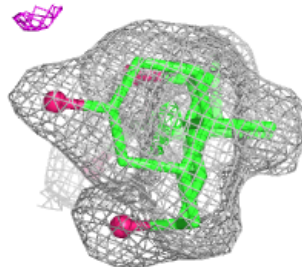
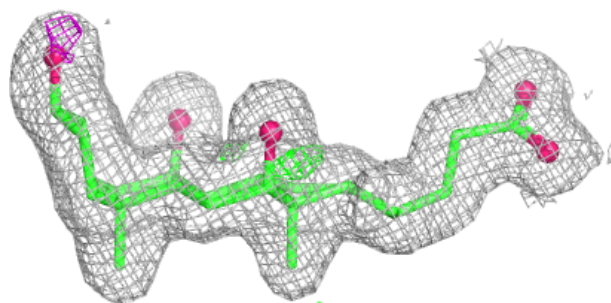
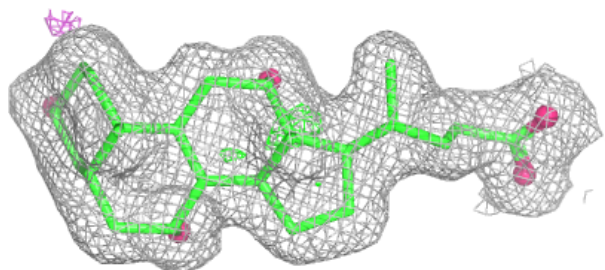


Electron density around PEK C 302:

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

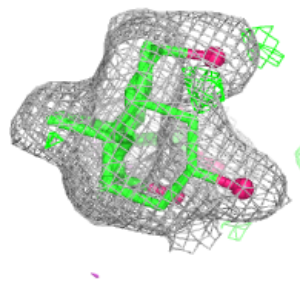
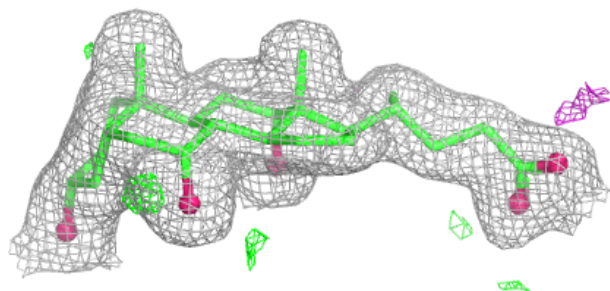
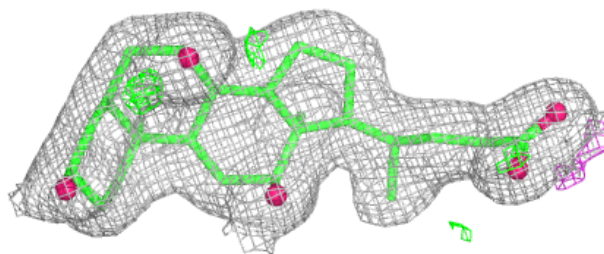
**Electron density around CHD B 303:**

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

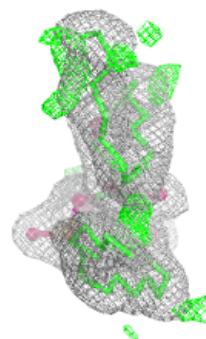
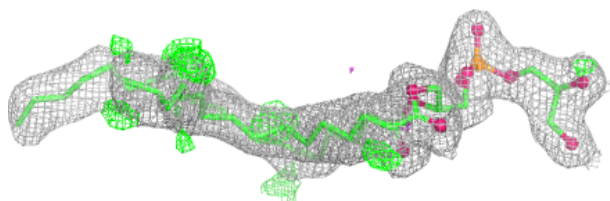
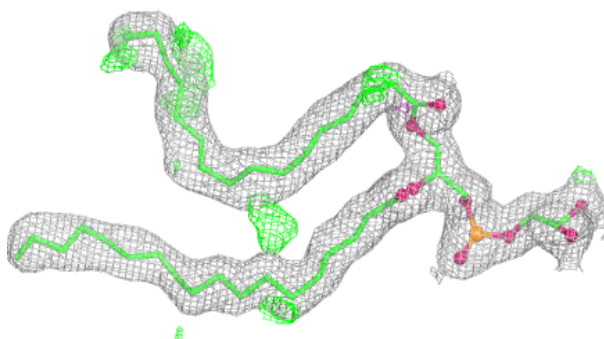


Electron density around CHD N 610:

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

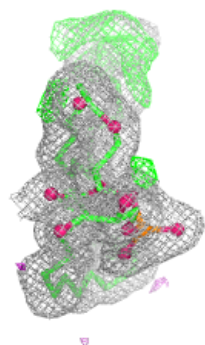
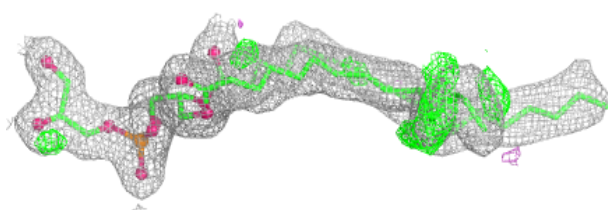
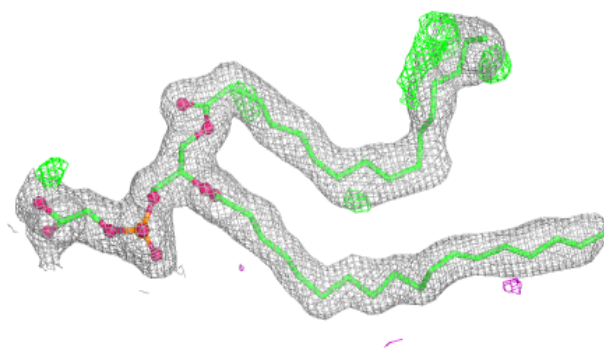
**Electron density around PGV N 609:**

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

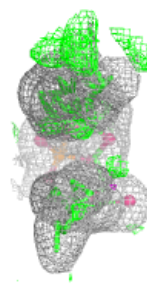
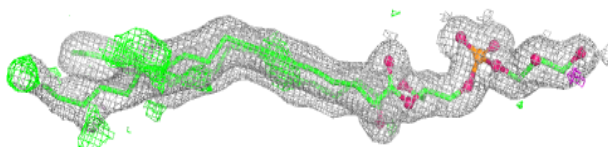
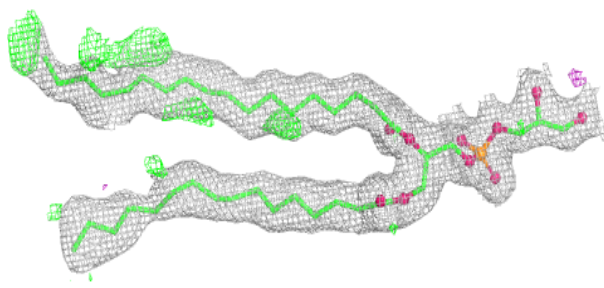


Electron density around PGV A 608:

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

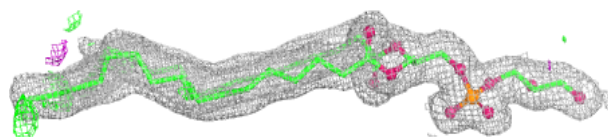
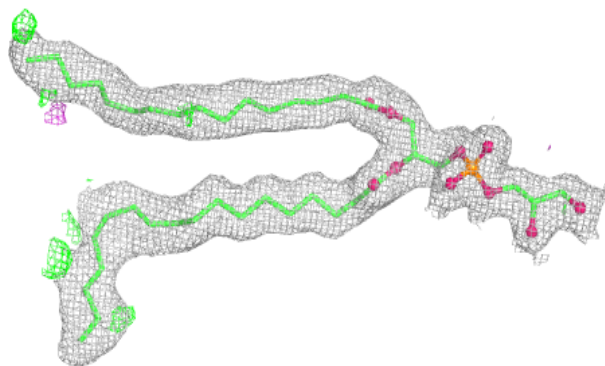
**Electron density around PGV C 304:**

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

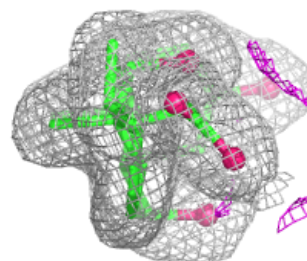
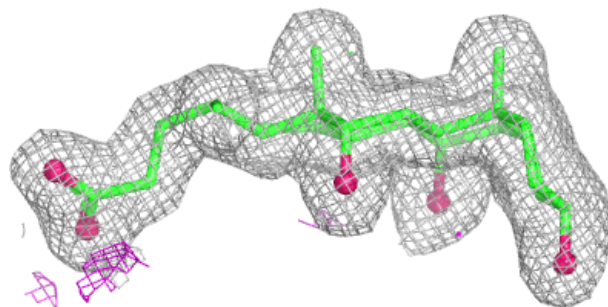
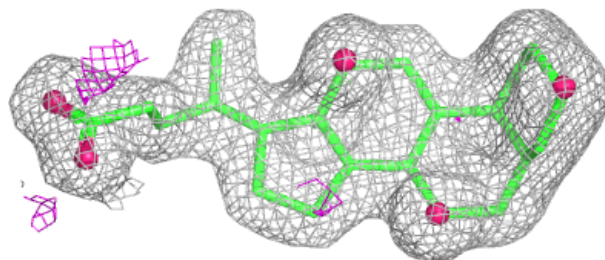


Electron density around PGV P 303:

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

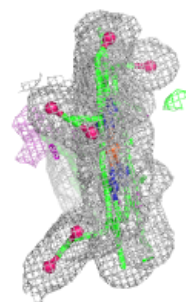
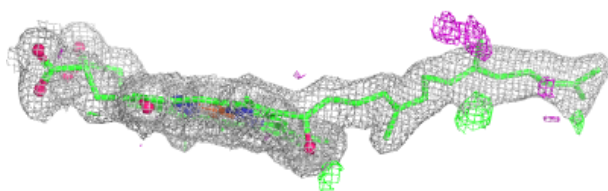
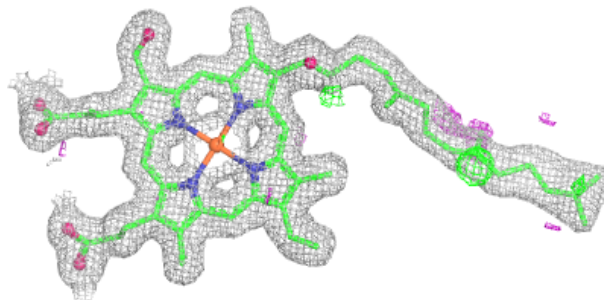
**Electron density around CHD O 301:**

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

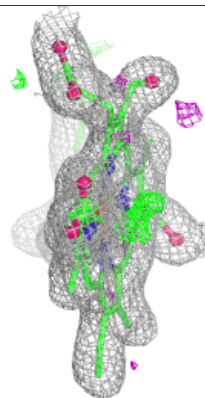
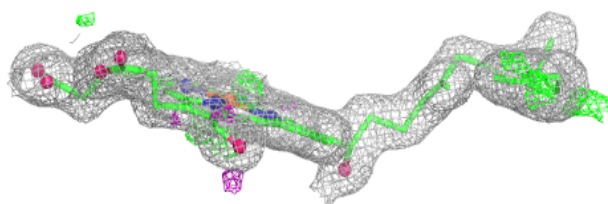
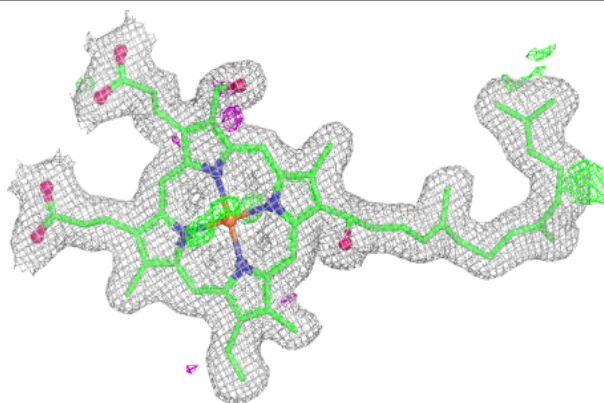


Electron density around HEA A 601:

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

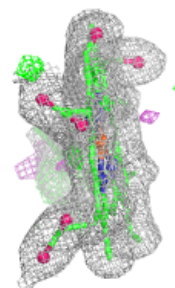
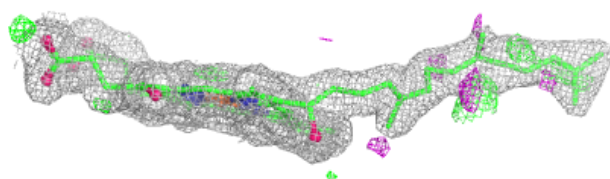
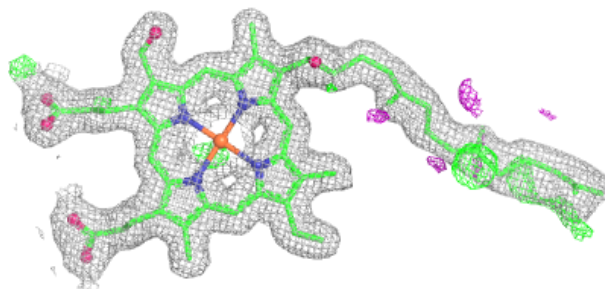
**Electron density around HEA A 602:**

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

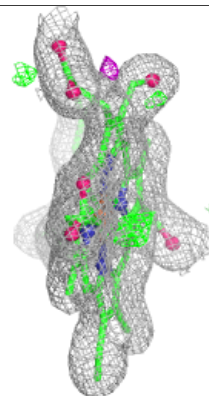
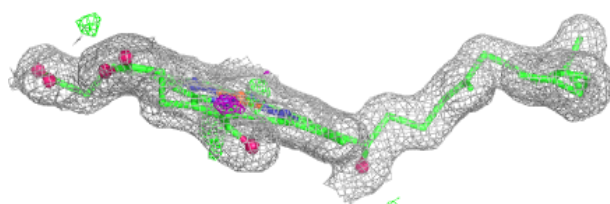
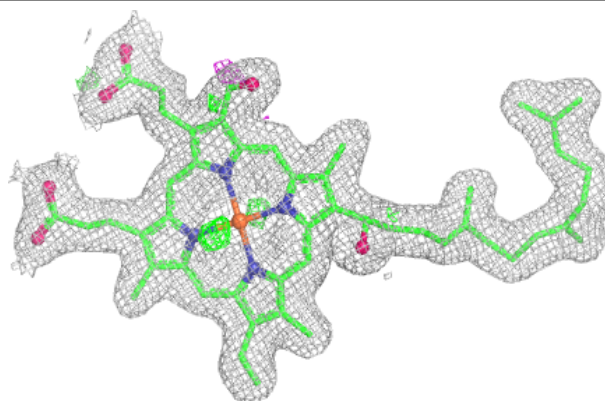


Electron density around HEA N 601:

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

**Electron density around HEA N 602:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.