



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:23 AM UTC

PDB ID : 3AG4 / pdb_00003ag4
Title : Bovine Heart Cytochrome c Oxidase in the Cyanide Ion-bound Fully Reduced State at 100 K
Authors : Muramoto, K.; Ohta, K.; Shinzawa-Itoh, K.; Kanda, K.; Taniguchi, M.; Nabekura, H.; Yamashita, E.; Tsukihara, T.; Yoshikawa, S.
Deposited on : 2010-03-19
Resolution : 2.05 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:

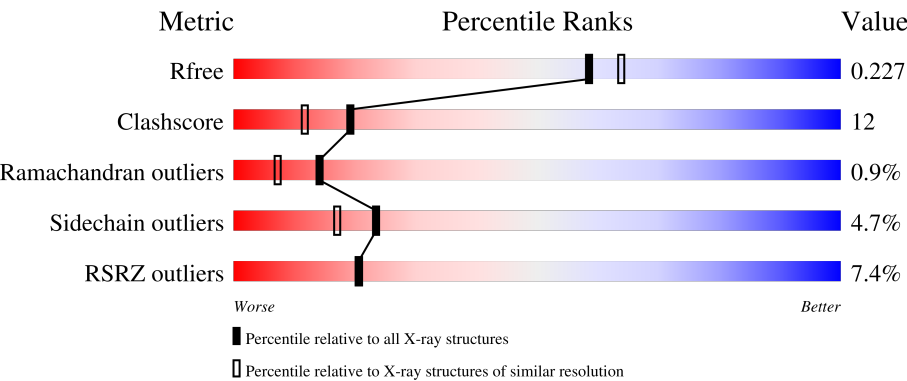
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	0% 65% 31% .
1	N	514	3% 70% 25% .
2	B	227	7% 72% 22% 5% .
2	O	227	12% 68% 26% 5% .

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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
15	CYN	N	520	-	-	X	-
22	CHD	C	271	X	-	-	-
22	CHD	J	60	X	-	-	-
22	CHD	P	1271	X	-	-	-
22	CHD	W	1059	X	-	-	-
23	UNX	C	262	-	-	-	X
23	UNX	P	262	-	-	-	X
25	CDL	C	270	-	-	X	-
25	CDL	G	269	-	-	X	-
25	CDL	T	1269	-	-	X	-
28	DMU	G	272	X	-	-	-
28	DMU	M	526	X	-	-	-
28	DMU	P	1272	X	-	-	-
28	DMU	Z	1526	X	-	-	-

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 32324 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	0	0
			4027	2691	623	678	35			
1	N	514	Total	C	N	O	S	0	0	0
			4027	2691	623	678	35			

- 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	0	0
			1824	1185	281	340	18			
2	O	227	Total	C	N	O	S	0	0	0
			1824	1185	281	340	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	0	0
			2110	1412	336	350	12			
3	P	259	Total	C	N	O	S	0	0	0
			2110	1412	336	350	12			

- 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	0	0
			1195	777	196	218	4			
4	Q	144	Total	C	N	O	S	0	0	0
			1195	777	196	218	4			

- 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	0	0
			852	544	144	162	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	0	0
			748	464	134	145	5			
6	S	98	Total	C	N	O	S	0	0	0
			748	464	134	145	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	84	Total	C	N	O	P	S	0	0
			675	431	129	113	1	1		
7	T	84	Total	C	N	O	P	S	0	0
			675	431	129	113	1	1		

- 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	0	0
			601	390	107	100	4			

- Molecule 10 is a protein called Cytochrome c oxidase polypeptide 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	0	0
			384	250	65	67	2			
11	X	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			

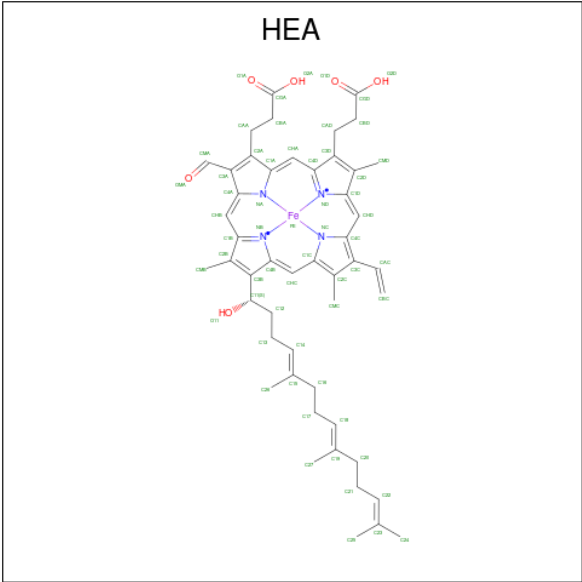
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C.

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.

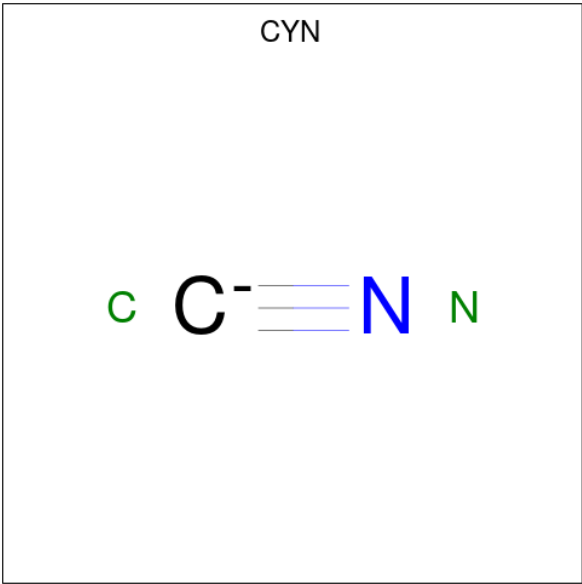
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			335	223	53	59			
13	Z	43	Total	C	N	O	0	0	0
			335	223	53	59			

- 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 CYANIDE ION (CCD ID: CYN) (formula: CN).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	1	Total C N 2 1 1	0	0
15	N	1	Total C N 2 1 1	0	0

- Molecule 16 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

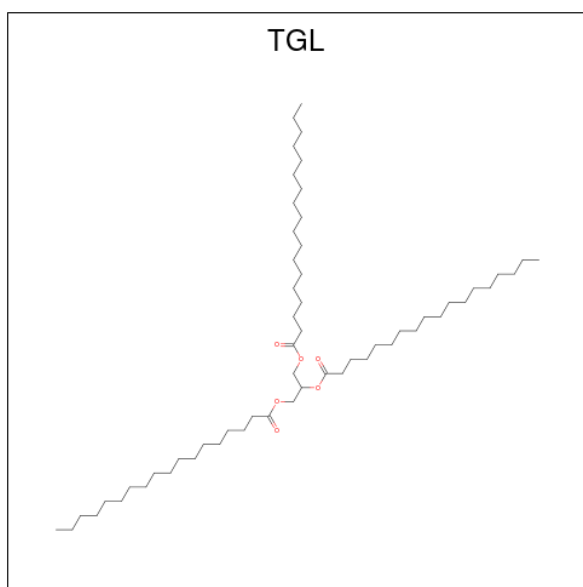
- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 18 is SODIUM ION (CCD ID: NA) (formula: Na).

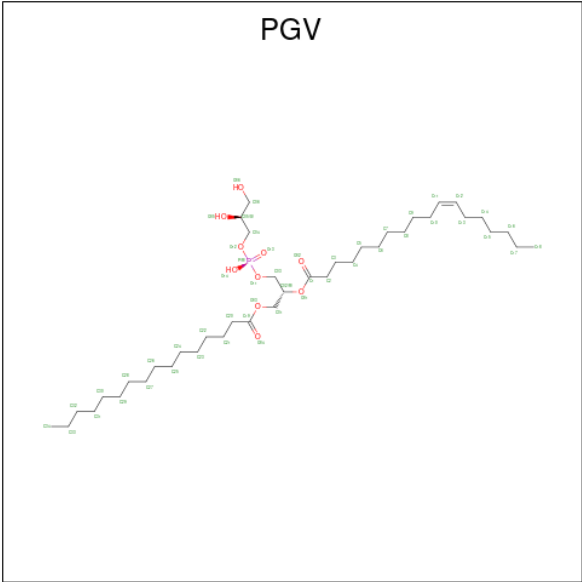
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total Na 1 1	0	0
18	N	1	Total Na 1 1	0	0

- Molecule 19 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: C₅₇H₁₁₀O₆).



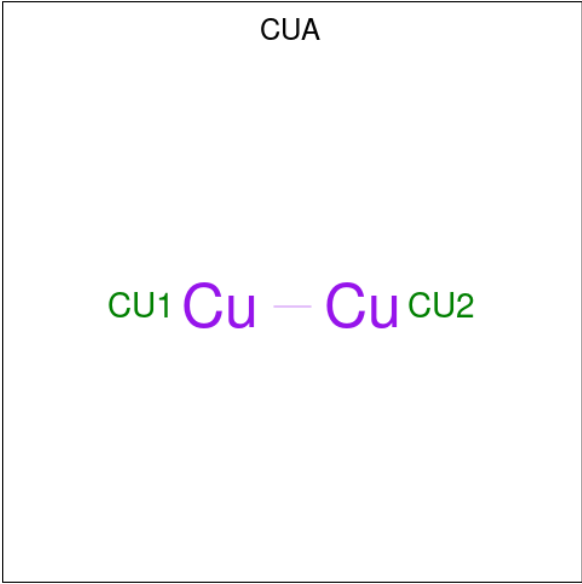
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			63	57	6		
19	D	1	Total	C	O	0	0
			63	57	6		
19	L	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	Q	1	Total	C	O	0	0
			63	57	6		

- Molecule 20 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



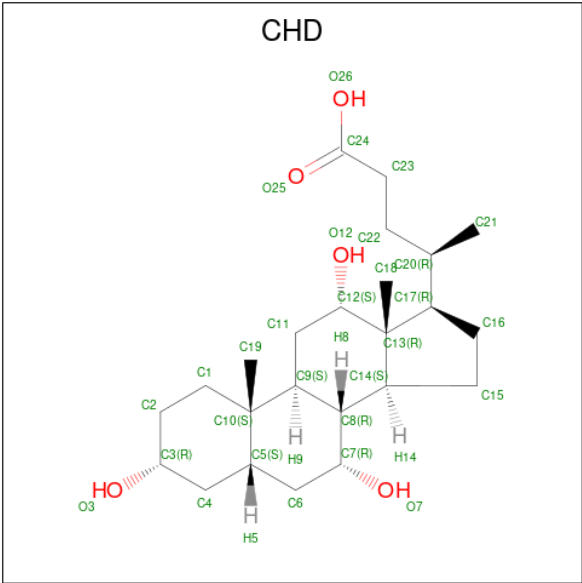
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0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

- 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	0
			29	24	5		
22	C	1	Total	C	O	0	0
			29	24	5		

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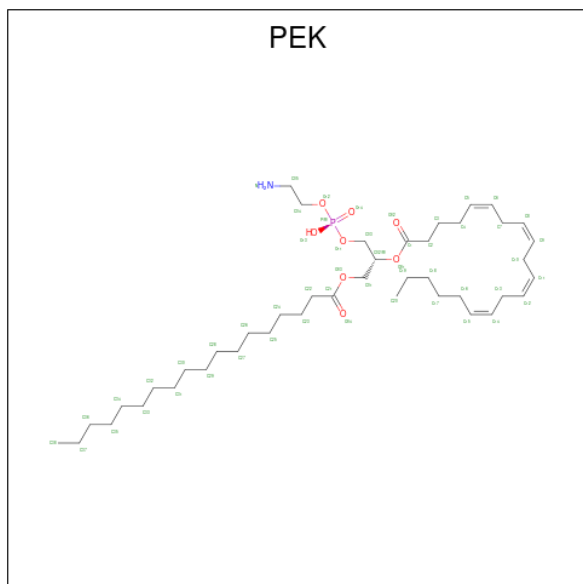
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	C	1	Total C O 29 24 5	0	0
22	J	1	Total C O 29 24 5	0	0
22	O	1	Total C O 29 24 5	0	0
22	P	1	Total C O 29 24 5	0	0
22	P	1	Total C O 29 24 5	0	0
22	W	1	Total C O 29 24 5	0	0

- Molecule 23 is UNKNOWN ATOM OR ION (CCD ID: UNX) (formula: X).

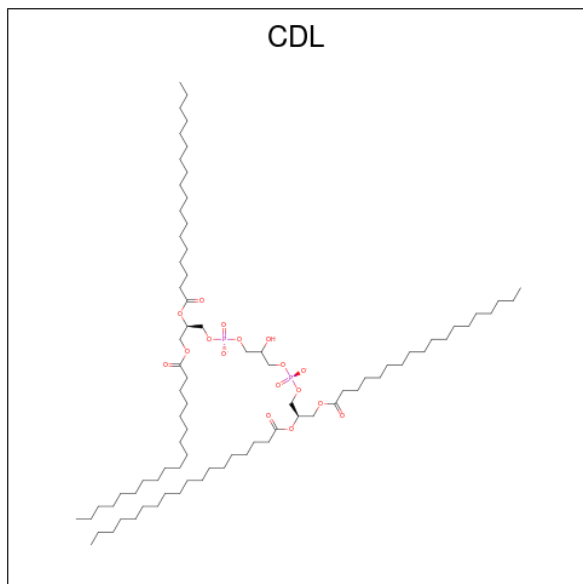
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	C	1	Total X 1 1	0	0
23	P	1	Total X 1 1	0	0

- Molecule 24 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).



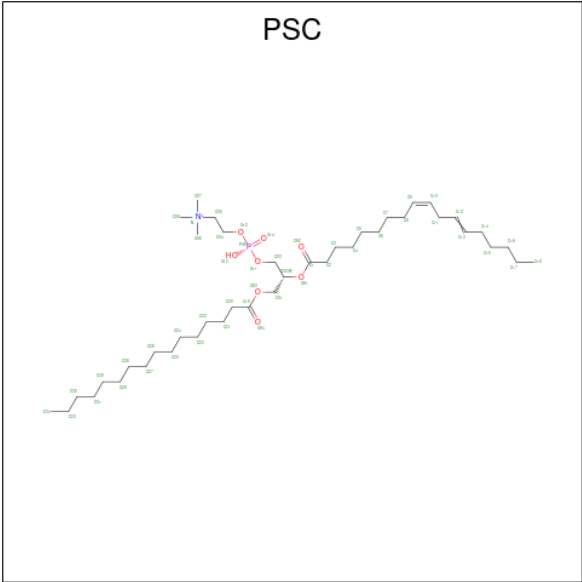
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	S	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 25 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

- 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: $C_{42}H_{81}NO_8P$).

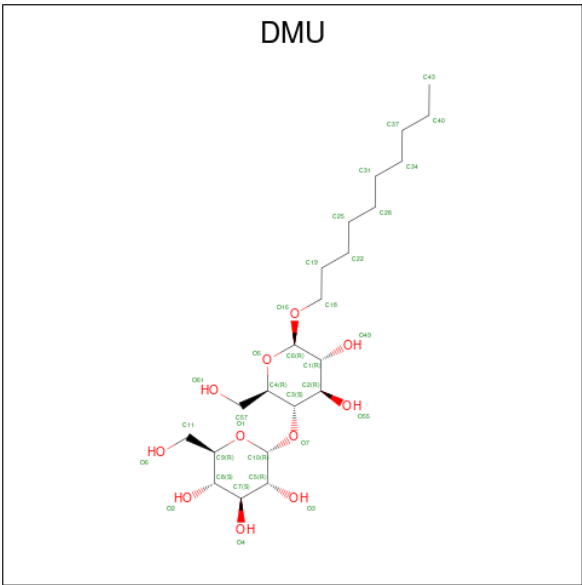


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	E	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
26	R	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- 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 DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: C₂₂H₄₂O₁₁).



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

- Molecule 29 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	225	Total	O	0	0
			225	225		
29	B	125	Total	O	0	0
			125	125		
29	C	106	Total	O	0	0
			106	106		
29	D	91	Total	O	0	0
			91	91		
29	E	62	Total	O	0	0
			62	62		
29	F	75	Total	O	0	0
			75	75		
29	G	41	Total	O	0	0
			41	41		
29	H	47	Total	O	0	0
			47	47		

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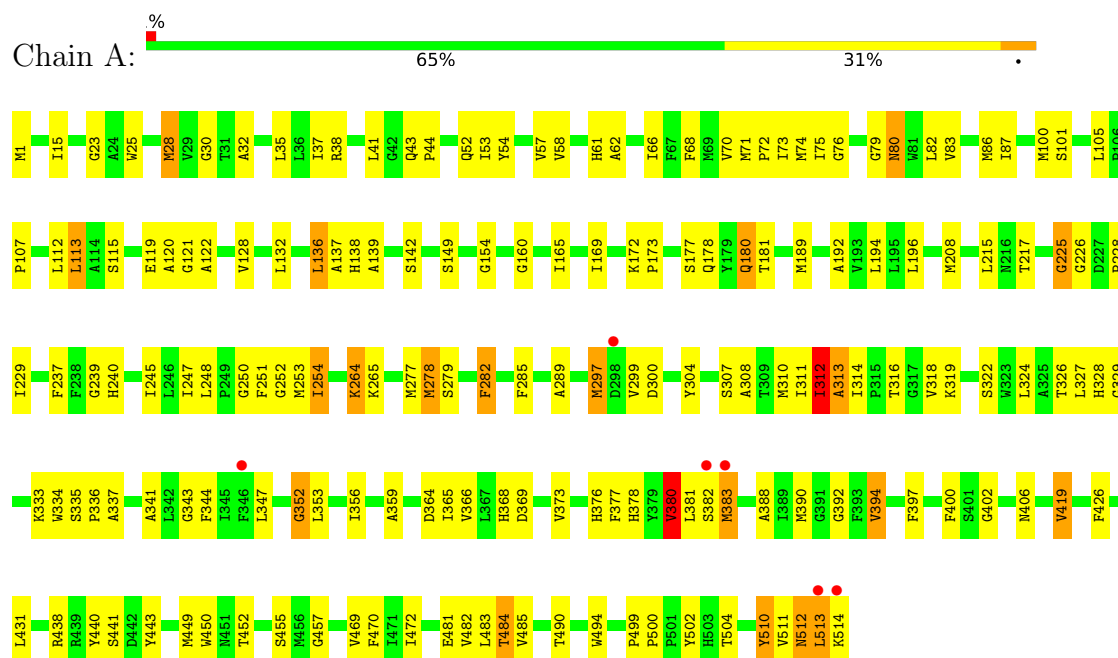
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	I	38	Total 38	O 38	0	0
29	J	20	Total 20	O 20	0	0
29	K	20	Total 20	O 20	0	0
29	L	22	Total 22	O 22	0	0
29	M	15	Total 15	O 15	0	0
29	N	199	Total 199	O 199	0	0
29	O	107	Total 107	O 107	0	0
29	P	100	Total 100	O 100	0	0
29	Q	55	Total 55	O 55	0	0
29	R	40	Total 40	O 40	0	0
29	S	56	Total 56	O 56	0	0
29	T	36	Total 36	O 36	0	0
29	U	41	Total 41	O 41	0	0
29	V	18	Total 18	O 18	0	0
29	W	12	Total 12	O 12	0	0
29	X	14	Total 14	O 14	0	0
29	Y	12	Total 12	O 12	0	0
29	Z	11	Total 11	O 11	0	0

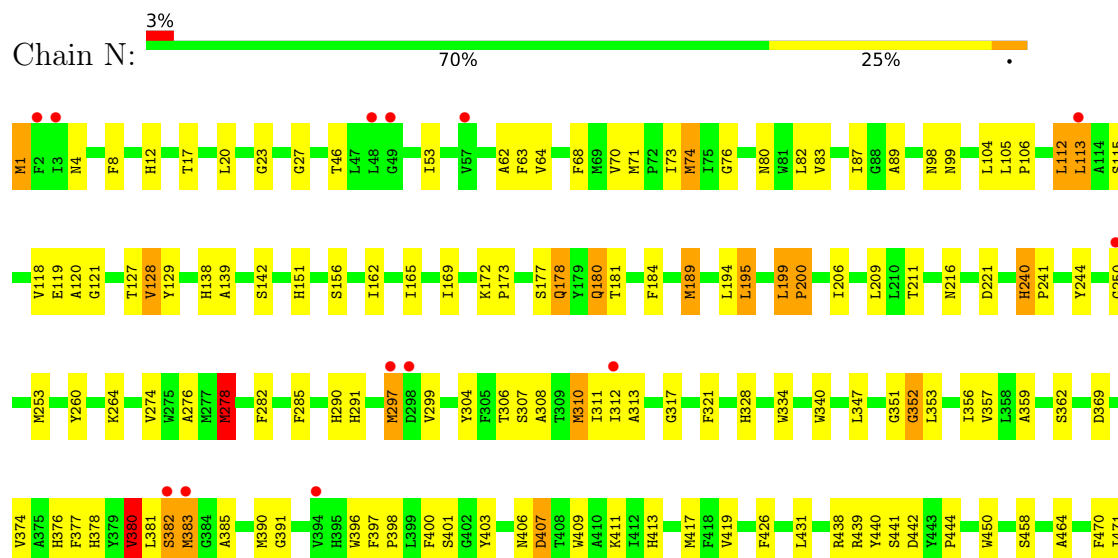
3 Residue-property plots

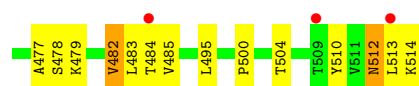
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

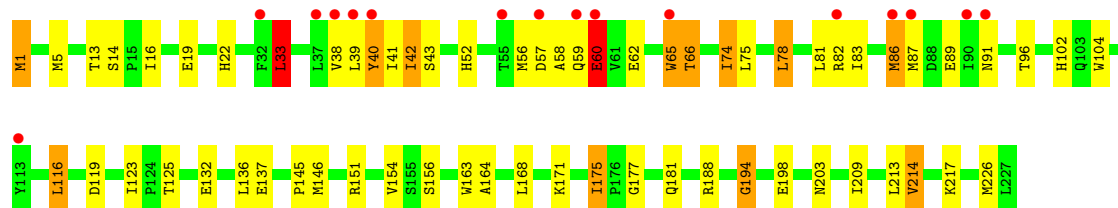


• Molecule 1: Cytochrome c oxidase subunit 1

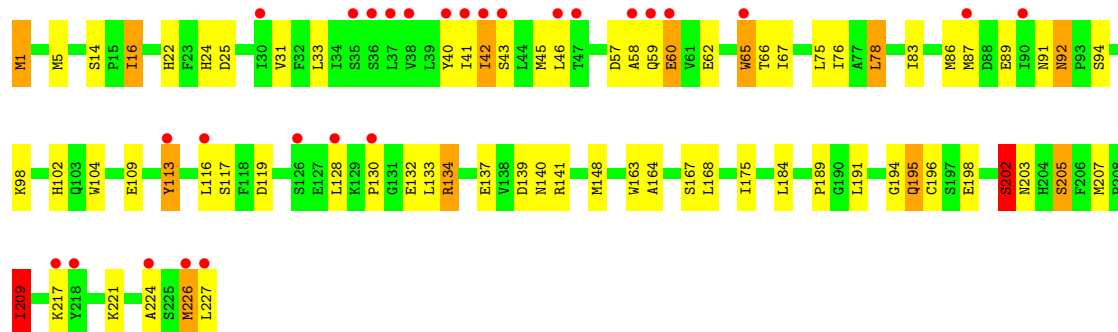




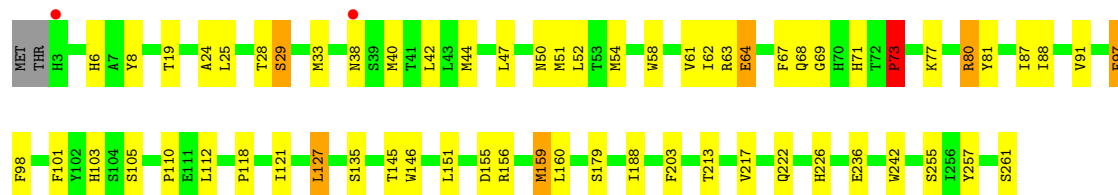
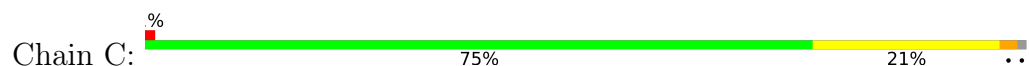
• Molecule 2: Cytochrome c oxidase subunit 2



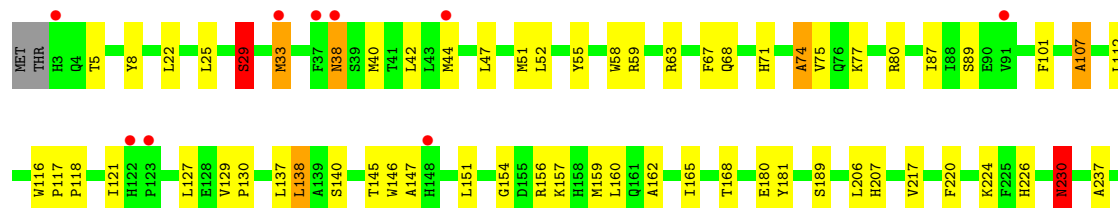
• Molecule 2: Cytochrome c oxidase subunit 2



• Molecule 3: Cytochrome c oxidase subunit 3

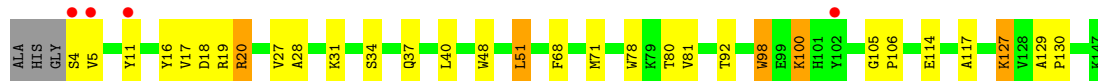
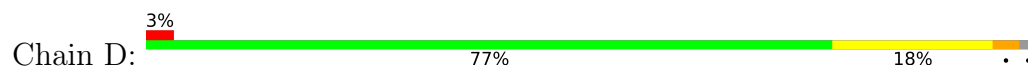


• Molecule 3: Cytochrome c oxidase subunit 3

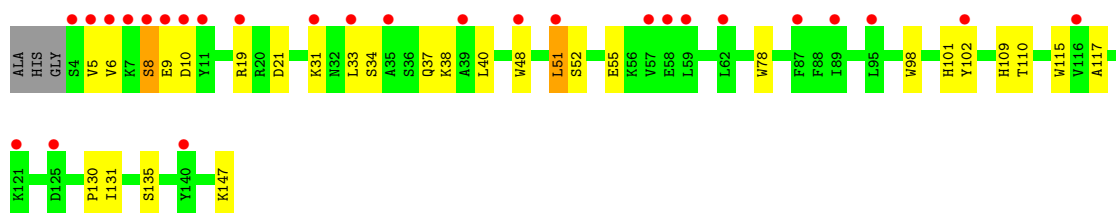
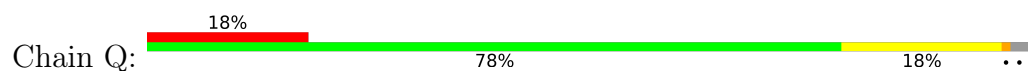




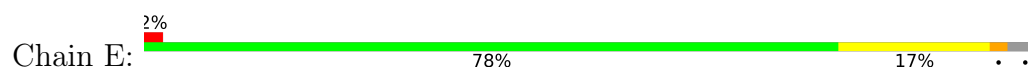
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



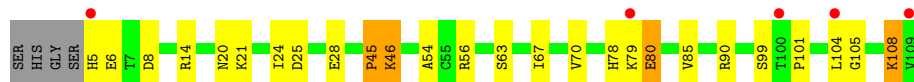
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



- Molecule 5: Cytochrome c oxidase subunit 5A



- Molecule 5: Cytochrome c oxidase subunit 5A



- Molecule 6: Cytochrome c oxidase subunit 5B

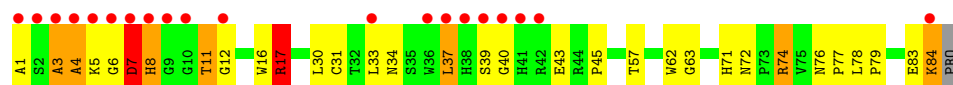


- Molecule 6: Cytochrome c oxidase subunit 5B

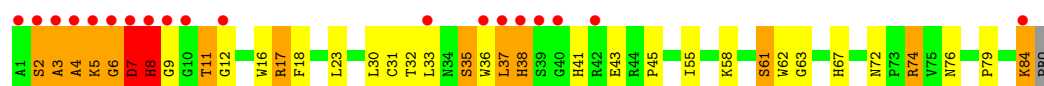




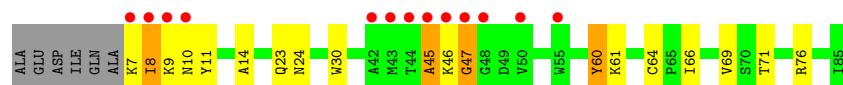
- Molecule 7: Cytochrome c oxidase subunit 6A2



- Molecule 7: Cytochrome c oxidase subunit 6A2



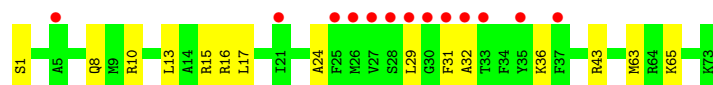
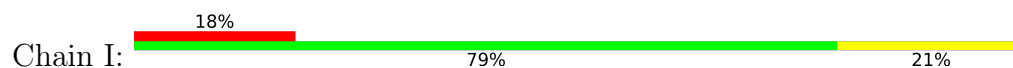
- Molecule 8: Cytochrome c oxidase subunit 6B1



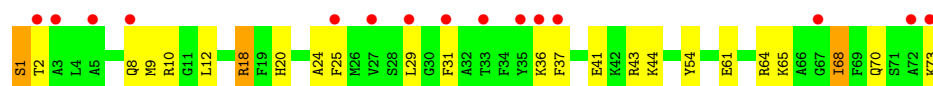
- Molecule 8: Cytochrome c oxidase subunit 6B1



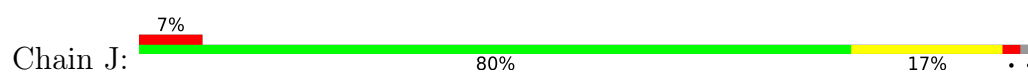
- Molecule 9: Cytochrome c oxidase subunit 6C



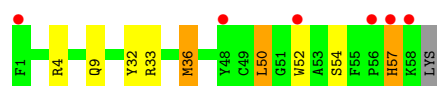
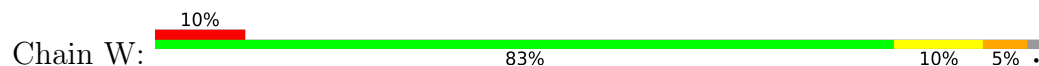
- Molecule 9: Cytochrome c oxidase subunit 6C



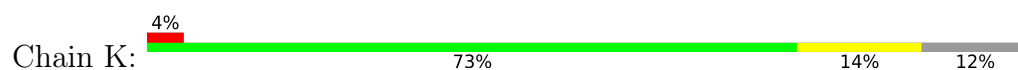
- Molecule 10: Cytochrome c oxidase polypeptide 7A1



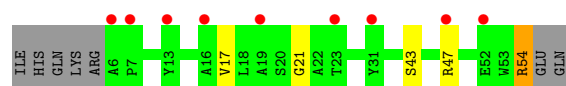
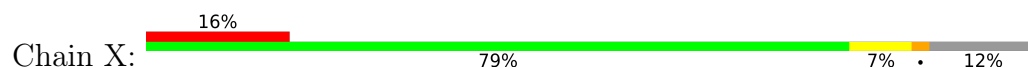
- Molecule 10: Cytochrome c oxidase polypeptide 7A1



- Molecule 11: Cytochrome c oxidase subunit 7B



- Molecule 11: Cytochrome c oxidase subunit 7B



- Molecule 12: Cytochrome c oxidase subunit 7C



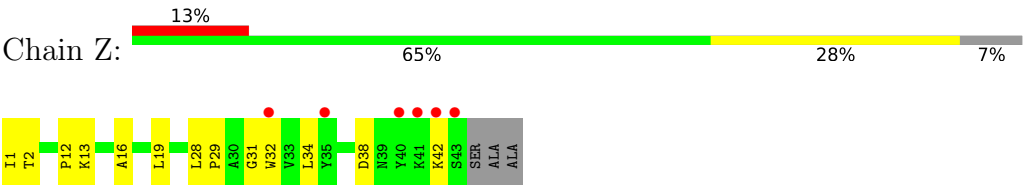
- Molecule 12: Cytochrome c oxidase subunit 7C



- 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	183.36Å 206.65Å 178.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.05 40.00 – 2.05	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.05) 99.8 (40.00-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.3	Depositor
R, R_{free}	0.186 , 0.219 (Not available) , 0.227	Depositor DCC
R_{free} test set	21002 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	34.5	Xtriage
Anisotropy	0.525	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.006 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	32324	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% 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: CU, TPO, TGL, FME, PGV, DMU, CUA, PSC, PEK, UNX, HEA, CHD, SAC, MG, CYN, CDL, NA, ZN

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	2.03	97/4156 (2.3%)	1.56	59/5678 (1.0%)
1	N	1.80	49/4156 (1.2%)	1.45	45/5678 (0.8%)
2	B	1.83	18/1860 (1.0%)	1.48	14/2534 (0.6%)
2	O	1.52	9/1860 (0.5%)	1.34	8/2534 (0.3%)
3	C	1.75	20/2197 (0.9%)	1.33	10/3005 (0.3%)
3	P	1.70	12/2197 (0.5%)	1.34	14/3005 (0.5%)
4	D	1.74	16/1229 (1.3%)	1.36	11/1658 (0.7%)
4	Q	1.32	5/1229 (0.4%)	1.22	2/1658 (0.1%)
5	E	1.74	9/871 (1.0%)	1.25	2/1182 (0.2%)
5	R	1.39	3/871 (0.3%)	1.20	0/1182
6	F	1.86	12/765 (1.6%)	1.49	7/1038 (0.7%)
6	S	1.60	6/765 (0.8%)	1.58	14/1038 (1.3%)
7	G	1.60	2/690 (0.3%)	1.34	4/937 (0.4%)
7	T	1.56	7/690 (1.0%)	1.46	6/937 (0.6%)
8	H	1.62	6/682 (0.9%)	1.38	3/921 (0.3%)
8	U	1.34	3/682 (0.4%)	1.32	5/921 (0.5%)
9	I	1.47	2/605 (0.3%)	1.36	3/802 (0.4%)
9	V	1.29	0/605	1.26	3/802 (0.4%)
10	J	1.45	0/471	1.29	2/636 (0.3%)
10	W	1.34	1/471 (0.2%)	1.20	1/636 (0.2%)
11	K	1.60	2/398 (0.5%)	1.40	4/546 (0.7%)
11	X	1.31	1/398 (0.3%)	1.31	3/546 (0.5%)
12	L	1.80	7/393 (1.8%)	1.44	4/526 (0.8%)
12	Y	1.56	2/393 (0.5%)	1.48	6/526 (1.1%)
13	M	1.80	6/345 (1.7%)	1.43	0/470
13	Z	1.43	0/345	1.29	0/470
All	All	1.70	295/29324 (1.0%)	1.40	230/39866 (0.6%)

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
10	J	0	1
10	W	0	1
12	L	0	1
All	All	0	5

All (295) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	198	GLU	C-O	12.55	1.37	1.23
1	A	388	ALA	CA-CB	11.34	1.71	1.53
2	B	198	GLU	C-O	11.09	1.37	1.23
1	N	139	ALA	CA-CB	10.72	1.70	1.53
1	A	419	VAL	CA-CB	9.76	1.65	1.54
2	B	40	TYR	N-CA	-9.48	1.35	1.46
1	N	195	LEU	C-O	9.10	1.34	1.24
1	A	122	ALA	CA-CB	8.62	1.64	1.53
1	N	419	VAL	CA-CB	8.61	1.64	1.54
1	A	83	VAL	CA-C	8.47	1.60	1.52
1	A	438	ARG	CB-CG	-8.39	1.27	1.52
1	A	248	LEU	CA-C	8.15	1.62	1.52
5	E	71	VAL	CA-CB	8.09	1.63	1.54
1	N	74	MET	CB-CG	8.06	1.76	1.52
1	A	316	THR	CA-CB	-7.91	1.41	1.53
8	H	66	ILE	CA-CB	7.91	1.64	1.54
3	P	74	ALA	CA-CB	7.89	1.65	1.53
1	A	113	LEU	CB-CG	7.80	1.69	1.53
1	A	352	GLY	N-CA	7.78	1.55	1.45
6	F	72	PHE	N-CA	7.73	1.55	1.46
1	N	89	ALA	C-O	7.70	1.34	1.23
1	N	383	MET	N-CA	7.65	1.55	1.46
1	N	297	MET	SD-CE	7.55	1.98	1.79
1	A	482	VAL	CA-CB	7.49	1.62	1.54
1	A	251	PHE	CA-C	7.43	1.62	1.52
1	A	299	VAL	CA-CB	7.27	1.63	1.54
1	A	240	HIS	N-CA	-7.09	1.41	1.46
13	M	22	THR	N-CA	7.03	1.54	1.46
1	N	181	THR	CA-CB	7.02	1.64	1.53
1	A	139	ALA	C-O	7.01	1.32	1.23
1	A	74	MET	CB-CG	6.99	1.73	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	308	ALA	CA-CB	-6.98	1.42	1.53
1	N	106	PRO	CA-C	6.94	1.58	1.52
1	N	340	TRP	N-CA	6.91	1.54	1.46
12	L	26	THR	CA-CB	6.88	1.64	1.53
6	F	20	VAL	CA-CB	6.77	1.62	1.54
1	A	312	ILE	CG1-CD1	6.73	1.78	1.51
6	S	2	SER	N-CA	6.72	1.54	1.46
4	D	117	ALA	CA-CB	6.72	1.63	1.53
13	M	11	SER	CA-C	6.71	1.62	1.53
1	A	70	VAL	C-O	6.69	1.31	1.24
7	G	71	HIS	N-CA	6.65	1.54	1.46
4	Q	117	ALA	CA-CB	6.65	1.63	1.53
1	A	226	GLY	N-CA	6.63	1.53	1.45
7	T	18	PHE	CA-C	6.63	1.61	1.52
4	D	92	THR	N-CA	6.58	1.54	1.46
4	D	100	LYS	CE-NZ	6.55	1.69	1.49
1	N	83	VAL	CA-CB	6.55	1.57	1.54
6	F	2	SER	CA-C	6.55	1.60	1.53
1	A	52	GLN	CA-C	6.52	1.61	1.52
2	B	171	LYS	N-CA	6.50	1.54	1.46
1	N	385	ALA	N-CA	6.50	1.54	1.46
3	P	87	ILE	C-O	6.49	1.31	1.24
4	D	27	VAL	C-O	6.49	1.30	1.23
1	N	120	ALA	CA-CB	6.47	1.62	1.53
2	O	134	ARG	CA-C	6.46	1.61	1.52
1	A	54	TYR	CA-C	6.43	1.61	1.52
1	A	112	LEU	CG-CD1	6.43	1.73	1.52
1	A	353	LEU	CA-C	6.40	1.61	1.52
12	L	34	ALA	N-CA	6.39	1.54	1.46
3	C	8	TYR	CA-C	-6.38	1.44	1.53
6	F	92	VAL	CA-CB	6.37	1.62	1.54
1	N	276	ALA	CA-CB	6.37	1.63	1.53
6	S	68	THR	N-CA	6.36	1.54	1.46
1	N	391	GLY	N-CA	6.35	1.53	1.45
1	A	443	TYR	CA-CB	6.28	1.62	1.54
2	O	175	ILE	N-CA	-6.27	1.40	1.46
1	A	38	ARG	CD-NE	6.26	1.55	1.46
3	P	33	MET	N-CA	6.25	1.53	1.46
1	N	482	VAL	CA-CB	6.24	1.60	1.54
1	N	396	TRP	N-CA	6.24	1.54	1.46
1	A	113	LEU	CG-CD1	6.23	1.73	1.52
1	N	260	TYR	CA-C	6.22	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	203	PHE	N-CA	6.21	1.53	1.46
8	H	71	THR	CA-CB	6.19	1.62	1.53
5	R	70	VAL	CA-CB	-6.18	1.46	1.54
1	A	366	VAL	CA-CB	6.17	1.62	1.54
13	M	7	LYS	CA-C	-6.16	1.44	1.52
3	C	69	GLY	CA-C	6.16	1.59	1.51
4	Q	5	VAL	CA-CB	6.16	1.60	1.53
1	A	457	GLY	N-CA	6.15	1.54	1.45
1	A	455	SER	C-O	6.13	1.31	1.24
1	A	264	LYS	CG-CD	-6.13	1.34	1.52
2	O	195	GLN	CA-C	6.13	1.60	1.52
2	B	74	ILE	CA-C	6.12	1.60	1.52
12	L	28	PHE	C-O	-6.12	1.17	1.24
1	A	37	ILE	CA-CB	6.08	1.61	1.54
1	A	318	VAL	CA-CB	6.08	1.62	1.54
2	B	125	THR	CA-CB	6.08	1.62	1.53
3	P	71	HIS	CA-CB	6.07	1.60	1.52
1	N	260	TYR	N-CA	-6.06	1.39	1.46
1	A	373	VAL	C-O	-6.06	1.17	1.24
1	A	327	LEU	N-CA	6.05	1.54	1.46
7	T	67	HIS	N-CA	6.04	1.53	1.46
1	N	162	ILE	CA-C	6.02	1.60	1.52
1	A	441	SER	C-O	6.01	1.31	1.24
1	A	192	ALA	CA-CB	5.99	1.62	1.53
8	H	14	ALA	CA-CB	5.99	1.62	1.53
1	A	80	ASN	N-CA	5.98	1.53	1.46
1	A	58	VAL	CA-CB	5.98	1.60	1.54
1	N	512	ASN	CA-CB	5.95	1.63	1.53
12	L	8	GLY	C-O	-5.94	1.16	1.24
1	N	113	LEU	CG-CD1	5.94	1.72	1.52
1	A	189	MET	SD-CE	-5.92	1.64	1.79
1	A	252	GLY	N-CA	5.91	1.53	1.45
1	N	64	VAL	CA-CB	5.89	1.61	1.54
2	B	209	ILE	CA-CB	-5.88	1.47	1.54
1	A	15	ILE	CA-C	5.86	1.60	1.52
1	N	113	LEU	CB-CG	5.85	1.65	1.53
1	A	120	ALA	CA-CB	5.85	1.61	1.53
1	A	313	ALA	CA-CB	5.83	1.63	1.53
1	A	322	SER	CA-C	-5.83	1.44	1.52
1	A	57	VAL	CA-CB	5.83	1.61	1.54
1	N	297	MET	CG-SD	5.83	1.95	1.80
3	C	6	HIS	CA-C	5.82	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	69	VAL	N-CA	5.81	1.53	1.46
5	E	29	LEU	C-O	-5.80	1.17	1.24
1	A	452	THR	CA-CB	5.80	1.62	1.53
8	U	24	ASN	C-O	5.80	1.31	1.24
1	N	172	LYS	C-N	5.78	1.40	1.33
1	A	300	ASP	C-O	-5.77	1.17	1.24
1	A	237	PHE	CA-C	5.76	1.60	1.52
1	A	165	ILE	CA-CB	5.74	1.60	1.54
1	N	464	ALA	N-CA	5.73	1.53	1.46
5	E	64	ALA	CA-CB	5.72	1.62	1.53
2	B	214	VAL	N-CA	5.71	1.53	1.46
2	O	175	ILE	CA-CB	5.71	1.58	1.54
1	A	359	ALA	CA-CB	5.70	1.62	1.53
6	F	1	ALA	C-N	5.69	1.38	1.33
1	A	279	SER	C-O	-5.68	1.17	1.24
5	E	82	TYR	CA-C	5.67	1.59	1.52
6	S	2	SER	CA-C	5.67	1.59	1.52
3	C	97	PHE	N-CA	5.66	1.53	1.46
3	P	29	SER	CB-OG	-5.66	1.30	1.42
3	C	61	VAL	CA-CB	5.65	1.61	1.54
6	S	54	ASN	CB-CG	-5.65	1.38	1.52
1	N	374	VAL	CA-C	5.64	1.59	1.52
2	B	154	VAL	C-O	5.64	1.29	1.24
2	B	136	LEU	N-CA	5.63	1.53	1.46
2	O	42	ILE	CA-CB	5.63	1.60	1.54
3	C	81	TYR	N-CA	5.62	1.53	1.46
1	A	376	HIS	C-O	5.61	1.30	1.24
2	B	123	ILE	CA-CB	5.61	1.61	1.54
3	C	19	THR	CA-C	5.61	1.60	1.52
7	T	55	ILE	CA-CB	5.60	1.60	1.54
3	C	222	GLN	C-O	-5.59	1.17	1.24
1	A	128	VAL	CA-CB	5.59	1.62	1.54
6	F	49	VAL	C-O	-5.58	1.18	1.24
1	N	98	ASN	C-O	5.58	1.30	1.24
7	G	17	ARG	CD-NE	-5.57	1.38	1.46
1	A	502	TYR	C-O	5.57	1.30	1.24
1	A	297	MET	CG-SD	5.56	1.94	1.80
1	N	206	ILE	N-CA	5.55	1.53	1.46
1	A	277	MET	C-O	5.55	1.30	1.24
1	N	477	ALA	N-CA	5.55	1.53	1.46
1	A	511	VAL	CA-CB	5.54	1.61	1.54
8	U	28	ASN	CA-C	5.54	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	240	HIS	CA-C	5.54	1.58	1.52
4	D	127	LYS	CB-CG	5.53	1.69	1.52
5	E	20	ASN	N-CA	5.50	1.53	1.46
1	A	172	LYS	CA-C	5.50	1.59	1.52
1	A	308	ALA	N-CA	5.49	1.53	1.46
1	A	253	MET	CA-C	-5.49	1.45	1.52
7	T	5	LYS	CB-CG	5.47	1.68	1.52
4	Q	6	VAL	CA-CB	5.46	1.63	1.54
1	A	469	VAL	N-CA	5.46	1.53	1.46
11	K	11	ASP	C-O	-5.46	1.17	1.24
3	C	242	TRP	CA-CB	5.45	1.61	1.53
2	O	78	LEU	CA-C	5.45	1.58	1.52
1	A	66	ILE	C-O	5.45	1.30	1.24
12	L	23	ALA	CA-CB	5.45	1.61	1.53
1	A	383	MET	CA-C	5.44	1.59	1.52
5	R	54	ALA	N-CA	5.44	1.52	1.46
12	L	21	LEU	CG-CD1	5.43	1.70	1.52
4	D	80	THR	CA-C	5.42	1.59	1.52
1	A	282	PHE	CA-C	5.41	1.59	1.52
1	N	70	VAL	C-O	5.41	1.30	1.24
1	N	178	GLN	N-CA	-5.41	1.39	1.46
1	A	75	ILE	CG1-CD1	5.41	1.72	1.51
1	A	341	ALA	CA-CB	5.41	1.61	1.53
5	E	77	PRO	CA-C	5.40	1.59	1.52
4	D	11	TYR	CA-CB	5.40	1.61	1.53
1	A	228	PRO	N-CA	-5.40	1.40	1.47
13	M	3	ALA	CA-CB	5.40	1.63	1.53
1	A	79	GLY	N-CA	5.39	1.52	1.45
1	A	438	ARG	CD-NE	5.39	1.53	1.46
1	A	196	LEU	C-O	5.39	1.30	1.24
3	C	121	ILE	CA-CB	5.39	1.60	1.54
1	N	200	PRO	C-O	5.39	1.30	1.24
6	F	61	ILE	CA-CB	5.39	1.59	1.53
4	Q	6	VAL	N-CA	5.39	1.53	1.46
3	C	24	ALA	N-CA	5.38	1.52	1.46
1	A	70	VAL	CA-CB	5.38	1.60	1.54
4	D	81	VAL	CA-C	5.37	1.59	1.52
1	N	128	VAL	N-CA	5.37	1.53	1.46
3	P	237	ALA	CA-CB	5.37	1.61	1.53
3	C	71	HIS	CA-C	-5.37	1.46	1.53
13	M	5	PRO	CA-CB	5.36	1.61	1.53
1	A	215	LEU	N-CA	5.35	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	297	MET	CA-CB	5.35	1.62	1.53
1	A	68	PHE	CD2-CE2	5.33	1.54	1.38
1	A	247	ILE	N-CA	5.33	1.53	1.46
3	C	80	ARG	CZ-NH1	5.33	1.40	1.32
1	A	245	ILE	CA-C	5.31	1.59	1.52
3	C	151	LEU	CA-C	5.31	1.59	1.52
1	A	484	THR	CA-C	5.31	1.58	1.52
1	N	441	SER	C-O	5.31	1.30	1.24
1	A	383	MET	CG-SD	5.30	1.94	1.80
5	E	81	ILE	C-O	5.30	1.30	1.24
2	B	163	TRP	N-CA	5.29	1.53	1.46
1	N	211	THR	CA-CB	5.29	1.61	1.53
1	N	253	MET	N-CA	5.29	1.52	1.46
4	D	20	ARG	CD-NE	-5.28	1.38	1.46
1	A	239	GLY	C-O	5.28	1.30	1.23
1	A	494	TRP	CA-C	5.28	1.59	1.52
2	B	38	VAL	C-O	5.28	1.30	1.24
5	R	85	VAL	C-O	-5.27	1.18	1.24
8	H	24	ASN	C-O	5.26	1.30	1.24
6	F	14	THR	CA-C	5.26	1.59	1.52
4	D	98	TRP	C-O	5.25	1.30	1.24
1	A	101	SER	N-CA	5.25	1.52	1.46
2	B	22	HIS	C-O	5.25	1.30	1.24
1	N	401	SER	N-CA	5.25	1.52	1.46
1	A	394	VAL	N-CA	5.24	1.52	1.46
1	A	392	GLY	CA-C	5.24	1.57	1.52
4	Q	6	VAL	CA-C	5.24	1.58	1.52
6	F	95	GLN	N-CA	5.24	1.52	1.46
1	N	63	PHE	C-O	-5.24	1.18	1.24
3	C	73	PRO	CB-CG	5.23	1.75	1.49
5	E	85	VAL	CA-CB	5.23	1.61	1.54
8	U	18	SER	C-O	-5.23	1.17	1.24
1	A	154	GLY	CA-C	5.22	1.57	1.52
4	D	19	ARG	CZ-NH2	5.21	1.40	1.33
9	I	63	MET	N-CA	5.21	1.52	1.46
1	N	216	ASN	CA-CB	5.19	1.61	1.53
1	A	196	LEU	N-CA	5.19	1.52	1.46
3	C	87	ILE	CA-C	5.19	1.59	1.52
7	T	32	THR	CA-C	5.19	1.59	1.52
1	A	426	PHE	C-O	5.19	1.29	1.24
1	A	113	LEU	CA-C	5.18	1.59	1.52
1	A	289	ALA	CA-CB	5.18	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	274	VAL	N-CA	5.18	1.52	1.46
1	A	149	SER	CA-CB	5.18	1.61	1.53
7	T	23	LEU	CA-CB	5.18	1.62	1.53
10	W	9	GLN	C-O	-5.18	1.18	1.24
2	B	194	GLY	C-O	5.17	1.29	1.23
2	O	209	ILE	CA-CB	5.17	1.60	1.54
6	S	92	VAL	CA-CB	5.17	1.60	1.54
1	A	368	HIS	CA-CB	5.16	1.61	1.53
12	Y	35	ALA	C-O	5.15	1.29	1.24
12	Y	8	GLY	N-CA	5.15	1.53	1.45
1	A	132	LEU	CA-C	5.15	1.59	1.52
4	D	28	ALA	CA-CB	5.14	1.61	1.53
4	D	100	LYS	CD-CE	5.14	1.67	1.52
12	L	35	ALA	N-CA	-5.13	1.41	1.46
3	P	181	TYR	CD1-CE1	5.13	1.54	1.38
1	A	121	GLY	N-CA	5.13	1.50	1.45
6	F	95	GLN	CA-C	5.13	1.59	1.52
11	K	31	TYR	C-O	5.12	1.29	1.24
3	C	88	ILE	N-CA	5.12	1.52	1.46
3	P	38	ASN	C-O	5.12	1.30	1.24
3	P	68	GLN	N-CA	5.12	1.52	1.45
1	N	63	PHE	N-CA	5.11	1.52	1.46
11	X	17	VAL	N-CA	5.10	1.52	1.46
1	N	165	ILE	N-CA	5.10	1.52	1.46
1	A	510	TYR	N-CA	-5.10	1.40	1.46
5	E	66	ARG	CD-NE	5.09	1.53	1.46
1	A	364	ASP	C-O	5.09	1.30	1.24
3	P	147	ALA	N-CA	5.09	1.52	1.46
1	N	426	PHE	CA-CB	5.08	1.60	1.53
8	H	64	CYS	C-N	5.08	1.40	1.33
1	A	254	ILE	CA-CB	5.07	1.60	1.54
1	A	181	THR	CA-CB	5.07	1.61	1.53
13	M	17	ILE	CA-C	5.07	1.59	1.52
3	P	145	THR	CA-CB	5.06	1.61	1.53
3	P	206	LEU	N-CA	-5.06	1.40	1.46
3	C	62	ILE	CA-C	5.05	1.59	1.52
4	D	11	TYR	CB-CG	5.05	1.62	1.51
4	D	40	LEU	C-O	5.04	1.29	1.24
2	B	43	SER	C-O	-5.04	1.17	1.24
3	C	101	PHE	C-O	5.03	1.29	1.24
7	T	79	PRO	CA-C	5.03	1.59	1.52
4	D	106	PRO	C-O	-5.02	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	70	ILE	CA-CB	5.02	1.60	1.54
2	B	52	HIS	C-O	5.02	1.29	1.23
2	O	119	ASP	C-O	5.02	1.30	1.23
2	B	116	LEU	CA-C	5.01	1.58	1.52
6	F	57	ILE	CA-CB	5.01	1.59	1.54
1	N	442	ASP	N-CA	5.01	1.51	1.46
1	A	53	ILE	CG1-CD1	5.01	1.71	1.51
1	A	469	VAL	CB-CG2	5.01	1.69	1.52
1	N	485	VAL	N-CA	-5.01	1.40	1.46
9	I	29	LEU	N-CA	5.01	1.52	1.46
2	B	96	THR	C-O	5.00	1.30	1.24
6	S	90	LYS	C-O	-5.00	1.18	1.24

All (230) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	240	HIS	N-CA-CB	11.78	121.58	110.39
1	A	310	MET	CG-SD-CE	-11.08	76.53	100.90
1	A	278	MET	CG-SD-CE	-10.50	77.80	100.90
1	N	278	MET	CG-SD-CE	-9.74	79.47	100.90
6	S	53	THR	CA-C-N	9.69	135.04	120.31
6	S	53	THR	C-N-CA	9.69	135.04	120.31
6	S	54	ASN	N-CA-C	8.57	121.76	111.82
1	A	380	VAL	CB-CA-C	-8.51	98.28	112.16
1	A	240	HIS	N-CA-CB	8.49	118.46	110.39
1	A	61	HIS	N-CA-C	-8.45	101.75	110.97
12	Y	29	PHE	N-CA-C	8.39	120.50	111.36
6	S	49	VAL	CA-C-N	-8.30	111.47	119.85
6	S	49	VAL	C-N-CA	-8.30	111.47	119.85
1	A	383	MET	CB-CA-C	-8.27	97.06	110.79
6	F	2	SER	N-CA-C	8.25	118.83	108.19
4	D	20	ARG	NE-CZ-NH2	-8.21	111.81	119.20
1	N	380	VAL	CB-CA-C	-8.21	100.89	112.22
1	N	299	VAL	N-CA-C	8.17	118.26	110.42
12	Y	11	ILE	CA-C-N	-7.75	110.15	119.84
12	Y	11	ILE	C-N-CA	-7.75	110.15	119.84
1	A	169	ILE	CB-CA-C	-7.73	101.88	112.24
6	S	94	HIS	N-CA-C	7.71	127.22	110.80
1	A	28	MET	N-CA-C	-7.56	103.05	111.82
1	A	310	MET	N-CA-C	7.36	118.94	111.07
3	C	38	ASN	N-CA-C	7.27	121.19	111.30
1	A	105	LEU	CA-C-N	-7.26	112.90	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	LEU	C-N-CA	-7.26	112.90	120.38
1	N	199	LEU	CA-C-N	-7.12	111.45	119.28
1	N	199	LEU	C-N-CA	-7.12	111.45	119.28
9	I	13	LEU	N-CA-C	-7.05	103.02	111.69
1	A	82	LEU	CA-C-N	-7.00	114.73	120.33
1	A	82	LEU	C-N-CA	-7.00	114.73	120.33
1	A	240	HIS	CA-CB-CG	-6.99	106.81	113.80
2	O	14	SER	CA-C-N	6.96	127.25	119.32
2	O	14	SER	C-N-CA	6.96	127.25	119.32
1	N	383	MET	CB-CA-C	-6.95	99.68	110.81
1	N	82	LEU	CA-C-N	-6.93	114.79	120.33
1	N	82	LEU	C-N-CA	-6.93	114.79	120.33
7	T	7	ASP	N-CA-C	6.91	125.52	110.80
7	T	58	LYS	CA-C-N	-6.80	112.98	119.85
7	T	58	LYS	C-N-CA	-6.80	112.98	119.85
4	Q	8	SER	N-CA-C	6.80	118.34	111.07
6	S	6	VAL	CA-C-N	-6.79	113.30	120.03
6	S	6	VAL	C-N-CA	-6.79	113.30	120.03
1	A	297	MET	CG-SD-CE	-6.78	85.98	100.90
3	P	138	LEU	N-CA-C	-6.78	103.82	111.14
1	A	449	MET	CA-CB-CG	-6.78	100.54	114.10
12	L	35	ALA	CA-C-N	-6.76	111.55	119.05
12	L	35	ALA	C-N-CA	-6.76	111.55	119.05
1	A	438	ARG	CB-CA-C	-6.75	96.44	110.40
3	C	255	SER	N-CA-C	6.74	118.51	111.03
1	N	12	HIS	N-CA-C	6.73	119.45	111.71
1	N	352	GLY	N-CA-C	-6.65	104.75	112.73
11	X	43	SER	CA-C-N	-6.60	112.90	120.89
11	X	43	SER	C-N-CA	-6.60	112.90	120.89
6	S	2	SER	N-CA-C	6.57	117.25	108.38
1	N	240	HIS	CA-CB-CG	-6.56	107.24	113.80
3	P	189	SER	N-CA-C	-6.54	105.17	113.02
1	N	357	VAL	N-CA-C	-6.53	104.15	110.42
2	B	38	VAL	N-CA-C	6.52	116.67	110.42
1	N	250	GLY	N-CA-C	-6.48	104.98	112.50
6	F	11	GLU	N-CA-C	6.43	118.37	111.36
6	F	93	PRO	CA-C-N	6.41	133.78	121.54
6	F	93	PRO	C-N-CA	6.41	133.78	121.54
3	C	236	GLU	CA-CB-CG	-6.39	101.33	114.10
12	Y	20	ARG	N-CA-C	-6.35	104.36	111.28
6	S	54	ASN	CB-CA-C	-6.33	98.52	110.67
1	N	407	ASP	N-CA-C	6.33	118.98	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	PRO	CA-C-N	6.29	126.77	119.47
1	A	173	PRO	C-N-CA	6.29	126.77	119.47
8	H	61	LYS	CB-CG-CD	-6.29	96.84	111.30
1	N	380	VAL	N-CA-CB	6.28	120.00	110.58
6	F	93	PRO	N-CA-C	6.27	120.81	111.41
5	E	108	LYS	CB-CA-C	6.26	120.09	109.50
1	A	189	MET	CG-SD-CE	-6.22	87.22	100.90
2	B	39	LEU	N-CA-C	-6.20	104.58	111.71
1	A	512	ASN	CB-CA-C	-6.17	98.10	109.46
3	P	80	ARG	CG-CD-NE	-6.17	98.43	112.00
3	P	217	VAL	N-CA-C	-6.17	104.50	110.42
1	A	319	LYS	N-CA-C	-6.12	103.94	111.40
2	O	226	MET	N-CA-C	-6.11	105.40	112.92
8	U	59	VAL	N-CA-C	6.08	116.74	110.36
1	N	209	LEU	N-CA-C	-6.07	104.66	111.28
1	A	74	MET	CB-CG-SD	-6.07	94.50	112.70
9	V	20	HIS	N-CA-C	6.04	117.94	111.36
8	U	73	ASP	N-CA-C	-6.02	104.64	111.14
5	E	26	ALA	N-CA-C	-6.01	104.81	111.36
8	H	14	ALA	CA-C-N	-6.00	114.58	120.52
8	H	14	ALA	C-N-CA	-6.00	114.58	120.52
1	A	79	GLY	N-CA-C	-6.00	105.23	112.49
1	N	200	PRO	N-CA-C	6.00	121.75	113.65
7	G	8	HIS	N-CA-C	6.00	123.57	110.80
6	S	53	THR	CB-CA-C	-5.99	98.50	110.42
1	A	472	ILE	N-CA-C	-5.98	104.68	110.72
4	D	5	VAL	N-CA-C	5.96	116.98	108.93
1	N	105	LEU	CA-C-N	-5.93	114.27	120.38
1	N	105	LEU	C-N-CA	-5.93	114.27	120.38
4	D	20	ARG	CB-CA-C	-5.90	100.65	110.68
9	I	29	LEU	N-CA-C	5.89	117.70	111.28
7	G	17	ARG	CB-CG-CD	-5.88	97.78	111.30
1	N	470	PHE	N-CA-C	-5.88	104.96	111.36
7	T	61	SER	CB-CA-C	-5.84	104.03	111.22
1	N	458	SER	N-CA-C	5.83	117.64	111.28
3	P	180	GLU	CB-CA-C	-5.83	101.11	110.79
1	A	87	ILE	N-CA-C	-5.81	107.08	112.43
1	A	438	ARG	CA-CB-CG	5.80	125.70	114.10
1	A	119	GLU	CB-CA-C	-5.79	109.89	116.54
3	P	151	LEU	N-CA-C	-5.78	104.88	111.07
2	O	202	SER	CB-CA-C	-5.74	98.99	110.42
2	O	65	TRP	N-CA-C	5.73	119.90	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	X	21	GLY	N-CA-C	-5.72	105.86	112.50
4	Q	10	ASP	N-CA-C	-5.71	105.66	113.30
4	D	105	GLY	CA-C-N	5.70	125.63	119.76
4	D	105	GLY	C-N-CA	5.70	125.63	119.76
2	B	175	ILE	N-CA-CB	-5.69	106.33	112.37
1	A	397	PHE	CA-C-N	-5.69	113.16	119.19
1	A	397	PHE	C-N-CA	-5.69	113.16	119.19
12	L	40	VAL	CB-CA-C	-5.69	104.46	112.14
1	A	278	MET	CA-CB-CG	-5.68	102.73	114.10
1	N	478	SER	N-CA-C	5.64	119.33	112.23
1	A	402	GLY	N-CA-C	-5.62	107.51	115.43
1	A	35	LEU	N-CA-C	-5.61	105.16	112.23
1	N	83	VAL	CA-C-N	-5.60	112.83	119.05
1	N	83	VAL	C-N-CA	-5.60	112.83	119.05
3	C	28	THR	N-CA-C	5.60	117.18	111.14
2	B	177	GLY	N-CA-C	-5.59	107.61	115.32
1	A	365	ILE	N-CA-C	-5.58	104.26	110.62
1	A	86	MET	CA-C-N	-5.57	113.07	122.88
1	A	86	MET	C-N-CA	-5.57	113.07	122.88
1	A	499	PRO	CA-C-N	-5.57	114.64	120.38
1	A	499	PRO	C-N-CA	-5.57	114.64	120.38
1	N	99	ASN	N-CA-C	-5.57	105.36	111.82
4	D	19	ARG	CA-C-N	5.57	128.01	120.38
4	D	19	ARG	C-N-CA	5.57	128.01	120.38
1	N	240	HIS	CA-C-N	-5.56	112.89	119.84
1	N	240	HIS	C-N-CA	-5.56	112.89	119.84
2	O	16	ILE	N-CA-C	5.55	115.75	110.42
11	K	35	GLN	CA-C-N	-5.55	112.15	122.69
11	K	35	GLN	C-N-CA	-5.55	112.15	122.69
3	P	230	ASN	N-CA-CB	-5.54	103.53	110.90
12	Y	13	PHE	N-CA-C	-5.54	100.94	109.52
1	A	237	PHE	N-CA-C	-5.53	105.35	111.71
1	N	206	ILE	N-CA-C	-5.53	104.92	113.16
1	A	380	VAL	CA-CB-CG2	5.53	119.80	110.40
1	A	500	PRO	CA-C-N	-5.51	114.58	120.03
1	A	500	PRO	C-N-CA	-5.51	114.58	120.03
1	N	27	GLY	N-CA-C	-5.51	105.99	113.37
7	T	2	SER	N-CA-C	-5.51	106.47	114.12
1	N	310	MET	N-CA-C	5.50	117.35	111.36
2	B	188	ARG	CA-C-N	-5.49	115.09	120.52
2	B	188	ARG	C-N-CA	-5.49	115.09	120.52
6	F	95	GLN	N-CA-C	5.44	122.39	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	495	LEU	N-CA-C	5.44	119.54	113.01
10	W	4	ARG	CB-CA-C	-5.43	101.98	110.94
10	J	28	ASP	N-CA-C	-5.42	105.37	111.28
7	G	57	THR	N-CA-C	-5.42	106.67	113.72
1	N	184	PHE	N-CA-C	-5.42	105.45	111.36
1	A	485	VAL	N-CA-C	-5.41	100.44	108.45
1	A	137	ALA	CA-C-N	-5.41	114.72	122.67
1	A	137	ALA	C-N-CA	-5.41	114.72	122.67
1	N	221	ASP	CB-CA-C	5.39	116.16	110.17
3	P	101	PHE	N-CA-C	5.38	116.83	111.07
1	A	225	GLY	N-CA-C	-5.38	107.84	115.43
1	A	470	PHE	N-CA-C	-5.37	105.51	111.36
3	P	29	SER	N-CA-C	-5.34	104.70	111.11
1	A	137	ALA	N-CA-C	-5.34	106.61	113.23
1	N	74	MET	CB-CG-SD	-5.34	96.69	112.70
4	D	129	ALA	CA-C-N	5.33	125.03	119.64
4	D	129	ALA	C-N-CA	5.33	125.03	119.64
3	C	105	SER	N-CA-C	5.33	118.94	112.23
7	T	8	HIS	N-CA-C	5.33	122.14	110.80
8	U	14	ALA	CA-C-N	5.32	125.29	120.03
8	U	14	ALA	C-N-CA	5.32	125.29	120.03
1	N	244	TYR	N-CA-C	-5.32	105.15	111.69
2	O	92	ASN	N-CA-C	5.27	121.45	109.81
3	P	140	SER	N-CA-C	-5.27	105.59	112.23
2	B	177	GLY	CA-C-N	-5.27	114.32	122.59
2	B	177	GLY	C-N-CA	-5.27	114.32	122.59
2	B	43	SER	N-CA-C	-5.26	105.72	111.82
2	B	13	THR	N-CA-C	-5.25	107.25	113.97
1	A	30	GLY	N-CA-C	-5.24	106.35	113.37
1	A	251	PHE	N-CA-C	-5.24	105.57	111.28
3	C	145	THR	N-CA-C	-5.24	105.25	111.69
1	N	485	VAL	N-CA-CB	-5.23	102.86	111.44
7	G	7	ASP	N-CA-C	5.23	121.95	110.80
1	A	52	GLN	N-CA-C	-5.23	105.58	111.28
1	A	380	VAL	CG1-CB-CG2	5.23	122.30	110.80
4	D	20	ARG	NE-CZ-NH1	5.22	126.72	121.50
12	Y	24	MET	CB-CA-C	-5.21	102.69	110.88
10	J	57	HIS	CB-CA-C	5.20	119.79	111.73
1	N	359	ALA	N-CA-C	-5.20	105.79	111.82
6	S	64	GLU	CA-C-N	-5.19	117.26	126.45
6	S	64	GLU	C-N-CA	-5.19	117.26	126.45
2	B	65	TRP	CB-CA-C	5.19	119.60	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	326	THR	N-CA-C	-5.18	105.71	111.36
3	C	236	GLU	N-CA-C	5.17	117.32	111.11
3	P	29	SER	CB-CA-C	-5.17	102.54	110.81
1	A	15	ILE	N-CA-C	-5.17	105.50	110.72
3	P	107	ALA	CA-C-O	-5.17	115.16	121.15
8	U	57	ARG	N-CA-C	-5.15	105.74	111.36
3	C	64	GLU	N-CA-C	-5.15	106.50	112.89
1	N	169	ILE	CB-CA-C	-5.15	105.45	111.94
4	D	130	PRO	N-CA-C	-5.15	107.03	114.18
1	N	308	ALA	N-CA-C	-5.15	105.67	111.28
1	A	359	ALA	N-CA-C	-5.14	105.86	111.82
1	N	113	LEU	CB-CA-C	5.14	119.59	110.85
2	B	119	ASP	N-CA-C	-5.13	102.19	110.14
11	K	19	ALA	CA-C-N	-5.13	111.97	120.68
11	K	19	ALA	C-N-CA	-5.13	111.97	120.68
1	N	383	MET	CA-CB-CG	5.13	124.35	114.10
6	F	87	THR	N-CA-CB	5.12	117.56	110.04
2	O	5	MET	N-CA-C	5.11	119.36	113.38
1	A	251	PHE	CB-CA-C	-5.11	102.31	110.79
3	P	75	VAL	N-CA-C	-5.11	105.73	110.53
1	N	8	PHE	N-CA-C	-5.09	105.80	112.41
1	N	500	PRO	CA-C-N	-5.09	114.99	120.03
1	N	500	PRO	C-N-CA	-5.09	114.99	120.03
1	A	314	ILE	CA-C-N	-5.08	113.69	119.28
1	A	314	ILE	C-N-CA	-5.08	113.69	119.28
3	C	29	SER	CA-CB-OG	-5.08	100.94	111.10
9	I	65	LYS	N-CA-C	5.06	117.53	111.71
3	C	135	SER	N-CA-C	-5.05	105.96	111.82
6	S	55	LYS	CB-CG-CD	-5.05	99.67	111.30
2	B	156	SER	CA-C-N	-5.04	114.74	122.60
2	B	156	SER	C-N-CA	-5.04	114.74	122.60
9	V	37	PHE	N-CA-C	-5.04	106.48	113.18
9	V	68	ILE	N-CA-C	5.03	117.34	111.05
12	L	44	LEU	N-CA-C	5.02	116.75	111.28
1	A	329	GLY	N-CA-C	-5.01	108.40	115.32
3	P	89	SER	N-CA-C	-5.01	105.95	111.71

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	F	93	PRO	Peptide

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Mol	Chain	Res	Type	Group
10	J	57	HIS	Peptide
12	L	2	HIS	Peptide
6	S	93	PRO	Peptide
10	W	57	HIS	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	4027	0	4001	74	0
1	N	4027	0	4001	89	0
2	B	1824	0	1833	38	0
2	O	1824	0	1833	61	0
3	C	2110	0	2027	37	0
3	P	2110	0	2027	46	0
4	D	1195	0	1183	18	0
4	Q	1195	0	1183	21	0
5	E	852	0	845	5	0
5	R	852	0	845	13	0
6	F	748	0	728	17	0
6	S	748	0	728	27	0
7	G	675	0	643	37	0
7	T	675	0	643	50	0
8	H	662	0	623	6	0
8	U	662	0	623	11	0
9	I	601	0	613	10	0
9	V	601	0	613	19	0
10	J	460	0	459	7	0
10	W	460	0	459	8	0
11	K	384	0	366	2	0
11	X	384	0	366	4	0
12	L	380	0	380	12	0
12	Y	380	0	380	15	0
13	M	335	0	352	9	0
13	Z	335	0	352	9	0
14	A	120	0	108	10	0
14	N	120	0	108	13	0
15	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	N	2	0	0	2	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	1	0	0	0	0
18	N	1	0	0	0	0
19	A	63	0	110	7	0
19	D	63	0	110	13	0
19	L	63	0	110	16	0
19	N	126	0	220	22	0
19	Q	63	0	110	10	0
20	A	102	0	152	11	0
20	C	102	0	152	6	0
20	N	102	0	152	7	0
20	P	102	0	152	5	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	29	0	36	3	0
22	C	58	0	70	4	0
22	J	29	0	36	2	0
22	O	29	0	36	1	0
22	P	58	0	73	5	0
22	W	29	0	35	6	0
23	C	1	0	0	0	0
23	P	1	0	0	0	0
24	C	53	0	77	3	0
24	G	106	0	154	23	0
24	S	53	0	77	17	0
24	T	106	0	154	28	0
25	C	100	0	156	21	0
25	G	100	0	156	28	0
25	P	100	0	156	19	0
25	T	100	0	156	35	0
26	E	52	0	80	16	0
26	R	52	0	80	14	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	G	33	0	38	3	0
28	M	33	0	38	1	0
28	P	33	0	38	5	0
28	Z	33	0	39	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	A	225	0	0	8	0
29	B	125	0	0	4	0
29	C	106	0	0	2	0
29	D	91	0	0	1	0
29	E	62	0	0	0	0
29	F	75	0	0	2	0
29	G	41	0	0	3	0
29	H	47	0	0	2	0
29	I	38	0	0	1	0
29	J	20	0	0	1	0
29	K	20	0	0	1	0
29	L	22	0	0	1	0
29	M	15	0	0	1	0
29	N	199	0	0	6	0
29	O	107	0	0	4	0
29	P	100	0	0	3	0
29	Q	55	0	0	2	0
29	R	40	0	0	1	0
29	S	56	0	0	5	0
29	T	36	0	0	4	0
29	U	41	0	0	4	0
29	V	18	0	0	1	0
29	W	12	0	0	0	0
29	X	14	0	0	0	0
29	Y	12	0	0	1	0
29	Z	11	0	0	0	0
All	All	32324	0	31275	725	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (725) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:74:MET:CB	1:N:74:MET:CG	1.76	1.56
1:A:312:ILE:CG1	1:A:312:ILE:CD1	1.78	1.54
4:D:100:LYS:CE	4:D:100:LYS:NZ	1.69	1.51
3:C:73:PRO:CG	3:C:73:PRO:CB	1.75	1.48
14:A:516:HEA:O11	14:A:516:HEA:C11	1.64	1.45
12:L:20:ARG:NH2	19:L:522:TGL:HC32	1.58	1.17
11:X:54:ARG:HH21	11:X:54:ARG:HG3	1.07	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:67:PHE:HE1	25:P:1270:CDL:H1	1.11	1.15
10:W:33:ARG:HG2	22:W:1059:CHD:H152	1.24	1.14
25:G:269:CDL:H241	25:G:269:CDL:H541	1.29	1.13
26:E:229:PSC:H072	9:I:10:ARG:HH21	1.13	1.09
6:S:52:ILE:O	6:S:94:HIS:CE1	2.07	1.08
2:B:41:ILE:HD13	26:E:229:PSC:H342	1.36	1.07
7:T:5:LYS:HD2	24:T:263:PEK:H383	1.37	1.07
6:F:1:ALA:HB2	29:G:4415:HOH:O	1.54	1.06
3:C:67:PHE:HE1	25:C:270:CDL:H1	1.19	1.06
26:E:229:PSC:C07	9:I:10:ARG:HH21	1.67	1.06
7:T:84:LYS:H	7:T:84:LYS:HD2	0.94	1.05
6:S:94:HIS:CD2	6:S:95:GLN:H	1.75	1.05
24:S:1265:PEK:C38	25:T:1269:CDL:H272	1.86	1.04
25:T:1269:CDL:HA21	25:T:1269:CDL:C11	1.87	1.04
6:F:85:CYS:SG	6:F:87:THR:HG23	1.97	1.03
25:G:269:CDL:H541	25:G:269:CDL:C24	1.89	1.02
25:G:269:CDL:C11	25:G:269:CDL:HA21	1.92	0.99
12:L:20:ARG:HH22	19:L:522:TGL:HC32	0.84	0.98
7:T:84:LYS:H	7:T:84:LYS:CD	1.76	0.98
6:F:1:ALA:N	24:G:265:PEK:H041	1.77	0.98
25:G:269:CDL:HA21	25:G:269:CDL:H112	1.45	0.97
7:T:5:LYS:CD	24:T:263:PEK:H383	1.94	0.96
7:T:84:LYS:HD2	7:T:84:LYS:N	1.79	0.96
20:C:267:PGV:H181	29:C:4710:HOH:O	1.62	0.96
20:N:1524:PGV:H22	20:N:1524:PGV:H011	1.46	0.96
19:L:522:TGL:H231	19:L:522:TGL:HA92	1.49	0.95
7:G:84:LYS:H	7:G:84:LYS:HD2	1.30	0.95
25:T:1269:CDL:HA21	25:T:1269:CDL:H111	1.49	0.95
12:Y:20:ARG:NH2	12:Y:24:MET:HG3	1.82	0.94
2:O:202:SER:HB2	2:O:203:ASN:HD22	1.32	0.93
7:G:5:LYS:HB3	1:N:278:MET:SD	2.07	0.93
6:F:1:ALA:H2	24:G:265:PEK:H041	1.31	0.93
3:P:67:PHE:CE1	25:P:1270:CDL:H1	2.04	0.91
7:T:5:LYS:CG	24:T:263:PEK:H383	2.01	0.91
7:T:31:CYS:SG	25:T:1269:CDL:H532	2.10	0.91
24:C:264:PEK:H32	24:C:264:PEK:H71	1.54	0.89
1:N:400:PHE:HB3	19:N:1522:TGL:H283	1.55	0.88
1:A:311:ILE:HD12	25:T:1269:CDL:H212	1.56	0.88
7:G:72:ASN:H	7:G:76:ASN:HD22	1.13	0.88
24:S:1265:PEK:H383	25:T:1269:CDL:H272	1.56	0.87
25:T:1269:CDL:HA21	25:T:1269:CDL:H112	1.53	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:74:MET:CB	1:N:74:MET:SD	2.62	0.87
7:G:84:LYS:H	7:G:84:LYS:CD	1.88	0.86
12:L:20:ARG:HH22	19:L:522:TGL:CC3	1.81	0.86
3:C:63:ARG:HE	25:C:270:CDL:HA22	1.40	0.85
4:D:34:SER:H	4:D:37:GLN:HE21	1.25	0.85
3:P:157:LYS:NZ	24:S:1265:PEK:H051	1.91	0.85
25:G:269:CDL:H601	25:G:269:CDL:H751	1.59	0.84
9:V:1:SAC:OAC	9:V:1:SAC:HB3	1.77	0.84
6:S:94:HIS:HD2	6:S:95:GLN:H	1.22	0.84
3:P:63:ARG:HE	25:P:1270:CDL:HA22	1.43	0.84
7:G:5:LYS:HG3	24:G:1263:PEK:H383	1.59	0.84
28:P:1272:DMU:H30	28:P:1272:DMU:O1	1.78	0.83
1:N:347:LEU:HD13	1:N:383:MET:SD	2.18	0.83
2:O:227:LEU:CB	29:O:4762:HOH:O	2.27	0.82
6:S:75:HIS:H	6:S:80:GLN:HE22	1.27	0.82
3:C:29:SER:HB3	3:C:42:LEU:HD13	1.61	0.82
3:C:160:LEU:HD13	22:C:271:CHD:H181	1.62	0.81
1:N:406:ASN:HD21	20:N:1524:PGV:H21	1.43	0.81
2:O:227:LEU:HB3	29:O:4762:HOH:O	1.78	0.81
8:U:9:LYS:O	8:U:10:ASN:HB2	1.79	0.81
3:C:80:ARG:NH1	24:T:263:PEK:H032	1.97	0.80
7:T:76:ASN:HD21	24:T:1264:PEK:HN2	1.26	0.80
24:S:1265:PEK:H381	25:T:1269:CDL:H272	1.62	0.80
7:T:31:CYS:SG	25:T:1269:CDL:H551	2.22	0.80
2:B:14:SER:HB3	2:B:168:LEU:HD23	1.64	0.79
7:T:37:LEU:HD23	25:T:1269:CDL:H352	1.63	0.79
25:G:269:CDL:H241	25:G:269:CDL:C54	2.12	0.79
8:H:23:GLN:HG3	29:H:4165:HOH:O	1.83	0.79
24:T:1264:PEK:H71	24:T:1264:PEK:H31	1.65	0.79
26:E:229:PSC:C07	9:I:10:ARG:NH2	2.45	0.79
3:C:67:PHE:CE1	25:C:270:CDL:H1	2.12	0.79
6:S:1:ALA:H2	24:S:1265:PEK:H041	1.47	0.77
3:C:63:ARG:HE	25:C:270:CDL:CA2	1.97	0.77
7:G:84:LYS:HD2	7:G:84:LYS:N	2.00	0.77
6:S:52:ILE:O	6:S:94:HIS:HE1	1.65	0.77
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.20	0.76
28:P:1272:DMU:H34	7:T:63:GLY:H	1.49	0.76
1:A:406:ASN:HD21	20:A:524:PGV:H22	1.49	0.76
2:B:82:ARG:NH1	2:B:86:MET:HE1	2.01	0.76
1:A:312:ILE:CD1	1:A:312:ILE:CG2	2.64	0.76
4:D:78:TRP:HB3	19:D:523:TGL:HB22	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:5:LYS:HG3	24:T:263:PEK:H383	1.69	0.75
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.68	0.75
7:T:72:ASN:H	7:T:76:ASN:HD22	1.35	0.74
3:C:50:ASN:ND2	3:C:54:MET:HE2	2.03	0.74
3:C:146:TRP:CZ2	7:G:17:ARG:HG3	2.23	0.74
7:G:72:ASN:H	7:G:76:ASN:ND2	1.84	0.74
6:S:85:CYS:SG	6:S:87:THR:HG23	2.28	0.74
1:A:484:THR:HB	13:M:2:THR:OG1	1.88	0.74
20:A:524:PGV:H311	13:M:19:LEU:HD23	1.69	0.73
24:S:1265:PEK:H381	25:T:1269:CDL:C27	2.18	0.73
3:C:80:ARG:HH11	24:T:263:PEK:H032	1.52	0.73
11:K:52:GLU:HG3	29:K:4738:HOH:O	1.87	0.73
7:T:5:LYS:HB2	24:T:263:PEK:H362	1.71	0.73
10:W:36:MET:HB3	22:W:1059:CHD:C18	2.19	0.73
2:B:41:ILE:HD13	26:E:229:PSC:C34	2.17	0.72
19:Q:1523:TGL:HC21	19:Q:1523:TGL:HG12	1.70	0.72
12:L:20:ARG:NH2	19:L:522:TGL:CC3	2.47	0.72
13:M:42:LYS:HE3	13:M:42:LYS:HA	1.70	0.72
1:N:381:LEU:HB2	14:N:516:HEA:CAC	2.20	0.72
2:B:82:ARG:HH11	2:B:86:MET:HE1	1.54	0.72
3:P:63:ARG:HE	25:P:1270:CDL:CA2	2.02	0.72
26:E:229:PSC:O01	26:E:229:PSC:H212	1.88	0.72
1:N:390:MET:HE2	1:N:413:HIS:HE1	1.52	0.72
6:S:76:LYS:HE3	6:S:93:PRO:HG2	1.72	0.72
24:G:265:PEK:H383	25:G:269:CDL:H272	1.72	0.72
19:N:1522:TGL:HA62	12:Y:25:MET:HG2	1.70	0.72
1:A:347:LEU:HD13	1:A:383:MET:HB3	1.72	0.71
4:D:78:TRP:CA	19:D:523:TGL:HB22	2.20	0.71
4:D:78:TRP:CB	19:D:523:TGL:HB22	2.20	0.71
10:J:52:TRP:O	10:J:57:HIS:HE1	1.72	0.71
7:T:5:LYS:HD2	24:T:263:PEK:C38	2.15	0.71
11:X:54:ARG:HG3	11:X:54:ARG:NH2	1.84	0.71
1:A:278:MET:SD	7:T:5:LYS:HB3	2.30	0.71
3:P:160:LEU:HD13	22:P:1271:CHD:H181	1.72	0.71
6:S:1:ALA:N	24:S:1265:PEK:C04	2.53	0.71
20:C:268:PGV:H31	29:C:4316:HOH:O	1.91	0.71
24:C:264:PEK:HN2	7:G:76:ASN:HD21	1.36	0.71
26:E:229:PSC:H32	26:E:229:PSC:H011	1.72	0.71
7:T:31:CYS:SG	25:T:1269:CDL:C55	2.79	0.71
25:T:1269:CDL:H222	25:T:1269:CDL:H522	1.73	0.70
6:F:1:ALA:N	24:G:265:PEK:C04	2.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:317:GLY:HA3	14:N:516:HEA:H202	1.72	0.70
12:L:24:MET:HE1	19:L:522:TGL:H152	1.72	0.70
1:A:324:LEU:HD22	2:B:42:ILE:HG13	1.74	0.69
25:P:1270:CDL:OB9	25:P:1270:CDL:H522	1.92	0.69
1:A:312:ILE:CD1	1:A:312:ILE:CB	2.69	0.69
14:N:516:HEA:NB	15:N:520:CYN:C	2.55	0.69
24:G:265:PEK:C38	25:G:269:CDL:H272	2.23	0.69
4:Q:78:TRP:HA	19:Q:1523:TGL:HB22	1.75	0.69
25:G:269:CDL:H511	25:G:269:CDL:H181	1.75	0.69
3:P:29:SER:HB3	3:P:42:LEU:HD13	1.75	0.69
1:N:334:TRP:HH2	2:O:46:LEU:HD13	1.56	0.68
5:E:6:GLU:OE1	5:E:14:ARG:NH2	2.27	0.68
7:G:5:LYS:HB2	24:G:1263:PEK:H362	1.76	0.68
6:S:1:ALA:N	24:S:1265:PEK:H041	2.09	0.68
25:T:1269:CDL:H241	25:T:1269:CDL:H541	1.76	0.68
26:E:229:PSC:H072	9:I:10:ARG:NH2	1.99	0.68
9:I:31:PHE:CD1	9:I:31:PHE:C	2.72	0.68
3:P:157:LYS:HZ1	24:S:1265:PEK:H051	1.59	0.68
14:N:516:HEA:HMD1	14:N:516:HEA:HBD2	1.74	0.68
2:O:67:ILE:HD11	29:O:4812:HOH:O	1.92	0.67
4:Q:34:SER:H	4:Q:37:GLN:NE2	1.93	0.67
3:P:52:LEU:HD21	25:P:1270:CDL:H412	1.77	0.67
6:F:1:ALA:H1	24:G:265:PEK:H041	1.60	0.66
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.77	0.66
25:G:269:CDL:H201	1:N:311:ILE:HD12	1.77	0.66
8:H:45:ALA:O	8:H:47:GLY:N	2.28	0.66
14:A:516:HEA:C11	14:A:516:HEA:HO1	2.07	0.66
7:T:5:LYS:HB2	24:T:263:PEK:C36	2.24	0.66
3:P:246:ASP:HB2	29:P:4260:HOH:O	1.95	0.66
1:A:229:ILE:HD11	2:B:175:ILE:HD13	1.76	0.66
1:N:151:HIS:CD2	24:T:1264:PEK:H382	2.30	0.66
1:N:113:LEU:CD1	19:N:1522:TGL:H292	2.25	0.66
11:X:54:ARG:HH21	11:X:54:ARG:CG	1.96	0.66
8:U:49:ASP:O	8:U:52:VAL:HG22	1.95	0.66
3:P:157:LYS:HZ2	24:S:1265:PEK:H051	1.57	0.66
3:P:224:LYS:HD3	25:P:1270:CDL:HB31	1.76	0.66
4:Q:52:SER:OG	4:Q:55:GLU:HG3	1.96	0.65
25:C:270:CDL:H661	25:C:270:CDL:H242	1.79	0.65
2:O:227:LEU:HB2	29:O:4762:HOH:O	1.94	0.65
25:C:270:CDL:H661	25:C:270:CDL:C24	2.26	0.65
25:T:1269:CDL:H562	25:T:1269:CDL:H762	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:113:LEU:HD12	19:N:1522:TGL:H292	1.79	0.64
26:E:229:PSC:H241	26:E:229:PSC:H62	1.79	0.64
7:T:38:HIS:HD1	7:T:38:HIS:N	1.95	0.64
7:T:3:ALA:HB3	24:T:263:PEK:H382	1.78	0.64
24:S:1265:PEK:C38	25:T:1269:CDL:C27	2.69	0.64
19:A:521:TGL:H102	19:A:521:TGL:H281	1.80	0.64
10:W:33:ARG:CG	22:W:1059:CHD:H152	2.14	0.64
7:G:3:ALA:HB1	24:G:1263:PEK:H382	1.80	0.64
6:S:64:GLU:O	6:S:65:ASP:HB2	1.96	0.64
2:O:42:ILE:HG22	19:Q:1523:TGL:H251	1.80	0.64
20:N:1524:PGV:H22	20:N:1524:PGV:C01	2.24	0.63
6:S:94:HIS:CD2	6:S:95:GLN:N	2.59	0.63
25:T:1269:CDL:H571	25:T:1269:CDL:H782	1.81	0.63
2:B:81:LEU:HD12	25:T:1269:CDL:H362	1.81	0.63
7:G:11:TPO:HG22	7:G:16:TRP:HE1	1.64	0.63
1:N:514:LYS:HE2	29:S:3514:HOH:O	1.99	0.63
7:G:5:LYS:CG	24:G:1263:PEK:H383	2.27	0.63
2:O:141:ARG:H	9:V:70:GLN:HE22	1.47	0.63
3:P:5:THR:HG22	6:S:96:LEU:HD13	1.80	0.63
3:P:55:TYR:CE1	25:P:1270:CDL:H521	2.34	0.63
2:B:83:ILE:O	2:B:87:MET:HG3	1.99	0.63
19:N:1522:TGL:HA22	12:Y:13:PHE:HB3	1.81	0.63
1:A:400:PHE:HB3	19:L:522:TGL:H283	1.81	0.62
25:G:269:CDL:HA21	25:G:269:CDL:H111	1.81	0.62
24:G:265:PEK:H381	25:G:269:CDL:C27	2.28	0.62
26:R:1229:PSC:C07	9:V:10:ARG:HH21	2.13	0.62
1:N:20:LEU:HB3	19:N:1522:TGL:H221	1.80	0.62
2:O:42:ILE:HG21	19:Q:1523:TGL:H232	1.82	0.62
4:D:78:TRP:HA	19:D:523:TGL:HB22	1.79	0.61
24:G:265:PEK:C38	25:G:269:CDL:C27	2.78	0.61
1:N:53:ILE:HG12	29:N:3704:HOH:O	1.99	0.61
1:N:177:SER:H	1:N:180:GLN:NE2	1.99	0.61
1:A:324:LEU:CD2	2:B:42:ILE:HG13	2.29	0.61
2:O:57:ASP:H	26:R:1229:PSC:H202	1.65	0.61
6:S:95:GLN:HB2	29:S:4526:HOH:O	2.01	0.61
7:T:8:HIS:ND1	24:T:263:PEK:H312	2.14	0.61
1:A:313:ALA:HB2	1:A:356:ILE:HD11	1.81	0.61
2:O:41:ILE:HD13	26:R:1229:PSC:H342	1.81	0.61
22:P:1271:CHD:H151	29:P:4657:HOH:O	2.00	0.61
5:R:6:GLU:OE1	5:R:14:ARG:NH2	2.32	0.61
1:A:513:LEU:O	1:A:514:LYS:HB2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:130:PRO:HD2	4:Q:131:ILE:HD12	1.84	0.60
6:S:1:ALA:H1	24:S:1265:PEK:C04	2.15	0.60
1:N:510:TYR:OH	1:N:512:ASN:ND2	2.34	0.60
1:A:265:LYS:HE3	29:F:4709:HOH:O	2.01	0.60
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.48	0.60
1:A:136:LEU:HB2	29:A:4376:HOH:O	2.02	0.60
14:A:516:HEA:HMD1	14:A:516:HEA:HBD2	1.82	0.60
10:W:36:MET:HG3	22:W:1059:CHD:H183	1.84	0.60
13:M:42:LYS:HA	13:M:42:LYS:CE	2.27	0.60
4:Q:101:HIS:HD2	4:Q:102:TYR:CD2	2.20	0.60
7:T:12:GLY:HA3	29:T:3372:HOH:O	2.02	0.60
7:T:30:LEU:HD12	25:T:1269:CDL:H261	1.84	0.60
1:N:87:ILE:O	1:N:173:PRO:HD3	2.02	0.59
1:N:74:MET:CG	1:N:74:MET:CA	2.75	0.59
7:T:3:ALA:CB	24:T:263:PEK:H382	2.33	0.59
1:A:312:ILE:CD1	1:A:312:ILE:HG23	2.31	0.59
7:T:37:LEU:CD2	25:T:1269:CDL:H352	2.31	0.59
20:A:524:PGV:H062	29:M:2126:HOH:O	2.02	0.59
24:G:265:PEK:H381	25:G:269:CDL:H273	1.84	0.59
3:P:226:HIS:CE1	25:P:1270:CDL:HB32	2.38	0.59
20:N:1524:PGV:H312	13:Z:16:ALA:HA	1.84	0.59
29:B:2562:HOH:O	19:D:523:TGL:HC72	2.02	0.59
1:A:378:HIS:HA	1:A:382:SER:HB2	1.85	0.58
26:E:229:PSC:H071	9:I:10:ARG:NH2	2.17	0.58
29:A:4410:HOH:O	4:D:100:LYS:HD3	2.01	0.58
1:N:381:LEU:HB2	14:N:516:HEA:HAC	1.83	0.58
25:P:1270:CDL:PA1	25:P:1270:CDL:HB22	2.42	0.58
20:A:522:PGV:H183	24:C:264:PEK:H332	1.85	0.58
1:N:53:ILE:HD12	12:Y:44:LEU:HD23	1.86	0.58
20:A:522:PGV:H343	29:A:4723:HOH:O	2.03	0.58
3:P:226:HIS:HE1	25:P:1270:CDL:HB32	1.69	0.58
6:F:90:LYS:HD2	29:F:4397:HOH:O	2.03	0.58
4:Q:19:ARG:HD2	4:Q:21:ASP:OD1	2.04	0.58
2:O:104:TRP:CD2	2:O:203:ASN:HB2	2.39	0.58
7:G:3:ALA:O	7:G:4:ALA:HB2	2.04	0.58
7:G:31:CYS:SG	25:G:269:CDL:H532	2.44	0.58
10:W:36:MET:HB3	22:W:1059:CHD:H183	1.86	0.58
7:G:7:ASP:HA	1:N:178:GLN:HG2	1.86	0.58
2:O:224:ALA:O	2:O:227:LEU:HG	2.03	0.57
6:F:1:ALA:H2	24:G:265:PEK:C04	2.10	0.57
12:L:12:PRO:HB2	19:L:522:TGL:HG2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:R:1229:PSC:H212	26:R:1229:PSC:C02	2.34	0.57
2:B:86:MET:O	2:B:89:GLU:HB2	2.04	0.57
3:C:127:LEU:HG	25:G:269:CDL:OB3	2.04	0.57
1:A:335:SER:HB2	1:A:336:PRO:HD2	1.87	0.57
25:G:269:CDL:H112	25:G:269:CDL:CA2	2.28	0.57
19:A:521:TGL:H241	19:A:521:TGL:H201	1.86	0.57
4:Q:130:PRO:HA	4:Q:135:SER:HB2	1.86	0.57
6:S:94:HIS:HD2	6:S:95:GLN:N	1.98	0.57
2:B:59:GLN:C	2:B:60:GLU:HG3	2.30	0.57
10:J:7:GLU:HG3	29:J:4595:HOH:O	2.04	0.57
12:L:14:SER:H	19:L:522:TGL:HC31	1.69	0.56
19:N:1522:TGL:HC31	12:Y:14:SER:H	1.71	0.56
8:U:61:LYS:HD3	29:U:4240:HOH:O	2.05	0.56
20:A:524:PGV:H02	20:A:524:PGV:O14	2.04	0.56
1:N:390:MET:HE2	1:N:413:HIS:CE1	2.38	0.56
19:N:1521:TGL:H111	19:N:1521:TGL:C28	2.36	0.56
3:P:40:MET:O	3:P:44:MET:HG2	2.05	0.56
2:O:116:LEU:HD12	2:O:117:SER:N	2.20	0.56
3:C:217:VAL:HG22	25:C:270:CDL:H732	1.86	0.56
25:G:269:CDL:H201	1:N:311:ILE:CD1	2.36	0.56
12:L:25:MET:HG2	19:L:522:TGL:HA62	1.87	0.56
7:G:45:PRO:HD2	29:G:2099:HOH:O	2.05	0.55
19:N:1522:TGL:H362	29:Y:4623:HOH:O	2.06	0.55
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.71	0.55
20:C:267:PGV:H182	25:C:270:CDL:H662	1.86	0.55
7:G:5:LYS:CD	24:G:1263:PEK:H383	2.36	0.55
1:A:337:ALA:HB2	1:A:394:VAL:HG23	1.88	0.55
7:G:37:LEU:HD21	25:G:269:CDL:H361	1.88	0.55
26:R:1229:PSC:H343	26:R:1229:PSC:H142	1.87	0.55
2:B:14:SER:HB3	2:B:168:LEU:CD2	2.35	0.55
4:Q:78:TRP:CA	19:Q:1523:TGL:HB22	2.37	0.55
1:A:311:ILE:CD1	25:T:1269:CDL:H212	2.35	0.55
10:J:56:PRO:HB2	10:J:58:LYS:HD3	1.89	0.55
14:N:516:HEA:HBD2	14:N:516:HEA:CMD	2.36	0.55
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.88	0.55
19:N:1521:TGL:H281	19:N:1521:TGL:H102	1.89	0.55
7:G:83:GLU:HG2	7:G:84:LYS:HZ2	1.72	0.54
1:N:397:PHE:HB3	1:N:398:PRO:HD3	1.89	0.54
7:G:30:LEU:CD2	25:G:269:CDL:H471	2.37	0.54
24:T:1264:PEK:H242	24:T:1264:PEK:H12	1.88	0.54
3:C:91:VAL:HG13	24:T:263:PEK:H15	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:62:TRP:HB3	28:G:272:DMU:H29	1.90	0.54
25:P:1270:CDL:H781	25:P:1270:CDL:H231	1.89	0.54
9:V:61:GLU:HG3	9:V:64:ARG:HH21	1.72	0.54
3:C:47:LEU:O	3:C:51:MET:HG2	2.07	0.54
8:U:36:PHE:CD1	8:U:57:ARG:HB2	2.43	0.54
1:A:312:ILE:CG2	1:A:312:ILE:HD12	2.39	0.53
2:B:217:LYS:HG2	29:B:4225:HOH:O	2.06	0.53
13:M:39:ASN:O	13:M:43:SER:HB2	2.07	0.53
1:N:351:GLY:C	1:N:380:VAL:HG13	2.33	0.53
9:V:61:GLU:OE1	9:V:64:ARG:NE	2.41	0.53
1:A:343:GLY:O	1:A:347:LEU:HG	2.08	0.53
7:G:30:LEU:HD23	25:G:269:CDL:H471	1.90	0.53
7:T:6:GLY:O	24:T:263:PEK:H311	2.08	0.53
1:A:32:ALA:HB3	12:L:36:PRO:HG2	1.90	0.53
7:T:3:ALA:O	7:T:4:ALA:HB2	2.08	0.53
1:A:347:LEU:HD22	1:A:383:MET:SD	2.48	0.53
1:N:76:GLY:O	1:N:80:ASN:HB2	2.08	0.53
26:R:1229:PSC:H212	26:R:1229:PSC:O01	2.09	0.53
1:A:483:LEU:HD21	13:M:4:LYS:HD3	1.91	0.53
2:O:164:ALA:O	2:O:194:GLY:HA3	2.08	0.53
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.90	0.53
19:D:523:TGL:H363	9:I:16:ARG:HH21	1.74	0.53
2:B:164:ALA:O	2:B:194:GLY:HA3	2.07	0.53
7:G:78:LEU:HB3	7:G:79:PRO:HD2	1.91	0.53
2:O:141:ARG:HG3	9:V:70:GLN:NE2	2.24	0.53
20:N:1524:PGV:H311	13:Z:19:LEU:HD23	1.90	0.53
4:D:114:GLU:OE1	11:K:51:LYS:NZ	2.40	0.52
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.45	0.52
1:A:73:ILE:CD1	14:A:515:HEA:H22	2.39	0.52
13:Z:28:LEU:N	13:Z:29:PRO:CD	2.73	0.52
2:O:191:LEU:HG	9:V:68:ILE:HD12	1.91	0.52
5:R:25:ASP:OD1	5:R:28:GLU:HG3	2.09	0.52
1:A:208:MET:HE2	3:C:97:PHE:CD1	2.44	0.52
4:D:78:TRP:HA	19:D:523:TGL:CB2	2.39	0.52
9:V:18:ARG:HG3	29:V:3588:HOH:O	2.09	0.52
1:N:317:GLY:CA	14:N:516:HEA:H202	2.39	0.52
24:T:1264:PEK:H42	24:T:1264:PEK:H222	1.90	0.52
12:Y:22:LEU:O	12:Y:26:THR:HB	2.09	0.52
4:D:34:SER:H	4:D:37:GLN:NE2	2.01	0.52
7:G:12:GLY:HA3	29:G:4330:HOH:O	2.08	0.52
4:Q:33:LEU:O	4:Q:38:LYS:HE2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:38:HIS:N	7:T:38:HIS:ND1	2.55	0.52
1:A:62:ALA:HB2	14:A:515:HEA:HBD1	1.92	0.52
5:E:48:ILE:O	5:E:52:LEU:HG	2.10	0.52
1:A:481:GLU:HB2	13:M:4:LYS:HE2	1.90	0.51
1:A:304:TYR:HD1	25:T:1269:CDL:HB32	1.74	0.51
1:N:151:HIS:HD2	24:T:1264:PEK:H382	1.72	0.51
3:C:226:HIS:CE1	25:C:270:CDL:HB31	2.45	0.51
1:N:378:HIS:HA	1:N:382:SER:HB2	1.93	0.51
7:T:31:CYS:HG	25:T:1269:CDL:H532	1.75	0.51
2:B:58:ALA:O	2:B:62:GLU:HG3	2.11	0.51
2:O:83:ILE:O	2:O:87:MET:HG3	2.10	0.51
7:G:4:ALA:CB	1:N:282:PHE:HA	2.39	0.51
1:N:479:LYS:NZ	29:N:3383:HOH:O	2.44	0.51
25:C:270:CDL:H151	25:C:270:CDL:H311	1.93	0.51
25:T:1269:CDL:H171	29:T:4401:HOH:O	2.10	0.51
7:T:12:GLY:CA	29:T:3372:HOH:O	2.58	0.51
12:Y:35:ALA:O	12:Y:39:ILE:HG13	2.11	0.51
1:N:310:MET:HE1	2:O:76:ILE:CG2	2.40	0.50
20:A:524:PGV:H212	29:A:4691:HOH:O	2.12	0.50
7:T:8:HIS:O	7:T:9:GLY:C	2.54	0.50
7:T:30:LEU:CD1	25:T:1269:CDL:H261	2.40	0.50
4:D:98:TRP:CE3	28:M:526:DMU:H12	2.46	0.50
7:T:37:LEU:HB3	7:T:38:HIS:HD1	1.75	0.50
20:N:1524:PGV:H252	13:Z:12:PRO:HG3	1.93	0.50
2:O:134:ARG:HB2	4:Q:110:THR:HG21	1.92	0.50
7:T:5:LYS:HG3	24:T:263:PEK:C38	2.39	0.50
1:N:406:ASN:ND2	20:N:1524:PGV:H032	2.26	0.50
20:P:1267:PGV:H172	25:P:1270:CDL:H662	1.94	0.50
7:G:5:LYS:HD2	24:G:1263:PEK:H383	1.94	0.50
1:N:112:LEU:HD23	1:N:112:LEU:C	2.36	0.50
1:N:514:LYS:NZ	29:N:3645:HOH:O	2.45	0.50
3:P:59:ARG:HB2	25:P:1270:CDL:H512	1.93	0.50
3:C:213:THR:HG23	25:C:270:CDL:H771	1.94	0.50
10:J:33:ARG:HG2	22:J:60:CHD:H151	1.92	0.50
1:N:307:SER:O	1:N:311:ILE:HG13	2.12	0.50
1:A:25:TRP:CE3	19:L:522:TGL:HB91	2.47	0.49
6:S:1:ALA:H2	24:S:1265:PEK:C04	2.15	0.49
2:O:89:GLU:O	2:O:91:ASN:ND2	2.46	0.49
2:B:19:GLU:OE2	2:B:19:GLU:HA	2.12	0.49
4:D:78:TRP:CA	19:D:523:TGL:CB2	2.89	0.49
3:P:168:THR:HG22	24:S:1265:PEK:H14	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:38:HIS:NE2	25:T:1269:CDL:H131	2.28	0.49
19:A:521:TGL:H281	19:A:521:TGL:C10	2.43	0.49
2:B:57:ASP:H	26:E:229:PSC:H201	1.78	0.49
28:P:1272:DMU:H30	28:P:1272:DMU:C10	2.42	0.49
2:O:40:TYR:CE2	9:V:24:ALA:HB2	2.48	0.49
1:A:229:ILE:HD11	2:B:175:ILE:CD1	2.43	0.49
1:A:347:LEU:HD13	1:A:383:MET:SD	2.52	0.49
10:J:52:TRP:O	10:J:57:HIS:CE1	2.61	0.49
3:P:107:ALA:HB2	20:P:1268:PGV:H031	1.94	0.49
7:T:2:SER:O	24:T:263:PEK:H331	2.12	0.49
1:A:510:TYR:OH	1:A:512:ASN:ND2	2.44	0.49
7:G:63:GLY:H	28:G:272:DMU:H40	1.77	0.49
2:O:168:LEU:HD13	2:O:184:LEU:HG	1.95	0.49
2:B:66:THR:HG21	22:B:1085:CHD:H42	1.95	0.49
4:Q:34:SER:N	4:Q:37:GLN:HE21	2.11	0.49
2:O:57:ASP:N	26:R:1229:PSC:H202	2.27	0.48
2:O:41:ILE:O	2:O:42:ILE:C	2.56	0.48
13:Z:32:TRP:N	28:Z:1526:DMU:H1	2.28	0.48
2:O:113:TYR:HD1	8:U:58:ARG:NH2	2.11	0.48
2:O:130:PRO:HA	4:Q:115:TRP:CH2	2.49	0.48
3:P:165:ILE:HG12	24:S:1265:PEK:H102	1.96	0.48
7:T:11:TPO:HG22	7:T:16:TRP:HE1	1.79	0.48
19:A:521:TGL:H122	19:A:521:TGL:H283	1.95	0.48
1:N:189:MET:O	1:N:189:MET:HG3	2.13	0.48
3:P:207:HIS:HD2	3:P:241:TYR:OH	1.97	0.48
4:Q:101:HIS:CD2	4:Q:102:TYR:CD2	3.02	0.48
3:C:103:HIS:HA	20:C:268:PGV:H012	1.95	0.48
1:N:377:PHE:CD1	14:N:516:HEA:HAD1	2.49	0.48
5:R:63:SER:O	5:R:67:ILE:HG13	2.13	0.48
1:N:113:LEU:HD13	19:N:1522:TGL:H292	1.95	0.48
14:N:516:HEA:NA	15:N:520:CYN:C	2.76	0.48
7:T:72:ASN:H	7:T:76:ASN:ND2	2.07	0.48
3:C:159:MET:SD	3:C:159:MET:C	2.97	0.48
22:O:229:CHD:H12	22:O:229:CHD:H212	1.95	0.48
3:C:52:LEU:HD23	25:C:270:CDL:H362	1.96	0.48
3:C:64:GLU:HA	3:C:68:GLN:HE21	1.79	0.48
25:G:269:CDL:HB32	1:N:304:TYR:HD1	1.79	0.48
1:N:1:FME:HCN	1:N:4:ASN:H	1.79	0.48
12:Y:20:ARG:NH2	12:Y:24:MET:CG	2.66	0.48
8:H:60:TYR:CD1	8:H:60:TYR:C	2.92	0.47
6:S:87:THR:HG22	29:S:4655:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:353:LEU:HB3	2:O:31:VAL:HG13	1.96	0.47
3:P:129:VAL:N	3:P:130:PRO:CD	2.76	0.47
1:A:347:LEU:HD13	1:A:383:MET:CB	2.42	0.47
26:E:229:PSC:H212	26:E:229:PSC:C02	2.43	0.47
1:N:334:TRP:HB2	19:Q:1523:TGL:HG11	1.94	0.47
1:N:438:ARG:O	1:N:439:ARG:HB2	2.14	0.47
24:T:1264:PEK:H11	24:T:1264:PEK:C15	2.44	0.47
26:E:229:PSC:H21	29:I:4186:HOH:O	2.15	0.47
4:Q:40:LEU:HD11	4:Q:55:GLU:HB3	1.95	0.47
4:Q:109:HIS:HD2	29:Q:3122:HOH:O	1.97	0.47
19:Q:1523:TGL:HG12	19:Q:1523:TGL:CC2	2.43	0.47
8:H:45:ALA:C	8:H:47:GLY:H	2.21	0.47
1:N:53:ILE:CD1	12:Y:44:LEU:HD23	2.45	0.47
3:P:112:LEU:HD13	3:P:118:PRO:HG3	1.97	0.47
26:R:1229:PSC:H222	26:R:1229:PSC:H32	1.97	0.47
6:S:55:LYS:HA	6:S:74:LEU:O	2.13	0.47
7:T:30:LEU:HD12	25:T:1269:CDL:C26	2.45	0.47
12:Y:8:GLY:HA2	12:Y:11:ILE:HD11	1.95	0.47
1:A:328:HIS:CE1	9:I:17:LEU:HD22	2.49	0.47
2:B:57:ASP:H	26:E:229:PSC:C20	2.28	0.47
5:R:78:HIS:CD2	9:V:12:LEU:HD13	2.49	0.47
1:A:177:SER:H	1:A:180:GLN:NE2	2.13	0.47
2:B:16:ILE:HD13	2:B:16:ILE:HA	1.77	0.47
2:B:74:ILE:HG13	25:T:1269:CDL:H441	1.97	0.47
3:C:63:ARG:NE	25:C:270:CDL:HA22	2.21	0.47
7:G:3:ALA:O	7:G:4:ALA:CB	2.61	0.47
25:G:269:CDL:H541	25:G:269:CDL:H242	1.87	0.47
24:G:1263:PEK:H042	3:P:77:LYS:NZ	2.29	0.47
14:N:515:HEA:HBC1	14:N:515:HEA:HMC3	1.97	0.47
2:O:40:TYR:HE2	9:V:24:ALA:HB2	1.79	0.47
7:T:41:HIS:HB3	7:T:74:ARG:NH1	2.30	0.47
8:U:9:LYS:HB2	8:U:9:LYS:HE2	1.68	0.47
8:U:27:ARG:NH1	29:U:3431:HOH:O	2.46	0.47
19:N:1521:TGL:H111	19:N:1521:TGL:H281	1.96	0.47
19:L:522:TGL:H231	19:L:522:TGL:CA9	2.29	0.47
2:O:163:TRP:NE1	2:O:209:ILE:HG12	2.30	0.47
28:P:1272:DMU:H29	7:T:62:TRP:HB3	1.97	0.47
1:A:73:ILE:HD11	14:A:515:HEA:H22	1.97	0.46
25:C:270:CDL:H621	25:C:270:CDL:H652	1.33	0.46
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.96	0.46
11:X:54:ARG:NH2	11:X:54:ARG:CG	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.97	0.46
3:P:47:LEU:O	3:P:51:MET:HG2	2.15	0.46
28:P:1272:DMU:H34	7:T:63:GLY:N	2.24	0.46
12:Y:35:ALA:HB3	12:Y:36:PRO:HD3	1.98	0.46
1:A:41:LEU:HD21	1:A:440:TYR:O	2.15	0.46
4:Q:98:TRP:CD2	28:Z:1526:DMU:H10	2.49	0.46
26:R:1229:PSC:H343	26:R:1229:PSC:C13	2.45	0.46
19:A:521:TGL:H122	19:A:521:TGL:C30	2.45	0.46
2:O:42:ILE:HG21	19:Q:1523:TGL:C23	2.45	0.46
1:N:407:ASP:O	1:N:411:LYS:HG3	2.16	0.46
3:C:257:TYR:O	3:C:261:SER:HB3	2.16	0.46
3:P:25:LEU:O	3:P:29:SER:HB2	2.15	0.46
3:P:230:ASN:HB2	29:S:3400:HOH:O	2.16	0.46
1:A:225:GLY:HA3	3:C:112:LEU:HD21	1.98	0.46
20:A:524:PGV:H41	20:A:524:PGV:H232	1.98	0.46
1:N:115:SER:HB2	1:N:142:SER:O	2.14	0.46
1:A:431:LEU:HD21	1:A:450:TRP:HB2	1.97	0.46
6:F:1:ALA:H1	24:G:265:PEK:C04	2.24	0.46
28:G:272:DMU:H30	28:G:272:DMU:O1	2.16	0.46
2:O:98:LYS:HB2	2:O:109:GLU:HB2	1.98	0.46
7:T:45:PRO:HD2	29:T:3099:HOH:O	2.16	0.46
5:E:12:ASP:OD1	5:E:44:GLU:HG3	2.16	0.46
5:R:46:LYS:HG2	29:R:4450:HOH:O	2.15	0.46
1:N:178:GLN:HB2	29:N:3430:HOH:O	2.16	0.45
9:V:31:PHE:CD1	9:V:31:PHE:C	2.94	0.45
19:N:1522:TGL:HG11	12:Y:12:PRO:HG2	1.97	0.45
3:C:146:TRP:CE2	7:G:17:ARG:HG3	2.51	0.45
1:N:313:ALA:HB2	1:N:356:ILE:HD11	1.97	0.45
5:R:80:GLU:H	5:R:80:GLU:CD	2.24	0.45
7:T:7:ASP:O	7:T:9:GLY:N	2.47	0.45
1:A:177:SER:H	1:A:180:GLN:HE21	1.65	0.45
1:A:194:LEU:HD22	1:A:285:PHE:HE2	1.81	0.45
1:A:307:SER:O	1:A:311:ILE:HG13	2.17	0.45
29:A:4735:HOH:O	4:D:17:VAL:CG1	2.65	0.45
1:A:23:GLY:HA3	1:A:73:ILE:HG13	1.98	0.45
22:C:525:CHD:H112	22:C:525:CHD:H12A	1.69	0.45
2:O:116:LEU:CD1	2:O:226:MET:HG3	2.46	0.45
7:T:35:SER:C	7:T:37:LEU:H	2.25	0.45
24:T:1264:PEK:H71	24:T:1264:PEK:C3	2.40	0.45
8:U:23:GLN:HG3	29:U:4336:HOH:O	2.15	0.45
1:A:344:PHE:CD1	1:A:344:PHE:C	2.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:51:SER:HB2	6:F:91:LEU:HD11	1.98	0.45
1:N:53:ILE:HD12	12:Y:44:LEU:CD2	2.46	0.45
2:O:58:ALA:O	2:O:62:GLU:HG3	2.16	0.45
26:R:1229:PSC:H251	26:R:1229:PSC:H221	1.72	0.45
1:A:304:TYR:CD2	1:A:304:TYR:C	2.94	0.45
29:B:3446:HOH:O	7:T:17:ARG:HD2	2.16	0.45
9:V:25:PHE:CE2	9:V:29:LEU:HD22	2.51	0.45
12:Y:27:LEU:O	12:Y:31:SER:HB3	2.17	0.45
1:A:514:LYS:HE3	29:A:2645:HOH:O	2.17	0.45
19:D:523:TGL:H332	19:D:523:TGL:H172	1.76	0.45
7:G:1:ALA:HB2	20:P:1268:PGV:H321	1.98	0.45
1:N:127:THR:HB	1:N:129:TYR:CE2	2.51	0.45
1:N:352:GLY:N	1:N:380:VAL:HG13	2.32	0.45
22:P:1525:CHD:H112	22:P:1525:CHD:H12A	1.55	0.45
2:B:56:MET:HG2	26:E:229:PSC:H211	1.99	0.44
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.98	0.44
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.99	0.44
25:G:269:CDL:H182	25:G:269:CDL:H152	1.33	0.44
4:D:68:PHE:HA	4:D:71:MET:HE3	1.98	0.44
25:P:1270:CDL:H232	25:P:1270:CDL:H262	1.79	0.44
1:A:390:MET:O	1:A:394:VAL:HG22	2.17	0.44
2:B:102:HIS:O	2:B:104:TRP:HA	2.17	0.44
1:N:17:THR:OG1	19:N:1522:TGL:H281	2.18	0.44
1:N:482:VAL:HG22	13:Z:1:ILE:HD11	1.98	0.44
6:S:52:ILE:C	6:S:94:HIS:CE1	2.90	0.44
29:B:3446:HOH:O	7:T:17:ARG:CD	2.66	0.44
25:G:269:CDL:H181	25:G:269:CDL:C51	2.46	0.44
20:P:1267:PGV:H152	20:P:1267:PGV:H12	1.20	0.44
19:D:523:TGL:H132	19:D:523:TGL:H302	1.69	0.44
1:N:113:LEU:HD12	19:N:1522:TGL:C29	2.46	0.44
3:P:253:TYR:CE2	25:T:1269:CDL:H641	2.52	0.44
22:P:1271:CHD:H112	22:P:1271:CHD:H12A	1.52	0.44
9:V:36:LYS:O	9:V:41:GLU:CG	2.65	0.44
1:A:250:GLY:O	1:A:254:ILE:HG12	2.17	0.44
1:A:282:PHE:CA	7:T:4:ALA:HB3	2.45	0.44
3:C:63:ARG:HE	25:C:270:CDL:HA21	1.81	0.44
7:G:34:ASN:HB2	25:G:269:CDL:H162	2.00	0.44
2:O:1:FME:SD	2:O:133:LEU:HD11	2.57	0.44
25:P:1270:CDL:HB22	25:P:1270:CDL:OA5	2.17	0.44
6:S:92:VAL:O	6:S:92:VAL:HG23	2.18	0.44
1:A:265:LYS:HB2	1:A:490:THR:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:199:LEU:N	1:N:200:PRO:CD	2.81	0.44
1:N:483:LEU:HD23	1:N:483:LEU:HA	1.90	0.44
19:N:1522:TGL:HC32	19:N:1522:TGL:HC62	1.43	0.44
3:P:207:HIS:CD2	3:P:241:TYR:OH	2.71	0.44
3:P:224:LYS:CD	25:P:1270:CDL:HB31	2.44	0.44
2:B:40:TYR:CE2	9:I:24:ALA:HB2	2.53	0.43
25:C:270:CDL:H661	25:C:270:CDL:H241	1.97	0.43
5:E:11:PHE:CG	26:E:229:PSC:H073	2.53	0.43
3:P:154:GLY:HA2	6:S:6:VAL:HB	2.00	0.43
19:Q:1523:TGL:HB92	19:Q:1523:TGL:H122	1.76	0.43
8:U:50:VAL:C	8:U:52:VAL:N	2.74	0.43
4:D:48:TRP:HA	4:D:51:LEU:HD22	1.99	0.43
2:O:139:ASP:OD2	2:O:140:ASN:N	2.50	0.43
6:S:70:ILE:HG13	6:S:84:SER:HB3	2.00	0.43
1:A:28:MET:HE2	14:A:515:HEA:H271	2.00	0.43
2:O:41:ILE:O	2:O:45:MET:HG2	2.17	0.43
6:F:64:GLU:O	6:F:65:ASP:HB2	2.18	0.43
7:G:72:ASN:OD1	7:G:74:ARG:HB2	2.18	0.43
22:J:60:CHD:H112	22:J:60:CHD:H12A	1.81	0.43
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.53	0.43
3:P:118:PRO:HD2	3:P:121:ILE:HG13	2.01	0.43
3:P:156:ARG:HE	22:P:1271:CHD:C24	2.31	0.43
1:A:113:LEU:CD1	19:L:522:TGL:H292	2.49	0.43
1:A:113:LEU:HD12	19:L:522:TGL:H292	2.00	0.43
1:A:115:SER:HB2	1:A:142:SER:O	2.18	0.43
1:N:118:VAL:O	1:N:119:GLU:C	2.60	0.43
1:N:290:HIS:CD2	1:N:291:HIS:CD2	3.06	0.43
1:N:484:THR:HB	13:Z:2:THR:OG1	2.18	0.43
19:N:1522:TGL:HC22	19:N:1522:TGL:HC82	2.00	0.43
1:A:347:LEU:CD1	1:A:383:MET:HB3	2.45	0.43
25:C:270:CDL:PA1	25:C:270:CDL:CB2	3.07	0.43
7:G:76:ASN:HA	7:G:77:PRO:HD2	1.93	0.43
1:N:104:LEU:HB2	1:N:156:SER:HB2	2.00	0.43
2:O:113:TYR:HD1	8:U:58:ARG:HH22	1.67	0.43
5:R:105:GLY:O	5:R:108:LYS:HG3	2.18	0.43
1:A:334:TRP:HB2	19:D:523:TGL:HG11	2.00	0.43
29:A:4735:HOH:O	4:D:17:VAL:HG11	2.19	0.43
6:F:65:ASP:O	6:F:66:ASN:C	2.59	0.43
12:L:41:ARG:HG3	13:M:40:TYR:CE1	2.54	0.43
1:N:46:THR:O	1:N:46:THR:HG23	2.18	0.43
26:R:1229:PSC:H232	26:R:1229:PSC:H201	1.28	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:4:GLU:HB3	12:Y:9:LYS:HB3	2.01	0.43
1:A:307:SER:CB	25:T:1269:CDL:H182	2.49	0.43
9:I:31:PHE:O	9:I:32:ALA:C	2.59	0.43
12:L:11:ILE:CG2	19:L:522:TGL:H272	2.48	0.43
1:N:440:TYR:CZ	2:O:205:SER:HA	2.53	0.43
19:N:1521:TGL:H111	19:N:1521:TGL:H283	2.00	0.43
19:N:1522:TGL:H282	19:N:1522:TGL:H251	1.41	0.43
2:O:189:PRO:HD2	9:V:54:TYR:OH	2.18	0.43
2:O:226:MET:HG3	2:O:226:MET:O	2.19	0.43
4:Q:48:TRP:CH2	5:R:56:ARG:HA	2.54	0.43
13:Z:1:ILE:HG23	13:Z:1:ILE:O	2.19	0.43
6:F:55:LYS:HA	6:F:74:LEU:O	2.19	0.43
12:L:20:ARG:HH22	19:L:522:TGL:HC62	1.84	0.43
4:Q:101:HIS:CD2	4:Q:102:TYR:CE2	3.07	0.43
5:R:45:PRO:HD3	9:V:9:MET:HE1	2.00	0.43
19:D:523:TGL:HB62	19:D:523:TGL:HA52	2.01	0.42
1:N:362:SER:OG	2:O:87:MET:HE2	2.19	0.42
14:N:516:HEA:HMC1	14:N:516:HEA:HHC	1.80	0.42
25:T:1269:CDL:H221	25:T:1269:CDL:H252	1.65	0.42
1:A:352:GLY:N	1:A:380:VAL:HG13	2.33	0.42
1:N:71:MET:CE	1:N:195:LEU:HD21	2.49	0.42
3:C:156:ARG:HE	22:C:271:CHD:C24	2.33	0.42
1:N:328:HIS:HB2	2:O:45:MET:SD	2.58	0.42
6:S:25:ARG:HD3	29:S:4617:HOH:O	2.19	0.42
10:W:50:LEU:HD22	10:W:54:SER:OG	2.19	0.42
20:C:267:PGV:H152	20:C:267:PGV:H12	1.12	0.42
4:D:20:ARG:HG3	29:D:4124:HOH:O	2.19	0.42
2:O:59:GLN:CG	2:O:59:GLN:O	2.67	0.42
14:A:516:HEA:HAD2	14:A:516:HEA:HHA	1.72	0.42
2:B:33:LEU:HA	2:B:33:LEU:HD12	1.36	0.42
1:N:177:SER:H	1:N:180:GLN:HE21	1.67	0.42
3:P:137:LEU:HD23	3:P:137:LEU:HA	1.83	0.42
19:Q:1523:TGL:H302	19:Q:1523:TGL:H132	1.85	0.42
24:G:265:PEK:H312	2:O:66:THR:HG23	2.01	0.42
29:L:4496:HOH:O	13:M:32:TRP:HH2	2.02	0.42
2:O:24:HIS:O	2:O:25:ASP:C	2.62	0.42
2:O:102:HIS:O	2:O:104:TRP:HA	2.20	0.42
2:O:202:SER:HB2	2:O:203:ASN:ND2	2.15	0.42
9:V:73:LYS:HB3	9:V:73:LYS:HE3	1.74	0.42
2:B:62:GLU:O	2:B:66:THR:HB	2.20	0.42
14:N:515:HEA:HHC	14:N:515:HEA:H11	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:22:HIS:CE1	9:V:43:ARG:HG2	2.55	0.42
5:R:20:ASN:O	5:R:21:LYS:C	2.63	0.42
22:B:1085:CHD:H11	24:S:1265:PEK:H271	2.01	0.42
10:J:31:LEU:HD12	10:J:31:LEU:HA	1.89	0.42
1:N:513:LEU:HD23	1:N:513:LEU:HA	1.91	0.42
29:N:3132:HOH:O	3:P:112:LEU:CD2	2.67	0.42
3:P:146:TRP:CD2	3:P:162:ALA:HB2	2.55	0.42
5:R:99:SER:HB2	5:R:104:LEU:HD21	2.02	0.42
25:T:1269:CDL:H391	25:T:1269:CDL:H161	2.02	0.42
2:B:116:LEU:HD11	2:B:226:MET:HB3	2.00	0.42
1:N:112:LEU:HD23	1:N:112:LEU:O	2.20	0.42
1:N:409:TRP:HB3	1:N:471:ILE:HG12	2.01	0.42
9:V:64:ARG:O	9:V:65:LYS:C	2.61	0.42
2:B:151:ARG:HD3	2:B:181:GLN:HE21	1.85	0.41
24:G:265:PEK:C38	25:G:269:CDL:H273	2.49	0.41
1:N:431:LEU:HD21	1:N:450:TRP:HB2	2.01	0.41
2:O:132:GLU:HB3	2:O:137:GLU:HG3	2.01	0.41
2:O:202:SER:CB	2:O:203:ASN:HD22	2.18	0.41
3:P:58:TRP:CG	20:P:1267:PGV:H41	2.56	0.41
25:T:1269:CDL:OB4	25:T:1269:CDL:H1	2.20	0.41
10:W:32:TYR:OH	22:W:1059:CHD:H213	2.20	0.41
13:Z:31:GLY:C	28:Z:1526:DMU:H1	2.45	0.41
1:A:419:VAL:HG23	19:D:523:TGL:H121	2.01	0.41
4:D:16:TYR:OH	4:D:18:ASP:OD2	2.32	0.41
1:N:240:HIS:O	1:N:241:PRO:C	2.61	0.41
2:O:40:TYR:O	2:O:43:SER:N	2.54	0.41
3:P:138:LEU:HD12	25:T:1269:CDL:H591	2.02	0.41
3:P:220:PHE:HB2	25:P:1270:CDL:H712	2.00	0.41
24:T:263:PEK:H312	24:T:263:PEK:H282	1.93	0.41
2:B:1:FME:HB3	2:B:1:FME:HE2	1.82	0.41
2:B:146:MET:HA	2:B:213:LEU:HD12	2.01	0.41
22:B:1085:CHD:H112	22:B:1085:CHD:H12A	1.64	0.41
3:C:58:TRP:HB2	25:C:270:CDL:H552	2.02	0.41
7:G:3:ALA:CB	24:G:1263:PEK:H382	2.50	0.41
4:Q:48:TRP:O	4:Q:51:LEU:HB2	2.20	0.41
10:W:52:TRP:CE2	10:W:57:HIS:CE1	3.08	0.41
1:A:76:GLY:O	1:A:80:ASN:HB2	2.21	0.41
14:A:515:HEA:HBC1	14:A:515:HEA:HMC1	2.02	0.41
2:B:78:LEU:HD12	2:B:78:LEU:HA	1.75	0.41
2:B:145:PRO:HA	2:B:214:VAL:O	2.19	0.41
1:N:62:ALA:HB2	14:N:515:HEA:HBD1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:130:PRO:HA	4:Q:115:TRP:CZ3	2.55	0.41
2:O:227:LEU:HD23	2:O:227:LEU:HA	1.93	0.41
25:P:1270:CDL:HB21	25:P:1270:CDL:OB6	2.21	0.41
24:T:1264:PEK:C15	24:T:1264:PEK:C11	2.98	0.41
1:A:217:THR:HG22	3:C:188:ILE:HG12	2.02	0.41
6:F:92:VAL:HG23	6:F:92:VAL:O	2.20	0.41
1:N:23:GLY:HA3	1:N:73:ILE:HG13	2.03	0.41
2:O:128:LEU:HD11	2:O:134:ARG:HA	2.03	0.41
3:P:157:LYS:HZ2	24:S:1265:PEK:C05	2.28	0.41
5:R:24:ILE:O	5:R:24:ILE:HG23	2.20	0.41
6:F:1:ALA:HB3	6:S:65:ASP:OD1	2.21	0.41
24:G:1263:PEK:H15	3:P:248:VAL:HG22	2.03	0.41
1:N:321:PHE:CD1	2:O:65:TRP:HB2	2.55	0.41
5:R:8:ASP:HA	26:R:1229:PSC:H071	2.03	0.41
1:A:378:HIS:HA	1:A:382:SER:CB	2.50	0.41
19:A:521:TGL:H102	19:A:521:TGL:C28	2.48	0.41
1:N:376:HIS:O	1:N:380:VAL:HG22	2.20	0.41
2:O:40:TYR:O	2:O:43:SER:OG	2.33	0.41
1:A:71:MET:HB2	1:A:72:PRO:HD3	2.02	0.41
2:B:42:ILE:HD13	2:B:42:ILE:HG21	1.78	0.41
25:C:270:CDL:H532	25:C:270:CDL:H561	1.41	0.41
1:N:115:SER:O	1:N:121:GLY:HA2	2.21	0.41
6:S:94:HIS:CG	6:S:95:GLN:N	2.86	0.41
1:A:377:PHE:O	1:A:381:LEU:HB3	2.21	0.41
1:A:406:ASN:ND2	20:A:524:PGV:H032	2.36	0.41
25:G:269:CDL:HB32	1:N:304:TYR:CD1	2.56	0.41
19:N:1521:TGL:H281	19:N:1521:TGL:C11	2.51	0.41
19:N:1521:TGL:HC22	29:Q:3606:HOH:O	2.21	0.41
7:T:31:CYS:SG	25:T:1269:CDL:C53	2.95	0.41
8:U:46:LYS:HD2	29:U:4404:HOH:O	2.20	0.41
3:C:112:LEU:HD13	3:C:118:PRO:HG3	2.02	0.41
3:C:155:ASP:OD2	6:F:2:SER:HA	2.20	0.41
1:A:43:GLN:HB2	1:A:44:PRO:HD2	2.03	0.40
1:A:100:MET:HE1	20:A:522:PGV:H81	2.02	0.40
14:A:515:HEA:HHC	14:A:515:HEA:H11	1.86	0.40
19:A:521:TGL:HB91	19:A:521:TGL:HB61	1.46	0.40
3:C:25:LEU:O	3:C:29:SER:HB2	2.21	0.40
3:C:40:MET:O	3:C:44:MET:HG2	2.21	0.40
25:C:270:CDL:PA1	25:C:270:CDL:HB22	2.56	0.40
25:C:270:CDL:H201	25:C:270:CDL:C64	2.50	0.40
8:H:76:ARG:HD2	29:H:4210:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:68:PHE:HE2	1:N:112:LEU:CD1	2.34	0.40
1:N:444:PRO:HD3	2:O:195:GLN:HE22	1.86	0.40
3:P:116:TRP:HA	3:P:117:PRO:C	2.46	0.40
3:P:249:TRP:HD1	29:P:3165:HOH:O	2.04	0.40
20:A:524:PGV:H152	20:A:524:PGV:C32	2.51	0.40
10:J:16:ASN:OD1	10:J:23:LYS:HE3	2.21	0.40
1:N:417:MET:HE3	29:N:3166:HOH:O	2.21	0.40
26:R:1229:PSC:H212	26:R:1229:PSC:C01	2.51	0.40
3:C:98:PHE:CD2	24:T:263:PEK:H182	2.56	0.40
20:C:268:PGV:H11	20:C:268:PGV:H241	2.03	0.40
1:N:398:PRO:HA	1:N:403:TYR:O	2.21	0.40
3:P:8:TYR:CE1	3:P:74:ALA:HB1	2.55	0.40
26:R:1229:PSC:H343	26:R:1229:PSC:C14	2.51	0.40
22:C:271:CHD:H112	22:C:271:CHD:H12A	1.66	0.40
7:G:5:LYS:HD2	24:G:1263:PEK:C38	2.52	0.40
24:T:263:PEK:H241	24:T:263:PEK:H271	1.96	0.40
1:A:160:GLY:HA3	29:A:2648:HOH:O	2.22	0.40
2:B:5:MET:HE2	2:B:5:MET:HB3	1.92	0.40
3:C:110:PRO:HB3	8:H:30:TRP:CE3	2.57	0.40
19:N:1521:TGL:H131	19:N:1521:TGL:H302	1.78	0.40
3:P:22:LEU:HA	3:P:22:LEU:HD23	1.85	0.40

There are no symmetry-related clashes.

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	512/514 (100%)	495 (97%)	17 (3%)	0	100	100
1	N	512/514 (100%)	495 (97%)	16 (3%)	1 (0%)	43	37
2	B	225/227 (99%)	212 (94%)	11 (5%)	2 (1%)	14	7
2	O	225/227 (99%)	211 (94%)	12 (5%)	2 (1%)	14	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	257/261 (98%)	251 (98%)	6 (2%)	0	100	100
3	P	257/261 (98%)	251 (98%)	5 (2%)	1 (0%)	30	22
4	D	142/147 (97%)	137 (96%)	5 (4%)	0	100	100
4	Q	142/147 (97%)	137 (96%)	5 (4%)	0	100	100
5	E	103/109 (94%)	97 (94%)	6 (6%)	0	100	100
5	R	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
6	F	96/98 (98%)	91 (95%)	3 (3%)	2 (2%)	5	1
6	S	96/98 (98%)	89 (93%)	4 (4%)	3 (3%)	3	0
7	G	81/85 (95%)	66 (82%)	7 (9%)	8 (10%)	0	0
7	T	81/85 (95%)	67 (83%)	9 (11%)	5 (6%)	1	0
8	H	77/85 (91%)	67 (87%)	4 (5%)	6 (8%)	1	0
8	U	77/85 (91%)	70 (91%)	5 (6%)	2 (3%)	4	0
9	I	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
9	V	71/73 (97%)	66 (93%)	5 (7%)	0	100	100
10	J	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
10	W	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
11	K	47/56 (84%)	46 (98%)	0	1 (2%)	5	1
11	X	47/56 (84%)	44 (94%)	3 (6%)	0	100	100
12	L	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
12	Y	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
13	M	41/46 (89%)	41 (100%)	0	0	100	100
13	Z	41/46 (89%)	38 (93%)	3 (7%)	0	100	100
All	All	3504/3614 (97%)	3336 (95%)	135 (4%)	33 (1%)	14	7

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	60	GLU
6	F	95	GLN
7	G	4	ALA
7	G	7	ASP
7	G	8	HIS
7	G	40	GLY
8	H	8	ILE

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Mol	Chain	Res	Type
8	H	46	LYS
3	P	38	ASN
6	S	94	HIS
6	S	95	GLN
7	T	4	ALA
7	T	7	ASP
7	T	8	HIS
8	U	8	ILE
8	U	10	ASN
7	G	39	SER
8	H	10	ASN
8	H	11	TYR
8	H	45	ALA
7	T	3	ALA
6	F	94	HIS
7	G	6	GLY
2	O	60	GLU
6	S	96	LEU
2	B	33	LEU
7	G	3	ALA
7	G	37	LEU
2	O	92	ASN
1	N	382	SER
11	K	14	GLY
7	T	6	GLY
8	H	47	GLY

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	426/426 (100%)	414 (97%)	12 (3%)	38	34
1	N	426/426 (100%)	413 (97%)	13 (3%)	35	30
2	B	210/210 (100%)	201 (96%)	9 (4%)	26	20
2	O	210/210 (100%)	195 (93%)	15 (7%)	13	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	224/226 (99%)	218 (97%)	6 (3%)	39	36
3	P	224/226 (99%)	219 (98%)	5 (2%)	45	44
4	D	128/129 (99%)	124 (97%)	4 (3%)	35	30
4	Q	128/129 (99%)	123 (96%)	5 (4%)	28	23
5	E	92/95 (97%)	90 (98%)	2 (2%)	45	44
5	R	92/95 (97%)	84 (91%)	8 (9%)	9	4
6	F	81/81 (100%)	76 (94%)	5 (6%)	16	9
6	S	81/81 (100%)	73 (90%)	8 (10%)	7	3
7	G	67/68 (98%)	62 (92%)	5 (8%)	12	6
7	T	67/68 (98%)	57 (85%)	10 (15%)	3	0
8	H	71/75 (95%)	67 (94%)	4 (6%)	19	12
8	U	71/75 (95%)	67 (94%)	4 (6%)	19	12
9	I	57/57 (100%)	53 (93%)	4 (7%)	14	7
9	V	57/57 (100%)	53 (93%)	4 (7%)	14	7
10	J	49/50 (98%)	48 (98%)	1 (2%)	48	48
10	W	49/50 (98%)	47 (96%)	2 (4%)	27	21
11	K	39/46 (85%)	38 (97%)	1 (3%)	40	37
11	X	39/46 (85%)	37 (95%)	2 (5%)	21	14
12	L	39/40 (98%)	38 (97%)	1 (3%)	40	37
12	Y	39/40 (98%)	37 (95%)	2 (5%)	21	14
13	M	37/38 (97%)	31 (84%)	6 (16%)	2	0
13	Z	37/38 (97%)	33 (89%)	4 (11%)	6	2
All	All	3040/3082 (99%)	2898 (95%)	142 (5%)	23	17

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	LEU
1	A	138	HIS
1	A	178	GLN
1	A	180	GLN
1	A	264	LYS
1	A	297	MET
1	A	312	ILE

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Mol	Chain	Res	Type
1	A	333	LYS
1	A	369	ASP
1	A	380	VAL
1	A	504	THR
1	A	513	LEU
2	B	33	LEU
2	B	42	ILE
2	B	60	GLU
2	B	65	TRP
2	B	66	THR
2	B	75	LEU
2	B	78	LEU
2	B	86	MET
2	B	91	ASN
3	C	33	MET
3	C	73	PRO
3	C	77	LYS
3	C	127	LEU
3	C	159	MET
3	C	179	SER
4	D	4	SER
4	D	31	LYS
4	D	51	LEU
4	D	127	LYS
5	E	14	ARG
5	E	90	ARG
6	F	37	LYS
6	F	48	LEU
6	F	78	GLU
6	F	87	THR
6	F	95	GLN
7	G	17	ARG
7	G	33	LEU
7	G	43	GLU
7	G	74	ARG
7	G	84	LYS
8	H	7	LYS
8	H	8	ILE
8	H	9	LYS
8	H	60	TYR
9	I	8	GLN
9	I	15	ARG

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Mol	Chain	Res	Type
9	I	36	LYS
9	I	43	ARG
10	J	50	LEU
11	K	54	ARG
12	L	26	THR
13	M	4	LYS
13	M	34	LEU
13	M	38	ASP
13	M	39	ASN
13	M	42	LYS
13	M	43	SER
1	N	112	LEU
1	N	128	VAL
1	N	138	HIS
1	N	180	GLN
1	N	189	MET
1	N	264	LYS
1	N	278	MET
1	N	297	MET
1	N	306	THR
1	N	312	ILE
1	N	369	ASP
1	N	380	VAL
1	N	504	THR
2	O	16	ILE
2	O	33	LEU
2	O	60	GLU
2	O	75	LEU
2	O	78	LEU
2	O	86	MET
2	O	94	SER
2	O	113	TYR
2	O	148	MET
2	O	167	SER
2	O	202	SER
2	O	205	SER
2	O	209	ILE
2	O	217	LYS
2	O	221	LYS
3	P	29	SER
3	P	33	MET
3	P	127	LEU

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Mol	Chain	Res	Type
3	P	159	MET
3	P	230	ASN
4	Q	8	SER
4	Q	9	GLU
4	Q	31	LYS
4	Q	51	LEU
4	Q	147	LYS
5	R	5	HIS
5	R	45	PRO
5	R	46	LYS
5	R	79	LYS
5	R	80	GLU
5	R	90	ARG
5	R	101	PRO
5	R	108	LYS
6	S	37	LYS
6	S	43	LYS
6	S	48	LEU
6	S	53	THR
6	S	64	GLU
6	S	80	GLN
6	S	94	HIS
6	S	98	HIS
7	T	17	ARG
7	T	33	LEU
7	T	35	SER
7	T	36	TRP
7	T	37	LEU
7	T	38	HIS
7	T	43	GLU
7	T	61	SER
7	T	74	ARG
7	T	84	LYS
8	U	9	LYS
8	U	12	GLN
8	U	41	LYS
8	U	60	TYR
9	V	2	THR
9	V	8	GLN
9	V	18	ARG
9	V	44	LYS
10	W	36	MET

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Mol	Chain	Res	Type
10	W	50	LEU
11	X	47	ARG
11	X	54	ARG
12	Y	20	ARG
12	Y	26	THR
13	Z	13	LYS
13	Z	34	LEU
13	Z	38	ASP
13	Z	42	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	98	ASN
1	A	178	GLN
1	A	180	GLN
1	A	422	ASN
1	A	512	ASN
2	B	181	GLN
3	C	50	ASN
3	C	68	GLN
3	C	161	GLN
4	D	29	HIS
4	D	37	GLN
4	D	101	HIS
4	D	143	ASN
5	E	78	HIS
5	E	94	ASN
6	F	88	HIS
7	G	34	ASN
7	G	76	ASN
8	H	31	GLN
10	J	57	HIS
11	K	35	GLN
13	M	36	HIS
1	N	178	GLN
1	N	180	GLN
1	N	406	ASN
1	N	512	ASN
2	O	10	GLN
2	O	59	GLN

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Mol	Chain	Res	Type
2	O	91	ASN
2	O	195	GLN
2	O	203	ASN
3	P	50	ASN
3	P	68	GLN
3	P	70	HIS
3	P	76	GLN
3	P	149	HIS
3	P	161	GLN
3	P	207	HIS
4	Q	37	GLN
4	Q	101	HIS
4	Q	109	HIS
4	Q	119	GLN
4	Q	143	ASN
5	R	5	HIS
5	R	78	HIS
5	R	94	ASN
6	S	80	GLN
6	S	94	HIS
6	S	95	GLN
7	T	76	ASN
8	U	31	GLN
8	U	37	HIS
9	V	70	GLN
10	W	57	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$
1	FME	A	1	1	8,9,10	0.77	0	8,9,11	5.42	5 (62%)
1	FME	N	1	1	8,9,10	1.24	1 (12%)	8,9,11	5.31	4 (50%)
2	FME	O	1	2	8,9,10	1.00	0	8,9,11	5.80	3 (37%)
7	TPO	G	11	7	8,10,11	2.49	4 (50%)	10,14,16	1.88	3 (30%)
9	SAC	V	1	9	7,8,9	3.08	2 (28%)	7,9,11	1.97	2 (28%)
9	SAC	I	1	9	7,8,9	2.30	2 (28%)	7,9,11	1.29	1 (14%)
2	FME	B	1	2	8,9,10	1.67	1 (12%)	8,9,11	6.22	4 (50%)
7	TPO	T	11	7	8,10,11	2.32	5 (62%)	10,14,16	2.18	2 (20%)

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

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	1	SAC	OAC-C1A	5.58	1.35	1.23
9	V	1	SAC	CA-N	5.48	1.54	1.46
9	I	1	SAC	OAC-C1A	4.31	1.32	1.23
7	G	11	TPO	P-OG1	4.29	1.67	1.59
7	G	11	TPO	P-O1P	4.04	1.63	1.50
9	I	1	SAC	CA-N	4.03	1.52	1.46
7	T	11	TPO	P-O1P	3.61	1.61	1.50
2	B	1	FME	O1-CN	-3.17	1.09	1.22
7	T	11	TPO	P-OG1	3.06	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	1	FME	CA-N	2.77	1.50	1.46
7	T	11	TPO	P-O3P	2.55	1.64	1.54
7	G	11	TPO	P-O2P	2.40	1.63	1.54
7	T	11	TPO	P-O2P	2.08	1.62	1.54
7	G	11	TPO	P-O3P	2.05	1.62	1.54
7	T	11	TPO	O-C	2.01	1.27	1.20

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-16.27	97.80	122.82
2	O	1	FME	CA-N-CN	-15.72	98.64	122.82
1	A	1	FME	CA-N-CN	-14.12	101.11	122.82
1	N	1	FME	CA-N-CN	-13.38	102.24	122.82
7	T	11	TPO	CG2-CB-CA	5.82	124.59	113.26
1	N	1	FME	CB-CA-N	5.30	120.17	110.52
2	B	1	FME	CG-CB-CA	-4.23	99.92	112.87
2	B	1	FME	C-CA-N	4.22	117.64	109.50
7	G	11	TPO	O2P-P-OG1	3.94	121.22	105.85
1	A	1	FME	CG-CB-CA	-3.65	101.71	112.87
9	V	1	SAC	C-CA-N	3.57	116.39	109.50
1	A	1	FME	CE-SD-CG	3.11	116.44	100.32
2	O	1	FME	CB-CA-N	-3.06	104.95	110.52
9	I	1	SAC	C-CA-N	2.99	115.26	109.50
1	N	1	FME	O1-CN-N	2.95	132.93	125.32
2	O	1	FME	C-CA-N	2.71	114.72	109.50
7	G	11	TPO	CG2-CB-CA	2.52	118.17	113.26
1	A	1	FME	CB-CA-N	2.48	115.03	110.52
1	A	1	FME	O-C-CA	-2.31	118.82	124.77
7	T	11	TPO	O-C-CA	-2.22	119.05	124.77
2	B	1	FME	O-C-CA	-2.21	119.07	124.77
9	V	1	SAC	OAC-C1A-C2A	-2.18	118.18	122.05
7	G	11	TPO	O-C-CA	-2.08	119.42	124.77
1	N	1	FME	O-C-CA	-2.05	119.51	124.77

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O1-CN-N-CA
1	A	1	FME	N-CA-CB-CG
2	B	1	FME	O1-CN-N-CA

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

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	N	1	FME	1	0
2	O	1	FME	1	0
7	G	11	TPO	1	0
9	V	1	SAC	1	0
2	B	1	FME	1	0
7	T	11	TPO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 56 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - leaving 46 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$
14	HEA	N	516	15,1	67,67,67	2.26	24 (35%)	81,103,103	3.04	40 (49%)
19	TGL	L	522	-	62,62,62	1.64	8 (12%)	65,65,65	1.85	16 (24%)
14	HEA	A	516	15,1	67,67,67	2.55	27 (40%)	81,103,103	3.52	39 (48%)
24	PEK	G	265	-	52,52,52	1.22	4 (7%)	55,57,57	1.26	3 (5%)
20	PGV	A	524	-	50,50,50	1.20	2 (4%)	53,56,56	1.35	6 (11%)
19	TGL	A	521	-	62,62,62	1.51	7 (11%)	65,65,65	2.41	17 (26%)
24	PEK	T	1264	-	52,52,52	0.95	2 (3%)	55,57,57	1.77	9 (16%)
22	CHD	B	1085	-	32,32,32	1.56	6 (18%)	51,51,51	5.66	37 (72%)
22	CHD	P	1525	-	32,32,32	1.55	6 (18%)	51,51,51	5.14	43 (84%)
20	PGV	N	1266	-	50,50,50	0.94	1 (2%)	53,56,56	1.38	6 (11%)
14	HEA	N	515	1	67,67,67	1.87	16 (23%)	81,103,103	2.06	21 (25%)
21	CUA	O	228	2	0,1,1	-	-	-	-	-
24	PEK	C	264	-	52,52,52	0.91	2 (3%)	55,57,57	1.70	12 (21%)
24	PEK	G	1263	-	52,52,52	1.19	2 (3%)	55,57,57	1.19	6 (10%)
14	HEA	A	515	1	67,67,67	2.16	20 (29%)	81,103,103	1.93	17 (20%)
26	PSC	R	1229	-	51,51,51	1.23	3 (5%)	57,59,59	1.03	5 (8%)
28	DMU	P	1272	-	34,34,34	1.24	1 (2%)	45,45,45	3.24	23 (51%)
20	PGV	A	522	-	50,50,50	0.99	2 (4%)	53,56,56	1.30	6 (11%)
22	CHD	C	525	-	32,32,32	1.88	7 (21%)	51,51,51	5.40	34 (66%)
22	CHD	O	229	-	32,32,32	1.27	2 (6%)	51,51,51	5.56	35 (68%)
22	CHD	W	1059	-	32,32,32	1.16	2 (6%)	51,51,51	5.10	34 (66%)
21	CUA	B	228	2	0,1,1	-	-	-	-	-
19	TGL	Q	1523	-	62,62,62	1.42	6 (9%)	65,65,65	1.26	9 (13%)
25	CDL	T	1269	-	99,99,99	1.47	12 (12%)	105,111,111	1.43	17 (16%)
20	PGV	C	268	-	50,50,50	1.31	3 (6%)	53,56,56	1.48	6 (11%)
22	CHD	C	271	-	32,32,32	0.96	2 (6%)	51,51,51	5.05	35 (68%)
26	PSC	E	229	-	51,51,51	1.29	3 (5%)	57,59,59	1.37	7 (12%)
19	TGL	D	523	-	62,62,62	1.66	7 (11%)	65,65,65	1.53	12 (18%)
28	DMU	Z	1526	-	34,34,34	0.96	2 (5%)	45,45,45	3.19	21 (46%)
28	DMU	G	272	-	34,34,34	1.29	4 (11%)	45,45,45	3.30	23 (51%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CDL	C	270	-	99,99,99	1.46	12 (12%)	105,111,111	1.44	15 (14%)
20	PGV	C	267	-	50,50,50	0.90	3 (6%)	53,56,56	1.37	5 (9%)
24	PEK	T	263	-	52,52,52	1.23	2 (3%)	55,57,57	1.19	5 (9%)
22	CHD	J	60	-	32,32,32	0.81	0	51,51,51	4.87	39 (76%)
20	PGV	P	1268	-	50,50,50	1.29	3 (6%)	53,56,56	1.53	7 (13%)
20	PGV	P	1267	-	50,50,50	0.87	2 (4%)	53,56,56	1.43	9 (16%)
25	CDL	P	1270	-	99,99,99	1.47	12 (12%)	105,111,111	1.40	14 (13%)
22	CHD	P	1271	-	32,32,32	0.82	1 (3%)	51,51,51	4.86	37 (72%)
24	PEK	S	1265	-	52,52,52	1.35	3 (5%)	55,57,57	1.32	5 (9%)
20	PGV	N	1524	-	50,50,50	1.23	2 (4%)	53,56,56	1.29	6 (11%)
28	DMU	M	526	-	34,34,34	0.84	1 (2%)	45,45,45	3.46	26 (57%)
15	CYN	A	520	16,14	1,1,1	0.25	0	-	-	-
19	TGL	N	1522	-	62,62,62	1.64	7 (11%)	65,65,65	1.63	15 (23%)
15	CYN	N	520	16,14	1,1,1	0.25	0	-	-	-
19	TGL	N	1521	-	62,62,62	1.39	6 (9%)	65,65,65	1.50	12 (18%)
25	CDL	G	269	-	99,99,99	1.58	14 (14%)	105,111,111	1.52	17 (16%)

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
14	HEA	N	516	15,1	-	12/36/76/76	-
19	TGL	L	522	-	-	35/65/65/65	-
14	HEA	A	516	15,1	-	8/36/76/76	-
24	PEK	G	265	-	-	26/56/56/56	-
20	PGV	A	524	-	-	32/55/55/55	-
19	TGL	A	521	-	-	35/65/65/65	-
24	PEK	T	1264	-	-	22/56/56/56	-
22	CHD	B	1085	-	-	2/9/74/74	0/4/4/4
22	CHD	P	1525	-	-	2/9/74/74	0/4/4/4
20	PGV	N	1266	-	-	13/55/55/55	-
14	HEA	N	515	1	-	8/36/76/76	-
24	PEK	C	264	-	-	21/56/56/56	-
24	PEK	G	1263	-	-	27/56/56/56	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	HEA	A	515	1	-	6/36/76/76	-
26	PSC	R	1229	-	-	39/55/55/55	-
28	DMU	P	1272	-	6/6/10/10	10/19/59/59	0/2/2/2
20	PGV	A	522	-	-	14/55/55/55	-
22	CHD	C	525	-	-	2/9/74/74	0/4/4/4
22	CHD	O	229	-	-	2/9/74/74	0/4/4/4
22	CHD	W	1059	-	2/2/12/12	7/9/74/74	0/4/4/4
19	TGL	Q	1523	-	-	36/65/65/65	-
25	CDL	T	1269	-	-	64/110/110/110	-
20	PGV	C	268	-	-	32/55/55/55	-
22	CHD	C	271	-	1/1/12/12	4/9/74/74	0/4/4/4
26	PSC	E	229	-	-	34/55/55/55	-
19	TGL	D	523	-	-	37/65/65/65	-
28	DMU	Z	1526	-	5/5/10/10	9/19/59/59	0/2/2/2
28	DMU	G	272	-	6/6/10/10	12/19/59/59	0/2/2/2
25	CDL	C	270	-	-	73/110/110/110	-
20	PGV	C	267	-	-	14/55/55/55	-
24	PEK	T	263	-	-	32/56/56/56	-
22	CHD	J	60	-	2/2/12/12	6/9/74/74	0/4/4/4
20	PGV	P	1268	-	-	28/55/55/55	-
20	PGV	P	1267	-	-	14/55/55/55	-
25	CDL	P	1270	-	-	68/110/110/110	-
22	CHD	P	1271	-	1/1/12/12	7/9/74/74	0/4/4/4
28	DMU	M	526	-	4/4/10/10	10/19/59/59	0/2/2/2
20	PGV	N	1524	-	-	35/55/55/55	-
24	PEK	S	1265	-	-	24/56/56/56	-
19	TGL	N	1522	-	-	39/65/65/65	-
19	TGL	N	1521	-	-	42/65/65/65	-
25	CDL	G	269	-	-	63/110/110/110	-

All (251) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	516	HEA	O11-C11	9.70	1.64	1.42
14	A	516	HEA	C11-C3B	7.86	1.61	1.51
14	N	516	HEA	O11-C11	7.34	1.59	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	N	1522	TGL	OG2-CB1	6.84	1.53	1.34
14	A	515	HEA	FE-NA	6.45	2.16	1.95
19	L	522	TGL	OG2-CB1	6.41	1.52	1.34
20	P	1268	PGV	O01-C1	6.26	1.52	1.34
20	C	268	PGV	O01-C1	6.09	1.51	1.34
24	S	1265	PEK	O03-C21	5.82	1.50	1.33
19	D	523	TGL	OG1-CA1	5.73	1.50	1.33
24	T	263	PEK	O03-C21	5.66	1.49	1.33
19	A	521	TGL	OG1-CA1	5.52	1.49	1.33
20	A	524	PGV	O03-C19	5.48	1.49	1.33
14	A	515	HEA	CHA-C1A	5.48	1.49	1.38
25	G	269	CDL	OB6-CB5	5.47	1.49	1.34
14	A	516	HEA	CHB-C4A	5.47	1.49	1.38
19	L	522	TGL	OG1-CA1	5.43	1.49	1.33
20	N	1524	PGV	O03-C19	5.42	1.49	1.33
19	D	523	TGL	OG2-CB1	5.34	1.49	1.34
25	G	269	CDL	OA8-CA7	5.34	1.48	1.33
25	P	1270	CDL	OA8-CA7	5.33	1.48	1.33
25	C	270	CDL	OA8-CA7	5.32	1.48	1.33
14	N	516	HEA	FE-NC	5.29	2.12	1.95
19	D	523	TGL	OB1-CB1	5.29	1.38	1.22
19	N	1522	TGL	OG3-CC1	5.25	1.48	1.33
19	N	1522	TGL	OG1-CA1	5.24	1.48	1.33
25	G	269	CDL	OA6-CA5	5.22	1.49	1.34
19	N	1521	TGL	OG2-CB1	5.22	1.49	1.34
14	N	515	HEA	C3A-C4A	-5.22	1.36	1.46
24	G	265	PEK	O03-C21	5.18	1.48	1.33
14	N	516	HEA	C11-C3B	5.13	1.57	1.51
25	T	1269	CDL	OB6-CB5	5.12	1.48	1.34
24	G	1263	PEK	O03-C21	5.07	1.48	1.33
19	Q	1523	TGL	OG1-CA1	5.06	1.48	1.33
22	C	525	CHD	C13-C12	-5.01	1.46	1.54
14	A	515	HEA	FE-NC	5.01	2.11	1.95
24	S	1265	PEK	O01-C1	4.97	1.48	1.34
24	G	265	PEK	O01-C1	4.95	1.48	1.34
24	T	263	PEK	O01-C1	4.95	1.48	1.34
14	N	516	HEA	C4D-C3D	-4.95	1.36	1.45
26	E	229	PSC	O01-C1	4.95	1.48	1.34
28	P	1272	DMU	O16-C6	4.93	1.48	1.40
20	C	268	PGV	O03-C19	4.91	1.47	1.33
22	C	525	CHD	C1-C10	-4.88	1.45	1.54
28	G	272	DMU	O16-C6	4.86	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Q	1523	TGL	OG3-CC1	4.85	1.47	1.33
25	T	1269	CDL	OA6-CA5	4.83	1.47	1.34
26	E	229	PSC	O03-C19	4.79	1.47	1.33
19	A	521	TGL	OG3-CC1	4.77	1.47	1.33
19	Q	1523	TGL	OG2-CB1	4.75	1.47	1.34
25	G	269	CDL	OB8-CB7	4.71	1.47	1.33
25	P	1270	CDL	OB6-CB5	4.70	1.47	1.34
19	N	1521	TGL	OG1-CA1	4.70	1.47	1.33
14	A	516	HEA	CHB-C1B	4.67	1.49	1.39
20	N	1266	PGV	O03-C19	4.65	1.46	1.33
24	G	1263	PEK	O01-C1	4.63	1.47	1.34
26	R	1229	PSC	O01-C1	4.62	1.47	1.34
25	T	1269	CDL	OB8-CB7	4.58	1.46	1.33
19	L	522	TGL	OG3-CC1	4.57	1.46	1.33
20	P	1268	PGV	O03-C19	4.57	1.46	1.33
14	N	515	HEA	FE-NC	4.53	2.10	1.95
14	A	516	HEA	FE-ND	-4.52	1.81	1.94
19	A	521	TGL	OG2-CB1	4.52	1.47	1.34
20	N	1524	PGV	O01-C1	4.50	1.47	1.34
14	A	515	HEA	CHD-C1D	4.49	1.47	1.38
25	C	270	CDL	OA6-CA5	4.47	1.46	1.34
19	N	1521	TGL	OG3-CC1	4.34	1.46	1.33
25	C	270	CDL	OB8-CB7	4.31	1.45	1.33
19	D	523	TGL	OG3-CC1	4.29	1.45	1.33
20	A	524	PGV	O01-C1	4.29	1.46	1.34
25	P	1270	CDL	OB8-CB7	4.25	1.45	1.33
26	R	1229	PSC	O03-C19	4.21	1.45	1.33
14	A	516	HEA	C4D-C3D	-4.17	1.38	1.45
25	T	1269	CDL	C59-C58	-4.16	1.31	1.51
14	A	516	HEA	FE-NA	4.14	2.08	1.95
25	P	1270	CDL	OA6-CA5	4.13	1.46	1.34
14	A	515	HEA	C3A-C4A	-4.12	1.38	1.46
26	R	1229	PSC	C13-C12	4.01	1.54	1.31
25	P	1270	CDL	C59-C58	-3.97	1.32	1.51
26	E	229	PSC	C13-C12	3.95	1.54	1.31
20	A	522	PGV	O03-C19	3.95	1.44	1.33
19	L	522	TGL	C20-CA9	-3.92	1.32	1.51
19	L	522	TGL	C10-CB9	-3.91	1.32	1.51
25	G	269	CDL	C59-C58	-3.90	1.32	1.51
14	A	515	HEA	C1D-ND	-3.89	1.33	1.40
25	C	270	CDL	OB6-CB5	3.85	1.45	1.34
14	N	516	HEA	FE-NB	-3.80	1.83	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	515	HEA	FE-ND	3.79	2.06	1.94
14	A	516	HEA	C4A-NA	-3.78	1.32	1.39
25	T	1269	CDL	C42-C41	-3.77	1.33	1.51
19	N	1522	TGL	C10-CB9	-3.76	1.33	1.51
25	T	1269	CDL	OA8-CA7	3.75	1.44	1.33
25	C	270	CDL	C62-C61	-3.75	1.33	1.51
14	N	515	HEA	CHD-C1D	3.71	1.45	1.38
22	O	229	CHD	C11-C9	3.71	1.59	1.53
25	T	1269	CDL	C62-C61	-3.68	1.33	1.51
25	C	270	CDL	C59-C58	-3.66	1.33	1.51
25	P	1270	CDL	C62-C61	-3.65	1.33	1.51
19	N	1522	TGL	C20-CA9	-3.63	1.33	1.51
14	N	515	HEA	C3B-C2B	3.61	1.43	1.34
14	N	516	HEA	C1C-NC	-3.59	1.32	1.39
19	A	521	TGL	OC1-CC1	-3.57	1.11	1.22
25	G	269	CDL	C42-C41	-3.55	1.34	1.51
14	N	515	HEA	CHC-C4B	3.53	1.45	1.38
14	A	515	HEA	CHC-C1C	3.52	1.47	1.39
14	N	516	HEA	CHD-C1D	3.52	1.45	1.38
25	P	1270	CDL	C19-C18	-3.51	1.34	1.51
19	A	521	TGL	C10-CB9	-3.50	1.34	1.51
19	N	1521	TGL	C10-CB9	-3.49	1.34	1.51
14	N	516	HEA	C3B-C2B	3.49	1.42	1.34
22	B	1085	CHD	C10-C5	-3.48	1.50	1.55
19	D	523	TGL	C15-CC9	-3.47	1.34	1.51
19	A	521	TGL	C20-CA9	-3.47	1.34	1.51
14	A	516	HEA	FE-NC	3.46	2.06	1.95
22	B	1085	CHD	C13-C14	-3.45	1.49	1.55
19	Q	1523	TGL	C20-CA9	-3.45	1.34	1.51
25	C	270	CDL	C19-C18	-3.45	1.34	1.51
25	G	269	CDL	C22-C21	-3.45	1.34	1.51
25	G	269	CDL	C62-C61	-3.44	1.34	1.51
14	N	516	HEA	C1D-C2D	-3.43	1.37	1.44
25	C	270	CDL	C79-C78	-3.42	1.34	1.51
14	A	516	HEA	C4B-C3B	-3.40	1.38	1.44
25	P	1270	CDL	C79-C78	-3.38	1.35	1.51
14	N	516	HEA	C1A-C2A	-3.37	1.39	1.45
25	T	1269	CDL	C22-C21	-3.37	1.35	1.51
25	T	1269	CDL	C79-C78	-3.36	1.35	1.51
24	T	1264	PEK	O01-C1	3.34	1.43	1.34
25	P	1270	CDL	C22-C21	-3.33	1.35	1.51
22	C	525	CHD	O12-C12	3.33	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	270	CDL	C22-C21	-3.33	1.35	1.51
25	C	270	CDL	C39-C38	-3.32	1.35	1.51
22	W	1059	CHD	C11-C9	3.32	1.59	1.53
25	C	270	CDL	C82-C81	-3.32	1.35	1.51
25	T	1269	CDL	C19-C18	-3.30	1.35	1.51
25	G	269	CDL	C39-C38	-3.29	1.35	1.51
14	A	515	HEA	O11-C11	3.29	1.50	1.42
19	Q	1523	TGL	C15-CC9	-3.28	1.35	1.51
25	P	1270	CDL	C82-C81	-3.28	1.35	1.51
19	Q	1523	TGL	C10-CB9	-3.28	1.35	1.51
22	P	1525	CHD	C16-C17	3.27	1.61	1.54
25	T	1269	CDL	C39-C38	-3.26	1.35	1.51
19	N	1521	TGL	C20-CA9	-3.24	1.35	1.51
14	A	515	HEA	C12-C13	3.18	1.63	1.53
14	N	515	HEA	CHA-C1A	3.18	1.44	1.38
14	A	515	HEA	CHB-C1B	3.15	1.46	1.39
14	N	515	HEA	C4B-C3B	-3.14	1.39	1.44
25	G	269	CDL	C19-C18	-3.14	1.36	1.51
14	A	515	HEA	CHB-C4A	3.13	1.44	1.38
25	P	1270	CDL	C39-C38	-3.13	1.36	1.51
19	L	522	TGL	C15-CC9	-3.13	1.36	1.51
14	A	516	HEA	CHA-C1A	3.09	1.44	1.38
19	D	523	TGL	C20-CA9	-3.07	1.36	1.51
25	C	270	CDL	C42-C41	-3.05	1.36	1.51
25	T	1269	CDL	C82-C81	-3.05	1.36	1.51
19	N	1521	TGL	C15-CC9	-3.05	1.36	1.51
20	C	267	PGV	O03-C19	3.05	1.42	1.33
19	N	1522	TGL	C15-CC9	-3.05	1.36	1.51
14	A	515	HEA	C1C-NC	-3.04	1.33	1.39
14	N	515	HEA	C1A-NA	-3.03	1.33	1.39
22	C	271	CHD	C20-C17	3.03	1.59	1.54
14	N	516	HEA	CHB-C4A	3.02	1.44	1.38
14	N	516	HEA	C4C-NC	-3.00	1.34	1.39
25	G	269	CDL	C17-C16	2.99	1.66	1.51
22	W	1059	CHD	C20-C17	2.98	1.59	1.54
25	P	1270	CDL	C42-C41	-2.98	1.37	1.51
25	G	269	CDL	C79-C78	-2.97	1.37	1.51
14	A	515	HEA	FE-ND	2.96	2.04	1.94
20	P	1267	PGV	O03-C19	2.95	1.42	1.33
25	G	269	CDL	C82-C81	-2.95	1.37	1.51
28	Z	1526	DMU	C3-C4	-2.94	1.44	1.52
14	A	516	HEA	C4C-NC	-2.91	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	515	HEA	CMB-C2B	2.90	1.56	1.50
19	D	523	TGL	C10-CB9	-2.90	1.37	1.51
22	B	1085	CHD	C4-C3	2.87	1.57	1.52
24	T	1264	PEK	O03-C01	-2.86	1.38	1.45
19	A	521	TGL	C15-CC9	-2.84	1.37	1.51
22	B	1085	CHD	C19-C10	2.84	1.59	1.54
14	A	516	HEA	C1B-NB	-2.82	1.33	1.38
22	O	229	CHD	C10-C5	-2.82	1.51	1.55
22	P	1525	CHD	O26-C24	-2.80	1.21	1.30
20	C	267	PGV	O01-C1	2.79	1.42	1.34
14	A	516	HEA	C1D-C2D	-2.73	1.39	1.44
14	A	516	HEA	C1A-NA	-2.72	1.34	1.39
14	N	516	HEA	C12-C11	2.72	1.57	1.53
14	N	515	HEA	FE-NA	2.71	2.04	1.95
14	N	515	HEA	CMB-C2B	2.69	1.56	1.50
24	C	264	PEK	O01-C1	2.69	1.41	1.34
14	N	516	HEA	C4B-C3B	-2.67	1.40	1.44
14	A	516	HEA	CMD-C2D	2.65	1.56	1.50
22	C	525	CHD	C19-C10	2.64	1.58	1.54
14	A	515	HEA	CMC-C2C	2.61	1.56	1.50
14	N	515	HEA	CHB-C4A	2.60	1.43	1.38
14	N	516	HEA	FE-ND	-2.57	1.87	1.94
24	S	1265	PEK	P-O11	2.56	1.69	1.59
22	P	1525	CHD	O12-C12	2.55	1.47	1.43
14	N	516	HEA	CMD-C2D	2.55	1.56	1.50
14	A	516	HEA	FE-NB	-2.54	1.87	1.94
24	C	264	PEK	O03-C21	2.50	1.40	1.33
14	N	516	HEA	C4A-NA	-2.48	1.34	1.39
14	A	516	HEA	CMB-C2B	2.47	1.55	1.50
28	M	526	DMU	C3-C4	-2.47	1.46	1.52
14	N	516	HEA	CMB-C2B	2.45	1.55	1.50
14	N	516	HEA	CHA-C1A	2.45	1.43	1.38
22	P	1525	CHD	C10-C5	-2.44	1.51	1.55
22	C	271	CHD	O26-C24	-2.43	1.22	1.30
22	C	525	CHD	C11-C12	2.42	1.57	1.53
14	A	516	HEA	C18-C19	2.39	1.38	1.33
14	A	515	HEA	C1A-NA	-2.38	1.35	1.39
14	A	515	HEA	CHD-C4C	2.38	1.44	1.39
22	B	1085	CHD	C18-C13	2.36	1.58	1.54
28	Z	1526	DMU	O16-C6	2.35	1.44	1.40
14	N	515	HEA	C4A-NA	-2.35	1.35	1.39
25	G	269	CDL	C16-C15	2.33	1.63	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	516	HEA	C3C-C2C	-2.30	1.33	1.41
14	N	515	HEA	C1D-ND	-2.26	1.36	1.40
14	A	516	HEA	CHC-C4B	2.26	1.43	1.38
22	C	525	CHD	C21-C20	2.25	1.58	1.53
14	N	515	HEA	CHD-C4C	2.25	1.44	1.39
14	N	516	HEA	CMC-C2C	2.25	1.55	1.50
20	A	522	PGV	O06-C06	2.25	1.51	1.42
24	G	265	PEK	P-O12	2.25	1.68	1.59
14	N	516	HEA	O1D-CGD	2.23	1.29	1.22
14	N	516	HEA	C18-C19	2.20	1.38	1.33
20	P	1267	PGV	O01-C1	2.20	1.40	1.34
22	C	525	CHD	O25-C24	2.17	1.29	1.22
14	A	516	HEA	CHD-C1D	2.16	1.42	1.38
14	N	516	HEA	CHC-C4B	2.16	1.42	1.38
20	C	268	PGV	P-O11	2.15	1.67	1.59
22	P	1525	CHD	C21-C20	2.15	1.58	1.53
14	A	515	HEA	C4D-ND	-2.14	1.34	1.38
28	G	272	DMU	C3-C4	-2.14	1.47	1.52
14	A	515	HEA	C22-C23	2.13	1.38	1.32
14	N	516	HEA	FE-NA	2.13	2.02	1.95
19	N	1522	TGL	CG3-CG2	2.13	1.57	1.50
20	C	267	PGV	C03-C02	2.10	1.57	1.50
22	B	1085	CHD	C1-C10	-2.09	1.50	1.54
14	A	516	HEA	C20-C19	2.09	1.55	1.51
14	A	516	HEA	CAA-C2A	2.08	1.56	1.51
28	G	272	DMU	O5-C6	2.08	1.47	1.41
14	A	516	HEA	C3A-C2A	2.08	1.41	1.37
20	P	1268	PGV	P-O11	2.08	1.67	1.59
14	A	516	HEA	C3D-C2D	2.07	1.41	1.36
14	N	515	HEA	C1A-C2A	-2.06	1.41	1.45
14	A	515	HEA	C4B-C3B	-2.03	1.41	1.44
19	L	522	TGL	CG3-CG2	2.02	1.57	1.50
22	P	1525	CHD	C11-C9	2.02	1.57	1.53
22	P	1271	CHD	C20-C17	2.02	1.57	1.54
28	G	272	DMU	O1-C10	2.01	1.47	1.41
14	A	516	HEA	C1C-NC	-2.01	1.35	1.39
24	G	265	PEK	P-O11	2.01	1.67	1.59
19	L	522	TGL	CG1-CG2	2.01	1.57	1.50

All (751) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1085	CHD	C18-C13-C12	-16.72	92.32	109.06
22	P	1271	CHD	C10-C9-C8	13.71	127.12	111.84
22	C	271	CHD	C10-C9-C8	13.17	126.52	111.84
22	B	1085	CHD	C1-C10-C5	12.87	126.22	107.75
22	C	525	CHD	C1-C10-C5	12.75	126.05	107.75
22	C	525	CHD	C6-C5-C10	12.66	126.13	112.66
22	B	1085	CHD	C6-C5-C10	12.28	125.73	112.66
22	P	1525	CHD	C14-C13-C12	12.27	118.63	107.42
22	O	229	CHD	C18-C13-C12	-12.26	96.78	109.06
22	O	229	CHD	C1-C10-C5	12.20	125.26	107.75
22	O	229	CHD	C14-C13-C12	12.00	118.38	107.42
22	B	1085	CHD	C17-C13-C12	11.16	127.71	117.67
22	C	525	CHD	C19-C10-C9	-10.96	96.45	111.18
22	P	1525	CHD	C1-C10-C5	10.87	123.35	107.75
22	W	1059	CHD	C10-C9-C8	10.71	123.78	111.84
22	O	229	CHD	C6-C5-C10	10.55	123.89	112.66
22	J	60	CHD	C10-C9-C8	10.43	123.46	111.84
22	C	525	CHD	C17-C13-C12	10.17	126.82	117.67
14	A	516	HEA	C3B-C4B-NB	9.98	121.31	109.84
22	W	1059	CHD	C13-C17-C20	9.97	131.56	119.48
22	B	1085	CHD	C14-C13-C12	9.96	116.52	107.42
22	O	229	CHD	C10-C9-C8	9.69	122.64	111.84
22	P	1525	CHD	C6-C5-C10	9.68	122.96	112.66
22	O	229	CHD	C19-C10-C9	-9.62	98.24	111.18
22	B	1085	CHD	C10-C9-C8	9.62	122.56	111.84
22	W	1059	CHD	C16-C17-C13	9.57	112.83	103.54
22	O	229	CHD	C5-C4-C3	9.46	126.98	112.71
22	C	525	CHD	C4-C3-C2	9.19	121.83	110.62
19	A	521	TGL	CG2-OG2-CB1	8.91	139.12	117.80
22	W	1059	CHD	C14-C8-C7	8.72	123.42	111.85
22	C	271	CHD	C15-C14-C8	8.69	130.27	118.36
22	P	1525	CHD	C18-C13-C12	-8.67	100.38	109.06
22	J	60	CHD	C14-C13-C12	8.65	115.33	107.42
22	C	271	CHD	C16-C17-C20	8.63	125.23	112.18
22	P	1525	CHD	C10-C9-C8	8.58	121.40	111.84
22	C	525	CHD	C10-C9-C8	8.52	121.33	111.84
22	C	271	CHD	C18-C13-C12	-8.44	100.61	109.06
14	A	516	HEA	C1D-ND-C4D	-8.40	95.26	105.21
22	C	271	CHD	C6-C5-C10	8.33	121.53	112.66
24	T	1264	PEK	C2-C3-C4	8.32	131.53	113.35
28	M	526	DMU	O1-C9-C8	8.32	124.69	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	J	60	CHD	C17-C13-C12	8.30	125.14	117.67
14	A	516	HEA	C2D-C1D-ND	8.27	119.34	109.84
22	O	229	CHD	C17-C13-C12	8.22	125.06	117.67
22	P	1271	CHD	C6-C5-C10	8.16	121.34	112.66
22	P	1525	CHD	C17-C13-C12	8.15	125.00	117.67
22	P	1525	CHD	C15-C14-C13	8.15	111.44	103.54
22	O	229	CHD	O12-C12-C13	-8.14	97.28	111.02
22	P	1271	CHD	C15-C14-C8	8.07	129.43	118.36
28	M	526	DMU	C18-O16-C6	7.97	127.29	113.68
28	M	526	DMU	O5-C6-C1	7.96	126.73	110.37
22	B	1085	CHD	C19-C10-C9	-7.94	100.50	111.18
22	B	1085	CHD	C15-C14-C13	7.94	111.24	103.54
14	A	516	HEA	CHA-C4D-C3D	-7.62	113.67	124.77
22	P	1525	CHD	C19-C10-C9	-7.59	100.97	111.18
22	W	1059	CHD	C5-C6-C7	7.56	123.39	114.40
22	J	60	CHD	C1-C2-C3	7.56	120.50	110.48
14	N	516	HEA	CMC-C2C-C1C	-7.51	113.99	125.42
14	A	516	HEA	C3D-C4D-ND	7.48	117.58	110.35
22	P	1271	CHD	C1-C10-C5	7.47	118.47	107.75
22	C	525	CHD	C18-C13-C12	-7.45	101.60	109.06
22	C	271	CHD	C14-C13-C12	7.44	114.22	107.42
22	O	229	CHD	C4-C3-C2	7.43	119.68	110.62
22	W	1059	CHD	C6-C5-C4	-7.38	102.80	111.23
22	B	1085	CHD	C5-C4-C3	7.31	123.74	112.71
22	C	271	CHD	C16-C17-C13	7.30	110.62	103.54
22	J	60	CHD	C18-C13-C12	-7.29	101.75	109.06
22	C	271	CHD	C5-C6-C7	7.28	123.06	114.40
22	C	271	CHD	C1-C10-C5	7.25	118.15	107.75
28	G	272	DMU	O1-C9-C8	7.25	122.76	109.70
28	Z	1526	DMU	O1-C9-C8	7.24	122.74	109.70
28	Z	1526	DMU	O1-C10-C5	7.23	125.23	110.37
22	B	1085	CHD	C18-C13-C17	-7.22	99.89	111.20
22	W	1059	CHD	C1-C2-C3	7.21	120.03	110.48
19	A	521	TGL	OG3-CC1-CC2	7.19	133.75	111.83
28	M	526	DMU	O1-C10-C5	7.19	125.14	110.37
22	W	1059	CHD	C15-C14-C13	7.17	110.49	103.54
22	P	1525	CHD	C18-C13-C14	-7.16	99.98	111.20
14	A	516	HEA	C26-C15-C16	7.15	127.64	115.23
22	C	525	CHD	C13-C17-C20	7.10	128.09	119.48
28	P	1272	DMU	O1-C10-C5	7.08	124.91	110.37
22	J	60	CHD	C6-C7-C8	7.07	119.22	111.50
14	N	516	HEA	C26-C15-C16	7.06	127.49	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	W	1059	CHD	C14-C13-C12	7.05	113.86	107.42
22	B	1085	CHD	C1-C2-C3	7.04	119.80	110.48
22	C	271	CHD	C15-C14-C13	7.03	110.36	103.54
22	P	1525	CHD	C6-C7-C8	7.03	119.17	111.50
14	N	515	HEA	CHC-C4B-NB	7.00	133.03	124.37
22	C	271	CHD	C1-C2-C3	6.99	119.75	110.48
28	P	1272	DMU	O16-C6-C1	6.98	118.87	108.27
22	W	1059	CHD	C15-C14-C8	6.97	127.92	118.36
22	C	271	CHD	C11-C12-C13	6.95	118.33	111.26
22	O	229	CHD	C17-C13-C14	6.91	107.05	100.11
22	J	60	CHD	C4-C5-C10	6.90	120.01	112.66
22	P	1525	CHD	C4-C3-C2	6.90	119.03	110.62
22	P	1271	CHD	C5-C6-C7	6.89	122.59	114.40
22	P	1525	CHD	C5-C4-C3	6.87	123.07	112.71
14	N	516	HEA	CMD-C2D-C1D	6.82	135.70	125.03
22	P	1271	CHD	C16-C17-C13	6.81	110.14	103.54
22	W	1059	CHD	C1-C10-C5	6.80	117.50	107.75
22	P	1271	CHD	C11-C9-C8	6.79	120.94	110.89
22	J	60	CHD	C1-C10-C5	6.78	117.48	107.75
14	N	516	HEA	C4A-CHB-C1B	-6.75	111.67	126.02
22	J	60	CHD	C6-C5-C10	6.74	119.83	112.66
22	C	525	CHD	O12-C12-C13	-6.70	99.71	111.02
22	P	1271	CHD	C1-C2-C3	6.69	119.34	110.48
22	J	60	CHD	C16-C17-C13	6.68	110.02	103.54
22	W	1059	CHD	C6-C5-C10	6.68	119.76	112.66
22	O	229	CHD	C15-C14-C8	6.68	127.51	118.36
28	Z	1526	DMU	O5-C6-C1	6.65	124.04	110.37
22	P	1271	CHD	C16-C17-C20	6.63	122.22	112.18
22	P	1271	CHD	C5-C4-C3	6.62	122.69	112.71
22	P	1271	CHD	C6-C7-C8	6.61	118.71	111.50
14	A	516	HEA	C4C-CHD-C1D	-6.59	110.74	126.25
28	P	1272	DMU	O1-C9-C8	6.57	121.53	109.70
28	G	272	DMU	O1-C10-C5	6.57	123.86	110.37
22	O	229	CHD	C11-C9-C8	6.53	120.55	110.89
22	P	1271	CHD	C18-C13-C12	-6.52	102.53	109.06
22	C	525	CHD	C15-C14-C13	6.52	109.87	103.54
22	C	525	CHD	C9-C8-C7	6.50	120.04	111.86
22	P	1271	CHD	C4-C3-C2	6.50	118.55	110.62
22	C	271	CHD	C5-C4-C3	6.50	122.51	112.71
22	C	525	CHD	C17-C13-C14	6.48	106.61	100.11
28	G	272	DMU	O16-C6-C1	6.47	118.10	108.27
22	C	271	CHD	C4-C5-C10	6.46	119.53	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	271	CHD	C6-C7-C8	6.43	118.53	111.50
22	W	1059	CHD	C5-C4-C3	6.43	122.41	112.71
14	N	515	HEA	C13-C12-C11	-6.39	104.19	114.39
22	W	1059	CHD	C6-C7-C8	6.37	118.45	111.50
22	J	60	CHD	C5-C6-C7	6.36	121.97	114.40
22	O	229	CHD	C18-C13-C17	-6.33	101.29	111.20
26	E	229	PSC	O01-C1-C2	6.33	125.17	111.48
14	N	516	HEA	CMC-C2C-C3C	6.31	141.38	126.55
25	G	269	CDL	OB6-CB5-C51	6.30	125.12	111.48
19	A	521	TGL	OG2-CB1-CB2	6.29	125.10	111.48
22	J	60	CHD	C15-C14-C13	6.28	109.63	103.54
19	A	521	TGL	OG3-CC1-OC1	-6.28	107.92	123.63
14	A	515	HEA	C13-C12-C11	-6.23	104.44	114.39
22	W	1059	CHD	C4-C3-C2	6.23	118.22	110.62
22	J	60	CHD	C16-C17-C20	6.22	121.58	112.18
22	P	1525	CHD	O7-C7-C6	-6.20	94.43	109.86
22	J	60	CHD	C4-C3-C2	6.20	118.18	110.62
14	A	516	HEA	CMD-C2D-C1D	6.16	134.66	125.03
22	J	60	CHD	C13-C17-C20	6.14	126.92	119.48
22	P	1525	CHD	C11-C9-C8	6.10	119.93	110.89
20	P	1268	PGV	O01-C1-C2	6.09	124.66	111.48
14	A	516	HEA	C4B-NB-C1B	-6.09	97.99	105.21
22	C	271	CHD	C17-C13-C12	6.08	123.14	117.67
22	P	1271	CHD	C14-C8-C7	6.07	119.91	111.85
22	C	525	CHD	C6-C5-C4	-6.07	104.30	111.23
22	W	1059	CHD	C4-C5-C10	6.06	119.11	112.66
22	O	229	CHD	C1-C10-C9	-6.05	101.94	111.34
22	W	1059	CHD	C9-C11-C12	6.03	122.18	114.29
22	J	60	CHD	C5-C4-C3	6.00	121.76	112.71
22	C	525	CHD	C14-C13-C12	5.97	112.87	107.42
19	N	1521	TGL	CG2-OG2-CB1	5.96	132.06	117.80
22	P	1271	CHD	C15-C14-C13	5.96	109.32	103.54
22	O	229	CHD	C11-C12-C13	5.95	117.32	111.26
14	N	516	HEA	C3B-C4B-NB	5.94	116.67	109.84
22	J	60	CHD	C11-C12-C13	5.94	117.30	111.26
22	W	1059	CHD	C2-C1-C10	5.92	122.73	112.74
28	M	526	DMU	C2-C3-C4	5.90	124.01	110.93
22	C	271	CHD	C4-C3-C2	5.88	117.80	110.62
28	G	272	DMU	O5-C4-C57	5.85	120.94	106.44
22	B	1085	CHD	C17-C13-C14	5.82	105.95	100.11
28	Z	1526	DMU	O16-C6-C1	5.80	117.08	108.27
28	G	272	DMU	C18-O16-C6	5.78	123.56	113.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	264	PEK	C2-C3-C4	5.77	125.96	113.35
22	P	1271	CHD	C14-C13-C12	5.76	112.68	107.42
22	W	1059	CHD	C1-C10-C9	-5.76	102.40	111.34
22	B	1085	CHD	C11-C12-C13	5.76	117.12	111.26
28	P	1272	DMU	O5-C4-C3	5.76	121.62	109.72
22	P	1271	CHD	C11-C12-C13	5.75	117.11	111.26
22	W	1059	CHD	C11-C12-C13	5.73	117.10	111.26
22	C	525	CHD	C11-C12-C13	5.73	117.09	111.26
22	C	525	CHD	C11-C9-C10	5.72	119.50	113.70
14	N	516	HEA	CHC-C4B-NB	5.69	131.41	124.37
22	B	1085	CHD	C14-C8-C9	5.69	117.70	109.75
14	N	516	HEA	CHB-C1B-C2B	-5.68	116.06	125.03
22	O	229	CHD	C2-C1-C10	5.68	122.32	112.74
14	A	516	HEA	C4B-C3B-C2B	-5.68	97.89	107.44
19	D	523	TGL	OG2-CB1-CB2	-5.63	99.29	111.48
22	O	229	CHD	C6-C5-C4	-5.61	104.82	111.23
22	C	271	CHD	C11-C9-C8	5.60	119.18	110.89
20	C	268	PGV	O01-C1-C2	5.57	123.54	111.48
22	P	1271	CHD	C2-C1-C10	5.57	122.14	112.74
28	P	1272	DMU	C8-C7-C5	5.55	120.57	110.83
22	J	60	CHD	C15-C14-C8	5.55	125.96	118.36
22	J	60	CHD	C2-C1-C10	5.52	122.06	112.74
22	W	1059	CHD	C9-C10-C5	5.51	116.17	108.51
25	T	1269	CDL	OB6-CB5-C51	5.51	123.40	111.48
22	O	229	CHD	C5-C6-C7	5.50	120.94	114.40
14	N	516	HEA	CHC-C4B-C3B	-5.50	111.92	125.80
20	P	1268	PGV	O03-C19-C20	5.48	128.55	111.83
22	P	1525	CHD	C18-C13-C17	-5.48	102.62	111.20
14	A	516	HEA	CHD-C1D-C2D	-5.47	111.40	126.95
22	C	525	CHD	O3-C3-C4	5.45	120.70	109.84
28	G	272	DMU	O5-C4-C3	5.45	120.98	109.72
22	O	229	CHD	C16-C17-C20	5.42	120.39	112.18
14	A	516	HEA	C17-C18-C19	5.42	140.04	127.62
22	C	525	CHD	C5-C4-C3	5.42	120.89	112.71
28	Z	1526	DMU	C8-C7-C5	5.40	120.32	110.83
22	B	1085	CHD	C6-C7-C8	5.40	117.39	111.50
22	C	525	CHD	C18-C13-C14	-5.39	102.75	111.20
22	C	271	CHD	C2-C1-C10	5.38	121.82	112.74
22	P	1525	CHD	C17-C13-C14	5.38	105.51	100.11
22	W	1059	CHD	C22-C20-C17	5.36	121.43	110.33
22	C	525	CHD	C18-C13-C17	-5.31	102.88	111.20
22	B	1085	CHD	O12-C12-C13	-5.31	102.05	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	516	HEA	O11-C11-C12	5.30	123.19	109.14
22	P	1271	CHD	C4-C5-C10	5.30	118.30	112.66
28	Z	1526	DMU	O5-C4-C3	5.27	120.62	109.72
22	O	229	CHD	C9-C8-C7	5.22	118.43	111.86
22	C	525	CHD	C4-C5-C10	-5.19	107.14	112.66
28	G	272	DMU	C8-C7-C5	5.18	119.93	110.83
14	A	516	HEA	C20-C19-C18	-5.18	109.55	121.17
22	P	1525	CHD	O12-C12-C11	-5.15	98.64	109.12
20	A	524	PGV	C02-O01-C1	5.15	130.11	117.80
22	B	1085	CHD	C4-C3-C2	5.14	116.89	110.62
22	J	60	CHD	C9-C11-C12	5.14	121.02	114.29
22	B	1085	CHD	C16-C17-C20	5.13	119.94	112.18
20	C	268	PGV	O03-C19-C20	5.12	127.44	111.83
28	Z	1526	DMU	O5-C4-C57	5.10	119.08	106.44
24	T	1264	PEK	O03-C01-C02	-5.09	93.73	108.40
22	J	60	CHD	C9-C10-C5	5.09	115.58	108.51
22	W	1059	CHD	C18-C13-C12	-5.04	104.02	109.06
24	G	265	PEK	O03-C21-C22	5.01	127.11	111.83
28	M	526	DMU	O5-C4-C3	5.01	120.08	109.72
14	A	516	HEA	CHC-C4B-C3B	-5.01	113.17	125.80
14	N	516	HEA	C2B-C1B-NB	5.01	115.69	109.90
25	C	270	CDL	OA6-CA5-C11	5.00	122.30	111.48
24	S	1265	PEK	O03-C21-C22	4.99	127.05	111.83
22	O	229	CHD	C18-C13-C14	-4.98	103.40	111.20
19	L	522	TGL	OG3-CC1-OC1	-4.96	111.22	123.63
28	G	272	DMU	O5-C6-C1	4.96	120.56	110.37
28	Z	1526	DMU	O1-C9-C11	4.95	118.70	106.44
28	P	1272	DMU	O1-C9-C11	4.94	118.67	106.44
22	W	1059	CHD	C11-C9-C10	4.93	118.70	113.70
22	C	271	CHD	C14-C8-C7	4.92	118.37	111.85
22	P	1525	CHD	O12-C12-C13	-4.91	102.72	111.02
22	C	271	CHD	C6-C5-C4	-4.90	105.63	111.23
22	C	525	CHD	C23-C22-C20	-4.88	105.35	114.46
22	J	60	CHD	C11-C9-C8	4.88	118.11	110.89
19	N	1522	TGL	CG2-OG2-CB1	4.87	129.45	117.80
19	L	522	TGL	CG2-OG2-CB1	4.86	129.44	117.80
22	C	271	CHD	C18-C13-C17	-4.86	103.58	111.20
14	A	516	HEA	C1D-C2D-C3D	-4.86	101.87	106.98
14	N	516	HEA	C4B-NB-C1B	-4.81	99.51	105.21
22	J	60	CHD	C14-C8-C7	4.81	118.23	111.85
28	G	272	DMU	C2-C3-C4	4.80	121.58	110.93
28	Z	1526	DMU	O7-C10-C5	-4.80	96.27	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	O	229	CHD	C14-C8-C9	4.80	116.45	109.75
28	P	1272	DMU	O5-C6-C1	4.79	120.21	110.37
14	A	515	HEA	CHC-C4B-NB	4.77	130.27	124.37
22	P	1271	CHD	C19-C10-C9	-4.75	104.80	111.18
22	C	271	CHD	C9-C11-C12	4.75	120.50	114.29
28	Z	1526	DMU	C2-C3-C4	4.72	121.39	110.93
28	P	1272	DMU	O5-C4-C57	4.70	118.08	106.44
19	L	522	TGL	OG3-CC1-CC2	4.67	126.08	111.83
22	P	1525	CHD	C2-C1-C10	4.66	120.61	112.74
14	N	516	HEA	C3C-C4C-NC	4.65	113.72	109.80
22	C	525	CHD	C2-C1-C10	4.65	120.59	112.74
25	G	269	CDL	OA6-CA5-C11	4.64	121.52	111.48
14	N	515	HEA	C27-C19-C20	4.64	123.28	115.23
14	A	515	HEA	C26-C15-C16	4.63	123.26	115.23
20	N	1524	PGV	O01-C1-C2	4.62	121.48	111.48
24	G	1263	PEK	O01-C1-C2	4.61	121.46	111.48
14	N	516	HEA	C12-C11-C3B	4.61	119.33	112.12
28	G	272	DMU	O1-C9-C11	4.61	117.86	106.44
22	J	60	CHD	C19-C10-C5	-4.61	102.74	110.44
22	C	271	CHD	C19-C10-C1	-4.58	101.02	108.31
25	P	1270	CDL	OB8-CB7-C71	4.57	125.76	111.83
19	N	1522	TGL	OG2-CB1-CB2	4.56	121.34	111.48
25	P	1270	CDL	OA6-CA5-C11	4.55	121.33	111.48
22	C	525	CHD	C9-C11-C12	4.49	120.17	114.29
28	P	1272	DMU	O7-C10-C5	4.47	119.09	108.09
14	A	516	HEA	CAA-CBA-CGA	-4.47	101.81	113.67
22	W	1059	CHD	C18-C13-C14	-4.45	104.22	111.20
14	A	515	HEA	C3C-C4C-NC	4.44	113.54	109.80
22	C	525	CHD	O7-C7-C6	-4.44	98.82	109.86
22	P	1271	CHD	O12-C12-C11	-4.43	100.11	109.12
19	L	522	TGL	OG1-CG1-CG2	4.42	121.15	108.40
28	M	526	DMU	O1-C9-C11	4.41	117.37	106.44
14	N	516	HEA	C2D-C1D-ND	4.41	114.91	109.84
22	P	1271	CHD	C9-C11-C12	4.39	120.04	114.29
28	M	526	DMU	O5-C4-C57	4.39	117.31	106.44
22	P	1525	CHD	O3-C3-C4	4.38	118.57	109.84
20	C	267	PGV	C27-C26-C25	-4.38	92.25	114.37
28	P	1272	DMU	C7-C8-C9	4.36	118.13	110.23
14	A	515	HEA	CHA-C4D-C3D	-4.36	118.42	124.77
22	C	525	CHD	C13-C14-C8	4.35	120.23	114.72
22	W	1059	CHD	C19-C10-C5	-4.34	103.18	110.44
22	P	1525	CHD	C1-C10-C9	-4.34	104.60	111.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	O	229	CHD	C4-C5-C10	-4.33	108.05	112.66
28	P	1272	DMU	C6-C1-C2	4.33	119.12	110.01
14	A	516	HEA	C4A-CHB-C1B	-4.33	116.82	126.02
22	B	1085	CHD	O12-C12-C11	-4.31	100.34	109.12
14	N	515	HEA	C17-C18-C19	-4.31	117.76	127.62
22	P	1271	CHD	O7-C7-C6	-4.30	99.17	109.86
22	W	1059	CHD	C9-C8-C7	4.29	117.25	111.86
22	P	1525	CHD	C22-C20-C17	-4.27	101.48	110.33
28	M	526	DMU	C8-C7-C5	4.27	118.32	110.83
22	J	60	CHD	C18-C13-C17	-4.25	104.55	111.20
22	C	525	CHD	C22-C20-C17	-4.25	101.52	110.33
22	B	1085	CHD	C11-C9-C8	4.23	117.16	110.89
14	A	516	HEA	C27-C19-C20	4.23	122.57	115.23
22	P	1271	CHD	C13-C17-C20	4.23	124.61	119.48
22	B	1085	CHD	C15-C14-C8	4.22	124.14	118.36
14	A	515	HEA	CHA-C4D-ND	4.20	128.94	124.42
20	N	1266	PGV	O01-C1-O02	-4.19	113.90	123.70
19	A	521	TGL	OG1-CA1-CA2	4.19	124.60	111.83
25	C	270	CDL	OB8-CB7-C71	4.18	124.58	111.83
25	T	1269	CDL	OA6-CA5-C11	4.16	120.48	111.48
14	N	515	HEA	C1C-CHC-C4B	-4.14	116.52	126.25
28	G	272	DMU	C7-C8-C9	4.13	117.72	110.23
22	P	1525	CHD	C19-C10-C5	-4.12	103.55	110.44
24	G	265	PEK	O01-C1-C2	4.12	120.38	111.48
22	W	1059	CHD	C17-C13-C12	4.11	121.37	117.67
25	G	269	CDL	OA8-CA7-C31	4.10	124.34	111.83
22	J	60	CHD	C22-C20-C17	4.10	118.82	110.33
22	B	1085	CHD	O3-C3-C4	4.09	118.00	109.84
28	G	272	DMU	C6-C1-C2	4.09	118.62	110.01
28	P	1272	DMU	C2-C3-C4	4.08	119.96	110.93
14	N	516	HEA	C4C-CHD-C1D	-4.07	116.67	126.25
24	T	263	PEK	O01-C1-C2	4.07	120.29	111.48
25	C	270	CDL	CB4-OB6-CB5	-4.04	108.13	117.80
14	N	516	HEA	C1D-ND-C4D	-4.04	100.42	105.21
22	B	1085	CHD	C9-C8-C7	4.02	116.92	111.86
22	P	1271	CHD	C17-C13-C14	4.02	104.14	100.11
22	P	1525	CHD	C1-C2-C3	4.01	115.79	110.48
22	B	1085	CHD	C6-C5-C4	-4.01	106.65	111.23
22	J	60	CHD	C19-C10-C9	-4.01	105.79	111.18
24	S	1265	PEK	O01-C1-C2	3.99	120.12	111.48
28	G	272	DMU	O7-C3-C4	3.99	119.95	109.48
28	M	526	DMU	O7-C3-C2	3.99	117.36	107.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	264	PEK	C24-C23-C22	-3.97	98.54	113.13
14	N	515	HEA	C3D-C4D-ND	3.96	114.18	110.35
19	L	522	TGL	OG1-CA1-CA2	3.96	123.92	111.83
14	N	516	HEA	C21-C20-C19	3.96	126.29	113.19
20	A	522	PGV	O03-C19-C20	3.93	123.82	111.83
22	C	525	CHD	C1-C10-C9	-3.91	105.27	111.34
14	A	515	HEA	CAA-CBA-CGA	-3.87	103.39	113.67
14	A	516	HEA	C3A-C2A-C1A	-3.87	103.38	107.05
14	N	515	HEA	C2A-C1A-NA	-3.85	106.61	110.32
22	P	1525	CHD	C11-C12-C13	3.85	115.18	111.26
20	P	1267	PGV	O03-C19-O04	-3.83	114.05	123.63
22	C	271	CHD	C21-C20-C17	3.81	118.60	112.88
22	B	1085	CHD	O7-C7-C6	-3.81	100.39	109.86
19	A	521	TGL	CG3-OG3-CC1	3.80	131.01	117.12
19	N	1521	TGL	CG3-OG3-CC1	3.80	131.01	117.12
28	M	526	DMU	O3-C5-C7	3.80	119.33	110.38
26	R	1229	PSC	O01-C1-C2	3.79	119.68	111.48
25	P	1270	CDL	OB8-CB7-OB9	-3.79	114.15	123.63
28	P	1272	DMU	C1-C2-C3	3.78	118.27	109.68
14	N	516	HEA	OMA-CMA-C3A	-3.78	117.08	125.62
19	A	521	TGL	OG2-CG2-CG1	3.76	121.83	108.34
20	N	1266	PGV	O03-C19-C20	3.75	123.27	111.83
14	A	515	HEA	C4C-C3C-C2C	-3.74	102.65	107.30
28	P	1272	DMU	C18-O16-C6	3.73	120.06	113.68
19	A	521	TGL	CB3-CB2-CB1	-3.73	100.03	113.69
28	G	272	DMU	C6-O5-C4	3.73	121.00	113.72
28	Z	1526	DMU	C7-C8-C9	3.72	116.98	110.23
22	J	60	CHD	C11-C9-C10	3.72	117.48	113.70
14	A	516	HEA	CHA-C4D-ND	3.72	128.42	124.42
28	Z	1526	DMU	C6-O5-C4	3.71	120.97	113.72
22	C	525	CHD	C11-C9-C8	3.71	116.38	110.89
25	C	270	CDL	OB8-CB7-OB9	-3.71	114.36	123.63
22	J	60	CHD	C6-C5-C4	-3.70	107.00	111.23
24	C	264	PEK	O01-C1-O02	-3.67	115.12	123.70
14	A	516	HEA	CHD-C1D-ND	3.67	128.91	124.37
28	M	526	DMU	O7-C10-C5	-3.67	99.07	108.09
22	J	60	CHD	C18-C13-C14	-3.64	105.50	111.20
28	G	272	DMU	O7-C3-C2	3.63	116.46	107.23
22	P	1271	CHD	C18-C13-C17	-3.62	105.52	111.20
22	P	1525	CHD	C13-C17-C20	3.62	123.86	119.48
19	A	521	TGL	OG1-CG1-CG2	3.60	118.77	108.40
19	L	522	TGL	OG2-CB1-CB2	3.59	119.25	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	P	1272	DMU	O5-C6-O16	3.58	118.51	110.04
22	B	1085	CHD	C1-C10-C9	-3.58	105.78	111.34
22	C	525	CHD	C14-C8-C9	3.57	114.74	109.75
14	A	516	HEA	C21-C20-C19	3.57	125.01	113.19
19	D	523	TGL	OG1-CA1-CA2	3.56	122.70	111.83
22	O	229	CHD	C15-C14-C13	3.56	107.00	103.54
28	M	526	DMU	C7-C8-C9	3.56	116.69	110.23
28	P	1272	DMU	C6-O5-C4	3.56	120.67	113.72
22	P	1525	CHD	C9-C11-C12	3.55	118.94	114.29
19	N	1521	TGL	OG1-CA1-CA2	3.55	122.67	111.83
19	Q	1523	TGL	OG3-CC1-CC2	3.55	122.67	111.83
28	G	272	DMU	O7-C10-C5	3.54	116.80	108.09
19	A	521	TGL	OG2-CG2-CG3	3.53	121.02	108.34
22	B	1085	CHD	C11-C9-C10	3.53	117.28	113.70
22	W	1059	CHD	C11-C9-C8	3.51	116.09	110.89
19	D	523	TGL	CG2-OG2-CB1	3.49	126.15	117.80
14	N	516	HEA	C26-C15-C14	-3.48	114.69	123.63
20	C	267	PGV	C8-C9-C10	-3.48	97.15	113.86
14	A	516	HEA	CHB-C4A-NA	3.45	128.22	124.45
22	C	271	CHD	O12-C12-C11	-3.45	102.09	109.12
22	B	1085	CHD	C9-C11-C12	3.45	118.81	114.29
14	N	516	HEA	C1D-C2D-C3D	-3.44	103.37	106.98
22	C	525	CHD	C15-C16-C17	3.43	111.86	105.14
20	P	1267	PGV	C8-C9-C10	-3.43	97.36	113.86
22	P	1271	CHD	C22-C23-C24	-3.43	103.34	112.49
22	C	525	CHD	C5-C6-C7	3.42	118.47	114.40
14	N	516	HEA	C2C-C1C-NC	3.40	115.59	110.14
28	P	1272	DMU	O7-C3-C4	3.39	118.38	109.48
20	N	1524	PGV	C01-O03-C19	3.39	129.51	117.12
14	A	516	HEA	C4A-NA-C1A	3.38	111.34	105.82
14	A	515	HEA	CHB-C4A-NA	-3.38	120.78	124.45
28	Z	1526	DMU	C1-C2-C3	3.34	117.27	109.68
14	A	516	HEA	C26-C15-C14	-3.34	115.05	123.63
28	G	272	DMU	C1-C2-C3	3.34	117.26	109.68
28	M	526	DMU	O7-C10-O1	-3.33	101.93	110.69
24	G	265	PEK	O03-C21-O04	-3.33	115.30	123.63
19	D	523	TGL	CG1-OG1-CA1	3.33	129.29	117.12
24	T	263	PEK	O03-C21-C22	3.32	121.95	111.83
22	P	1271	CHD	O12-C12-C13	-3.30	105.45	111.02
22	P	1525	CHD	C14-C8-C9	3.30	114.35	109.75
14	A	516	HEA	CMB-C2B-C1B	-3.29	119.89	125.03
26	E	229	PSC	O01-C1-O02	-3.28	116.04	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	M	526	DMU	C57-C4-C3	3.27	122.57	113.38
14	N	515	HEA	C1B-C2B-C3B	-3.27	103.01	106.80
14	A	516	HEA	O1A-CGA-CBA	-3.26	112.76	123.09
28	M	526	DMU	C10-C5-C7	3.25	116.85	110.01
22	P	1271	CHD	C6-C5-C4	-3.25	107.51	111.23
22	C	271	CHD	C22-C23-C24	-3.25	103.82	112.49
24	G	1263	PEK	O03-C21-C22	3.24	121.73	111.83
28	P	1272	DMU	C10-O1-C9	3.24	120.05	113.72
20	N	1266	PGV	O03-C01-C02	3.24	117.73	108.40
22	P	1525	CHD	C11-C9-C10	3.23	116.98	113.70
22	J	60	CHD	O7-C7-C6	-3.22	101.86	109.86
19	L	522	TGL	CC3-CC2-CC1	3.20	125.44	113.69
14	N	516	HEA	C3D-C4D-ND	3.20	113.45	110.35
22	B	1085	CHD	C19-C10-C5	-3.19	105.11	110.44
22	B	1085	CHD	C21-C20-C17	3.18	117.66	112.88
28	M	526	DMU	O16-C6-C1	3.17	113.09	108.27
22	J	60	CHD	C9-C8-C7	3.16	115.83	111.86
14	N	516	HEA	CHA-C1A-NA	3.15	127.89	124.45
20	C	268	PGV	O04-C19-C20	-3.13	111.53	123.78
26	R	1229	PSC	O03-C19-C20	3.13	121.38	111.83
19	N	1522	TGL	OG3-CG3-CG2	3.13	117.41	108.40
19	N	1522	TGL	OG1-CA1-CA2	3.08	121.22	111.83
19	N	1522	TGL	OG3-CC1-CC2	3.07	121.19	111.83
20	A	524	PGV	O01-C02-C03	3.03	119.23	108.34
24	S	1265	PEK	O03-C01-C02	3.02	117.11	108.40
14	N	516	HEA	CHA-C4D-C3D	-3.02	120.37	124.77
19	D	523	TGL	OG2-CB1-OB1	3.01	130.74	123.70
28	P	1272	DMU	O16-C18-C19	3.01	119.57	109.37
14	N	516	HEA	C25-C23-C24	-2.99	107.70	114.59
19	Q	1523	TGL	OG2-CG2-CG3	2.99	119.06	108.34
25	G	269	CDL	C80-C79-C78	2.97	129.40	114.37
20	P	1268	PGV	C03-C02-C01	-2.96	104.88	111.78
19	N	1522	TGL	CG3-OG3-CC1	2.96	127.93	117.12
14	N	516	HEA	CBC-CAC-C3C	-2.96	112.76	127.53
28	G	272	DMU	C10-O1-C9	2.95	119.49	113.72
22	C	525	CHD	O12-C12-C11	-2.95	103.12	109.12
19	N	1521	TGL	OG3-CC1-CC2	2.95	120.82	111.83
14	N	516	HEA	CHB-C1B-NB	2.94	127.59	124.42
24	T	1264	PEK	O01-C1-O02	-2.94	116.83	123.70
28	G	272	DMU	O5-C6-O16	2.93	116.97	110.04
22	P	1525	CHD	C16-C17-C13	2.93	106.38	103.54
20	A	524	PGV	C3-C2-C1	-2.91	103.02	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	P	1271	CHD	C17-C13-C12	2.91	120.29	117.67
20	C	267	PGV	O14-P-O13	2.91	125.98	112.44
14	A	516	HEA	CAA-C2A-C1A	2.91	130.76	124.85
25	C	270	CDL	C52-C51-CB5	-2.91	103.04	113.69
22	P	1271	CHD	C23-C22-C20	-2.90	109.04	114.46
20	A	522	PGV	O03-C19-O04	-2.89	116.39	123.63
20	P	1268	PGV	O04-C19-C20	-2.89	112.47	123.78
14	N	516	HEA	C20-C21-C22	2.89	126.32	112.02
28	M	526	DMU	C31-C28-C25	-2.89	99.75	114.37
20	P	1267	PGV	C27-C26-C25	-2.89	99.77	114.37
28	G	272	DMU	C10-C5-C7	2.89	116.08	110.01
20	N	1524	PGV	C02-O01-C1	2.88	124.68	117.80
25	G	269	CDL	CA6-OA8-CA7	2.88	127.63	117.12
19	N	1522	TGL	OG1-CG1-CG2	2.88	116.69	108.40
20	A	522	PGV	C02-O01-C1	2.87	124.67	117.80
22	P	1525	CHD	C9-C8-C7	2.87	115.47	111.86
25	G	269	CDL	C82-C81-C80	2.87	128.86	114.37
28	Z	1526	DMU	O3-C5-C7	2.86	117.13	110.38
26	E	229	PSC	C02-O01-C1	2.86	124.64	117.80
25	P	1270	CDL	OB6-CB4-CB6	2.86	118.59	108.34
22	B	1085	CHD	C4-C5-C10	-2.85	109.62	112.66
24	C	264	PEK	O04-C21-C22	2.85	134.93	123.78
19	Q	1523	TGL	CG2-OG2-CB1	2.84	124.60	117.80
22	W	1059	CHD	O7-C7-C6	-2.84	102.79	109.86
14	A	515	HEA	CHC-C4B-C3B	-2.83	118.66	125.80
20	A	524	PGV	O03-C19-C20	2.83	120.45	111.83
20	P	1267	PGV	O03-C19-C20	2.81	120.40	111.83
24	C	264	PEK	O03-C21-C22	-2.80	103.28	111.83
14	N	516	HEA	O2A-CGA-CBA	2.80	122.86	114.00
25	G	269	CDL	OB8-CB7-C71	2.80	120.37	111.83
22	P	1271	CHD	C19-C10-C1	-2.80	103.86	108.31
14	A	515	HEA	C2D-C1D-ND	2.77	113.02	109.84
19	N	1522	TGL	OG3-CC1-OC1	-2.76	116.71	123.63
25	T	1269	CDL	CA4-OA6-CA5	-2.76	111.19	117.80
28	P	1272	DMU	C11-C9-C8	2.76	119.79	113.02
22	O	229	CHD	O12-C12-C11	-2.76	103.51	109.12
25	T	1269	CDL	OB8-CB6-CB4	2.75	116.33	108.40
14	A	516	HEA	C17-C16-C15	-2.74	104.09	113.19
22	C	271	CHD	C17-C13-C14	2.74	102.87	100.11
14	N	516	HEA	CHD-C1D-C2D	-2.74	119.16	126.95
24	G	1263	PEK	O03-C21-O04	-2.73	116.81	123.63
22	P	1525	CHD	C4-C5-C10	-2.73	109.76	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	O	229	CHD	C14-C8-C7	2.72	115.46	111.85
22	B	1085	CHD	C2-C1-C10	2.71	117.31	112.74
25	P	1270	CDL	OA8-CA7-C31	2.71	120.10	111.83
25	T	1269	CDL	C83-C82-C81	2.70	128.03	114.37
22	C	271	CHD	C19-C10-C9	-2.70	107.55	111.18
14	A	516	HEA	C2B-C1B-NB	2.70	113.03	109.90
24	T	1264	PEK	C24-C23-C22	-2.69	103.24	113.13
22	P	1525	CHD	C21-C20-C22	-2.68	106.19	110.34
14	A	516	HEA	CBD-CAD-C3D	2.68	119.95	112.53
19	L	522	TGL	CB4-CB3-CB2	-2.67	103.32	113.13
24	S	1265	PEK	O03-C21-O04	-2.66	116.97	123.63
20	A	524	PGV	O01-C1-C2	2.65	117.22	111.48
28	Z	1526	DMU	C10-C5-C7	2.65	115.58	110.01
25	T	1269	CDL	OB8-CB7-C71	2.63	119.87	111.83
22	J	60	CHD	C14-C8-C9	2.63	113.43	109.75
19	A	521	TGL	C15-CC9-CC8	2.63	127.64	114.37
14	A	515	HEA	O11-C11-C3B	-2.62	106.45	111.26
24	T	1264	PEK	C3-C2-C1	2.62	123.31	113.69
19	A	521	TGL	CG3-CG2-CG1	-2.62	105.68	111.78
28	Z	1526	DMU	O5-C6-O16	2.62	116.23	110.04
24	G	1263	PEK	C02-O01-C1	2.61	124.05	117.80
19	N	1522	TGL	OB1-CB1-CB2	-2.61	113.58	123.78
22	C	271	CHD	C19-C10-C5	-2.61	106.08	110.44
20	N	1524	PGV	O03-C19-C20	2.60	119.77	111.83
22	O	229	CHD	C6-C7-C8	2.60	114.34	111.50
22	P	1525	CHD	C14-C8-C7	2.60	115.30	111.85
25	T	1269	CDL	OA8-CA7-C31	2.59	119.74	111.83
19	D	523	TGL	C10-CB9-CB8	2.59	127.45	114.37
28	G	272	DMU	C11-C9-C8	2.59	119.37	113.02
19	N	1522	TGL	C15-CC9-CC8	2.58	127.43	114.37
26	E	229	PSC	C32-C31-C30	-2.58	101.33	114.37
20	P	1267	PGV	O14-P-O13	2.58	124.44	112.44
14	N	515	HEA	O11-C11-C3B	-2.57	106.54	111.26
22	C	271	CHD	C9-C10-C5	2.57	112.09	108.51
25	T	1269	CDL	C39-C38-C37	2.57	127.36	114.37
14	N	515	HEA	CHA-C4D-C3D	-2.57	121.03	124.77
25	G	269	CDL	C19-C18-C17	2.57	127.33	114.37
19	Q	1523	TGL	OG2-CB1-CB2	2.56	117.02	111.48
25	P	1270	CDL	OA6-CA5-OA7	-2.56	117.72	123.70
14	N	515	HEA	CHC-C1C-C2C	-2.56	120.00	127.43
14	A	516	HEA	C13-C14-C15	-2.56	121.77	127.62
20	P	1268	PGV	O02-C1-C2	-2.56	113.78	123.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	Z	1526	DMU	O7-C3-C2	2.56	113.73	107.23
20	C	268	PGV	C01-O03-C19	2.55	126.45	117.12
25	G	269	CDL	OB8-CB7-OB9	-2.55	117.25	123.63
28	M	526	DMU	O5-C6-O16	2.53	116.02	110.04
24	C	264	PEK	C30-C29-C28	-2.53	101.60	114.37
22	J	60	CHD	C17-C13-C14	2.52	102.65	100.11
25	T	1269	CDL	CB6-CB4-CB3	-2.52	105.91	111.78
25	T	1269	CDL	OB8-CB7-OB9	-2.52	117.32	123.63
24	C	264	PEK	O01-C02-C01	-2.51	99.34	108.34
25	C	270	CDL	OA8-CA7-C31	2.51	119.49	111.83
22	P	1271	CHD	C19-C10-C5	-2.51	106.24	110.44
19	L	522	TGL	OB1-CB1-CB2	-2.51	113.98	123.78
28	M	526	DMU	C6-C1-C2	2.50	115.28	110.01
20	N	1266	PGV	O03-C19-O04	-2.50	117.37	123.63
28	M	526	DMU	C6-O5-C4	2.50	118.60	113.72
22	O	229	CHD	C9-C11-C12	2.50	117.56	114.29
14	A	515	HEA	C27-C19-C18	-2.49	117.22	123.63
20	N	1266	PGV	C23-C22-C21	-2.49	101.77	114.37
14	N	516	HEA	C4C-NC-C1C	-2.49	101.76	105.82
25	G	269	CDL	CB6-CB4-CB3	-2.49	105.98	111.78
19	L	522	TGL	CA5-CA4-CA3	-2.49	101.80	114.37
20	C	268	PGV	O02-C1-C2	-2.48	114.08	123.78
14	A	516	HEA	C1B-C2B-C3B	2.48	109.67	106.80
14	N	516	HEA	CAA-CBA-CGA	-2.48	107.08	113.67
22	J	60	CHD	C13-C14-C8	2.48	117.86	114.72
19	Q	1523	TGL	OG1-CA1-CA2	2.48	119.38	111.83
28	P	1272	DMU	C57-C4-C3	2.46	120.29	113.38
22	P	1271	CHD	C9-C10-C5	2.46	111.92	108.51
28	M	526	DMU	O4-C7-C5	2.45	116.16	110.38
25	G	269	CDL	OB7-CB5-C51	-2.45	114.19	123.78
14	N	515	HEA	CHC-C4B-C3B	-2.45	119.62	125.80
22	O	229	CHD	C19-C10-C5	-2.44	106.35	110.44
20	N	1524	PGV	O01-C1-O02	-2.44	117.99	123.70
28	Z	1526	DMU	C57-C4-C3	2.44	120.25	113.38
25	C	270	CDL	O1-C1-CB2	2.44	118.14	109.70
14	N	516	HEA	C4C-C3C-C2C	-2.44	104.27	107.30
20	A	522	PGV	O03-C01-C02	2.43	115.40	108.40
25	T	1269	CDL	C82-C81-C80	2.43	126.65	114.37
20	P	1267	PGV	O01-C1-O02	-2.43	118.03	123.70
28	G	272	DMU	O4-C7-C5	2.43	116.10	110.38
22	P	1271	CHD	C21-C20-C17	2.42	116.52	112.88
28	Z	1526	DMU	C6-C1-C2	2.42	115.10	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	515	HEA	C26-C15-C14	-2.42	117.42	123.63
25	G	269	CDL	C17-C16-C15	-2.42	102.16	114.37
19	N	1521	TGL	OG2-CG2-CG3	2.41	116.98	108.34
14	A	515	HEA	OMA-CMA-C3A	-2.41	120.19	125.62
25	C	270	CDL	C53-C52-C51	-2.40	104.30	113.13
22	P	1525	CHD	C5-C6-C7	2.40	117.25	114.40
19	Q	1523	TGL	OG3-CC1-OC1	-2.40	117.63	123.63
14	A	515	HEA	O1A-CGA-CBA	-2.39	115.51	123.09
19	N	1521	TGL	OG2-CG2-CG1	2.39	116.91	108.34
19	N	1521	TGL	OG1-CA1-OA1	-2.38	117.67	123.63
22	O	229	CHD	O25-C24-C23	-2.38	115.54	123.09
22	O	229	CHD	O26-C24-C23	2.38	121.51	114.00
19	D	523	TGL	CB3-CB2-CB1	2.37	122.39	113.69
25	C	270	CDL	C82-C81-C80	2.37	126.34	114.37
14	N	515	HEA	C27-C19-C18	-2.36	117.57	123.63
22	C	271	CHD	C23-C22-C20	-2.36	110.06	114.46
25	T	1269	CDL	CB6-OB8-CB7	2.36	125.73	117.12
28	Z	1526	DMU	C10-O1-C9	2.35	118.31	113.72
19	N	1521	TGL	OG2-CB1-CB2	2.35	116.57	111.48
24	T	1264	PEK	C03-C02-C01	-2.35	106.30	111.78
22	J	60	CHD	C1-C10-C9	-2.35	107.69	111.34
26	R	1229	PSC	O03-C19-O04	-2.35	117.75	123.63
19	Q	1523	TGL	CG1-OG1-CA1	2.35	125.70	117.12
24	C	264	PEK	O03-C01-C02	-2.35	101.63	108.40
24	C	264	PEK	C32-C31-C30	-2.35	102.50	114.37
25	G	269	CDL	OA8-CA7-OA9	-2.35	117.76	123.63
25	G	269	CDL	CB6-OB8-CB7	2.35	125.70	117.12
22	C	271	CHD	C9-C8-C7	2.35	114.81	111.86
19	N	1522	TGL	CC3-CC2-CC1	2.35	122.29	113.69
19	A	521	TGL	CB4-CB3-CB2	2.35	121.75	113.13
25	T	1269	CDL	CB2-C1-CA2	-2.34	105.90	112.65
22	W	1059	CHD	C19-C10-C1	-2.34	104.58	108.31
28	M	526	DMU	O55-C2-C3	2.34	115.94	109.94
22	B	1085	CHD	C14-C8-C7	2.34	114.95	111.85
22	O	229	CHD	C16-C17-C13	2.34	105.81	103.54
25	G	269	CDL	OA6-CA5-OA7	-2.33	118.26	123.70
24	T	263	PEK	O03-C01-C02	2.32	115.09	108.40
19	N	1522	TGL	C10-CB9-CB8	2.32	126.10	114.37
25	C	270	CDL	C42-C41-C40	2.32	126.09	114.37
28	M	526	DMU	C1-C2-C3	2.31	114.93	109.68
14	N	515	HEA	C2D-C1D-ND	2.31	112.50	109.84
14	A	516	HEA	CAD-CBD-CGD	2.30	119.77	113.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	P	1270	CDL	C39-C38-C37	2.29	125.95	114.37
22	W	1059	CHD	C21-C20-C17	2.29	116.32	112.88
19	N	1522	TGL	OG2-CG2-CG3	2.29	116.56	108.34
19	Q	1523	TGL	CG3-OG3-CC1	2.29	125.48	117.12
28	M	526	DMU	C25-C22-C19	-2.29	102.81	114.37
19	L	522	TGL	C15-CC9-CC8	2.28	125.89	114.37
19	N	1522	TGL	CA5-CA4-CA3	-2.27	102.87	114.37
24	T	263	PEK	C01-O03-C21	2.27	125.42	117.12
14	A	516	HEA	C1A-CHA-C4D	-2.27	121.19	126.02
22	P	1525	CHD	O7-C7-C8	-2.27	104.32	109.52
25	T	1269	CDL	C43-C42-C41	2.26	125.81	114.37
22	B	1085	CHD	O26-C24-C23	2.26	121.15	114.00
22	C	525	CHD	C21-C20-C17	-2.26	109.49	112.88
14	N	516	HEA	C4B-C3B-C2B	-2.26	103.65	107.44
22	C	271	CHD	C14-C8-C9	2.26	112.90	109.75
24	C	264	PEK	C11-C10-C9	2.26	123.13	112.02
24	T	263	PEK	C02-O01-C1	2.25	123.19	117.80
19	L	522	TGL	C26-C25-C24	-2.25	102.98	114.37
19	L	522	TGL	CA3-CA2-CA1	-2.25	105.45	113.69
14	N	516	HEA	C3A-C2A-C1A	-2.25	104.92	107.05
20	C	268	PGV	O01-C02-C01	2.25	116.41	108.34
20	C	267	PGV	C14-C13-C12	-2.25	100.01	112.60
28	G	272	DMU	O61-C57-C4	2.25	118.98	111.33
19	D	523	TGL	CG3-OG3-CC1	2.24	125.30	117.12
22	P	1271	CHD	C11-C9-C10	-2.24	111.43	113.70
22	B	1085	CHD	C22-C23-C24	-2.23	106.53	112.49
20	A	524	PGV	C01-O03-C19	2.23	125.28	117.12
19	D	523	TGL	C13-C12-C11	2.23	125.65	114.37
20	P	1267	PGV	O02-C1-C2	2.23	132.51	123.78
25	P	1270	CDL	CB4-OB6-CB5	-2.23	112.46	117.80
20	A	522	PGV	C7-C6-C5	-2.23	103.11	114.37
25	T	1269	CDL	OA8-CA7-OA9	-2.23	118.06	123.63
22	B	1085	CHD	C16-C17-C13	2.23	105.70	103.54
22	P	1525	CHD	C15-C14-C8	2.23	121.41	118.36
25	P	1270	CDL	C40-C39-C38	2.23	125.62	114.37
14	N	516	HEA	C3C-C2C-C1C	-2.22	104.55	107.17
26	R	1229	PSC	O01-C1-O02	-2.22	118.51	123.70
22	J	60	CHD	O12-C12-C11	-2.22	104.60	109.12
28	Z	1526	DMU	C11-C9-C8	2.22	118.47	113.02
25	C	270	CDL	OA8-CA6-CA4	2.22	114.79	108.40
14	N	515	HEA	C12-C11-C3B	2.22	115.59	112.12
24	S	1265	PEK	P-O11-C03	2.22	134.06	121.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	264	PEK	C26-C25-C24	-2.22	103.16	114.37
22	P	1525	CHD	C22-C23-C24	-2.22	106.58	112.49
19	A	521	TGL	C16-C15-CC9	2.21	125.56	114.37
28	P	1272	DMU	C10-C5-C7	2.21	114.67	110.01
14	N	515	HEA	C26-C15-C16	2.21	119.06	115.23
14	A	516	HEA	CHC-C1C-C2C	-2.21	121.02	127.43
19	A	521	TGL	OB1-CB1-CB2	-2.21	115.15	123.78
20	P	1268	PGV	O01-C02-C03	2.21	116.26	108.34
14	N	515	HEA	C4B-NB-C1B	2.20	107.82	105.21
14	N	515	HEA	C2C-C1C-NC	2.20	113.67	110.14
22	P	1525	CHD	C9-C10-C5	2.19	111.56	108.51
24	G	1263	PEK	C01-O03-C21	2.19	125.13	117.12
25	P	1270	CDL	C42-C41-C40	2.19	125.45	114.37
14	N	515	HEA	C3B-C4B-NB	-2.19	107.32	109.84
20	N	1266	PGV	O02-C1-C2	2.19	132.34	123.78
25	G	269	CDL	C43-C42-C41	2.18	125.41	114.37
14	N	516	HEA	O2A-CGA-O1A	-2.18	117.72	123.33
19	D	523	TGL	OG1-CA1-OA1	-2.17	118.19	123.63
28	P	1272	DMU	O61-C57-C4	2.17	118.73	111.33
25	T	1269	CDL	OA6-CA5-OA7	-2.17	118.63	123.70
25	P	1270	CDL	C52-C51-CB5	-2.17	105.74	113.69
19	Q	1523	TGL	OG1-CA1-OA1	-2.17	118.20	123.63
19	D	523	TGL	OG3-CC1-CC2	2.16	118.44	111.83
24	T	1264	PEK	C30-C29-C28	-2.16	103.43	114.37
22	P	1525	CHD	C21-C20-C17	2.16	116.13	112.88
14	N	515	HEA	C3C-C4C-NC	2.16	111.62	109.80
22	O	229	CHD	C19-C10-C1	2.15	111.72	108.31
14	A	516	HEA	CHB-C1B-NB	-2.14	122.12	124.42
25	C	270	CDL	OA6-CA5-OA7	-2.14	118.70	123.70
19	L	522	TGL	C24-C23-C22	-2.14	103.56	114.37
26	E	229	PSC	O01-C02-C03	2.13	116.00	108.34
19	N	1521	TGL	CC4-CC3-CC2	-2.13	105.30	113.13
25	P	1270	CDL	OA8-CA6-CA4	2.13	114.54	108.40
25	C	270	CDL	C57-C56-C55	-2.13	103.61	114.37
22	J	60	CHD	O7-C7-C8	-2.13	104.64	109.52
26	R	1229	PSC	O01-C02-C03	2.13	115.98	108.34
22	O	229	CHD	O7-C7-C6	-2.12	104.57	109.86
14	N	516	HEA	CHA-C1A-C2A	-2.12	121.51	124.86
22	W	1059	CHD	C23-C22-C20	-2.12	110.50	114.46
19	N	1521	TGL	C16-C15-CC9	2.11	125.05	114.37
19	L	522	TGL	OG3-CG3-CG2	2.11	114.47	108.40
20	N	1524	PGV	O03-C19-O04	-2.10	118.37	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	D	523	TGL	OG3-CC1-OC1	-2.10	118.37	123.63
22	W	1059	CHD	C16-C17-C20	2.10	115.35	112.18
25	C	270	CDL	C61-C60-C59	-2.10	103.77	114.37
19	N	1521	TGL	OG3-CC1-OC1	-2.10	118.39	123.63
20	P	1268	PGV	O12-P-O13	-2.09	100.63	108.94
19	N	1522	TGL	C16-C15-CC9	2.09	124.92	114.37
19	L	522	TGL	CB9-CB8-CB7	-2.08	103.84	114.37
24	C	264	PEK	C27-C26-C25	-2.08	103.85	114.37
14	A	515	HEA	CMC-C2C-C1C	-2.08	122.25	125.42
22	P	1271	CHD	C13-C14-C8	2.08	117.35	114.72
22	P	1525	CHD	C16-C17-C20	2.08	115.32	112.18
14	A	516	HEA	CBA-CAA-C2A	-2.07	106.80	112.53
19	N	1521	TGL	CG1-OG1-CA1	2.07	124.69	117.12
19	A	521	TGL	OA1-CA1-CA2	-2.07	115.69	123.78
22	B	1085	CHD	O25-C24-C23	-2.07	116.54	123.09
20	P	1267	PGV	O06-C06-C05	-2.06	101.08	110.38
14	N	515	HEA	C4A-NA-C1A	2.06	109.18	105.82
28	M	526	DMU	O49-C1-C2	2.06	115.24	110.38
20	A	522	PGV	C21-C20-C19	-2.06	106.14	113.69
25	C	270	CDL	C79-C78-C77	2.05	124.75	114.37
25	P	1270	CDL	C82-C81-C80	2.05	124.72	114.37
26	E	229	PSC	O03-C19-C20	2.05	118.08	111.83
25	P	1270	CDL	C55-C54-C53	-2.05	104.03	114.37
24	T	1264	PEK	O13-P-O14	2.04	121.94	112.44
20	C	267	PGV	C02-O01-C1	2.04	122.68	117.80
19	A	521	TGL	CC3-CC2-CC1	2.04	121.16	113.69
14	N	516	HEA	C1B-C2B-C3B	-2.04	104.44	106.80
25	G	269	CDL	C18-C17-C16	-2.03	104.12	114.37
22	P	1525	CHD	O26-C24-O25	-2.03	118.12	123.33
14	N	516	HEA	CMD-C2D-C3D	-2.03	120.67	126.15
24	G	1263	PEK	O01-C1-O02	-2.02	118.98	123.70
22	J	60	CHD	O12-C12-C13	-2.02	107.61	111.02
22	P	1525	CHD	C6-C5-C4	-2.02	108.92	111.23
25	T	1269	CDL	C80-C79-C78	2.01	124.55	114.37
20	P	1267	PGV	C02-O01-C1	2.01	122.62	117.80
24	T	1264	PEK	C28-C27-C26	-2.01	104.19	114.37
22	C	271	CHD	C13-C17-C20	2.01	121.92	119.48
26	E	229	PSC	C3-C2-C1	2.00	121.04	113.69

All (27) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
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Mol	Chain	Res	Type	Atom
22	C	271	CHD	C9
22	J	60	CHD	C17
22	J	60	CHD	C9
22	P	1271	CHD	C9
22	W	1059	CHD	C17
22	W	1059	CHD	C9
28	G	272	DMU	C9
28	G	272	DMU	C4
28	G	272	DMU	C3
28	G	272	DMU	C6
28	G	272	DMU	C5
28	G	272	DMU	C2
28	M	526	DMU	C5
28	M	526	DMU	C9
28	M	526	DMU	C4
28	M	526	DMU	C2
28	P	1272	DMU	C9
28	P	1272	DMU	C4
28	P	1272	DMU	C10
28	P	1272	DMU	C6
28	P	1272	DMU	C5
28	P	1272	DMU	C2
28	Z	1526	DMU	C9
28	Z	1526	DMU	C4
28	Z	1526	DMU	C6
28	Z	1526	DMU	C5
28	Z	1526	DMU	C2

All (1006) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	516	HEA	C2A-C3A-CMA-OMA
14	A	516	HEA	C4A-C3A-CMA-OMA
14	A	516	HEA	C2D-C3D-CAD-CBD
14	N	515	HEA	C2A-C3A-CMA-OMA
14	N	515	HEA	C4A-C3A-CMA-OMA
14	N	515	HEA	C26-C15-C16-C17
14	N	516	HEA	C2D-C3D-CAD-CBD
14	N	516	HEA	C4D-C3D-CAD-CBD
19	A	521	TGL	OB1-CB1-OG2-CG2
19	A	521	TGL	CC2-CC1-OG3-CG3

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Mol	Chain	Res	Type	Atoms
19	A	521	TGL	OC1-CC1-OG3-CG3
19	Q	1523	TGL	CC2-CC1-OG3-CG3
20	A	524	PGV	C04-O12-P-O11
20	A	524	PGV	C04-O12-P-O13
20	A	524	PGV	C04-O12-P-O14
20	A	524	PGV	C02-C03-O11-P
20	A	524	PGV	C04-C05-C06-O06
20	A	524	PGV	O02-C1-O01-C02
20	C	268	PGV	C04-C05-C06-O06
20	C	268	PGV	C2-C1-O01-C02
20	N	1524	PGV	C03-O11-P-O13
20	N	1524	PGV	C04-O12-P-O11
20	N	1524	PGV	C02-C03-O11-P
20	N	1524	PGV	O02-C1-O01-C02
20	N	1524	PGV	C2-C1-O01-C02
20	P	1268	PGV	O12-C04-C05-C06
20	P	1268	PGV	C2-C1-O01-C02
22	W	1059	CHD	C13-C17-C20-C22
22	W	1059	CHD	C16-C17-C20-C21
22	W	1059	CHD	C16-C17-C20-C22
24	C	264	PEK	O12-C04-C05-N
24	C	264	PEK	C11-C12-C13-C14
24	G	265	PEK	O12-C04-C05-N
24	G	1263	PEK	C03-O11-P-O12
24	G	1263	PEK	C03-O11-P-O13
24	G	1263	PEK	O12-C04-C05-N
24	S	1265	PEK	C04-O12-P-O11
24	S	1265	PEK	C04-O12-P-O13
24	S	1265	PEK	C04-O12-P-O14
24	S	1265	PEK	O12-C04-C05-N
24	T	263	PEK	C03-O11-P-O12
24	T	263	PEK	C03-O11-P-O13
24	T	263	PEK	C04-O12-P-O13
24	T	1264	PEK	C11-C12-C13-C14
24	T	1264	PEK	C12-C13-C14-C15
25	C	270	CDL	CB2-C1-CA2-OA2
25	C	270	CDL	O1-C1-CB2-OB2
25	C	270	CDL	CA2-OA2-PA1-OA3
25	C	270	CDL	CA2-OA2-PA1-OA4
25	C	270	CDL	CA2-OA2-PA1-OA5
25	C	270	CDL	CA3-OA5-PA1-OA2
25	C	270	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
25	G	269	CDL	O1-C1-CA2-OA2
25	G	269	CDL	CA2-C1-CB2-OB2
25	G	269	CDL	OA9-CA7-OA8-CA6
25	G	269	CDL	C31-CA7-OA8-CA6
25	G	269	CDL	C1-CB2-OB2-PB2
25	G	269	CDL	CB3-OB5-PB2-OB2
25	G	269	CDL	CB3-OB5-PB2-OB3
25	G	269	CDL	CB3-OB5-PB2-OB4
25	P	1270	CDL	CA2-OA2-PA1-OA3
25	P	1270	CDL	CA2-OA2-PA1-OA4
25	P	1270	CDL	CA2-OA2-PA1-OA5
25	P	1270	CDL	CA3-OA5-PA1-OA2
25	P	1270	CDL	C11-CA5-OA6-CA4
25	P	1270	CDL	CB2-OB2-PB2-OB3
25	P	1270	CDL	CB2-OB2-PB2-OB4
25	T	1269	CDL	C1-CB2-OB2-PB2
25	T	1269	CDL	CB3-OB5-PB2-OB2
25	T	1269	CDL	CB3-OB5-PB2-OB3
25	T	1269	CDL	CB3-OB5-PB2-OB4
26	E	229	PSC	C04-O12-P-O11
26	E	229	PSC	C04-O12-P-O13
26	E	229	PSC	C04-O12-P-O14
26	E	229	PSC	C2-C1-O01-C02
26	R	1229	PSC	C03-O11-P-O14
26	R	1229	PSC	C04-O12-P-O11
26	R	1229	PSC	C04-O12-P-O13
26	R	1229	PSC	C04-O12-P-O14
26	R	1229	PSC	O02-C1-O01-C02
28	G	272	DMU	C1-C6-O16-C18
28	M	526	DMU	O5-C6-O16-C18
28	Z	1526	DMU	C19-C18-O16-C6
19	Q	1523	TGL	OC1-CC1-OG3-CG3
20	A	524	PGV	O04-C19-O03-C01
19	D	523	TGL	CC2-CC1-OG3-CG3
20	A	524	PGV	C20-C19-O03-C01
19	D	523	TGL	OC1-CC1-OG3-CG3
22	C	271	CHD	C16-C17-C20-C21
22	P	1271	CHD	C16-C17-C20-C21
22	P	1271	CHD	C16-C17-C20-C22
26	R	1229	PSC	O04-C19-O03-C01
19	L	522	TGL	OB1-CB1-OG2-CG2
25	C	270	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
25	P	1270	CDL	OA7-CA5-OA6-CA4
25	P	1270	CDL	OB7-CB5-OB6-CB4
26	E	229	PSC	O02-C1-O01-C02
20	N	1524	PGV	C20-C19-O03-C01
19	L	522	TGL	CB2-CB1-OG2-CG2
20	A	524	PGV	C2-C1-O01-C02
25	P	1270	CDL	C51-CB5-OB6-CB4
26	R	1229	PSC	C2-C1-O01-C02
22	J	60	CHD	C16-C17-C20-C22
14	N	515	HEA	C14-C15-C16-C17
19	L	522	TGL	CA2-CA1-OG1-CG1
19	N	1522	TGL	CA2-CA1-OG1-CG1
26	E	229	PSC	C20-C19-O03-C01
26	R	1229	PSC	C20-C19-O03-C01
20	C	267	PGV	C10-C11-C12-C13
20	P	1267	PGV	C10-C11-C12-C13
24	C	264	PEK	C10-C11-C12-C13
24	C	264	PEK	C13-C14-C15-C16
24	G	1263	PEK	C7-C8-C9-C10
24	T	263	PEK	C4-C5-C6-C7
24	T	1264	PEK	C7-C8-C9-C10
19	N	1522	TGL	OA1-CA1-OG1-CG1
20	N	1524	PGV	O04-C19-O03-C01
14	A	516	HEA	C4D-C3D-CAD-CBD
20	C	268	PGV	O02-C1-O01-C02
20	P	1268	PGV	O02-C1-O01-C02
28	G	272	DMU	O6-C11-C9-O1
20	N	1524	PGV	O12-C04-C05-O05
25	T	1269	CDL	O1-C1-CA2-OA2
25	T	1269	CDL	C31-CA7-OA8-CA6
25	T	1269	CDL	C71-CB7-OB8-CB6
28	M	526	DMU	O5-C4-C57-O61
28	Z	1526	DMU	O5-C4-C57-O61
28	P	1272	DMU	C3-C4-C57-O61
19	A	521	TGL	CB2-CB1-OG2-CG2
25	T	1269	CDL	C11-CA5-OA6-CA4
22	P	1271	CHD	C21-C20-C22-C23
26	E	229	PSC	O04-C19-O03-C01
28	Z	1526	DMU	O6-C11-C9-O1
24	T	1264	PEK	C1-C2-C3-C4
22	C	271	CHD	C16-C17-C20-C22
26	R	1229	PSC	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
25	T	1269	CDL	OA9-CA7-OA8-CA6
25	T	1269	CDL	OB9-CB7-OB8-CB6
19	N	1522	TGL	CC1-CC2-CC3-CC4
19	L	522	TGL	OA1-CA1-OG1-CG1
28	P	1272	DMU	O5-C6-O16-C18
19	A	521	TGL	C13-C14-C29-C30
19	N	1522	TGL	CC3-CC4-CC5-CC6
25	C	270	CDL	C62-C63-C64-C65
19	L	522	TGL	CC1-CC2-CC3-CC4
22	C	271	CHD	C17-C20-C22-C23
20	P	1268	PGV	C10-C11-C12-C13
24	G	1263	PEK	C4-C5-C6-C7
24	S	1265	PEK	C4-C5-C6-C7
24	T	263	PEK	C7-C8-C9-C10
24	T	263	PEK	C13-C14-C15-C16
24	T	1264	PEK	C13-C14-C15-C16
24	S	1265	PEK	C34-C35-C36-C37
25	C	270	CDL	C38-C39-C40-C41
19	N	1522	TGL	CB2-CB1-OG2-CG2
26	R	1229	PSC	C20-C21-C22-C23
19	N	1522	TGL	OB1-CB1-OG2-CG2
25	T	1269	CDL	OA7-CA5-OA6-CA4
20	A	524	PGV	O12-C04-C05-C06
20	N	1524	PGV	O12-C04-C05-C06
25	C	270	CDL	CA2-C1-CB2-OB2
25	P	1270	CDL	CB2-C1-CA2-OA2
20	C	268	PGV	C20-C19-O03-C01
19	A	521	TGL	CB6-CB7-CB8-CB9
19	D	523	TGL	C17-C18-C19-C33
19	L	522	TGL	CB3-CB4-CB5-CB6
19	L	522	TGL	CC3-CC4-CC5-CC6
20	C	268	PGV	C20-C21-C22-C23
26	E	229	PSC	C20-C21-C22-C23
22	P	1271	CHD	C17-C20-C22-C23
19	A	521	TGL	C21-C20-CA9-CA8
19	N	1521	TGL	C13-C14-C29-C30
25	T	1269	CDL	C79-C80-C81-C82
19	N	1521	TGL	CB1-CB2-CB3-CB4
22	C	271	CHD	C21-C20-C22-C23
20	P	1268	PGV	O12-C04-C05-O05
25	G	269	CDL	O1-C1-CB2-OB2
25	P	1270	CDL	O1-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
20	C	268	PGV	O01-C02-C03-O11
25	P	1270	CDL	C23-C24-C25-C26
19	D	523	TGL	OG1-CG1-CG2-OG2
25	G	269	CDL	C71-CB7-OB8-CB6
19	D	523	TGL	CB9-C10-C11-C12
24	C	264	PEK	C7-C8-C9-C10
24	S	1265	PEK	C10-C11-C12-C13
20	N	1524	PGV	O05-C05-C06-O06
25	T	1269	CDL	CA5-C11-C12-C13
26	R	1229	PSC	C1-C2-C3-C4
20	P	1267	PGV	C12-C13-C14-C15
20	C	268	PGV	O04-C19-O03-C01
22	J	60	CHD	C13-C17-C20-C22
19	D	523	TGL	C13-C14-C29-C30
19	Q	1523	TGL	C13-C14-C29-C30
25	G	269	CDL	C78-C79-C80-C81
19	A	521	TGL	CA2-CA1-OG1-CG1
28	M	526	DMU	O6-C11-C9-O1
20	N	1524	PGV	C20-C21-C22-C23
25	P	1270	CDL	C40-C41-C42-C43
24	G	1263	PEK	C33-C34-C35-C36
28	P	1272	DMU	O6-C11-C9-C8
25	C	270	CDL	C14-C15-C16-C17
28	M	526	DMU	O6-C11-C9-C8
25	P	1270	CDL	CA5-C11-C12-C13
25	P	1270	CDL	CB7-C71-C72-C73
25	T	1269	CDL	CB5-C51-C52-C53
26	R	1229	PSC	C19-C20-C21-C22
25	T	1269	CDL	CB4-CB3-OB5-PB2
20	C	268	PGV	C1-C2-C3-C4
25	G	269	CDL	CB5-C51-C52-C53
25	T	1269	CDL	CA7-C31-C32-C33
26	E	229	PSC	C1-C2-C3-C4
28	Z	1526	DMU	O5-C6-O16-C18
19	Q	1523	TGL	CB9-C10-C11-C12
20	A	524	PGV	O12-C04-C05-O05
20	C	268	PGV	O12-C04-C05-O05
25	C	270	CDL	O1-C1-CA2-OA2
25	P	1270	CDL	O1-C1-CB2-OB2
25	T	1269	CDL	O1-C1-CB2-OB2
19	N	1521	TGL	OC1-CC1-OG3-CG3
25	G	269	CDL	CA5-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
24	T	263	PEK	C33-C34-C35-C36
24	T	1264	PEK	C4-C5-C6-C7
26	R	1229	PSC	C11-C10-C9-C8
19	A	521	TGL	OA1-CA1-OG1-CG1
28	P	1272	DMU	O16-C18-C19-C22
19	N	1521	TGL	CC2-CC1-OG3-CG3
22	J	60	CHD	C16-C17-C20-C21
22	J	60	CHD	C13-C17-C20-C21
19	D	523	TGL	CB1-CB2-CB3-CB4
20	C	268	PGV	O12-C04-C05-C06
25	P	1270	CDL	CA2-C1-CB2-OB2
25	T	1269	CDL	CA2-C1-CB2-OB2
26	R	1229	PSC	C04-C05-N-C06
20	C	267	PGV	C12-C13-C14-C15
28	G	272	DMU	C3-C4-C57-O61
20	A	524	PGV	C2-C3-C4-C5
25	C	270	CDL	C53-C54-C55-C56
28	P	1272	DMU	C1-C6-O16-C18
24	G	265	PEK	C13-C14-C15-C16
25	C	270	CDL	C60-C61-C62-C63
20	A	524	PGV	C19-C20-C21-C22
14	N	516	HEA	C19-C20-C21-C22
25	G	269	CDL	OB9-CB7-OB8-CB6
20	N	1524	PGV	C04-C05-C06-O06
19	Q	1523	TGL	CG3-CG2-OG2-CB1
25	G	269	CDL	C15-C16-C17-C18
28	G	272	DMU	O5-C4-C57-O61
22	W	1059	CHD	C17-C20-C22-C23
25	G	269	CDL	C11-CA5-OA6-CA4
26	R	1229	PSC	C04-C05-N-C07
19	N	1522	TGL	C12-C13-C14-C29
19	Q	1523	TGL	CC6-CC7-CC8-CC9
25	T	1269	CDL	C36-C37-C38-C39
19	N	1521	TGL	CA7-CA8-CA9-C20
19	N	1522	TGL	CA2-CA3-CA4-CA5
19	Q	1523	TGL	C11-C10-CB9-CB8
24	C	264	PEK	C16-C17-C18-C19
25	C	270	CDL	C23-C24-C25-C26
25	P	1270	CDL	C11-C12-C13-C14
26	R	1229	PSC	C2-C3-C4-C5
19	Q	1523	TGL	CB1-CB2-CB3-CB4
24	G	265	PEK	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
26	E	229	PSC	C11-C10-C9-C8
19	A	521	TGL	CA3-CA4-CA5-CA6
19	N	1521	TGL	CA4-CA5-CA6-CA7
20	C	268	PGV	C23-C24-C25-C26
25	C	270	CDL	C35-C36-C37-C38
25	C	270	CDL	C39-C40-C41-C42
25	C	270	CDL	C51-C52-C53-C54
26	E	229	PSC	C29-C30-C31-C32
24	G	1263	PEK	C22-C21-O03-C01
19	D	523	TGL	C10-C11-C12-C13
19	L	522	TGL	CC6-CC7-CC8-CC9
19	N	1521	TGL	C12-C13-C14-C29
19	Q	1523	TGL	C21-C22-C23-C24
19	Q	1523	TGL	C23-C24-C25-C26
20	P	1268	PGV	C22-C23-C24-C25
25	G	269	CDL	C72-C73-C74-C75
25	G	269	CDL	C77-C78-C79-C80
25	P	1270	CDL	C13-C14-C15-C16
25	P	1270	CDL	C16-C17-C18-C19
25	P	1270	CDL	C79-C80-C81-C82
26	R	1229	PSC	C3-C4-C5-C6
20	A	524	PGV	O05-C05-C06-O06
20	C	268	PGV	O05-C05-C06-O06
19	D	523	TGL	CA6-CA7-CA8-CA9
19	N	1522	TGL	CB4-CB5-CB6-CB7
19	N	1522	TGL	CC4-CC5-CC6-CC7
20	A	524	PGV	C22-C23-C24-C25
20	A	522	PGV	C23-C24-C25-C26
24	G	265	PEK	C26-C27-C28-C29
24	T	263	PEK	C16-C17-C18-C19
25	C	270	CDL	C41-C42-C43-C44
26	R	1229	PSC	C4-C5-C6-C7
19	N	1521	TGL	CB3-CB4-CB5-CB6
24	G	265	PEK	C28-C29-C30-C31
25	P	1270	CDL	C83-C84-C85-C86
28	G	272	DMU	C28-C31-C34-C37
25	C	270	CDL	C51-CB5-OB6-CB4
20	N	1524	PGV	C4-C5-C6-C7
19	N	1522	TGL	C21-C22-C23-C24
25	P	1270	CDL	C77-C78-C79-C80
19	N	1522	TGL	C23-C24-C25-C26
20	P	1268	PGV	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
25	P	1270	CDL	C72-C73-C74-C75
25	P	1270	CDL	C73-C74-C75-C76
25	P	1270	CDL	C82-C83-C84-C85
25	T	1269	CDL	C54-C55-C56-C57
25	T	1269	CDL	C55-C56-C57-C58
25	T	1269	CDL	C56-C57-C58-C59
19	L	522	TGL	C12-C13-C14-C29
20	A	522	PGV	C29-C30-C31-C32
25	P	1270	CDL	C74-C75-C76-C77
19	N	1521	TGL	CB6-CB7-CB8-CB9
25	P	1270	CDL	C58-C59-C60-C61
25	T	1269	CDL	C19-C20-C21-C22
25	G	269	CDL	OA7-CA5-OA6-CA4
24	T	263	PEK	C22-C21-O03-C01
25	P	1270	CDL	CA3-CA4-CA6-OA8
19	N	1521	TGL	CA3-CA4-CA5-CA6
24	G	1263	PEK	C25-C26-C27-C28
25	T	1269	CDL	C59-C60-C61-C62
20	C	268	PGV	C5-C6-C7-C8
20	C	268	PGV	C22-C23-C24-C25
20	P	1267	PGV	C13-C14-C15-C16
24	G	265	PEK	C29-C30-C31-C32
24	S	1265	PEK	C29-C30-C31-C32
25	C	270	CDL	C43-C44-C45-C46
25	C	270	CDL	C81-C82-C83-C84
25	G	269	CDL	C79-C80-C81-C82
19	N	1521	TGL	C20-C21-C22-C23
25	G	269	CDL	C55-C56-C57-C58
28	P	1272	DMU	C25-C28-C31-C34
19	N	1522	TGL	CC9-C15-C16-C17
20	C	267	PGV	C7-C8-C9-C10
24	G	265	PEK	C25-C26-C27-C28
24	G	265	PEK	C31-C32-C33-C34
26	R	1229	PSC	C04-C05-N-C08
19	N	1522	TGL	C10-C11-C12-C13
20	C	268	PGV	C14-C15-C16-C17
28	G	272	DMU	C31-C34-C37-C40
19	N	1521	TGL	C21-C20-CA9-CA8
24	G	1263	PEK	C16-C17-C18-C19
24	T	263	PEK	C31-C32-C33-C34
25	C	270	CDL	C21-C22-C23-C24
25	T	1269	CDL	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
20	A	524	PGV	C11-C10-C9-C8
19	N	1522	TGL	C25-C26-C27-C28
24	G	1263	PEK	C10-C11-C12-C13
24	S	1265	PEK	C7-C8-C9-C10
26	R	1229	PSC	C11-C12-C13-C14
20	N	1524	PGV	C14-C15-C16-C17
24	G	1263	PEK	C23-C24-C25-C26
24	T	263	PEK	C34-C35-C36-C37
25	P	1270	CDL	C81-C82-C83-C84
19	A	521	TGL	C16-C17-C18-C19
22	P	1271	CHD	C20-C22-C23-C24
19	L	522	TGL	C25-C26-C27-C28
19	D	523	TGL	C14-C29-C30-C31
19	Q	1523	TGL	CB2-CB3-CB4-CB5
24	G	1263	PEK	O04-C21-O03-C01
19	Q	1523	TGL	C10-C11-C12-C13
20	C	267	PGV	C13-C14-C15-C16
20	P	1267	PGV	C7-C8-C9-C10
25	T	1269	CDL	C17-C18-C19-C20
19	N	1521	TGL	OB1-CB1-OG2-CG2
25	C	270	CDL	OB7-CB5-OB6-CB4
20	A	522	PGV	C4-C5-C6-C7
20	N	1266	PGV	C7-C8-C9-C10
25	C	270	CDL	C18-C19-C20-C21
25	C	270	CDL	C61-C62-C63-C64
25	P	1270	CDL	C42-C43-C44-C45
25	T	1269	CDL	C40-C41-C42-C43
19	D	523	TGL	C11-C10-CB9-CB8
19	N	1521	TGL	CC7-CC8-CC9-C15
19	Q	1523	TGL	CC7-CC8-CC9-C15
24	T	263	PEK	C25-C26-C27-C28
25	P	1270	CDL	C36-C37-C38-C39
28	P	1272	DMU	C5-C10-O7-C3
24	G	1263	PEK	C24-C25-C26-C27
19	A	521	TGL	C17-C18-C19-C33
19	Q	1523	TGL	C12-C13-C14-C29
20	N	1266	PGV	C6-C7-C8-C9
24	T	263	PEK	C30-C31-C32-C33
25	C	270	CDL	C31-C32-C33-C34
25	C	270	CDL	C72-C73-C74-C75
25	P	1270	CDL	C38-C39-C40-C41
28	G	272	DMU	O5-C6-O16-C18

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Mol	Chain	Res	Type	Atoms
19	A	521	TGL	CG2-CG3-OG3-CC1
19	Q	1523	TGL	CC9-C15-C16-C17
20	C	268	PGV	C30-C31-C32-C33
25	C	270	CDL	C63-C64-C65-C66
19	N	1521	TGL	C11-C12-C13-C14
25	G	269	CDL	C61-C62-C63-C64
19	L	522	TGL	C22-C23-C24-C25
25	P	1270	CDL	C59-C60-C61-C62
25	G	269	CDL	C76-C77-C78-C79
28	P	1272	DMU	O6-C11-C9-O1
19	N	1521	TGL	CB2-CB1-OG2-CG2
19	N	1521	TGL	C17-C18-C19-C33
19	N	1522	TGL	C21-C20-CA9-CA8
19	N	1522	TGL	CA9-C20-C21-C22
20	C	268	PGV	C12-C13-C14-C15
20	P	1268	PGV	C11-C10-C9-C8
24	G	265	PEK	C2-C3-C4-C5
19	N	1521	TGL	C25-C26-C27-C28
24	T	263	PEK	O04-C21-O03-C01
19	Q	1523	TGL	C18-C19-C33-C34
20	A	522	PGV	C19-C20-C21-C22
20	P	1267	PGV	C1-C2-C3-C4
24	S	1265	PEK	C33-C34-C35-C36
25	G	269	CDL	C56-C57-C58-C59
25	G	269	CDL	C57-C58-C59-C60
25	T	1269	CDL	C12-C13-C14-C15
25	T	1269	CDL	C63-C64-C65-C66
19	L	522	TGL	CA5-CA6-CA7-CA8
28	Z	1526	DMU	C28-C31-C34-C37
22	W	1059	CHD	C13-C17-C20-C21
19	L	522	TGL	C17-C18-C19-C33
28	Z	1526	DMU	C25-C28-C31-C34
19	A	521	TGL	C15-C16-C17-C18
25	C	270	CDL	C16-C17-C18-C19
25	G	269	CDL	C18-C19-C20-C21
19	L	522	TGL	C16-C15-CC9-CC8
25	C	270	CDL	C40-C41-C42-C43
19	Q	1523	TGL	C21-C20-CA9-CA8
20	N	1524	PGV	C2-C3-C4-C5
20	P	1268	PGV	O01-C02-C03-O11
19	D	523	TGL	C21-C20-CA9-CA8
19	D	523	TGL	CB2-CB3-CB4-CB5

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Mol	Chain	Res	Type	Atoms
19	N	1521	TGL	C16-C17-C18-C19
20	A	524	PGV	C24-C25-C26-C27
25	G	269	CDL	C33-C34-C35-C36
25	G	269	CDL	C62-C63-C64-C65
19	A	521	TGL	CA4-CA5-CA6-CA7
19	N	1521	TGL	C14-C29-C30-C31
25	C	270	CDL	C11-C12-C13-C14
19	Q	1523	TGL	OG1-CG1-CG2-OG2
24	C	264	PEK	C15-C16-C17-C18
24	G	265	PEK	C15-C16-C17-C18
24	G	1263	PEK	O03-C01-C02-O01
24	G	1263	PEK	C2-C3-C4-C5
19	Q	1523	TGL	CA4-CA5-CA6-CA7
20	N	1524	PGV	C7-C8-C9-C10
20	N	1266	PGV	C29-C30-C31-C32
25	C	270	CDL	C71-C72-C73-C74
25	G	269	CDL	C83-C84-C85-C86
24	G	265	PEK	C22-C21-O03-C01
19	D	523	TGL	C23-C24-C25-C26
19	N	1521	TGL	CB9-C10-C11-C12
25	P	1270	CDL	C35-C36-C37-C38
25	T	1269	CDL	C71-C72-C73-C74
25	T	1269	CDL	CB7-C71-C72-C73
19	D	523	TGL	C16-C17-C18-C19
19	L	522	TGL	C10-C11-C12-C13
26	E	229	PSC	C5-C6-C7-C8
19	A	521	TGL	CC4-CC5-CC6-CC7
19	L	522	TGL	C21-C22-C23-C24
24	T	263	PEK	C22-C23-C24-C25
24	T	1264	PEK	C26-C27-C28-C29
25	T	1269	CDL	C35-C36-C37-C38
19	N	1522	TGL	C22-C23-C24-C25
20	N	1266	PGV	C5-C6-C7-C8
24	C	264	PEK	C34-C35-C36-C37
24	G	1263	PEK	C31-C32-C33-C34
25	G	269	CDL	C14-C15-C16-C17
20	P	1268	PGV	C30-C31-C32-C33
25	C	270	CDL	C19-C20-C21-C22
25	G	269	CDL	C37-C38-C39-C40
25	G	269	CDL	C38-C39-C40-C41
24	T	1264	PEK	C10-C11-C12-C13
19	Q	1523	TGL	C17-C18-C19-C33

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Mol	Chain	Res	Type	Atoms
25	T	1269	CDL	C74-C75-C76-C77
20	C	268	PGV	C11-C10-C9-C8
19	D	523	TGL	CA4-CA5-CA6-CA7
20	C	268	PGV	C4-C5-C6-C7
24	T	1264	PEK	C25-C26-C27-C28
20	C	268	PGV	C01-C02-C03-O11
24	T	263	PEK	C01-C02-C03-O11
25	T	1269	CDL	OB5-CB3-CB4-CB6
19	A	521	TGL	CB5-CB6-CB7-CB8
25	G	269	CDL	C54-C55-C56-C57
25	C	270	CDL	C59-C60-C61-C62
26	E	229	PSC	C24-C25-C26-C27
19	L	522	TGL	C11-C10-CB9-CB8
24	G	265	PEK	C1-C2-C3-C4
19	L	522	TGL	CB5-CB6-CB7-CB8
20	A	524	PGV	C26-C27-C28-C29
24	G	265	PEK	C24-C25-C26-C27
25	G	269	CDL	C36-C37-C38-C39
25	G	269	CDL	C59-C60-C61-C62
24	G	265	PEK	C10-C11-C12-C13
19	A	521	TGL	OG1-CG1-CG2-CG3
19	D	523	TGL	OG1-CG1-CG2-CG3
19	Q	1523	TGL	OG1-CG1-CG2-CG3
20	N	1524	PGV	O03-C01-C02-C03
25	C	270	CDL	CB3-CB4-CB6-OB8
26	E	229	PSC	O03-C01-C02-C03
26	R	1229	PSC	O03-C01-C02-C03
20	P	1267	PGV	C28-C29-C30-C31
25	C	270	CDL	C79-C80-C81-C82
20	N	1524	PGV	C12-C13-C14-C15
26	R	1229	PSC	C24-C25-C26-C27
19	L	522	TGL	C21-C20-CA9-CA8
20	N	1524	PGV	C5-C6-C7-C8
25	C	270	CDL	C71-CB7-OB8-CB6
19	N	1521	TGL	CA6-CA7-CA8-CA9
20	N	1266	PGV	C26-C27-C28-C29
24	C	264	PEK	C25-C26-C27-C28
26	R	1229	PSC	C27-C28-C29-C30
25	G	269	CDL	C13-C14-C15-C16
25	G	269	CDL	C40-C41-C42-C43
25	P	1270	CDL	C19-C20-C21-C22
20	A	522	PGV	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
25	T	1269	CDL	C62-C63-C64-C65
20	P	1267	PGV	C25-C26-C27-C28
25	T	1269	CDL	C16-C17-C18-C19
24	G	265	PEK	O04-C21-O03-C01
25	C	270	CDL	C17-C18-C19-C20
25	C	270	CDL	C42-C43-C44-C45
20	P	1267	PGV	C20-C21-C22-C23
20	P	1268	PGV	C1-C2-C3-C4
24	G	1263	PEK	C1-C2-C3-C4
19	A	521	TGL	CA5-CA6-CA7-CA8
19	A	521	TGL	CC7-CC8-CC9-C15
19	N	1521	TGL	C15-C16-C17-C18
19	D	523	TGL	CG3-CG2-OG2-CB1
20	A	524	PGV	C03-C02-O01-C1
26	R	1229	PSC	C03-C02-O01-C1
24	T	1264	PEK	C22-C23-C24-C25
25	C	270	CDL	C76-C77-C78-C79
20	A	524	PGV	C12-C13-C14-C15
14	N	516	HEA	C2A-C3A-CMA-OMA
20	A	522	PGV	C5-C6-C7-C8
20	P	1268	PGV	C23-C24-C25-C26
25	P	1270	CDL	C18-C19-C20-C21
24	C	264	PEK	C4-C5-C6-C7
24	G	265	PEK	C34-C35-C36-C37
20	P	1268	PGV	C3-C4-C5-C6
28	P	1272	DMU	C22-C25-C28-C31
26	R	1229	PSC	C31-C32-C33-C34
25	T	1269	CDL	C20-C21-C22-C23
19	L	522	TGL	C23-C24-C25-C26
25	P	1270	CDL	C22-C23-C24-C25
26	E	229	PSC	C23-C24-C25-C26
24	T	1264	PEK	C33-C34-C35-C36
25	P	1270	CDL	C12-C13-C14-C15
25	P	1270	CDL	C60-C61-C62-C63
19	L	522	TGL	OG2-CG2-CG3-OG3
19	N	1521	TGL	OG1-CG1-CG2-OG2
24	T	263	PEK	O03-C01-C02-O01
25	G	269	CDL	OA6-CA4-CA6-OA8
25	T	1269	CDL	OB6-CB4-CB6-OB8
19	D	523	TGL	CC4-CC5-CC6-CC7
25	C	270	CDL	C83-C84-C85-C86
19	A	521	TGL	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
20	N	1524	PGV	O03-C19-C20-C21
25	C	270	CDL	C58-C59-C60-C61
25	G	269	CDL	C31-C32-C33-C34
25	T	1269	CDL	C77-C78-C79-C80
14	A	516	HEA	C3B-C11-C12-C13
14	N	516	HEA	C3B-C11-C12-C13
19	N	1521	TGL	CB7-CB8-CB9-C10
19	Q	1523	TGL	CA6-CA7-CA8-CA9
20	P	1268	PGV	C20-C19-O03-C01
19	A	521	TGL	C29-C30-C31-C32
24	T	263	PEK	C29-C30-C31-C32
19	L	522	TGL	C11-C12-C13-C14
26	E	229	PSC	C31-C32-C33-C34
19	D	523	TGL	CC2-CC3-CC4-CC5
19	D	523	TGL	C18-C19-C33-C34
25	P	1270	CDL	C43-C44-C45-C46
20	C	268	PGV	C31-C32-C33-C34
20	N	1524	PGV	C10-C11-C12-C13
19	L	522	TGL	C29-C30-C31-C32
24	T	1264	PEK	C35-C36-C37-C38
19	N	1522	TGL	CA5-CA6-CA7-CA8
26	E	229	PSC	C26-C27-C28-C29
20	A	524	PGV	C05-C04-O12-P
20	P	1268	PGV	C02-C03-O11-P
25	C	270	CDL	OB9-CB7-OB8-CB6
25	G	269	CDL	C24-C25-C26-C27
28	G	272	DMU	C5-C10-O7-C3
25	T	1269	CDL	C24-C25-C26-C27
26	E	229	PSC	C3-C4-C5-C6
19	A	521	TGL	C21-C22-C23-C24
20	P	1267	PGV	C15-C16-C17-C18
20	A	524	PGV	C01-C02-C03-O11
20	P	1268	PGV	C01-C02-C03-O11
25	C	270	CDL	OA5-CA3-CA4-CA6
25	C	270	CDL	OB5-CB3-CB4-CB6
25	P	1270	CDL	OB5-CB3-CB4-CB6
25	T	1269	CDL	OA5-CA3-CA4-CA6
20	C	267	PGV	C25-C26-C27-C28
24	G	1263	PEK	C30-C31-C32-C33
25	G	269	CDL	C20-C21-C22-C23
20	A	524	PGV	C31-C32-C33-C34
19	Q	1523	TGL	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
20	P	1267	PGV	C31-C32-C33-C34
20	P	1268	PGV	C14-C15-C16-C17
28	G	272	DMU	C4-C3-O7-C10
25	P	1270	CDL	C44-C45-C46-C47
20	A	524	PGV	C20-C21-C22-C23
19	L	522	TGL	CA4-CA5-CA6-CA7
19	L	522	TGL	CC5-CC6-CC7-CC8
19	Q	1523	TGL	C19-C33-C34-C35
19	A	521	TGL	CG1-CG2-CG3-OG3
20	A	524	PGV	O03-C01-C02-C03
24	G	1263	PEK	O03-C01-C02-C03
25	C	270	CDL	CA3-CA4-CA6-OA8
25	P	1270	CDL	CB3-CB4-CB6-OB8
25	T	1269	CDL	CA3-CA4-CA6-OA8
25	T	1269	CDL	CB3-CB4-CB6-OB8
19	N	1521	TGL	CC4-CC5-CC6-CC7
25	T	1269	CDL	C81-C82-C83-C84
20	A	522	PGV	C31-C32-C33-C34
25	C	270	CDL	C80-C81-C82-C83
20	P	1268	PGV	C24-C25-C26-C27
20	N	1266	PGV	C31-C32-C33-C34
25	C	270	CDL	C1-CA2-OA2-PA1
25	C	270	CDL	CA4-CA3-OA5-PA1
25	G	269	CDL	CB4-CB3-OB5-PB2
24	T	263	PEK	C10-C11-C12-C13
19	L	522	TGL	CB2-CB3-CB4-CB5
19	N	1522	TGL	C14-C29-C30-C31
28	G	272	DMU	O16-C18-C19-C22
19	L	522	TGL	CA9-C20-C21-C22
19	Q	1523	TGL	CB6-CB7-CB8-CB9
28	G	272	DMU	C25-C28-C31-C34
19	N	1522	TGL	OG2-CB1-CB2-CB3
19	A	521	TGL	OG1-CG1-CG2-OG2
20	C	268	PGV	O03-C01-C02-O01
19	N	1521	TGL	CA5-CA6-CA7-CA8
24	C	264	PEK	C9-C10-C11-C12
24	G	265	PEK	C5-C6-C7-C8
24	G	265	PEK	C11-C10-C9-C8
24	G	265	PEK	C9-C10-C11-C12
24	G	1263	PEK	C12-C13-C14-C15
24	S	1265	PEK	C5-C6-C7-C8
24	S	1265	PEK	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
24	T	263	PEK	C6-C7-C8-C9
24	T	263	PEK	C9-C10-C11-C12
24	T	1264	PEK	C11-C10-C9-C8
26	R	1229	PSC	C9-C10-C11-C12
26	R	1229	PSC	C10-C11-C12-C13
19	A	521	TGL	CA6-CA7-CA8-CA9
20	C	268	PGV	C21-C22-C23-C24
28	M	526	DMU	C34-C37-C40-C43
24	C	264	PEK	C23-C24-C25-C26
20	C	267	PGV	C1-C2-C3-C4
19	D	523	TGL	CA5-CA6-CA7-CA8
20	N	1266	PGV	C25-C26-C27-C28
20	C	267	PGV	C22-C23-C24-C25
20	P	1268	PGV	C13-C14-C15-C16
24	S	1265	PEK	C25-C26-C27-C28
19	N	1522	TGL	C29-C30-C31-C32
20	C	267	PGV	C15-C16-C17-C18
24	G	1263	PEK	C34-C35-C36-C37
25	C	270	CDL	C73-C74-C75-C76
24	C	264	PEK	C27-C28-C29-C30
25	C	270	CDL	C12-C13-C14-C15
25	T	1269	CDL	C64-C65-C66-C67
19	L	522	TGL	CB7-CB8-CB9-C10
25	T	1269	CDL	C23-C24-C25-C26
25	T	1269	CDL	C11-C12-C13-C14
25	T	1269	CDL	C33-C34-C35-C36
19	D	523	TGL	OG2-CB1-CB2-CB3
25	T	1269	CDL	C38-C39-C40-C41
19	A	521	TGL	CA7-CA8-CA9-C20
20	N	1266	PGV	C23-C24-C25-C26
25	G	269	CDL	CB2-C1-CA2-OA2
25	C	270	CDL	C37-C38-C39-C40
19	Q	1523	TGL	CC4-CC5-CC6-CC7
25	P	1270	CDL	OA5-CA3-CA4-CA6
20	A	524	PGV	C28-C29-C30-C31
28	P	1272	DMU	C4-C3-O7-C10
20	C	268	PGV	C25-C26-C27-C28
20	P	1268	PGV	C31-C32-C33-C34
20	A	522	PGV	C10-C11-C12-C13
20	C	268	PGV	C28-C29-C30-C31
24	S	1265	PEK	C31-C32-C33-C34
25	P	1270	CDL	C71-C72-C73-C74

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Mol	Chain	Res	Type	Atoms
19	D	523	TGL	OB1-CB1-OG2-CG2
20	P	1268	PGV	O04-C19-O03-C01
25	P	1270	CDL	C63-C64-C65-C66
25	G	269	CDL	C34-C35-C36-C37
28	M	526	DMU	C28-C31-C34-C37
26	E	229	PSC	C03-C02-O01-C1
20	N	1524	PGV	C31-C32-C33-C34
25	T	1269	CDL	C41-C42-C43-C44
24	G	1263	PEK	O01-C02-C03-O11
24	T	263	PEK	O01-C02-C03-O11
25	C	270	CDL	OB5-CB3-CB4-OB6
25	P	1270	CDL	OA5-CA3-CA4-OA6
20	N	1524	PGV	C15-C16-C17-C18
24	T	263	PEK	O03-C01-C02-C03
19	Q	1523	TGL	C29-C30-C31-C32
19	D	523	TGL	CB2-CB1-OG2-CG2
14	A	515	HEA	C14-C15-C16-C17
26	E	229	PSC	C4-C5-C6-C7
19	N	1522	TGL	OG2-CG2-CG3-OG3
25	C	270	CDL	OB6-CB4-CB6-OB8
25	P	1270	CDL	OA6-CA4-CA6-OA8
25	P	1270	CDL	OB6-CB4-CB6-OB8
25	T	1269	CDL	OA6-CA4-CA6-OA8
26	E	229	PSC	O03-C01-C02-O01
20	P	1268	PGV	C28-C29-C30-C31
24	T	263	PEK	C27-C28-C29-C30
24	S	1265	PEK	C30-C31-C32-C33
25	C	270	CDL	C55-C56-C57-C58
19	N	1522	TGL	CC5-CC6-CC7-CC8
20	P	1267	PGV	C22-C23-C24-C25
20	C	268	PGV	C02-C03-O11-P
25	G	269	CDL	C35-C36-C37-C38
20	C	268	PGV	C15-C16-C17-C18
25	P	1270	CDL	C24-C25-C26-C27
26	R	1229	PSC	O12-C04-C05-N
24	S	1265	PEK	C23-C24-C25-C26
19	Q	1523	TGL	CA5-CA6-CA7-CA8
19	L	522	TGL	CC4-CC5-CC6-CC7
24	S	1265	PEK	C22-C23-C24-C25
19	N	1521	TGL	C10-C11-C12-C13
24	T	1264	PEK	C31-C32-C33-C34
24	C	264	PEK	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
19	N	1522	TGL	CB5-CB6-CB7-CB8
24	T	1264	PEK	C23-C24-C25-C26
25	C	270	CDL	C32-C33-C34-C35
20	N	1524	PGV	C24-C25-C26-C27
24	G	1263	PEK	C01-C02-C03-O11
26	E	229	PSC	C01-C02-C03-O11
20	N	1524	PGV	C30-C31-C32-C33
28	G	272	DMU	C34-C37-C40-C43
19	L	522	TGL	C14-C29-C30-C31
19	N	1521	TGL	C18-C19-C33-C34
28	M	526	DMU	C25-C28-C31-C34
28	M	526	DMU	C19-C22-C25-C28
24	G	1263	PEK	C13-C14-C15-C16
20	P	1267	PGV	C02-C03-O11-P
19	D	523	TGL	CA3-CA4-CA5-CA6
25	C	270	CDL	OA5-CA3-CA4-OA6
25	T	1269	CDL	OB5-CB3-CB4-OB6
26	E	229	PSC	O01-C02-C03-O11
19	N	1521	TGL	C23-C24-C25-C26
14	A	515	HEA	C4A-C3A-CMA-OMA
14	N	516	HEA	C4A-C3A-CMA-OMA
19	A	521	TGL	OG2-CG2-CG3-OG3
20	N	1524	PGV	O03-C01-C02-O01
25	C	270	CDL	OA6-CA4-CA6-OA8
26	R	1229	PSC	O03-C01-C02-O01
25	T	1269	CDL	C14-C15-C16-C17
24	T	263	PEK	C26-C27-C28-C29
24	C	264	PEK	C32-C33-C34-C35
24	G	265	PEK	C3-C4-C5-C6
25	C	270	CDL	CA7-C31-C32-C33
19	L	522	TGL	C33-C34-C35-C36
24	T	1264	PEK	C17-C18-C19-C20
20	N	1524	PGV	C21-C22-C23-C24
26	E	229	PSC	C22-C23-C24-C25
19	Q	1523	TGL	CB4-CB5-CB6-CB7
20	N	1524	PGV	C04-O12-P-O13
24	G	265	PEK	C03-O11-P-O12
24	G	265	PEK	C04-O12-P-O14
24	T	263	PEK	C04-O12-P-O11
24	T	263	PEK	C04-O12-P-O14
25	C	270	CDL	CA3-OA5-PA1-OA3
25	C	270	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
25	C	270	CDL	CB2-OB2-PB2-OB5
25	G	269	CDL	CA3-OA5-PA1-OA4
25	P	1270	CDL	CA3-OA5-PA1-OA3
25	P	1270	CDL	CB2-OB2-PB2-OB5
25	T	1269	CDL	CB2-OB2-PB2-OB3
26	R	1229	PSC	C03-O11-P-O12
26	R	1229	PSC	C03-O11-P-O13
19	N	1522	TGL	C13-C14-C29-C30
24	C	264	PEK	C28-C29-C30-C31
20	C	267	PGV	C02-C03-O11-P
20	C	268	PGV	C05-C04-O12-P
20	N	1524	PGV	C05-C04-O12-P
25	P	1270	CDL	CA4-CA3-OA5-PA1
19	Q	1523	TGL	C16-C17-C18-C19
25	C	270	CDL	C13-C14-C15-C16
19	N	1522	TGL	C11-C12-C13-C14
25	T	1269	CDL	C13-C14-C15-C16
19	L	522	TGL	OG2-CB1-CB2-CB3
19	N	1522	TGL	CB1-CB2-CB3-CB4
20	N	1524	PGV	C01-C02-O01-C1
24	G	265	PEK	C35-C36-C37-C38
25	G	269	CDL	C41-C42-C43-C44
28	Z	1526	DMU	C31-C34-C37-C40
19	A	521	TGL	C18-C19-C33-C34
24	S	1265	PEK	C35-C36-C37-C38
20	C	268	PGV	C24-C25-C26-C27
20	A	524	PGV	C25-C26-C27-C28
19	N	1522	TGL	C17-C18-C19-C33
20	C	267	PGV	C29-C30-C31-C32
26	R	1229	PSC	C26-C27-C28-C29
24	S	1265	PEK	O03-C01-C02-O01
24	G	265	PEK	C27-C28-C29-C30
25	P	1270	CDL	C41-C42-C43-C44
25	T	1269	CDL	C32-C33-C34-C35
26	R	1229	PSC	C15-C16-C17-C18
20	A	522	PGV	C6-C7-C8-C9
20	C	267	PGV	C20-C21-C22-C23
19	L	522	TGL	OG1-CA1-CA2-CA3
19	L	522	TGL	CG1-CG2-CG3-OG3
19	N	1522	TGL	CG1-CG2-CG3-OG3
25	G	269	CDL	CA3-CA4-CA6-OA8
25	T	1269	CDL	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
20	N	1266	PGV	C24-C25-C26-C27
19	D	523	TGL	CA9-C20-C21-C22
26	R	1229	PSC	O03-C19-C20-C21
24	S	1265	PEK	C17-C18-C19-C20
25	G	269	CDL	C23-C24-C25-C26
25	G	269	CDL	C71-C72-C73-C74
20	N	1266	PGV	C12-C13-C14-C15
24	C	264	PEK	C2-C3-C4-C5
24	T	263	PEK	C15-C16-C17-C18
25	T	1269	CDL	C34-C35-C36-C37
20	P	1268	PGV	C05-C04-O12-P
19	D	523	TGL	CC5-CC6-CC7-CC8
24	G	265	PEK	C4-C5-C6-C7
24	G	1263	PEK	C29-C30-C31-C32
25	P	1270	CDL	C75-C76-C77-C78
19	A	521	TGL	C11-C12-C13-C14
20	N	1524	PGV	C11-C12-C13-C14
24	S	1265	PEK	C3-C4-C5-C6
24	S	1265	PEK	C14-C15-C16-C17
24	T	1264	PEK	C3-C4-C5-C6
26	R	1229	PSC	C12-C13-C14-C15
20	N	1524	PGV	C11-C10-C9-C8
19	N	1522	TGL	CA6-CA7-CA8-CA9
26	E	229	PSC	C27-C28-C29-C30
25	G	269	CDL	C21-C22-C23-C24
19	A	521	TGL	CB7-CB8-CB9-C10
26	E	229	PSC	C04-C05-N-C08
19	N	1521	TGL	CC6-CC7-CC8-CC9
19	N	1522	TGL	CA3-CA4-CA5-CA6
22	J	60	CHD	C22-C23-C24-O25
19	N	1521	TGL	CB4-CB5-CB6-CB7
20	A	524	PGV	C10-C11-C12-C13
20	C	268	PGV	C10-C11-C12-C13
20	N	1266	PGV	C10-C11-C12-C13
22	O	229	CHD	C22-C23-C24-O25
25	T	1269	CDL	C15-C16-C17-C18
22	J	60	CHD	C22-C23-C24-O26
20	N	1524	PGV	C13-C14-C15-C16
22	O	229	CHD	C22-C23-C24-O26
24	C	264	PEK	C14-C15-C16-C17
20	C	267	PGV	C05-C04-O12-P
25	P	1270	CDL	C1-CA2-OA2-PA1

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Mol	Chain	Res	Type	Atoms
19	A	521	TGL	C14-C29-C30-C31
14	A	516	HEA	CAA-CBA-CGA-O1A
24	G	265	PEK	C01-C02-C03-O11
25	G	269	CDL	OB5-CB3-CB4-CB6
19	N	1522	TGL	CC6-CC7-CC8-CC9
14	A	516	HEA	CAA-CBA-CGA-O2A
14	N	516	HEA	CAA-CBA-CGA-O1A
20	N	1266	PGV	C9-C10-C11-C12
24	G	1263	PEK	C9-C10-C11-C12
26	E	229	PSC	C9-C10-C11-C12
26	E	229	PSC	C10-C11-C12-C13
26	R	1229	PSC	C21-C22-C23-C24
14	N	515	HEA	CAD-CBD-CGD-O1D
22	B	1085	CHD	C22-C23-C24-O25
19	A	521	TGL	CB2-CB3-CB4-CB5
19	N	1522	TGL	C20-C21-C22-C23
28	M	526	DMU	C31-C34-C37-C40
24	G	1263	PEK	C17-C18-C19-C20
25	T	1269	CDL	C53-C54-C55-C56
14	N	516	HEA	CAA-CBA-CGA-O2A
22	P	1271	CHD	C22-C23-C24-O26
20	C	267	PGV	C24-C25-C26-C27
19	L	522	TGL	C19-C33-C34-C35
19	N	1521	TGL	CB2-CB3-CB4-CB5
14	A	516	HEA	C26-C15-C16-C17
14	N	516	HEA	C26-C15-C16-C17
25	G	269	CDL	C12-C13-C14-C15
22	B	1085	CHD	C22-C23-C24-O26
26	R	1229	PSC	C28-C29-C30-C31
20	A	522	PGV	O03-C19-C20-C21
19	Q	1523	TGL	CB3-CB4-CB5-CB6
14	A	515	HEA	CAD-CBD-CGD-O1D
19	N	1522	TGL	CA4-CA5-CA6-CA7
19	D	523	TGL	C12-C13-C14-C29
25	P	1270	CDL	C57-C58-C59-C60
19	Q	1523	TGL	OG2-CB1-CB2-CB3
14	N	515	HEA	CAD-CBD-CGD-O2D
20	N	1524	PGV	O04-C19-C20-C21
25	T	1269	CDL	CB2-C1-CA2-OA2
26	R	1229	PSC	O01-C1-C2-C3
19	D	523	TGL	C11-C12-C13-C14
19	Q	1523	TGL	CC2-CC3-CC4-CC5

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Mol	Chain	Res	Type	Atoms
26	R	1229	PSC	C7-C8-C9-C10
25	G	269	CDL	C52-C53-C54-C55
26	E	229	PSC	C30-C31-C32-C33
25	C	270	CDL	C74-C75-C76-C77
20	A	522	PGV	C30-C31-C32-C33
19	N	1521	TGL	CB5-CB6-CB7-CB8
19	N	1521	TGL	OA1-CA1-OG1-CG1
19	N	1522	TGL	C16-C17-C18-C19
19	A	521	TGL	C10-C11-C12-C13
22	P	1271	CHD	C22-C23-C24-O25
25	G	269	CDL	C64-C65-C66-C67
19	N	1521	TGL	CG1-CG2-OG2-CB1
20	A	522	PGV	C11-C12-C13-C14
24	T	263	PEK	C14-C15-C16-C17
24	T	1264	PEK	C15-C16-C17-C18
14	N	516	HEA	CAD-CBD-CGD-O2D
22	C	525	CHD	C22-C23-C24-O25
20	C	268	PGV	C9-C10-C11-C12
14	N	516	HEA	CAD-CBD-CGD-O1D
20	P	1267	PGV	C05-C04-O12-P
22	P	1525	CHD	C22-C23-C24-O26
20	P	1268	PGV	O05-C05-C06-O06
25	C	270	CDL	C34-C35-C36-C37
25	G	269	CDL	C53-C54-C55-C56
20	A	524	PGV	C11-C12-C13-C14
20	A	522	PGV	C9-C10-C11-C12
24	T	1264	PEK	C14-C15-C16-C17
24	T	1264	PEK	O01-C1-C2-C3
19	N	1521	TGL	C11-C10-CB9-CB8
25	P	1270	CDL	C21-C22-C23-C24
25	C	270	CDL	C52-C53-C54-C55
22	P	1525	CHD	C22-C23-C24-O25
20	P	1268	PGV	C11-C12-C13-C14
25	T	1269	CDL	C37-C38-C39-C40
20	C	267	PGV	C28-C29-C30-C31
24	C	264	PEK	C24-C25-C26-C27
22	C	525	CHD	C22-C23-C24-O26
28	Z	1526	DMU	O6-C11-C9-C8
19	N	1521	TGL	CC5-CC6-CC7-CC8
28	Z	1526	DMU	C22-C25-C28-C31
19	D	523	TGL	OG3-CC1-CC2-CC3
19	A	521	TGL	CC6-CC7-CC8-CC9

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Mol	Chain	Res	Type	Atoms
26	E	229	PSC	O12-C04-C05-N
19	N	1522	TGL	C11-C10-CB9-CB8
24	C	264	PEK	O01-C1-C2-C3
20	C	268	PGV	C29-C30-C31-C32
24	T	263	PEK	C24-C25-C26-C27
24	T	263	PEK	O01-C1-C2-C3
25	C	270	CDL	C12-C11-CA5-OA6
25	T	1269	CDL	C84-C85-C86-C87
25	P	1270	CDL	C17-C18-C19-C20
19	N	1521	TGL	OG3-CC1-CC2-CC3
22	W	1059	CHD	C22-C23-C24-O25
19	N	1522	TGL	CB7-CB8-CB9-C10
19	D	523	TGL	CC1-CC2-CC3-CC4
19	D	523	TGL	CC7-CC8-CC9-C15
28	M	526	DMU	C19-C18-O16-C6
25	C	270	CDL	C77-C78-C79-C80
25	T	1269	CDL	C80-C81-C82-C83
14	N	515	HEA	CAA-CBA-CGA-O2A
19	Q	1523	TGL	C11-C12-C13-C14
24	S	1265	PEK	O01-C1-C2-C3
14	N	516	HEA	C27-C19-C20-C21
20	P	1268	PGV	O01-C1-C2-C3
19	N	1521	TGL	CC9-C15-C16-C17
20	P	1267	PGV	C27-C28-C29-C30
14	A	515	HEA	CAD-CBD-CGD-O2D
19	Q	1523	TGL	C20-C21-C22-C23
20	P	1268	PGV	C2-C3-C4-C5
25	P	1270	CDL	C32-C31-CA7-OA8
20	A	524	PGV	C4-C5-C6-C7
25	C	270	CDL	C36-C37-C38-C39
22	W	1059	CHD	C22-C23-C24-O26
25	P	1270	CDL	C76-C77-C78-C79
20	N	1266	PGV	O03-C19-C20-C21
20	N	1524	PGV	C29-C30-C31-C32
19	Q	1523	TGL	CA7-CA8-CA9-C20
26	E	229	PSC	C19-C20-C21-C22
14	N	515	HEA	CAA-CBA-CGA-O1A
25	G	269	CDL	C84-C85-C86-C87
25	P	1270	CDL	OB5-CB3-CB4-OB6
20	A	522	PGV	C27-C28-C29-C30
19	D	523	TGL	OB1-CB1-CB2-CB3
19	N	1521	TGL	OC1-CC1-CC2-CC3

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Mol	Chain	Res	Type	Atoms
25	C	270	CDL	C12-C11-CA5-OA7
26	E	229	PSC	C04-C05-N-C06
26	E	229	PSC	C04-C05-N-C07
25	G	269	CDL	C32-C31-CA7-OA8
19	N	1522	TGL	OB1-CB1-CB2-CB3
25	G	269	CDL	C63-C64-C65-C66
19	D	523	TGL	OC1-CC1-CC2-CC3
24	T	263	PEK	O02-C1-C2-C3
25	G	269	CDL	C16-C17-C18-C19
25	G	269	CDL	C51-C52-C53-C54
24	S	1265	PEK	O02-C1-C2-C3
25	G	269	CDL	C32-C31-CA7-OA9
25	P	1270	CDL	C84-C85-C86-C87
14	A	515	HEA	CAA-CBA-CGA-O2A
20	P	1268	PGV	O02-C1-C2-C3
25	P	1270	CDL	C12-C11-CA5-OA6
26	E	229	PSC	O03-C19-C20-C21
20	A	524	PGV	O02-C1-C2-C3
25	G	269	CDL	C44-C45-C46-C47
19	D	523	TGL	OG1-CA1-CA2-CA3
24	C	264	PEK	O02-C1-C2-C3
24	T	1264	PEK	C24-C25-C26-C27
25	P	1270	CDL	C32-C31-CA7-OA9
24	T	1264	PEK	O02-C1-C2-C3
20	A	524	PGV	O01-C1-C2-C3
25	P	1270	CDL	C52-C51-CB5-OB6
14	A	515	HEA	CAA-CBA-CGA-O1A
25	C	270	CDL	C52-C51-CB5-OB6
19	D	523	TGL	CA1-CA2-CA3-CA4
19	N	1521	TGL	C16-C15-CC9-CC8

There are no ring outliers.

42 monomers are involved in 342 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	N	516	HEA	10	0
19	L	522	TGL	16	0
14	A	516	HEA	4	0
24	G	265	PEK	13	0
20	A	524	PGV	8	0
19	A	521	TGL	7	0
24	T	1264	PEK	9	0

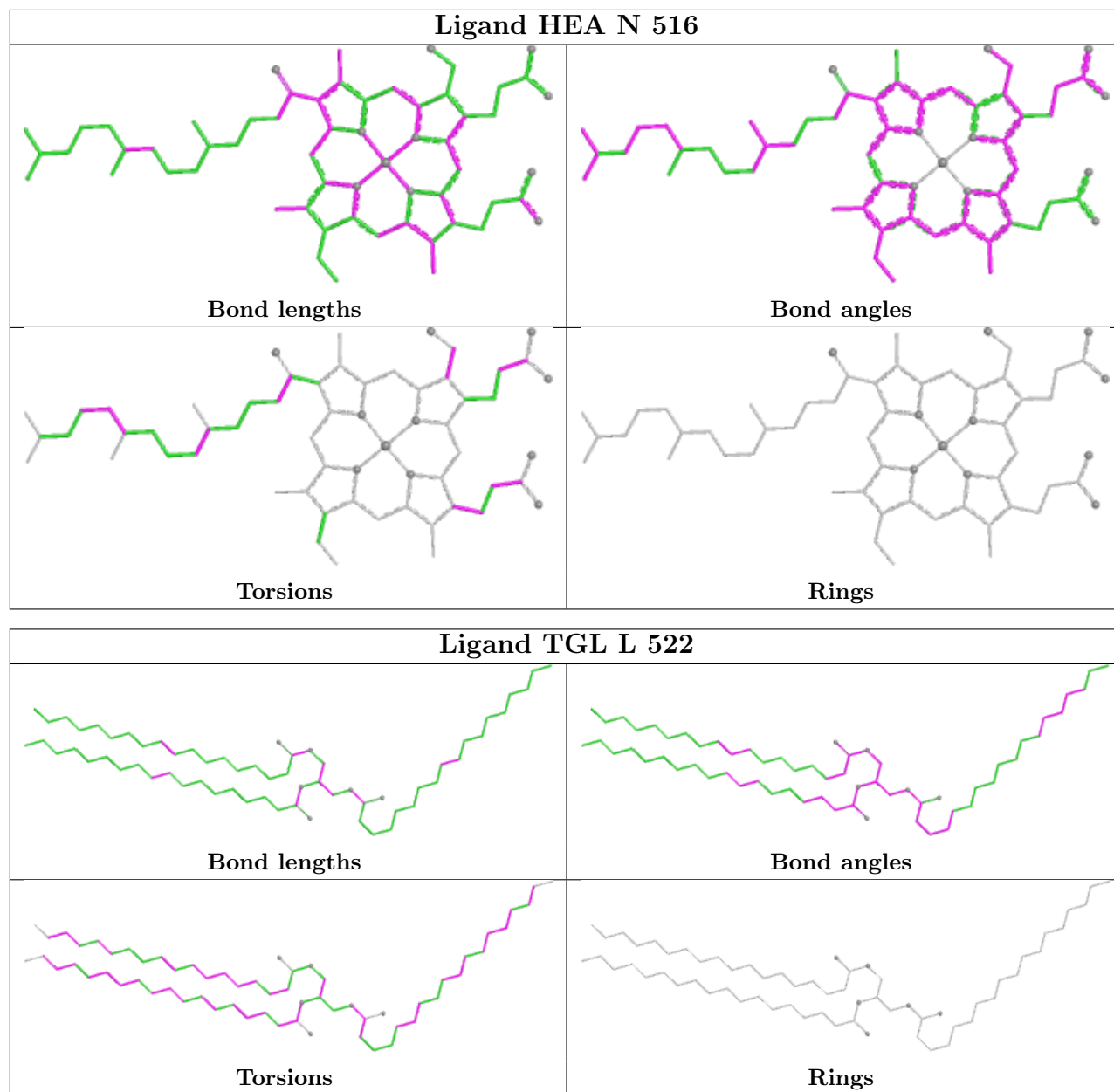
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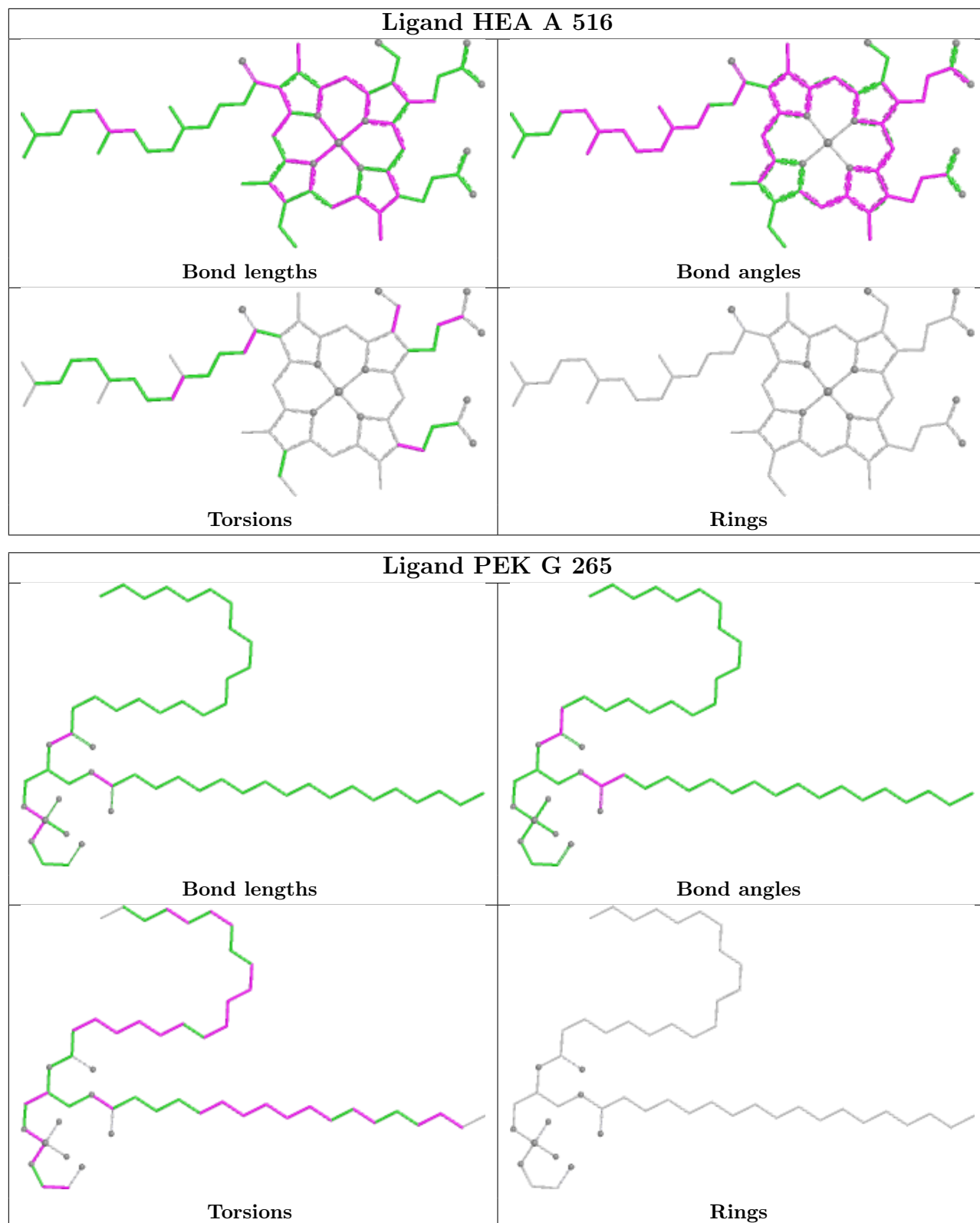
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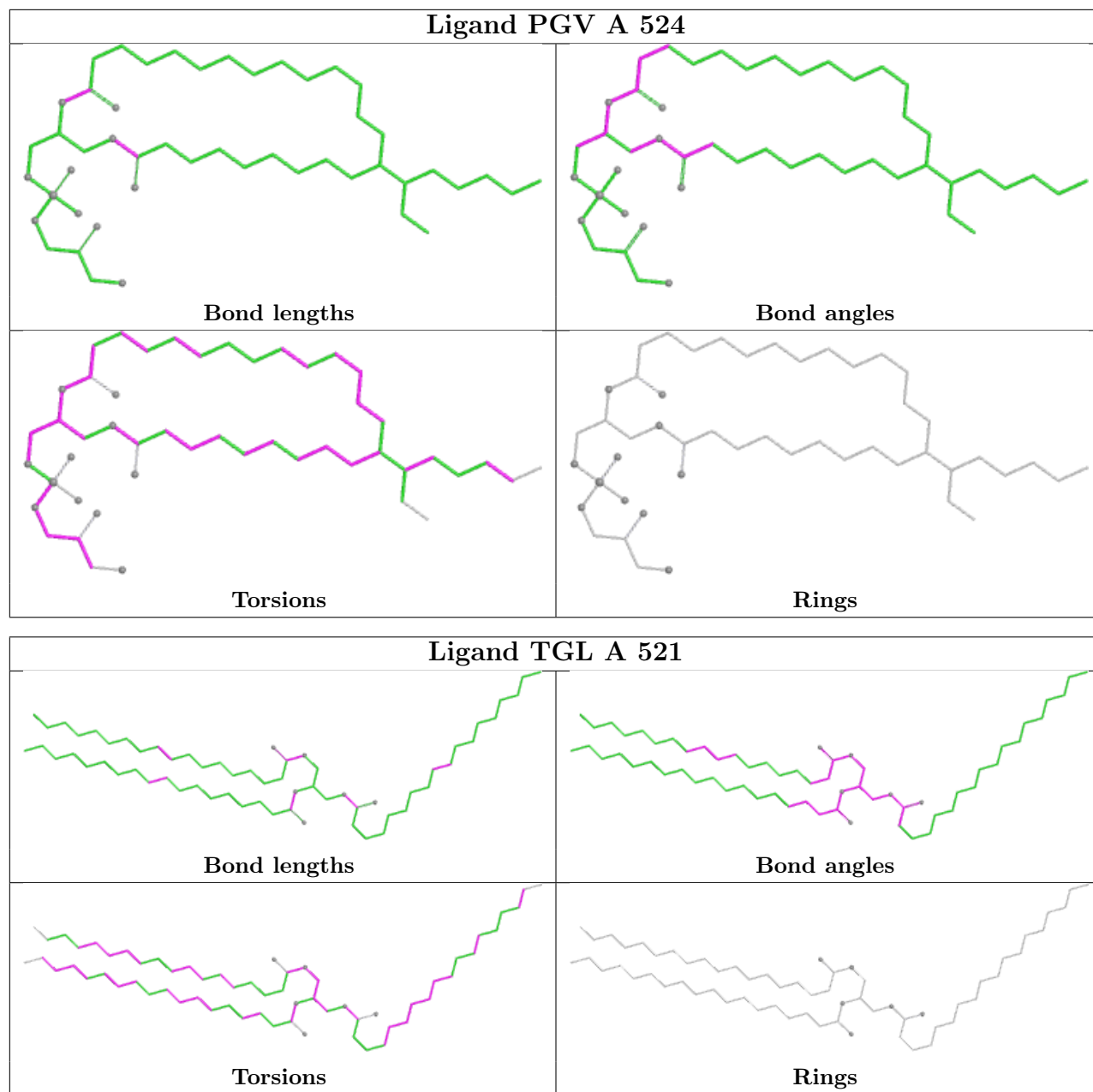
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	1085	CHD	3	0
22	P	1525	CHD	1	0
14	N	515	HEA	3	0
24	C	264	PEK	3	0
24	G	1263	PEK	10	0
14	A	515	HEA	6	0
26	R	1229	PSC	14	0
28	P	1272	DMU	5	0
20	A	522	PGV	3	0
22	C	525	CHD	1	0
22	O	229	CHD	1	0
22	W	1059	CHD	6	0
19	Q	1523	TGL	10	0
25	T	1269	CDL	35	0
20	C	268	PGV	3	0
22	C	271	CHD	3	0
26	E	229	PSC	16	0
19	D	523	TGL	13	0
28	Z	1526	DMU	3	0
28	G	272	DMU	3	0
25	C	270	CDL	21	0
20	C	267	PGV	3	0
24	T	263	PEK	19	0
22	J	60	CHD	2	0
20	P	1268	PGV	2	0
20	P	1267	PGV	3	0
25	P	1270	CDL	19	0
22	P	1271	CHD	4	0
24	S	1265	PEK	17	0
20	N	1524	PGV	7	0
28	M	526	DMU	1	0
19	N	1522	TGL	15	0
15	N	520	CYN	2	0
19	N	1521	TGL	7	0
25	G	269	CDL	28	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

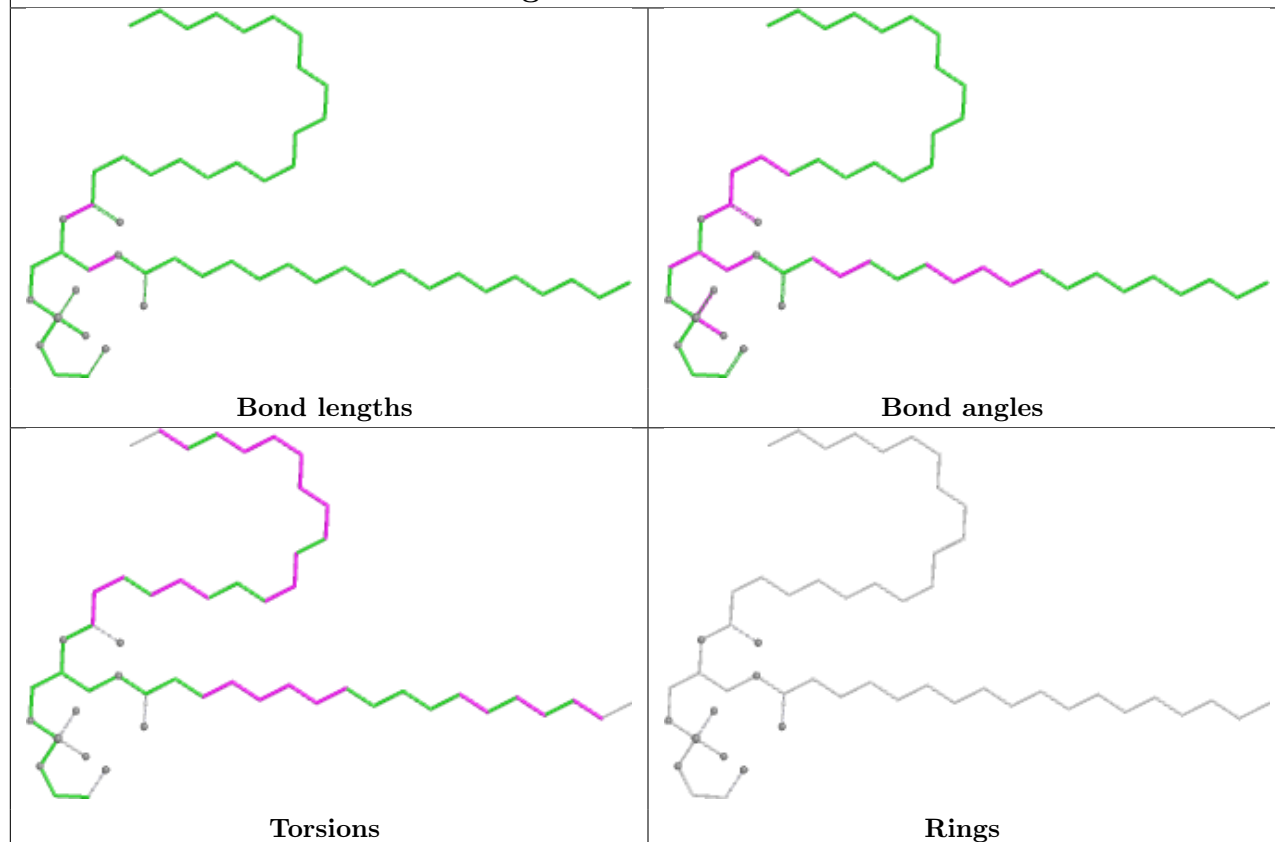
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



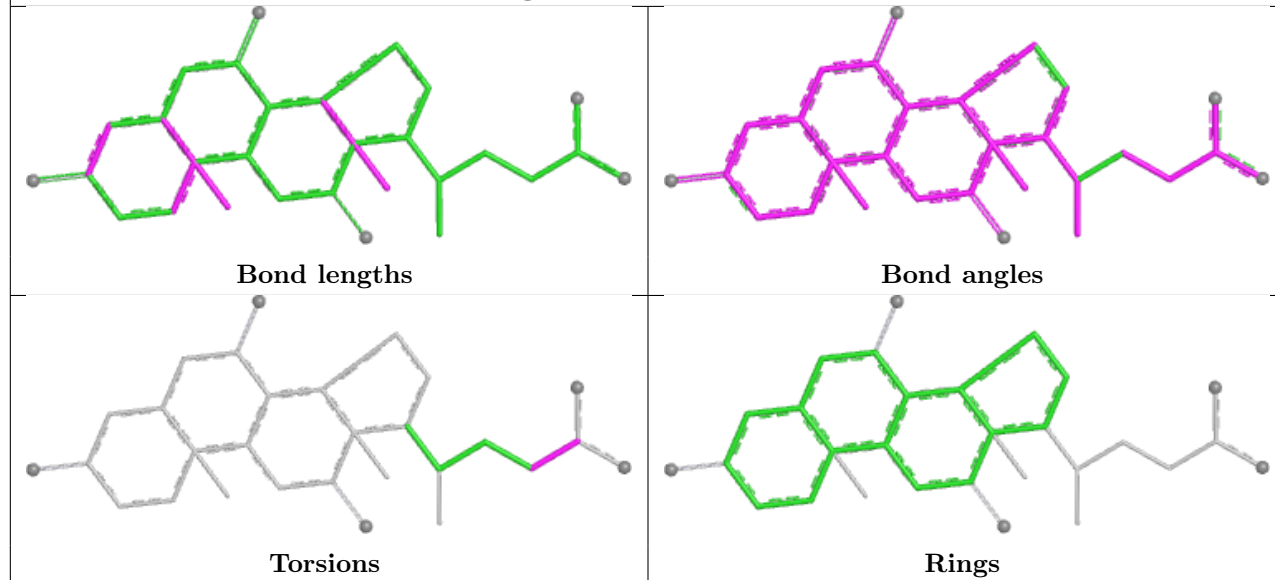


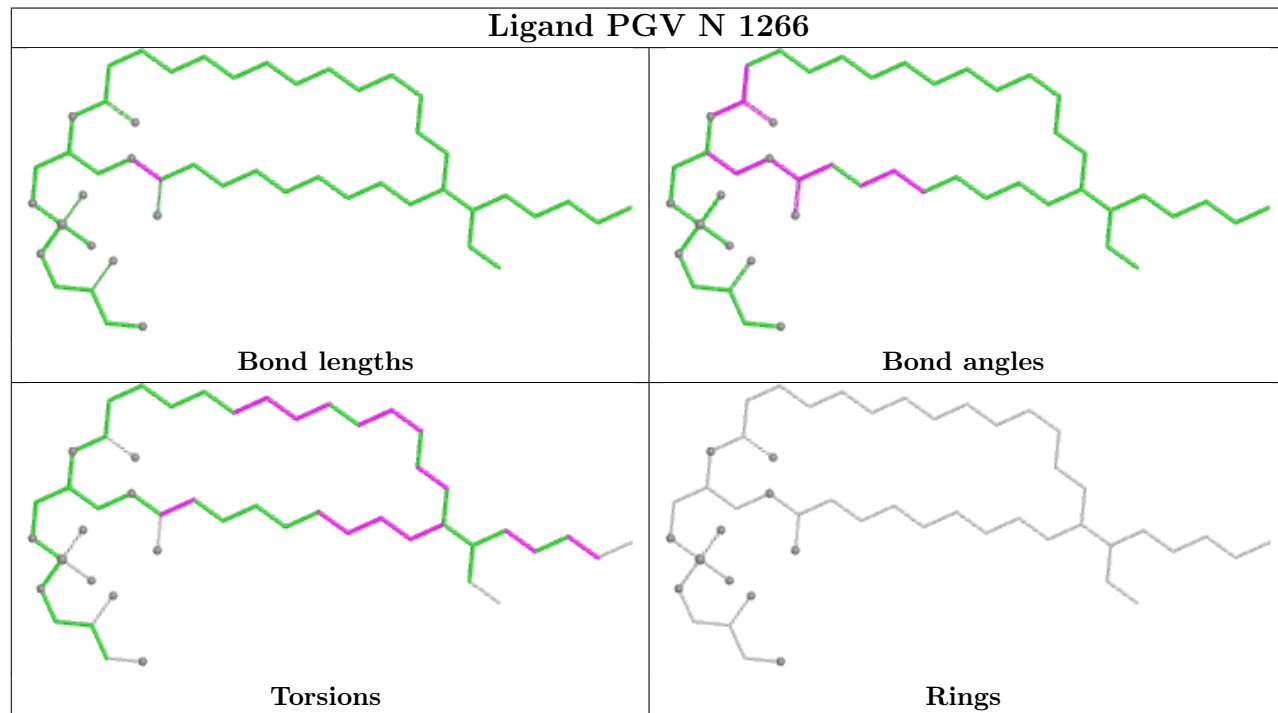
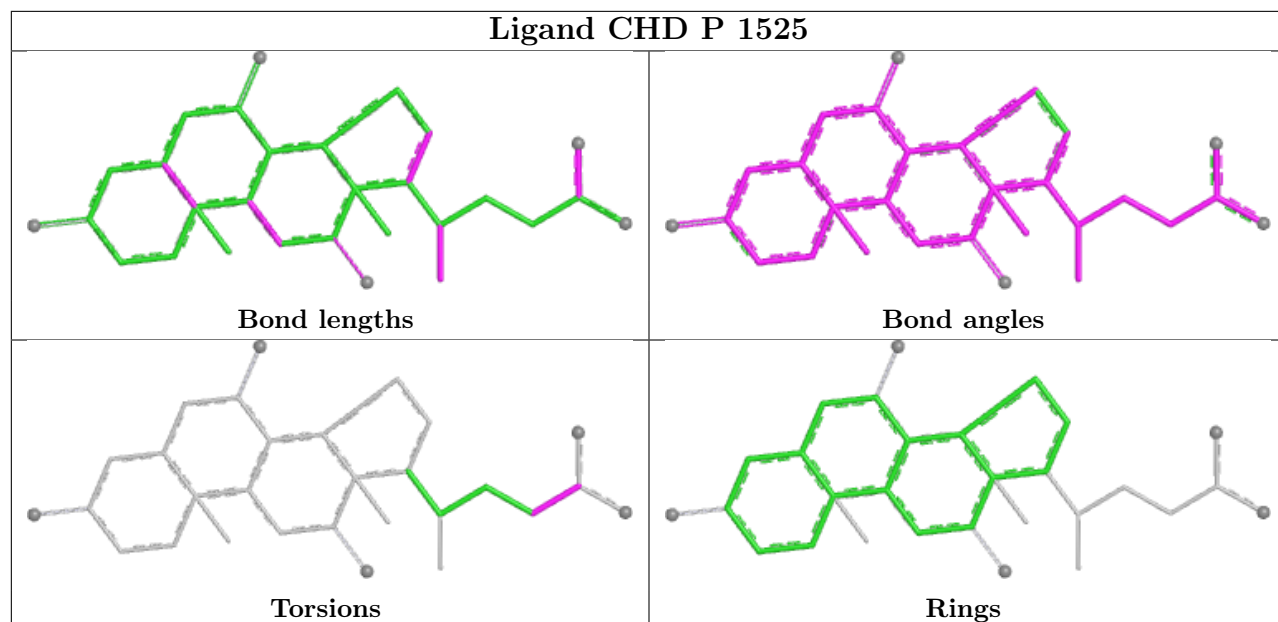


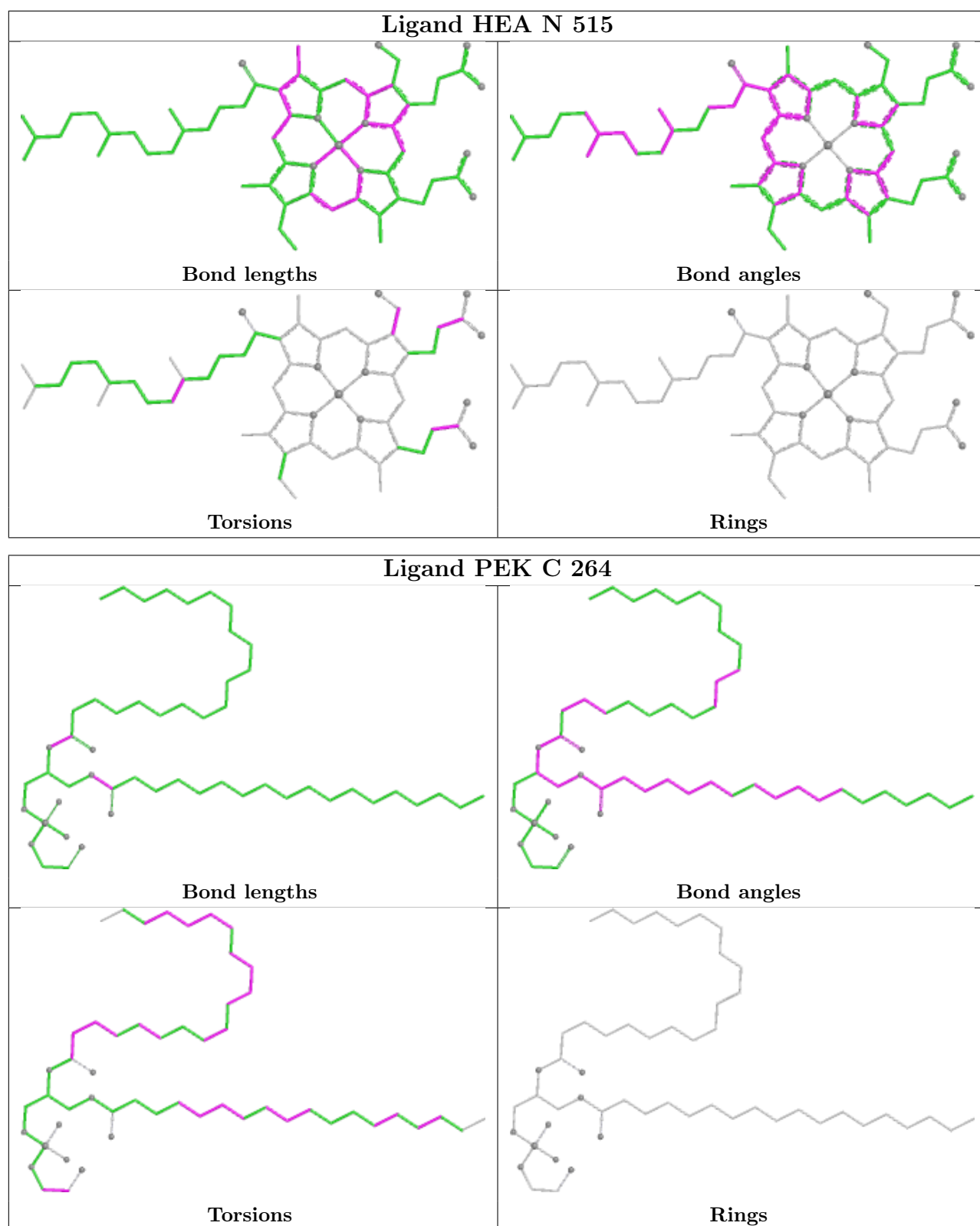
Ligand PEK T 1264

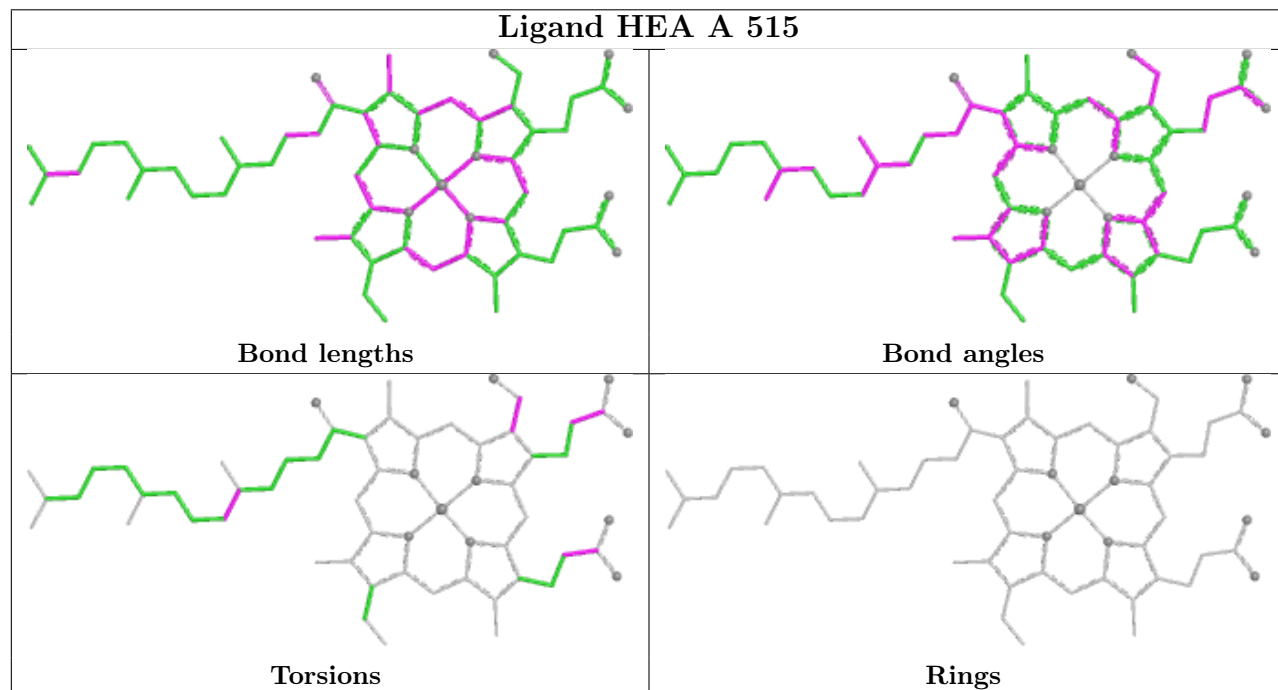
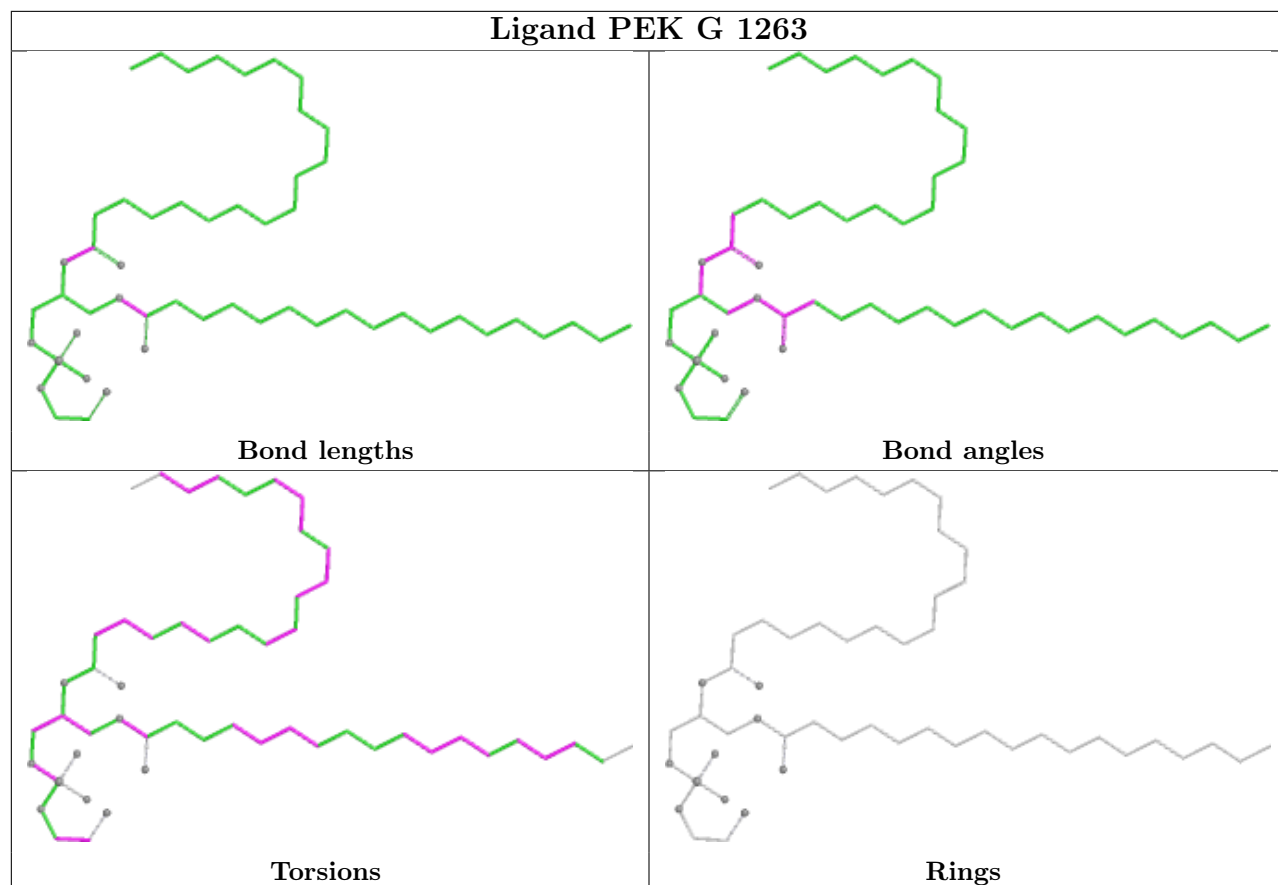


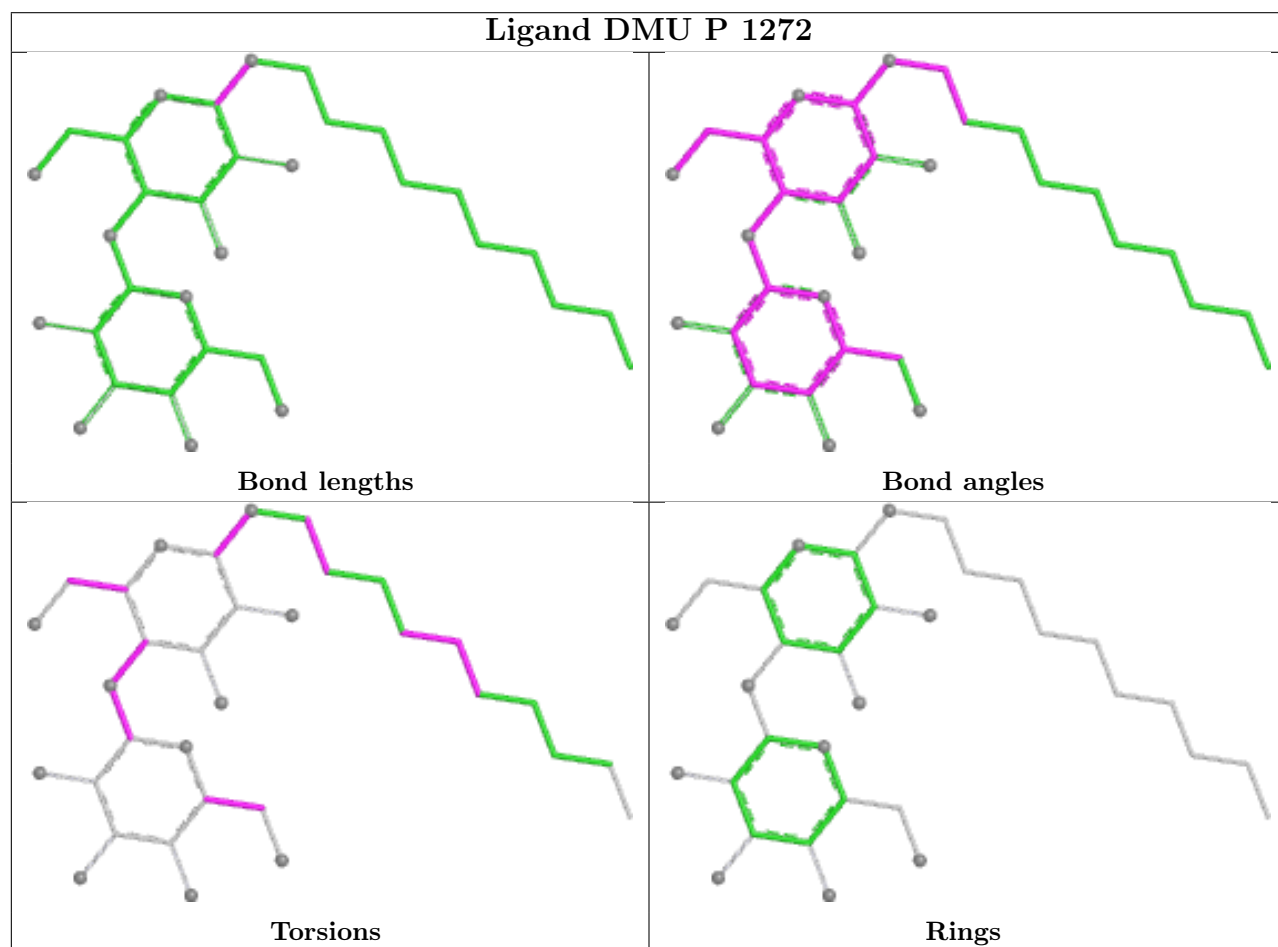
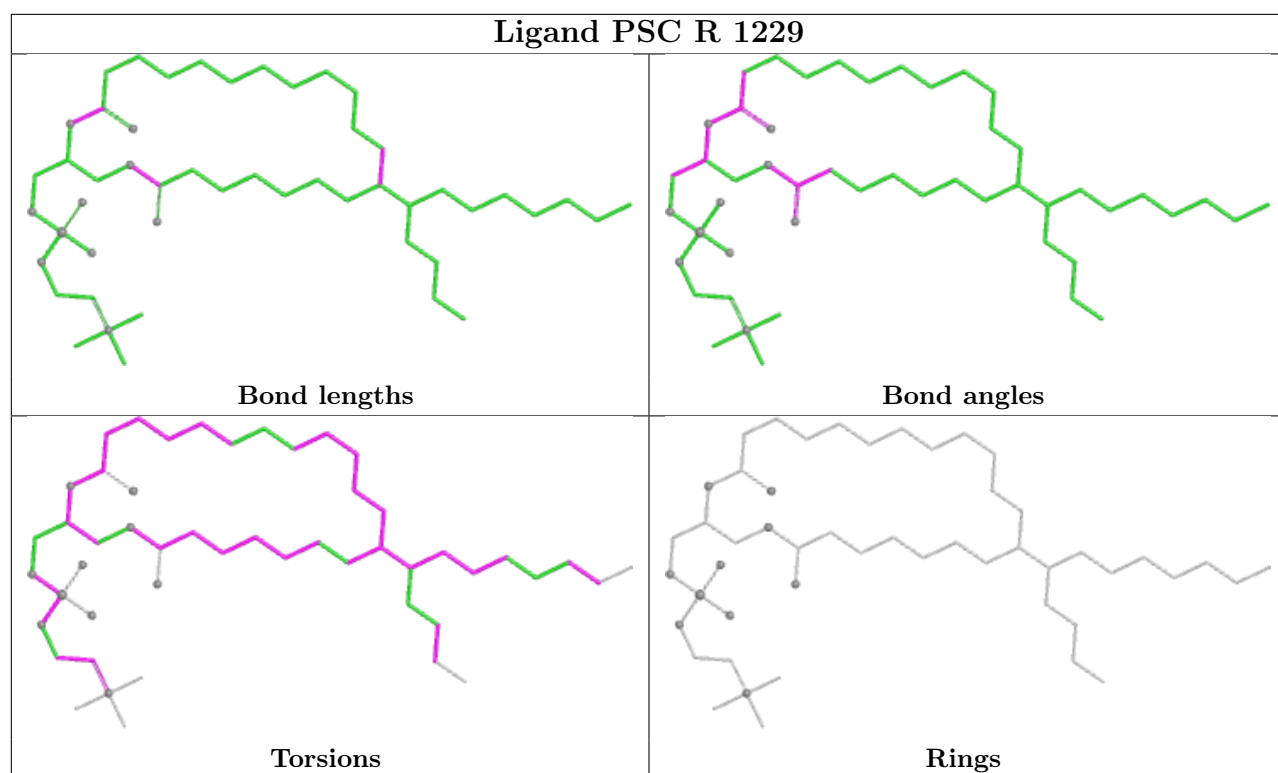
Ligand CHD B 1085

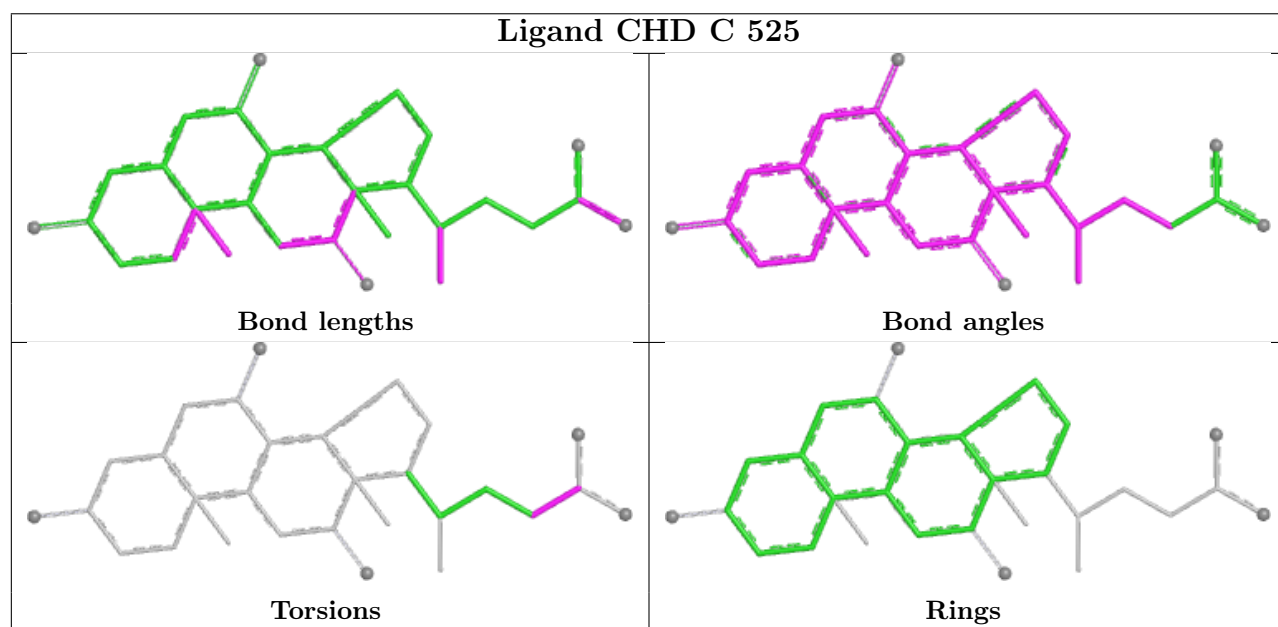
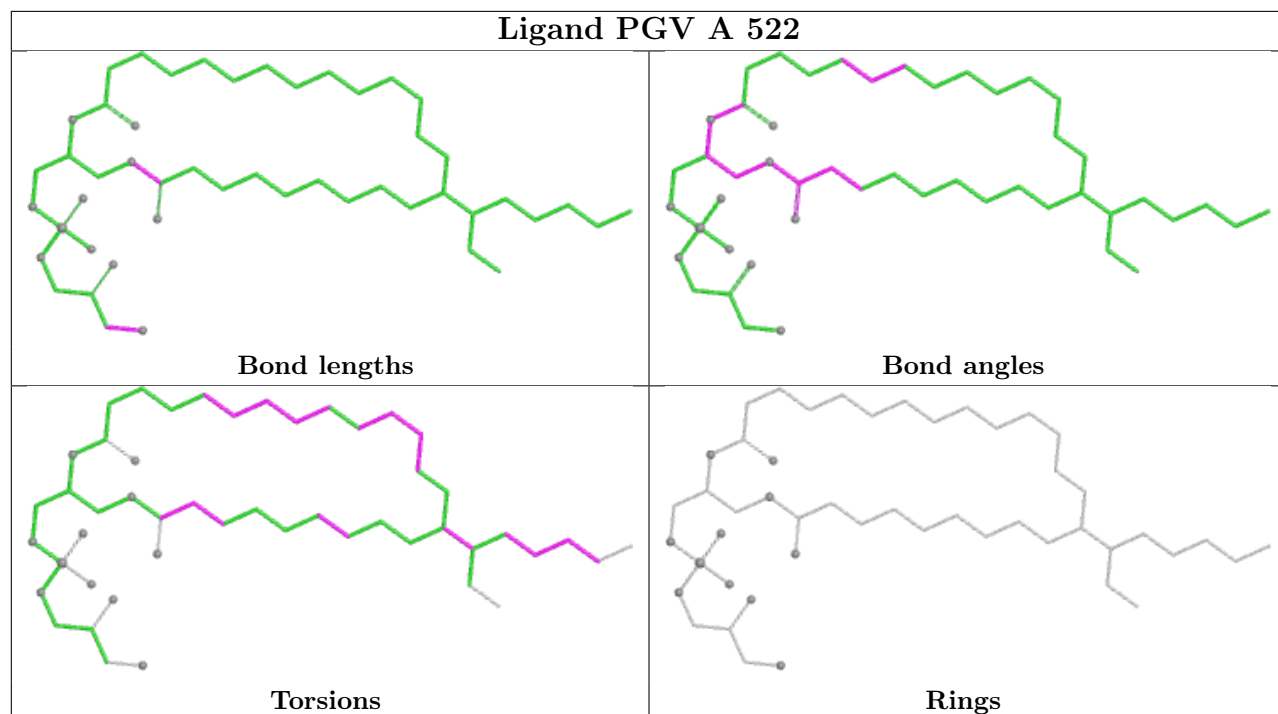


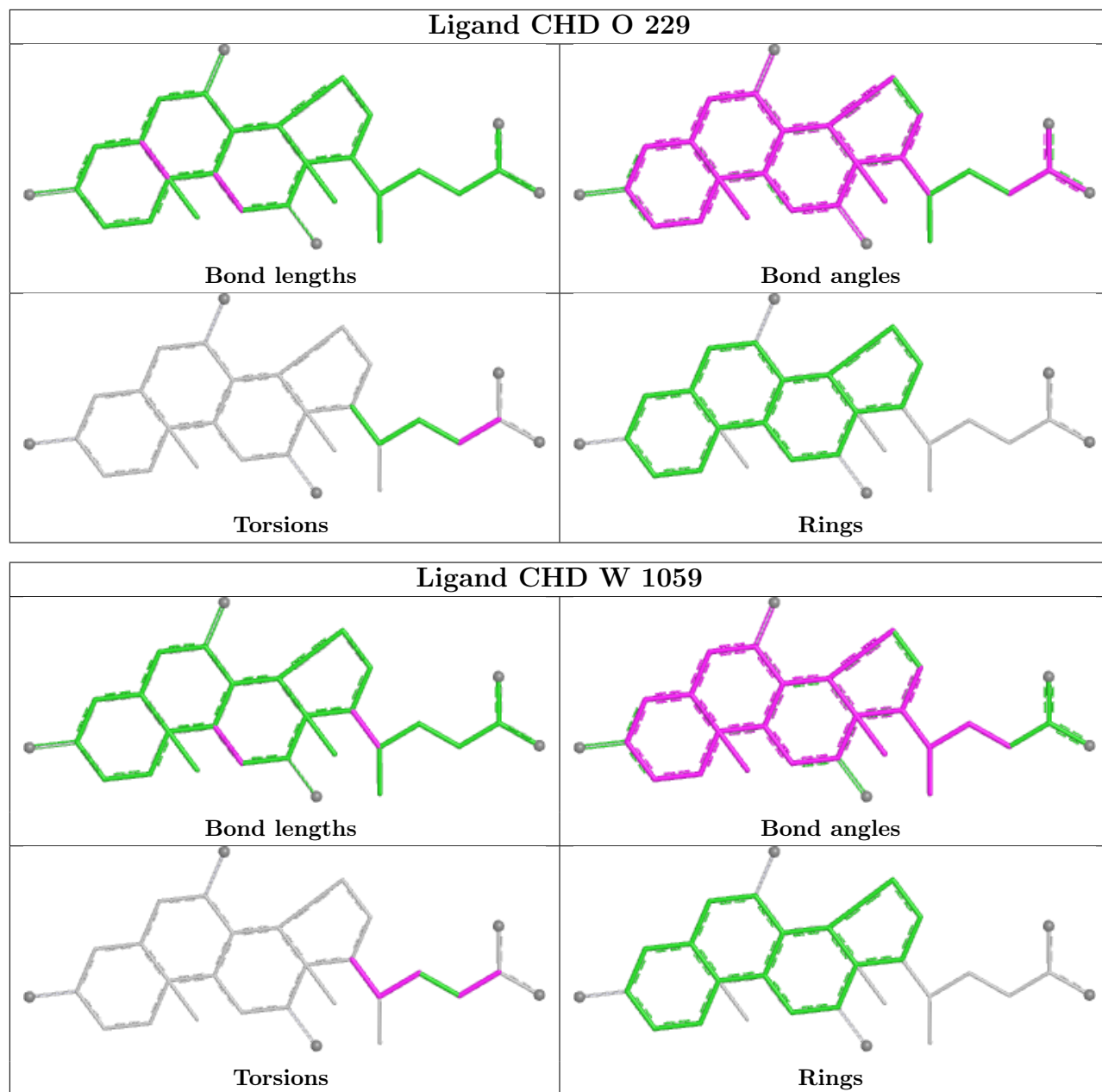


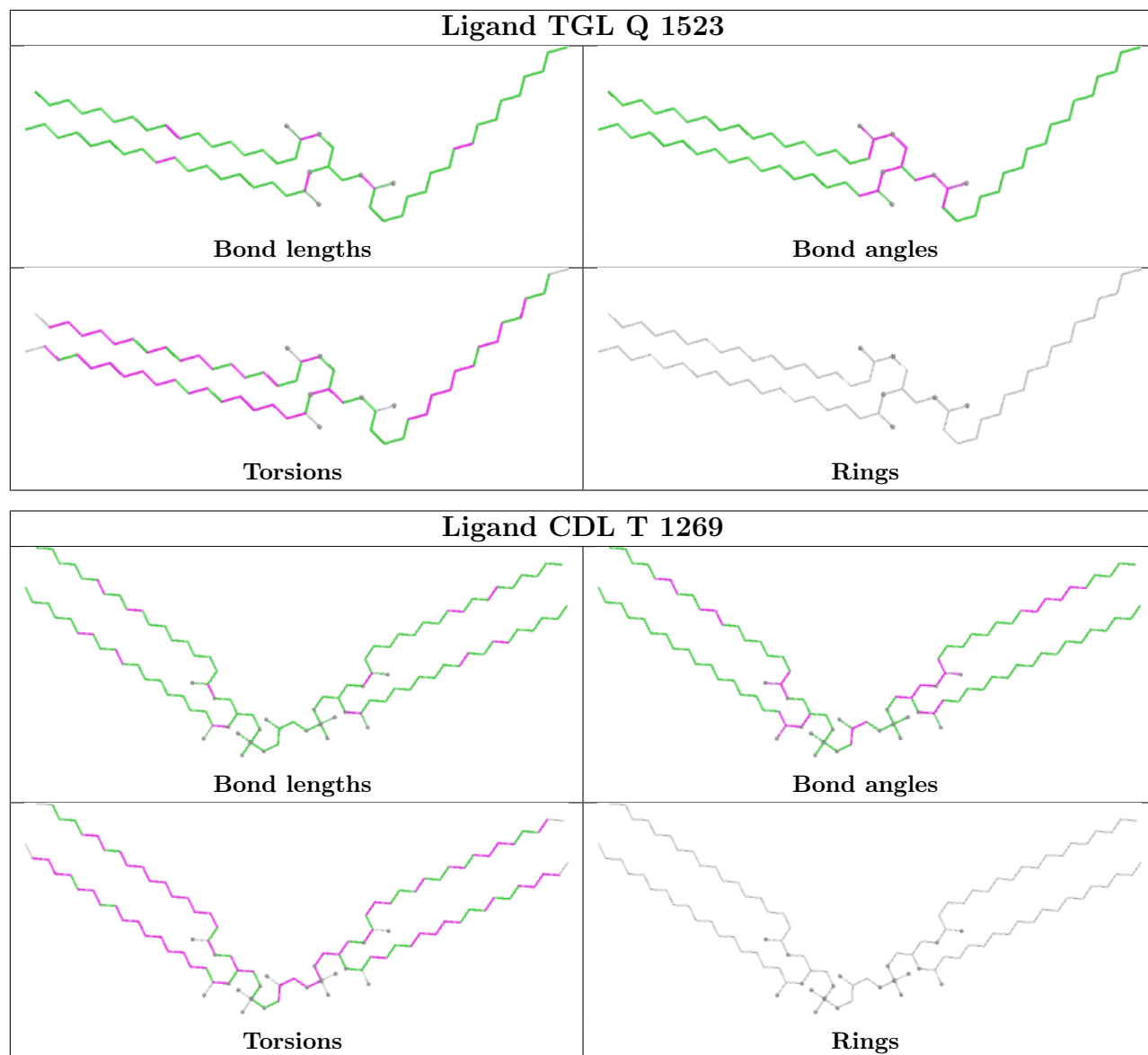


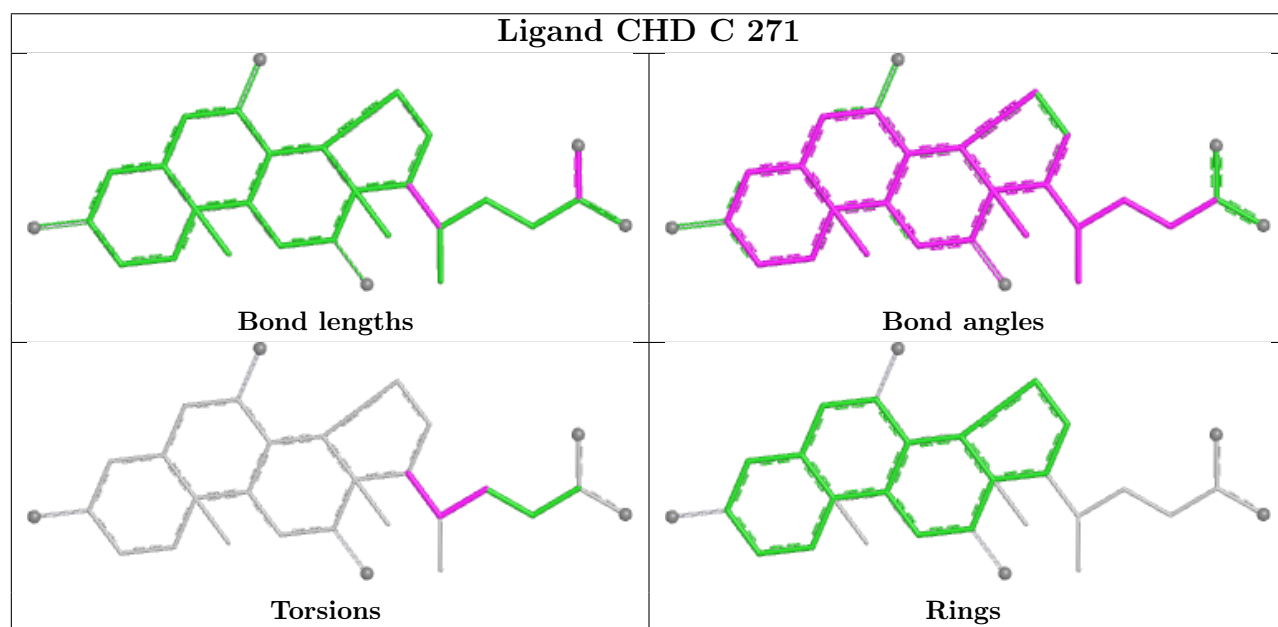
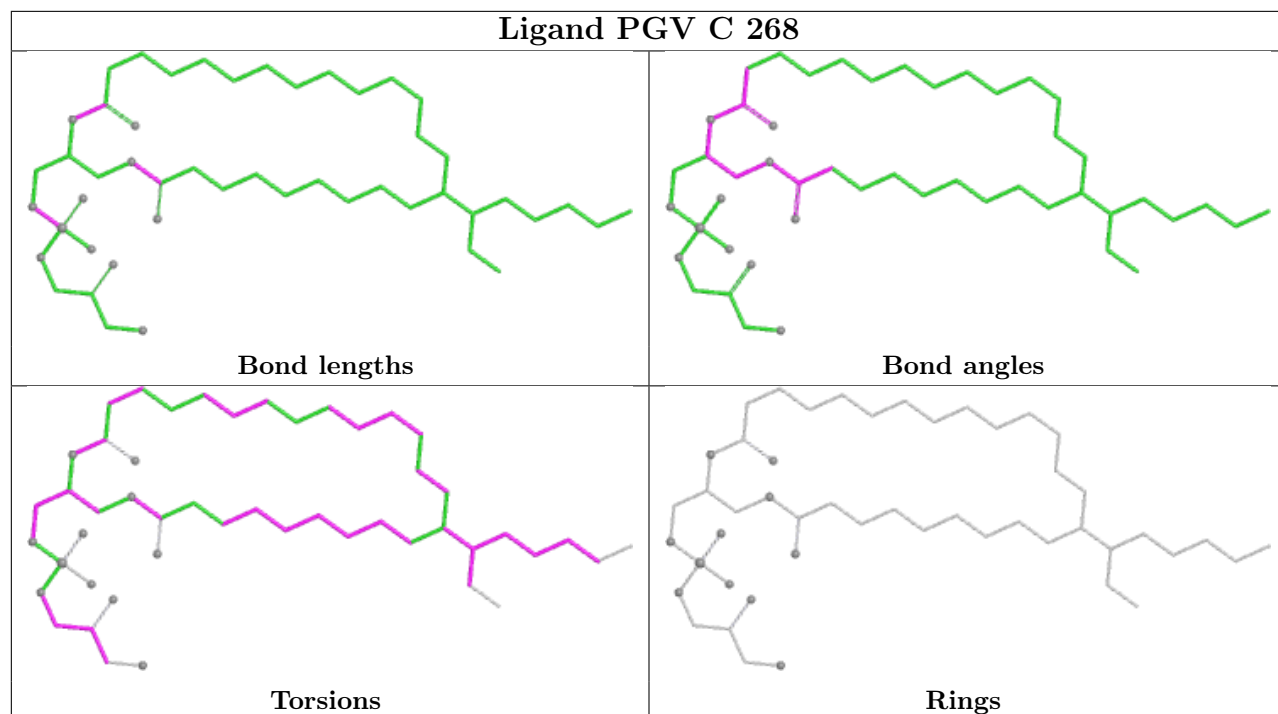




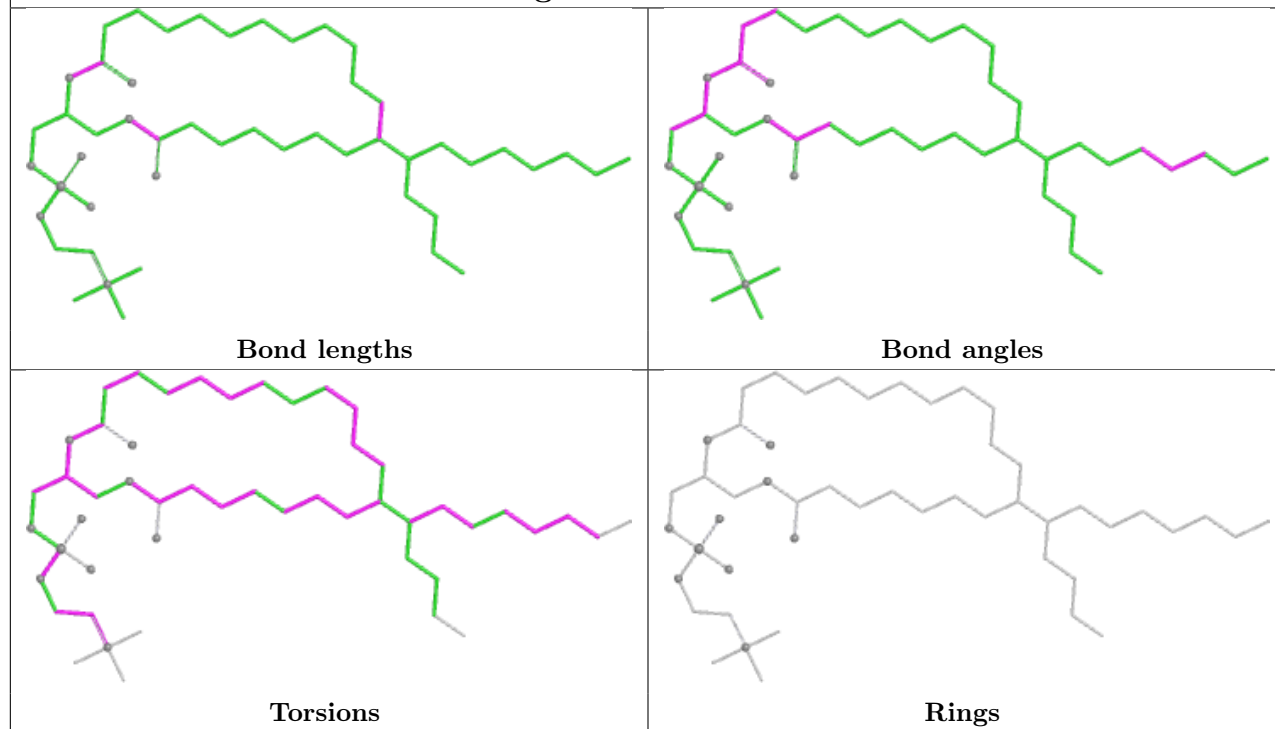




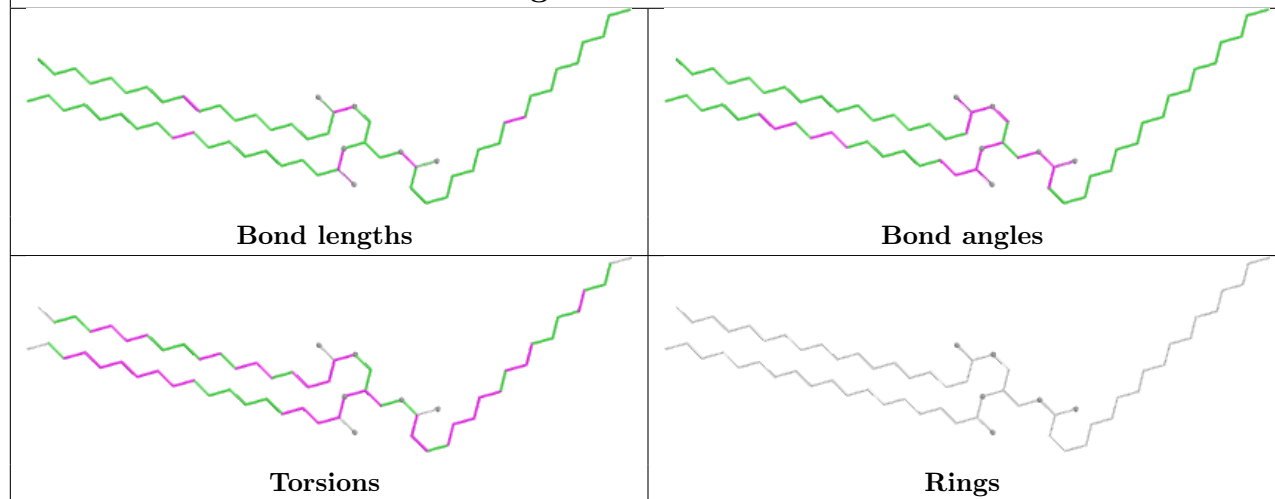


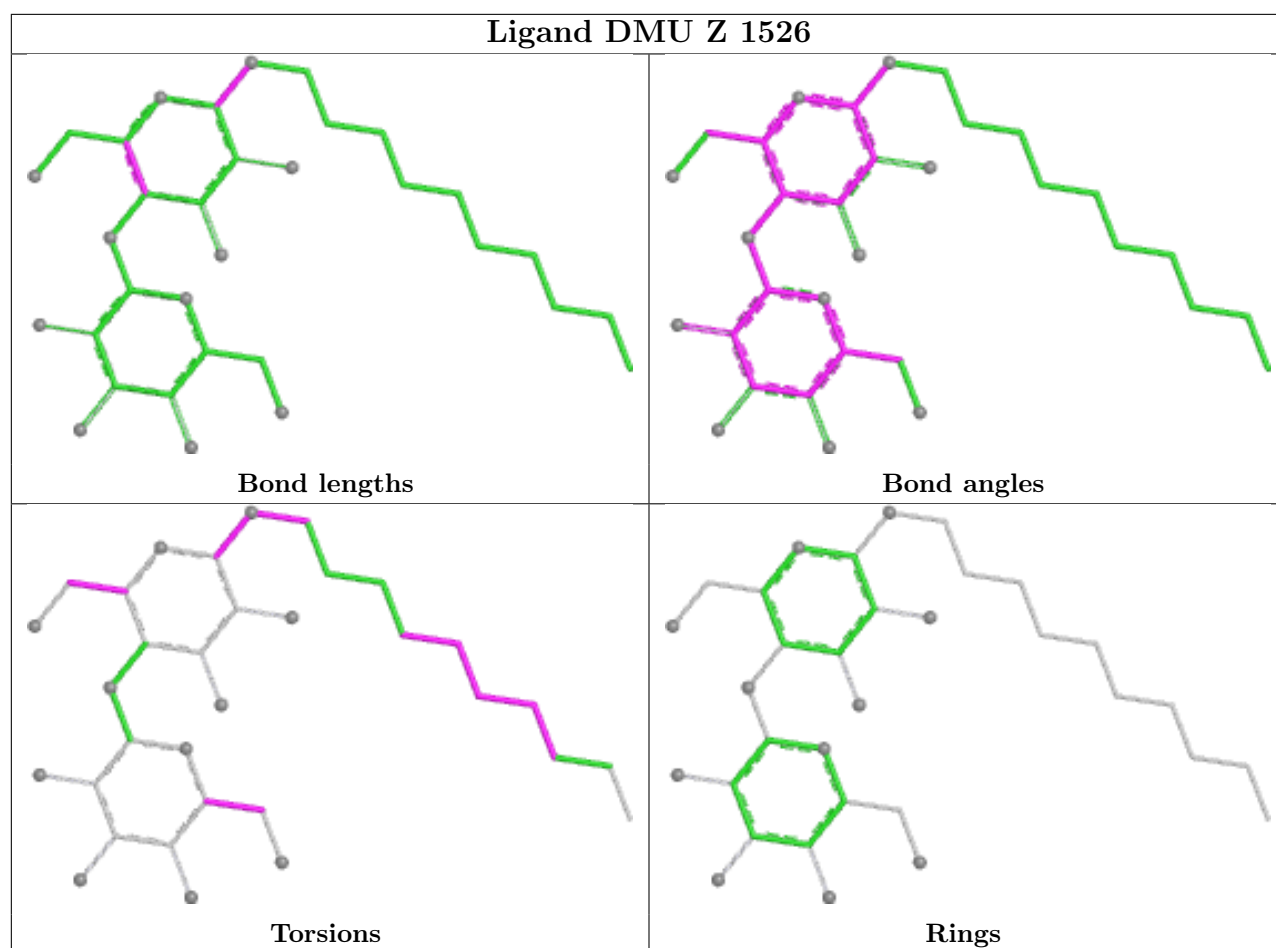


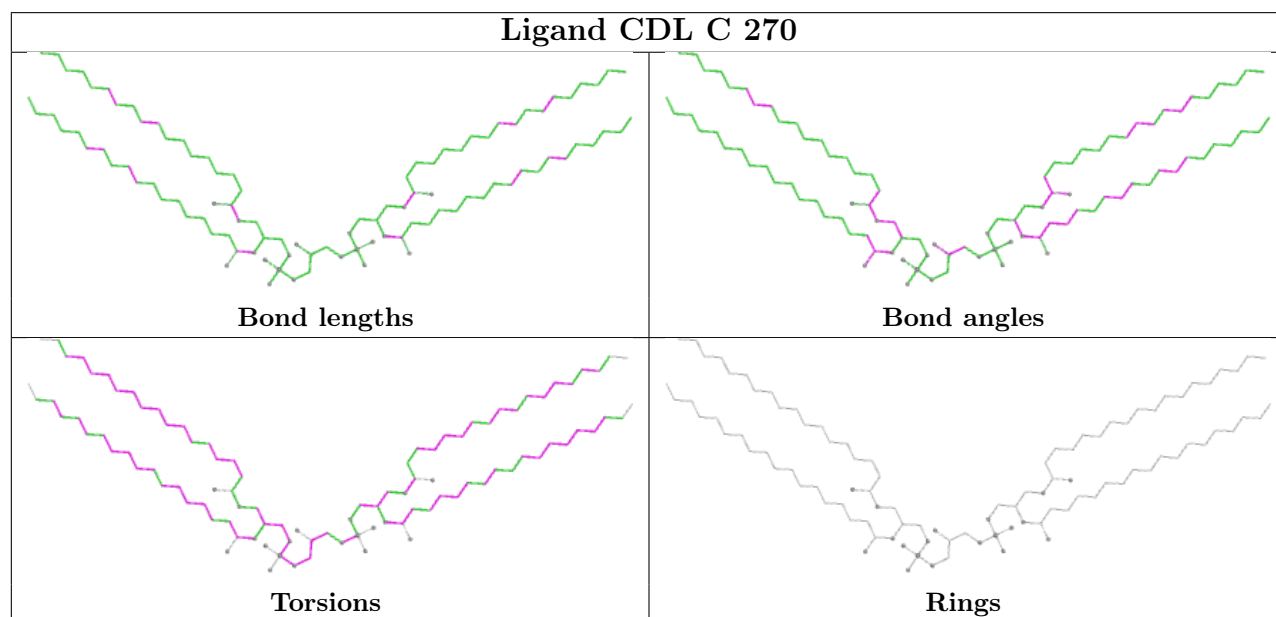
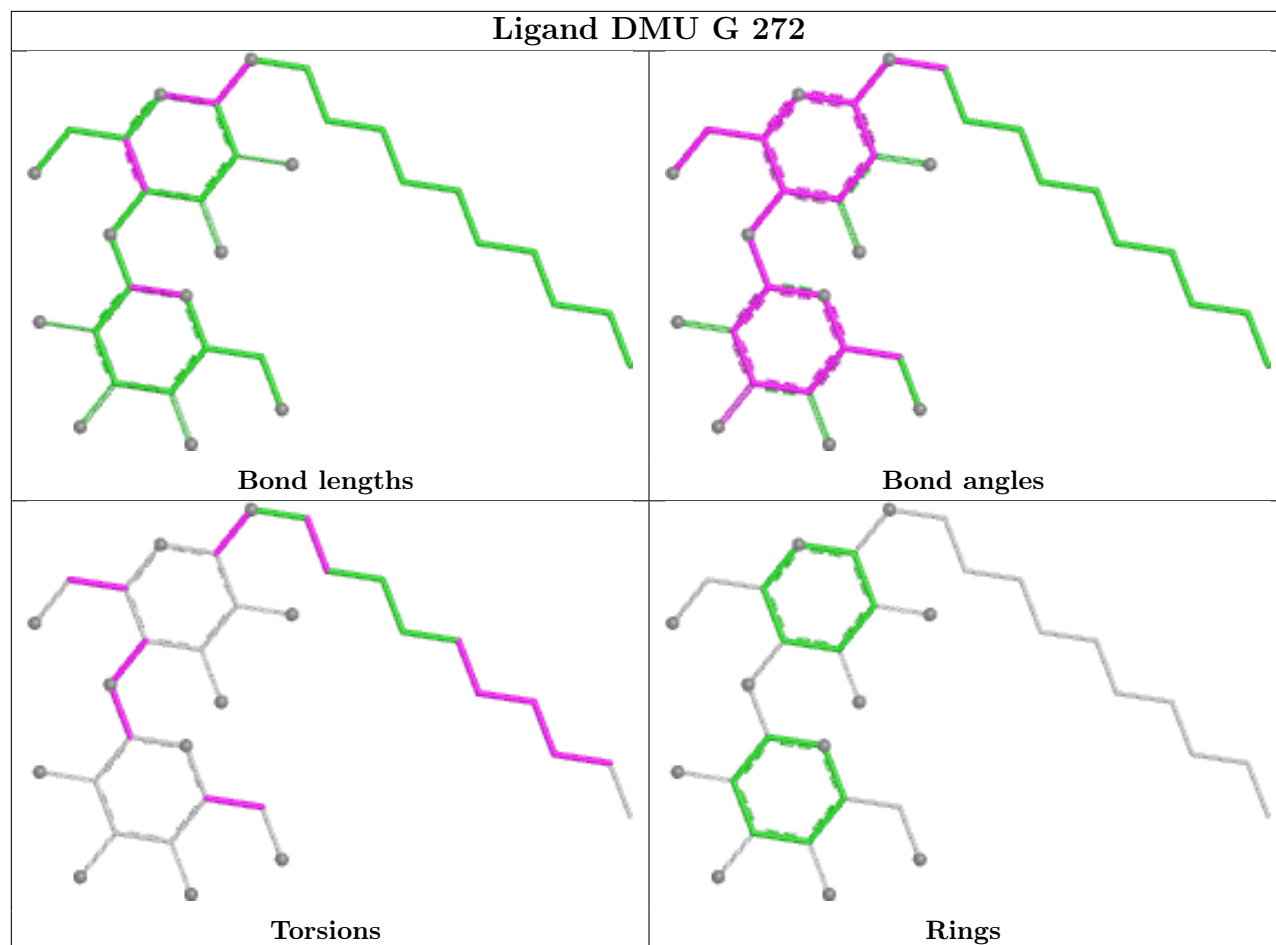
Ligand PSC E 229

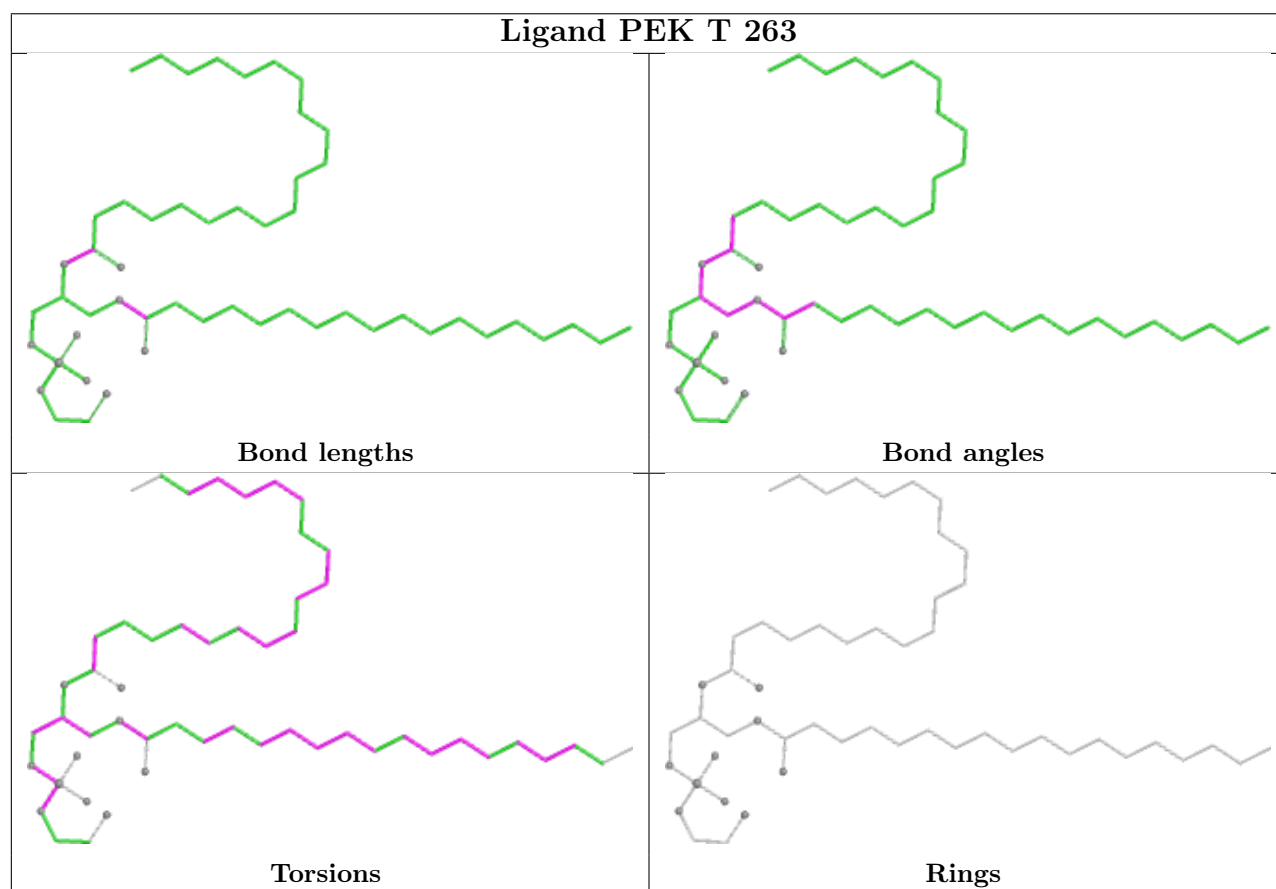
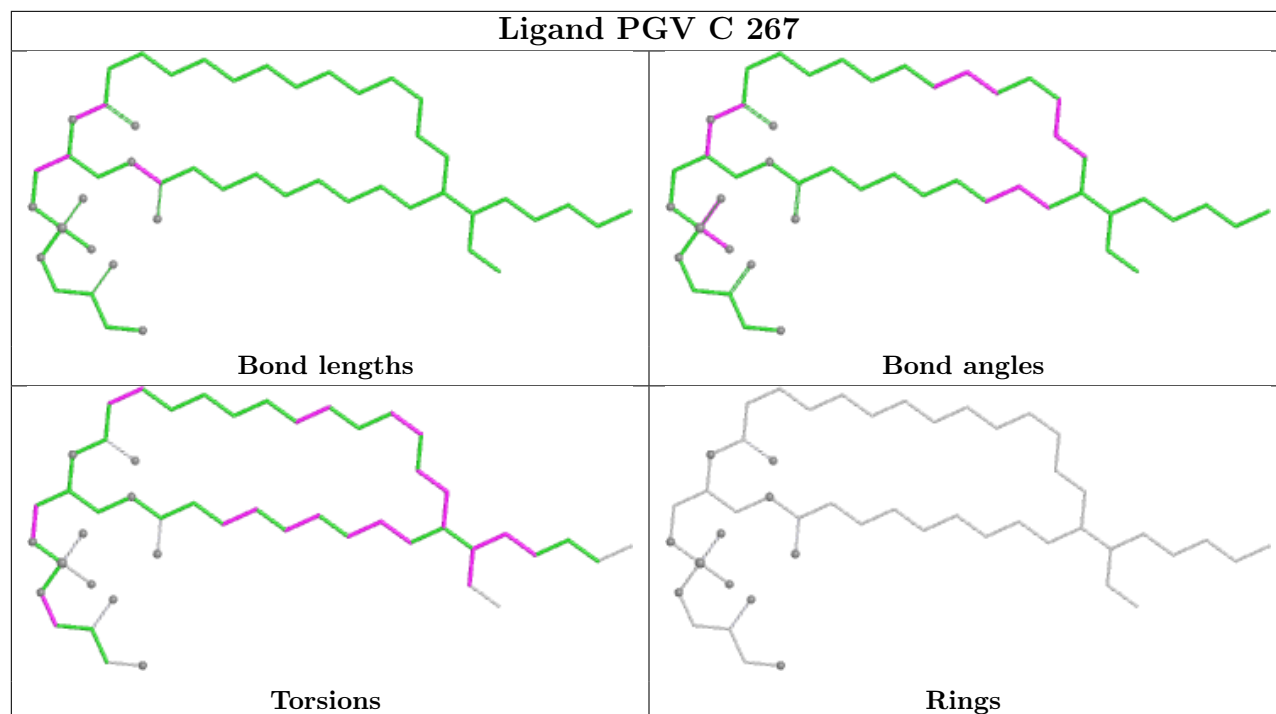


Ligand TGL D 523

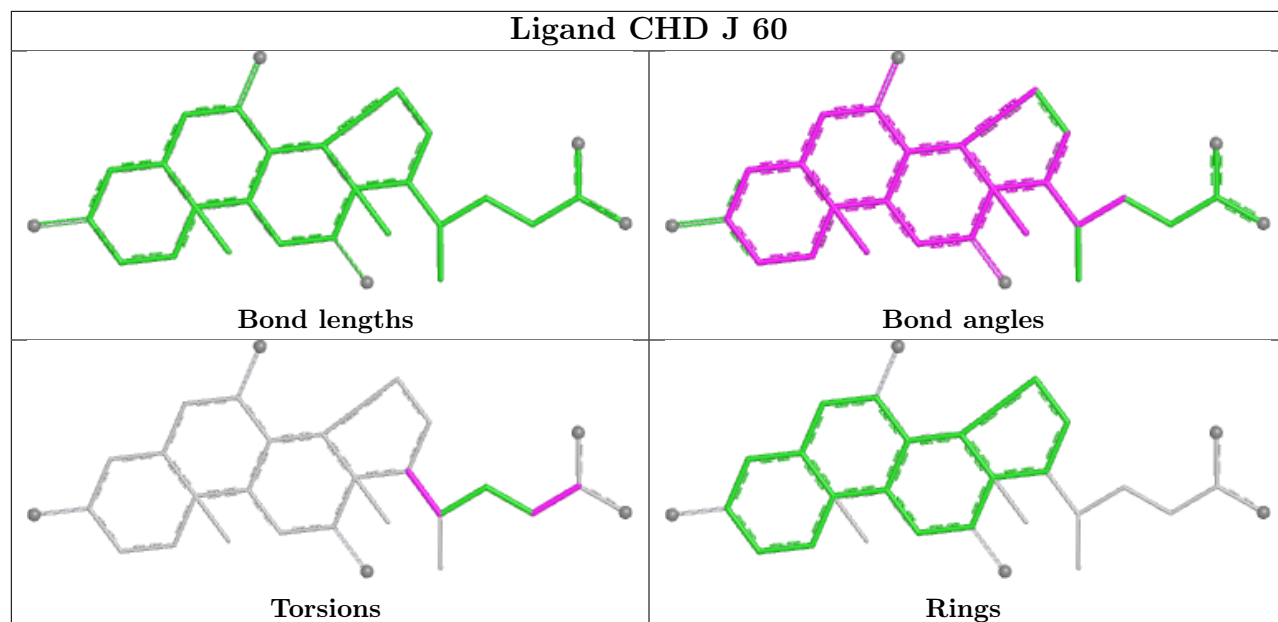




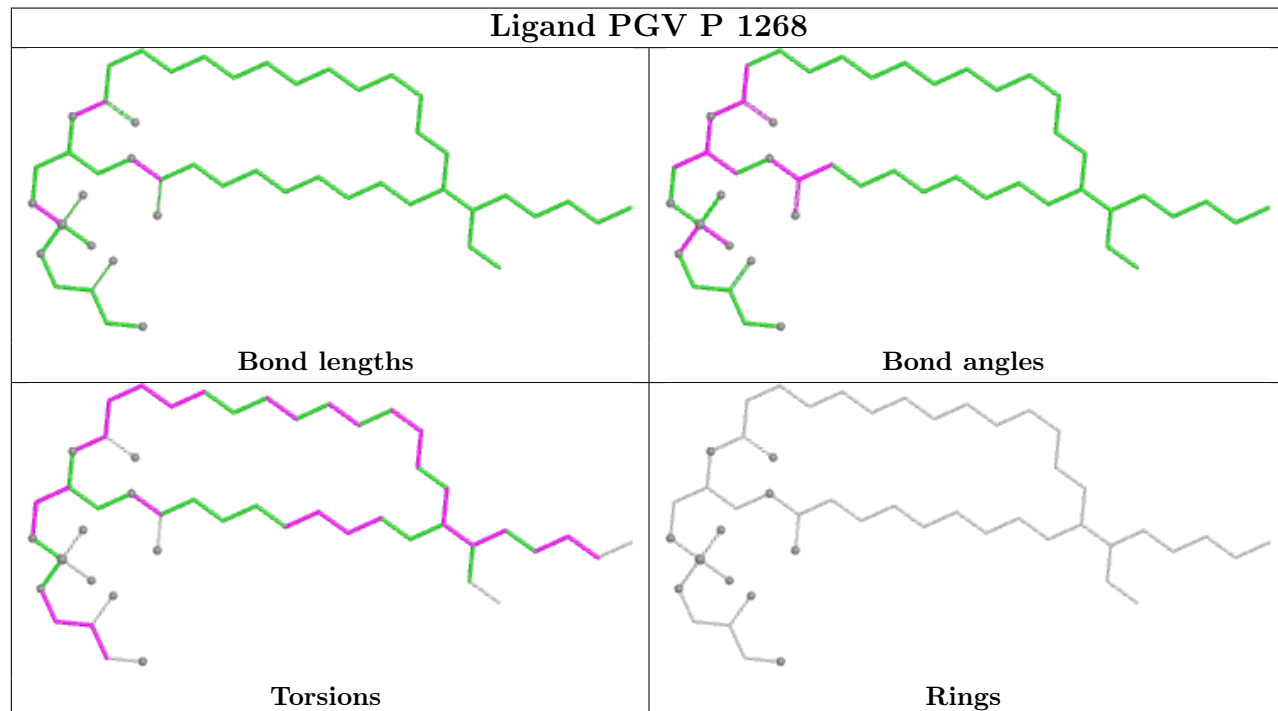


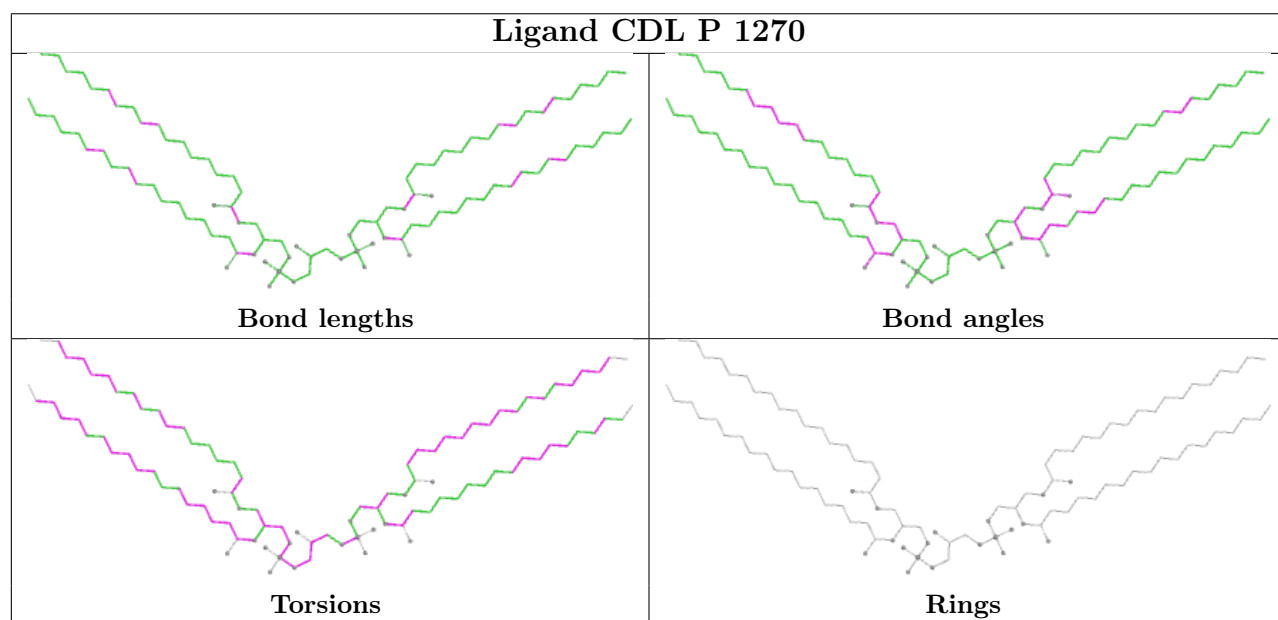
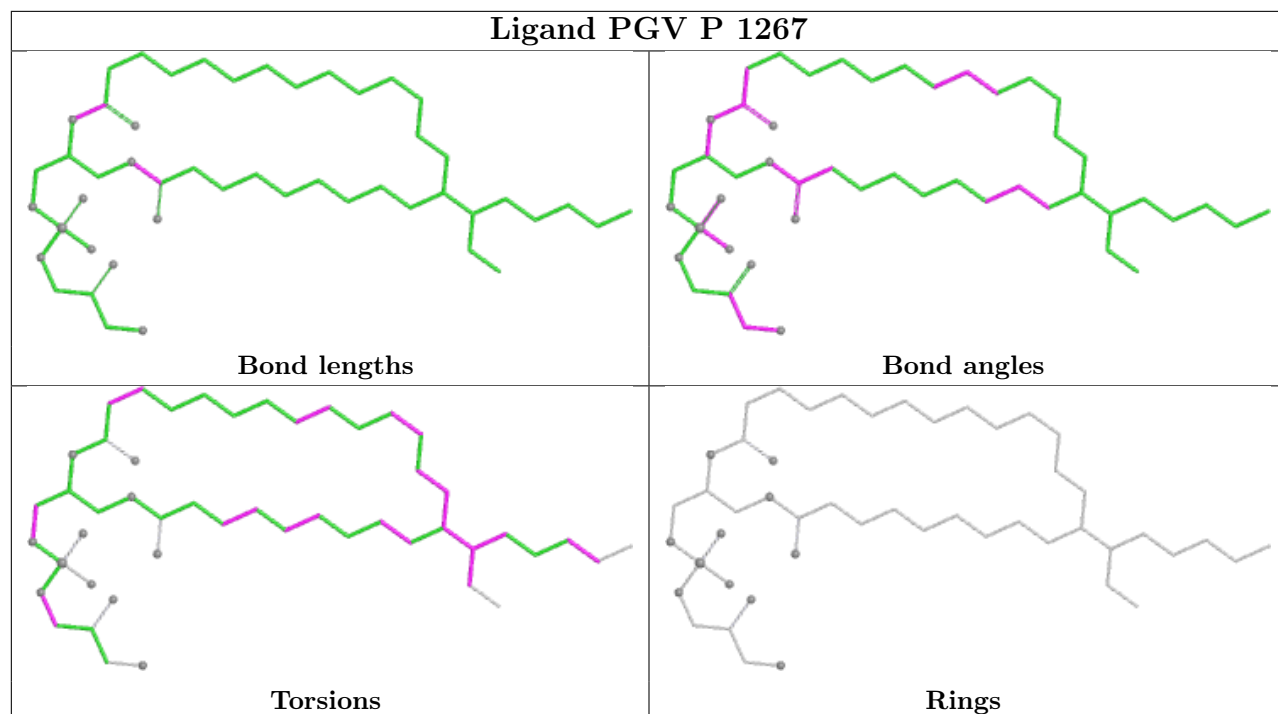


Ligand CHD J 60

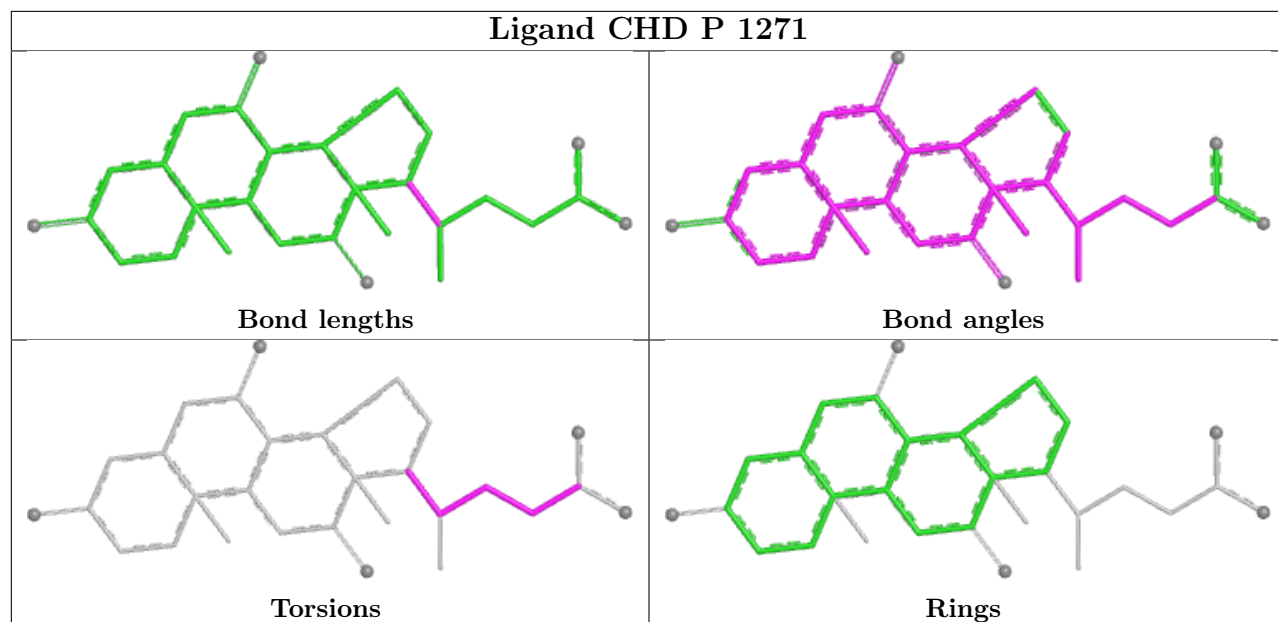


Ligand PGV P 1268

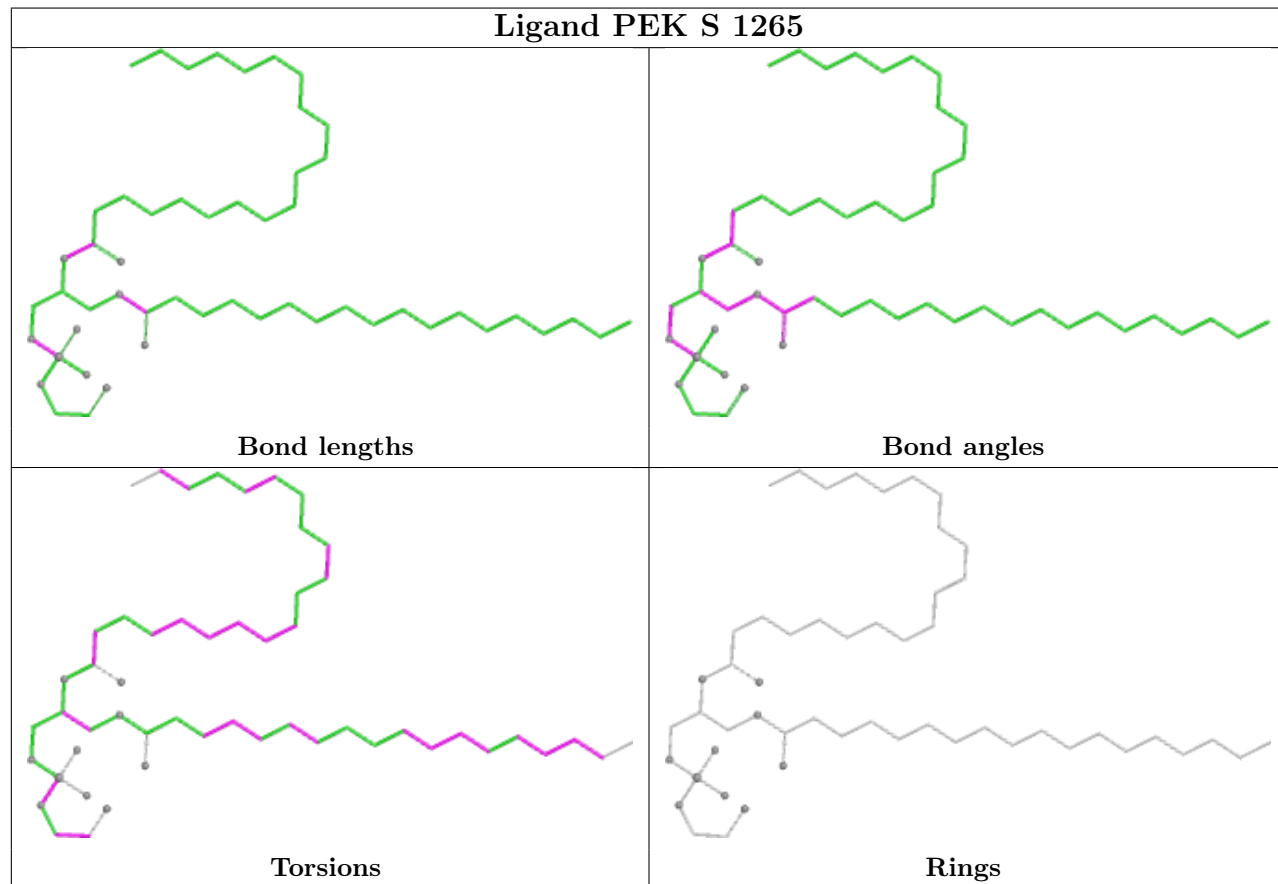


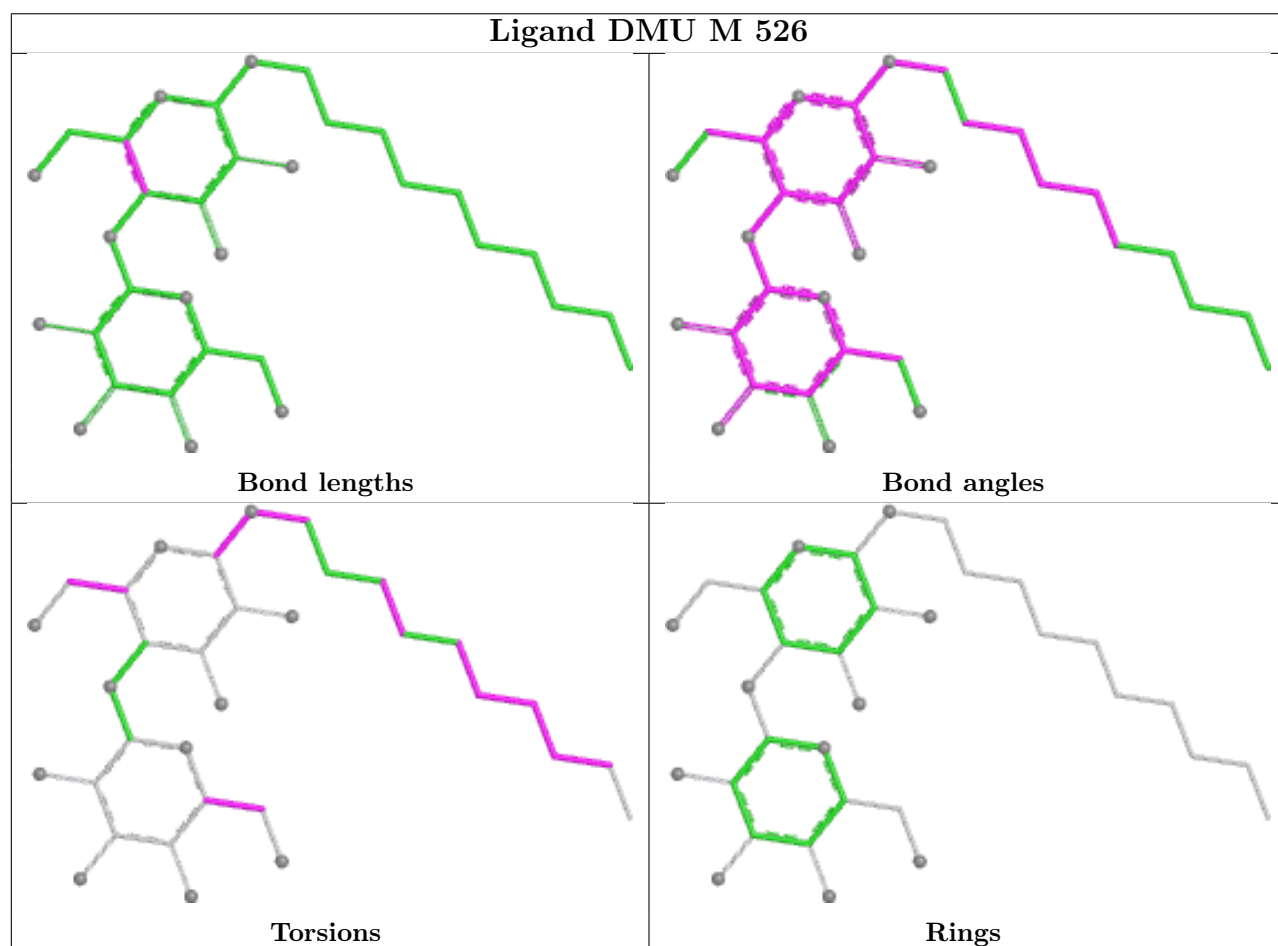
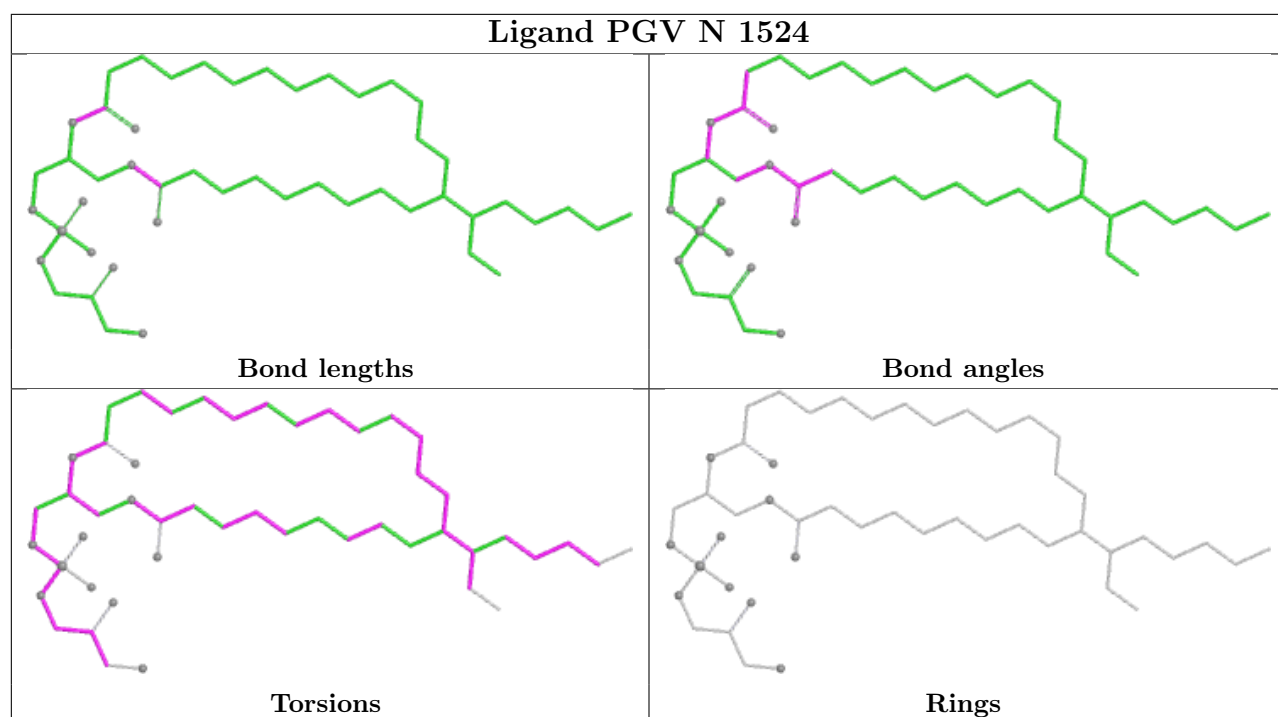


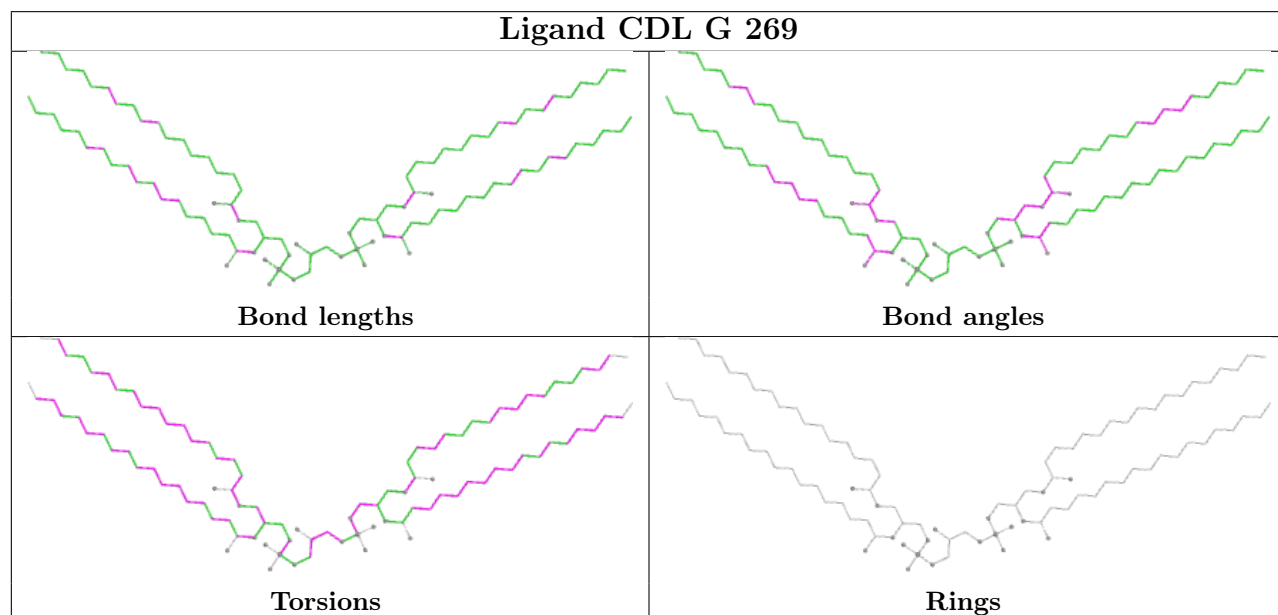
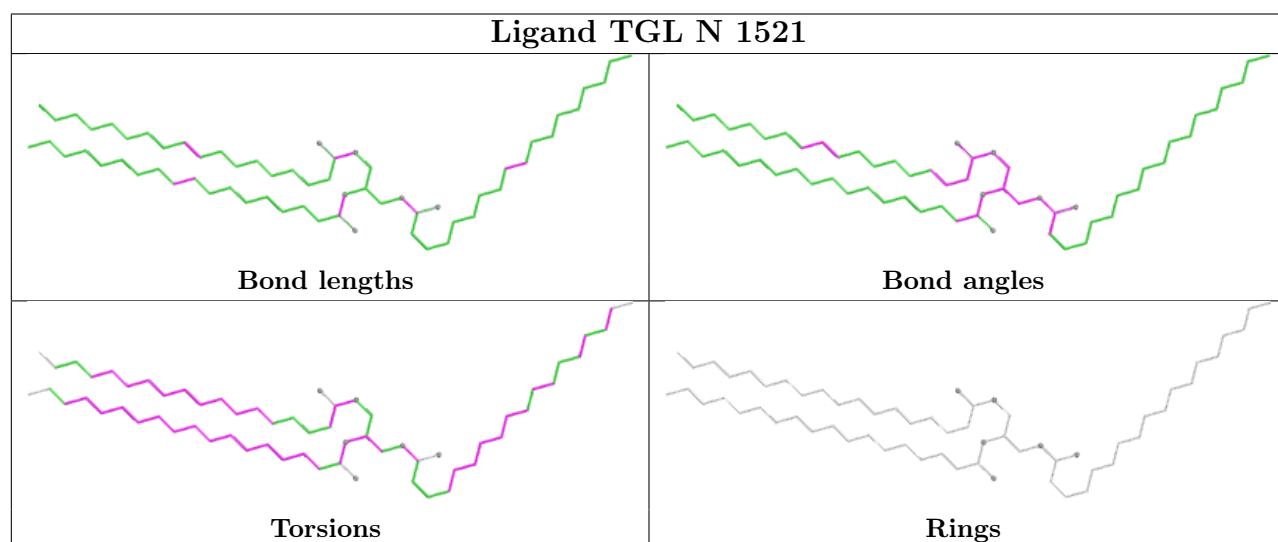
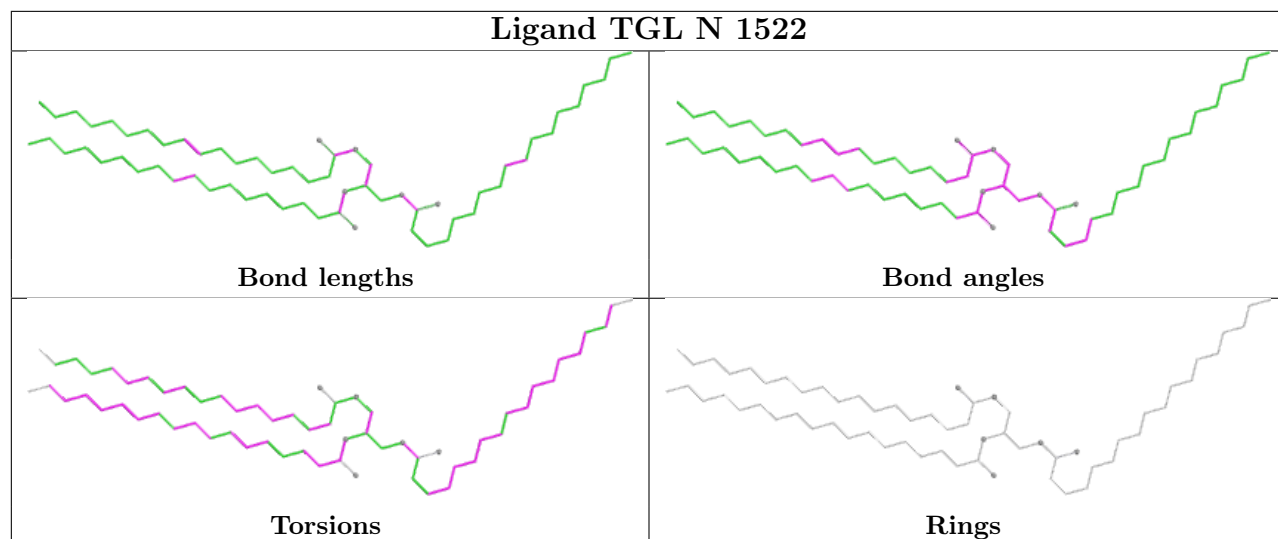
Ligand CHD P 1271



Ligand PEK S 1265







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%)	-0.28	6 (1%) 76 78	23, 29, 40, 63	0
1	N	513/514 (99%)	0.36	16 (3%) 51 52	30, 36, 47, 68	0
2	B	226/227 (99%)	0.26	16 (7%) 22 22	24, 35, 59, 78	0
2	O	226/227 (99%)	0.87	27 (11%) 9 8	33, 45, 70, 88	0
3	C	259/261 (99%)	-0.09	2 (0%) 82 84	26, 32, 43, 62	0
3	P	259/261 (99%)	0.30	9 (3%) 47 48	29, 36, 47, 67	0
4	D	144/147 (97%)	0.19	4 (2%) 55 57	30, 37, 56, 70	0
4	Q	144/147 (97%)	1.44	27 (18%) 3 2	39, 52, 76, 118	0
5	E	105/109 (96%)	0.25	2 (1%) 66 68	31, 38, 63, 99	0
5	R	105/109 (96%)	0.84	5 (4%) 35 36	36, 43, 68, 103	0
6	F	98/98 (100%)	0.58	9 (9%) 14 14	29, 39, 80, 127	0
6	S	98/98 (100%)	1.12	12 (12%) 8 7	34, 43, 86, 123	0
7	G	83/85 (97%)	1.30	20 (24%) 2 1	29, 39, 110, 113	0
7	T	83/85 (97%)	1.33	19 (22%) 2 1	29, 42, 102, 110	0
8	H	79/85 (92%)	0.75	13 (16%) 4 4	30, 41, 90, 112	0
8	U	79/85 (92%)	0.97	11 (13%) 6 6	37, 48, 94, 113	0
9	I	72/73 (98%)	0.83	13 (18%) 3 3	34, 46, 80, 83	0
9	V	72/73 (98%)	1.37	15 (20%) 2 2	39, 55, 82, 85	0
10	J	58/59 (98%)	0.60	4 (6%) 23 23	31, 41, 65, 96	0
10	W	58/59 (98%)	0.95	6 (10%) 12 11	34, 45, 69, 107	0
11	K	49/56 (87%)	0.49	2 (4%) 41 41	33, 41, 52, 62	0
11	X	49/56 (87%)	1.36	9 (18%) 3 2	44, 51, 64, 76	0
12	L	46/47 (97%)	0.19	2 (4%) 40 40	29, 34, 50, 79	0
12	Y	46/47 (97%)	0.96	3 (6%) 25 24	34, 45, 61, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	0.31	4 (9%) 14 14	30, 34, 71, 101	0
13	Z	43/46 (93%)	1.29	6 (13%) 6 5	41, 46, 90, 112	0
All	All	3550/3614 (98%)	0.47	262 (7%) 20 21	23, 38, 69, 127	0

All (262) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	6	VAL	11.5
6	S	1	ALA	10.8
4	Q	5	VAL	10.2
6	F	1	ALA	9.9
6	S	97	ALA	9.9
7	G	5	LYS	9.2
8	H	8	ILE	8.1
6	S	94	HIS	8.1
6	F	96	LEU	7.9
7	T	5	LYS	7.8
8	U	8	ILE	7.4
7	G	4	ALA	7.3
6	S	96	LEU	7.3
7	G	2	SER	7.1
7	G	7	ASP	6.7
4	Q	8	SER	6.7
7	G	3	ALA	6.6
6	S	93	PRO	6.5
7	T	4	ALA	6.3
6	F	2	SER	6.0
6	S	98	HIS	6.0
7	T	36	TRP	6.0
6	F	97	ALA	6.0
7	T	9	GLY	6.0
7	T	2	SER	5.5
7	G	1	ALA	5.4
4	Q	7	LYS	5.3
8	H	47	GLY	5.2
7	G	9	GLY	5.1
6	S	3	GLY	5.1
12	L	2	HIS	5.1
7	G	36	TRP	4.9
7	T	37	LEU	4.9
7	G	37	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
3	P	3	HIS	4.8
8	H	44	THR	4.7
6	S	95	GLN	4.7
10	J	1	PHE	4.7
4	Q	4	SER	4.7
2	B	59	GLN	4.7
9	V	3	ALA	4.6
6	S	2	SER	4.6
7	T	1	ALA	4.5
2	O	227	LEU	4.5
7	T	3	ALA	4.5
7	G	10	GLY	4.5
2	O	226	MET	4.4
13	Z	43	SER	4.4
2	O	113	TYR	4.3
13	M	43	SER	4.3
7	T	7	ASP	4.3
8	H	46	LYS	4.2
9	V	2	THR	4.2
7	G	12	GLY	4.0
2	O	47	THR	4.0
7	G	6	GLY	4.0
9	V	37	PHE	3.9
6	F	94	HIS	3.9
9	I	27	VAL	3.8
13	Z	32	TRP	3.8
4	D	4	SER	3.7
13	Z	40	TYR	3.7
7	T	33	LEU	3.7
10	W	1	PHE	3.7
7	T	6	GLY	3.7
8	U	44	THR	3.7
7	T	8	HIS	3.6
8	H	7	LYS	3.6
8	H	9	LYS	3.6
8	U	47	GLY	3.6
6	F	98	HIS	3.6
9	V	31	PHE	3.6
9	I	29	LEU	3.6
1	N	513	LEU	3.6
1	N	3	ILE	3.5
3	C	38	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
10	J	58	LYS	3.5
12	Y	2	HIS	3.5
13	M	40	TYR	3.5
6	F	3	GLY	3.5
7	T	12	GLY	3.5
7	G	38	HIS	3.5
7	T	42	ARG	3.4
13	Z	42	LYS	3.4
4	Q	11	TYR	3.4
2	O	90	ILE	3.4
7	T	10	GLY	3.4
10	W	58	LYS	3.4
9	I	25	PHE	3.4
9	I	31	PHE	3.4
7	G	8	HIS	3.3
2	B	87	MET	3.3
8	U	46	LYS	3.3
8	H	48	GLY	3.3
7	T	38	HIS	3.3
1	N	2	PHE	3.3
4	Q	9	GLU	3.3
1	A	383	MET	3.3
2	O	59	GLN	3.3
8	H	10	ASN	3.3
6	S	92	VAL	3.2
1	N	113	LEU	3.2
7	T	84	LYS	3.2
10	J	52	TRP	3.2
4	D	5	VAL	3.2
2	O	65	TRP	3.2
11	K	47	ARG	3.2
6	F	95	GLN	3.2
2	O	217	LYS	3.1
4	Q	35	ALA	3.1
8	H	42	ALA	3.1
1	A	298	ASP	3.1
11	K	6	ALA	3.1
2	O	30	ILE	3.1
13	Z	41	LYS	3.1
4	Q	33	LEU	3.0
2	B	65	TRP	3.0
7	G	41	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
1	N	382	SER	3.0
5	R	109	VAL	3.0
8	U	7	LYS	3.0
9	V	36	LYS	2.9
3	P	122	HIS	2.9
1	A	513	LEU	2.9
2	O	38	VAL	2.9
9	V	27	VAL	2.9
1	N	49	GLY	2.9
1	N	383	MET	2.8
1	N	312	ILE	2.8
2	B	60	GLU	2.8
10	W	52	TRP	2.8
8	U	50	VAL	2.8
1	N	297	MET	2.8
10	J	48	TYR	2.8
11	X	13	TYR	2.8
4	Q	39	ALA	2.8
9	I	32	ALA	2.8
11	X	23	THR	2.8
7	G	84	LYS	2.8
12	L	47	LYS	2.8
7	T	39	SER	2.8
11	X	47	ARG	2.8
4	Q	10	ASP	2.8
4	Q	125	ASP	2.8
7	G	42	ARG	2.7
5	E	5	HIS	2.7
11	X	52	GLU	2.7
2	B	90	ILE	2.7
3	P	38	ASN	2.7
7	G	39	SER	2.7
8	H	43	MET	2.7
2	B	57	ASP	2.7
8	U	45	ALA	2.7
9	V	25	PHE	2.7
5	E	109	VAL	2.7
12	Y	20	ARG	2.7
2	O	130	PRO	2.7
7	G	40	GLY	2.7
9	I	37	PHE	2.6
2	B	113	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
2	O	218	TYR	2.6
1	A	514	LYS	2.6
1	N	250	GLY	2.6
7	T	40	GLY	2.6
2	B	91	ASN	2.6
9	V	33	THR	2.6
2	O	35	SER	2.6
4	Q	57	VAL	2.6
9	I	30	GLY	2.6
9	V	29	LEU	2.6
12	Y	47	LYS	2.6
8	H	45	ALA	2.6
2	O	37	LEU	2.6
8	U	9	LYS	2.5
11	X	6	ALA	2.5
3	P	33	MET	2.5
4	Q	58	GLU	2.5
2	O	58	ALA	2.5
9	V	5	ALA	2.5
5	R	5	HIS	2.5
2	O	41	ILE	2.5
4	Q	89	ILE	2.5
2	O	43	SER	2.4
5	R	100	THR	2.4
3	C	3	HIS	2.4
4	Q	87	PHE	2.4
9	V	8	GLN	2.4
9	I	33	THR	2.4
1	A	346	PHE	2.4
3	P	44	MET	2.4
1	N	484	THR	2.4
9	V	35	TYR	2.4
2	B	39	LEU	2.4
4	Q	95	LEU	2.4
13	M	39	ASN	2.4
1	N	298	ASP	2.4
2	B	37	LEU	2.3
3	P	37	PHE	2.3
9	I	26	MET	2.3
2	O	116	LEU	2.3
2	O	126	SER	2.3
9	I	21	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	38	VAL	2.3
2	B	40	TYR	2.3
2	O	128	LEU	2.3
4	D	11	TYR	2.3
4	Q	102	TYR	2.3
5	R	79	LYS	2.3
9	V	67	GLY	2.3
9	V	73	LYS	2.3
13	M	42	LYS	2.3
2	O	87	MET	2.3
4	Q	59	LEU	2.3
5	R	104	LEU	2.3
10	W	57	HIS	2.2
9	I	28	SER	2.2
4	Q	51	LEU	2.2
4	Q	62	LEU	2.2
2	O	40	TYR	2.2
4	Q	48	TRP	2.2
1	A	382	SER	2.2
3	P	123	PRO	2.2
11	X	16	ALA	2.2
2	O	46	LEU	2.2
7	G	33	LEU	2.2
3	P	148	HIS	2.2
2	B	32	PHE	2.2
8	H	50	VAL	2.2
9	V	72	ALA	2.2
11	X	19	ALA	2.2
9	I	35	TYR	2.2
10	W	48	TYR	2.2
13	Z	35	TYR	2.2
4	Q	31	LYS	2.2
8	H	55	TRP	2.2
2	B	55	THR	2.2
6	S	52	ILE	2.1
8	U	11	TYR	2.1
2	O	60	GLU	2.1
8	U	55	TRP	2.1
1	N	394	VAL	2.1
4	Q	116	VAL	2.1
4	Q	121	LYS	2.1
2	B	86	MET	2.1

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Mol	Chain	Res	Type	RSRZ
4	Q	19	ARG	2.1
3	P	91	VAL	2.1
1	N	48	LEU	2.1
2	O	36	SER	2.1
6	S	53	THR	2.1
10	W	56	PRO	2.1
11	X	7	PRO	2.1
11	X	31	TYR	2.1
2	O	42	ILE	2.1
1	N	57	VAL	2.1
9	I	5	ALA	2.1
6	F	93	PRO	2.0
2	O	224	ALA	2.0
8	U	10	ASN	2.0
2	B	82	ARG	2.0
1	N	509	THR	2.0
4	D	102	TYR	2.0
4	Q	140	TYR	2.0

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

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	0.03	0.23	88,90,92,93	0
7	TPO	T	11	11/12	0.52	0.24	75,82,101,102	0
7	TPO	G	11	11/12	0.52	0.29	74,82,105,105	0
9	SAC	I	1	9/10	0.70	0.18	77,82,84,85	0
1	FME	N	1	10/11	0.81	0.24	50,54,74,77	0
1	FME	A	1	10/11	0.85	0.15	46,51,63,76	0
2	FME	O	1	10/11	0.94	0.12	41,42,49,55	0
2	FME	B	1	10/11	0.96	0.09	31,33,40,56	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
23	UNX	C	262	1/1	0.68	0.58	49,49,49,49	0
24	PEK	T	263	53/53	0.68	0.31	54,103,127,128	0
23	UNX	P	262	1/1	0.71	0.58	49,49,49,49	0
22	CHD	W	1059	29/29	0.72	0.25	107,115,119,120	0
24	PEK	G	265	53/53	0.73	0.27	51,91,109,114	0
28	DMU	P	1272	33/33	0.73	0.25	104,118,124,125	0
24	PEK	G	1263	53/53	0.74	0.32	59,107,131,132	0
19	TGL	N	1522	63/63	0.74	0.29	54,76,92,95	0
20	PGV	N	1524	51/51	0.74	0.26	54,81,117,119	0
20	PGV	P	1268	51/51	0.76	0.29	64,100,119,121	0
24	PEK	S	1265	53/53	0.76	0.27	50,87,111,114	0
26	PSC	R	1229	52/52	0.77	0.28	53,109,133,136	0
25	CDL	G	269	100/100	0.77	0.28	72,99,122,124	0
25	CDL	T	1269	100/100	0.78	0.28	66,96,122,126	0
26	PSC	E	229	52/52	0.78	0.26	53,106,131,133	0
19	TGL	Q	1523	63/63	0.78	0.28	67,83,98,100	0
22	CHD	J	60	29/29	0.78	0.21	105,109,113,114	0
19	TGL	A	521	63/63	0.79	0.25	49,82,106,110	0
28	DMU	G	272	33/33	0.79	0.23	85,116,119,121	0
25	CDL	P	1270	100/100	0.79	0.28	46,100,119,122	0
20	PGV	C	268	51/51	0.80	0.28	60,91,117,117	0
19	TGL	D	523	63/63	0.80	0.27	48,70,93,94	0
20	PGV	A	524	51/51	0.80	0.26	45,75,117,118	0
19	TGL	N	1521	63/63	0.81	0.26	71,92,105,109	0
19	TGL	L	522	63/63	0.81	0.26	43,68,84,87	0
25	CDL	C	270	100/100	0.82	0.23	49,96,120,122	0
28	DMU	Z	1526	33/33	0.82	0.15	44,59,75,75	0
22	CHD	C	271	29/29	0.83	0.19	72,84,87,90	0
15	CYN	N	520	2/2	0.87	0.16	42,42,42,43	0
22	CHD	P	1271	29/29	0.87	0.17	68,86,90,91	0
28	DMU	M	526	33/33	0.91	0.11	36,51,69,71	0
24	PEK	T	1264	53/53	0.93	0.16	30,54,83,85	0
22	CHD	P	1525	29/29	0.94	0.09	28,38,43,51	0
22	CHD	O	229	29/29	0.94	0.08	27,34,42,45	0
20	PGV	N	1266	51/51	0.95	0.12	28,43,70,75	0
18	NA	N	519	1/1	0.95	0.10	40,40,40,40	0
24	PEK	C	264	53/53	0.95	0.14	27,50,76,79	0

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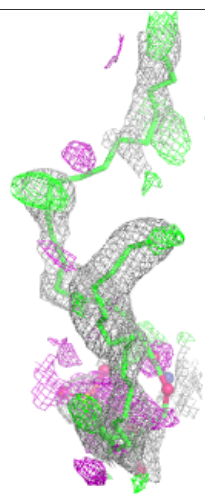
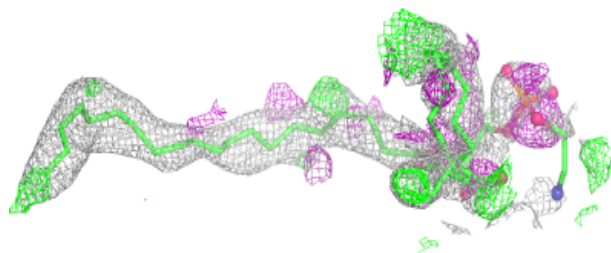
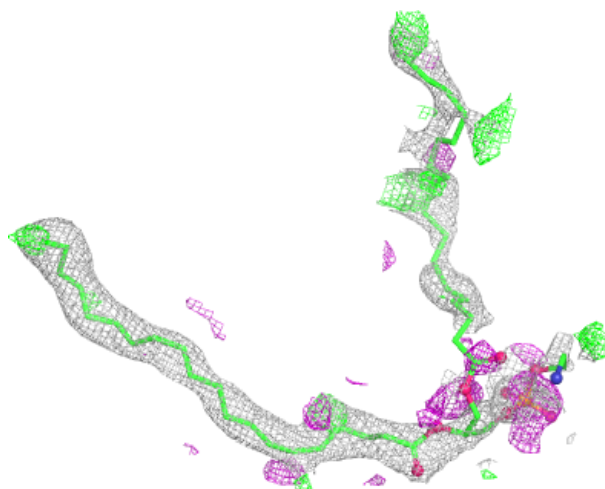
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	CHD	B	1085	29/29	0.95	0.08	29,34,40,50	0
22	CHD	C	525	29/29	0.95	0.08	25,35,39,46	0
14	HEA	N	516	60/60	0.95	0.12	32,40,54,57	0
17	MG	N	518	1/1	0.96	0.05	33,33,33,33	0
20	PGV	A	522	51/51	0.96	0.11	25,36,68,72	0
20	PGV	P	1267	51/51	0.96	0.12	29,40,77,85	0
20	PGV	C	267	51/51	0.96	0.12	23,36,72,75	0
15	CYN	A	520	2/2	0.96	0.08	31,31,31,31	0
21	CUA	O	228	2/2	0.97	0.04	36,36,36,37	0
18	NA	A	519	1/1	0.97	0.05	30,30,30,30	0
14	HEA	A	516	60/60	0.97	0.10	23,35,51,52	0
14	HEA	N	515	60/60	0.98	0.08	30,36,50,52	0
14	HEA	A	515	60/60	0.98	0.06	18,27,40,45	0
27	ZN	F	99	1/1	0.99	0.02	35,35,35,35	0
27	ZN	S	99	1/1	0.99	0.02	38,38,38,38	0
21	CUA	B	228	2/2	0.99	0.03	28,28,28,28	0
17	MG	A	518	1/1	0.99	0.03	25,25,25,25	0
16	CU	A	517	1/1	0.99	0.04	31,31,31,31	0
16	CU	N	517	1/1	0.99	0.04	37,37,37,37	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.

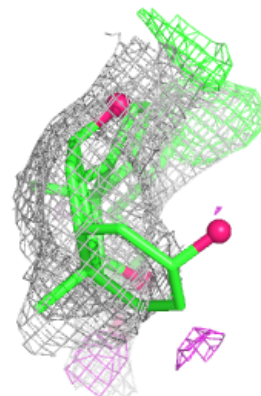
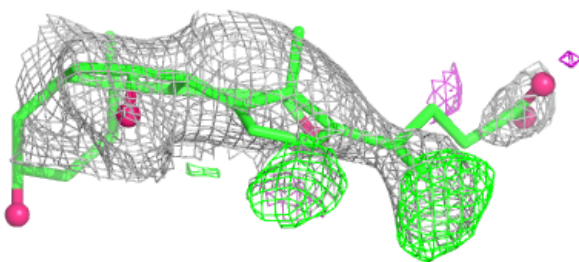
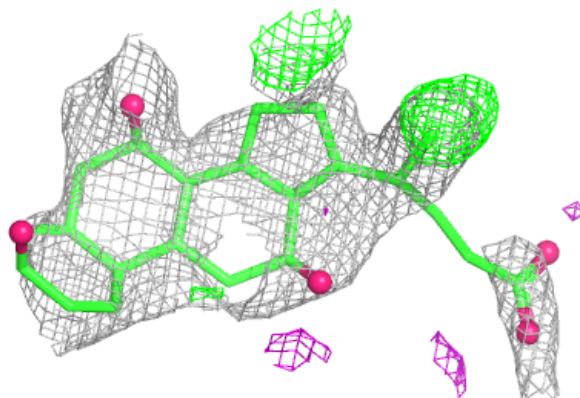
Electron density around PEK T 263:

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



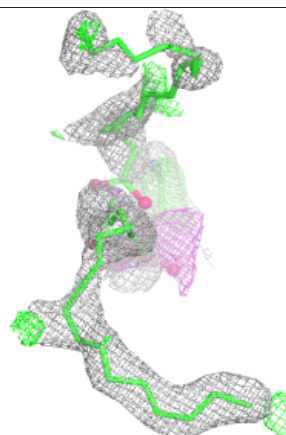
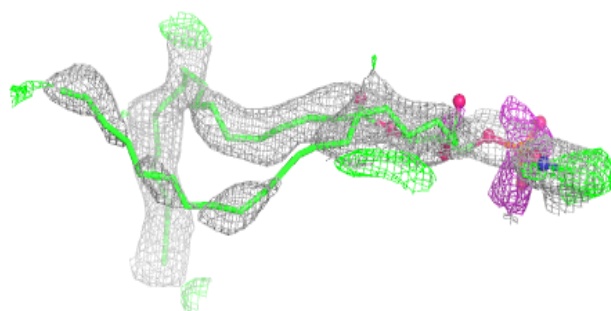
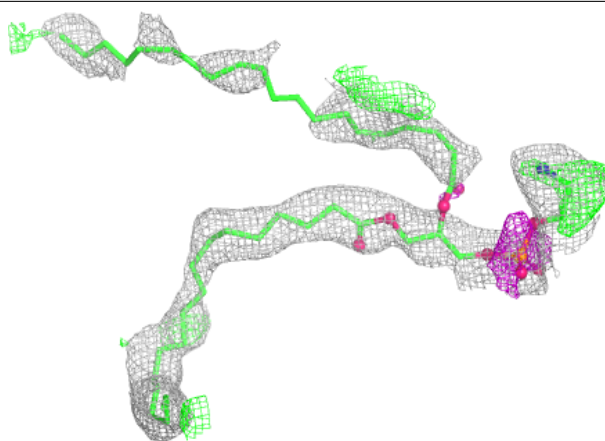
Electron density around CHD W 1059:

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



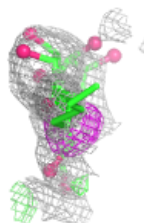
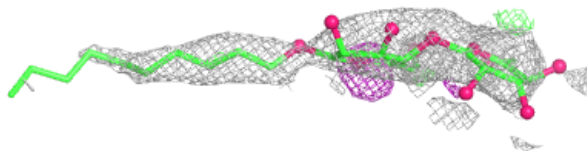
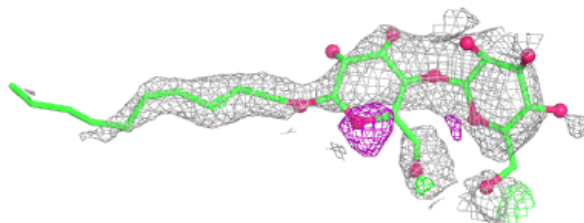
Electron density around PEK G 265:

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



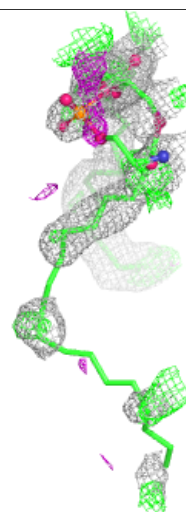
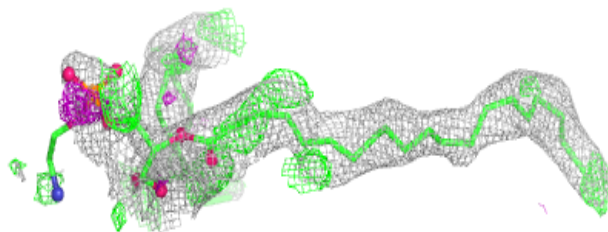
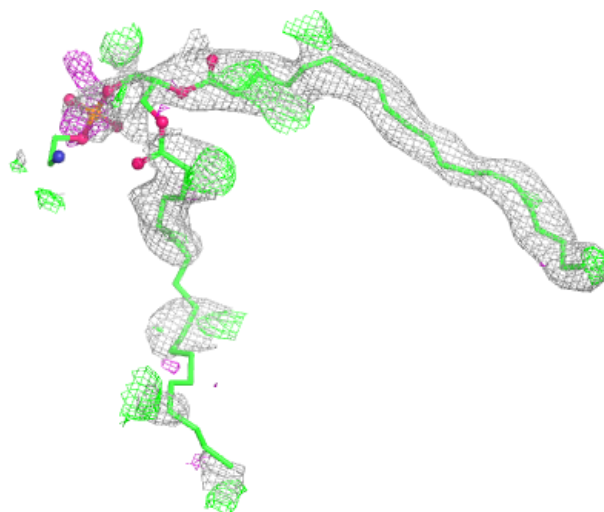
Electron density around DMU P 1272:

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



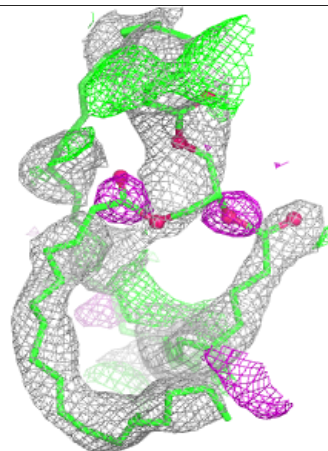
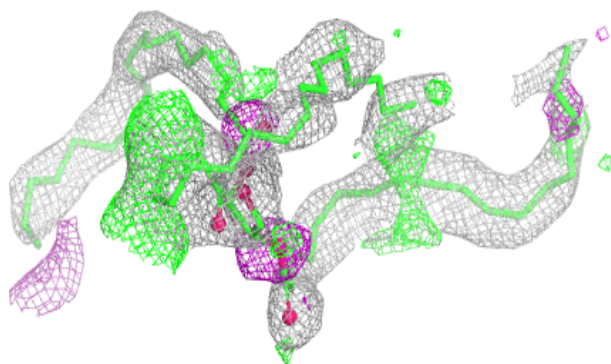
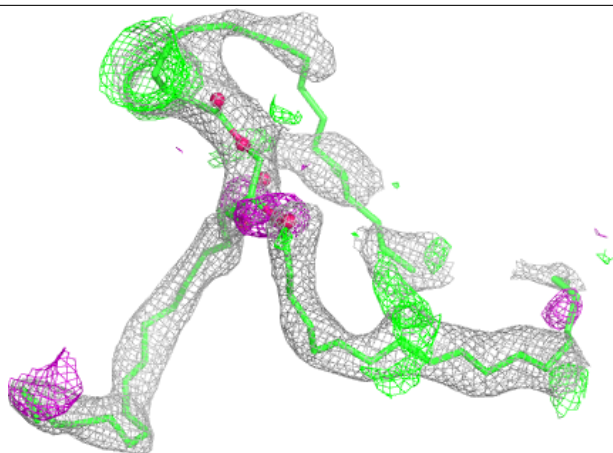
Electron density around PEK G 1263:

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

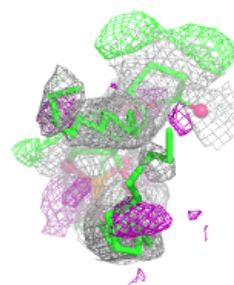
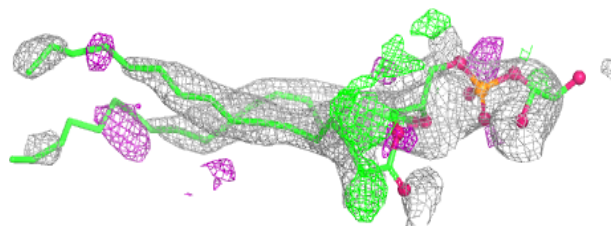
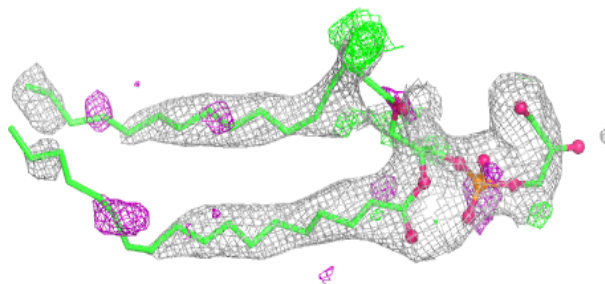


Electron density around TGL N 1522:

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

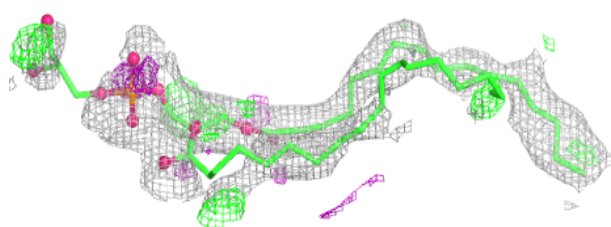
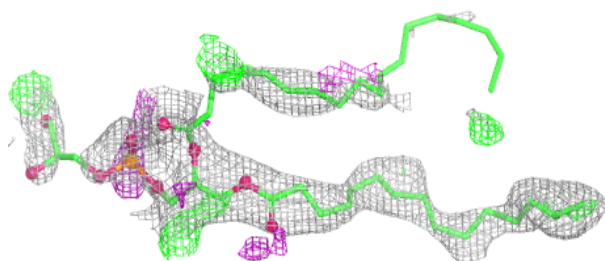
**Electron density around PGV N 1524:**

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

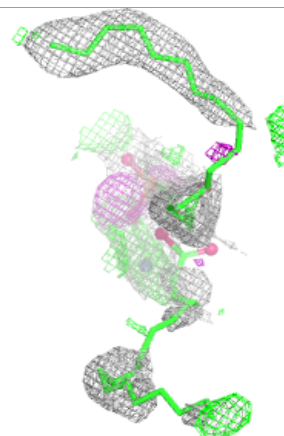
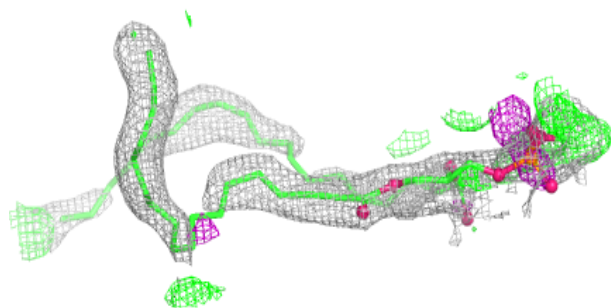
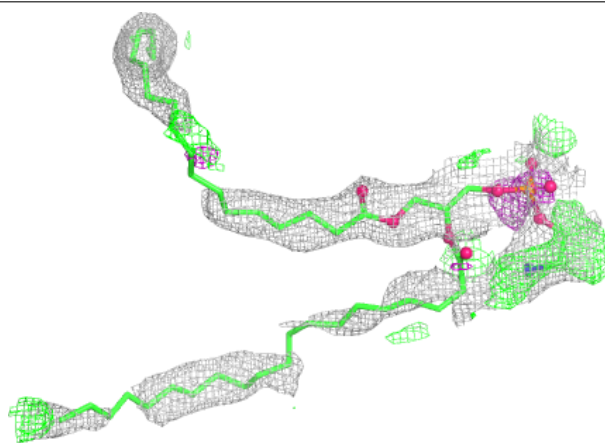


Electron density around PGV P 1268:

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

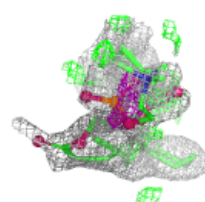
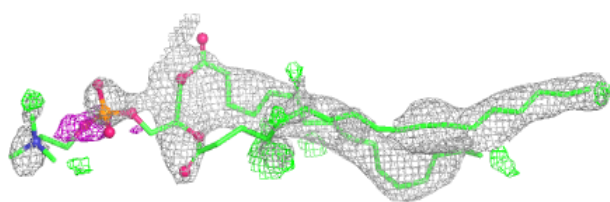
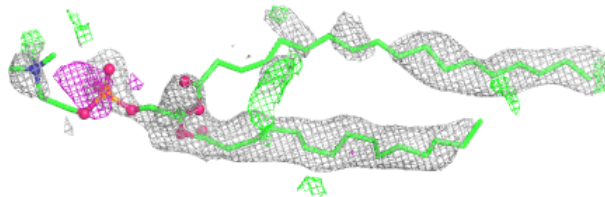
**Electron density around PEK S 1265:**

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

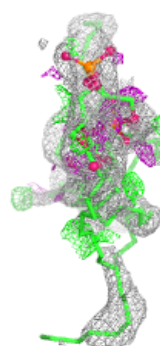
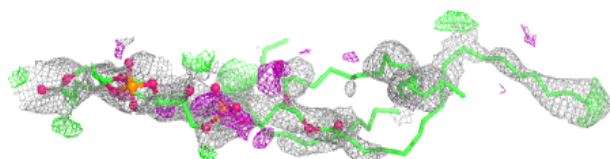
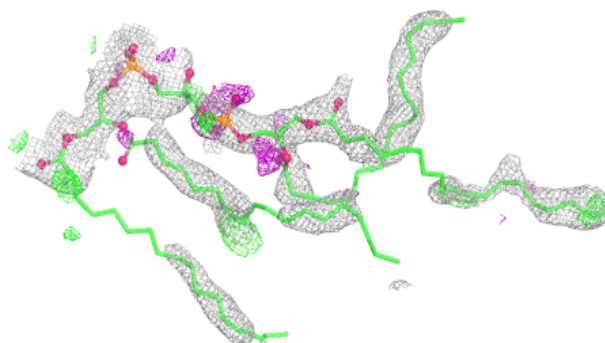


Electron density around PSC R 1229:

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

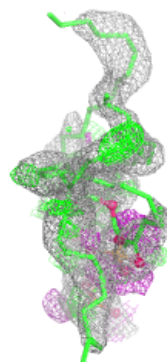
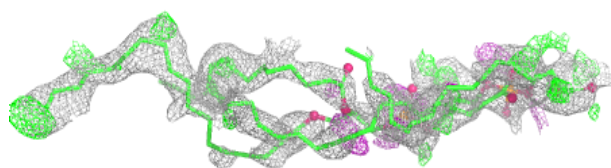
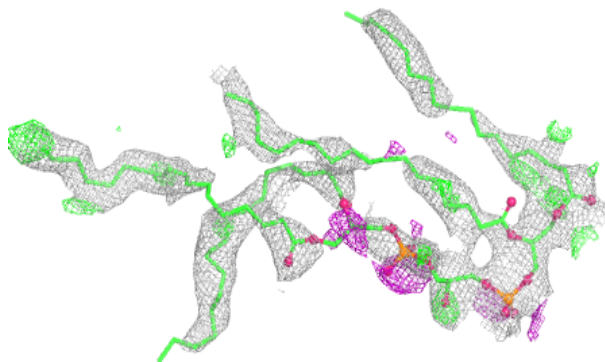
**Electron density around CDL G 269:**

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

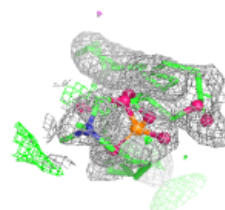
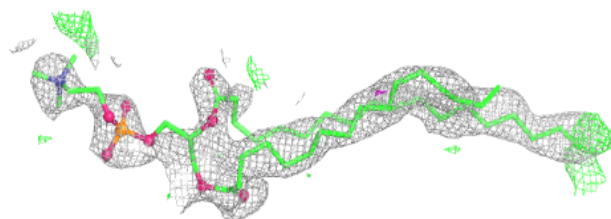
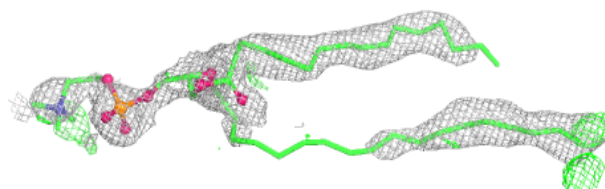


Electron density around CDL T 1269:

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

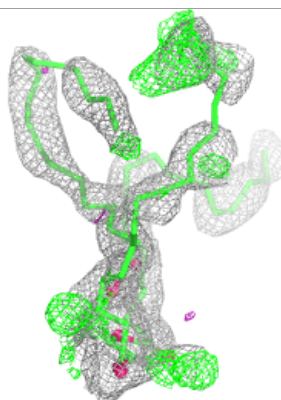
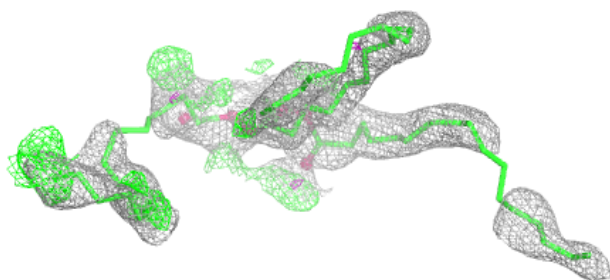
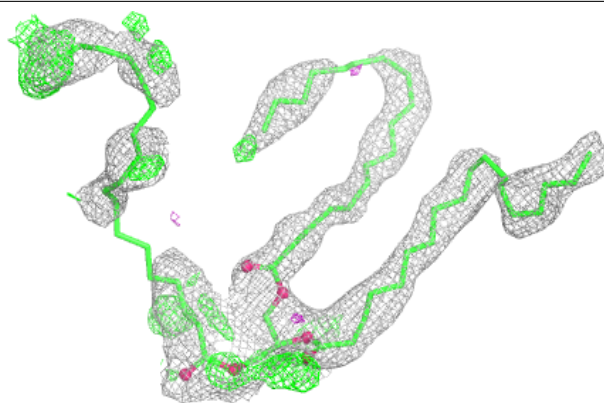
**Electron density around PSC E 229:**

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

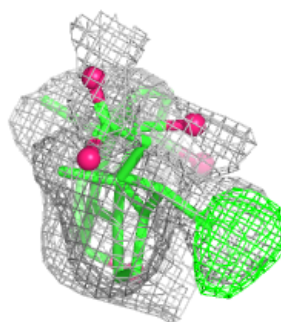
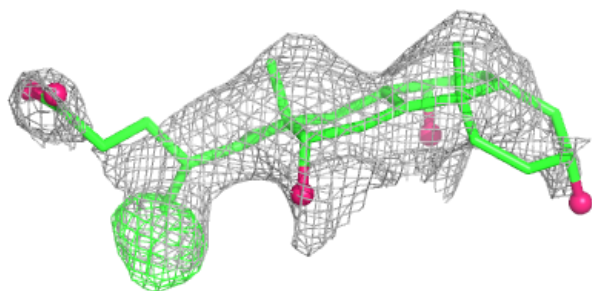
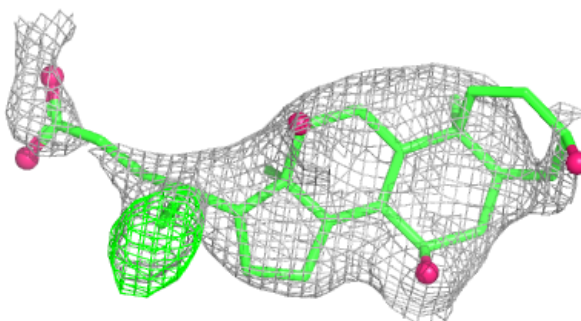


Electron density around TGL Q 1523:

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

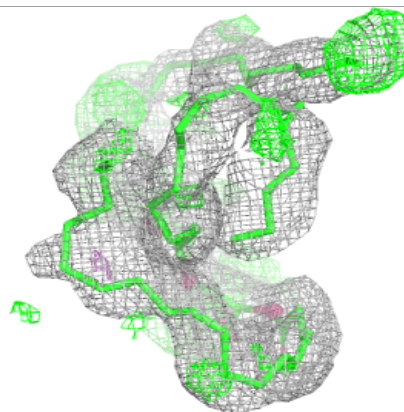
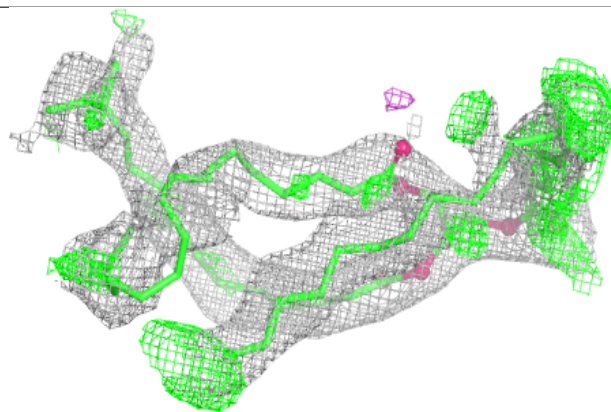
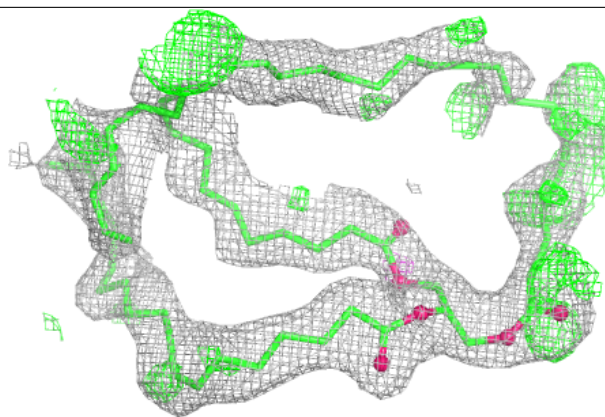
**Electron density around CHD J 60:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

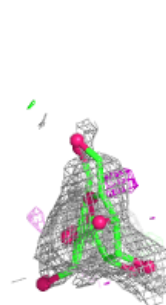
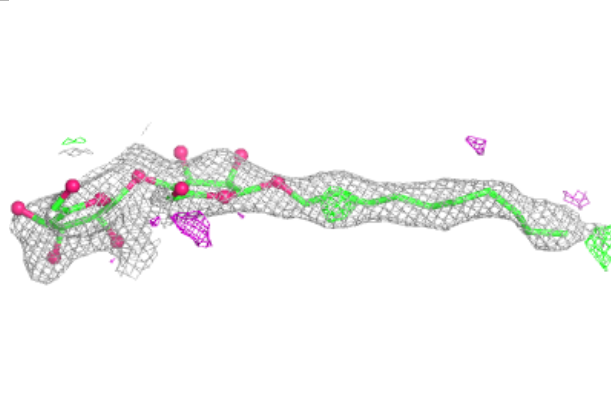
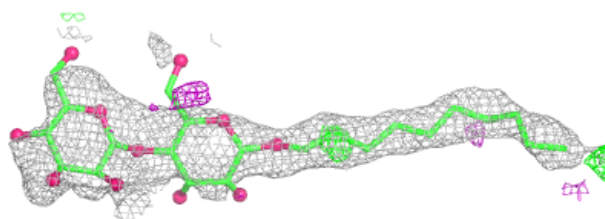


Electron density around TGL A 521:

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

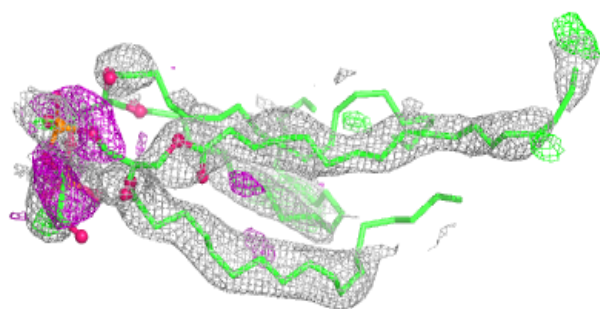
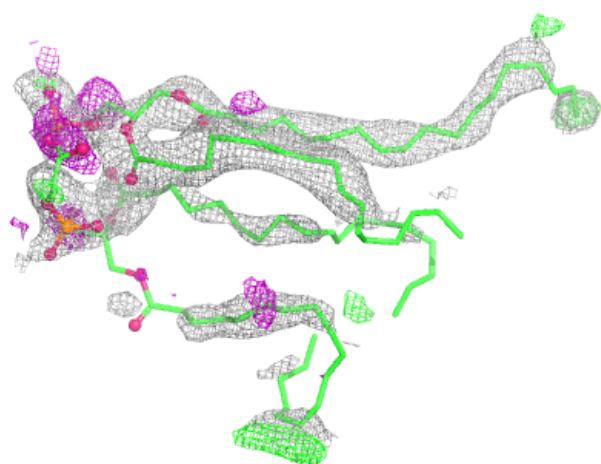
**Electron density around DMU G 272:**

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



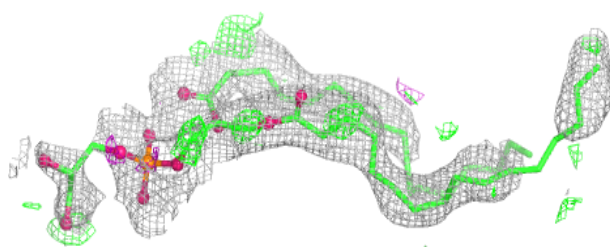
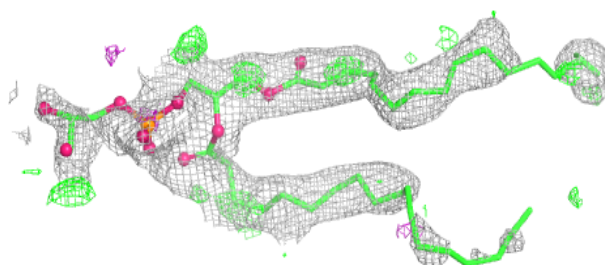
Electron density around CDL P 1270:

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

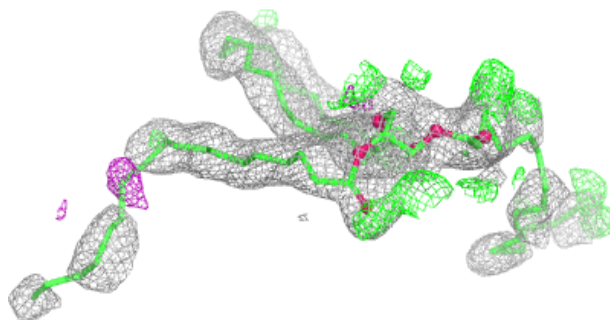
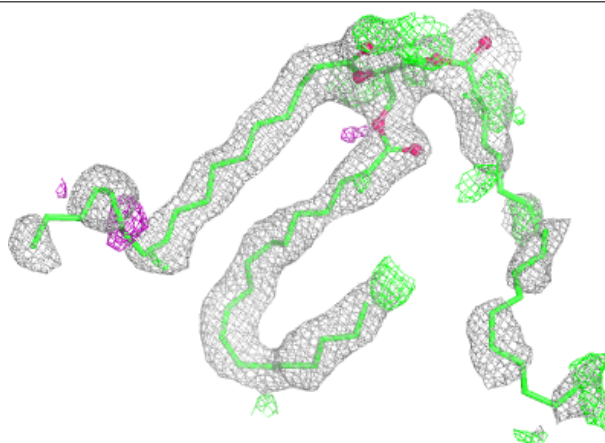


Electron density around PGV C 268:

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

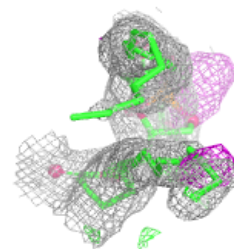
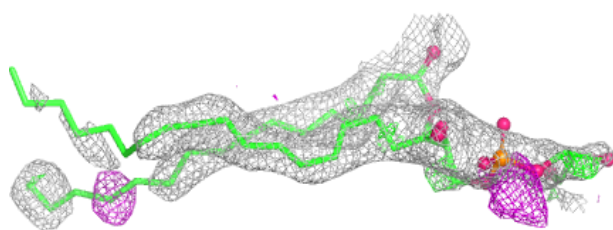
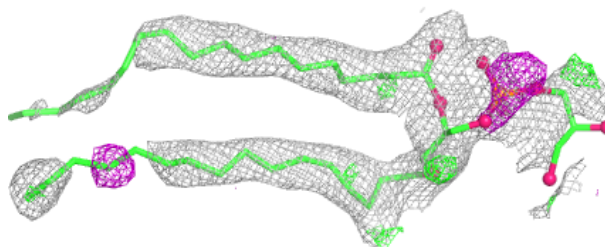
**Electron density around TGL D 523:**

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

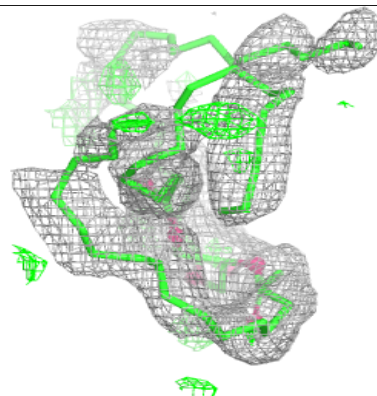
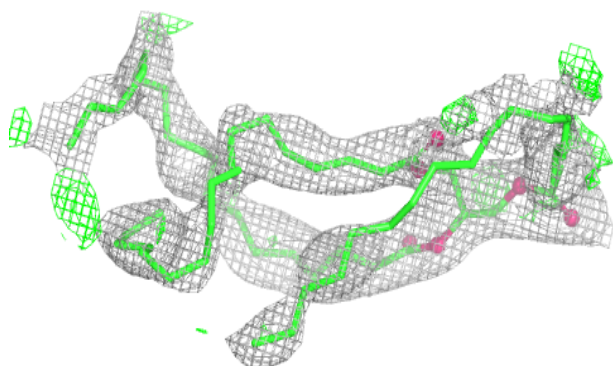
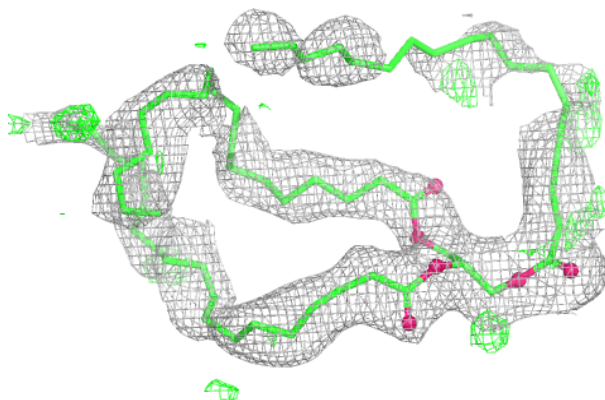


Electron density around PGV A 524:

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

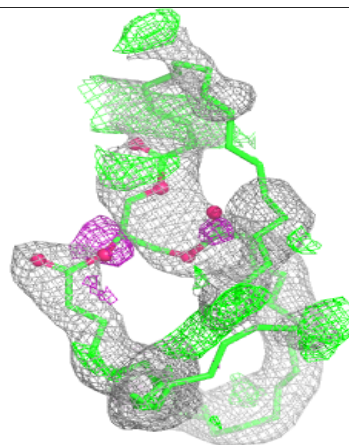
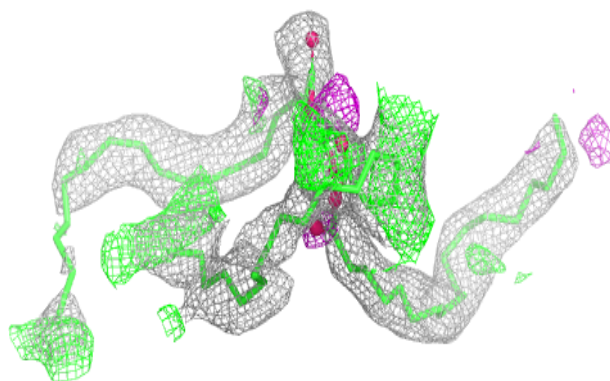
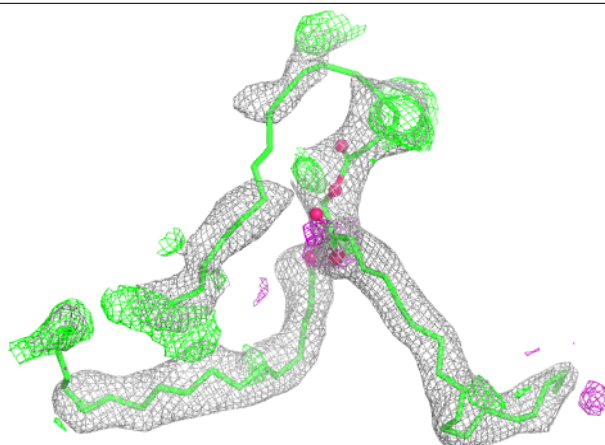
**Electron density around TGL N 1521:**

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and green (positive)



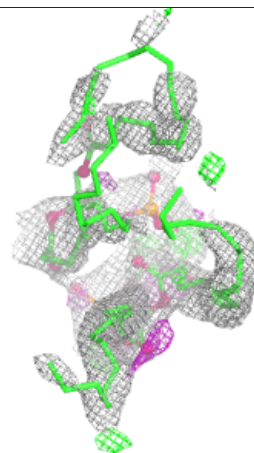
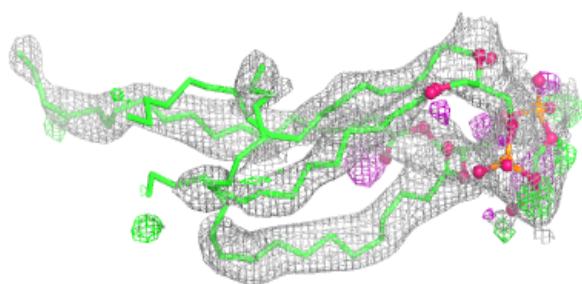
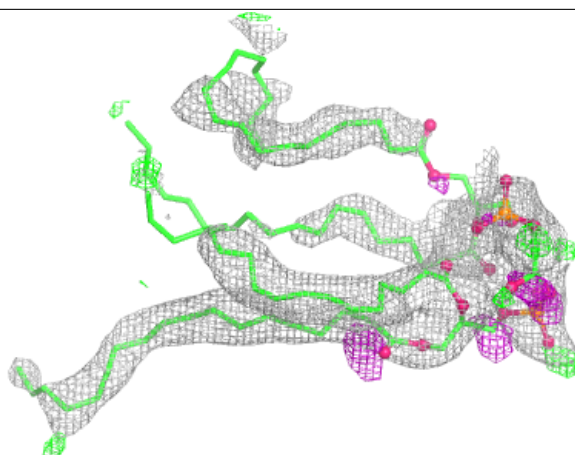
Electron density around TGL L 522:

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



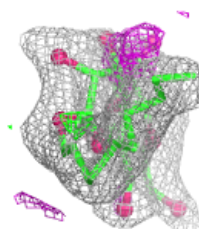
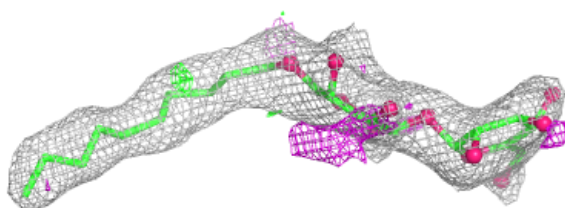
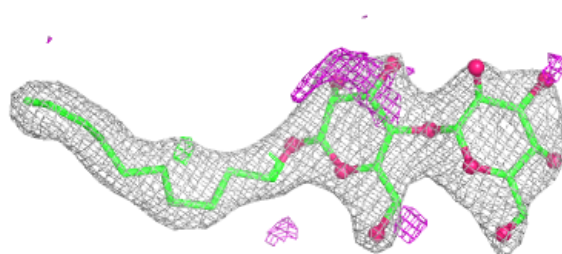
Electron density around CDL C 270:

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

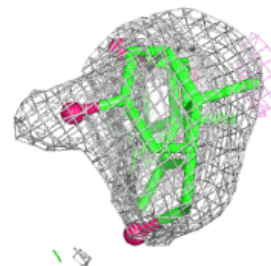
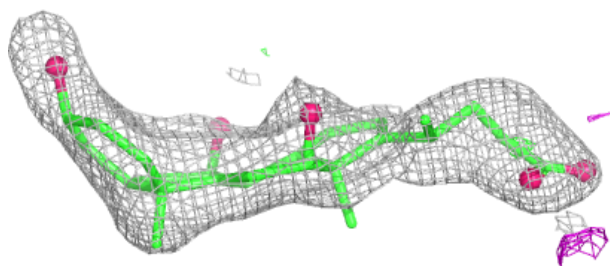
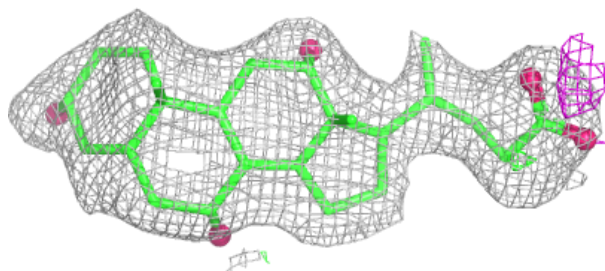


Electron density around DMU Z 1526:

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

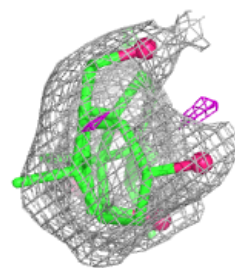
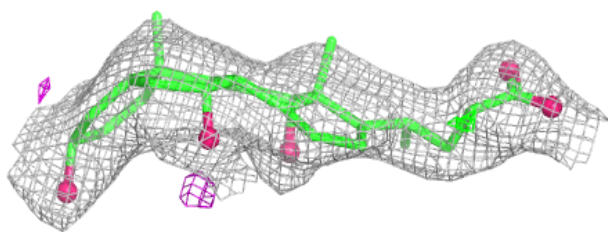
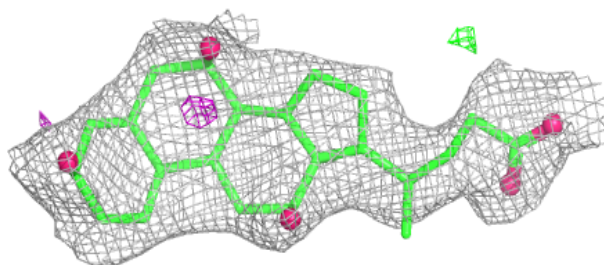
**Electron density around CHD C 271:**

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

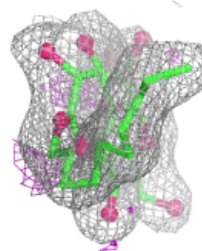
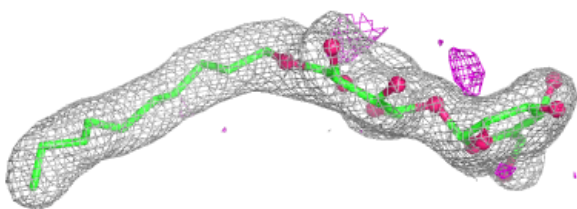
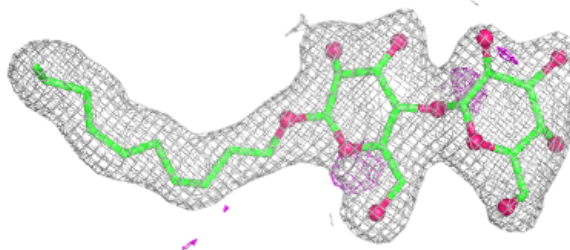


Electron density around CHD P 1271:

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

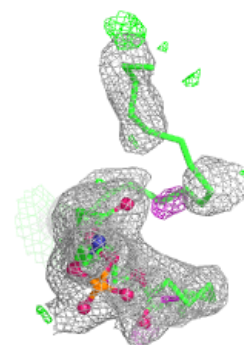
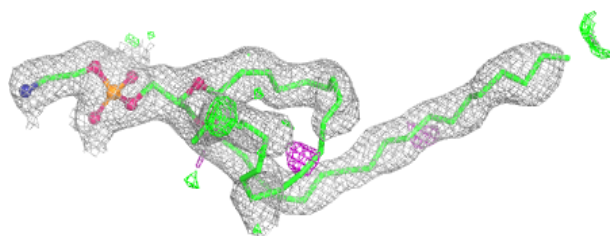
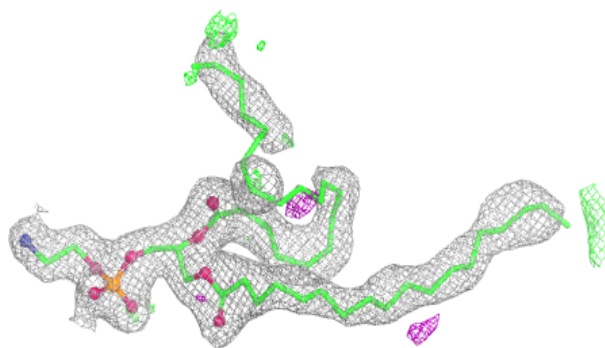
**Electron density around DMU M 526:**

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

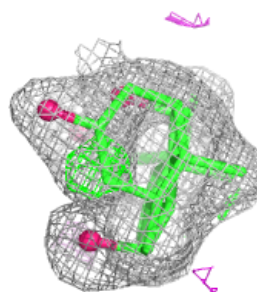
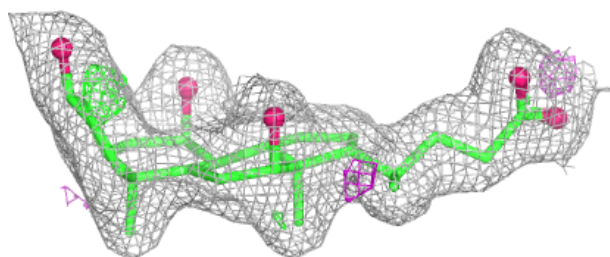


Electron density around PEK T 1264:

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

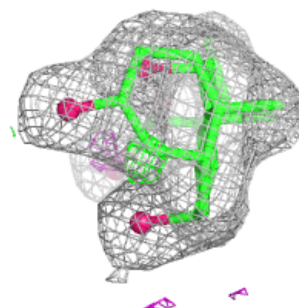
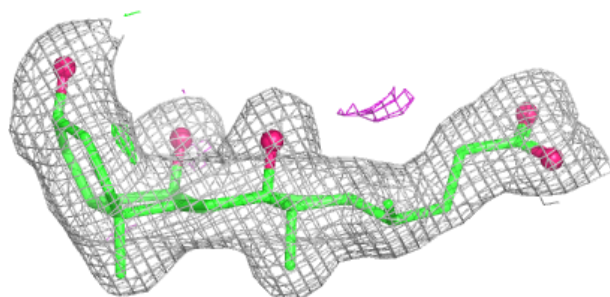
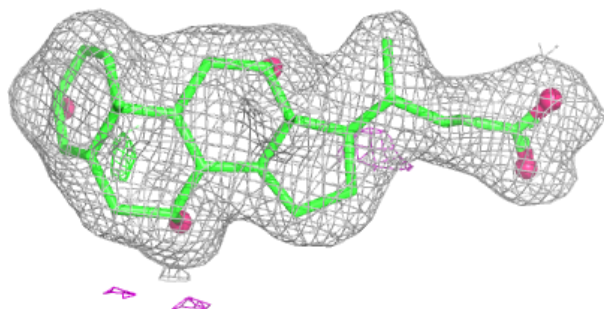
**Electron density around CHD P 1525:**

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

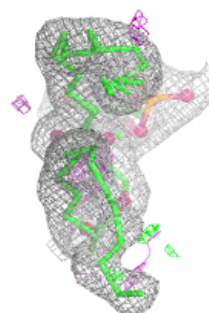
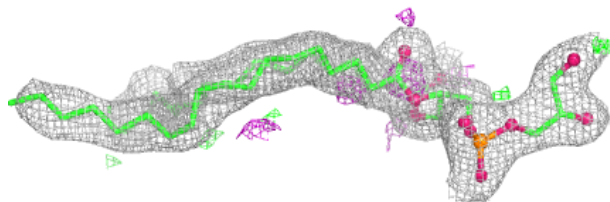
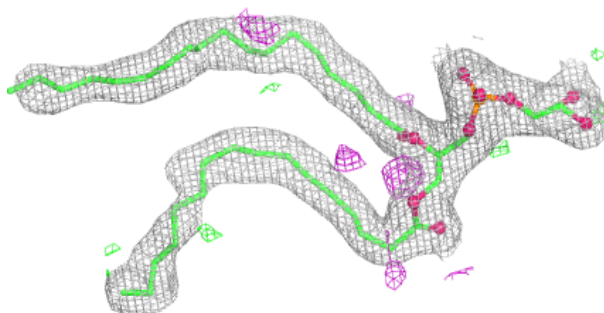


Electron density around CHD O 229:

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

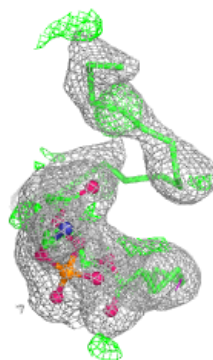
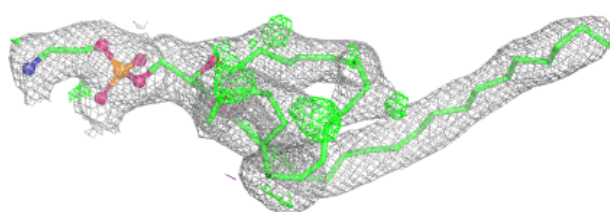
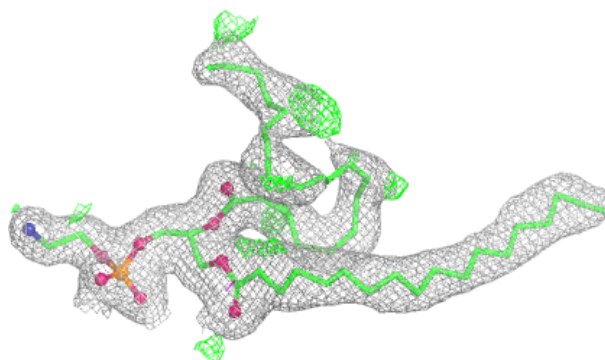
**Electron density around PGV N 1266:**

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

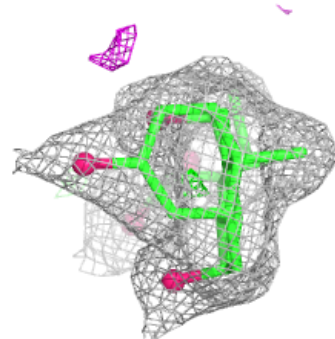
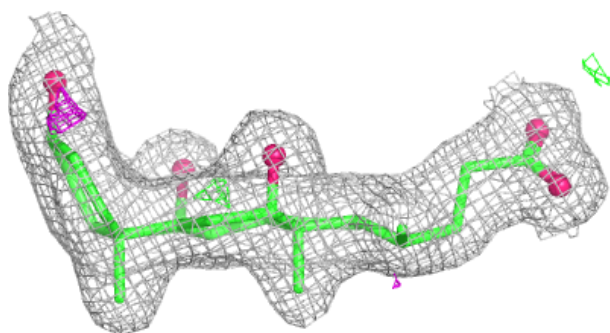
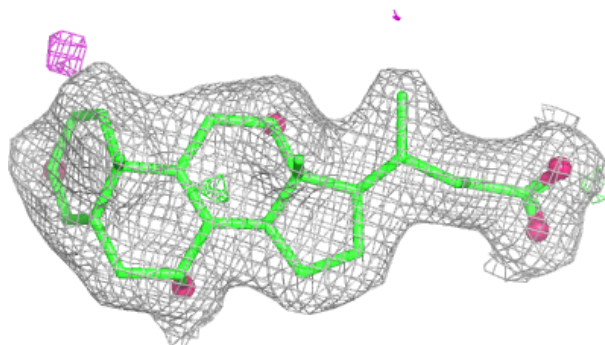


Electron density around PEK C 264:

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

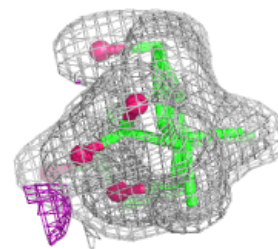
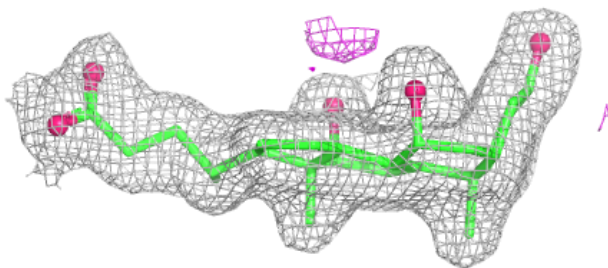
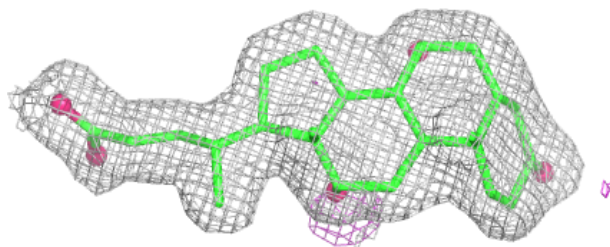
**Electron density around CHD B 1085:**

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

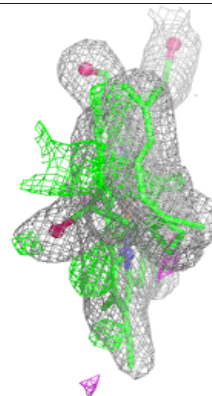
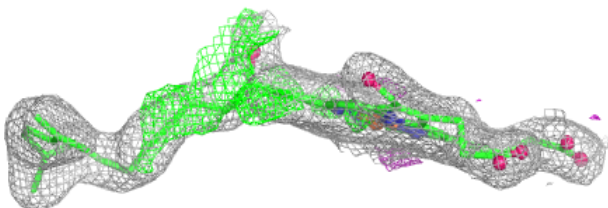
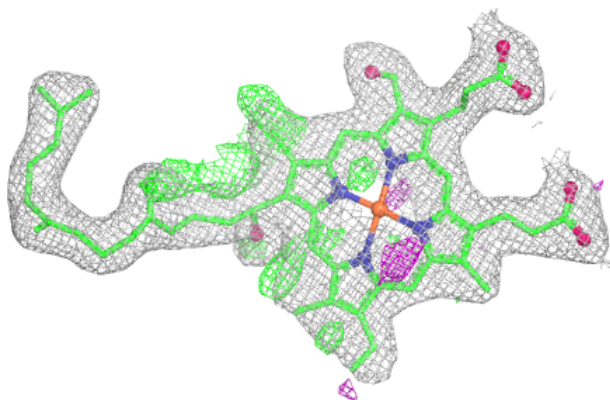


Electron density around CHD C 525:

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

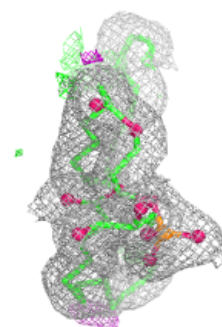
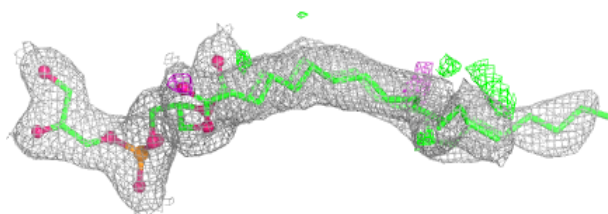
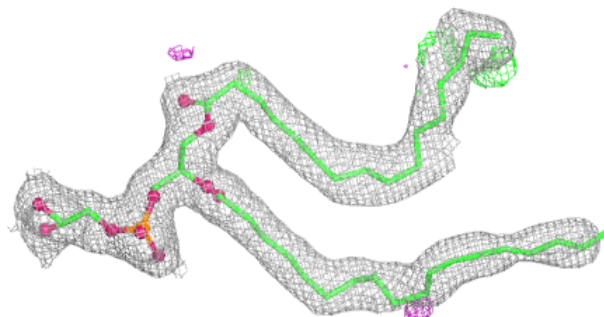
**Electron density around HEA N 516:**

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

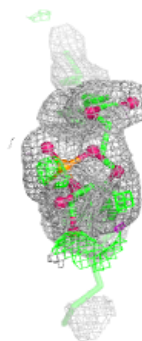
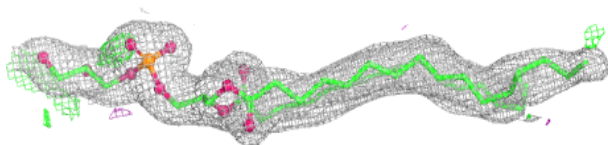
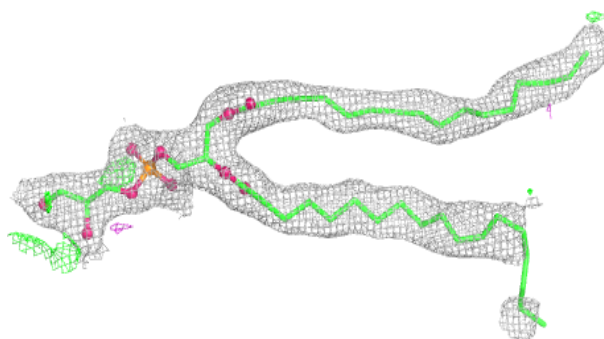


Electron density around PGV A 522:

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

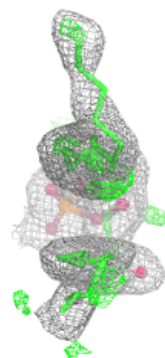
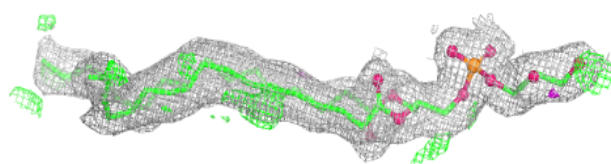
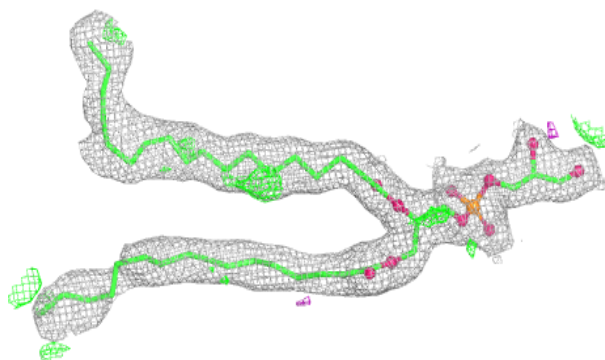
**Electron density around PGV P 1267:**

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

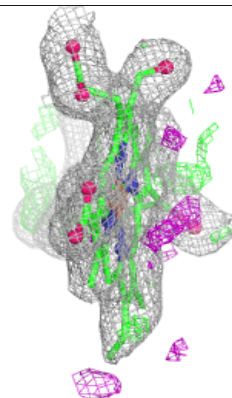
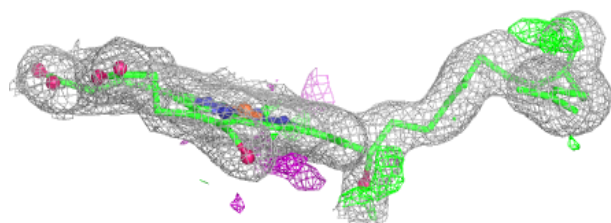
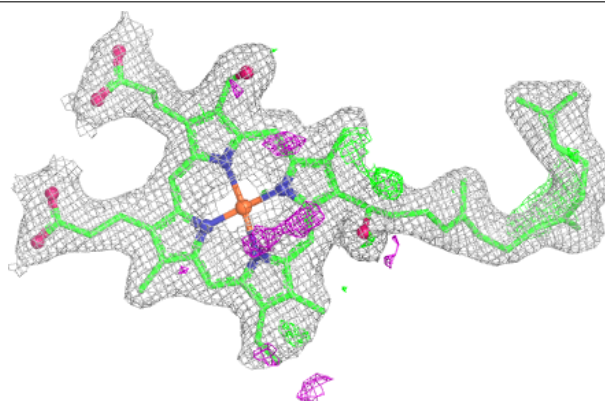


Electron density around PGV C 267:

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

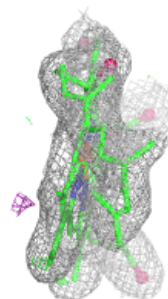
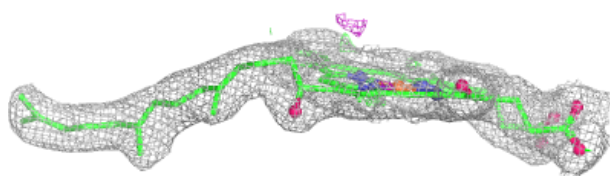
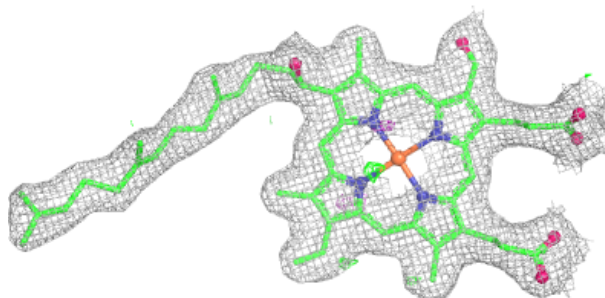
**Electron density around HEA A 516:**

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

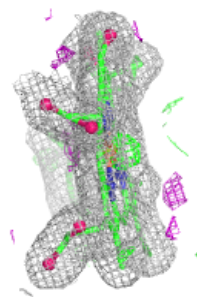
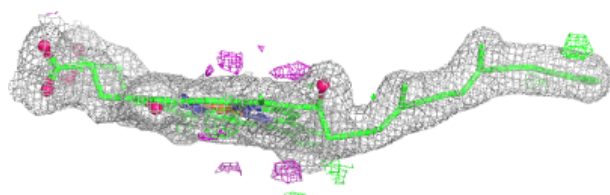
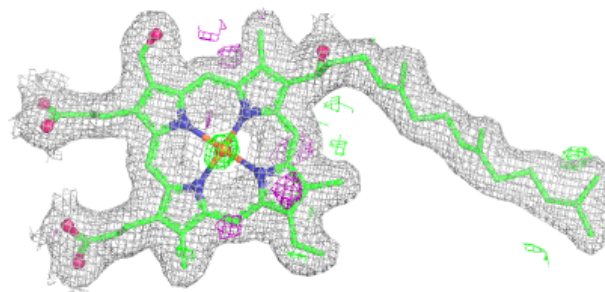


Electron density around HEA N 515:

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

**Electron density around HEA A 515:**

$2mF_o-DF_c$ (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.