Full wwPDB X-ray Structure Validation Report ⓘ

Dec 12, 2023 – 10:31 AM EST

PDB ID	:	1V55
Title	:	Bovine heart cytochrome c oxidase at the fully reduced state
Authors	:	Tsukihara, T.; Shimokata, K.; Katayama, Y.; Shimada, H.; Muramoto, K.; Aoyama, H.; Mochizuki, M.; Shinzawa-Itoh, K.; Yamashita, E.; Yao, M.; Ishimura, Y.; Yoshikawa, S.
Deposited on	:	2003-11-21
Resolution	:	1.90 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

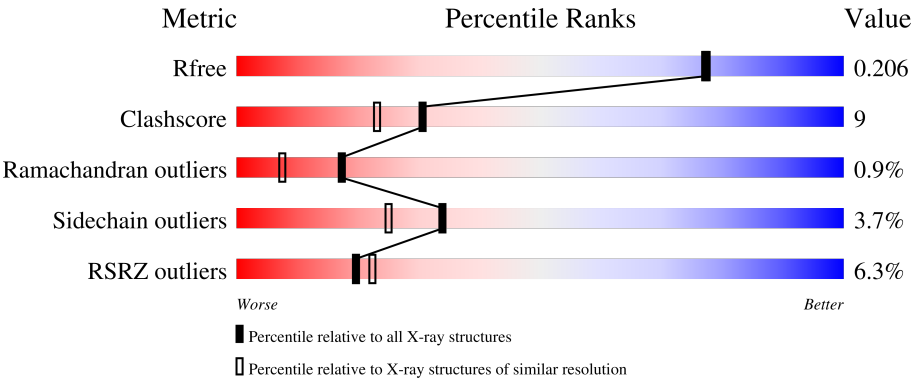
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

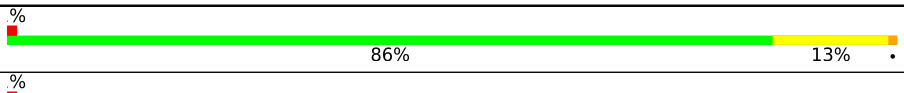
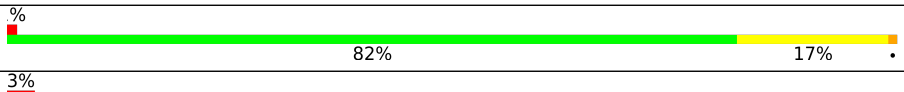
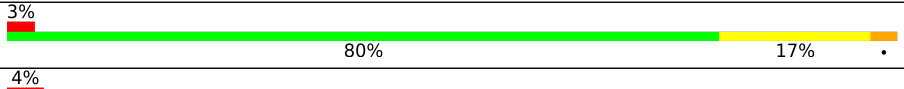
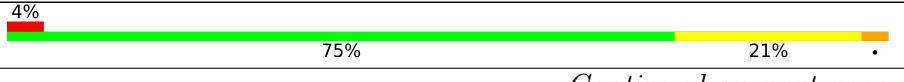
The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	
1	N	514	
2	B	227	
2	O	227	

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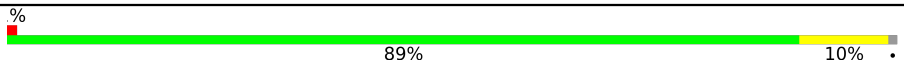
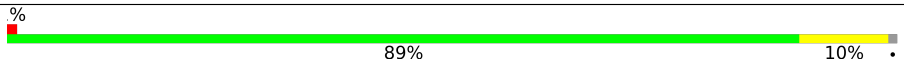
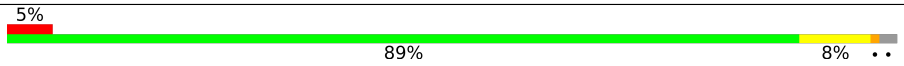
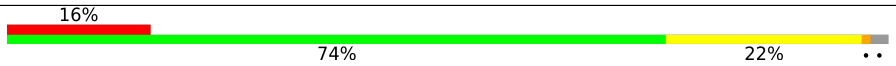
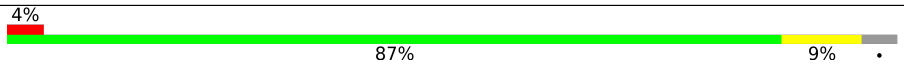
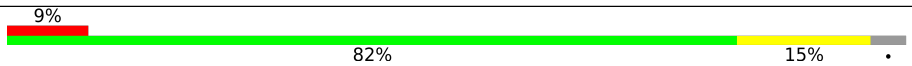
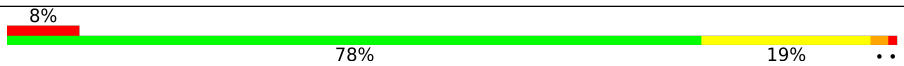
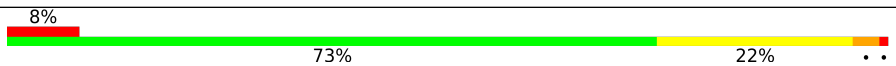
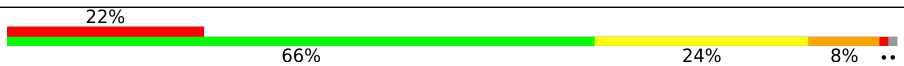
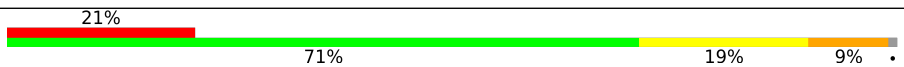
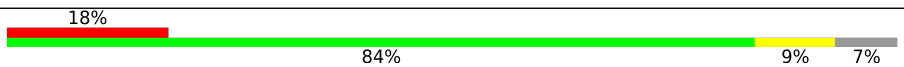
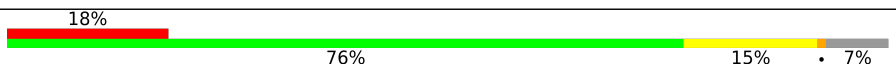
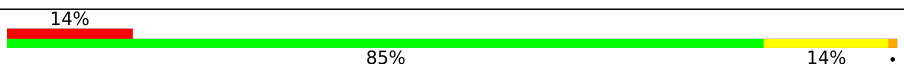
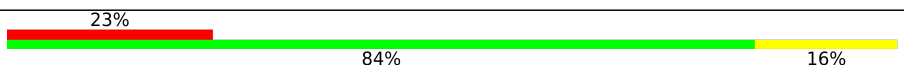
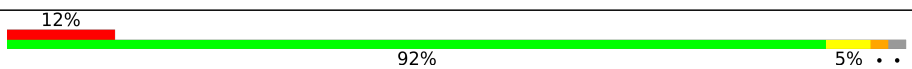
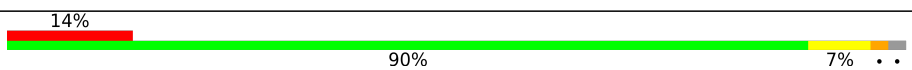
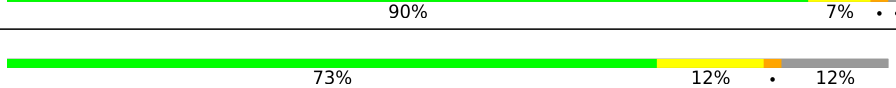
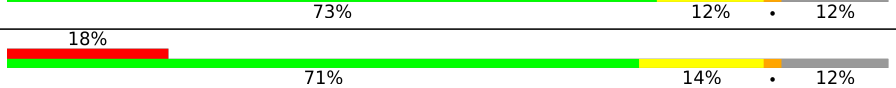
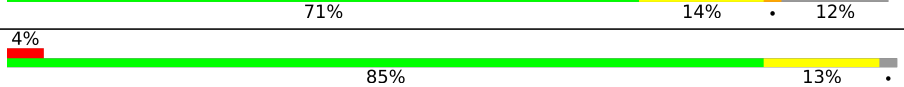
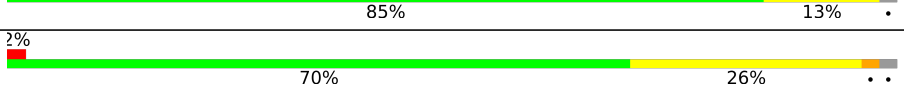
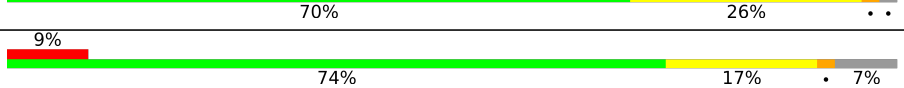
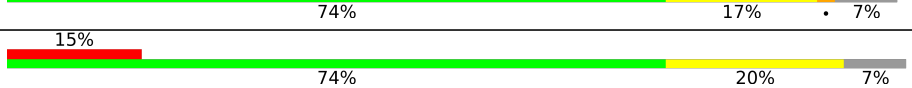
Mol	Chain	Length	Quality of chain
3	C	261	
3	P	261	
4	D	147	
4	Q	147	
5	E	109	
5	R	109	
6	F	98	
6	S	98	
7	G	85	
7	T	85	
8	H	85	
8	U	85	
9	I	73	
9	V	73	
10	J	59	
10	W	59	
11	K	56	
11	X	56	
12	L	47	
12	Y	47	
13	M	46	
13	Z	46	

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
18	TGL	A	3522	-	-	X	-
18	TGL	N	4521	-	-	X	-
21	CHD	C	3271	X	-	-	-
21	CHD	J	3060	X	-	-	X
21	CHD	P	4271	X	-	-	-
21	CHD	W	4060	X	-	-	X
22	CDL	C	3270	-	-	X	-
23	PEK	T	3263	-	-	-	X
27	DMU	M	3526	X	-	-	-
27	DMU	Z	4526	X	-	-	-
9	SAC	I	1	-	X	-	-
9	SAC	V	1	-	X	-	X

2 Entry composition (i)

There are 28 unique types of molecules in this entry. The entry contains 32609 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 polypeptide I.

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 polypeptide II.

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 polypeptide III.

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 IV 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 polypeptide Va.

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 polypeptide Vb.

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 polypeptide VIa-heart.

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

- Molecule 8 is a protein called Cytochrome c oxidase polypeptide VIb.

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 polypeptide VIc.

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 VIIa-heart.

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 polypeptide VIIb.

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 polypeptide VIIc.

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 polypeptide VIII-heart.

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 COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

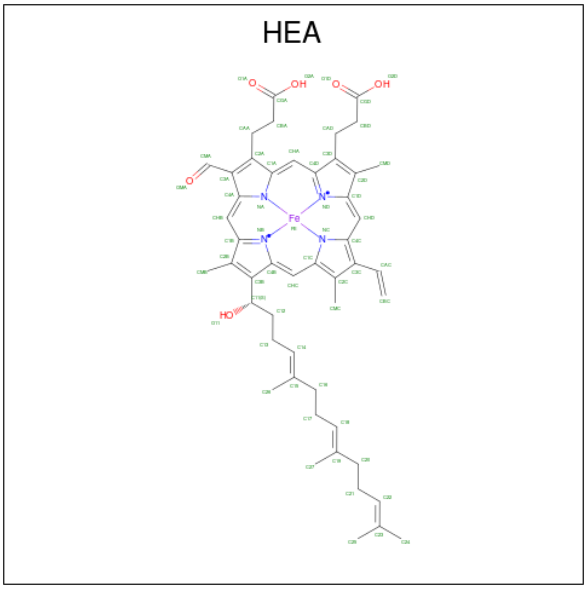
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 16 is SODIUM ION (three-letter code: NA) (formula: Na).

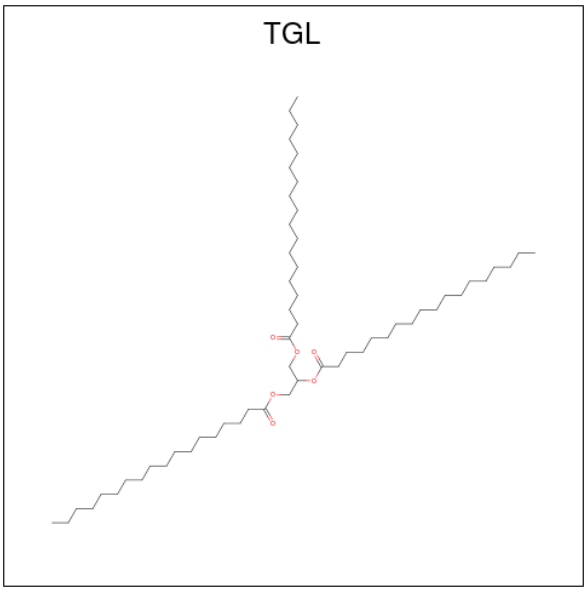
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	1	Total Na 1 1	0	0
16	N	1	Total Na 1 1	0	0

- Molecule 17 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



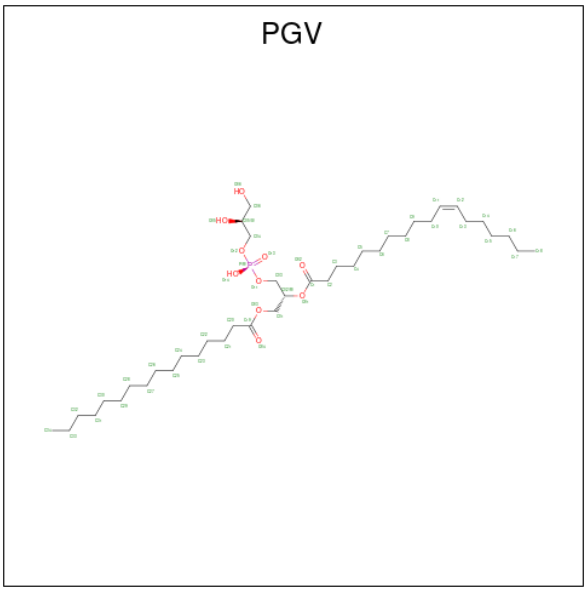
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total C Fe N O 60 49 1 4 6	0	0
17	A	1	Total C Fe N O 60 49 1 4 6	0	0
17	N	1	Total C Fe N O 60 49 1 4 6	0	0
17	N	1	Total C Fe N O 60 49 1 4 6	0	0

- Molecule 18 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: $C_{57}H_{110}O_6$).



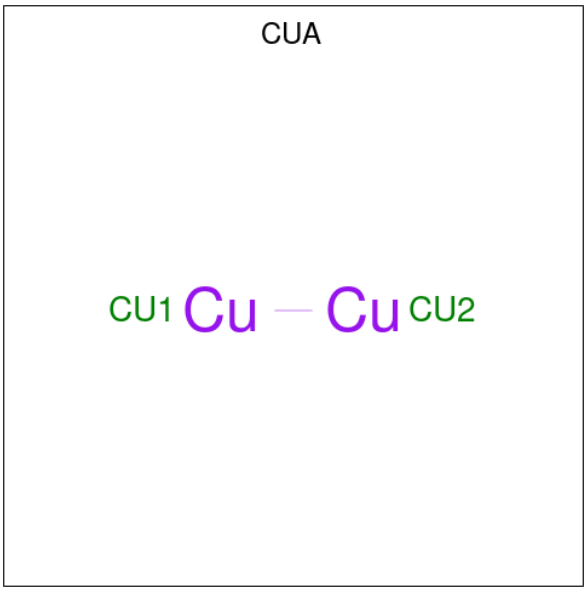
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total C O 63 57 6	0	0
18	A	1	Total C O 63 57 6	0	0
18	A	1	Total C O 63 57 6	0	0
18	N	1	Total C O 63 57 6	0	0
18	N	1	Total C O 63 57 6	0	0
18	Q	1	Total C O 63 57 6	0	0

- Molecule 19 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: $C_{40}H_{77}O_{10}P$).



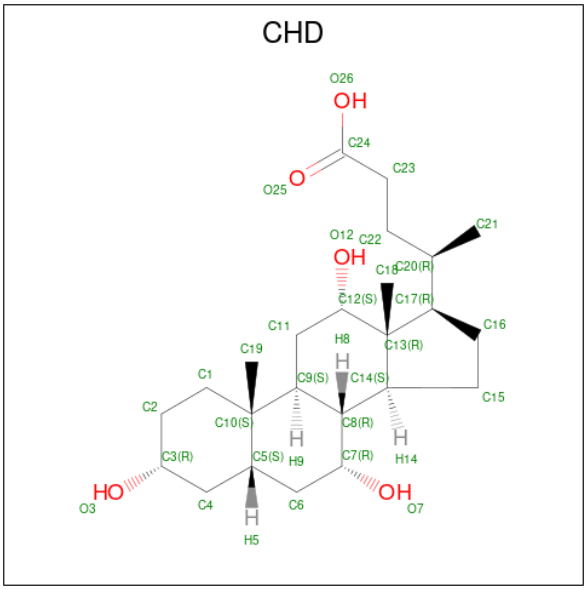
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0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

- Molecule 20 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).



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

- Molecule 21 is CHOLIC ACID (three-letter code: CHD) (formula: $C_{24}H_{40}O_5$).



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

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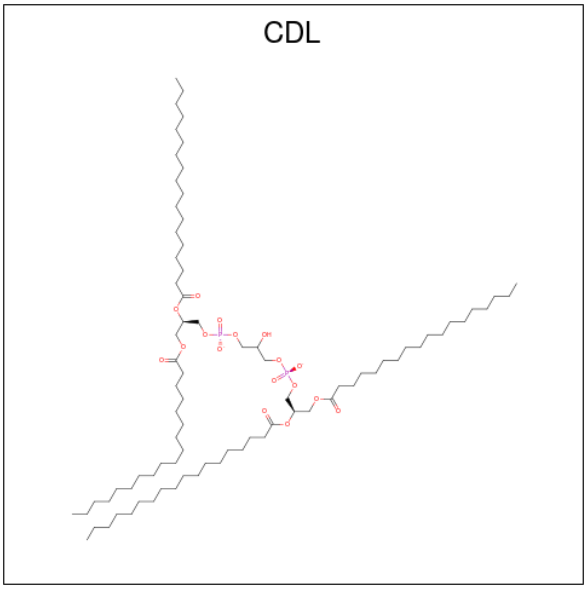
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	C	1	Total C O 29 24 5	0	0
21	J	1	Total C O 29 24 5	0	0
21	O	1	Total C O 29 24 5	0	0
21	P	1	Total C O 29 24 5	0	0
21	P	1	Total C O 29 24 5	0	0
21	W	1	Total C O 29 24 5	0	0

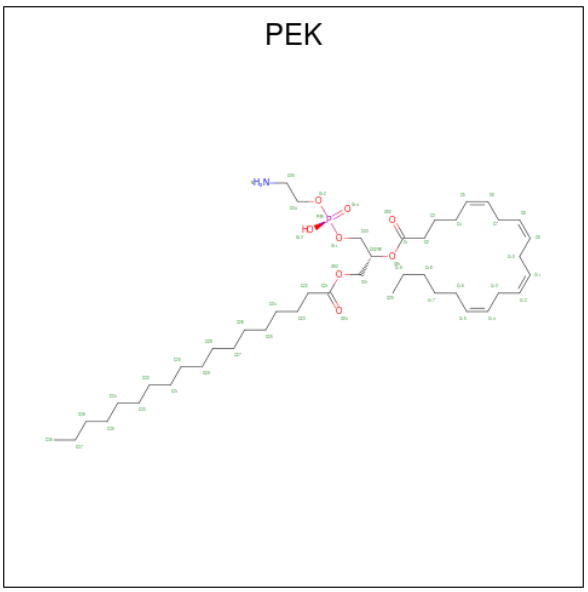
- Molecule 22 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

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

(three-letter code: PEK) (formula: $C_{43}H_{78}NO_8P$).

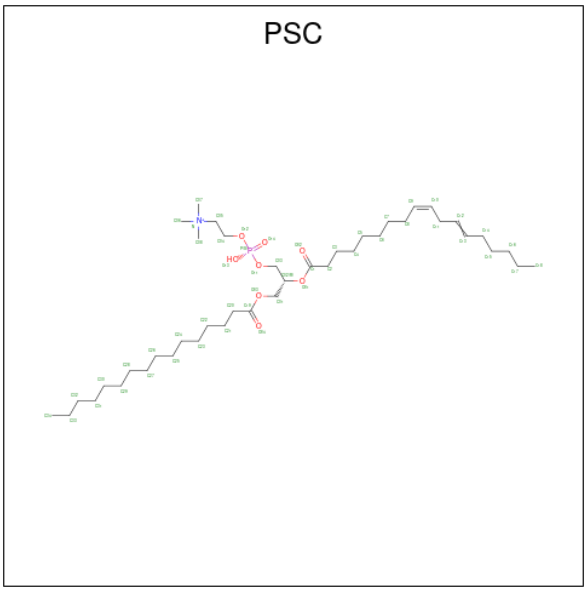


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 24 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

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

- Molecule 25 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 (three-letter code: PSC) (formula: $C_{42}H_{81}NO_8P$).

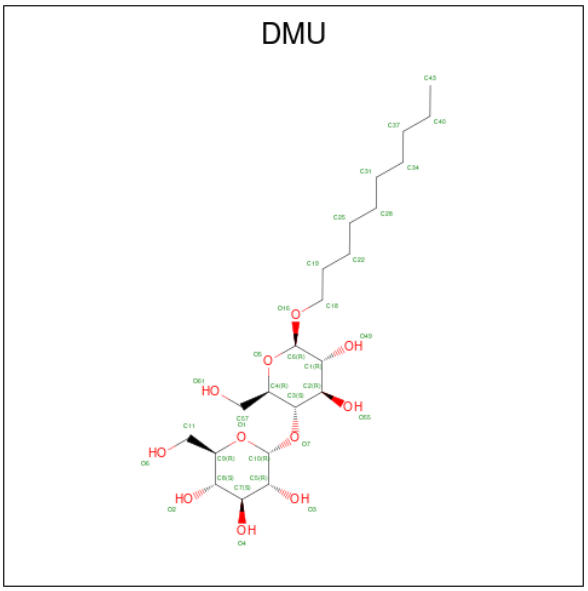


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	E	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
25	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 27 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).



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

- Molecule 28 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	229	Total O 229 229	0	0
28	B	167	Total O 167 167	0	0
28	C	107	Total O 107 107	0	0
28	D	112	Total O 112 112	0	0
28	E	90	Total O 90 90	0	0
28	F	109	Total O 109 109	0	0
28	G	54	Total O 54 54	0	0
28	H	61	Total O 61 61	0	0
28	I	50	Total O 50 50	0	0
28	J	34	Total O 34 34	0	0

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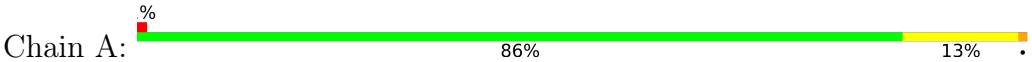
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	K	28	Total O 28 28	0	0
28	L	21	Total O 21 21	0	0
28	M	33	Total O 33 33	0	0
28	N	214	Total O 214 214	0	0
28	O	116	Total O 116 116	0	0
28	P	112	Total O 112 112	0	0
28	Q	72	Total O 72 72	0	0
28	R	48	Total O 48 48	0	0
28	S	77	Total O 77 77	0	0
28	T	48	Total O 48 48	0	0
28	U	54	Total O 54 54	0	0
28	V	32	Total O 32 32	0	0
28	W	20	Total O 20 20	0	0
28	X	20	Total O 20 20	0	0
28	Y	22	Total O 22 22	0	0
28	Z	13	Total O 13 13	0	0

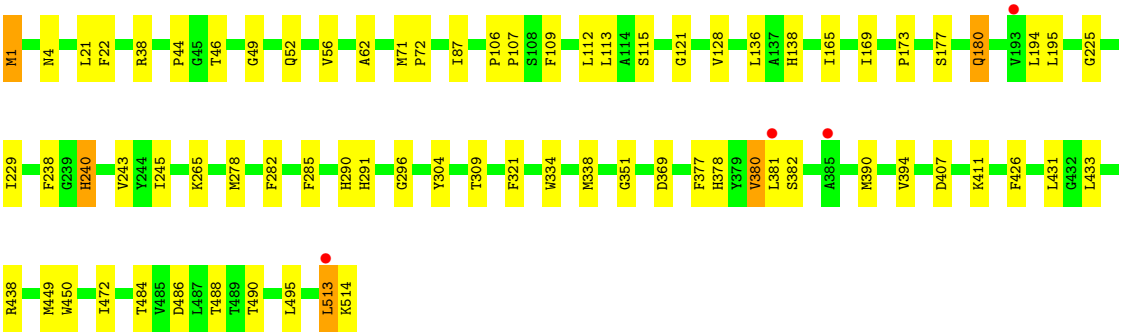
3 Residue-property plots (i)

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 polypeptide I

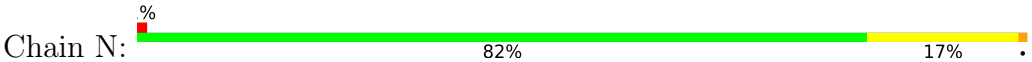
Chain A:

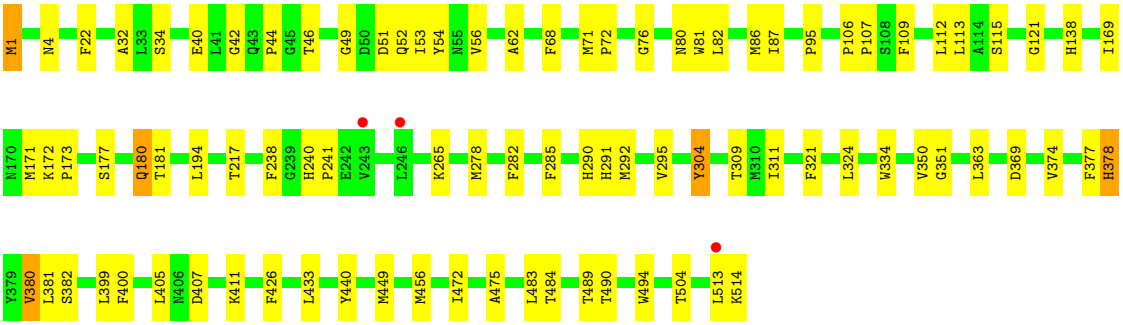




• Molecule 1: Cytochrome c oxidase polypeptide I

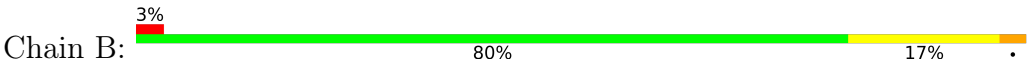
Chain N:

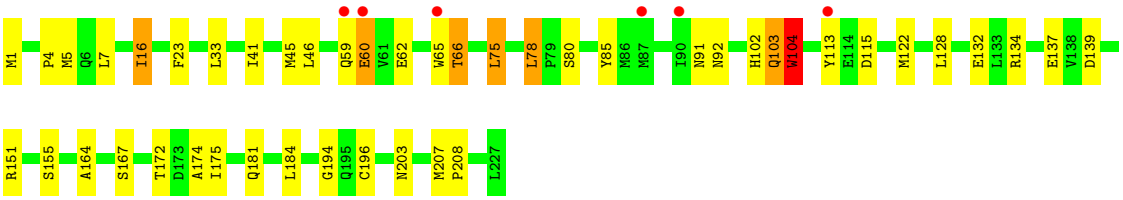




• Molecule 2: Cytochrome c oxidase polypeptide II

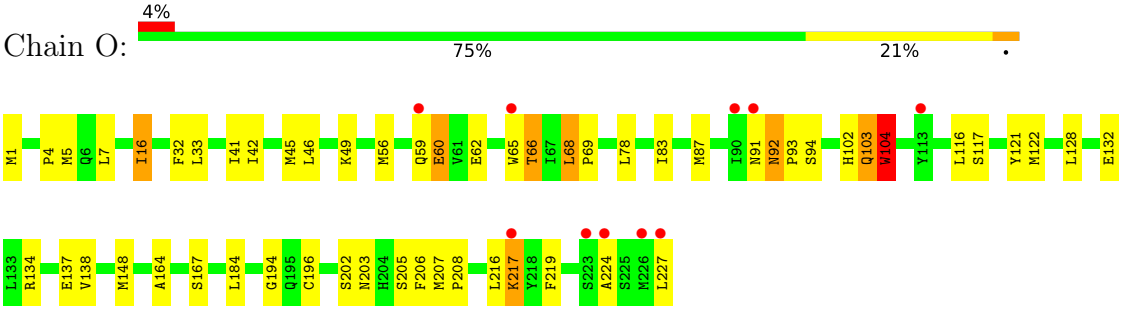
Chain B:





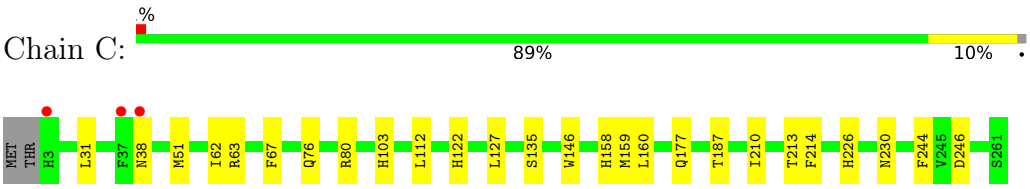
• Molecule 2: Cytochrome c oxidase polypeptide II

Chain O:



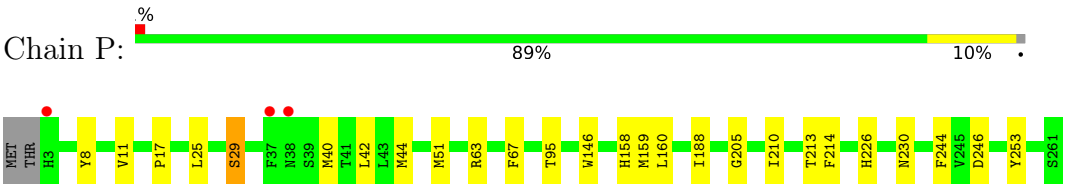
• Molecule 3: Cytochrome c oxidase polypeptide III

Chain C:



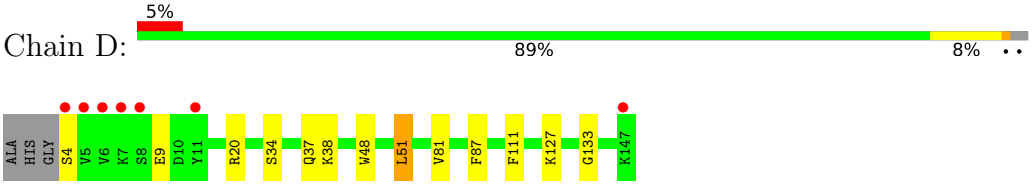
• Molecule 3: Cytochrome c oxidase polypeptide III

Chain P:



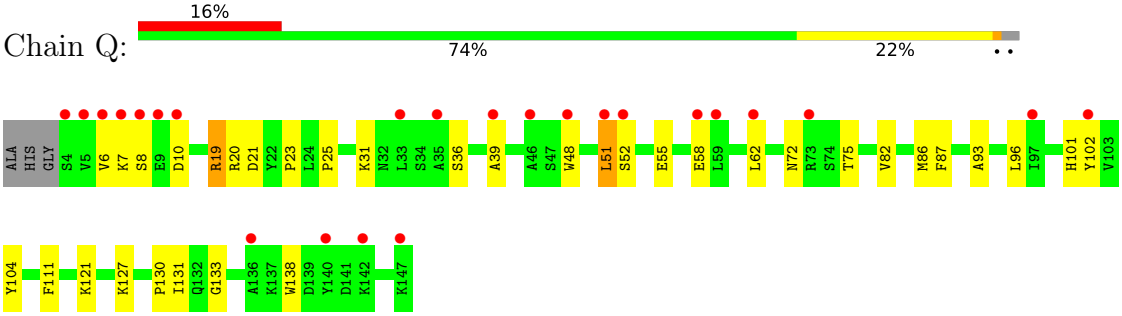
• Molecule 4: Cytochrome c oxidase subunit IV isoform 1

Chain D:



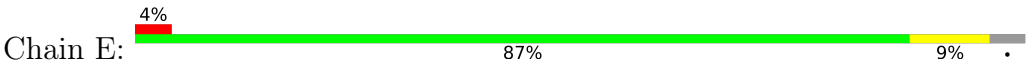
• Molecule 4: Cytochrome c oxidase subunit IV isoform 1

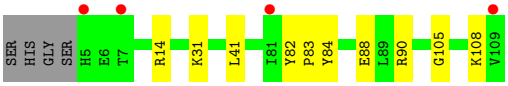
Chain Q:



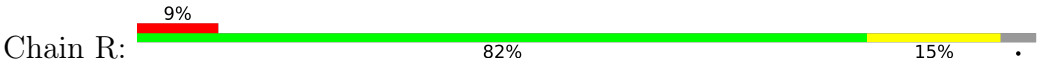
• Molecule 5: Cytochrome c oxidase polypeptide Va

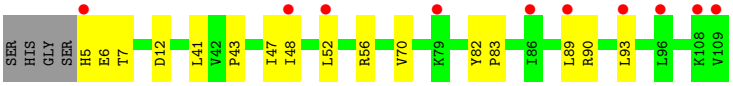
Chain E:



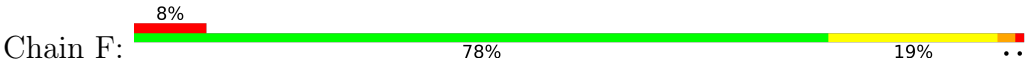


• Molecule 5: Cytochrome c oxidase polypeptide Va

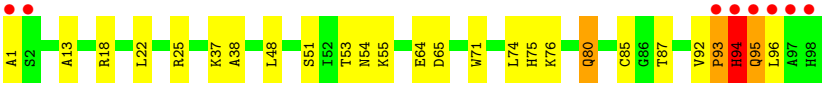




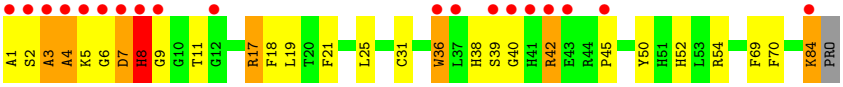
• Molecule 6: Cytochrome c oxidase polypeptide Vb



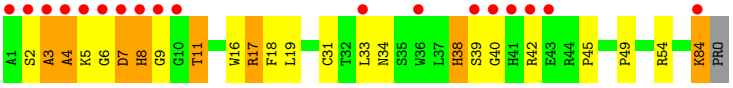
• Molecule 6: Cytochrome c oxidase polypeptide Vb



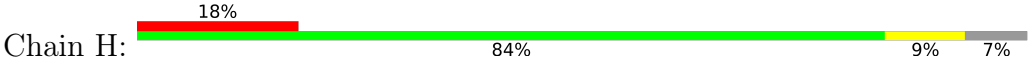
• Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

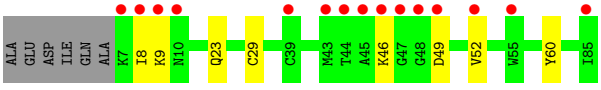


• Molecule 7: Cytochrome c oxidase polypeptide VIa-heart



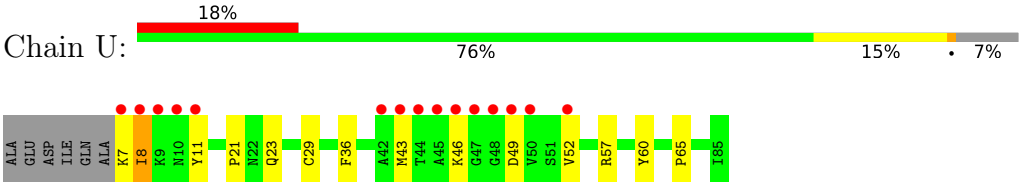
• Molecule 8: Cytochrome c oxidase polypeptide VIb





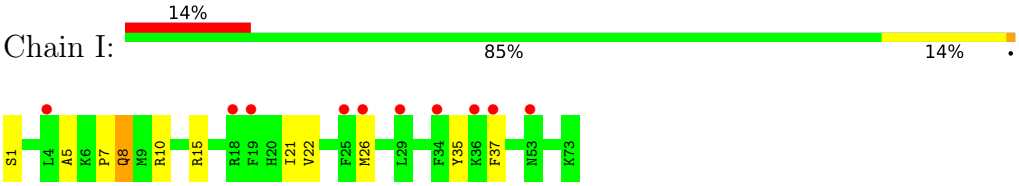
• Molecule 8: Cytochrome c oxidase polypeptide VIb

Chain U:



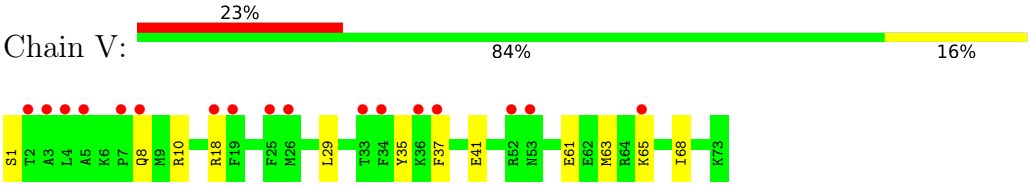
• Molecule 9: Cytochrome c oxidase polypeptide VIc

Chain I:



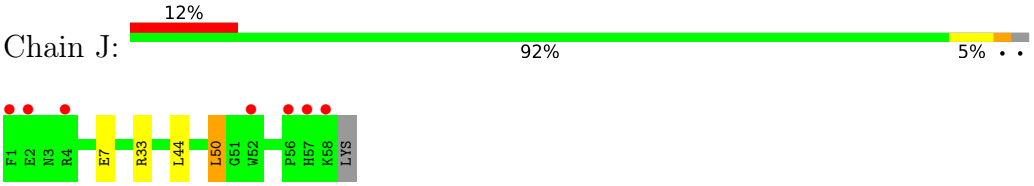
• Molecule 9: Cytochrome c oxidase polypeptide VIc

Chain V:



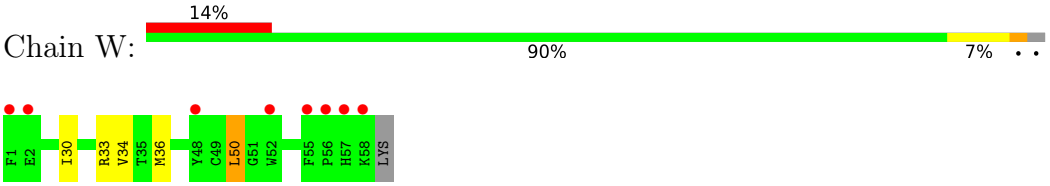
• Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart

Chain J:



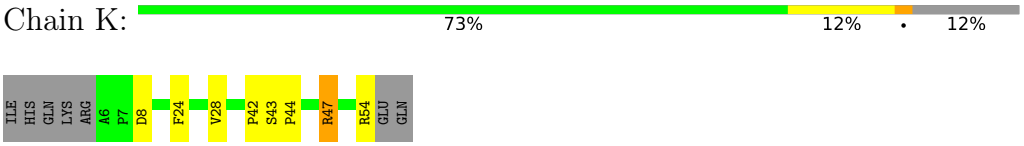
• Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart

Chain W:



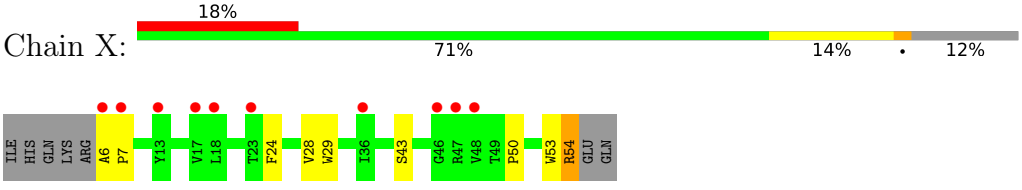
• Molecule 11: Cytochrome c oxidase polypeptide VIIb

Chain K:



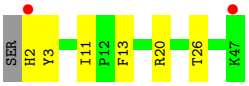
• Molecule 11: Cytochrome c oxidase polypeptide VIIb

Chain X:



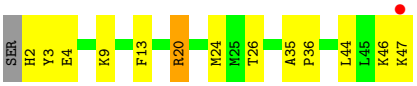
• Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain L:



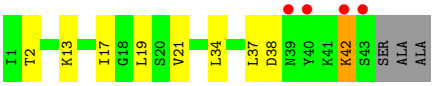
• Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain Y:



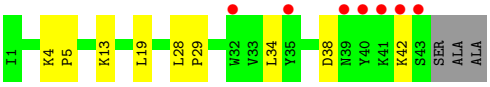
• Molecule 13: Cytochrome c oxidase polypeptide VIII-heart

Chain M:



• Molecule 13: Cytochrome c oxidase polypeptide VIII-heart

Chain Z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	183.06Å 206.58Å 178.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.90 64.24 – 1.89	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-1.90) 98.1 (64.24-1.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 1.90Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.203 , 0.230 0.205 , 0.206	Depositor DCC
R_{free} test set	26086 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	25.3	Xtriage
Anisotropy	0.539	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 65.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.007 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	32609	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: TPO, PSC, PEK, MG, PGV, ZN, DMU, TGL, NA, HEA, CDL, CHD, CUA, SAC, UNX, CU, FME

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.53	0/4156	0.69	1/5678 (0.0%)
1	N	0.53	0/4156	0.68	1/5678 (0.0%)
2	B	0.52	0/1860	0.82	4/2534 (0.2%)
2	O	0.52	0/1860	0.82	3/2534 (0.1%)
3	C	0.53	0/2197	0.61	0/3005
3	P	0.52	0/2197	0.63	0/3005
4	D	0.50	0/1229	0.67	1/1658 (0.1%)
4	Q	0.51	0/1229	0.65	1/1658 (0.1%)
5	E	0.51	0/871	0.66	0/1182
5	R	0.51	0/871	0.67	0/1182
6	F	0.50	0/765	0.81	2/1038 (0.2%)
6	S	0.47	0/765	0.82	2/1038 (0.2%)
7	G	0.53	0/690	0.71	0/937
7	T	0.54	0/690	0.72	1/937 (0.1%)
8	H	0.48	0/682	0.67	0/921
8	U	0.51	0/682	0.69	0/921
9	I	0.52	0/605	0.64	0/802
9	V	0.53	0/605	0.61	0/802
10	J	0.47	0/471	0.63	0/636
10	W	0.49	0/471	0.66	0/636
11	K	0.54	0/398	0.68	0/546
11	X	0.56	0/398	0.68	0/546
12	L	0.54	0/393	0.55	0/526
12	Y	0.55	0/393	0.58	0/526
13	M	0.47	0/345	0.62	0/470
13	Z	0.45	0/345	0.62	0/470
All	All	0.52	0/29324	0.69	16/39866 (0.0%)

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
1	A	0	1
1	N	0	2
2	B	0	2
2	O	0	1
8	U	0	1
All	All	0	7

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	103	GLN	CA-C-N	-6.93	101.94	117.20
6	S	94	HIS	N-CA-C	6.19	127.71	111.00
4	D	133	GLY	N-CA-C	6.09	128.33	113.10
2	O	103	GLN	CA-C-N	-6.04	103.91	117.20
6	F	94	HIS	N-CA-C	5.98	127.14	111.00
4	Q	133	GLY	N-CA-C	5.94	127.95	113.10
2	B	104	TRP	N-CA-C	5.87	126.85	111.00
7	T	33	LEU	CA-CB-CG	5.83	128.72	115.30
6	F	93	PRO	N-CA-C	5.77	127.10	112.10
1	N	378	HIS	CA-CB-CG	-5.58	104.11	113.60
2	O	104	TRP	N-CA-C	5.47	125.77	111.00
2	B	184	LEU	CA-CB-CG	5.46	127.86	115.30
2	O	184	LEU	CA-CB-CG	5.35	127.61	115.30
6	S	93	PRO	N-CA-C	5.32	125.92	112.10
1	A	438	ARG	CB-CA-C	-5.28	99.84	110.40
2	B	103	GLN	C-N-CA	5.12	134.51	121.70

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
2	B	103	GLN	Mainchain
2	B	85	TYR	Sidechain
1	N	240	HIS	Sidechain
1	N	304	TYR	Sidechain
2	O	103	GLN	Mainchain
8	U	11	TYR	Sidechain

5.2 Too-close contacts (i)

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	60	0
1	N	4027	0	4001	80	0
2	B	1824	0	1833	27	0
2	O	1824	0	1833	42	0
3	C	2110	0	2027	27	0
3	P	2110	0	2027	26	0
4	D	1195	0	1183	13	0
4	Q	1195	0	1183	28	0
5	E	852	0	845	6	0
5	R	852	0	845	8	0
6	F	748	0	728	13	0
6	S	748	0	728	19	0
7	G	675	0	643	26	0
7	T	675	0	643	25	0
8	H	662	0	623	3	0
8	U	662	0	623	6	0
9	I	601	0	613	7	0
9	V	601	0	613	6	0
10	J	460	0	459	4	0
10	W	460	0	459	4	0
11	K	384	0	366	5	0
11	X	384	0	366	10	0
12	L	380	0	380	13	0
12	Y	380	0	380	11	0
13	M	335	0	352	6	0
13	Z	335	0	352	3	0
14	A	1	0	0	0	0
14	N	1	0	0	0	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	120	0	108	5	0
17	N	120	0	108	6	0
18	A	189	0	330	47	0
18	N	126	0	220	41	0
18	Q	63	0	110	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	A	102	0	152	7	0
19	C	102	0	152	9	0
19	N	102	0	152	6	0
19	P	102	0	152	6	0
20	B	2	0	0	0	0
20	O	2	0	0	0	0
21	B	29	0	39	1	0
21	C	58	0	78	4	0
21	J	29	0	39	3	0
21	O	29	0	39	0	0
21	P	58	0	78	2	0
21	W	29	0	39	3	0
22	C	100	0	156	23	0
22	G	100	0	156	17	0
22	P	100	0	156	20	0
22	T	100	0	156	20	0
23	C	106	0	154	13	0
23	G	53	0	77	6	0
23	P	106	0	154	8	0
23	T	53	0	77	8	0
24	C	1	0	0	0	0
24	P	1	0	0	0	0
25	E	52	0	80	12	0
25	O	52	0	80	11	0
26	F	1	0	0	0	0
26	S	1	0	0	0	0
27	M	33	0	37	0	0
27	Z	33	0	37	0	0
28	A	229	0	0	6	0
28	B	167	0	0	2	0
28	C	107	0	0	4	0
28	D	112	0	0	3	0
28	E	90	0	0	1	0
28	F	109	0	0	1	0
28	G	54	0	0	3	0
28	H	61	0	0	2	0
28	I	50	0	0	3	0
28	J	34	0	0	2	0
28	K	28	0	0	0	0
28	L	21	0	0	1	0
28	M	33	0	0	1	0
28	N	214	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	O	116	0	0	1	0
28	P	112	0	0	4	0
28	Q	72	0	0	3	0
28	R	48	0	0	0	0
28	S	77	0	0	3	0
28	T	48	0	0	2	0
28	U	54	0	0	1	0
28	V	32	0	0	2	0
28	W	20	0	0	0	0
28	X	20	0	0	1	0
28	Y	22	0	0	0	0
28	Z	13	0	0	1	0
All	All	32609	0	31222	568	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 9.

All (568) 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)
7:T:84:LYS:HD2	7:T:84:LYS:H	1.21	1.03
7:G:84:LYS:H	7:G:84:LYS:HD2	1.21	1.03
10:W:33:ARG:HG2	21:W:4060:CHD:H152	1.42	0.99
18:A:3522:TGL:HC32	12:L:20:ARG:HH22	1.29	0.98
4:D:34:SER:H	4:D:37:GLN:HE21	1.14	0.92
10:J:33:ARG:HG2	21:J:3060:CHD:H152	1.51	0.92
22:C:3270:CDL:H242	22:C:3270:CDL:H661	1.54	0.89
22:P:4270:CDL:H242	22:P:4270:CDL:H661	1.54	0.89
6:S:94:HIS:CD2	6:S:95:GLN:H	1.89	0.89
25:O:4230:PSC:H21	25:O:4230:PSC:H222	1.55	0.88
18:A:3522:TGL:HC72	28:L:2344:HOH:O	1.73	0.88
18:A:3522:TGL:HC61	12:L:20:ARG:HH12	1.39	0.87
7:G:8:HIS:HD2	23:G:4263:PEK:H252	1.42	0.85
18:N:4522:TGL:HC31	12:Y:13:PHE:HA	1.59	0.85
25:E:3230:PSC:H222	25:E:3230:PSC:H21	1.59	0.84
18:A:3522:TGL:CC6	12:L:20:ARG:HH12	1.91	0.84
6:S:85:CYS:SG	6:S:87:THR:HG23	2.19	0.82
8:H:23:GLN:HG3	28:H:2104:HOH:O	1.79	0.81
2:O:41:ILE:HD13	25:O:4230:PSC:H342	1.62	0.81
3:C:67:PHE:HE1	22:C:3270:CDL:H1	1.44	0.80
3:C:63:ARG:HE	22:C:3270:CDL:HA22	1.43	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:67:PHE:HE1	22:P:4270:CDL:H1	1.47	0.80
1:N:1:FME:HCN	1:N:4:ASN:H	1.48	0.79
6:S:94:HIS:CG	6:S:95:GLN:H	2.02	0.78
3:P:63:ARG:HE	22:P:4270:CDL:HA22	1.47	0.78
1:N:112:LEU:HG	28:N:1379:HOH:O	1.85	0.76
18:A:3522:TGL:HC31	12:L:13:PHE:HA	1.66	0.76
6:S:76:LYS:HE3	6:S:93:PRO:HG3	1.68	0.76
23:P:4264:PEK:H102	23:P:4264:PEK:H161	1.68	0.76
18:A:3521:TGL:HA91	18:A:3521:TGL:H241	1.68	0.76
23:C:3264:PEK:H102	23:C:3264:PEK:H161	1.65	0.75
1:A:229:ILE:HD11	2:B:175:ILE:HD13	1.66	0.75
7:T:5:LYS:HD2	23:T:3263:PEK:H382	1.69	0.75
3:C:210:ILE:HG23	19:C:3267:PGV:H102	1.68	0.75
18:N:4522:TGL:HC62	18:N:4522:TGL:HC22	1.68	0.74
7:G:5:LYS:HB3	1:N:278:MET:SD	2.27	0.74
1:N:334:TRP:CZ3	18:Q:4523:TGL:HA42	2.23	0.74
6:F:85:CYS:SG	6:F:87:THR:HG23	2.28	0.73
1:N:68:PHE:HE2	1:N:112:LEU:HD13	1.50	0.73
18:A:3522:TGL:HC22	18:A:3522:TGL:HC62	1.69	0.73
3:C:160:LEU:HD13	21:C:3271:CHD:H181	1.69	0.73
19:A:3524:PGV:H162	19:A:3524:PGV:H321	1.71	0.72
19:N:4524:PGV:H162	19:N:4524:PGV:H321	1.70	0.72
3:P:210:ILE:HG23	19:P:4267:PGV:H102	1.72	0.72
18:N:4521:TGL:HA91	18:N:4521:TGL:H241	1.70	0.71
18:N:4521:TGL:HB91	2:O:32:PHE:CE2	2.25	0.71
3:P:160:LEU:HD13	21:P:4271:CHD:H181	1.73	0.70
13:M:42:LYS:HE3	13:M:42:LYS:HA	1.74	0.70
23:G:4263:PEK:H9	3:P:244:PHE:HA	1.73	0.70
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.74	0.69
1:A:296:GLY:HA2	8:H:23:GLN:OE1	1.91	0.69
1:N:426:PHE:CE1	18:N:4521:TGL:H282	2.28	0.69
22:P:4270:CDL:H391	28:P:2645:HOH:O	1.91	0.69
6:S:75:HIS:H	6:S:80:GLN:HE22	1.41	0.68
3:P:29:SER:HB3	3:P:42:LEU:HD13	1.74	0.68
7:T:31:CYS:SG	22:T:4269:CDL:H532	2.33	0.68
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.75	0.68
1:N:113:LEU:HB3	28:N:2240:HOH:O	1.93	0.68
19:A:3524:PGV:H032	28:A:3752:HOH:O	1.93	0.67
1:A:278:MET:SD	7:T:5:LYS:HB3	2.35	0.67
18:A:3522:TGL:HC61	12:L:20:ARG:NH1	2.09	0.67
2:O:217:LYS:HA	2:O:217:LYS:HE2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:89:LEU:O	5:R:93:LEU:HG	1.94	0.67
1:A:177:SER:H	1:A:180:GLN:HE21	1.43	0.67
19:C:3267:PGV:H161	19:C:3267:PGV:H12	1.78	0.66
1:N:456:MET:HG2	4:Q:96:LEU:HD13	1.78	0.66
7:T:84:LYS:HD2	7:T:84:LYS:N	2.03	0.66
4:D:34:SER:H	4:D:37:GLN:NE2	1.89	0.66
3:C:244:PHE:HA	23:T:3263:PEK:H9	1.77	0.66
23:P:4265:PEK:H383	22:T:4269:CDL:H272	1.77	0.66
18:Q:4523:TGL:HC21	18:Q:4523:TGL:HG12	1.76	0.66
2:O:56:MET:HA	25:O:4230:PSC:H202	1.78	0.65
18:A:3522:TGL:HC32	12:L:20:ARG:NH2	2.09	0.65
23:C:3264:PEK:H71	23:C:3264:PEK:H32	1.79	0.65
6:F:8:THR:OG1	6:F:11:GLU:HG3	1.99	0.63
7:G:36:TRP:HB3	28:G:628:HOH:O	1.97	0.63
6:S:94:HIS:CD2	6:S:95:GLN:N	2.64	0.63
18:A:3523:TGL:HC21	18:A:3523:TGL:HG12	1.79	0.63
7:G:84:LYS:H	7:G:84:LYS:CD	2.02	0.63
1:N:378:HIS:O	1:N:382:SER:HB2	1.99	0.63
1:N:53:ILE:HG12	28:N:1382:HOH:O	1.98	0.63
3:C:63:ARG:HE	22:C:3270:CDL:CA2	2.11	0.63
7:G:84:LYS:HD2	7:G:84:LYS:N	2.04	0.62
23:C:3265:PEK:H383	22:G:3269:CDL:H272	1.82	0.62
19:P:4267:PGV:H161	19:P:4267:PGV:H12	1.80	0.62
1:A:426:PHE:CE1	18:A:3521:TGL:H282	2.34	0.62
3:C:146:TRP:CZ2	7:G:17:ARG:HG3	2.34	0.62
1:N:449:MET:SD	2:O:5:MET:HG2	2.39	0.61
3:P:63:ARG:HE	22:P:4270:CDL:CA2	2.12	0.61
1:N:433:LEU:HD11	18:N:4521:TGL:OB1	2.00	0.61
25:O:4230:PSC:C07	9:V:10:ARG:HH21	2.13	0.61
1:A:472:ILE:HG21	18:A:3522:TGL:HA81	1.81	0.61
18:A:3523:TGL:HA81	18:A:3523:TGL:H242	1.80	0.61
3:P:67:PHE:CE1	22:P:4270:CDL:H1	2.32	0.61
22:C:3270:CDL:H312	22:C:3270:CDL:H151	1.81	0.61
1:A:449:MET:SD	2:B:5:MET:HG2	2.41	0.61
22:P:4270:CDL:H312	22:P:4270:CDL:H151	1.83	0.61
2:B:62:GLU:O	2:B:66:THR:HB	2.00	0.61
3:P:146:TRP:CZ2	7:T:17:ARG:HG3	2.36	0.61
2:O:41:ILE:CD1	25:O:4230:PSC:H342	2.30	0.60
3:P:246:ASP:HB2	28:P:1272:HOH:O	2.01	0.60
1:N:472:ILE:HD13	18:N:4522:TGL:HA92	1.83	0.60
18:A:3523:TGL:HC31	28:A:3753:HOH:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:58:GLU:O	4:Q:62:LEU:HG	2.02	0.60
7:T:17:ARG:HD2	28:T:1509:HOH:O	2.02	0.60
18:A:3522:TGL:H271	12:L:11:ILE:HG22	1.82	0.60
19:A:3524:PGV:H311	13:M:19:LEU:HD23	1.83	0.60
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.37	0.60
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.36	0.60
18:Q:4523:TGL:HA81	18:Q:4523:TGL:H242	1.83	0.59
9:V:63:MET:HB3	9:V:68:ILE:HD11	1.84	0.59
3:C:213:THR:HG23	22:C:3270:CDL:H762	1.82	0.59
8:U:49:ASP:O	8:U:52:VAL:HG22	2.03	0.59
1:A:484:THR:HB	13:M:2:THR:OG1	2.02	0.59
4:Q:127:LYS:O	4:Q:130:PRO:HD3	2.03	0.59
7:G:31:CYS:SG	22:G:3269:CDL:H532	2.43	0.59
11:K:24:PHE:O	11:K:28:VAL:HG12	2.02	0.59
1:A:1:FME:HCN	1:A:4:ASN:H	1.68	0.58
22:G:3269:CDL:HB32	1:N:304:TYR:HD1	1.68	0.58
23:P:4264:PEK:H71	23:P:4264:PEK:H32	1.83	0.58
6:S:87:THR:HG21	28:S:1303:HOH:O	2.02	0.58
7:T:38:HIS:NE2	22:T:4269:CDL:H111	2.18	0.58
22:P:4270:CDL:H112	28:P:2598:HOH:O	2.03	0.58
4:Q:82:VAL:O	4:Q:86:MET:HG3	2.03	0.58
17:N:515:HEA:HMC1	17:N:515:HEA:HBC1	1.86	0.58
6:F:92:VAL:HG23	6:F:92:VAL:O	2.03	0.58
1:A:177:SER:H	1:A:180:GLN:NE2	2.02	0.58
7:G:45:PRO:HD2	28:G:132:HOH:O	2.03	0.58
10:J:7:GLU:HG3	28:J:2487:HOH:O	2.03	0.58
5:R:43:PRO:HB2	5:R:48:ILE:HD11	1.86	0.58
1:A:113:LEU:HD12	18:A:3522:TGL:H292	1.85	0.57
7:T:45:PRO:HD2	28:T:1132:HOH:O	2.04	0.57
19:N:4524:PGV:H141	4:Q:87:PHE:CE2	2.39	0.57
19:A:3524:PGV:H141	4:D:87:PHE:CE2	2.39	0.57
3:P:51:MET:HB3	22:P:4270:CDL:H622	1.87	0.57
7:T:5:LYS:CD	23:T:3263:PEK:H382	2.33	0.57
1:A:229:ILE:HD11	2:B:175:ILE:CD1	2.33	0.57
1:N:350:VAL:HG11	18:N:4521:TGL:H281	1.87	0.57
23:C:3265:PEK:H041	6:F:1:ALA:N	2.20	0.56
1:N:68:PHE:CE2	1:N:112:LEU:HD13	2.37	0.56
1:N:113:LEU:CD1	18:N:4522:TGL:H292	2.35	0.56
18:N:4521:TGL:HB91	2:O:32:PHE:HE2	1.71	0.56
3:C:51:MET:HB3	22:C:3270:CDL:H622	1.87	0.56
6:S:22:LEU:HD12	28:S:2496:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.88	0.56
2:O:224:ALA:O	2:O:227:LEU:HG	2.06	0.56
1:N:113:LEU:HD12	18:N:4522:TGL:H292	1.88	0.56
2:O:49:LYS:NZ	18:Q:4523:TGL:HC71	2.21	0.56
3:C:246:ASP:HB2	28:C:3557:HOH:O	2.04	0.56
17:N:516:HEA:HMD1	17:N:516:HEA:HBD2	1.88	0.56
3:P:25:LEU:O	3:P:29:SER:HB2	2.06	0.56
3:P:226:HIS:CE1	22:P:4270:CDL:HB31	2.41	0.56
25:E:3230:PSC:H072	9:I:10:ARG:HH21	1.70	0.55
18:N:4521:TGL:H283	18:N:4521:TGL:H101	1.86	0.55
3:C:158:HIS:NE2	23:C:3265:PEK:H051	2.22	0.55
22:C:3270:CDL:H662	19:C:3267:PGV:H182	1.88	0.55
7:G:17:ARG:HD2	28:G:2008:HOH:O	2.06	0.55
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.88	0.55
1:A:136:LEU:HB2	28:A:3740:HOH:O	2.06	0.55
17:A:516:HEA:HMD1	17:A:516:HEA:HBD2	1.87	0.55
2:B:139:ASP:HB2	28:B:4220:HOH:O	2.07	0.55
18:N:4522:TGL:HG12	12:Y:13:PHE:HB3	1.88	0.55
1:A:377:PHE:O	1:A:381:LEU:HB3	2.07	0.55
3:C:67:PHE:CE1	22:C:3270:CDL:H1	2.34	0.55
2:O:83:ILE:O	2:O:87:MET:HG3	2.07	0.55
9:V:65:LYS:O	11:X:54:ARG:NH1	2.36	0.55
4:Q:20:ARG:HD2	4:Q:72:ASN:OD1	2.07	0.54
2:O:59:GLN:O	2:O:59:GLN:HG3	2.08	0.54
4:Q:86:MET:HE1	28:X:2287:HOH:O	2.06	0.54
1:A:113:LEU:CD1	18:A:3522:TGL:H292	2.37	0.54
18:A:3523:TGL:HB82	18:A:3523:TGL:H122	1.89	0.54
1:N:52:GLN:O	1:N:56:VAL:HG23	2.07	0.54
1:A:321:PHE:CD2	25:E:3230:PSC:H341	2.43	0.54
7:G:8:HIS:CD2	23:G:4263:PEK:H252	2.32	0.54
4:Q:19:ARG:HD2	4:Q:21:ASP:OD1	2.07	0.54
18:A:3521:TGL:H283	18:A:3521:TGL:H101	1.89	0.54
22:G:3269:CDL:H332	28:O:1358:HOH:O	2.08	0.54
1:N:51:ASP:OD1	2:O:206:PHE:HE1	1.90	0.54
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.90	0.53
22:P:4270:CDL:H121	28:P:2392:HOH:O	2.07	0.53
1:N:177:SER:H	1:N:180:GLN:NE2	2.06	0.53
18:N:4522:TGL:HC22	18:N:4522:TGL:CC6	2.37	0.53
2:O:62:GLU:O	2:O:66:THR:HB	2.08	0.53
7:T:38:HIS:CD2	22:T:4269:CDL:HA21	2.42	0.53
18:A:3522:TGL:HC62	12:L:20:ARG:HH12	1.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.72	0.53
2:B:102:HIS:O	2:B:104:TRP:N	2.41	0.53
1:N:334:TRP:HZ3	18:Q:4523:TGL:HA62	1.72	0.53
3:P:213:THR:HG23	22:P:4270:CDL:H762	1.91	0.53
9:I:8:GLN:HE22	9:I:10:ARG:H	1.57	0.53
1:N:483:LEU:HD13	4:Q:6:VAL:HB	1.89	0.53
4:D:20:ARG:HG3	28:D:168:HOH:O	2.09	0.53
1:A:514:LYS:HE3	28:A:3750:HOH:O	2.08	0.53
28:B:4144:HOH:O	22:T:4269:CDL:H332	2.09	0.53
18:N:4522:TGL:CG1	12:Y:13:PHE:HB3	2.39	0.53
18:N:4521:TGL:H101	18:N:4521:TGL:C28	2.39	0.52
2:O:122:MET:HB2	2:O:208:PRO:HD2	1.92	0.52
18:Q:4523:TGL:HB82	18:Q:4523:TGL:H122	1.90	0.52
1:A:304:TYR:HD1	22:T:4269:CDL:HB32	1.75	0.52
1:A:194:LEU:HD22	1:A:285:PHE:HE2	1.74	0.52
2:B:164:ALA:O	2:B:194:GLY:HA3	2.09	0.52
1:A:21:LEU:HD23	18:A:3522:TGL:H211	1.92	0.52
2:O:49:LYS:O	4:Q:20:ARG:NH2	2.39	0.52
6:F:64:GLU:O	6:F:65:ASP:HB2	2.10	0.52
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.44	0.52
7:T:3:ALA:O	7:T:4:ALA:HB2	2.10	0.52
8:U:7:LYS:O	8:U:8:ILE:HG22	2.09	0.52
7:T:11:TPO:HG22	7:T:16:TRP:HE1	1.74	0.52
2:B:122:MET:HB2	2:B:208:PRO:HD2	1.92	0.52
23:P:4265:PEK:H041	6:S:1:ALA:N	2.24	0.52
1:N:472:ILE:HG21	18:N:4522:TGL:HA81	1.91	0.52
18:A:3522:TGL:CC6	18:A:3522:TGL:HC22	2.37	0.51
4:D:4:SER:N	28:D:257:HOH:O	2.44	0.51
22:G:3269:CDL:H612	22:G:3269:CDL:H751	1.92	0.51
6:S:92:VAL:O	6:S:92:VAL:HG23	2.11	0.51
2:O:116:LEU:HD12	2:O:117:SER:N	2.26	0.51
22:T:4269:CDL:H612	22:T:4269:CDL:H751	1.91	0.51
1:A:87:ILE:O	1:A:173:PRO:HD3	2.11	0.51
4:D:4:SER:HB2	28:D:257:HOH:O	2.09	0.51
5:E:84:TYR:O	5:E:88:GLU:HG2	2.11	0.51
6:F:75:HIS:H	6:F:80:GLN:HE22	1.58	0.51
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.93	0.51
1:A:472:ILE:HD13	18:A:3522:TGL:HA92	1.93	0.51
7:G:3:ALA:O	7:G:4:ALA:HB2	2.11	0.51
1:N:22:PHE:HA	18:N:4522:TGL:HB72	1.93	0.51
1:A:282:PHE:HA	7:T:4:ALA:CB	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:P:4264:PEK:H102	23:P:4264:PEK:C16	2.40	0.51
1:A:1:FME:HCN	1:A:4:ASN:HB2	1.92	0.50
1:N:400:PHE:HB3	18:N:4522:TGL:H282	1.93	0.50
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.93	0.50
4:Q:121:LYS:HG2	11:X:53:TRP:CD1	2.46	0.50
18:A:3521:TGL:HC52	2:B:7:LEU:HD12	1.94	0.50
6:S:51:SER:O	6:S:94:HIS:N	2.45	0.50
3:C:103:HIS:HA	19:C:3268:PGV:H012	1.94	0.50
1:N:106:PRO:HB2	1:N:107:PRO:HD3	1.94	0.50
18:N:4521:TGL:H283	18:N:4521:TGL:CB9	2.42	0.50
3:P:158:HIS:NE2	23:P:4265:PEK:H051	2.26	0.50
18:A:3521:TGL:OB1	18:A:3521:TGL:HB42	2.11	0.50
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.94	0.50
13:M:17:ILE:O	13:M:21:VAL:HG23	2.12	0.50
22:T:4269:CDL:H322	22:T:4269:CDL:HA62	1.94	0.50
2:O:68:LEU:CB	2:O:69:PRO:HD3	2.42	0.50
7:T:34:ASN:ND2	22:T:4269:CDL:H151	2.26	0.50
13:Z:28:LEU:HB2	13:Z:29:PRO:HD3	1.93	0.50
2:B:128:LEU:HD11	2:B:134:ARG:HA	1.94	0.50
1:N:290:HIS:CD2	1:N:291:HIS:CD2	3.00	0.50
22:C:3270:CDL:H192	22:C:3270:CDL:H372	1.94	0.50
18:A:3521:TGL:HC22	28:I:346:HOH:O	2.12	0.49
22:G:3269:CDL:HB32	1:N:304:TYR:CD1	2.47	0.49
9:I:22:VAL:O	9:I:26:MET:HG2	2.12	0.49
18:A:3521:TGL:H101	18:A:3521:TGL:C28	2.42	0.49
25:E:3230:PSC:C07	9:I:10:ARG:HH21	2.25	0.49
22:C:3270:CDL:H651	22:C:3270:CDL:H771	1.95	0.49
23:C:3264:PEK:H102	23:C:3264:PEK:C16	2.38	0.49
12:Y:20:ARG:HH21	12:Y:24:MET:HG3	1.78	0.49
3:C:122:HIS:HD2	28:C:3562:HOH:O	1.95	0.49
1:N:62:ALA:HB2	17:N:515:HEA:HBD1	1.93	0.49
2:O:102:HIS:O	2:O:104:TRP:N	2.45	0.49
1:A:52:GLN:O	1:A:56:VAL:HG23	2.12	0.49
5:E:41:LEU:HA	28:I:301:HOH:O	2.12	0.49
1:N:350:VAL:CG1	18:N:4521:TGL:H281	2.42	0.49
1:N:472:ILE:HG21	18:N:4522:TGL:CA8	2.42	0.49
7:T:2:SER:O	7:T:3:ALA:HB3	2.13	0.49
1:N:42:GLY:HA3	4:Q:104:TYR:OH	2.12	0.49
18:N:4521:TGL:OB1	18:N:4521:TGL:HB42	2.12	0.49
18:N:4521:TGL:H283	18:N:4521:TGL:HB92	1.94	0.49
22:P:4270:CDL:H231	22:P:4270:CDL:H641	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:46:LYS:O	12:Y:47:LYS:HB2	2.12	0.49
2:B:172:THR:HG23	28:H:2574:HOH:O	2.12	0.49
3:C:226:HIS:CE1	22:C:3270:CDL:HB31	2.48	0.48
1:N:407:ASP:O	1:N:411:LYS:HG3	2.13	0.48
22:P:4270:CDL:H372	22:P:4270:CDL:H192	1.93	0.48
12:Y:2:HIS:ND1	12:Y:3:TYR:N	2.58	0.48
28:A:3691:HOH:O	19:C:3268:PGV:H12	2.13	0.48
6:F:92:VAL:O	6:F:92:VAL:CG2	2.61	0.48
18:A:3521:TGL:H283	18:A:3521:TGL:HB92	1.95	0.48
18:N:4522:TGL:HB52	18:N:4522:TGL:HB81	1.59	0.48
1:A:472:ILE:HG21	18:A:3522:TGL:CA8	2.44	0.48
1:N:87:ILE:O	1:N:173:PRO:HD3	2.13	0.48
2:O:164:ALA:O	2:O:194:GLY:HA3	2.13	0.48
1:N:377:PHE:O	1:N:381:LEU:HB3	2.14	0.48
18:N:4522:TGL:OA1	18:N:4522:TGL:H181	2.14	0.48
22:P:4270:CDL:H651	22:P:4270:CDL:H771	1.95	0.48
4:Q:23:PRO:O	4:Q:25:PRO:HD3	2.14	0.48
4:Q:36:SER:O	4:Q:39:ALA:HB3	2.14	0.48
10:W:30:ILE:O	10:W:34:VAL:HG23	2.13	0.48
18:A:3521:TGL:H241	18:A:3521:TGL:CA9	2.43	0.48
23:C:3265:PEK:H301	2:O:66:THR:CG2	2.44	0.47
2:O:68:LEU:HD22	25:O:4230:PSC:H171	1.95	0.47
18:A:3521:TGL:H283	18:A:3521:TGL:CB9	2.44	0.47
18:A:3522:TGL:CG1	12:L:13:PHE:HB3	2.44	0.47
3:C:177:GLN:HA	3:C:177:GLN:OE1	2.14	0.47
7:G:5:LYS:HD2	23:G:4263:PEK:H382	1.95	0.47
9:I:35:TYR:C	9:I:37:PHE:H	2.18	0.47
1:N:172:LYS:HD2	1:N:181:THR:CG2	2.44	0.47
3:P:253:TYR:CE2	22:T:4269:CDL:H641	2.49	0.47
22:G:3269:CDL:H172	22:G:3269:CDL:H511	1.97	0.47
22:G:3269:CDL:H322	22:G:3269:CDL:HA62	1.95	0.47
2:B:59:GLN:HG3	2:B:59:GLN:O	2.14	0.47
5:E:14:ARG:HD2	28:E:3271:HOH:O	2.14	0.47
6:F:90:LYS:HD2	28:F:187:HOH:O	2.14	0.47
22:G:3269:CDL:H212	1:N:311:ILE:HD12	1.97	0.47
2:O:203:ASN:N	2:O:203:ASN:HD22	2.12	0.47
6:S:22:LEU:O	6:S:25:ARG:HB3	2.15	0.47
9:V:35:TYR:C	9:V:37:PHE:H	2.18	0.47
1:A:378:HIS:O	1:A:382:SER:HB2	2.15	0.47
1:N:115:SER:O	1:N:121:GLY:HA2	2.15	0.47
18:N:4521:TGL:HB91	2:O:32:PHE:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:N:4524:PGV:H211	28:Z:2192:HOH:O	2.14	0.47
2:O:202:SER:HB2	2:O:203:ASN:HD22	1.80	0.47
11:X:24:PHE:O	11:X:28:VAL:HG12	2.14	0.47
22:G:3269:CDL:H252	22:G:3269:CDL:H222	1.73	0.47
2:O:128:LEU:HD11	2:O:134:ARG:HA	1.96	0.47
1:A:1:FME:CE	1:A:1:FME:HA	2.45	0.47
25:O:4230:PSC:C14	25:O:4230:PSC:H343	2.45	0.47
4:Q:101:HIS:HD2	4:Q:102:TYR:CE2	2.33	0.47
23:C:3265:PEK:H232	7:G:21:PHE:CD2	2.49	0.46
8:H:49:ASP:O	8:H:52:VAL:HG22	2.15	0.46
1:N:76:GLY:O	1:N:80:ASN:HB2	2.14	0.46
7:T:8:HIS:CD2	23:T:3263:PEK:H231	2.50	0.46
2:B:41:ILE:HD13	25:E:3230:PSC:H342	1.97	0.46
1:N:177:SER:H	1:N:180:GLN:HE21	1.63	0.46
11:X:54:ARG:NH2	11:X:54:ARG:HG3	2.29	0.46
1:A:390:MET:O	1:A:394:VAL:HG13	2.15	0.46
1:A:433:LEU:HD11	18:A:3521:TGL:OB1	2.15	0.46
2:B:151:ARG:HD3	2:B:181:GLN:HE21	1.80	0.46
7:G:50:TYR:HB3	7:G:52:HIS:CE1	2.50	0.46
4:Q:131:ILE:HD12	4:Q:131:ILE:H	1.81	0.46
11:X:54:ARG:HG3	11:X:54:ARG:HH21	1.80	0.46
25:E:3230:PSC:C14	25:E:3230:PSC:H343	2.46	0.46
1:N:95:PRO:HG2	3:P:11:VAL:CG2	2.46	0.46
4:Q:75:THR:HG22	28:Q:1438:HOH:O	2.14	0.46
22:C:3270:CDL:H652	22:C:3270:CDL:H621	1.59	0.46
23:C:3265:PEK:H102	23:C:3265:PEK:H131	1.76	0.46
1:N:426:PHE:CD1	18:N:4521:TGL:H282	2.50	0.46
18:N:4521:TGL:H101	18:N:4521:TGL:C27	2.46	0.46
13:Z:4:LYS:HB2	13:Z:5:PRO:CD	2.46	0.46
1:A:195:LEU:HD23	1:A:245:ILE:HD13	1.97	0.46
2:B:4:PRO:HB2	11:K:43:SER:HA	1.98	0.46
22:T:4269:CDL:H172	22:T:4269:CDL:H511	1.96	0.46
1:N:324:LEU:HD13	2:O:41:ILE:CG2	2.46	0.46
4:Q:7:LYS:O	4:Q:10:ASP:HB2	2.15	0.46
1:A:426:PHE:CD1	18:A:3521:TGL:H282	2.51	0.46
17:A:515:HEA:HBC1	17:A:515:HEA:HMC1	1.97	0.46
1:A:62:ALA:HB2	17:A:515:HEA:HBD1	1.98	0.46
1:A:290:HIS:CD2	1:A:291:HIS:CD2	3.04	0.46
4:Q:101:HIS:HD2	4:Q:102:TYR:CD2	2.34	0.46
7:G:84:LYS:CD	7:G:84:LYS:N	2.74	0.45
7:T:31:CYS:SG	22:T:4269:CDL:C53	3.03	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:187:THR:HG22	23:C:3264:PEK:H052	1.97	0.45
4:D:127:LYS:HD2	28:I:353:HOH:O	2.17	0.45
7:G:7:ASP:O	1:N:169:ILE:HD12	2.15	0.45
1:N:426:PHE:HE1	18:N:4521:TGL:H282	1.78	0.45
22:P:4270:CDL:HB21	22:P:4270:CDL:CB3	2.47	0.45
7:G:69:PHE:HD1	7:G:70:PHE:CE1	2.35	0.45
7:T:7:ASP:O	7:T:9:GLY:N	2.48	0.45
8:U:23:GLN:HG3	28:U:1462:HOH:O	2.17	0.45
9:V:18:ARG:HD3	28:V:1387:HOH:O	2.16	0.45
1:A:377:PHE:CD1	17:A:516:HEA:HAD1	2.52	0.45
3:C:63:ARG:NE	22:C:3270:CDL:HA22	2.23	0.45
1:A:334:TRP:CZ2	2:B:46:LEU:HB3	2.52	0.45
1:N:82:LEU:O	1:N:86:MET:HG3	2.17	0.45
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.99	0.45
11:X:54:ARG:HH21	11:X:54:ARG:CG	2.29	0.45
1:A:22:PHE:HA	18:A:3522:TGL:HB72	1.99	0.45
1:A:71:MET:HB2	1:A:72:PRO:HD3	1.99	0.45
18:A:3522:TGL:HG12	12:L:13:PHE:HB3	1.98	0.45
2:B:41:ILE:O	2:B:45:MET:HG2	2.17	0.45
2:B:78:LEU:HD12	2:B:78:LEU:HA	1.78	0.45
3:C:210:ILE:HD13	19:C:3267:PGV:H301	1.99	0.45
22:C:3270:CDL:H632	22:C:3270:CDL:H602	1.64	0.45
23:C:3265:PEK:H041	6:F:1:ALA:H1	1.79	0.45
1:N:489:THR:HA	6:S:71:TRP:O	2.17	0.45
1:A:225:GLY:HA3	3:C:112:LEU:HD21	1.98	0.45
7:T:84:LYS:H	7:T:84:LYS:CD	2.05	0.45
18:N:4521:TGL:HA91	18:N:4521:TGL:H222	1.57	0.45
1:A:165:ILE:O	1:A:169:ILE:HG12	2.15	0.45
3:P:67:PHE:HE1	22:P:4270:CDL:C1	2.23	0.45
1:A:1:FME:HA	1:A:1:FME:HE2	1.98	0.44
1:A:1:FME:HE2	12:L:3:TYR:HE1	1.81	0.44
1:A:106:PRO:HB2	1:A:107:PRO:HD3	1.99	0.44
21:J:3060:CHD:H3	28:J:2631:HOH:O	2.17	0.44
13:M:42:LYS:HA	13:M:42:LYS:CE	2.41	0.44
18:N:4521:TGL:H101	18:N:4521:TGL:H271	1.98	0.44
19:C:3268:PGV:H231	19:C:3268:PGV:H202	1.80	0.44
2:O:4:PRO:HB2	11:X:43:SER:HA	1.99	0.44
1:A:194:LEU:HD22	1:A:285:PHE:CE2	2.52	0.44
18:A:3522:TGL:HB81	18:A:3522:TGL:HB52	1.60	0.44
19:A:3524:PGV:H211	28:M:2318:HOH:O	2.17	0.44
22:G:3269:CDL:H181	22:G:3269:CDL:H152	1.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:LEU:HD21	1:A:450:TRP:HB2	1.99	0.44
3:C:158:HIS:CE1	23:C:3265:PEK:H051	2.53	0.44
1:N:44:PRO:HG2	4:Q:111:PHE:CZ	2.53	0.44
1:N:171:MET:HG2	3:P:8:TYR:CE1	2.52	0.44
1:N:378:HIS:CD2	1:N:382:SER:OG	2.71	0.44
1:A:513:LEU:HD22	1:A:513:LEU:HA	1.75	0.44
9:I:5:ALA:O	9:I:7:PRO:HD3	2.18	0.44
2:O:216:LEU:O	2:O:219:PHE:HB3	2.18	0.44
11:X:6:ALA:HA	11:X:7:PRO:HD2	1.89	0.44
7:G:42:ARG:O	7:G:42:ARG:HD3	2.18	0.44
5:R:5:HIS:HB3	5:R:6:GLU:H	1.63	0.44
22:G:3269:CDL:H571	22:G:3269:CDL:H601	1.80	0.44
19:P:4268:PGV:H231	19:P:4268:PGV:H202	1.82	0.44
19:A:3524:PGV:H141	4:D:87:PHE:CD2	2.52	0.44
22:T:4269:CDL:H252	22:T:4269:CDL:H222	1.73	0.44
2:O:92:ASN:HA	2:O:93:PRO:HD2	1.83	0.43
22:C:3270:CDL:HB21	22:C:3270:CDL:CB3	2.48	0.43
2:O:41:ILE:O	2:O:45:MET:HG2	2.17	0.43
22:P:4270:CDL:H662	19:P:4267:PGV:H182	2.00	0.43
1:A:407:ASP:O	1:A:411:LYS:HG3	2.19	0.43
22:P:4270:CDL:H621	22:P:4270:CDL:H652	1.62	0.43
18:A:3522:TGL:H271	12:L:11:ILE:CG2	2.49	0.43
4:Q:48:TRP:O	4:Q:51:LEU:HB2	2.19	0.43
5:R:12:ASP:HA	5:R:47:ILE:HD11	2.01	0.43
12:Y:35:ALA:HB3	12:Y:36:PRO:HD3	2.00	0.43
18:A:3521:TGL:HG11	2:B:7:LEU:HB3	2.00	0.43
25:E:3230:PSC:H252	25:E:3230:PSC:H221	1.79	0.43
1:N:440:TYR:CZ	2:O:205:SER:HA	2.53	0.43
18:N:4522:TGL:H272	18:N:4522:TGL:H232	1.99	0.43
1:A:309:THR:HG22	17:A:516:HEA:HMB2	2.01	0.43
18:A:3522:TGL:OA1	18:A:3522:TGL:H181	2.19	0.43
22:C:3270:CDL:H231	22:C:3270:CDL:H641	2.00	0.43
25:E:3230:PSC:H201	25:E:3230:PSC:H232	1.84	0.43
7:G:25:LEU:HD23	7:G:25:LEU:HA	1.88	0.43
6:S:94:HIS:CG	6:S:95:GLN:N	2.78	0.43
12:Y:20:ARG:NH2	12:Y:24:MET:HG3	2.33	0.43
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.54	0.43
7:G:7:ASP:O	7:G:9:GLY:N	2.47	0.43
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.99	0.43
1:N:363:LEU:HD23	1:N:363:LEU:HA	1.87	0.43
19:N:4524:PGV:H141	4:Q:87:PHE:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:50:LEU:O	10:W:50:LEU:HD22	2.18	0.43
10:J:50:LEU:HD22	10:J:50:LEU:O	2.18	0.43
5:R:48:ILE:O	5:R:52:LEU:HG	2.19	0.43
21:C:3271:CHD:H161	28:C:3628:HOH:O	2.18	0.43
21:C:3271:CHD:H222	21:C:3271:CHD:H162	1.72	0.43
7:G:1:ALA:HB2	19:P:4268:PGV:H321	2.00	0.43
22:G:3269:CDL:H522	22:G:3269:CDL:H202	2.01	0.43
12:Y:4:GLU:HB3	12:Y:9:LYS:HB3	2.01	0.43
1:A:115:SER:O	1:A:121:GLY:HA2	2.19	0.43
1:A:240:HIS:O	1:A:243:VAL:HG22	2.19	0.43
22:C:3270:CDL:H532	22:C:3270:CDL:H561	1.84	0.43
4:D:48:TRP:HA	4:D:51:LEU:HD22	2.00	0.43
18:N:4521:TGL:H283	18:N:4521:TGL:C10	2.49	0.43
25:O:4230:PSC:H241	25:O:4230:PSC:H62	2.00	0.43
7:T:5:LYS:HG3	23:T:3263:PEK:H382	2.01	0.43
19:A:3524:PGV:H012	19:A:3524:PGV:C4	2.50	0.42
25:E:3230:PSC:H62	25:E:3230:PSC:H241	2.01	0.42
21:J:3060:CHD:H212	21:J:3060:CHD:H161	1.70	0.42
1:N:399:LEU:HB2	1:N:494:TRP:CZ3	2.54	0.42
2:O:132:GLU:HB3	2:O:137:GLU:HG3	2.00	0.42
25:O:4230:PSC:H231	25:O:4230:PSC:H42	2.01	0.42
28:A:3743:HOH:O	11:K:8:ASP:HB2	2.19	0.42
3:C:135:SER:HB3	22:G:3269:CDL:H581	2.01	0.42
4:D:9:GLU:CD	4:D:9:GLU:H	2.23	0.42
18:N:4521:TGL:HG11	2:O:7:LEU:HB3	2.00	0.42
4:Q:138:TRP:CH2	11:X:50:PRO:HG2	2.54	0.42
7:T:8:HIS:ND1	23:T:3263:PEK:H311	2.34	0.42
5:E:31:LYS:HE3	6:F:83:PRO:O	2.19	0.42
1:N:426:PHE:CE1	18:N:4521:TGL:C28	3.01	0.42
5:R:82:TYR:N	5:R:83:PRO:CD	2.82	0.42
1:A:282:PHE:HZ	22:T:4269:CDL:H761	1.84	0.42
22:P:4270:CDL:H522	22:P:4270:CDL:OB9	2.19	0.42
4:Q:52:SER:OG	4:Q:55:GLU:HG3	2.20	0.42
6:S:64:GLU:O	6:S:65:ASP:HB2	2.19	0.42
18:A:3521:TGL:HA91	18:A:3521:TGL:H222	1.60	0.42
3:C:146:TRP:CE2	7:G:17:ARG:HG3	2.54	0.42
22:C:3270:CDL:PA1	22:C:3270:CDL:HB22	2.60	0.42
11:K:42:PRO:HG2	11:K:47:ARG:HE	1.85	0.42
1:N:81:TRP:HZ2	18:N:4522:TGL:C28	2.33	0.42
1:N:292:MET:O	1:N:295:VAL:HG22	2.20	0.42
1:N:374:VAL:HA	1:N:377:PHE:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:3521:TGL:H101	18:A:3521:TGL:C27	2.49	0.42
13:M:37:LEU:HA	13:M:37:LEU:HD23	1.72	0.42
10:W:36:MET:HB3	21:W:4060:CHD:H181	2.01	0.42
21:C:3271:CHD:H222	28:C:3628:HOH:O	2.19	0.42
25:E:3230:PSC:H062	25:E:3230:PSC:H042	1.75	0.42
9:I:21:ILE:HD13	9:I:21:ILE:HA	1.93	0.42
1:N:351:GLY:C	1:N:380:VAL:HG13	2.40	0.42
8:U:36:PHE:CE1	8:U:57:ARG:HB2	2.54	0.42
1:N:53:ILE:HD12	12:Y:44:LEU:HD23	2.01	0.42
1:N:71:MET:HB2	1:N:72:PRO:HD3	2.02	0.42
2:O:217:LYS:HE2	2:O:217:LYS:CA	2.49	0.42
7:T:5:LYS:CG	23:T:3263:PEK:H382	2.50	0.42
1:A:128:VAL:O	1:A:128:VAL:HG12	2.20	0.42
22:C:3270:CDL:H812	19:C:3267:PGV:H181	2.02	0.42
6:F:51:SER:O	6:F:94:HIS:N	2.53	0.42
1:N:46:THR:OG1	1:N:49:GLY:HA2	2.20	0.42
2:O:16:ILE:HD13	2:O:16:ILE:HA	1.96	0.42
3:P:253:TYR:HE2	22:T:4269:CDL:H641	1.83	0.42
4:Q:131:ILE:HD12	4:Q:131:ILE:N	2.34	0.42
7:T:19:LEU:HD21	23:T:3263:PEK:H362	2.02	0.42
22:T:4269:CDL:H432	22:T:4269:CDL:H402	1.78	0.42
22:T:4269:CDL:H662	22:T:4269:CDL:H631	1.88	0.42
8:U:43:MET:HE1	8:U:52:VAL:HG21	2.02	0.42
21:W:4060:CHD:H161	21:W:4060:CHD:H212	1.71	0.42
1:A:46:THR:OG1	1:A:49:GLY:HA2	2.20	0.41
1:A:351:GLY:HA3	1:A:380:VAL:HG13	2.01	0.41
18:A:3522:TGL:H272	18:A:3522:TGL:H232	2.02	0.41
4:D:34:SER:O	4:D:38:LYS:HG3	2.20	0.41
6:F:55:LYS:HA	6:F:74:LEU:O	2.19	0.41
2:O:104:TRP:HA	2:O:207:MET:SD	2.60	0.41
1:N:217:THR:HG22	3:P:188:ILE:HG12	2.01	0.41
1:A:44:PRO:HG2	4:D:111:PHE:CZ	2.56	0.41
25:E:3230:PSC:H343	25:E:3230:PSC:H141	2.02	0.41
11:K:43:SER:HA	11:K:44:PRO:HD3	1.96	0.41
2:B:16:ILE:HD13	2:B:16:ILE:HA	1.91	0.41
3:C:31:LEU:HD23	3:C:31:LEU:HA	1.92	0.41
1:N:40:GLU:HG2	1:N:54:TYR:CD2	2.55	0.41
1:N:95:PRO:HG2	3:P:11:VAL:HG23	2.01	0.41
1:N:324:LEU:HD13	2:O:41:ILE:HG22	2.01	0.41
19:N:4524:PGV:H311	13:Z:19:LEU:HD23	2.02	0.41
6:S:13:ALA:O	6:S:18:ARG:HD2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:C:3270:CDL:OB9	22:C:3270:CDL:H522	2.21	0.41
1:N:405:LEU:HD23	1:N:475:ALA:HB2	2.02	0.41
18:N:4521:TGL:H281	18:N:4521:TGL:HB81	2.03	0.41
3:P:40:MET:O	3:P:44:MET:HG2	2.20	0.41
18:A:3521:TGL:H101	18:A:3521:TGL:H271	2.01	0.41
22:G:3269:CDL:OA7	22:G:3269:CDL:H331	2.20	0.41
10:J:44:LEU:HD23	10:J:44:LEU:HA	1.96	0.41
18:N:4521:TGL:H241	18:N:4521:TGL:CA9	2.44	0.41
21:P:4271:CHD:H162	21:P:4271:CHD:H222	1.71	0.41
4:Q:93:ALA:HB2	11:X:29:TRP:CE2	2.55	0.41
7:G:2:SER:OG	23:G:4263:PEK:H291	2.21	0.41
22:G:3269:CDL:H402	22:G:3269:CDL:H432	1.76	0.41
17:N:516:HEA:HHA	17:N:516:HEA:HAD2	1.88	0.41
6:S:55:LYS:HA	6:S:74:LEU:O	2.21	0.41
22:T:4269:CDL:H551	22:T:4269:CDL:H582	1.77	0.41
3:C:62:ILE:HG13	19:C:3267:PGV:H21	2.02	0.41
1:N:68:PHE:HE2	1:N:112:LEU:CD1	2.27	0.41
1:N:321:PHE:CD2	25:O:4230:PSC:H341	2.56	0.41
2:O:42:ILE:O	2:O:46:LEU:HG	2.20	0.41
2:O:121:TYR:O	2:O:138:VAL:HA	2.20	0.41
1:A:334:TRP:CZ3	18:A:3523:TGL:HA62	2.55	0.41
2:B:23:PHE:CZ	2:B:80:SER:HB2	2.56	0.41
2:B:75:LEU:HA	2:B:75:LEU:HD12	1.79	0.41
18:N:4521:TGL:HC22	28:Q:1346:HOH:O	2.21	0.41
19:N:4524:PGV:H012	19:N:4524:PGV:C4	2.50	0.41
3:P:205:GLY:HA3	23:P:4264:PEK:H181	2.02	0.41
23:P:4265:PEK:H041	6:S:1:ALA:H1	1.84	0.41
4:Q:48:TRP:CH2	5:R:56:ARG:HA	2.56	0.41
5:R:41:LEU:HA	28:V:1301:HOH:O	2.21	0.41
22:T:4269:CDL:H561	22:T:4269:CDL:H611	2.02	0.41
3:C:67:PHE:HE1	22:C:3270:CDL:C1	2.25	0.41
6:F:52:ILE:HA	6:F:94:HIS:HA	2.02	0.41
1:N:34:SER:HB2	17:N:515:HEA:C2B	2.51	0.41
25:O:4230:PSC:H343	25:O:4230:PSC:H141	2.03	0.41
8:U:8:ILE:HD12	8:U:8:ILE:HA	1.98	0.41
2:B:155:SER:O	2:B:174:ALA:HB1	2.21	0.40
21:B:4085:CHD:H12	21:B:4085:CHD:H212	2.03	0.40
18:A:3522:TGL:H291	18:A:3522:TGL:H122	1.90	0.40
18:A:3523:TGL:HB51	4:D:81:VAL:HG11	2.03	0.40
22:C:3270:CDL:HB22	22:C:3270:CDL:OA5	2.22	0.40
7:G:19:LEU:HD21	23:G:4263:PEK:H362	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:2:HIS:CG	12:L:3:TYR:H	2.39	0.40
1:A:265:LYS:HB2	1:A:490:THR:HG21	2.02	0.40
1:A:488:THR:HB	1:A:495:LEU:HD13	2.03	0.40
22:T:4269:CDL:H601	22:T:4269:CDL:H571	1.76	0.40
9:V:37:PHE:HA	9:V:41:GLU:HB2	2.03	0.40
3:C:76:GLN:O	3:C:80:ARG:HG3	2.21	0.40
1:N:514:LYS:HE2	28:S:1303:HOH:O	2.22	0.40
4:Q:31:LYS:HB3	28:Q:2391:HOH:O	2.21	0.40
23:C:3265:PEK:H383	22:G:3269:CDL:C27	2.50	0.40
5:E:105:GLY:O	5:E:108:LYS:HG2	2.22	0.40
25:E:3230:PSC:H231	25:E:3230:PSC:H42	2.03	0.40
1:N:309:THR:HG22	17:N:516:HEA:HMB2	2.04	0.40
1:N:400:PHE:O	18:N:4522:TGL:H283	2.22	0.40
3:P:95:THR:HG21	19:P:4268:PGV:H282	2.04	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%)	500 (98%)	12 (2%)	0	100 100
1	N	512/514 (100%)	500 (98%)	12 (2%)	0	100 100
2	B	225/227 (99%)	210 (93%)	12 (5%)	3 (1%)	12 4
2	O	225/227 (99%)	208 (92%)	14 (6%)	3 (1%)	12 4
3	C	257/261 (98%)	251 (98%)	5 (2%)	1 (0%)	34 24
3	P	257/261 (98%)	251 (98%)	6 (2%)	0	100 100
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100 100
4	Q	142/147 (97%)	139 (98%)	3 (2%)	0	100 100
5	E	103/109 (94%)	103 (100%)	0	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	R	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
6	F	96/98 (98%)	89 (93%)	4 (4%)	3 (3%)	4	0
6	S	96/98 (98%)	91 (95%)	2 (2%)	3 (3%)	4	0
7	G	81/85 (95%)	66 (82%)	8 (10%)	7 (9%)	1	0
7	T	81/85 (95%)	65 (80%)	9 (11%)	7 (9%)	1	0
8	H	77/85 (91%)	70 (91%)	4 (5%)	3 (4%)	3	0
8	U	77/85 (91%)	70 (91%)	5 (6%)	2 (3%)	5	1
9	I	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
9	V	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
10	J	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
10	W	56/59 (95%)	56 (100%)	0	0	100	100
11	K	47/56 (84%)	47 (100%)	0	0	100	100
11	X	47/56 (84%)	47 (100%)	0	0	100	100
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
12	Y	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
13	Z	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
All	All	3504/3614 (97%)	3360 (96%)	112 (3%)	32 (1%)	17	7

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	95	GLN
7	G	4	ALA
7	G	7	ASP
7	G	8	HIS
7	G	39	SER
6	S	94	HIS
6	S	95	GLN
7	T	3	ALA
7	T	4	ALA
7	T	7	ASP
7	T	8	HIS
7	T	39	SER
2	B	104	TRP
6	F	94	HIS

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Mol	Chain	Res	Type
7	G	3	ALA
7	G	40	GLY
8	H	8	ILE
8	H	46	LYS
2	O	104	TRP
7	T	40	GLY
8	U	8	ILE
8	U	46	LYS
2	B	60	GLU
2	O	60	GLU
6	F	96	LEU
6	S	96	LEU
3	C	38	ASN
8	H	9	LYS
7	G	6	GLY
7	T	6	GLY
2	B	92	ASN
2	O	92	ASN

5.3.2 Protein sidechains (i)

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%)	415 (97%)	11 (3%)	46	39
1	N	426/426 (100%)	416 (98%)	10 (2%)	50	45
2	B	210/210 (100%)	198 (94%)	12 (6%)	20	11
2	O	210/210 (100%)	198 (94%)	12 (6%)	20	11
3	C	224/226 (99%)	220 (98%)	4 (2%)	59	55
3	P	224/226 (99%)	219 (98%)	5 (2%)	52	47
4	D	128/129 (99%)	127 (99%)	1 (1%)	81	82
4	Q	128/129 (99%)	125 (98%)	3 (2%)	50	45
5	E	92/95 (97%)	91 (99%)	1 (1%)	73	73
5	R	92/95 (97%)	89 (97%)	3 (3%)	38	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	F	81/81 (100%)	77 (95%)	4 (5%)	25 15
6	S	81/81 (100%)	76 (94%)	5 (6%)	18 9
7	G	67/68 (98%)	59 (88%)	8 (12%)	5 1
7	T	67/68 (98%)	60 (90%)	7 (10%)	7 2
8	H	71/75 (95%)	69 (97%)	2 (3%)	43 36
8	U	71/75 (95%)	67 (94%)	4 (6%)	21 11
9	I	57/57 (100%)	55 (96%)	2 (4%)	36 27
9	V	57/57 (100%)	54 (95%)	3 (5%)	22 13
10	J	49/50 (98%)	48 (98%)	1 (2%)	55 51
10	W	49/50 (98%)	48 (98%)	1 (2%)	55 51
11	K	39/46 (85%)	37 (95%)	2 (5%)	24 14
11	X	39/46 (85%)	38 (97%)	1 (3%)	46 39
12	L	39/40 (98%)	38 (97%)	1 (3%)	46 39
12	Y	39/40 (98%)	37 (95%)	2 (5%)	24 14
13	M	37/38 (97%)	33 (89%)	4 (11%)	6 2
13	Z	37/38 (97%)	33 (89%)	4 (11%)	6 2
All	All	3040/3082 (99%)	2927 (96%)	113 (4%)	34 25

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	109	PHE
1	A	112	LEU
1	A	138	HIS
1	A	180	GLN
1	A	238	PHE
1	A	338	MET
1	A	369	ASP
1	A	380	VAL
1	A	486	ASP
1	A	513	LEU
2	B	16	ILE
2	B	33	LEU
2	B	60	GLU
2	B	65	TRP

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Mol	Chain	Res	Type
2	B	66	THR
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	104	TRP
2	B	113	TYR
2	B	115	ASP
2	B	167	SER
3	C	127	LEU
3	C	159	MET
3	C	214	PHE
3	C	230	ASN
4	D	51	LEU
5	E	90	ARG
6	F	48	LEU
6	F	78	GLU
6	F	95	GLN
6	F	96	LEU
7	G	8	HIS
7	G	17	ARG
7	G	18	PHE
7	G	36	TRP
7	G	38	HIS
7	G	42	ARG
7	G	54	ARG
7	G	84	LYS
8	H	29	CYS
8	H	60	TYR
9	I	8	GLN
9	I	15	ARG
10	J	50	LEU
11	K	47	ARG
11	K	54	ARG
12	L	26	THR
13	M	13	LYS
13	M	34	LEU
13	M	38	ASP
13	M	42	LYS
1	N	109	PHE
1	N	138	HIS
1	N	180	GLN
1	N	238	PHE

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Mol	Chain	Res	Type
1	N	241	PRO
1	N	369	ASP
1	N	380	VAL
1	N	484	THR
1	N	504	THR
1	N	513	LEU
2	O	16	ILE
2	O	33	LEU
2	O	60	GLU
2	O	65	TRP
2	O	66	THR
2	O	68	LEU
2	O	78	LEU
2	O	91	ASN
2	O	94	SER
2	O	148	MET
2	O	167	SER
2	O	217	LYS
3	P	17	PRO
3	P	29	SER
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	8	SER
4	Q	19	ARG
4	Q	51	LEU
5	R	7	THR
5	R	70	VAL
5	R	90	ARG
6	S	37	LYS
6	S	48	LEU
6	S	53	THR
6	S	54	ASN
6	S	80	GLN
7	T	17	ARG
7	T	18	PHE
7	T	38	HIS
7	T	42	ARG
7	T	49	PRO
7	T	54	ARG
7	T	84	LYS
8	U	21	PRO

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Mol	Chain	Res	Type
8	U	29	CYS
8	U	60	TYR
8	U	65	PRO
9	V	8	GLN
9	V	29	LEU
9	V	61	GLU
10	W	50	LEU
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 (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	98	ASN
1	A	99	ASN
1	A	178	GLN
1	A	180	GLN
1	A	512	ASN
2	B	91	ASN
2	B	181	GLN
2	B	195	GLN
3	C	50	ASN
3	C	68	GLN
4	D	37	GLN
4	D	143	ASN
5	E	78	HIS
5	E	94	ASN
6	F	80	GLN
7	G	8	HIS
9	I	8	GLN
11	K	35	GLN
1	N	80	ASN
1	N	98	ASN
1	N	180	GLN
1	N	512	ASN
2	O	10	GLN

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Mol	Chain	Res	Type
2	O	91	ASN
2	O	181	GLN
2	O	195	GLN
2	O	203	ASN
3	P	68	GLN
4	Q	37	GLN
4	Q	101	HIS
5	R	94	ASN
6	S	54	ASN
6	S	80	GLN
6	S	94	HIS
7	T	71	HIS
9	V	8	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	SAC	V	1	9	7,8,9	2.78	2 (28%)	8,9,11	3.15	5 (62%)
2	FME	O	1	2	8,9,10	0.72	0	7,9,11	2.27	2 (28%)
2	FME	B	1	2	8,9,10	0.85	0	7,9,11	1.71	2 (28%)
7	TPO	T	11	7	8,10,11	1.40	1 (12%)	10,14,16	1.00	0
1	FME	N	1	1	8,9,10	0.77	0	7,9,11	1.83	2 (28%)
7	TPO	G	11	7	8,10,11	1.31	1 (12%)	10,14,16	1.02	0
1	FME	A	1	1	8,9,10	0.68	0	7,9,11	1.26	1 (14%)
9	SAC	I	1	9	7,8,9	2.46	2 (28%)	8,9,11	2.99	5 (62%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	SAC	V	1	9	-	3/7/8/10	-
2	FME	O	1	2	-	1/7/9/11	-
2	FME	B	1	2	-	1/7/9/11	-
7	TPO	T	11	7	-	5/9/11/13	-
1	FME	N	1	1	-	3/7/9/11	-
7	TPO	G	11	7	-	4/9/11/13	-
1	FME	A	1	1	-	3/7/9/11	-
9	SAC	I	1	9	-	3/7/8/10	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	1	SAC	OAC-C1A	5.17	1.34	1.23
9	I	1	SAC	OAC-C1A	4.97	1.34	1.23
9	V	1	SAC	CA-N	4.80	1.53	1.46
9	I	1	SAC	CA-N	3.93	1.51	1.46
7	T	11	TPO	CB-CA	2.65	1.59	1.53
7	G	11	TPO	CB-CA	2.17	1.58	1.53

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	V	1	SAC	CA-N-C1A	-6.58	111.00	123.15
9	I	1	SAC	CA-N-C1A	-6.27	111.58	123.15
2	O	1	FME	C-CA-N	4.38	117.64	109.73
1	N	1	FME	CA-N-CN	-4.22	116.33	122.82
2	O	1	FME	CA-N-CN	-3.93	116.77	122.82
9	I	1	SAC	C-CA-N	-3.44	103.53	109.73
9	V	1	SAC	C-CA-N	-3.28	103.82	109.73
9	I	1	SAC	CB-CA-N	3.10	117.50	110.55
9	V	1	SAC	CB-CA-N	3.00	117.27	110.55
9	V	1	SAC	C2A-C1A-N	2.93	121.05	116.10
2	B	1	FME	C-CA-N	2.84	114.85	109.73
2	B	1	FME	CA-N-CN	-2.74	118.61	122.82
1	A	1	FME	CA-N-CN	-2.44	119.08	122.82
9	V	1	SAC	OAC-C1A-C2A	-2.18	118.01	122.06
9	I	1	SAC	C2A-C1A-N	2.17	119.78	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	1	SAC	OAC-C1A-C2A	-2.13	118.10	122.06
1	N	1	FME	O-C-CA	-2.09	119.30	124.78

There are no chirality outliers.

All (23) 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
7	G	11	TPO	N-CA-CB-CG2
7	G	11	TPO	N-CA-CB-OG1
7	G	11	TPO	C-CA-CB-CG2
7	G	11	TPO	O-C-CA-CB
9	I	1	SAC	OAC-C1A-N-CA
9	I	1	SAC	CB-CA-N-C1A
1	N	1	FME	O1-CN-N-CA
1	N	1	FME	N-CA-CB-CG
1	N	1	FME	C-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
7	T	11	TPO	O-C-CA-CB
9	V	1	SAC	C2A-C1A-N-CA
9	V	1	SAC	OAC-C1A-N-CA
9	V	1	SAC	CB-CA-N-C1A
9	I	1	SAC	C2A-C1A-N-CA
1	A	1	FME	C-CA-CB-CG
7	T	11	TPO	CB-OG1-P-O1P

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	T	11	TPO	1	0
1	N	1	FME	1	0
1	A	1	FME	5	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 52 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - leaving 42 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	$\#\|Z\| > 2$
18	TGL	A	3522	-	62,62,62	1.39	6 (9%)	65,65,65	1.20	5 (7%)
23	PEK	P	4265	-	52,52,52	1.64	11 (21%)	55,57,57	0.95	4 (7%)
20	CUA	O	228	2	0,1,1	-	-	-		
23	PEK	T	3263	-	52,52,52	1.64	10 (19%)	55,57,57	0.97	3 (5%)
23	PEK	P	4264	-	52,52,52	1.42	6 (11%)	55,57,57	1.23	7 (12%)
17	HEA	N	515	1	57,67,67	1.16	5 (8%)	61,103,103	1.16	5 (8%)
18	TGL	A	3523	-	62,62,62	1.07	3 (4%)	65,65,65	1.06	4 (6%)
19	PGV	N	4266	-	50,50,50	0.90	2 (4%)	53,56,56	0.79	3 (5%)
27	DMU	M	3526	-	34,34,34	3.26	8 (23%)	45,45,45	4.08	20 (44%)
21	CHD	W	4060	-	32,32,32	1.16	3 (9%)	51,51,51	3.30	26 (50%)
19	PGV	A	3524	-	50,50,50	1.08	3 (6%)	53,56,56	1.05	6 (11%)
22	CDL	G	3269	-	99,99,99	0.97	7 (7%)	105,111,111	0.88	6 (5%)
22	CDL	P	4270	-	99,99,99	0.75	1 (1%)	105,111,111	0.86	5 (4%)
23	PEK	G	4263	-	52,52,52	1.60	9 (17%)	55,57,57	0.99	3 (5%)
18	TGL	N	4521	-	62,62,62	1.12	4 (6%)	65,65,65	1.09	5 (7%)
19	PGV	P	4268	-	50,50,50	1.07	3 (6%)	53,56,56	0.69	0
17	HEA	A	515	1	57,67,67	1.12	4 (7%)	61,103,103	1.30	6 (9%)
25	PSC	E	3230	-	51,51,51	1.20	3 (5%)	57,59,59	1.05	4 (7%)
19	PGV	N	4524	-	50,50,50	1.11	4 (8%)	53,56,56	1.02	3 (5%)
23	PEK	C	3264	-	52,52,52	1.42	5 (9%)	55,57,57	1.19	7 (12%)
17	HEA	N	516	1	57,67,67	1.11	5 (8%)	61,103,103	1.33	9 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CHD	P	4271	-	32,32,32	0.82	0	51,51,51	3.57	24 (47%)
19	PGV	A	3266	-	50,50,50	0.86	1 (2%)	53,56,56	0.72	0
19	PGV	C	3267	-	50,50,50	0.80	1 (2%)	53,56,56	0.86	2 (3%)
22	CDL	C	3270	-	99,99,99	0.74	1 (1%)	105,111,111	0.86	5 (4%)
23	PEK	C	3265	-	52,52,52	1.61	8 (15%)	55,57,57	0.96	4 (7%)
18	TGL	A	3521	-	62,62,62	1.09	4 (6%)	65,65,65	1.12	5 (7%)
21	CHD	B	4085	-	32,32,32	0.80	1 (3%)	51,51,51	1.83	15 (29%)
21	CHD	P	4525	-	32,32,32	0.82	1 (3%)	51,51,51	1.62	9 (17%)
18	TGL	Q	4523	-	62,62,62	1.10	3 (4%)	65,65,65	1.04	5 (7%)
21	CHD	J	3060	-	32,32,32	1.12	2 (6%)	51,51,51	3.26	26 (50%)
21	CHD	C	3271	-	32,32,32	0.87	0	51,51,51	3.59	24 (47%)
22	CDL	T	4269	-	99,99,99	0.96	5 (5%)	105,111,111	0.90	6 (5%)
25	PSC	O	4230	-	51,51,51	1.20	3 (5%)	57,59,59	1.04	4 (7%)
21	CHD	O	3085	-	32,32,32	0.84	1 (3%)	51,51,51	1.88	16 (31%)
19	PGV	C	3268	-	50,50,50	1.07	3 (6%)	53,56,56	0.69	1 (1%)
19	PGV	P	4267	-	50,50,50	0.83	1 (2%)	53,56,56	0.86	1 (1%)
27	DMU	Z	4526	-	34,34,34	3.22	9 (26%)	45,45,45	4.06	20 (44%)
18	TGL	N	4522	-	62,62,62	1.44	8 (12%)	65,65,65	1.18	4 (6%)
20	CUA	B	228	2	0,1,1	-	-	-		
21	CHD	C	3525	-	32,32,32	0.89	0	51,51,51	1.66	11 (21%)
17	HEA	A	516	1	57,67,67	1.15	5 (8%)	61,103,103	1.35	9 (14%)

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
18	TGL	A	3522	-	-	32/65/65/65	-
23	PEK	P	4265	-	-	20/56/56/56	-
23	PEK	T	3263	-	-	25/56/56/56	-
23	PEK	P	4264	-	-	21/56/56/56	-
17	HEA	N	515	1	-	2/32/76/76	-
18	TGL	A	3523	-	-	25/65/65/65	-
27	DMU	M	3526	-	5/5/10/10	10/19/59/59	0/2/2/2
19	PGV	N	4266	-	-	13/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CHD	W	4060	-	5/5/12/12	8/9/74/74	0/4/4/4
19	PGV	A	3524	-	-	30/55/55/55	-
22	CDL	G	3269	-	-	66/110/110/110	-
22	CDL	P	4270	-	-	77/110/110/110	-
23	PEK	G	4263	-	-	25/56/56/56	-
18	TGL	N	4521	-	-	31/65/65/65	-
19	PGV	P	4268	-	-	29/55/55/55	-
17	HEA	A	515	1	-	3/32/76/76	-
25	PSC	E	3230	-	-	34/55/55/55	-
19	PGV	N	4524	-	-	31/55/55/55	-
23	PEK	C	3264	-	-	21/56/56/56	-
17	HEA	N	516	1	-	7/32/76/76	-
21	CHD	P	4271	-	5/5/12/12	8/9/74/74	0/4/4/4
19	PGV	A	3266	-	-	13/55/55/55	-
19	PGV	C	3267	-	-	16/55/55/55	-
22	CDL	C	3270	-	-	77/110/110/110	-
23	PEK	C	3265	-	-	20/56/56/56	-
18	TGL	A	3521	-	-	31/65/65/65	-
21	CHD	B	4085	-	-	2/9/74/74	0/4/4/4
21	CHD	P	4525	-	-	2/9/74/74	0/4/4/4
18	TGL	Q	4523	-	-	25/65/65/65	-
21	CHD	J	3060	-	5/5/12/12	8/9/74/74	0/4/4/4
21	CHD	C	3271	-	5/5/12/12	8/9/74/74	0/4/4/4
22	CDL	T	4269	-	-	67/110/110/110	-
25	PSC	O	4230	-	-	33/55/55/55	-
21	CHD	O	3085	-	-	2/9/74/74	0/4/4/4
19	PGV	C	3268	-	-	29/55/55/55	-
19	PGV	P	4267	-	-	16/55/55/55	-
27	DMU	Z	4526	-	5/5/10/10	10/19/59/59	0/2/2/2
18	TGL	N	4522	-	-	32/65/65/65	-
21	CHD	C	3525	-	-	2/9/74/74	0/4/4/4
17	HEA	A	516	1	-	7/32/76/76	-

All (159) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	M	3526	DMU	O7-C3	-8.12	1.22	1.43
27	Z	4526	DMU	O16-C6	-7.94	1.26	1.40
27	M	3526	DMU	O16-C6	-7.77	1.26	1.40
27	Z	4526	DMU	O7-C3	-7.61	1.24	1.43
27	M	3526	DMU	O5-C4	-7.12	1.27	1.44
27	Z	4526	DMU	O16-C18	-6.79	1.24	1.43
27	M	3526	DMU	O16-C18	-6.75	1.24	1.43
27	Z	4526	DMU	O5-C4	-6.47	1.28	1.44
27	M	3526	DMU	O1-C9	-6.26	1.29	1.44
27	Z	4526	DMU	O1-C9	-6.13	1.29	1.44
27	Z	4526	DMU	O7-C10	-6.11	1.24	1.41
27	M	3526	DMU	O7-C10	-5.95	1.25	1.41
18	A	3522	TGL	OG2-CB1	5.85	1.50	1.34
18	N	4522	TGL	OG2-CB1	5.57	1.50	1.34
27	Z	4526	DMU	O1-C10	-5.48	1.27	1.41
27	M	3526	DMU	O1-C10	-5.38	1.28	1.41
27	M	3526	DMU	O5-C6	-5.05	1.29	1.41
27	Z	4526	DMU	O5-C6	-4.94	1.29	1.41
18	N	4522	TGL	OG1-CA1	4.91	1.47	1.33
18	N	4521	TGL	OG2-CB1	4.84	1.48	1.34
23	C	3264	PEK	C15-C14	4.68	1.58	1.31
23	G	4263	PEK	C12-C11	4.66	1.58	1.31
23	P	4264	PEK	C15-C14	4.65	1.58	1.31
23	P	4264	PEK	C12-C11	4.63	1.58	1.31
18	A	3522	TGL	OG1-CA1	4.56	1.46	1.33
18	N	4522	TGL	OG3-CC1	4.53	1.46	1.33
23	C	3264	PEK	C12-C11	4.51	1.57	1.31
23	T	3263	PEK	C12-C11	4.50	1.57	1.31
18	A	3523	TGL	OG1-CA1	4.40	1.46	1.33
18	Q	4523	TGL	OG1-CA1	4.30	1.45	1.33
23	T	3263	PEK	C9-C8	4.26	1.56	1.31
23	C	3265	PEK	C15-C14	4.26	1.56	1.31
23	C	3265	PEK	C12-C11	4.26	1.56	1.31
23	P	4265	PEK	C12-C11	4.25	1.56	1.31
25	O	4230	PSC	C10-C9	4.24	1.56	1.31
18	A	3521	TGL	OG2-CB1	4.21	1.46	1.34
23	P	4265	PEK	C6-C5	4.21	1.56	1.31
23	P	4265	PEK	C15-C14	4.18	1.56	1.31
23	T	3263	PEK	C6-C5	4.16	1.55	1.31
23	C	3265	PEK	C6-C5	4.16	1.55	1.31
19	N	4524	PGV	C12-C11	4.15	1.55	1.31
19	A	3524	PGV	C12-C11	4.15	1.55	1.31
23	G	4263	PEK	C9-C8	4.14	1.55	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	3522	TGL	OG3-CC1	4.14	1.45	1.33
19	P	4268	PGV	C12-C11	4.13	1.55	1.31
25	O	4230	PSC	C13-C12	4.13	1.55	1.31
23	P	4265	PEK	C9-C8	4.13	1.55	1.31
23	C	3265	PEK	C9-C8	4.13	1.55	1.31
18	Q	4523	TGL	OG2-CB1	4.10	1.45	1.34
25	E	3230	PSC	C10-C9	4.09	1.55	1.31
25	E	3230	PSC	C13-C12	4.09	1.55	1.31
23	G	4263	PEK	C15-C14	4.09	1.55	1.31
23	G	4263	PEK	C6-C5	4.08	1.55	1.31
19	C	3268	PGV	C12-C11	4.05	1.55	1.31
23	T	3263	PEK	C15-C14	4.03	1.55	1.31
23	C	3264	PEK	C9-C8	4.01	1.55	1.31
18	A	3523	TGL	OG3-CC1	3.99	1.45	1.33
19	N	4266	PGV	C12-C11	3.94	1.54	1.31
23	P	4264	PEK	C9-C8	3.94	1.54	1.31
23	P	4264	PEK	C6-C5	3.93	1.54	1.31
23	C	3264	PEK	C6-C5	3.88	1.54	1.31
19	A	3266	PGV	C12-C11	3.87	1.54	1.31
18	A	3521	TGL	OG1-CA1	3.80	1.44	1.33
18	N	4521	TGL	OG1-CA1	3.80	1.44	1.33
18	Q	4523	TGL	OG3-CC1	3.78	1.44	1.33
18	A	3523	TGL	OG2-CB1	3.74	1.44	1.34
21	W	4060	CHD	C13-C17	3.68	1.61	1.55
23	G	4263	PEK	C03-C02	3.63	1.61	1.50
22	T	4269	CDL	CB6-CB4	3.54	1.61	1.50
23	T	3263	PEK	C03-C02	3.54	1.61	1.50
21	J	3060	CHD	C13-C17	3.47	1.61	1.55
18	A	3521	TGL	OG3-CC1	3.45	1.43	1.33
18	N	4521	TGL	OG3-CC1	3.34	1.43	1.33
22	G	3269	CDL	CB6-CB4	3.15	1.60	1.50
17	N	515	HEA	C4C-NC	3.13	1.42	1.36
18	N	4522	TGL	OG3-CG3	3.06	1.52	1.45
19	P	4267	PGV	C12-C11	3.05	1.49	1.31
23	P	4265	PEK	O03-C21	3.04	1.42	1.33
17	A	515	HEA	CHC-C4B	3.01	1.42	1.35
19	C	3267	PGV	C12-C11	3.01	1.49	1.31
17	A	515	HEA	C3A-CMA	-3.01	1.39	1.46
17	N	516	HEA	C3A-CMA	-2.99	1.39	1.46
25	O	4230	PSC	C2-C1	2.95	1.59	1.50
23	G	4263	PEK	C01-C02	2.94	1.59	1.50
22	G	3269	CDL	OA6-CA5	2.93	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	3265	PEK	O03-C21	2.91	1.41	1.33
23	T	3263	PEK	C01-C02	2.90	1.59	1.50
17	N	515	HEA	C1C-NC	2.86	1.42	1.36
22	T	4269	CDL	CB3-CB4	2.84	1.59	1.50
23	T	3263	PEK	O03-C21	2.84	1.41	1.33
23	C	3265	PEK	C03-C02	2.75	1.59	1.50
17	A	515	HEA	C1C-NC	2.74	1.41	1.36
22	G	3269	CDL	CB3-CB4	2.74	1.59	1.50
23	T	3263	PEK	C22-C21	2.72	1.58	1.50
19	P	4268	PGV	O01-C1	2.71	1.42	1.34
19	C	3268	PGV	O01-C1	2.69	1.41	1.34
23	P	4265	PEK	C03-C02	2.68	1.58	1.50
17	A	516	HEA	C3C-C2C	-2.68	1.36	1.40
19	N	4524	PGV	C20-C19	2.65	1.58	1.50
17	A	516	HEA	C3A-C2A	-2.64	1.36	1.40
25	E	3230	PSC	C2-C1	2.60	1.58	1.50
18	A	3522	TGL	OG2-CG2	2.58	1.53	1.46
23	G	4263	PEK	O03-C21	2.56	1.40	1.33
17	N	515	HEA	C3A-CMA	-2.54	1.40	1.46
22	C	3270	CDL	C71-CB7	2.53	1.58	1.50
17	A	516	HEA	C3A-CMA	-2.52	1.40	1.46
23	P	4265	PEK	C01-C02	2.52	1.58	1.50
19	A	3524	PGV	C20-C19	2.51	1.58	1.50
19	N	4266	PGV	C01-C02	2.50	1.58	1.50
22	T	4269	CDL	OA6-CA5	2.49	1.41	1.34
17	A	515	HEA	C4C-NC	2.45	1.41	1.36
19	P	4268	PGV	C2-C1	2.45	1.57	1.50
18	A	3522	TGL	OG3-CG3	2.43	1.50	1.45
23	G	4263	PEK	C22-C21	2.43	1.57	1.50
19	N	4524	PGV	P-O11	2.41	1.69	1.59
17	A	516	HEA	C4D-ND	2.37	1.43	1.38
22	G	3269	CDL	OB6-CB5	2.37	1.41	1.34
23	C	3265	PEK	C01-C02	2.33	1.57	1.50
22	P	4270	CDL	C71-CB7	2.33	1.57	1.50
18	N	4522	TGL	CG3-CG2	2.31	1.57	1.50
19	C	3268	PGV	C2-C1	2.31	1.57	1.50
18	N	4522	TGL	CC2-CC1	2.30	1.57	1.50
19	A	3524	PGV	P-O11	2.28	1.68	1.59
22	T	4269	CDL	CB2-C1	2.28	1.59	1.51
17	N	515	HEA	CHC-C4B	2.22	1.40	1.35
21	W	4060	CHD	C8-C7	2.22	1.57	1.53
27	Z	4526	DMU	C8-C9	2.22	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	P	4264	PEK	O03-C01	-2.21	1.40	1.45
17	N	516	HEA	C3A-C2A	-2.21	1.37	1.40
17	N	515	HEA	C3A-C2A	-2.21	1.37	1.40
17	A	516	HEA	CHC-C4B	2.21	1.40	1.35
18	A	3521	TGL	OG1-CG1	-2.19	1.40	1.45
21	B	4085	CHD	C13-C12	-2.19	1.51	1.54
23	P	4265	PEK	P-O11	2.18	1.68	1.59
22	G	3269	CDL	C11-CA5	2.18	1.57	1.50
22	T	4269	CDL	C11-CA5	2.17	1.57	1.50
18	N	4522	TGL	OG2-CG2	2.17	1.52	1.46
23	P	4265	PEK	C22-C21	2.17	1.57	1.50
17	N	516	HEA	C3C-C2C	-2.16	1.37	1.40
23	P	4265	PEK	P-O12	2.15	1.68	1.59
23	G	4263	PEK	P-O11	2.14	1.68	1.59
22	G	3269	CDL	C71-CB7	2.13	1.56	1.50
23	P	4265	PEK	O01-C1	2.13	1.40	1.34
18	N	4521	TGL	OG1-CG1	-2.12	1.40	1.45
22	G	3269	CDL	CB2-C1	2.12	1.58	1.51
23	T	3263	PEK	P-O11	2.12	1.67	1.59
23	C	3265	PEK	P-O11	2.10	1.67	1.59
19	N	4524	PGV	C03-C02	2.10	1.57	1.50
18	N	4522	TGL	CB2-CB1	2.09	1.56	1.50
21	P	4525	CHD	C8-C9	2.07	1.57	1.53
18	A	3522	TGL	CG3-CG2	2.06	1.57	1.50
17	N	516	HEA	CHC-C4B	2.06	1.40	1.35
21	O	3085	CHD	C8-C9	2.05	1.57	1.53
23	T	3263	PEK	C2-C1	2.04	1.56	1.50
21	J	3060	CHD	C8-C7	2.03	1.57	1.53
23	P	4264	PEK	C2-C1	2.03	1.56	1.50
23	C	3264	PEK	O03-C01	-2.01	1.40	1.45
17	N	516	HEA	C3C-CAC	2.01	1.52	1.47
21	W	4060	CHD	C20-C17	2.00	1.57	1.54

All (322) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	M	3526	DMU	C10-C5-C7	10.25	131.34	110.00
27	Z	4526	DMU	C10-C5-C7	10.20	131.24	110.00
21	P	4271	CHD	C17-C13-C14	9.90	110.08	100.09
21	C	3271	CHD	C17-C13-C14	9.71	109.88	100.09
21	P	4271	CHD	C10-C9-C8	8.91	121.38	111.82
21	C	3271	CHD	C10-C9-C8	8.88	121.36	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	J	3060	CHD	C17-C13-C14	8.87	109.03	100.09
21	W	4060	CHD	C17-C13-C14	8.78	108.95	100.09
21	P	4271	CHD	C17-C13-C12	-8.63	109.78	117.67
21	C	3271	CHD	C17-C13-C12	-8.31	110.08	117.67
27	Z	4526	DMU	C8-C7-C5	-8.03	96.81	110.82
21	C	3271	CHD	C19-C10-C9	-8.00	100.16	111.18
27	Z	4526	DMU	C7-C8-C9	7.90	124.34	110.24
27	M	3526	DMU	C8-C7-C5	-7.83	97.16	110.82
27	M	3526	DMU	O1-C9-C11	7.82	125.87	106.44
21	P	4271	CHD	C19-C10-C9	-7.78	100.46	111.18
27	Z	4526	DMU	O1-C9-C11	7.75	125.70	106.44
27	M	3526	DMU	C7-C8-C9	7.68	123.94	110.24
27	M	3526	DMU	O5-C4-C3	7.51	125.58	109.75
27	Z	4526	DMU	O5-C6-O16	7.49	127.72	109.97
27	Z	4526	DMU	O5-C4-C3	7.41	125.36	109.75
27	M	3526	DMU	O1-C9-C8	7.17	122.71	109.69
27	M	3526	DMU	O5-C6-O16	7.02	126.60	109.97
27	Z	4526	DMU	O1-C9-C8	6.93	122.29	109.69
21	W	4060	CHD	C13-C17-C20	6.93	127.77	119.50
27	M	3526	DMU	C6-O5-C4	6.92	127.27	113.69
27	Z	4526	DMU	C6-O5-C4	6.89	127.22	113.69
27	Z	4526	DMU	O5-C4-C57	6.75	123.23	106.44
21	J	3060	CHD	C13-C17-C20	6.65	127.44	119.50
27	M	3526	DMU	O5-C4-C57	6.56	122.74	106.44
27	M	3526	DMU	O7-C3-C2	6.41	124.34	107.28
21	C	3271	CHD	C14-C13-C12	6.36	113.32	107.40
27	Z	4526	DMU	O7-C3-C2	6.16	123.67	107.28
21	P	4271	CHD	C14-C13-C12	6.04	113.02	107.40
21	J	3060	CHD	C4-C3-C2	6.03	117.75	110.55
21	P	4271	CHD	C9-C8-C7	5.99	119.04	111.88
21	C	3271	CHD	C19-C10-C1	-5.94	98.69	108.26
21	C	3271	CHD	C9-C8-C7	5.92	118.95	111.88
21	C	3271	CHD	C1-C10-C5	5.84	116.41	107.77
21	P	4271	CHD	C1-C10-C5	5.80	116.35	107.77
27	M	3526	DMU	C18-O16-C6	5.79	123.44	113.84
21	P	4271	CHD	C19-C10-C1	-5.69	99.10	108.26
21	W	4060	CHD	C4-C3-C2	5.66	117.31	110.55
21	W	4060	CHD	C18-C13-C14	-5.66	102.36	111.21
21	J	3060	CHD	C11-C12-C13	5.65	117.04	111.24
21	W	4060	CHD	C5-C6-C7	5.55	120.58	114.46
21	J	3060	CHD	C11-C9-C10	5.55	119.45	113.73
21	J	3060	CHD	C5-C6-C7	5.48	120.51	114.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	J	3060	CHD	C15-C14-C8	-5.42	110.76	118.33
21	W	4060	CHD	C11-C12-C13	5.40	116.79	111.24
21	W	4060	CHD	C15-C14-C8	-5.40	110.79	118.33
21	W	4060	CHD	C6-C5-C10	5.30	118.29	112.66
21	P	4271	CHD	C4-C3-C2	5.29	116.87	110.55
21	J	3060	CHD	C18-C13-C14	-5.24	103.02	111.21
21	C	3271	CHD	C4-C3-C2	5.23	116.80	110.55
27	Z	4526	DMU	C18-O16-C6	5.21	122.48	113.84
21	W	4060	CHD	C11-C9-C10	5.19	119.08	113.73
21	W	4060	CHD	C10-C9-C8	5.03	117.22	111.82
21	P	4271	CHD	C15-C14-C8	-5.03	111.30	118.33
21	C	3271	CHD	C15-C14-C8	-4.99	111.35	118.33
21	J	3060	CHD	C6-C5-C10	4.99	117.95	112.66
18	A	3521	TGL	OG2-CB1-CB2	4.78	121.79	111.50
21	J	3060	CHD	C10-C9-C8	4.73	116.90	111.82
18	N	4521	TGL	OG2-CB1-CB2	4.70	121.64	111.50
21	P	4525	CHD	C13-C17-C20	4.69	125.09	119.50
21	W	4060	CHD	C2-C1-C10	4.59	120.66	112.78
18	N	4522	TGL	OG3-CG3-CG2	4.52	121.58	108.43
18	A	3523	TGL	OG2-CB1-CB2	4.45	121.10	111.50
18	A	3522	TGL	OG3-CG3-CG2	4.44	121.37	108.43
21	C	3271	CHD	C4-C5-C10	4.44	117.37	112.66
21	C	3525	CHD	C13-C17-C20	4.44	124.79	119.50
27	M	3526	DMU	O16-C6-C1	4.44	115.23	108.30
21	J	3060	CHD	C9-C8-C7	4.35	117.08	111.88
21	J	3060	CHD	C2-C1-C10	4.30	120.16	112.78
21	J	3060	CHD	C1-C10-C5	4.26	114.07	107.77
27	M	3526	DMU	C10-O7-C3	4.25	128.47	117.96
21	O	3085	CHD	C10-C9-C8	4.24	116.38	111.82
21	P	4271	CHD	C4-C5-C10	4.21	117.13	112.66
21	W	4060	CHD	C9-C8-C7	4.18	116.87	111.88
27	Z	4526	DMU	C6-C1-C2	4.08	118.50	110.00
18	Q	4523	TGL	OG2-CB1-CB2	4.08	120.30	111.50
21	W	4060	CHD	C1-C10-C5	4.07	113.79	107.77
27	M	3526	DMU	C6-C1-C2	4.05	118.44	110.00
27	Z	4526	DMU	C10-O7-C3	4.02	127.91	117.96
21	J	3060	CHD	C13-C14-C8	3.96	119.80	114.74
21	W	4060	CHD	C13-C14-C8	3.95	119.78	114.74
21	B	4085	CHD	C15-C14-C8	-3.90	112.88	118.33
18	N	4522	TGL	OG2-CB1-CB2	3.89	119.89	111.50
18	A	3522	TGL	OG2-CB1-CB2	3.88	119.86	111.50
21	O	3085	CHD	C16-C17-C13	-3.84	99.79	103.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	Z	4526	DMU	O16-C6-C1	3.81	114.26	108.30
21	O	3085	CHD	C15-C14-C13	-3.80	99.83	103.55
21	B	4085	CHD	C15-C14-C13	-3.80	99.83	103.55
27	Z	4526	DMU	O7-C10-O1	3.74	121.12	110.67
21	W	4060	CHD	C5-C4-C3	3.70	118.19	112.76
17	A	515	HEA	CMC-C2C-C3C	3.70	131.59	124.68
21	C	3525	CHD	C15-C14-C8	-3.69	113.17	118.33
27	M	3526	DMU	O5-C6-C1	3.67	118.11	110.35
21	P	4525	CHD	C5-C6-C7	3.66	118.50	114.46
21	C	3271	CHD	C18-C13-C12	-3.65	105.35	109.07
17	A	515	HEA	CMC-C2C-C1C	-3.65	122.86	128.46
27	Z	4526	DMU	O5-C6-C1	3.62	118.02	110.35
27	Z	4526	DMU	O7-C3-C4	3.61	119.34	109.45
21	O	3085	CHD	C15-C14-C8	-3.60	113.30	118.33
27	M	3526	DMU	O7-C10-O1	3.58	120.69	110.67
21	W	4060	CHD	C9-C11-C12	3.57	119.01	114.30
21	P	4525	CHD	C15-C14-C8	-3.57	113.35	118.33
21	P	4271	CHD	C1-C10-C9	3.57	116.96	111.35
23	T	3263	PEK	C03-C02-C01	3.55	120.19	111.79
27	M	3526	DMU	C10-O1-C9	3.55	120.65	113.69
21	C	3271	CHD	C1-C10-C9	3.53	116.91	111.35
19	A	3524	PGV	P-O11-C03	3.51	142.25	121.68
21	J	3060	CHD	C1-C2-C3	3.49	114.94	110.47
21	W	4060	CHD	C1-C2-C3	3.45	114.89	110.47
23	C	3264	PEK	O03-C21-C22	-3.43	101.14	111.91
21	C	3271	CHD	C5-C6-C7	3.43	118.25	114.46
21	P	4271	CHD	C6-C5-C10	3.40	116.27	112.66
21	B	4085	CHD	C16-C17-C13	-3.39	100.23	103.55
23	G	4263	PEK	C03-C02-C01	3.37	119.77	111.79
21	O	3085	CHD	C19-C10-C9	-3.37	106.54	111.18
23	P	4264	PEK	O03-C21-C22	-3.36	101.37	111.91
21	B	4085	CHD	C10-C9-C8	3.36	115.42	111.82
21	P	4271	CHD	C14-C8-C7	3.32	116.21	111.81
21	J	3060	CHD	C9-C11-C12	3.32	118.68	114.30
21	O	3085	CHD	C5-C6-C7	3.31	118.11	114.46
21	P	4271	CHD	C5-C4-C3	3.29	117.59	112.76
19	N	4524	PGV	P-O11-C03	3.28	140.93	121.68
21	C	3525	CHD	C5-C6-C7	3.25	118.05	114.46
21	P	4271	CHD	C18-C13-C12	-3.25	105.76	109.07
27	M	3526	DMU	O7-C3-C4	3.24	118.32	109.45
21	J	3060	CHD	C5-C4-C3	3.23	117.50	112.76
27	Z	4526	DMU	C10-O1-C9	3.21	119.99	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	4085	CHD	C14-C8-C9	-3.21	105.31	109.71
21	B	4085	CHD	C1-C10-C5	3.21	112.51	107.77
21	C	3271	CHD	C5-C4-C3	3.19	117.45	112.76
23	T	3263	PEK	P-O11-C03	3.19	140.38	121.68
21	B	4085	CHD	C18-C13-C12	-3.19	105.82	109.07
27	M	3526	DMU	O7-C10-C5	3.17	116.31	108.10
21	C	3271	CHD	C6-C5-C10	3.16	116.02	112.66
23	G	4263	PEK	P-O11-C03	3.16	140.24	121.68
21	C	3271	CHD	C14-C8-C7	3.16	116.00	111.81
21	W	4060	CHD	C18-C13-C12	-3.15	105.86	109.07
21	W	4060	CHD	C17-C13-C12	-3.15	114.79	117.67
21	P	4525	CHD	C1-C10-C5	3.15	112.43	107.77
21	W	4060	CHD	C14-C13-C12	3.14	110.32	107.40
25	E	3230	PSC	C16-C15-C14	3.12	127.41	113.79
21	P	4271	CHD	C5-C6-C7	3.10	117.88	114.46
21	B	4085	CHD	C1-C2-C3	3.06	114.40	110.47
25	O	4230	PSC	C16-C15-C14	3.03	127.01	113.79
27	Z	4526	DMU	C1-C2-C3	3.03	116.60	109.68
25	O	4230	PSC	C01-O03-C19	-3.00	106.01	117.12
25	E	3230	PSC	C01-O03-C19	-2.97	106.11	117.12
21	W	4060	CHD	C16-C15-C14	2.97	111.02	105.13
27	Z	4526	DMU	O7-C10-C5	2.95	115.74	108.10
27	M	3526	DMU	C1-C2-C3	2.91	116.33	109.68
21	C	3525	CHD	C10-C9-C8	2.90	114.94	111.82
23	C	3265	PEK	P-O11-C03	2.89	138.65	121.68
21	B	4085	CHD	C9-C11-C12	2.88	118.11	114.30
17	A	516	HEA	CMB-C2B-C3B	-2.88	124.85	130.34
21	P	4525	CHD	C14-C8-C9	-2.87	105.77	109.71
17	A	515	HEA	C2D-C1D-ND	2.87	113.25	109.84
17	N	516	HEA	C1D-ND-C4D	-2.87	102.11	105.07
21	J	3060	CHD	C16-C15-C14	2.86	110.81	105.13
23	P	4265	PEK	P-O11-C03	2.86	138.46	121.68
21	P	4525	CHD	C1-C2-C3	2.85	114.13	110.47
21	J	3060	CHD	C18-C13-C12	-2.85	106.17	109.07
19	A	3524	PGV	C3-C2-C1	-2.84	103.31	113.62
21	C	3525	CHD	C16-C17-C13	-2.83	100.78	103.55
21	C	3271	CHD	C1-C2-C3	2.82	114.08	110.47
21	J	3060	CHD	C17-C13-C12	-2.81	115.10	117.67
19	N	4524	PGV	C03-C02-C01	2.80	118.42	111.79
17	N	515	HEA	CMC-C2C-C3C	2.80	129.92	124.68
21	O	3085	CHD	C9-C11-C12	2.79	117.99	114.30
17	A	516	HEA	C4B-NB-C1B	-2.79	102.19	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	C	3525	CHD	C14-C13-C12	-2.78	104.81	107.40
21	B	4085	CHD	C17-C13-C14	2.77	102.88	100.09
23	P	4264	PEK	O03-C21-O04	2.76	130.57	123.59
21	B	4085	CHD	O3-C3-C4	-2.76	104.36	109.85
21	C	3525	CHD	C14-C8-C9	-2.76	105.92	109.71
17	N	516	HEA	C27-C19-C20	2.76	119.91	115.27
21	C	3271	CHD	C18-C13-C14	-2.74	106.92	111.21
22	P	4270	CDL	CB6-OB8-CB7	-2.74	106.97	117.12
21	J	3060	CHD	C15-C16-C17	2.73	110.55	105.13
21	P	4271	CHD	C15-C16-C17	2.73	110.55	105.13
23	G	4263	PEK	O03-C01-C02	2.73	116.38	108.43
18	A	3521	TGL	OG3-CC1-OC1	-2.72	116.72	123.59
21	P	4525	CHD	C9-C11-C12	2.71	117.88	114.30
21	C	3271	CHD	C15-C16-C17	2.70	110.49	105.13
23	P	4264	PEK	C3-C2-C1	-2.70	103.81	113.62
17	A	516	HEA	C1D-ND-C4D	-2.70	102.29	105.07
22	C	3270	CDL	OB6-CB5-C51	-2.69	105.71	111.50
21	P	4271	CHD	C18-C13-C14	-2.69	107.01	111.21
21	O	3085	CHD	C5-C4-C3	2.68	116.69	112.76
25	O	4230	PSC	C15-C14-C13	2.67	127.75	112.43
21	C	3271	CHD	C13-C17-C20	-2.66	116.31	119.50
21	P	4271	CHD	C1-C2-C3	2.66	113.88	110.47
21	O	3085	CHD	C14-C13-C12	-2.66	104.93	107.40
22	C	3270	CDL	CB6-OB8-CB7	-2.63	107.38	117.12
21	O	3085	CHD	C1-C2-C3	2.63	113.84	110.47
21	O	3085	CHD	C17-C13-C14	2.63	102.74	100.09
21	W	4060	CHD	C15-C16-C17	2.63	110.34	105.13
23	C	3264	PEK	O03-C21-O04	2.63	130.22	123.59
25	E	3230	PSC	C15-C14-C13	2.60	127.35	112.43
21	C	3525	CHD	C1-C10-C5	2.60	111.61	107.77
21	J	3060	CHD	C19-C10-C9	-2.58	107.63	111.18
23	C	3264	PEK	C3-C2-C1	-2.57	104.29	113.62
21	J	3060	CHD	C14-C8-C9	2.56	113.23	109.71
23	T	3263	PEK	O03-C01-C02	2.56	115.90	108.43
18	N	4521	TGL	OG3-CC1-OC1	-2.56	117.14	123.59
21	C	3271	CHD	C16-C15-C14	2.55	110.18	105.13
21	P	4271	CHD	C13-C17-C20	-2.52	116.48	119.50
21	O	3085	CHD	C14-C8-C9	-2.52	106.26	109.71
17	A	515	HEA	C1D-ND-C4D	-2.51	102.48	105.07
21	P	4271	CHD	C16-C15-C14	2.50	110.08	105.13
19	N	4524	PGV	C3-C2-C1	-2.49	104.55	113.62
17	A	516	HEA	C2B-C1B-NB	2.49	112.87	109.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	W	4060	CHD	C14-C8-C9	2.49	113.13	109.71
21	P	4271	CHD	C9-C11-C12	2.49	117.59	114.30
23	P	4265	PEK	P-O12-C04	2.49	133.83	121.59
21	O	3085	CHD	C18-C13-C12	-2.48	106.55	109.07
19	C	3267	PGV	C9-C10-C11	-2.48	98.25	112.43
17	N	516	HEA	CHA-C4D-C3D	-2.47	121.20	124.84
21	J	3060	CHD	C14-C13-C12	2.47	109.70	107.40
17	A	515	HEA	C26-C15-C16	2.46	119.41	115.27
21	J	3060	CHD	C4-C5-C10	2.46	115.27	112.66
18	Q	4523	TGL	CB6-CB5-CB4	2.44	126.84	114.42
18	A	3522	TGL	OG1-CA1-CA2	2.44	119.56	111.91
21	B	4085	CHD	C5-C6-C7	2.41	117.12	114.46
19	P	4267	PGV	C9-C10-C11	-2.41	98.62	112.43
18	A	3522	TGL	OG3-CC1-OC1	-2.40	117.54	123.59
21	J	3060	CHD	O7-C7-C6	2.39	115.88	109.94
17	N	516	HEA	CMB-C2B-C3B	-2.38	125.80	130.34
21	O	3085	CHD	O3-C3-C4	-2.38	105.11	109.85
23	C	3265	PEK	O03-C01-C02	2.38	115.36	108.43
23	C	3264	PEK	C30-C29-C28	-2.38	102.37	114.42
18	A	3523	TGL	CB6-CB5-CB4	2.37	126.47	114.42
18	N	4522	TGL	OG1-CA1-CA2	2.36	119.32	111.91
23	P	4264	PEK	C30-C29-C28	-2.36	102.45	114.42
21	O	3085	CHD	C1-C10-C5	2.34	111.23	107.77
19	A	3524	PGV	C03-C02-C01	2.34	117.32	111.79
22	T	4269	CDL	OB8-CB6-CB4	2.34	115.24	108.43
17	N	515	HEA	C2D-C1D-ND	2.33	112.60	109.84
21	C	3271	CHD	C9-C11-C12	2.32	117.36	114.30
18	N	4522	TGL	OG3-CC1-OC1	-2.32	117.75	123.59
19	N	4266	PGV	O03-C01-C02	2.31	115.15	108.43
21	C	3271	CHD	C9-C10-C5	2.31	111.82	108.58
23	C	3265	PEK	P-O12-C04	2.29	132.87	121.59
22	T	4269	CDL	C22-C21-C20	2.29	126.06	114.42
22	G	3269	CDL	C22-C21-C20	2.28	126.01	114.42
22	T	4269	CDL	C23-C22-C21	2.28	125.98	114.42
17	A	515	HEA	C26-C15-C14	-2.26	117.89	123.68
21	B	4085	CHD	C18-C13-C14	2.25	114.74	111.21
21	W	4060	CHD	O7-C7-C6	2.25	115.53	109.94
23	P	4264	PEK	C24-C23-C22	-2.25	105.11	113.19
22	G	3269	CDL	C23-C22-C21	2.24	125.82	114.42
23	P	4265	PEK	O03-C01-C02	2.24	114.96	108.43
23	P	4264	PEK	C32-C31-C30	-2.24	103.07	114.42
21	W	4060	CHD	C4-C5-C10	2.24	115.03	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	N	516	HEA	C17-C18-C19	2.23	133.04	127.66
22	P	4270	CDL	OB6-CB5-C51	-2.23	106.69	111.50
22	G	3269	CDL	C19-C18-C17	2.23	125.72	114.42
22	T	4269	CDL	C19-C18-C17	2.22	125.70	114.42
18	A	3521	TGL	CB6-CB5-CB4	2.22	125.69	114.42
21	P	4525	CHD	C19-C10-C9	-2.21	108.13	111.18
22	G	3269	CDL	OB8-CB6-CB4	2.21	114.88	108.43
21	C	3525	CHD	C19-C10-C9	-2.20	108.15	111.18
23	C	3265	PEK	C11-C10-C9	2.20	122.87	112.02
23	C	3264	PEK	C23-C22-C21	-2.20	105.62	113.62
21	W	4060	CHD	C19-C10-C9	-2.18	108.17	111.18
17	N	516	HEA	C20-C19-C18	-2.18	116.70	121.12
17	A	516	HEA	CHA-C4D-C3D	-2.18	121.63	124.84
17	A	516	HEA	C27-C19-C20	2.18	118.94	115.27
25	E	3230	PSC	C14-C13-C12	-2.17	108.11	124.73
21	C	3525	CHD	C15-C14-C13	-2.16	101.43	103.55
21	B	4085	CHD	C5-C4-C3	2.16	115.93	112.76
23	C	3264	PEK	C24-C23-C22	-2.16	105.43	113.19
21	B	4085	CHD	C19-C10-C9	-2.15	108.22	111.18
19	N	4266	PGV	C01-O03-C19	-2.14	109.18	117.12
21	C	3525	CHD	C9-C11-C12	2.14	117.13	114.30
22	T	4269	CDL	C83-C82-C81	2.14	125.29	114.42
18	A	3521	TGL	CB5-CB4-CB3	2.14	125.29	114.42
23	P	4265	PEK	C11-C10-C9	2.14	122.55	112.02
17	N	515	HEA	CMC-C2C-C1C	-2.14	125.18	128.46
19	N	4266	PGV	O01-C1-C2	-2.13	106.90	111.50
21	P	4271	CHD	C9-C10-C5	2.13	111.58	108.58
23	C	3264	PEK	C32-C31-C30	-2.13	103.62	114.42
22	C	3270	CDL	C79-C78-C77	2.12	125.21	114.42
22	P	4270	CDL	C82-C81-C80	2.12	125.20	114.42
17	N	516	HEA	CHA-C4D-ND	2.12	126.73	124.43
22	P	4270	CDL	OB6-CB5-OB7	2.12	128.82	123.70
21	O	3085	CHD	C2-C1-C10	2.12	116.41	112.78
18	N	4521	TGL	CB6-CB5-CB4	2.11	125.14	114.42
17	A	516	HEA	C20-C19-C18	-2.11	116.85	121.12
18	A	3523	TGL	CB5-CB4-CB3	2.10	125.11	114.42
18	A	3521	TGL	CC6-CC5-CC4	2.10	125.10	114.42
18	A	3523	TGL	OG1-CA1-CA2	2.10	118.50	111.91
17	N	515	HEA	C26-C15-C16	2.10	118.80	115.27
19	C	3268	PGV	C21-C20-C19	-2.10	105.99	113.62
21	P	4525	CHD	C10-C9-C8	2.09	114.07	111.82
17	N	515	HEA	C3C-C4C-NC	2.08	111.90	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	T	4269	CDL	C79-C78-C77	2.07	124.95	114.42
22	C	3270	CDL	C82-C81-C80	2.07	124.95	114.42
18	Q	4523	TGL	CB5-CB4-CB3	2.07	124.92	114.42
17	N	516	HEA	C4B-NB-C1B	-2.06	102.95	105.07
18	N	4521	TGL	CB5-CB4-CB3	2.05	124.84	114.42
22	P	4270	CDL	C79-C78-C77	2.05	124.83	114.42
17	A	516	HEA	C3D-C4D-ND	2.05	112.34	110.36
19	C	3267	PGV	O01-C1-C2	-2.05	107.08	111.50
19	A	3524	PGV	O01-C02-C03	2.05	115.82	108.40
25	O	4230	PSC	C14-C13-C12	-2.04	109.05	124.73
19	A	3524	PGV	P-O12-C04	2.04	133.66	121.68
22	G	3269	CDL	C79-C78-C77	2.04	124.78	114.42
18	N	4521	TGL	CC6-CC5-CC4	2.04	124.78	114.42
17	A	516	HEA	CMC-C2C-C1C	-2.03	125.35	128.46
22	C	3270	CDL	OB6-CB5-OB7	2.03	128.60	123.70
19	A	3524	PGV	C02-O01-C1	2.02	122.76	117.79
18	Q	4523	TGL	OG1-CA1-CA2	2.02	118.23	111.91
23	P	4264	PEK	C2-C3-C4	2.01	116.82	113.23
17	N	516	HEA	CMC-C2C-C1C	-2.01	125.38	128.46
18	Q	4523	TGL	CG3-OG3-CC1	-2.00	109.71	117.12
18	A	3522	TGL	CC6-CC5-CC4	2.00	124.58	114.42
22	G	3269	CDL	C83-C82-C81	2.00	124.58	114.42

All (30) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	C	3271	CHD	C8
21	C	3271	CHD	C3
21	C	3271	CHD	C14
21	C	3271	CHD	C9
21	C	3271	CHD	C12
21	J	3060	CHD	C8
21	J	3060	CHD	C14
21	J	3060	CHD	C17
21	J	3060	CHD	C9
21	J	3060	CHD	C12
21	P	4271	CHD	C8
21	P	4271	CHD	C3
21	P	4271	CHD	C14
21	P	4271	CHD	C9
21	P	4271	CHD	C12
21	W	4060	CHD	C8

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Mol	Chain	Res	Type	Atom
21	W	4060	CHD	C14
21	W	4060	CHD	C17
21	W	4060	CHD	C9
21	W	4060	CHD	C12
27	M	3526	DMU	C2
27	M	3526	DMU	C9
27	M	3526	DMU	C5
27	M	3526	DMU	C6
27	M	3526	DMU	C4
27	Z	4526	DMU	C2
27	Z	4526	DMU	C9
27	Z	4526	DMU	C5
27	Z	4526	DMU	C6
27	Z	4526	DMU	C4

All (918) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	3521	TGL	CB2-CB1-OG2-CG2
18	A	3521	TGL	OB1-CB1-OG2-CG2
18	A	3523	TGL	OB1-CB1-OG2-CG2
18	N	4521	TGL	CB2-CB1-OG2-CG2
18	N	4521	TGL	OB1-CB1-OG2-CG2
18	Q	4523	TGL	OB1-CB1-OG2-CG2
19	A	3524	PGV	C03-O11-P-O13
19	A	3524	PGV	C02-C03-O11-P
19	A	3524	PGV	C05-C04-O12-P
19	A	3524	PGV	C2-C1-O01-C02
19	C	3268	PGV	C04-O12-P-O14
19	C	3268	PGV	O12-C04-C05-C06
19	C	3268	PGV	C04-C05-C06-O06
19	N	4524	PGV	C03-O11-P-O13
19	N	4524	PGV	C02-C03-O11-P
19	N	4524	PGV	C05-C04-O12-P
19	N	4524	PGV	C2-C1-O01-C02
19	P	4268	PGV	C04-O12-P-O14
19	P	4268	PGV	O12-C04-C05-C06
19	P	4268	PGV	C04-C05-C06-O06
21	J	3060	CHD	C16-C17-C20-C21
21	J	3060	CHD	C16-C17-C20-C22
21	W	4060	CHD	C16-C17-C20-C21
21	W	4060	CHD	C16-C17-C20-C22

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Mol	Chain	Res	Type	Atoms
22	C	3270	CDL	CA2-C1-CB2-OB2
22	C	3270	CDL	CA2-OA2-PA1-OA3
22	C	3270	CDL	CA2-OA2-PA1-OA4
22	C	3270	CDL	C11-CA5-OA6-CA4
22	G	3269	CDL	CB2-C1-CA2-OA2
22	G	3269	CDL	CA2-OA2-PA1-OA3
22	G	3269	CDL	C1-CB2-OB2-PB2
22	G	3269	CDL	CB3-OB5-PB2-OB3
22	G	3269	CDL	CB3-OB5-PB2-OB4
22	G	3269	CDL	OB6-CB4-CB6-OB8
22	P	4270	CDL	CA2-C1-CB2-OB2
22	P	4270	CDL	CA2-OA2-PA1-OA3
22	P	4270	CDL	CA2-OA2-PA1-OA4
22	P	4270	CDL	C11-CA5-OA6-CA4
22	T	4269	CDL	CB2-C1-CA2-OA2
22	T	4269	CDL	CA2-OA2-PA1-OA3
22	T	4269	CDL	C1-CB2-OB2-PB2
22	T	4269	CDL	CB3-OB5-PB2-OB2
22	T	4269	CDL	CB3-OB5-PB2-OB3
22	T	4269	CDL	CB3-OB5-PB2-OB4
22	T	4269	CDL	OB6-CB4-CB6-OB8
23	C	3264	PEK	O12-C04-C05-N
23	G	4263	PEK	C04-O12-P-O13
23	G	4263	PEK	O12-C04-C05-N
23	P	4264	PEK	O12-C04-C05-N
23	P	4265	PEK	C04-O12-P-O13
23	T	3263	PEK	C04-O12-P-O13
23	T	3263	PEK	O12-C04-C05-N
25	E	3230	PSC	C04-O12-P-O14
25	E	3230	PSC	O02-C1-O01-C02
25	E	3230	PSC	C13-C14-C15-C16
25	O	4230	PSC	C04-O12-P-O14
25	O	4230	PSC	O02-C1-O01-C02
25	O	4230	PSC	C13-C14-C15-C16
27	M	3526	DMU	O5-C6-O16-C18
27	Z	4526	DMU	O5-C6-O16-C18
18	A	3522	TGL	CG2-CG3-OG3-CC1
18	N	4522	TGL	CG2-CG3-OG3-CC1
18	A	3521	TGL	OC1-CC1-OG3-CG3
18	A	3523	TGL	OC1-CC1-OG3-CG3
18	N	4521	TGL	OC1-CC1-OG3-CG3
18	Q	4523	TGL	OC1-CC1-OG3-CG3

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Mol	Chain	Res	Type	Atoms
19	A	3524	PGV	O02-C1-O01-C02
19	N	4524	PGV	O02-C1-O01-C02
22	C	3270	CDL	OA7-CA5-OA6-CA4
22	P	4270	CDL	OA7-CA5-OA6-CA4
18	A	3523	TGL	CB2-CB1-OG2-CG2
18	Q	4523	TGL	CB2-CB1-OG2-CG2
27	Z	4526	DMU	O6-C11-C9-O1
18	A	3521	TGL	CB3-CB4-CB5-CB6
18	A	3522	TGL	CB3-CB4-CB5-CB6
18	A	3523	TGL	CB3-CB4-CB5-CB6
18	N	4521	TGL	CB3-CB4-CB5-CB6
18	N	4522	TGL	CB3-CB4-CB5-CB6
18	Q	4523	TGL	CB3-CB4-CB5-CB6
22	C	3270	CDL	C17-C18-C19-C20
22	C	3270	CDL	C20-C21-C22-C23
22	C	3270	CDL	C37-C38-C39-C40
22	C	3270	CDL	C40-C41-C42-C43
22	C	3270	CDL	C57-C58-C59-C60
22	C	3270	CDL	C80-C81-C82-C83
22	G	3269	CDL	C17-C18-C19-C20
22	G	3269	CDL	C20-C21-C22-C23
22	G	3269	CDL	C37-C38-C39-C40
22	G	3269	CDL	C40-C41-C42-C43
22	G	3269	CDL	C57-C58-C59-C60
22	G	3269	CDL	C60-C61-C62-C63
22	G	3269	CDL	C77-C78-C79-C80
22	G	3269	CDL	C80-C81-C82-C83
22	P	4270	CDL	C17-C18-C19-C20
22	P	4270	CDL	C20-C21-C22-C23
22	P	4270	CDL	C37-C38-C39-C40
22	P	4270	CDL	C40-C41-C42-C43
22	P	4270	CDL	C57-C58-C59-C60
22	P	4270	CDL	C80-C81-C82-C83
22	T	4269	CDL	C17-C18-C19-C20
22	T	4269	CDL	C20-C21-C22-C23
22	T	4269	CDL	C37-C38-C39-C40
22	T	4269	CDL	C40-C41-C42-C43
22	T	4269	CDL	C57-C58-C59-C60
22	T	4269	CDL	C60-C61-C62-C63
22	T	4269	CDL	C77-C78-C79-C80
18	A	3521	TGL	CC2-CC1-OG3-CG3
18	A	3523	TGL	CC2-CC1-OG3-CG3

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Mol	Chain	Res	Type	Atoms
18	N	4521	TGL	CC2-CC1-OG3-CG3
18	N	4522	TGL	CA2-CA1-OG1-CG1
18	Q	4523	TGL	CC2-CC1-OG3-CG3
22	C	3270	CDL	C77-C78-C79-C80
22	P	4270	CDL	C77-C78-C79-C80
22	T	4269	CDL	C80-C81-C82-C83
22	C	3270	CDL	C60-C61-C62-C63
22	P	4270	CDL	C60-C61-C62-C63
18	A	3523	TGL	CC2-CC3-CC4-CC5
27	M	3526	DMU	O6-C11-C9-O1
19	C	3268	PGV	O12-C04-C05-O05
19	P	4268	PGV	O12-C04-C05-O05
22	C	3270	CDL	O1-C1-CB2-OB2
22	G	3269	CDL	O1-C1-CA2-OA2
22	P	4270	CDL	O1-C1-CB2-OB2
22	T	4269	CDL	O1-C1-CA2-OA2
18	A	3522	TGL	CA2-CA1-OG1-CG1
22	G	3269	CDL	C31-CA7-OA8-CA6
22	T	4269	CDL	C31-CA7-OA8-CA6
18	Q	4523	TGL	CC2-CC3-CC4-CC5
22	G	3269	CDL	OA9-CA7-OA8-CA6
22	T	4269	CDL	OA9-CA7-OA8-CA6
18	N	4521	TGL	CA9-C20-C21-C22
18	N	4522	TGL	CC3-CC4-CC5-CC6
22	C	3270	CDL	C62-C63-C64-C65
22	P	4270	CDL	C62-C63-C64-C65
18	A	3521	TGL	CA9-C20-C21-C22
18	A	3522	TGL	CC3-CC4-CC5-CC6
21	C	3271	CHD	C13-C17-C20-C22
21	P	4271	CHD	C13-C17-C20-C22
22	C	3270	CDL	C23-C24-C25-C26
22	P	4270	CDL	C23-C24-C25-C26
22	T	4269	CDL	C52-C53-C54-C55
18	A	3522	TGL	OA1-CA1-OG1-CG1
18	N	4522	TGL	OA1-CA1-OG1-CG1
19	N	4524	PGV	C20-C21-C22-C23
22	G	3269	CDL	C52-C53-C54-C55
19	A	3524	PGV	C20-C21-C22-C23
18	A	3522	TGL	OC1-CC1-OG3-CG3
18	N	4522	TGL	OC1-CC1-OG3-CG3
22	G	3269	CDL	C15-C16-C17-C18
22	G	3269	CDL	C73-C74-C75-C76

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Mol	Chain	Res	Type	Atoms
25	E	3230	PSC	C20-C21-C22-C23
25	E	3230	PSC	C20-C19-O03-C01
25	O	4230	PSC	C20-C19-O03-C01
18	A	3522	TGL	CB5-CB6-CB7-CB8
22	T	4269	CDL	C15-C16-C17-C18
22	T	4269	CDL	C73-C74-C75-C76
25	O	4230	PSC	C20-C21-C22-C23
21	C	3271	CHD	C17-C20-C22-C23
18	N	4522	TGL	CB5-CB6-CB7-CB8
17	A	516	HEA	C4D-C3D-CAD-CBD
17	N	516	HEA	C4D-C3D-CAD-CBD
22	C	3270	CDL	CB2-C1-CA2-OA2
22	P	4270	CDL	CB2-C1-CA2-OA2
18	A	3521	TGL	CA2-CA1-OG1-CG1
18	N	4521	TGL	CA2-CA1-OG1-CG1
23	C	3265	PEK	C22-C21-O03-C01
23	P	4265	PEK	C22-C21-O03-C01
21	J	3060	CHD	C13-C17-C20-C22
21	W	4060	CHD	C13-C17-C20-C22
21	P	4271	CHD	C17-C20-C22-C23
19	P	4268	PGV	C7-C8-C9-C10
22	G	3269	CDL	O1-C1-CB2-OB2
22	T	4269	CDL	O1-C1-CB2-OB2
19	C	3268	PGV	C7-C8-C9-C10
22	G	3269	CDL	CA7-C31-C32-C33
22	G	3269	CDL	CB7-C71-C72-C73
22	T	4269	CDL	CA7-C31-C32-C33
22	T	4269	CDL	CB7-C71-C72-C73
23	C	3264	PEK	C1-C2-C3-C4
23	G	4263	PEK	C1-C2-C3-C4
23	C	3265	PEK	O04-C21-O03-C01
27	M	3526	DMU	O5-C4-C57-O61
21	C	3271	CHD	C21-C20-C22-C23
21	P	4271	CHD	C21-C20-C22-C23
19	A	3524	PGV	C1-C2-C3-C4
23	T	3263	PEK	C1-C2-C3-C4
25	E	3230	PSC	C22-C23-C24-C25
23	P	4265	PEK	O04-C21-O03-C01
18	A	3522	TGL	CB1-CB2-CB3-CB4
18	A	3523	TGL	CA1-CA2-CA3-CA4
18	N	4522	TGL	CB1-CB2-CB3-CB4
18	Q	4523	TGL	CA1-CA2-CA3-CA4

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Mol	Chain	Res	Type	Atoms
19	N	4524	PGV	C1-C2-C3-C4
23	P	4264	PEK	C1-C2-C3-C4
25	E	3230	PSC	C1-C2-C3-C4
25	O	4230	PSC	C1-C2-C3-C4
17	A	516	HEA	C2D-C3D-CAD-CBD
27	Z	4526	DMU	O5-C4-C57-O61
23	C	3265	PEK	C1-C2-C3-C4
23	P	4265	PEK	C1-C2-C3-C4
19	C	3268	PGV	C20-C21-C22-C23
19	P	4268	PGV	C20-C21-C22-C23
25	O	4230	PSC	C22-C23-C24-C25
18	A	3521	TGL	OA1-CA1-OG1-CG1
18	N	4521	TGL	OA1-CA1-OG1-CG1
22	C	3270	CDL	O1-C1-CA2-OA2
19	A	3524	PGV	C20-C19-O03-C01
21	J	3060	CHD	C13-C17-C20-C21
21	P	4271	CHD	C13-C17-C20-C21
21	W	4060	CHD	C13-C17-C20-C21
25	E	3230	PSC	O04-C19-O03-C01
25	O	4230	PSC	O04-C19-O03-C01
25	E	3230	PSC	C11-C12-C13-C14
25	O	4230	PSC	C11-C12-C13-C14
27	Z	4526	DMU	C3-C4-C57-O61
22	T	4269	CDL	C11-CA5-OA6-CA4
25	E	3230	PSC	C2-C1-O01-C02
25	O	4230	PSC	C2-C1-O01-C02
19	A	3524	PGV	C03-O11-P-O12
19	C	3268	PGV	C04-O12-P-O11
19	N	4524	PGV	C03-O11-P-O12
19	P	4268	PGV	C04-O12-P-O11
22	C	3270	CDL	CA2-OA2-PA1-OA5
22	C	3270	CDL	CA3-OA5-PA1-OA2
22	C	3270	CDL	CB2-OB2-PB2-OB5
22	G	3269	CDL	CA2-OA2-PA1-OA5
22	G	3269	CDL	CB3-OB5-PB2-OB2
22	P	4270	CDL	CA2-OA2-PA1-OA5
22	P	4270	CDL	CA3-OA5-PA1-OA2
22	P	4270	CDL	CB2-OB2-PB2-OB5
22	T	4269	CDL	CA2-OA2-PA1-OA5
23	C	3265	PEK	C04-O12-P-O11
23	P	4265	PEK	C04-O12-P-O11
19	N	4524	PGV	C20-C19-O03-C01

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Mol	Chain	Res	Type	Atoms
21	C	3271	CHD	C13-C17-C20-C21
22	G	3269	CDL	CA2-C1-CB2-OB2
22	T	4269	CDL	CA2-C1-CB2-OB2
22	G	3269	CDL	OA7-CA5-OA6-CA4
22	T	4269	CDL	OA7-CA5-OA6-CA4
22	G	3269	CDL	C22-C23-C24-C25
22	T	4269	CDL	C63-C64-C65-C66
22	G	3269	CDL	C63-C64-C65-C66
22	G	3269	CDL	C82-C83-C84-C85
22	T	4269	CDL	C22-C23-C24-C25
27	M	3526	DMU	C25-C28-C31-C34
22	G	3269	CDL	C11-CA5-OA6-CA4
18	A	3523	TGL	C12-C13-C14-C29
18	Q	4523	TGL	C12-C13-C14-C29
19	A	3266	PGV	C6-C7-C8-C9
19	C	3268	PGV	C30-C31-C32-C33
19	N	4266	PGV	C6-C7-C8-C9
19	P	4268	PGV	C30-C31-C32-C33
22	C	3270	CDL	C51-C52-C53-C54
22	C	3270	CDL	C63-C64-C65-C66
22	C	3270	CDL	C72-C73-C74-C75
23	C	3264	PEK	C23-C24-C25-C26
23	C	3265	PEK	C29-C30-C31-C32
23	P	4264	PEK	C23-C24-C25-C26
27	Z	4526	DMU	C25-C28-C31-C34
18	A	3523	TGL	C16-C15-CC9-CC8
19	A	3524	PGV	C22-C23-C24-C25
19	C	3268	PGV	C24-C25-C26-C27
19	N	4524	PGV	C22-C23-C24-C25
22	P	4270	CDL	C51-C52-C53-C54
22	P	4270	CDL	C63-C64-C65-C66
22	P	4270	CDL	C72-C73-C74-C75
22	T	4269	CDL	C82-C83-C84-C85
23	P	4265	PEK	C29-C30-C31-C32
18	N	4521	TGL	C22-C23-C24-C25
18	N	4521	TGL	C23-C24-C25-C26
18	Q	4523	TGL	C16-C15-CC9-CC8
19	C	3268	PGV	C14-C15-C16-C17
19	P	4268	PGV	C14-C15-C16-C17
22	C	3270	CDL	C61-C62-C63-C64
19	C	3268	PGV	C02-C03-O11-P
19	P	4268	PGV	C02-C03-O11-P

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Mol	Chain	Res	Type	Atoms
18	A	3521	TGL	C22-C23-C24-C25
18	A	3521	TGL	C23-C24-C25-C26
19	P	4268	PGV	C2-C3-C4-C5
19	P	4268	PGV	C24-C25-C26-C27
22	P	4270	CDL	O1-C1-CA2-OA2
18	A	3522	TGL	C17-C18-C19-C33
22	C	3270	CDL	C73-C74-C75-C76
22	G	3269	CDL	C41-C42-C43-C44
22	T	4269	CDL	C13-C14-C15-C16
22	T	4269	CDL	C41-C42-C43-C44
18	A	3522	TGL	C21-C20-CA9-CA8
18	A	3522	TGL	C24-C25-C26-C27
18	N	4522	TGL	C17-C18-C19-C33
19	A	3266	PGV	C29-C30-C31-C32
19	C	3268	PGV	C2-C3-C4-C5
19	N	4266	PGV	C29-C30-C31-C32
22	G	3269	CDL	C79-C80-C81-C82
22	P	4270	CDL	C61-C62-C63-C64
22	T	4269	CDL	C79-C80-C81-C82
18	A	3522	TGL	C16-C15-CC9-CC8
18	N	4521	TGL	CB4-CB5-CB6-CB7
18	N	4522	TGL	C16-C15-CC9-CC8
18	N	4522	TGL	C24-C25-C26-C27
19	A	3524	PGV	C14-C15-C16-C17
22	G	3269	CDL	C13-C14-C15-C16
22	G	3269	CDL	C33-C34-C35-C36
22	C	3270	CDL	CB7-C71-C72-C73
18	A	3521	TGL	CB4-CB5-CB6-CB7
18	A	3521	TGL	CC4-CC5-CC6-CC7
18	A	3522	TGL	CC6-CC7-CC8-CC9
18	A	3522	TGL	C22-C23-C24-C25
18	N	4521	TGL	CC4-CC5-CC6-CC7
18	N	4522	TGL	C22-C23-C24-C25
19	C	3268	PGV	C23-C24-C25-C26
19	N	4524	PGV	C14-C15-C16-C17
22	P	4270	CDL	C73-C74-C75-C76
22	T	4269	CDL	C33-C34-C35-C36
23	T	3263	PEK	C31-C32-C33-C34
25	E	3230	PSC	C2-C3-C4-C5
25	O	4230	PSC	C2-C3-C4-C5
18	A	3521	TGL	C12-C13-C14-C29
18	N	4522	TGL	CC6-CC7-CC8-CC9

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Mol	Chain	Res	Type	Atoms
18	Q	4523	TGL	CB6-CB7-CB8-CB9
19	P	4268	PGV	C23-C24-C25-C26
23	G	4263	PEK	C31-C32-C33-C34
19	A	3524	PGV	C04-C05-C06-O06
19	N	4524	PGV	C04-C05-C06-O06
18	A	3523	TGL	CB6-CB7-CB8-CB9
18	N	4521	TGL	C12-C13-C14-C29
18	N	4522	TGL	C21-C20-CA9-CA8
19	C	3267	PGV	C11-C10-C9-C8
19	P	4267	PGV	C11-C10-C9-C8
22	P	4270	CDL	CB7-C71-C72-C73
19	A	3524	PGV	C24-C25-C26-C27
19	C	3267	PGV	C22-C23-C24-C25
19	N	4524	PGV	C24-C25-C26-C27
19	P	4267	PGV	C22-C23-C24-C25
22	C	3270	CDL	C74-C75-C76-C77
23	P	4265	PEK	C25-C26-C27-C28
23	T	3263	PEK	C22-C23-C24-C25
19	N	4266	PGV	C15-C16-C17-C18
22	P	4270	CDL	C74-C75-C76-C77
23	C	3265	PEK	C25-C26-C27-C28
23	G	4263	PEK	C22-C23-C24-C25
19	A	3266	PGV	C23-C24-C25-C26
25	E	3230	PSC	C29-C30-C31-C32
25	O	4230	PSC	C29-C30-C31-C32
19	A	3266	PGV	C5-C6-C7-C8
19	N	4266	PGV	C5-C6-C7-C8
22	C	3270	CDL	C13-C14-C15-C16
18	A	3522	TGL	C21-C22-C23-C24
18	N	4521	TGL	C14-C29-C30-C31
27	Z	4526	DMU	C19-C18-O16-C6
18	A	3521	TGL	C14-C29-C30-C31
18	A	3522	TGL	C18-C19-C33-C34
19	N	4266	PGV	C23-C24-C25-C26
22	C	3270	CDL	C55-C56-C57-C58
22	P	4270	CDL	C13-C14-C15-C16
23	T	3263	PEK	C27-C28-C29-C30
19	A	3524	PGV	O04-C19-O03-C01
18	N	4522	TGL	C18-C19-C33-C34
19	C	3267	PGV	C25-C26-C27-C28
19	P	4267	PGV	C25-C26-C27-C28
22	P	4270	CDL	C55-C56-C57-C58

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Mol	Chain	Res	Type	Atoms
23	T	3263	PEK	C25-C26-C27-C28
18	A	3523	TGL	OG1-CG1-CG2-CG3
18	Q	4523	TGL	OG1-CG1-CG2-CG3
23	C	3264	PEK	O03-C01-C02-C03
18	N	4522	TGL	C21-C22-C23-C24
23	G	4263	PEK	C27-C28-C29-C30
22	G	3269	CDL	C23-C24-C25-C26
22	P	4270	CDL	C75-C76-C77-C78
22	T	4269	CDL	C23-C24-C25-C26
19	N	4524	PGV	O04-C19-O03-C01
22	P	4270	CDL	C51-CB5-OB6-CB4
19	A	3266	PGV	C15-C16-C17-C18
23	P	4264	PEK	C16-C17-C18-C19
21	W	4060	CHD	C21-C20-C22-C23
19	A	3524	PGV	O05-C05-C06-O06
19	C	3268	PGV	O05-C05-C06-O06
19	N	4524	PGV	O05-C05-C06-O06
19	P	4268	PGV	O05-C05-C06-O06
18	A	3523	TGL	CB5-CB6-CB7-CB8
22	C	3270	CDL	C16-C17-C18-C19
22	P	4270	CDL	C16-C17-C18-C19
23	G	4263	PEK	C25-C26-C27-C28
27	Z	4526	DMU	O16-C18-C19-C22
18	Q	4523	TGL	CB5-CB6-CB7-CB8
22	C	3270	CDL	C75-C76-C77-C78
23	C	3264	PEK	C16-C17-C18-C19
22	T	4269	CDL	OB9-CB7-OB8-CB6
22	C	3270	CDL	C32-C33-C34-C35
22	P	4270	CDL	C32-C33-C34-C35
22	C	3270	CDL	OB7-CB5-OB6-CB4
22	P	4270	CDL	OB7-CB5-OB6-CB4
19	N	4266	PGV	C7-C8-C9-C10
22	C	3270	CDL	C19-C20-C21-C22
22	G	3269	CDL	OB9-CB7-OB8-CB6
18	A	3521	TGL	C16-C15-CC9-CC8
22	P	4270	CDL	C19-C20-C21-C22
22	G	3269	CDL	CA5-C11-C12-C13
22	P	4270	CDL	CA5-C11-C12-C13
22	T	4269	CDL	CA5-C11-C12-C13
22	C	3270	CDL	C11-C12-C13-C14
22	T	4269	CDL	C56-C57-C58-C59
23	P	4264	PEK	O04-C21-O03-C01

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Mol	Chain	Res	Type	Atoms
19	P	4268	PGV	C19-C20-C21-C22
22	C	3270	CDL	CA5-C11-C12-C13
19	A	3266	PGV	C7-C8-C9-C10
19	P	4267	PGV	C7-C8-C9-C10
22	G	3269	CDL	C56-C57-C58-C59
22	P	4270	CDL	C11-C12-C13-C14
18	N	4521	TGL	C16-C15-CC9-CC8
18	N	4521	TGL	C20-C21-C22-C23
23	C	3264	PEK	O04-C21-O03-C01
18	A	3521	TGL	C20-C21-C22-C23
22	G	3269	CDL	C39-C40-C41-C42
22	T	4269	CDL	C39-C40-C41-C42
27	M	3526	DMU	O16-C18-C19-C22
19	P	4268	PGV	O02-C1-O01-C02
23	T	3263	PEK	O02-C1-O01-C02
19	C	3268	PGV	C19-C20-C21-C22
18	N	4522	TGL	CC2-CC1-OG3-CG3
23	C	3264	PEK	C22-C21-O03-C01
18	N	4522	TGL	C19-C33-C34-C35
22	G	3269	CDL	C19-C20-C21-C22
18	A	3522	TGL	C19-C33-C34-C35
22	T	4269	CDL	C19-C20-C21-C22
22	T	4269	CDL	C72-C73-C74-C75
21	J	3060	CHD	C21-C20-C22-C23
19	C	3268	PGV	C25-C26-C27-C28
22	G	3269	CDL	C72-C73-C74-C75
22	T	4269	CDL	C62-C63-C64-C65
18	A	3522	TGL	CA7-CA8-CA9-C20
19	C	3267	PGV	C7-C8-C9-C10
18	A	3522	TGL	CC2-CC1-OG3-CG3
18	A	3523	TGL	CB4-CB5-CB6-CB7
22	C	3270	CDL	C51-CB5-OB6-CB4
23	G	4263	PEK	C2-C1-O01-C02
23	T	3263	PEK	C2-C1-O01-C02
18	N	4522	TGL	CA7-CA8-CA9-C20
22	C	3270	CDL	C78-C79-C80-C81
23	C	3265	PEK	C16-C17-C18-C19
19	C	3268	PGV	C29-C30-C31-C32
19	C	3268	PGV	O02-C1-O01-C02
19	P	4268	PGV	C25-C26-C27-C28
18	A	3521	TGL	OG1-CG1-CG2-OG2
18	A	3523	TGL	OG1-CG1-CG2-OG2

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Mol	Chain	Res	Type	Atoms
18	N	4521	TGL	OG1-CG1-CG2-OG2
18	Q	4523	TGL	OG1-CG1-CG2-OG2
22	G	3269	CDL	C62-C63-C64-C65
22	P	4270	CDL	C78-C79-C80-C81
18	A	3521	TGL	C13-C14-C29-C30
18	A	3521	TGL	C17-C18-C19-C33
18	Q	4523	TGL	CB4-CB5-CB6-CB7
19	P	4267	PGV	C13-C14-C15-C16
22	P	4270	CDL	C18-C19-C20-C21
23	C	3265	PEK	C2-C3-C4-C5
23	P	4265	PEK	C2-C3-C4-C5
23	P	4265	PEK	C16-C17-C18-C19
18	N	4521	TGL	C13-C14-C29-C30
18	N	4521	TGL	C17-C18-C19-C33
18	Q	4523	TGL	C23-C24-C25-C26
19	C	3267	PGV	C13-C14-C15-C16
22	C	3270	CDL	C18-C19-C20-C21
22	P	4270	CDL	C14-C15-C16-C17
22	C	3270	CDL	C36-C37-C38-C39
22	G	3269	CDL	C14-C15-C16-C17
18	A	3522	TGL	CB9-C10-C11-C12
18	N	4521	TGL	CC2-CC3-CC4-CC5
23	G	4263	PEK	O02-C1-O01-C02
18	A	3521	TGL	CC2-CC3-CC4-CC5
18	A	3522	TGL	CC4-CC5-CC6-CC7
18	N	4522	TGL	CB9-C10-C11-C12
19	P	4267	PGV	C24-C25-C26-C27
19	P	4268	PGV	C29-C30-C31-C32
22	C	3270	CDL	C14-C15-C16-C17
22	T	4269	CDL	C14-C15-C16-C17
27	Z	4526	DMU	C22-C25-C28-C31
25	O	4230	PSC	C04-O12-P-O11
27	M	3526	DMU	C3-C4-C57-O61
25	E	3230	PSC	C21-C22-C23-C24
22	T	4269	CDL	C71-CB7-OB8-CB6
19	A	3524	PGV	C01-C02-C03-O11
19	N	4524	PGV	C01-C02-C03-O11
22	C	3270	CDL	OA5-CA3-CA4-CA6
22	P	4270	CDL	OA5-CA3-CA4-CA6
22	C	3270	CDL	C71-C72-C73-C74
22	G	3269	CDL	C38-C39-C40-C41
25	E	3230	PSC	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
19	N	4524	PGV	C5-C6-C7-C8
25	O	4230	PSC	C3-C4-C5-C6
18	N	4522	TGL	CC4-CC5-CC6-CC7
22	P	4270	CDL	C71-C72-C73-C74
25	O	4230	PSC	C21-C22-C23-C24
18	A	3523	TGL	C23-C24-C25-C26
18	N	4522	TGL	CC2-CC3-CC4-CC5
18	Q	4523	TGL	CA9-C20-C21-C22
19	N	4524	PGV	C2-C3-C4-C5
22	P	4270	CDL	C36-C37-C38-C39
23	P	4264	PEK	C22-C23-C24-C25
22	G	3269	CDL	C71-CB7-OB8-CB6
27	M	3526	DMU	C22-C25-C28-C31
18	A	3523	TGL	CA9-C20-C21-C22
19	C	3267	PGV	C24-C25-C26-C27
22	C	3270	CDL	C59-C60-C61-C62
21	P	4271	CHD	C16-C17-C20-C21
22	P	4270	CDL	C12-C13-C14-C15
22	T	4269	CDL	C38-C39-C40-C41
17	N	516	HEA	C2D-C3D-CAD-CBD
22	C	3270	CDL	CA3-CA4-CA6-OA8
22	C	3270	CDL	CB3-CB4-CB6-OB8
22	P	4270	CDL	CA3-CA4-CA6-OA8
22	P	4270	CDL	CB3-CB4-CB6-OB8
23	C	3264	PEK	C22-C23-C24-C25
23	C	3265	PEK	O03-C01-C02-C03
23	P	4264	PEK	O03-C01-C02-C03
23	P	4265	PEK	O03-C01-C02-C03
21	C	3271	CHD	C16-C17-C20-C22
21	P	4271	CHD	C16-C17-C20-C22
23	P	4264	PEK	C22-C21-O03-C01
18	A	3521	TGL	C25-C26-C27-C28
19	A	3524	PGV	C5-C6-C7-C8
22	C	3270	CDL	C12-C13-C14-C15
21	W	4060	CHD	C17-C20-C22-C23
18	N	4521	TGL	C25-C26-C27-C28
19	N	4524	PGV	C13-C14-C15-C16
18	N	4521	TGL	CA1-CA2-CA3-CA4
22	T	4269	CDL	C44-C45-C46-C47
21	C	3271	CHD	C16-C17-C20-C21
19	P	4267	PGV	C15-C16-C17-C18
22	G	3269	CDL	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
22	P	4270	CDL	C59-C60-C61-C62
22	P	4270	CDL	C84-C85-C86-C87
19	C	3267	PGV	C15-C16-C17-C18
22	C	3270	CDL	C84-C85-C86-C87
23	P	4265	PEK	C31-C32-C33-C34
19	A	3524	PGV	C2-C3-C4-C5
19	A	3524	PGV	C13-C14-C15-C16
19	A	3524	PGV	C31-C32-C33-C34
23	C	3265	PEK	C31-C32-C33-C34
27	M	3526	DMU	C34-C37-C40-C43
18	A	3521	TGL	CA1-CA2-CA3-CA4
22	G	3269	CDL	CB5-C51-C52-C53
22	T	4269	CDL	CB5-C51-C52-C53
22	G	3269	CDL	C44-C45-C46-C47
18	A	3522	TGL	C29-C30-C31-C32
18	N	4522	TGL	C29-C30-C31-C32
19	N	4524	PGV	C31-C32-C33-C34
27	Z	4526	DMU	C34-C37-C40-C43
19	A	3524	PGV	C03-C02-O01-C1
19	N	4524	PGV	C03-C02-O01-C1
18	A	3521	TGL	C16-C17-C18-C19
18	A	3522	TGL	CC2-CC3-CC4-CC5
18	N	4521	TGL	C16-C17-C18-C19
22	T	4269	CDL	C12-C13-C14-C15
18	A	3521	TGL	CC7-CC8-CC9-C15
18	N	4522	TGL	C33-C34-C35-C36
18	A	3522	TGL	C33-C34-C35-C36
18	N	4521	TGL	CC7-CC8-CC9-C15
21	J	3060	CHD	C17-C20-C22-C23
23	P	4264	PEK	C24-C25-C26-C27
22	G	3269	CDL	C24-C25-C26-C27
22	T	4269	CDL	C24-C25-C26-C27
19	P	4268	PGV	C2-C1-O01-C02
19	A	3524	PGV	C12-C13-C14-C15
19	N	4524	PGV	C12-C13-C14-C15
19	C	3268	PGV	C13-C14-C15-C16
23	C	3264	PEK	C24-C25-C26-C27
23	G	4263	PEK	C21-C22-C23-C24
23	C	3265	PEK	O12-C04-C05-N
23	T	3263	PEK	C21-C22-C23-C24
19	P	4268	PGV	C13-C14-C15-C16
22	G	3269	CDL	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
18	A	3521	TGL	C21-C20-CA9-CA8
19	A	3266	PGV	C31-C32-C33-C34
19	C	3268	PGV	C2-C1-O01-C02
22	P	4270	CDL	CA4-CA3-OA5-PA1
19	A	3266	PGV	C4-C5-C6-C7
19	N	4266	PGV	C31-C32-C33-C34
23	C	3265	PEK	C30-C31-C32-C33
27	M	3526	DMU	C19-C18-O16-C6
22	P	4270	CDL	C39-C40-C41-C42
22	T	4269	CDL	C58-C59-C60-C61
18	N	4521	TGL	C21-C20-CA9-CA8
23	P	4265	PEK	C30-C31-C32-C33
23	P	4265	PEK	C32-C33-C34-C35
22	G	3269	CDL	C58-C59-C60-C61
22	T	4269	CDL	C35-C36-C37-C38
25	O	4230	PSC	C4-C5-C6-C7
18	A	3521	TGL	OG1-CG1-CG2-CG3
18	N	4521	TGL	OG1-CG1-CG2-CG3
22	G	3269	CDL	CA3-CA4-CA6-OA8
22	T	4269	CDL	CA3-CA4-CA6-OA8
25	E	3230	PSC	C4-C5-C6-C7
25	E	3230	PSC	C14-C15-C16-C17
27	Z	4526	DMU	C28-C31-C34-C37
23	C	3264	PEK	C5-C6-C7-C8
23	C	3264	PEK	C9-C10-C11-C12
23	P	4264	PEK	C5-C6-C7-C8
23	P	4264	PEK	C9-C10-C11-C12
25	E	3230	PSC	C9-C10-C11-C12
25	O	4230	PSC	C9-C10-C11-C12
18	A	3521	TGL	CC5-CC6-CC7-CC8
19	N	4524	PGV	C26-C27-C28-C29
23	C	3265	PEK	C32-C33-C34-C35
19	N	4266	PGV	C4-C5-C6-C7
19	A	3524	PGV	O01-C02-C03-O11
19	C	3268	PGV	O01-C02-C03-O11
19	P	4268	PGV	O01-C02-C03-O11
22	C	3270	CDL	OA5-CA3-CA4-OA6
22	P	4270	CDL	OA5-CA3-CA4-OA6
18	A	3522	TGL	CC7-CC8-CC9-C15
19	A	3524	PGV	C26-C27-C28-C29
19	P	4267	PGV	C30-C31-C32-C33
22	C	3270	CDL	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
22	G	3269	CDL	C43-C44-C45-C46
22	C	3270	CDL	OB6-CB4-CB6-OB8
22	P	4270	CDL	OB6-CB4-CB6-OB8
25	O	4230	PSC	C14-C15-C16-C17
18	N	4522	TGL	CC7-CC8-CC9-C15
22	T	4269	CDL	C43-C44-C45-C46
19	P	4267	PGV	C31-C32-C33-C34
22	P	4270	CDL	C56-C57-C58-C59
22	C	3270	CDL	C1-CA2-OA2-PA1
22	C	3270	CDL	CA4-CA3-OA5-PA1
22	G	3269	CDL	CB4-CB3-OB5-PB2
22	P	4270	CDL	C1-CA2-OA2-PA1
22	T	4269	CDL	CB4-CB3-OB5-PB2
23	P	4264	PEK	C26-C27-C28-C29
19	C	3267	PGV	C31-C32-C33-C34
23	C	3265	PEK	C22-C23-C24-C25
23	C	3264	PEK	C26-C27-C28-C29
25	O	4230	PSC	C15-C16-C17-C18
22	C	3270	CDL	C56-C57-C58-C59
22	G	3269	CDL	C21-C22-C23-C24
25	E	3230	PSC	C15-C16-C17-C18
22	C	3270	CDL	OB5-CB3-CB4-CB6
22	P	4270	CDL	OB5-CB3-CB4-CB6
22	T	4269	CDL	C21-C22-C23-C24
23	G	4263	PEK	C28-C29-C30-C31
23	G	4263	PEK	C2-C3-C4-C5
19	N	4266	PGV	C30-C31-C32-C33
18	N	4521	TGL	CC5-CC6-CC7-CC8
25	O	4230	PSC	C04-C05-N-C08
22	C	3270	CDL	C38-C39-C40-C41
23	T	3263	PEK	C28-C29-C30-C31
19	C	3267	PGV	C23-C24-C25-C26
25	O	4230	PSC	C03-C02-O01-C1
19	C	3267	PGV	C30-C31-C32-C33
19	P	4268	PGV	C11-C10-C9-C8
22	G	3269	CDL	CB3-CB4-CB6-OB8
25	E	3230	PSC	O03-C01-C02-C03
25	O	4230	PSC	O03-C01-C02-C03
19	A	3266	PGV	C30-C31-C32-C33
23	P	4265	PEK	C22-C23-C24-C25
22	C	3270	CDL	OA6-CA4-CA6-OA8
22	G	3269	CDL	OA6-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
22	P	4270	CDL	OA6-CA4-CA6-OA8
22	T	4269	CDL	OA6-CA4-CA6-OA8
23	G	4263	PEK	O03-C01-C02-O01
23	T	3263	PEK	O03-C01-C02-O01
25	E	3230	PSC	O03-C01-C02-O01
25	O	4230	PSC	O03-C01-C02-O01
18	A	3523	TGL	C18-C19-C33-C34
19	C	3268	PGV	C11-C10-C9-C8
22	G	3269	CDL	C54-C55-C56-C57
25	O	4230	PSC	C27-C28-C29-C30
22	P	4270	CDL	C38-C39-C40-C41
27	M	3526	DMU	C28-C31-C34-C37
18	A	3522	TGL	OB1-CB1-OG2-CG2
18	Q	4523	TGL	C18-C19-C33-C34
22	G	3269	CDL	CB2-OB2-PB2-OB5
22	T	4269	CDL	CB2-OB2-PB2-OB5
23	G	4263	PEK	C04-O12-P-O11
23	T	3263	PEK	C04-O12-P-O11
25	E	3230	PSC	C04-O12-P-O11
22	T	4269	CDL	C54-C55-C56-C57
19	C	3267	PGV	C02-C03-O11-P
19	P	4267	PGV	C02-C03-O11-P
19	A	3524	PGV	C03-O11-P-O14
19	N	4524	PGV	C03-O11-P-O14
22	C	3270	CDL	CA3-OA5-PA1-OA3
22	C	3270	CDL	CB2-OB2-PB2-OB3
22	C	3270	CDL	CB2-OB2-PB2-OB4
22	G	3269	CDL	CA2-OA2-PA1-OA4
22	P	4270	CDL	CA3-OA5-PA1-OA3
22	P	4270	CDL	CB2-OB2-PB2-OB3
22	P	4270	CDL	CB2-OB2-PB2-OB4
22	T	4269	CDL	CA2-OA2-PA1-OA4
23	C	3265	PEK	C04-O12-P-O13
23	G	4263	PEK	C04-O12-P-O14
23	T	3263	PEK	C04-O12-P-O14
25	E	3230	PSC	C04-O12-P-O13
25	O	4230	PSC	C04-O12-P-O13
25	O	4230	PSC	C04-C05-N-C07
25	E	3230	PSC	C27-C28-C29-C30
19	C	3268	PGV	C01-C02-C03-O11
18	N	4522	TGL	C25-C26-C27-C28
23	P	4265	PEK	O12-C04-C05-N

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Mol	Chain	Res	Type	Atoms
18	A	3522	TGL	C25-C26-C27-C28
23	C	3265	PEK	C17-C18-C19-C20
19	P	4267	PGV	C23-C24-C25-C26
18	A	3522	TGL	CB2-CB1-OG2-CG2
23	P	4265	PEK	C17-C18-C19-C20
23	T	3263	PEK	C2-C3-C4-C5
18	N	4522	TGL	OB1-CB1-OG2-CG2
19	N	4524	PGV	O01-C02-C03-O11
22	C	3270	CDL	OB5-CB3-CB4-OB6
22	P	4270	CDL	OB5-CB3-CB4-OB6
22	C	3270	CDL	C34-C35-C36-C37
25	E	3230	PSC	C04-C05-N-C07
25	O	4230	PSC	C04-C05-N-C06
23	C	3264	PEK	C17-C18-C19-C20
22	T	4269	CDL	CB3-CB4-CB6-OB8
23	C	3264	PEK	O03-C01-C02-O01
23	C	3265	PEK	O03-C01-C02-O01
23	P	4264	PEK	O03-C01-C02-O01
23	P	4265	PEK	O03-C01-C02-O01
22	P	4270	CDL	C31-C32-C33-C34
19	N	4266	PGV	C25-C26-C27-C28
22	P	4270	CDL	C34-C35-C36-C37
19	A	3266	PGV	C25-C26-C27-C28
22	C	3270	CDL	C31-C32-C33-C34
25	E	3230	PSC	C04-C05-N-C06
25	E	3230	PSC	C04-C05-N-C08
23	P	4264	PEK	C17-C18-C19-C20
18	N	4522	TGL	CB4-CB5-CB6-CB7
19	C	3267	PGV	C20-C21-C22-C23
19	P	4267	PGV	C20-C21-C22-C23
22	G	3269	CDL	C84-C85-C86-C87
25	E	3230	PSC	C03-C02-O01-C1
19	P	4268	PGV	C01-C02-C03-O11
19	P	4268	PGV	C3-C4-C5-C6
18	N	4522	TGL	C13-C14-C29-C30
19	P	4268	PGV	C4-C5-C6-C7
22	P	4270	CDL	C42-C43-C44-C45
18	A	3522	TGL	CB4-CB5-CB6-CB7
18	A	3522	TGL	C13-C14-C29-C30
23	G	4263	PEK	C33-C34-C35-C36
18	N	4522	TGL	CB2-CB1-OG2-CG2
23	G	4263	PEK	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
23	T	3263	PEK	C33-C34-C35-C36
18	N	4521	TGL	C21-C22-C23-C24
23	T	3263	PEK	C24-C25-C26-C27
18	A	3523	TGL	C15-C16-C17-C18
23	P	4264	PEK	C25-C26-C27-C28
19	C	3268	PGV	C3-C4-C5-C6
23	C	3264	PEK	C25-C26-C27-C28
23	T	3263	PEK	C14-C15-C16-C17
18	Q	4523	TGL	CB9-C10-C11-C12
22	P	4270	CDL	C44-C45-C46-C47
22	C	3270	CDL	C42-C43-C44-C45
23	P	4264	PEK	C31-C32-C33-C34
22	T	4269	CDL	C84-C85-C86-C87
23	T	3263	PEK	C35-C36-C37-C38
18	Q	4523	TGL	C15-C16-C17-C18
22	C	3270	CDL	C44-C45-C46-C47
23	T	3263	PEK	C32-C33-C34-C35
23	P	4264	PEK	C3-C4-C5-C6
21	J	3060	CHD	C22-C23-C24-O25
23	C	3264	PEK	C31-C32-C33-C34
23	C	3264	PEK	C3-C4-C5-C6
17	A	515	HEA	CAD-CBD-CGD-O1D
21	W	4060	CHD	C22-C23-C24-O25
18	A	3521	TGL	C21-C22-C23-C24
19	A	3524	PGV	C21-C22-C23-C24
18	Q	4523	TGL	C33-C34-C35-C36
23	G	4263	PEK	C32-C33-C34-C35
23	G	4263	PEK	C24-C25-C26-C27
17	N	516	HEA	CAA-CBA-CGA-O1A
21	O	3085	CHD	C22-C23-C24-O25
17	N	515	HEA	CAD-CBD-CGD-O1D
19	C	3267	PGV	C05-C04-O12-P
21	B	4085	CHD	C22-C23-C24-O25
18	A	3523	TGL	C33-C34-C35-C36
17	A	516	HEA	CAA-CBA-CGA-O1A
18	N	4521	TGL	CB1-CB2-CB3-CB4
19	C	3268	PGV	C4-C5-C6-C7
22	T	4269	CDL	C32-C33-C34-C35
19	N	4524	PGV	C21-C22-C23-C24
22	P	4270	CDL	C54-C55-C56-C57
23	P	4264	PEK	C28-C29-C30-C31
22	G	3269	CDL	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
23	G	4263	PEK	C35-C36-C37-C38
19	C	3268	PGV	C28-C29-C30-C31
19	P	4268	PGV	C28-C29-C30-C31
17	N	516	HEA	CAA-CBA-CGA-O2A
19	A	3266	PGV	C9-C10-C11-C12
19	N	4266	PGV	C9-C10-C11-C12
23	C	3265	PEK	C26-C27-C28-C29
23	G	4263	PEK	C6-C7-C8-C9
23	T	3263	PEK	C6-C7-C8-C9
22	P	4270	CDL	C43-C44-C45-C46
17	A	516	HEA	CAA-CBA-CGA-O2A
21	W	4060	CHD	C22-C23-C24-O26
18	A	3523	TGL	CB9-C10-C11-C12
22	P	4270	CDL	C33-C34-C35-C36
21	J	3060	CHD	C22-C23-C24-O26
18	Q	4523	TGL	C11-C10-CB9-CB8
22	C	3270	CDL	C54-C55-C56-C57
21	C	3271	CHD	C22-C23-C24-O25
21	C	3271	CHD	C22-C23-C24-O26
22	C	3270	CDL	C33-C34-C35-C36
17	A	515	HEA	CAD-CBD-CGD-O2D
17	N	515	HEA	CAD-CBD-CGD-O2D
21	P	4271	CHD	C22-C23-C24-O25
22	C	3270	CDL	C43-C44-C45-C46
23	P	4265	PEK	C26-C27-C28-C29
21	P	4271	CHD	C22-C23-C24-O26
18	A	3522	TGL	OG1-CA1-CA2-CA3
19	A	3266	PGV	O03-C19-C20-C21
19	P	4267	PGV	C05-C04-O12-P
22	C	3270	CDL	C76-C77-C78-C79
25	O	4230	PSC	C31-C32-C33-C34
19	P	4268	PGV	C22-C23-C24-C25
22	P	4270	CDL	C76-C77-C78-C79
21	B	4085	CHD	C22-C23-C24-O26
19	C	3267	PGV	C29-C30-C31-C32
18	A	3523	TGL	OG1-CA1-CA2-CA3
23	C	3265	PEK	C3-C4-C5-C6
21	O	3085	CHD	C22-C23-C24-O26
19	C	3268	PGV	C31-C32-C33-C34
18	N	4522	TGL	OG1-CA1-CA2-CA3
19	C	3268	PGV	C22-C23-C24-C25
23	C	3264	PEK	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
18	Q	4523	TGL	OG1-CA1-CA2-CA3
22	P	4270	CDL	C15-C16-C17-C18
23	C	3264	PEK	C28-C29-C30-C31
22	T	4269	CDL	C53-C54-C55-C56
23	T	3263	PEK	C3-C4-C5-C6
25	E	3230	PSC	C31-C32-C33-C34
19	N	4266	PGV	O03-C19-C20-C21
19	P	4268	PGV	C31-C32-C33-C34
19	P	4267	PGV	C29-C30-C31-C32
19	A	3524	PGV	O01-C1-C2-C3
25	O	4230	PSC	O03-C19-C20-C21
22	C	3270	CDL	C15-C16-C17-C18
18	A	3523	TGL	OG3-CC1-CC2-CC3
23	C	3264	PEK	O01-C1-C2-C3
23	P	4264	PEK	C27-C28-C29-C30
18	Q	4523	TGL	OG3-CC1-CC2-CC3
19	N	4524	PGV	O01-C1-C2-C3
19	C	3267	PGV	C9-C10-C11-C12
19	C	3267	PGV	C11-C12-C13-C14
19	C	3268	PGV	C9-C10-C11-C12
19	N	4266	PGV	C11-C12-C13-C14
19	P	4267	PGV	C11-C12-C13-C14
23	G	4263	PEK	C3-C4-C5-C6
23	P	4265	PEK	C3-C4-C5-C6
21	C	3525	CHD	C22-C23-C24-O26
21	P	4525	CHD	C22-C23-C24-O26
25	E	3230	PSC	O03-C19-C20-C21
17	A	516	HEA	CAD-CBD-CGD-O2D
18	N	4522	TGL	OG2-CB1-CB2-CB3
22	G	3269	CDL	C53-C54-C55-C56
23	P	4264	PEK	O01-C1-C2-C3
18	A	3522	TGL	OG2-CB1-CB2-CB3
17	A	516	HEA	CAD-CBD-CGD-O1D
17	N	516	HEA	CAD-CBD-CGD-O2D
21	P	4525	CHD	C22-C23-C24-O25
19	P	4268	PGV	C9-C10-C11-C12
25	E	3230	PSC	C7-C8-C9-C10
25	O	4230	PSC	C7-C8-C9-C10
17	N	516	HEA	CAD-CBD-CGD-O1D
18	A	3521	TGL	CB1-CB2-CB3-CB4
22	G	3269	CDL	C78-C79-C80-C81
21	C	3525	CHD	C22-C23-C24-O25

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Mol	Chain	Res	Type	Atoms
22	C	3270	CDL	C52-C51-CB5-OB6
18	A	3521	TGL	OG3-CC1-CC2-CC3
18	A	3523	TGL	OG2-CB1-CB2-CB3
18	Q	4523	TGL	OG2-CB1-CB2-CB3
22	G	3269	CDL	C11-C12-C13-C14
23	G	4263	PEK	C30-C31-C32-C33
18	N	4521	TGL	OG3-CC1-CC2-CC3
22	C	3270	CDL	C12-C11-CA5-OA6
22	P	4270	CDL	C12-C11-CA5-OA6
22	P	4270	CDL	C52-C51-CB5-OB6
25	O	4230	PSC	O01-C1-C2-C3
22	T	4269	CDL	C11-C12-C13-C14
19	A	3266	PGV	C11-C12-C13-C14
19	P	4267	PGV	C9-C10-C11-C12
25	E	3230	PSC	O01-C1-C2-C3
19	A	3524	PGV	C3-C4-C5-C6
19	N	4524	PGV	C3-C4-C5-C6
23	T	3263	PEK	O01-C1-C2-C3
25	O	4230	PSC	O02-C1-C2-C3
23	T	3263	PEK	C30-C31-C32-C33
17	N	516	HEA	C26-C15-C16-C17
22	T	4269	CDL	C78-C79-C80-C81
25	E	3230	PSC	O02-C1-C2-C3
23	G	4263	PEK	O01-C1-C2-C3
23	C	3264	PEK	O02-C1-C2-C3
25	E	3230	PSC	O04-C19-C20-C21
23	C	3265	PEK	C24-C25-C26-C27
19	N	4524	PGV	O02-C1-C2-C3
18	A	3523	TGL	C11-C10-CB9-CB8
25	O	4230	PSC	O04-C19-C20-C21
22	C	3270	CDL	C12-C11-CA5-OA7
23	P	4264	PEK	O02-C1-C2-C3
23	P	4265	PEK	C24-C25-C26-C27
22	P	4270	CDL	C12-C11-CA5-OA7
18	A	3523	TGL	OB1-CB1-CB2-CB3
17	A	516	HEA	C26-C15-C16-C17
22	C	3270	CDL	C24-C25-C26-C27
19	N	4524	PGV	C28-C29-C30-C31
19	A	3524	PGV	O03-C19-C20-C21
19	N	4524	PGV	O03-C19-C20-C21
18	Q	4523	TGL	OB1-CB1-CB2-CB3
17	A	515	HEA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
22	T	4269	CDL	C55-C56-C57-C58
22	P	4270	CDL	C32-C31-CA7-OA8
19	A	3524	PGV	O02-C1-C2-C3
22	C	3270	CDL	C41-C42-C43-C44
25	E	3230	PSC	C6-C7-C8-C9
22	P	4270	CDL	C32-C31-CA7-OA9
23	G	4263	PEK	O02-C1-C2-C3
18	A	3521	TGL	OG2-CB1-CB2-CB3
18	N	4521	TGL	OG2-CB1-CB2-CB3
22	C	3270	CDL	C32-C31-CA7-OA8
22	P	4270	CDL	C24-C25-C26-C27
23	T	3263	PEK	O02-C1-C2-C3

There are no ring outliers.

33 monomers are involved in 278 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	3522	TGL	25	0
23	P	4265	PEK	4	0
23	T	3263	PEK	8	0
23	P	4264	PEK	4	0
17	N	515	HEA	3	0
18	A	3523	TGL	6	0
21	W	4060	CHD	3	0
19	A	3524	PGV	7	0
22	G	3269	CDL	17	0
22	P	4270	CDL	20	0
23	G	4263	PEK	6	0
18	N	4521	TGL	24	0
19	P	4268	PGV	3	0
17	A	515	HEA	2	0
25	E	3230	PSC	12	0
19	N	4524	PGV	6	0
23	C	3264	PEK	4	0
17	N	516	HEA	3	0
21	P	4271	CHD	2	0
19	C	3267	PGV	6	0
22	C	3270	CDL	23	0
23	C	3265	PEK	9	0
18	A	3521	TGL	16	0
21	B	4085	CHD	1	0
18	Q	4523	TGL	6	0

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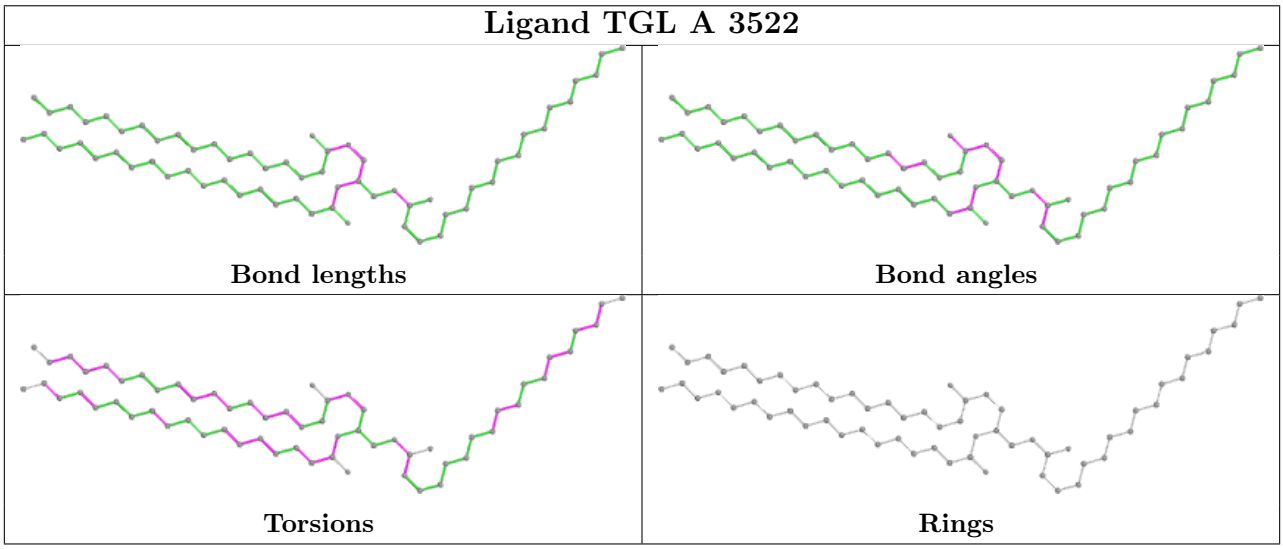
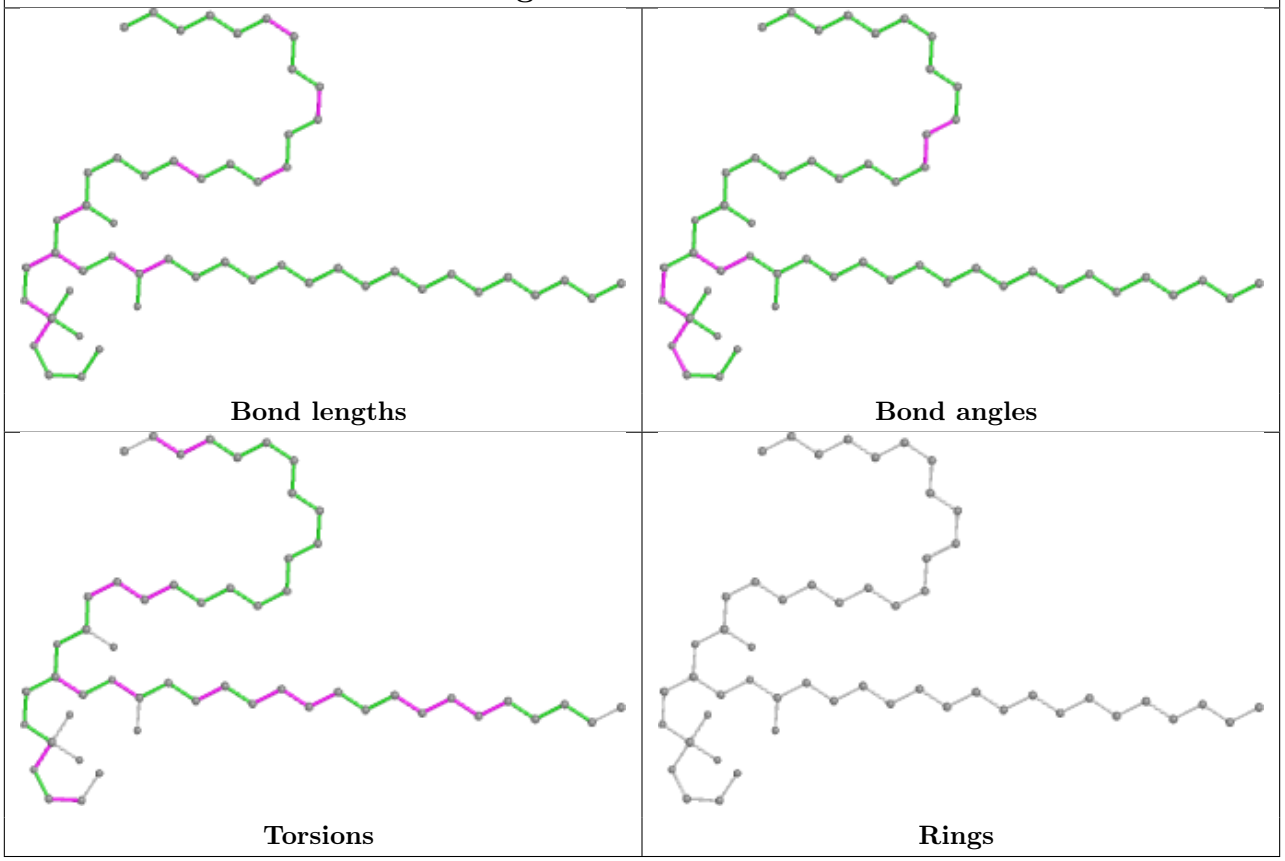
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	J	3060	CHD	3	0
21	C	3271	CHD	4	0
22	T	4269	CDL	20	0
25	O	4230	PSC	11	0
19	C	3268	PGV	3	0
19	P	4267	PGV	3	0
18	N	4522	TGL	17	0
17	A	516	HEA	3	0

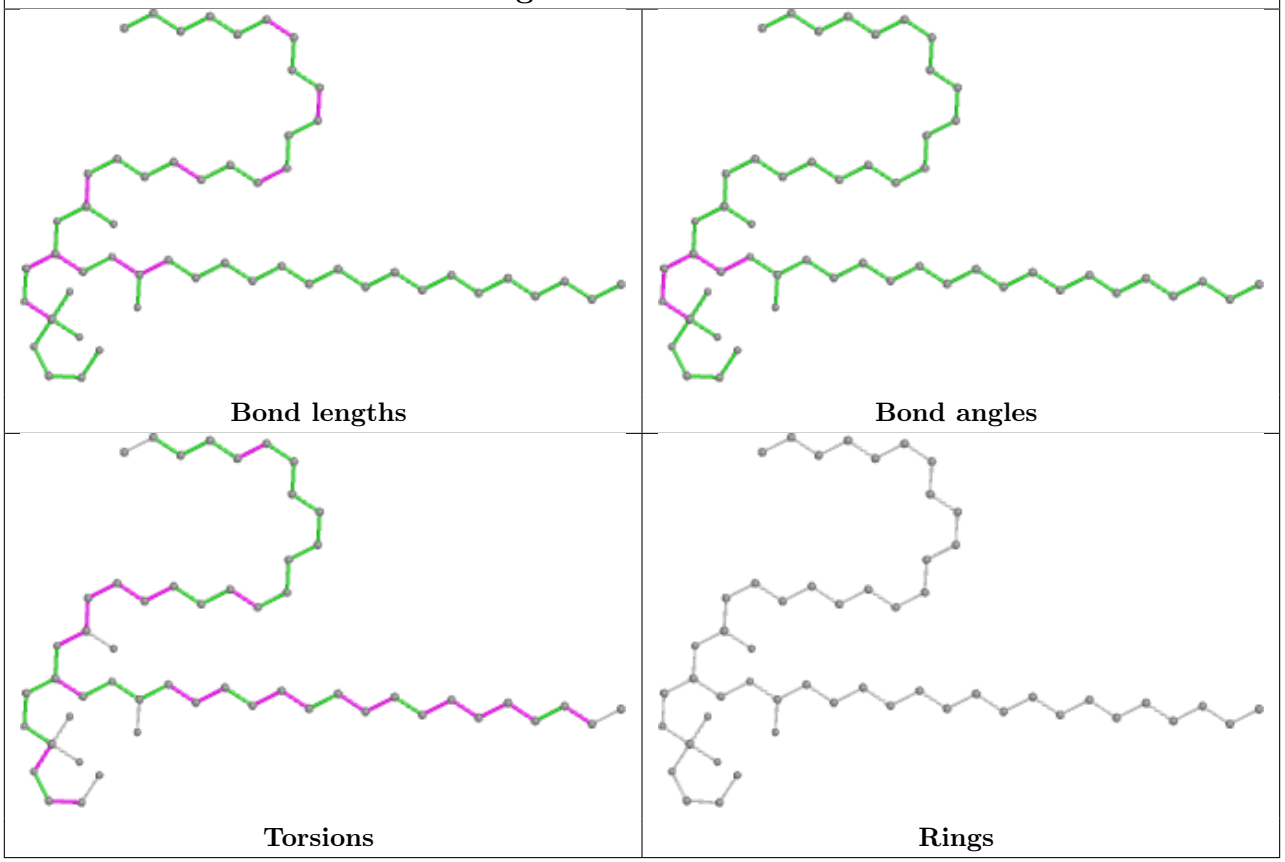
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



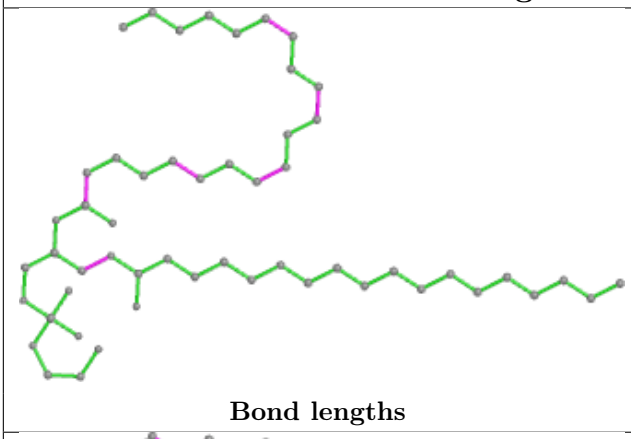
Ligand PEK P 4265



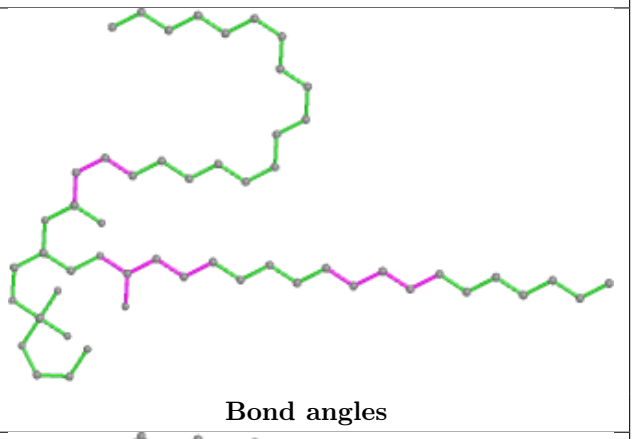
Ligand PEK T 3263



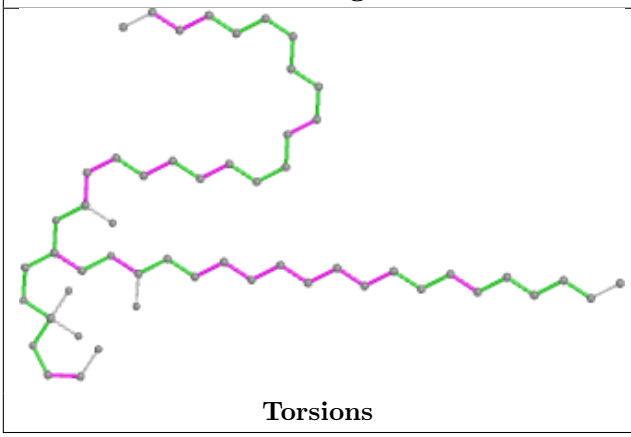
Ligand PEK P 4264



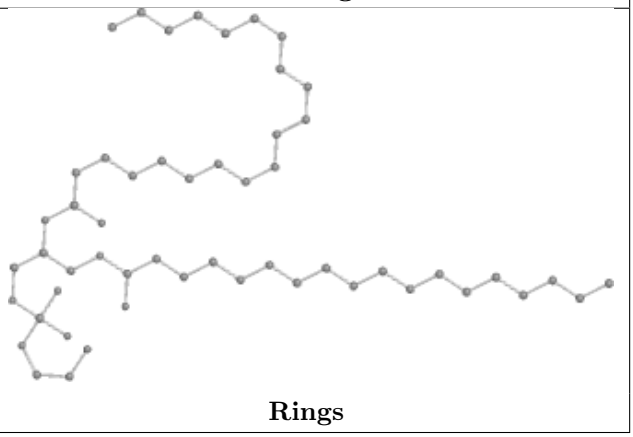
Bond lengths



Bond angles

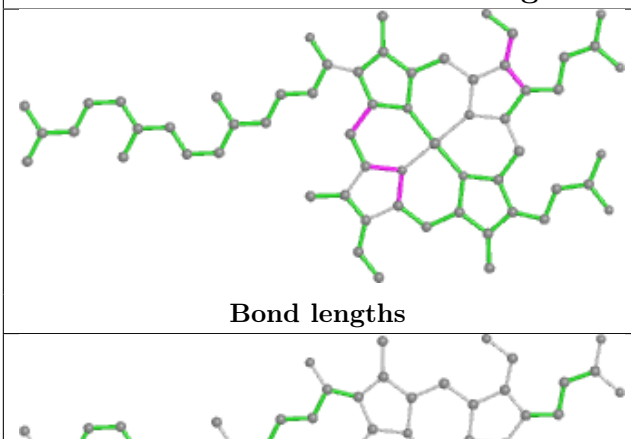


Torsions

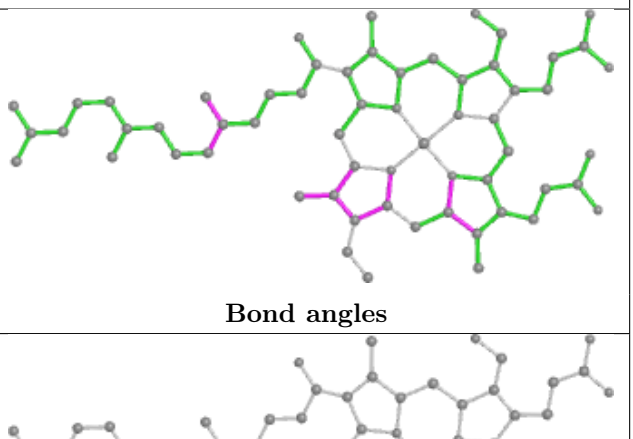


Rings

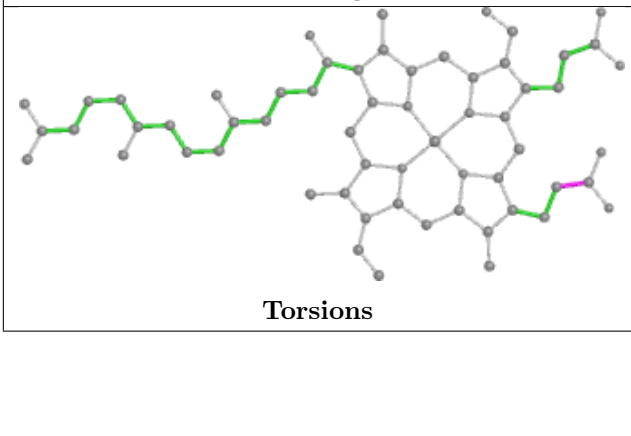
Ligand HEA N 515



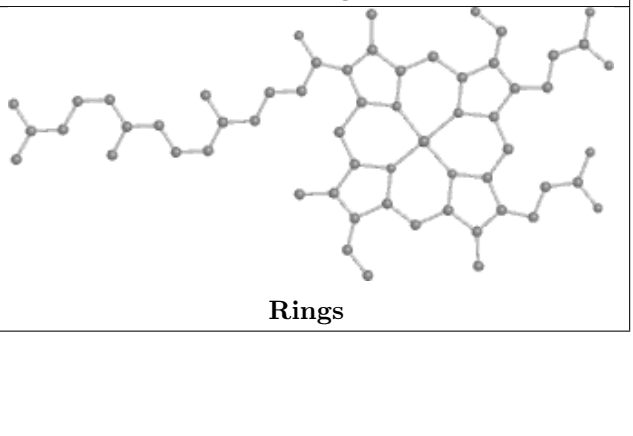
Bond lengths



Bond angles

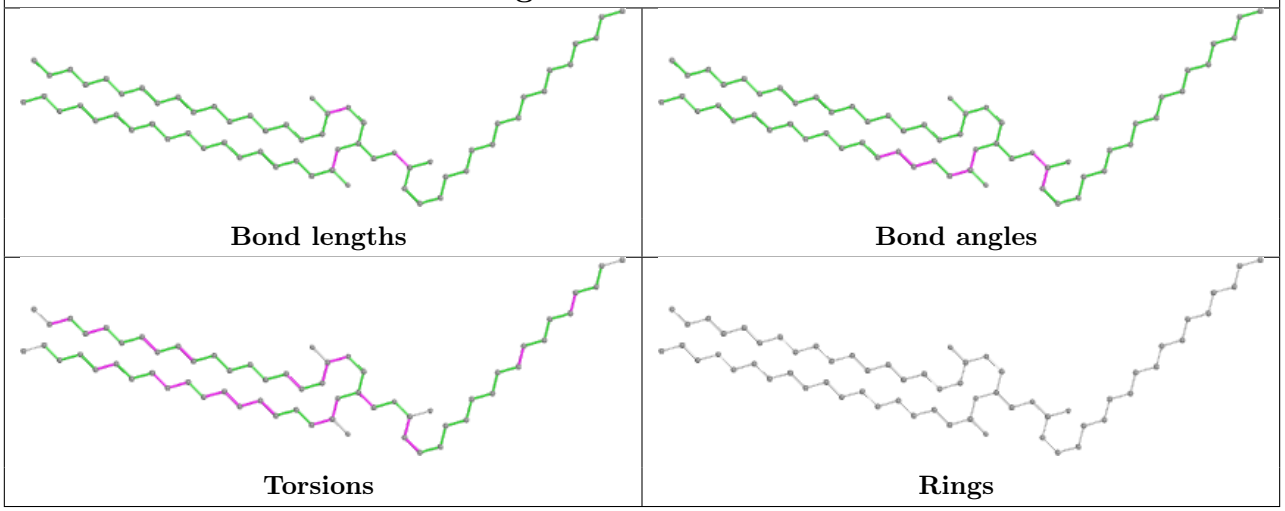


Torsions

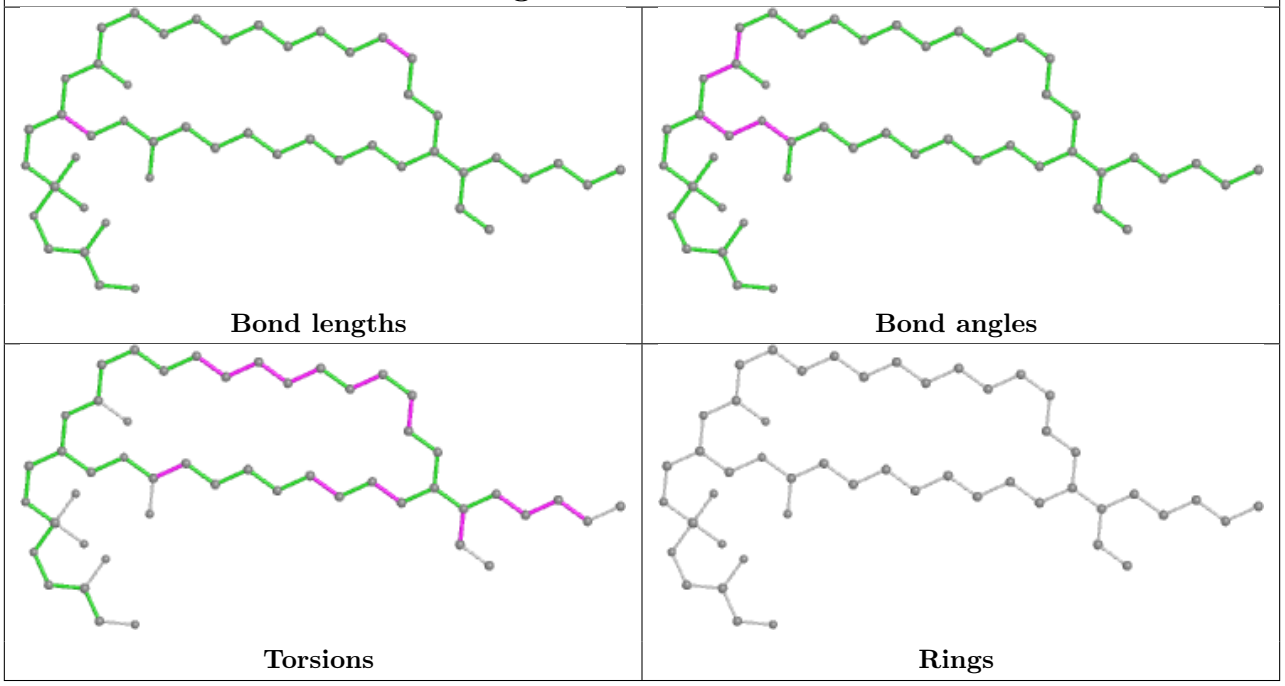


Rings

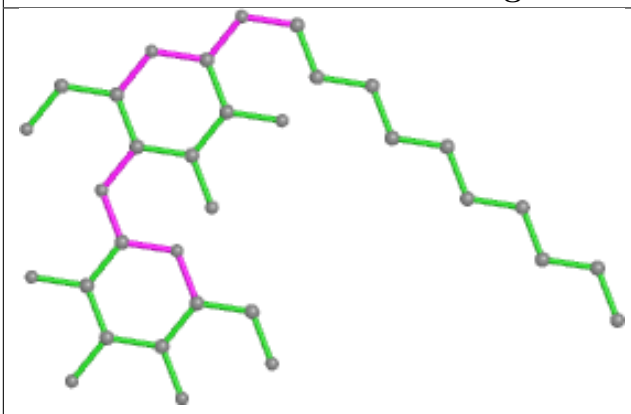
Ligand TGL A 3523



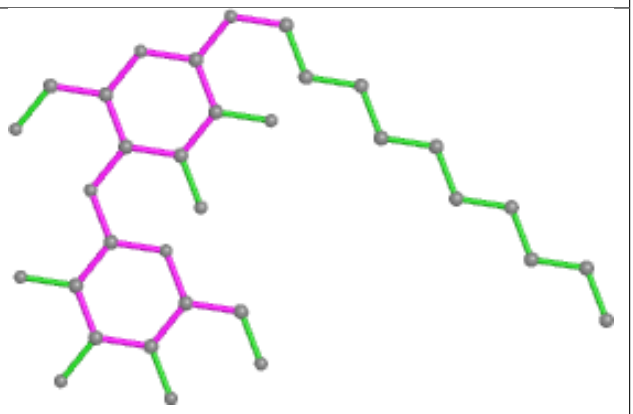
Ligand PGV N 4266



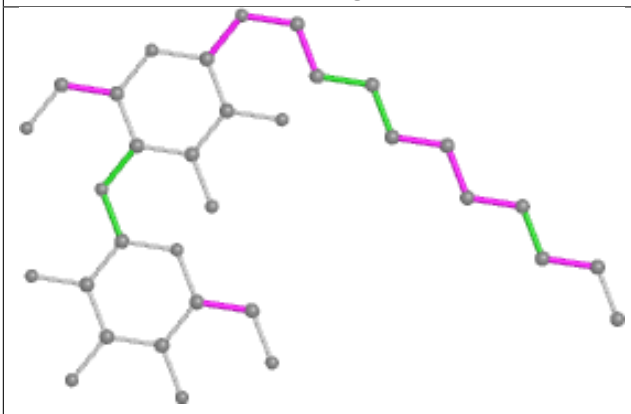
Ligand DMU M 3526



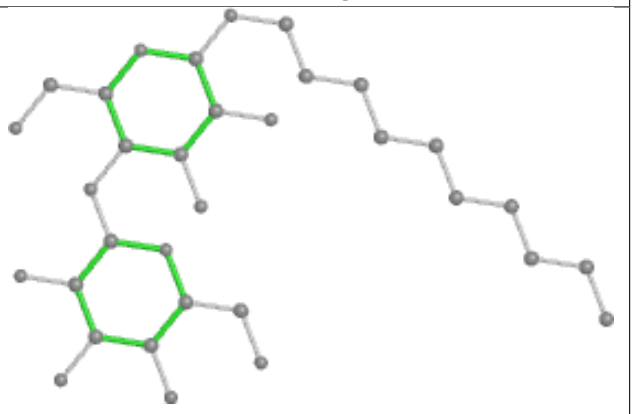
Bond lengths



Bond angles

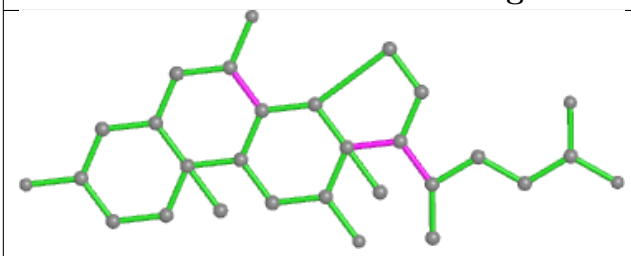


Torsions

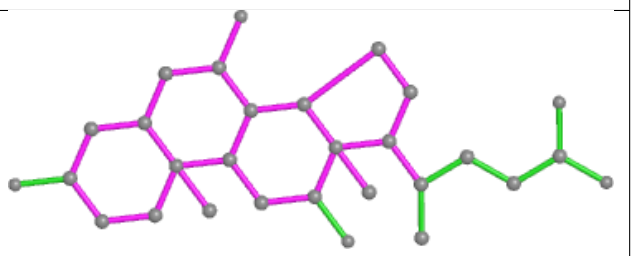


Rings

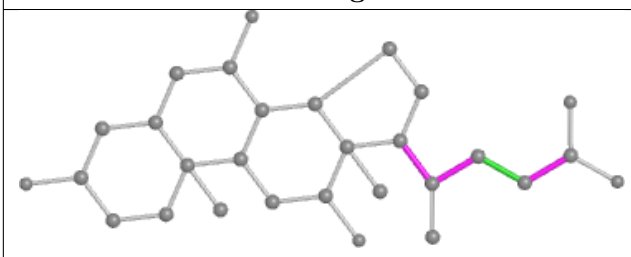
Ligand CHD W 4060



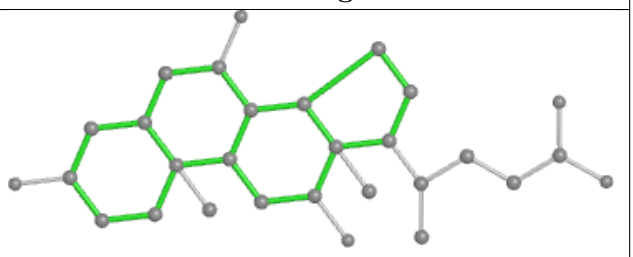
Bond lengths



Bond angles

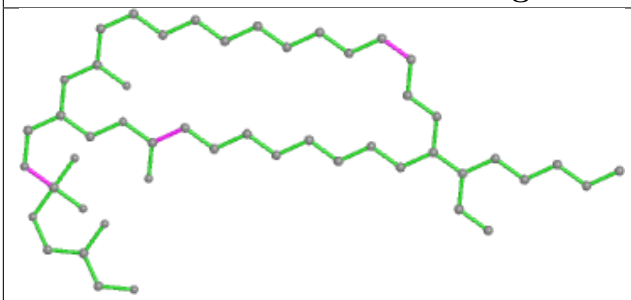


Torsions

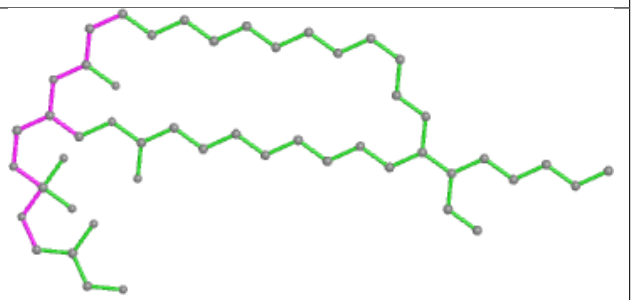


Rings

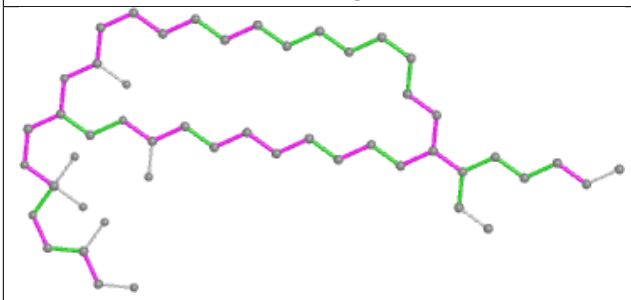
Ligand PGV A 3524



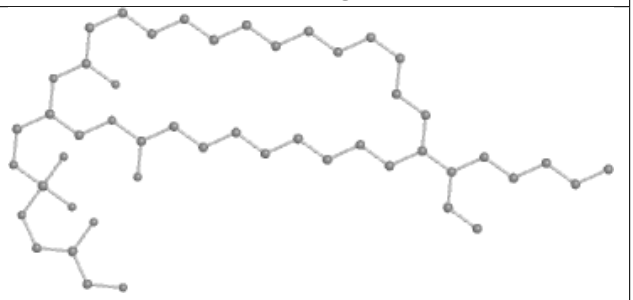
Bond lengths



Bond angles

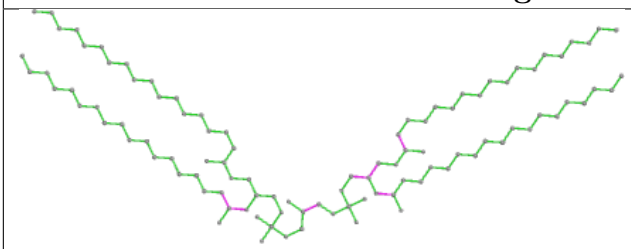


Torsions

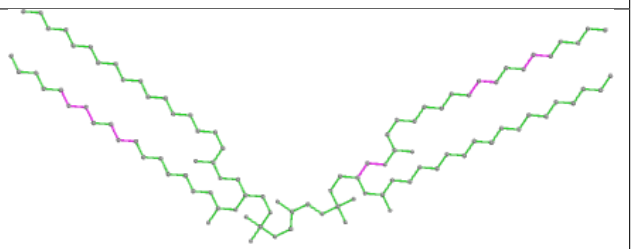


Rings

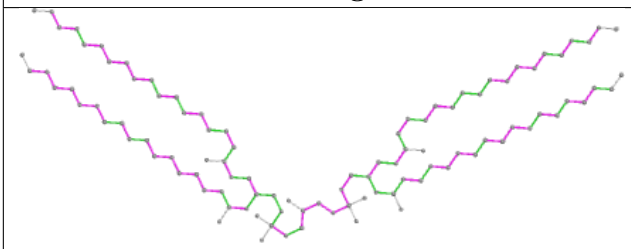
Ligand CDL G 3269



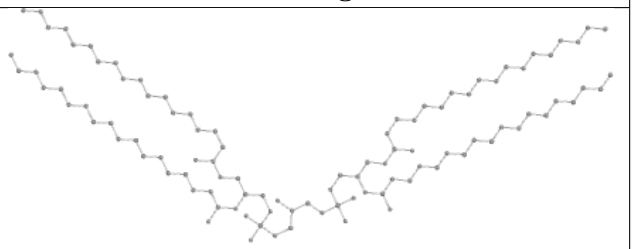
Bond lengths



Bond angles

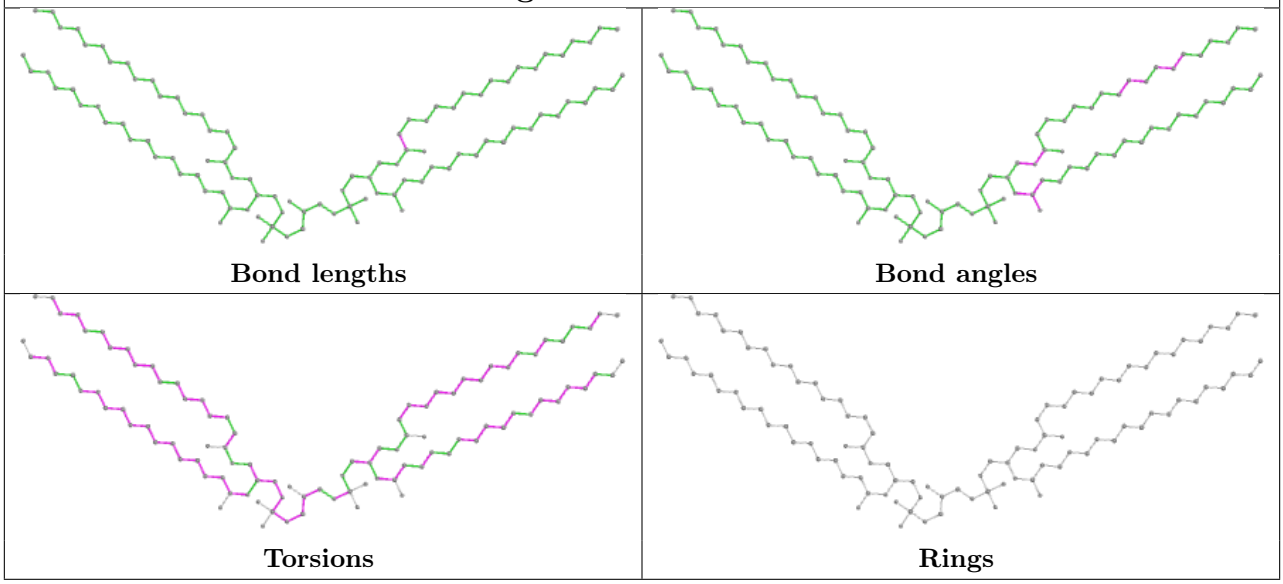


Torsions

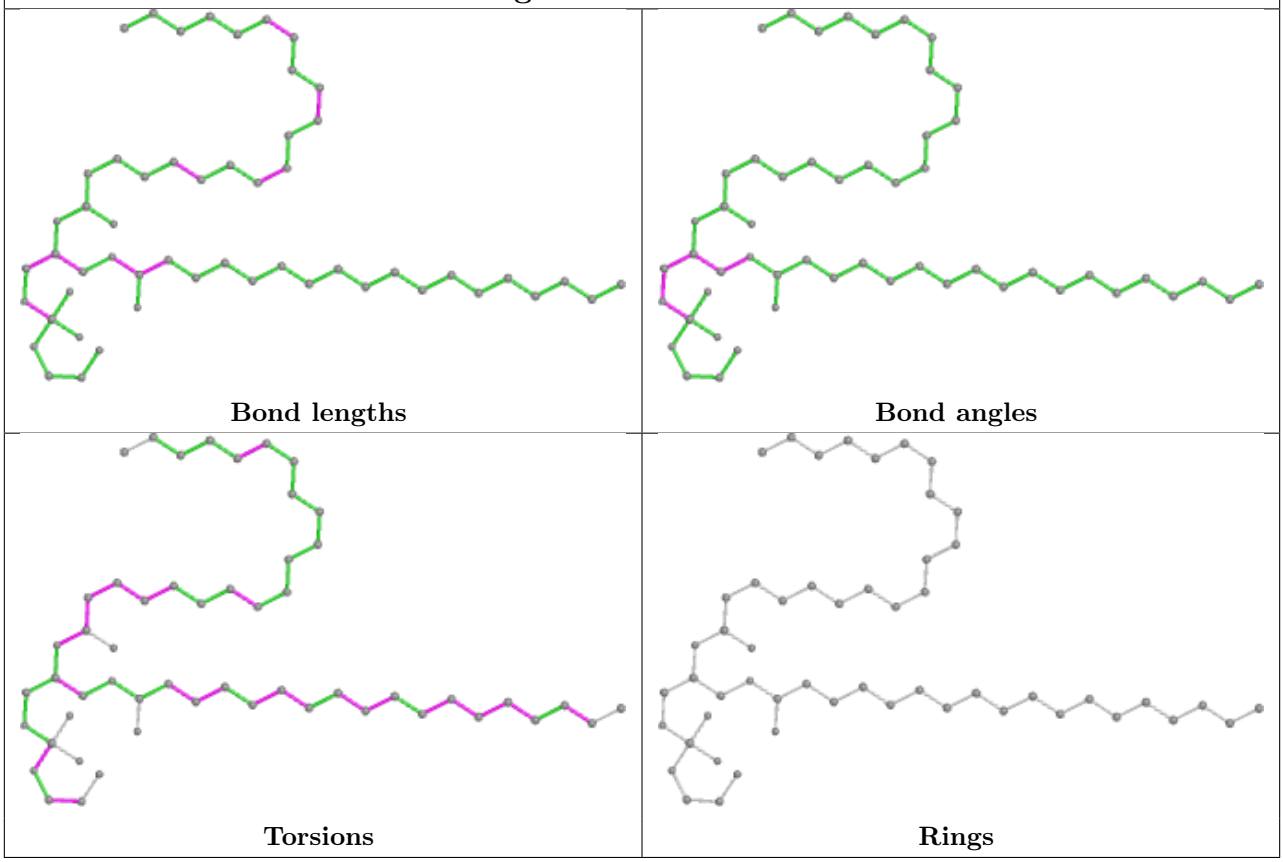


Rings

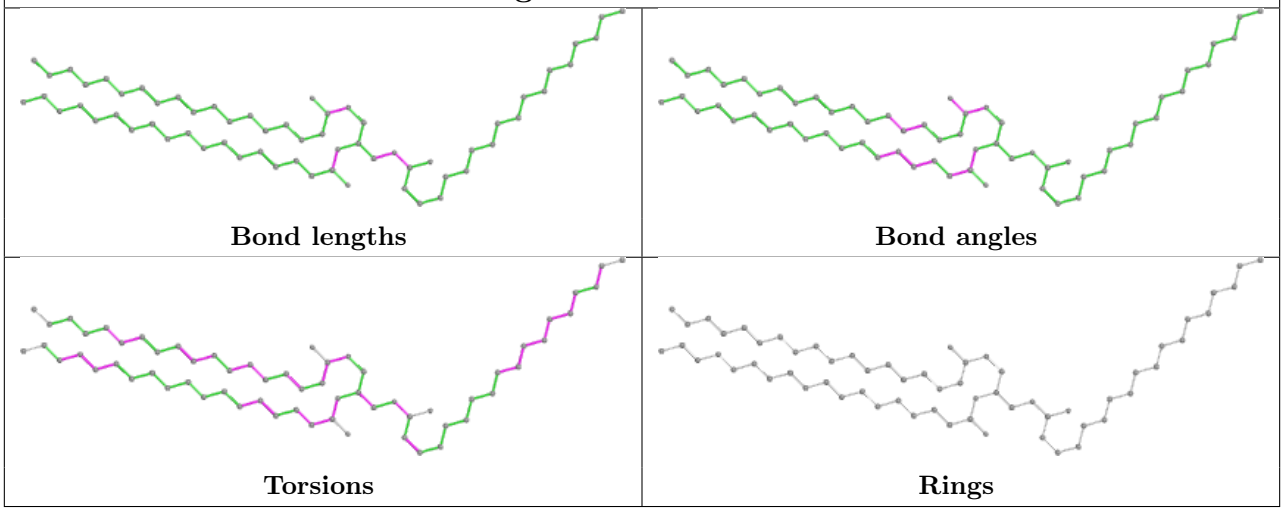
Ligand CDL P 4270



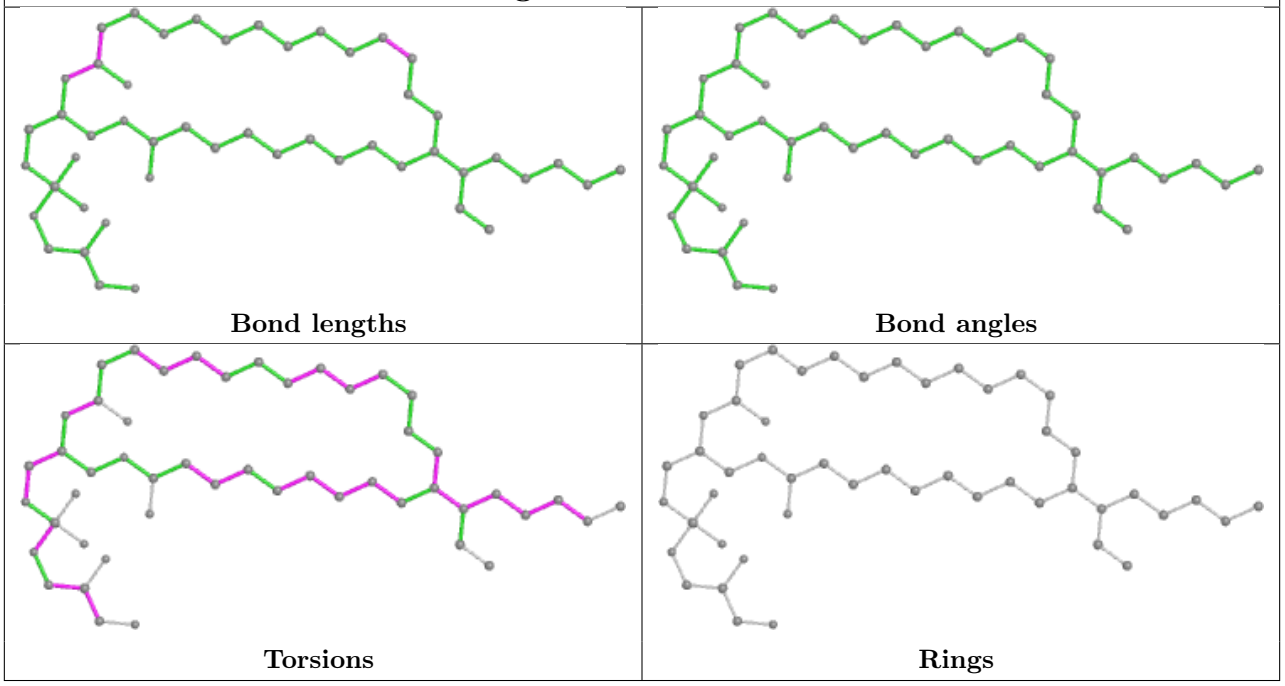
Ligand PEK G 4263



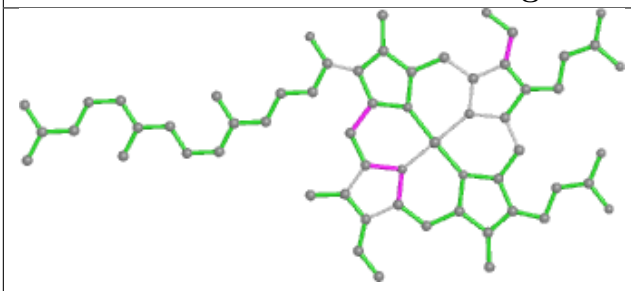
Ligand TGL N 4521



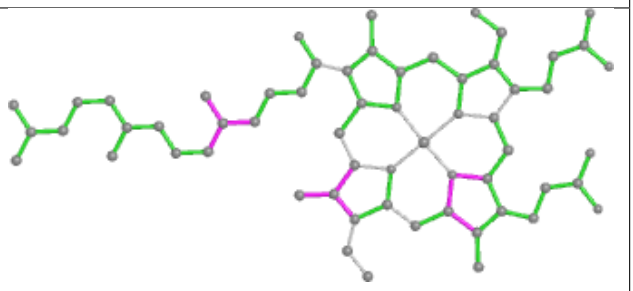
Ligand PGV P 4268



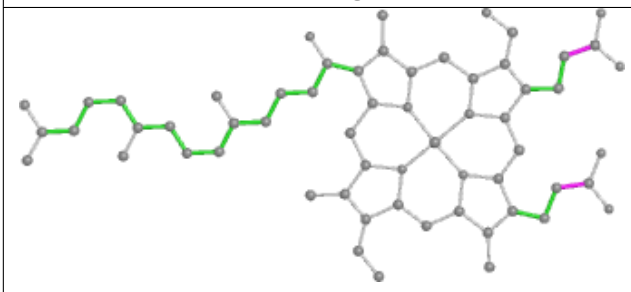
Ligand HEA A 515



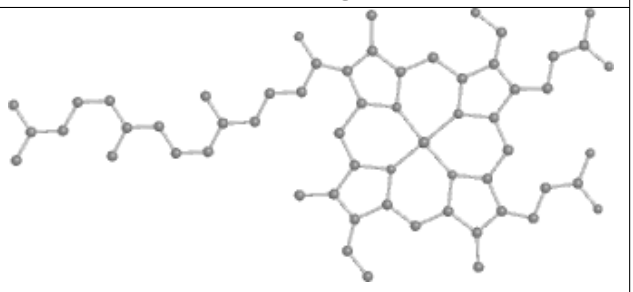
Bond lengths



Bond angles

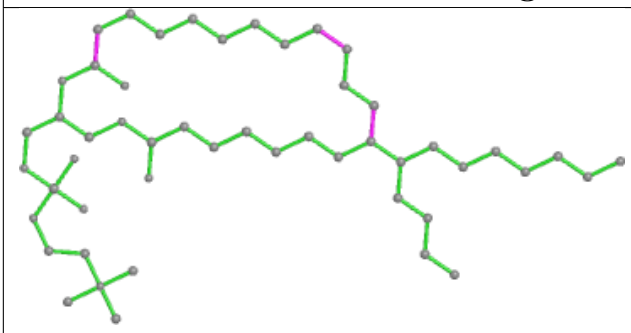


Torsions

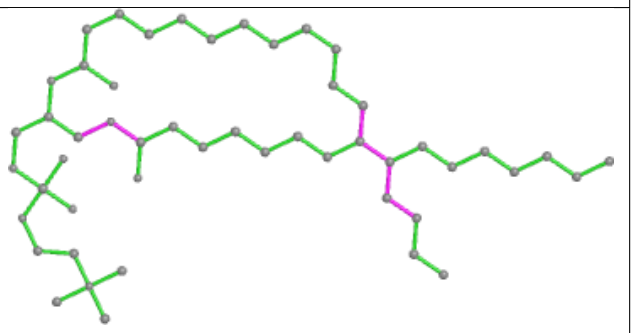


Rings

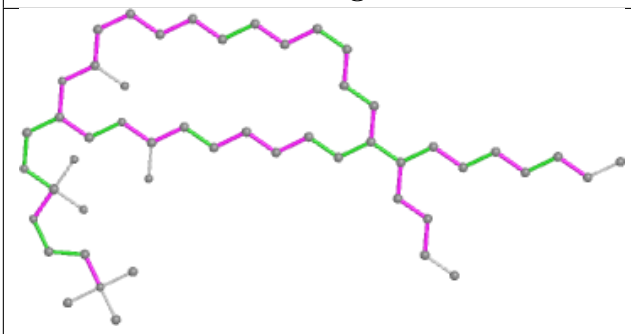
Ligand PSC E 3230



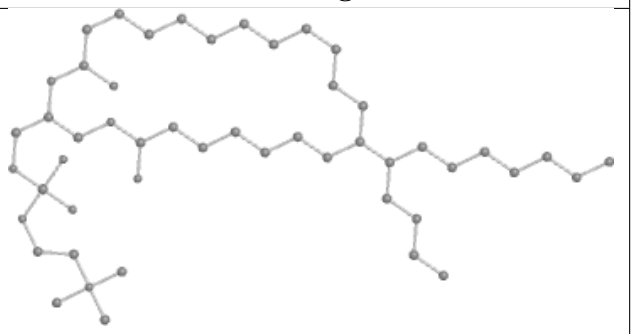
Bond lengths



Bond angles

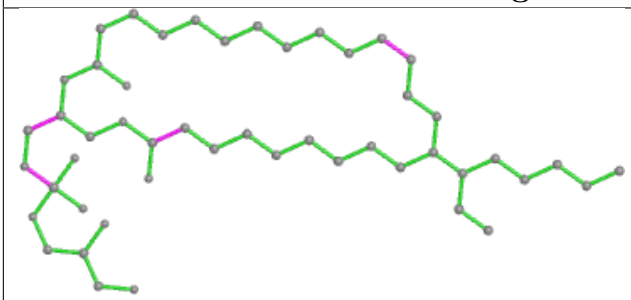


Torsions

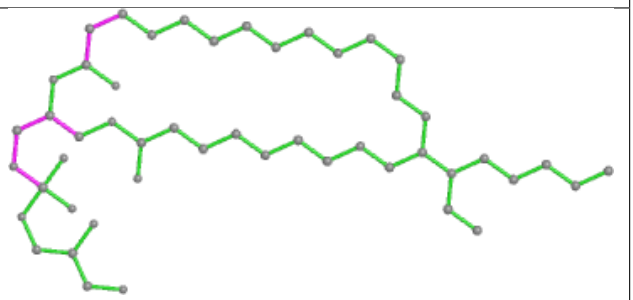


Rings

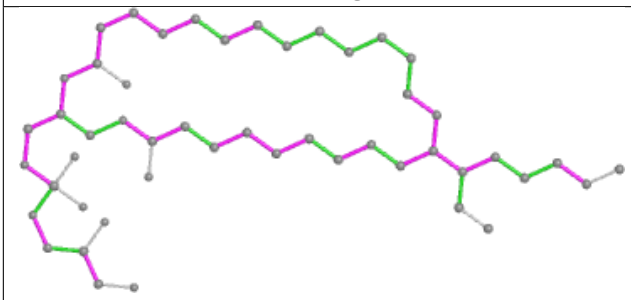
Ligand PGV N 4524



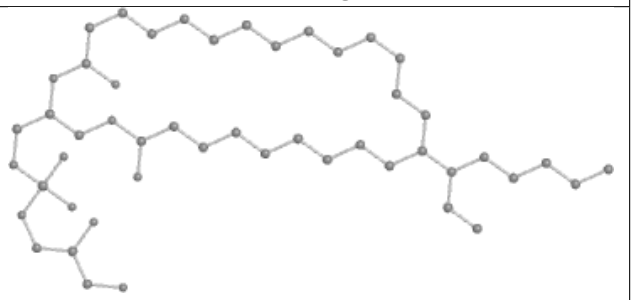
Bond lengths



Bond angles

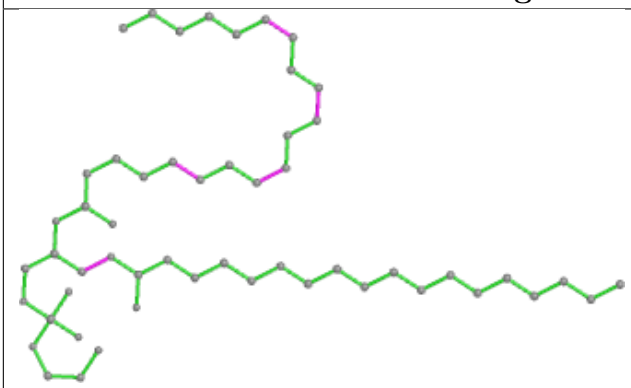


Torsions

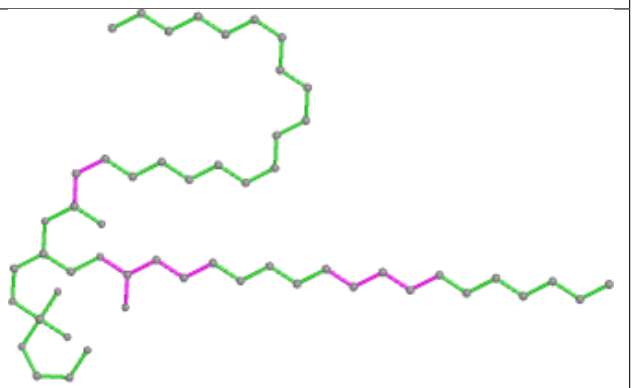


Rings

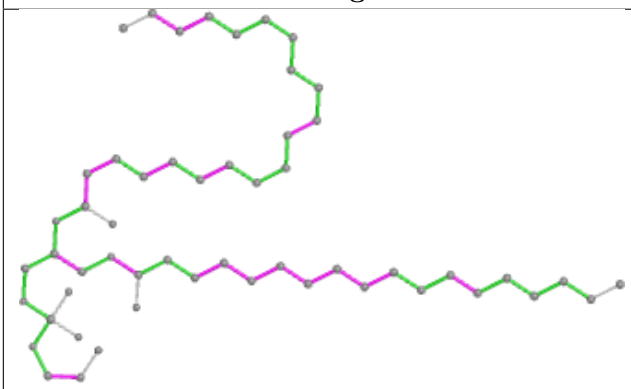
Ligand PEK C 3264



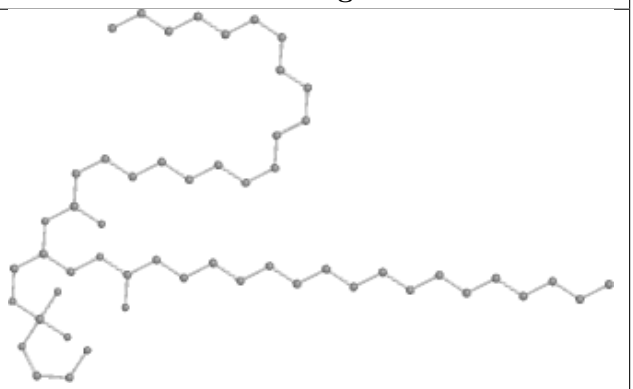
Bond lengths



Bond angles

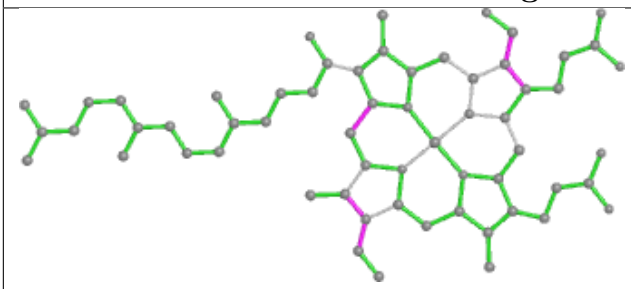


Torsions

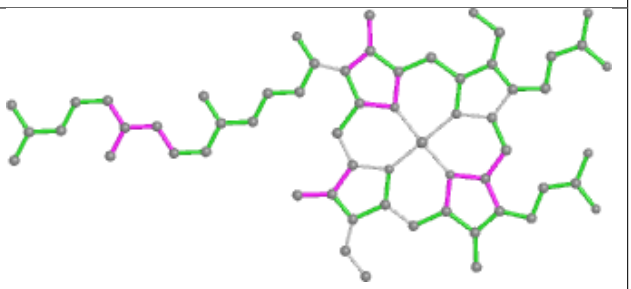


Rings

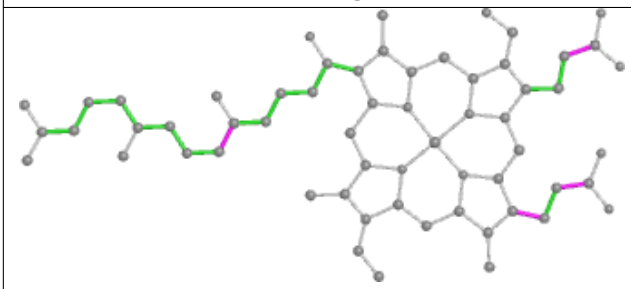
Ligand HEA N 516



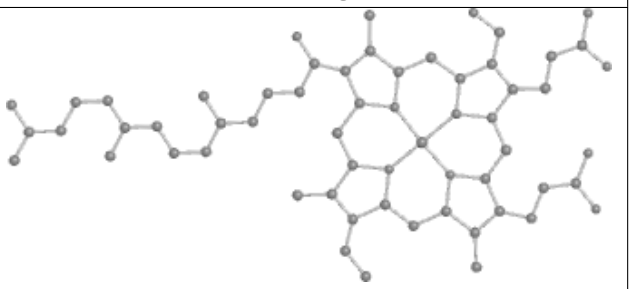
Bond lengths



Bond angles

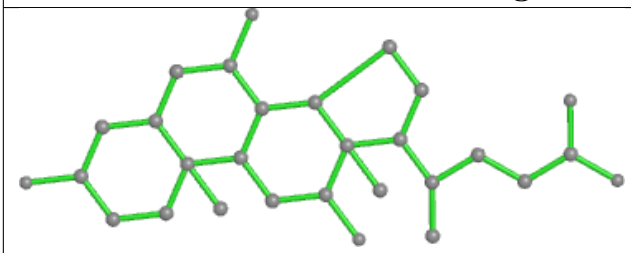


Torsions

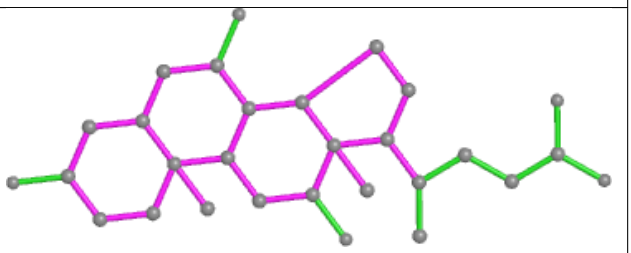


Rings

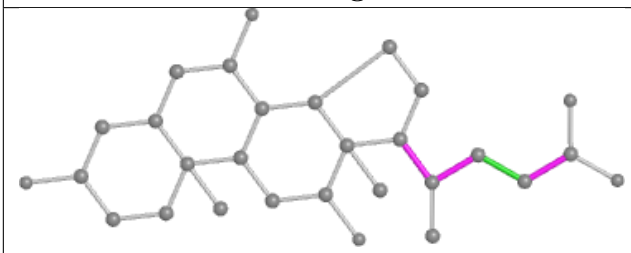
Ligand CHD P 4271



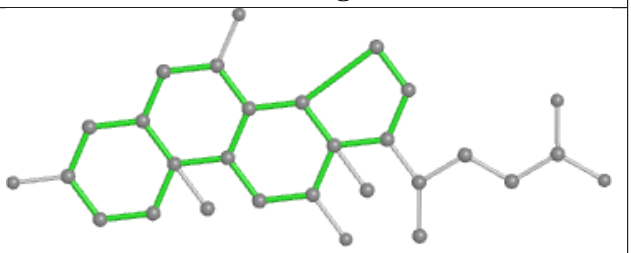
Bond lengths



Bond angles

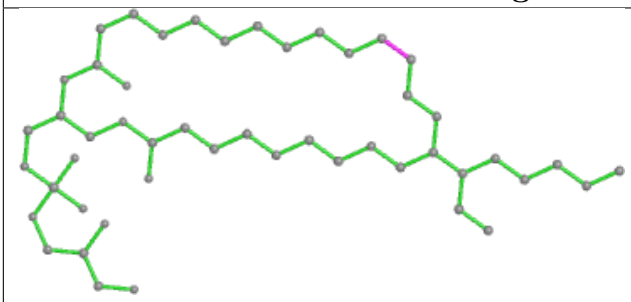


Torsions

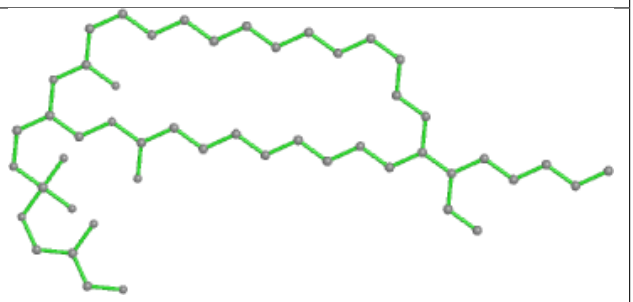


Rings

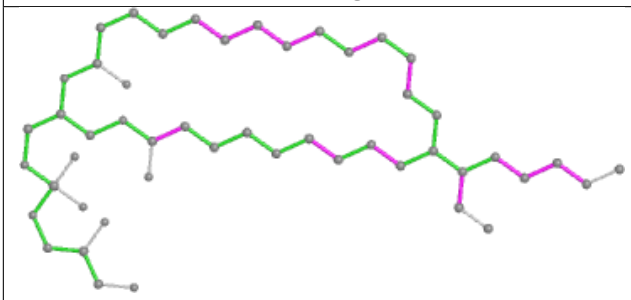
Ligand PGV A 3266



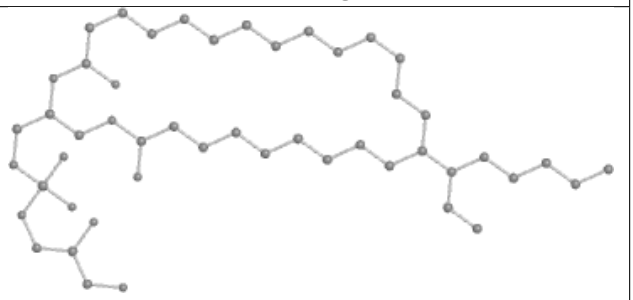
Bond lengths



Bond angles

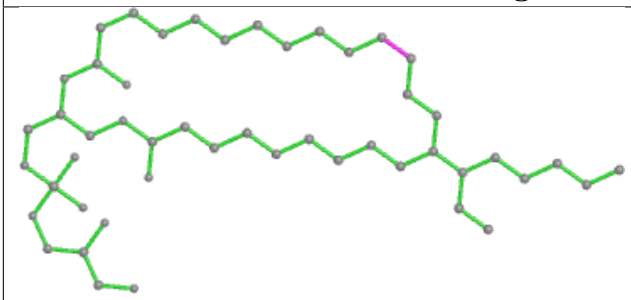


Torsions

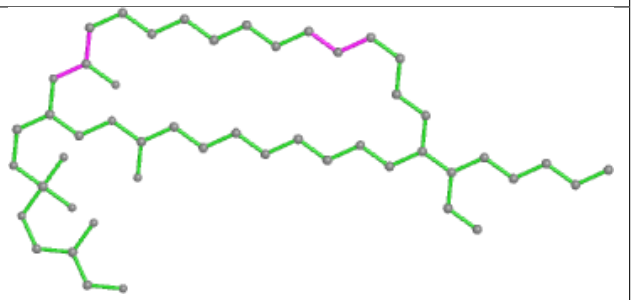


Rings

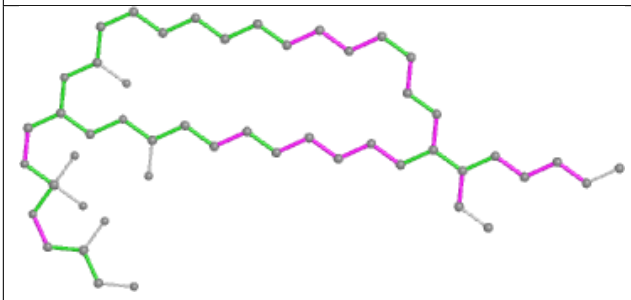
Ligand PGV C 3267



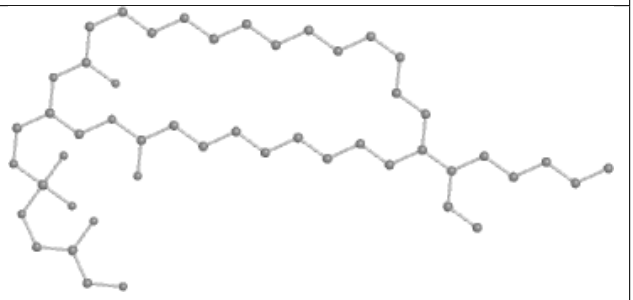
Bond lengths



Bond angles

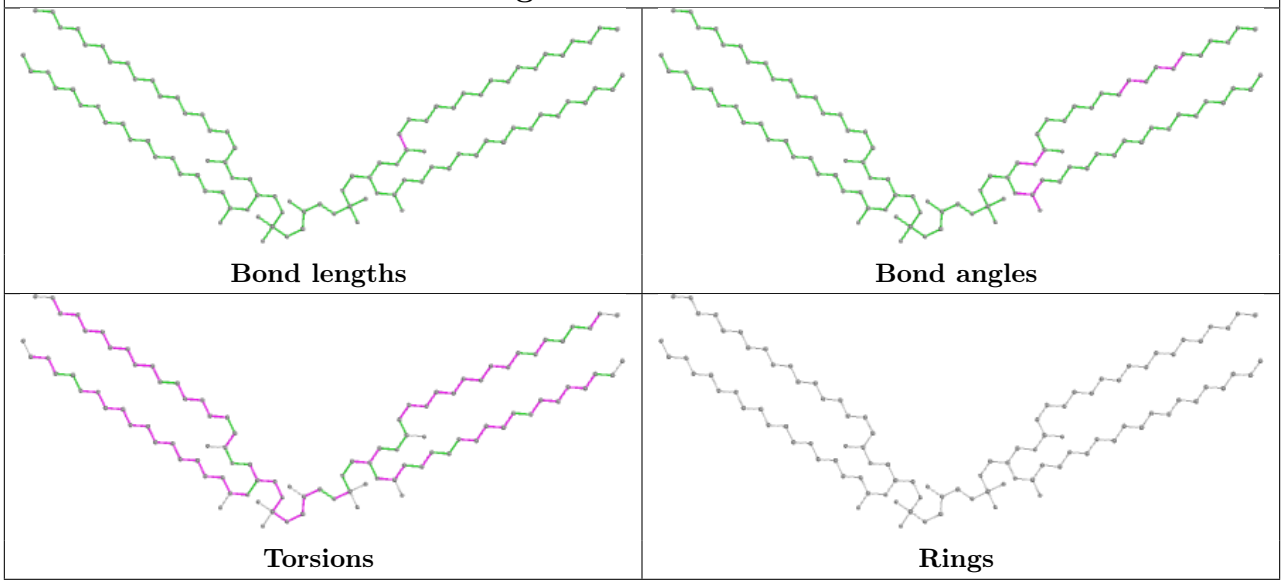


Torsions

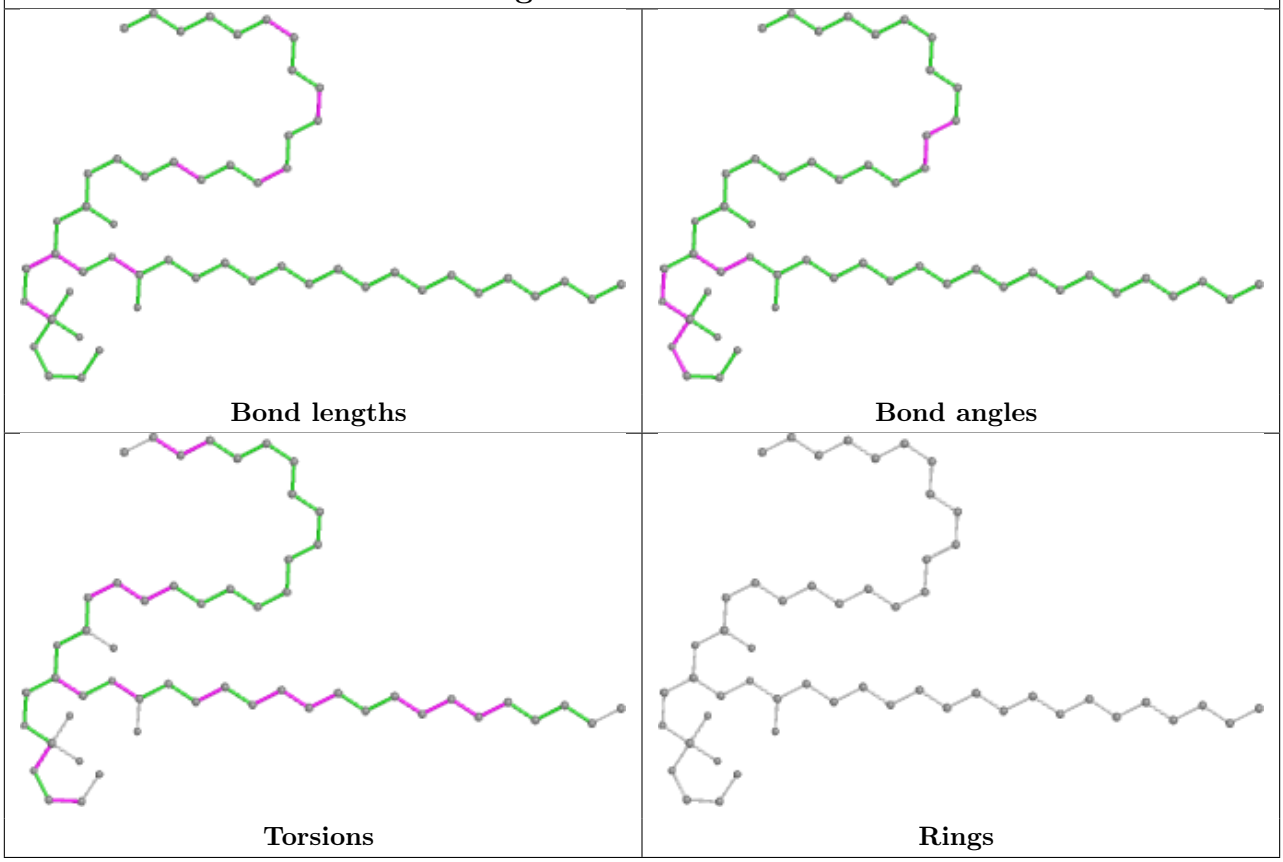


Rings

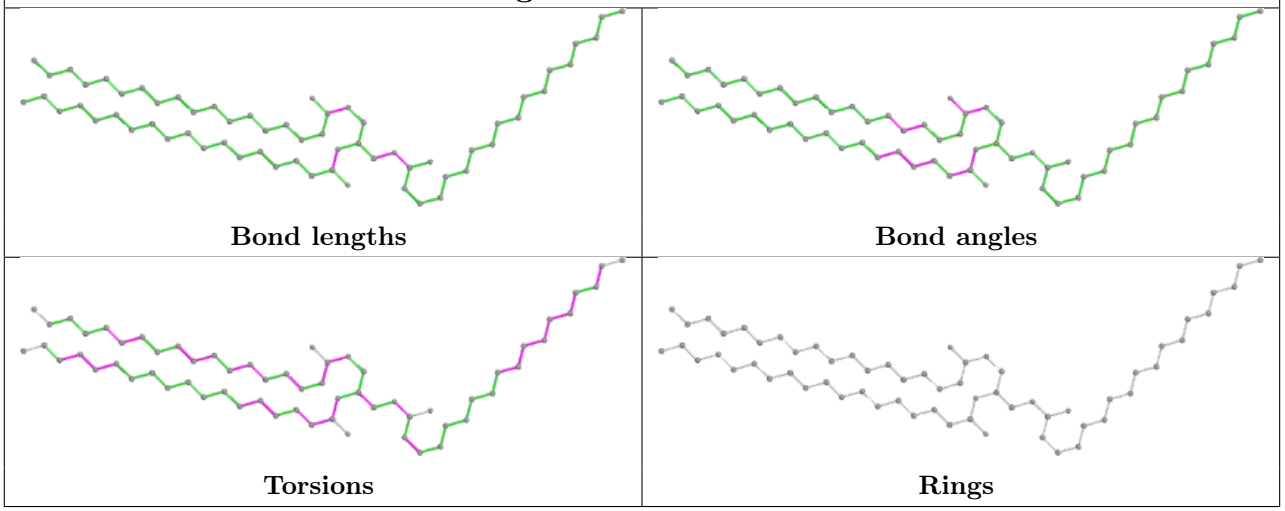
Ligand CDL C 3270



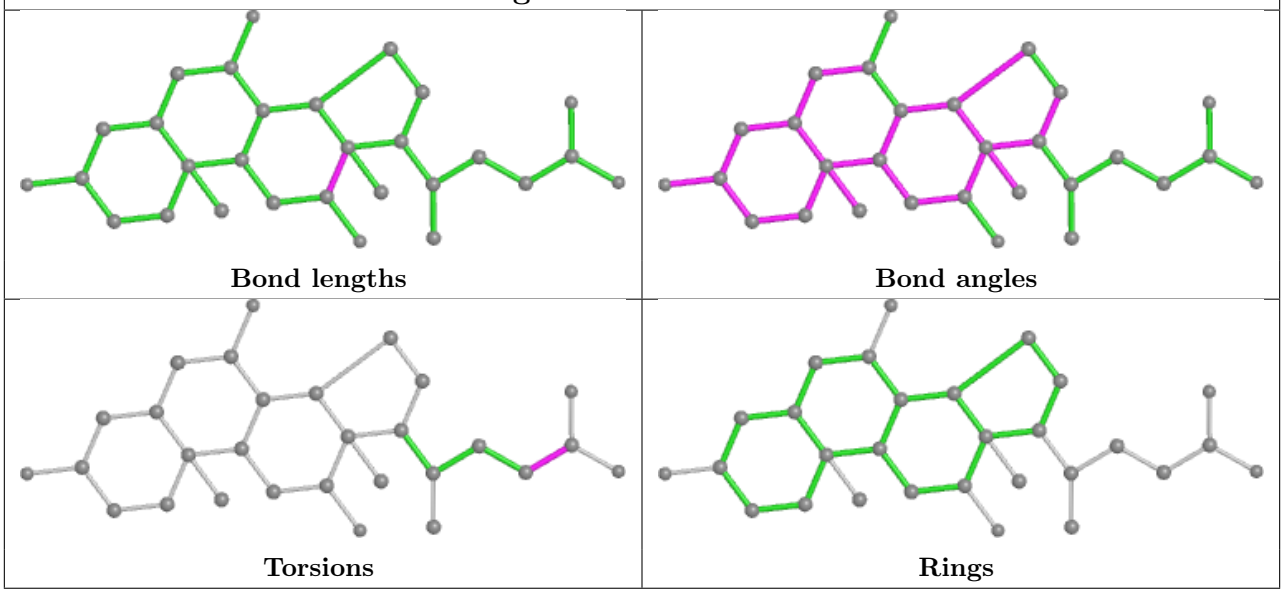
Ligand PEK C 3265



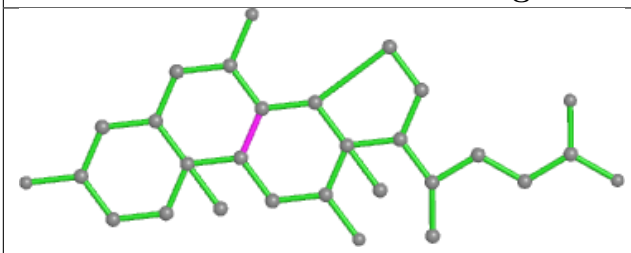
Ligand TGL A 3521



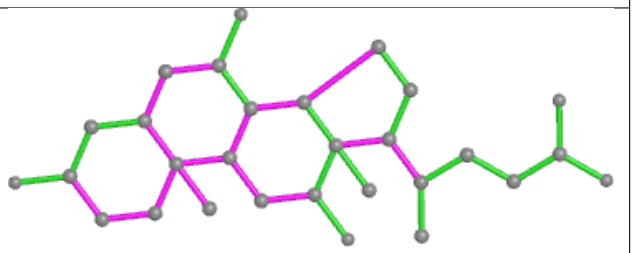
Ligand CHD B 4085



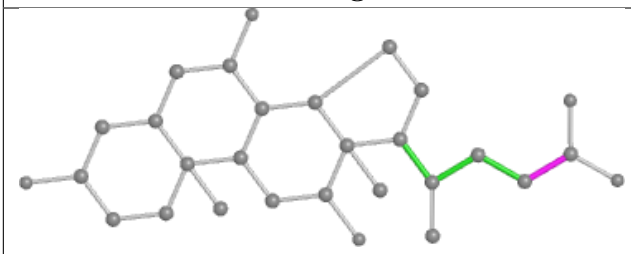
Ligand CHD P 4525



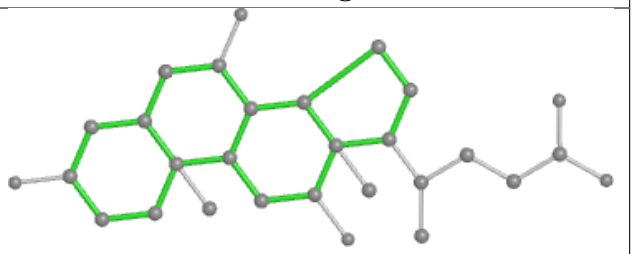
Bond lengths



Bond angles

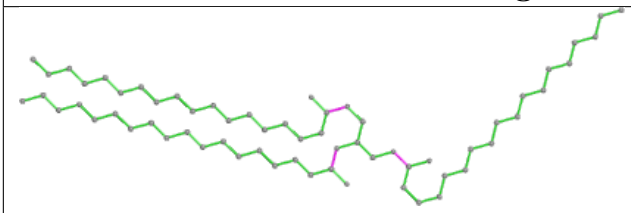


Torsions

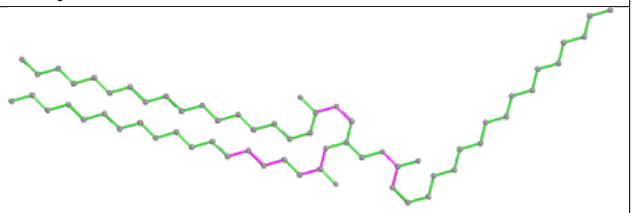


Rings

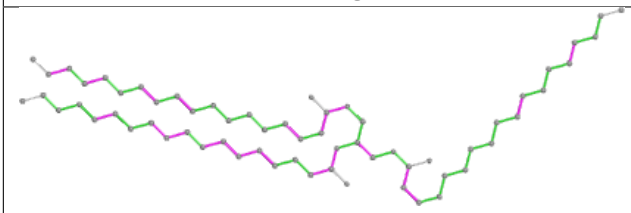
Ligand TGL Q 4523



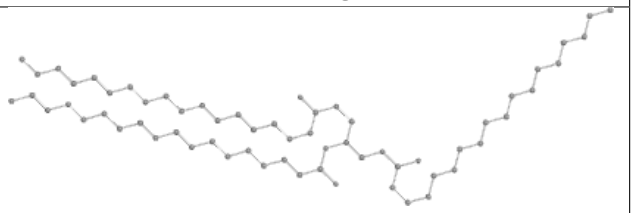
Bond lengths



Bond angles

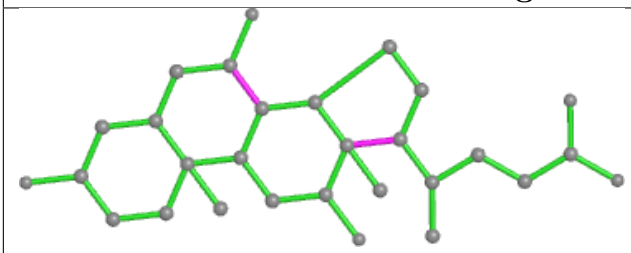


Torsions

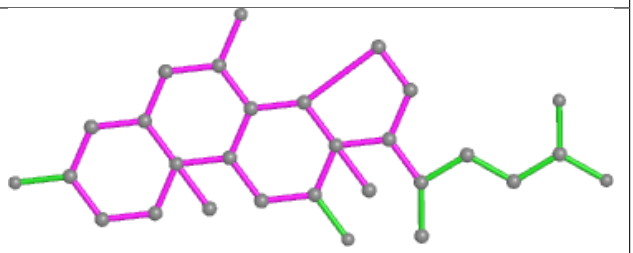


Rings

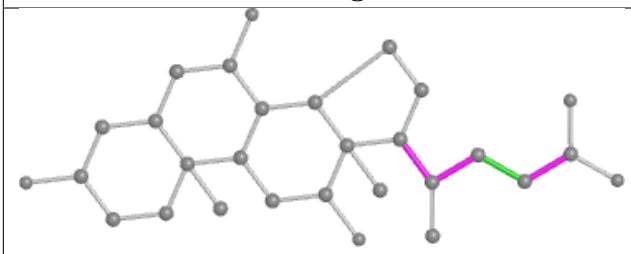
Ligand CHD J 3060



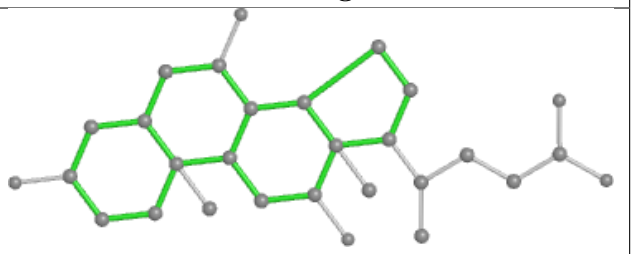
Bond lengths



Bond angles

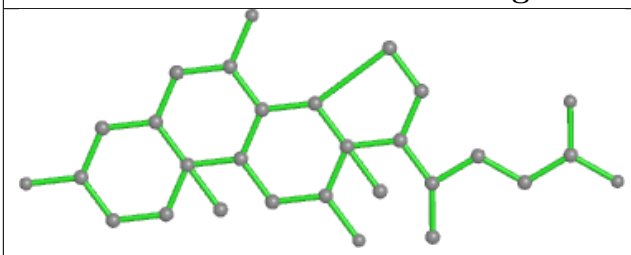


Torsions

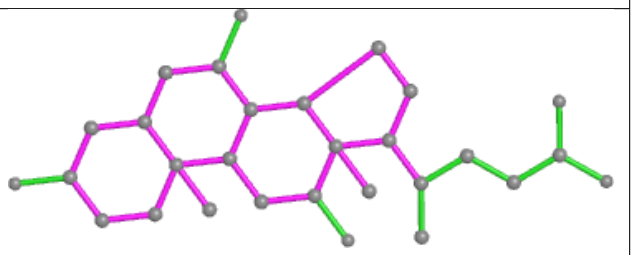


Rings

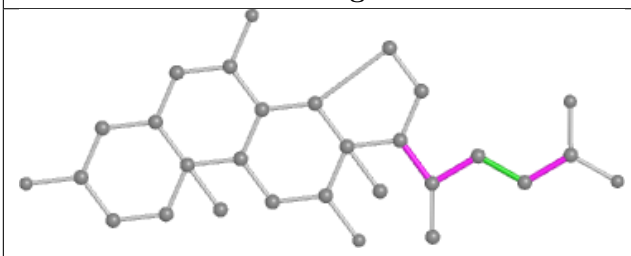
Ligand CHD C 3271



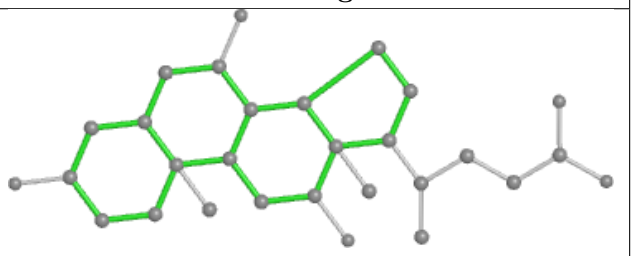
Bond lengths



Bond angles

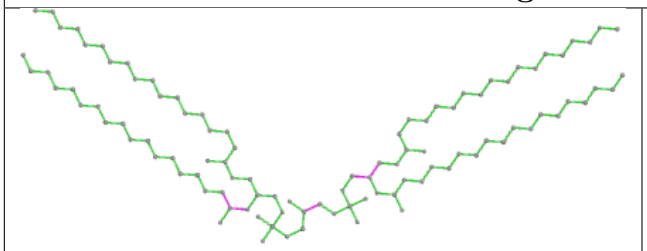


Torsions

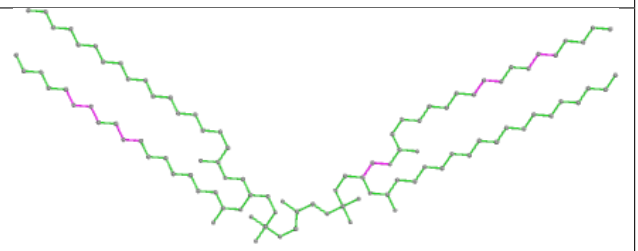


Rings

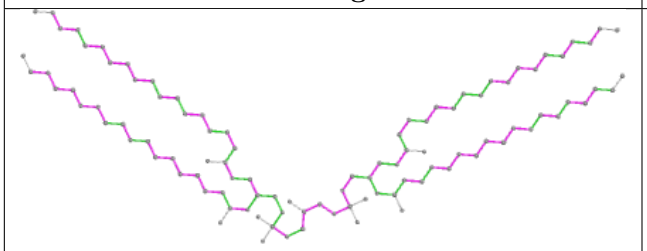
Ligand CDL T 4269



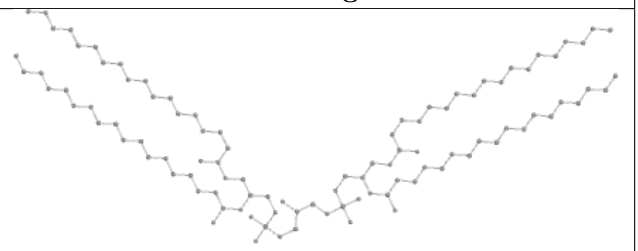
Bond lengths



Bond angles

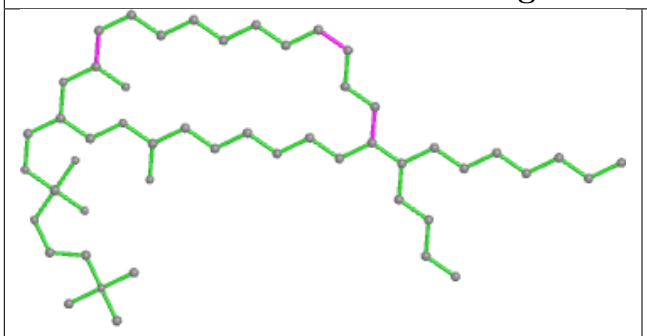


Torsions

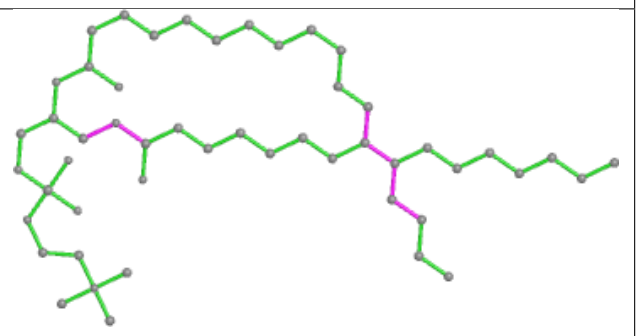


Rings

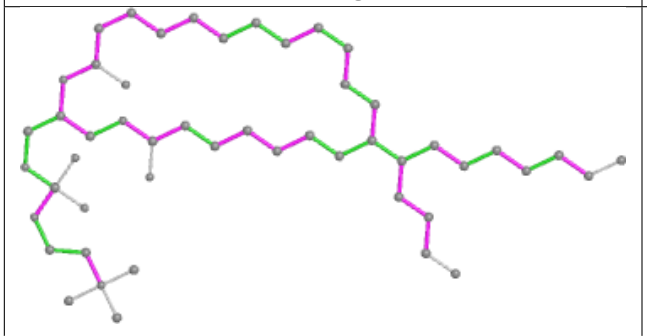
Ligand PSC O 4230



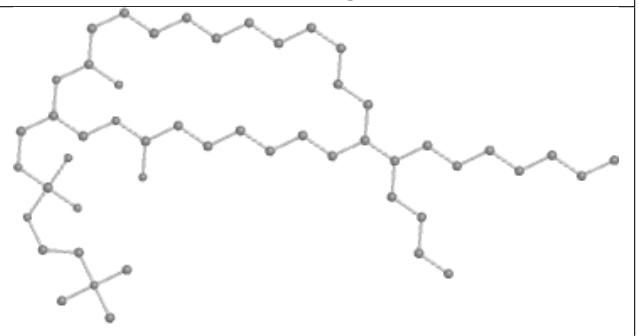
Bond lengths



Bond angles

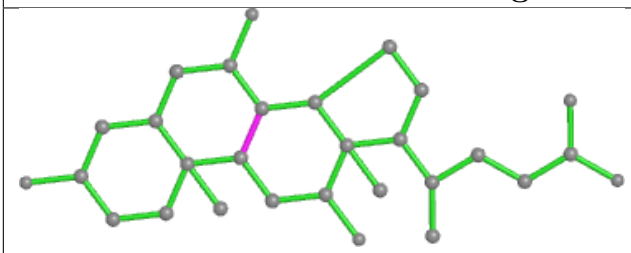


Torsions

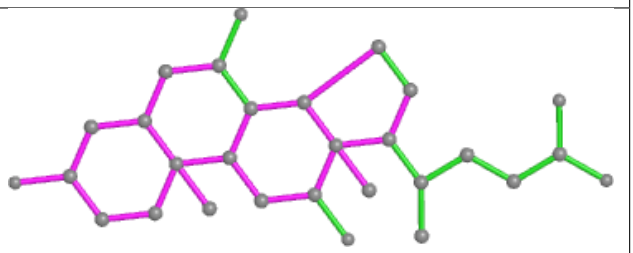


Rings

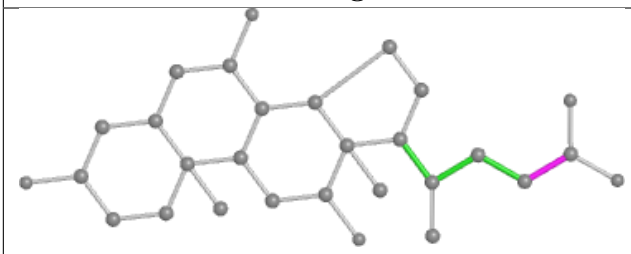
Ligand CHD O 3085



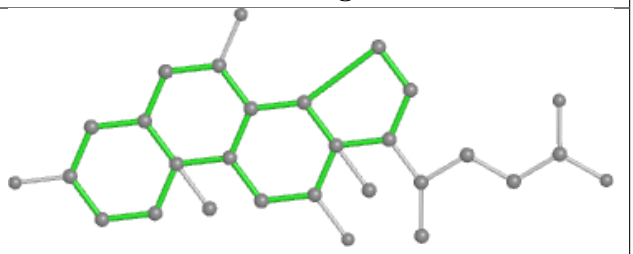
Bond lengths



Bond angles

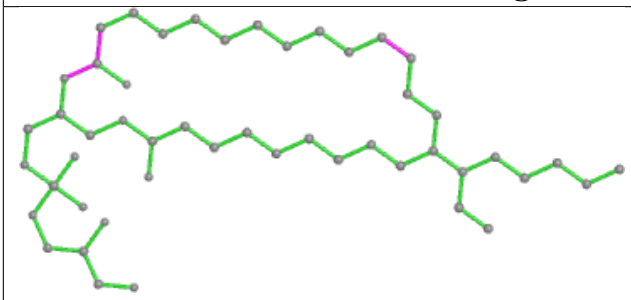


Torsions

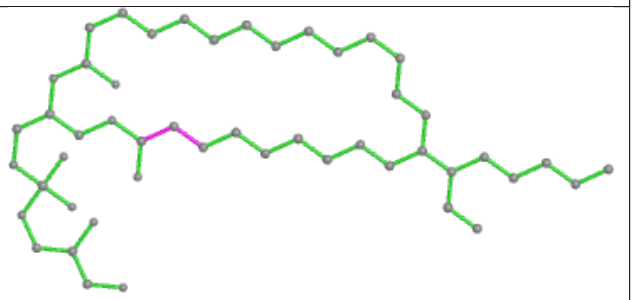


Rings

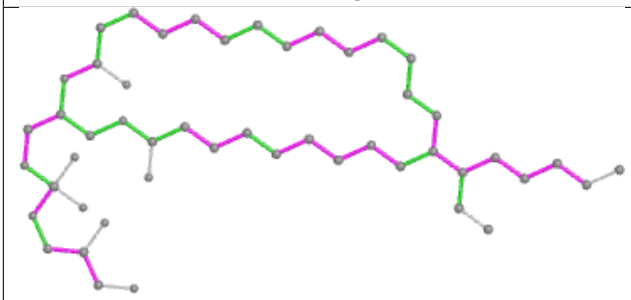
Ligand PGV C 3268



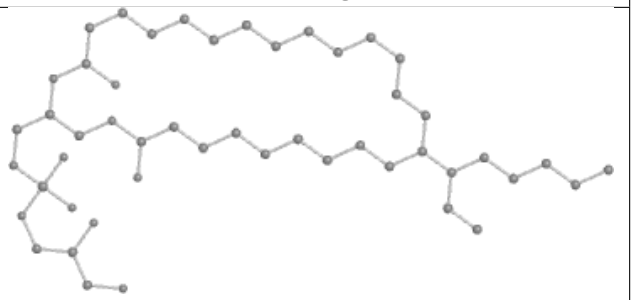
Bond lengths



Bond angles

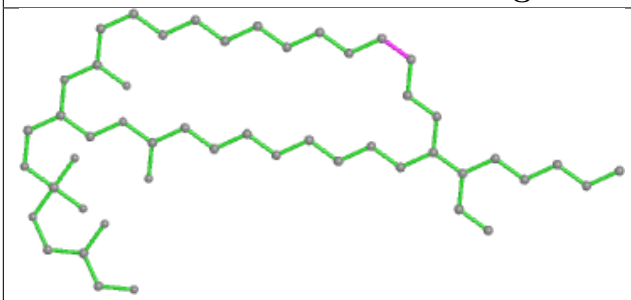


Torsions

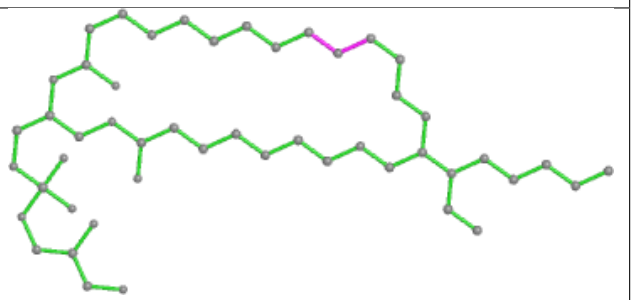


Rings

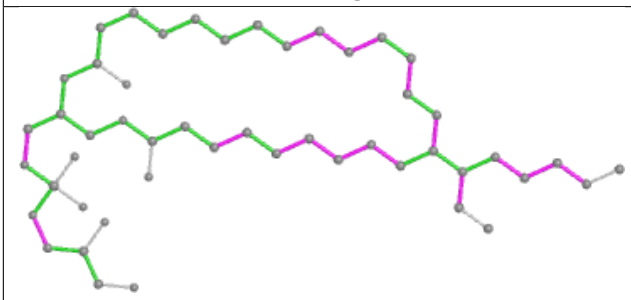
Ligand PGV P 4267



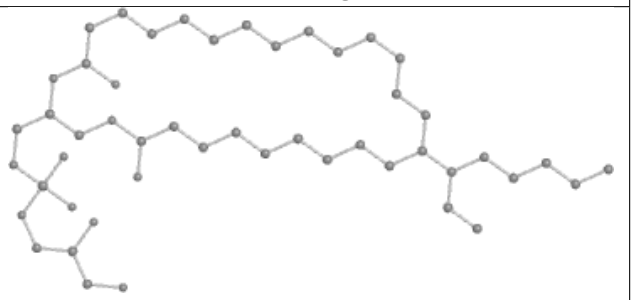
Bond lengths



Bond angles

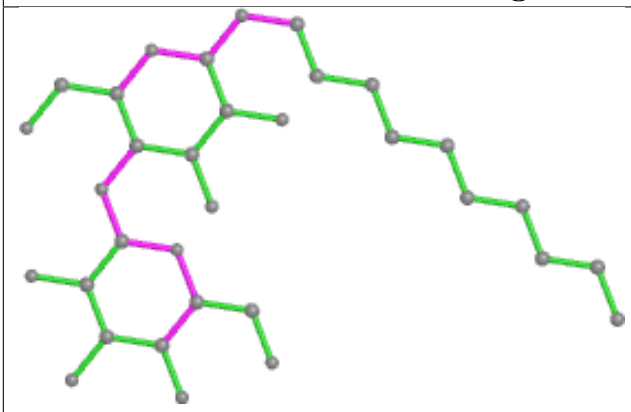


Torsions

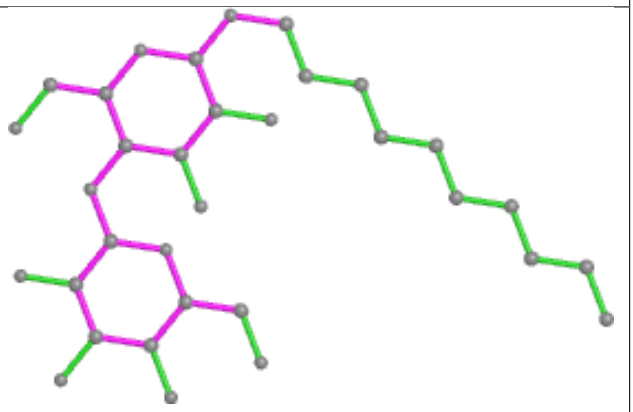


Rings

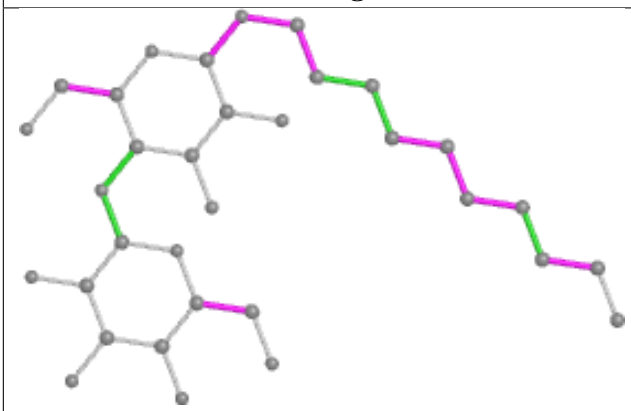
Ligand DMU Z 4526



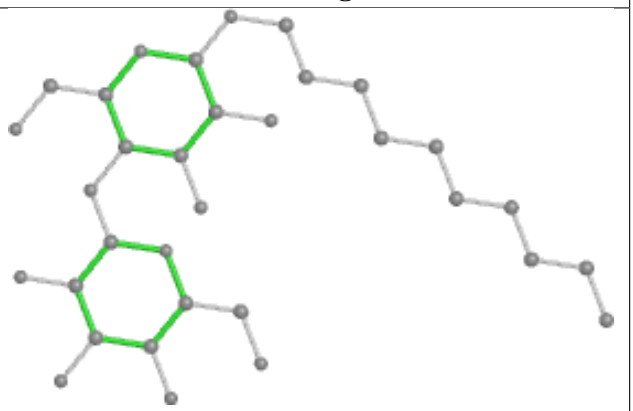
Bond lengths



Bond angles

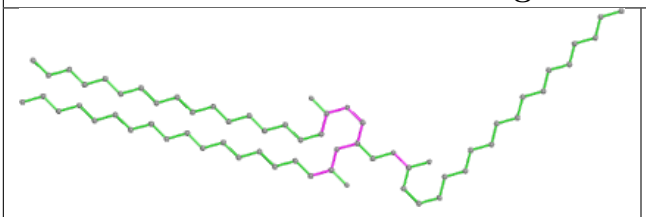


Torsions

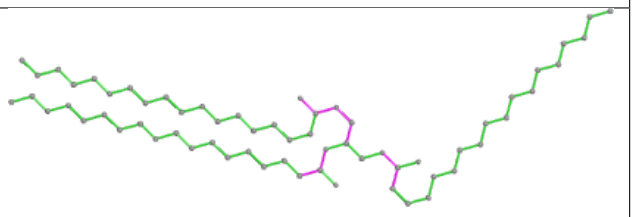


Rings

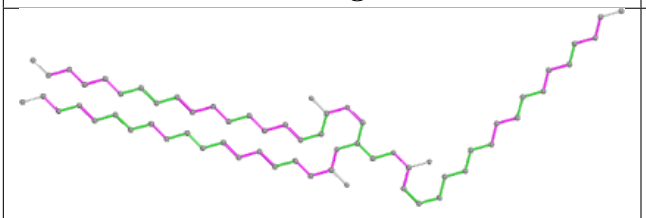
Ligand TGL N 4522



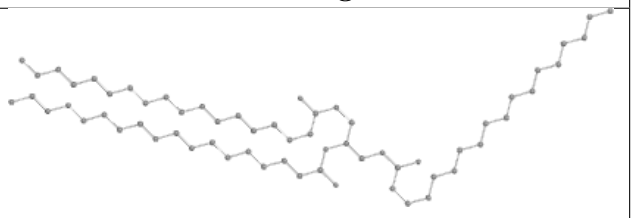
Bond lengths



Bond angles

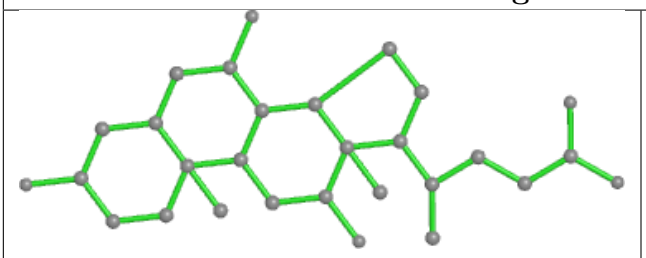


Torsions

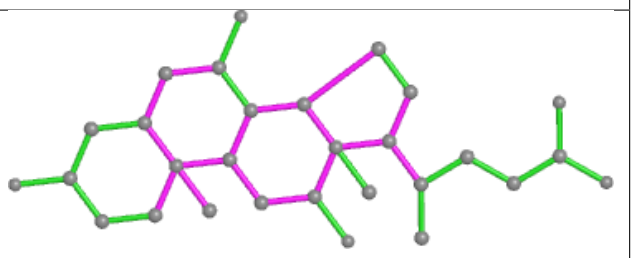


Rings

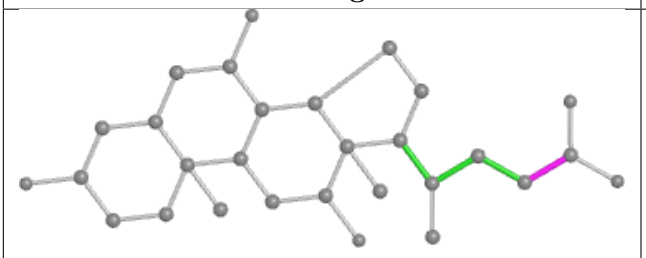
Ligand CHD C 3525



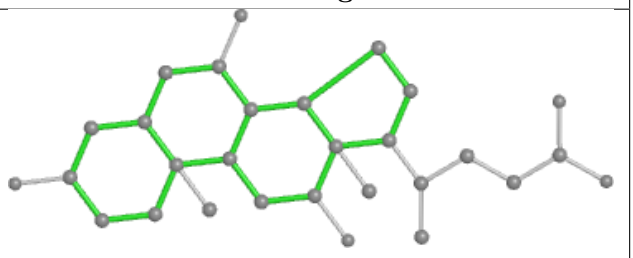
Bond lengths



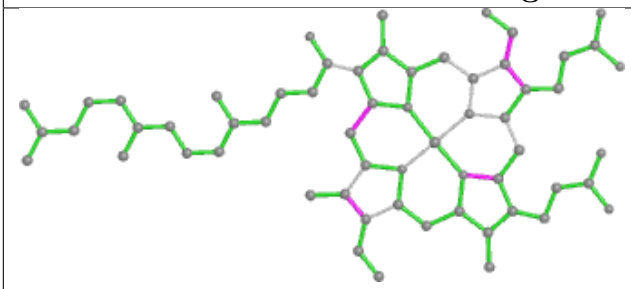
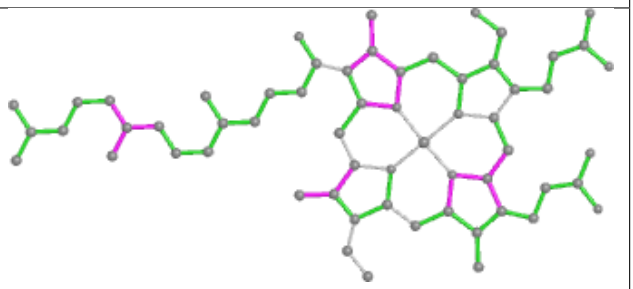
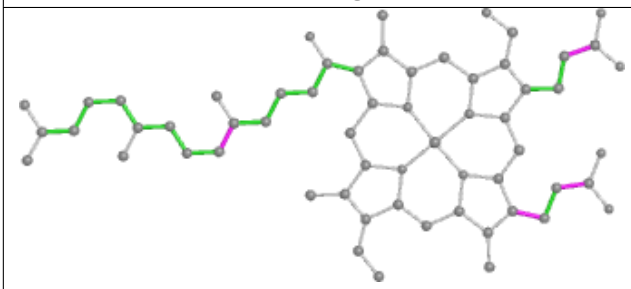
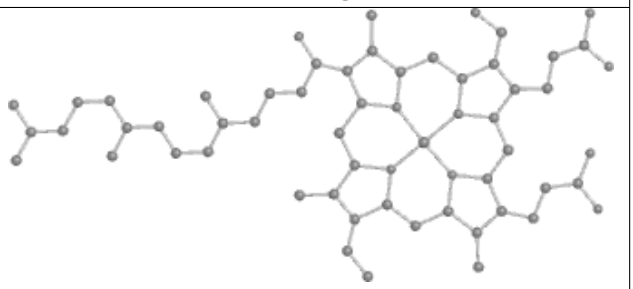
Bond angles



Torsions



Rings

Ligand HEA A 516	
	
Bond lengths	Bond angles
	
Torsions	Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	0.20	4 (0%) 86 87	13, 19, 29, 66	0
1	N	513/514 (99%)	0.02	3 (0%) 89 90	17, 24, 34, 67	0
2	B	226/227 (99%)	-0.09	6 (2%) 54 57	14, 27, 52, 83	0
2	O	226/227 (99%)	0.14	10 (4%) 34 37	21, 33, 60, 87	0
3	C	259/261 (99%)	-0.40	3 (1%) 79 81	16, 23, 37, 65	0
3	P	259/261 (99%)	-0.34	3 (1%) 79 81	18, 25, 39, 65	0
4	D	144/147 (97%)	-0.04	7 (4%) 29 33	20, 30, 56, 81	0
4	Q	144/147 (97%)	1.41	24 (16%) 1 1	29, 41, 67, 98	0
5	E	105/109 (96%)	0.34	4 (3%) 40 43	23, 31, 57, 97	0
5	R	105/109 (96%)	0.87	10 (9%) 8 9	27, 37, 60, 97	0
6	F	98/98 (100%)	0.66	8 (8%) 11 13	20, 29, 85, 100	0
6	S	98/98 (100%)	0.65	8 (8%) 11 13	21, 31, 91, 100	0
7	G	83/85 (97%)	1.06	19 (22%) 0 0	21, 31, 97, 99	0
7	T	83/85 (97%)	1.06	18 (21%) 0 0	20, 35, 94, 98	0
8	H	79/85 (92%)	0.83	15 (18%) 1 1	21, 34, 89, 100	0
8	U	79/85 (92%)	1.04	15 (18%) 1 1	27, 38, 91, 100	0
9	I	72/73 (98%)	0.73	10 (13%) 2 3	24, 41, 64, 81	0
9	V	72/73 (98%)	1.19	17 (23%) 0 0	27, 47, 66, 91	0
10	J	58/59 (98%)	0.48	7 (12%) 4 4	23, 32, 73, 94	0
10	W	58/59 (98%)	0.87	8 (13%) 2 3	26, 38, 76, 100	0
11	K	49/56 (87%)	-0.08	0 100 100	24, 34, 46, 67	0
11	X	49/56 (87%)	1.31	10 (20%) 1 1	33, 41, 58, 75	0
12	L	46/47 (97%)	-0.18	2 (4%) 35 38	20, 25, 44, 92	0
12	Y	46/47 (97%)	-0.05	1 (2%) 62 64	26, 33, 58, 85	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	43/46 (93%)	0.17	4 (9%) 8 10	21, 26, 77, 99	0
13	Z	43/46 (93%)	0.66	7 (16%) 1 1	28, 35, 84, 100	0
All	All	3550/3614 (98%)	0.28	223 (6%) 20 22	13, 28, 62, 100	0

All (223) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	4	SER	21.0
4	Q	6	VAL	19.3
4	Q	5	VAL	19.0
6	S	97	ALA	15.5
6	F	97	ALA	14.5
4	Q	8	SER	13.9
6	F	98	HIS	13.7
6	F	96	LEU	13.4
13	Z	43	SER	12.1
10	W	58	LYS	12.0
6	S	94	HIS	11.6
6	F	1	ALA	10.4
6	S	96	LEU	10.3
8	U	7	LYS	9.3
8	U	8	ILE	9.3
6	F	95	GLN	8.9
5	R	5	HIS	8.8
2	O	227	LEU	8.8
6	S	1	ALA	8.7
7	T	8	HIS	8.3
4	Q	7	LYS	8.1
7	G	3	ALA	8.1
8	H	7	LYS	8.0
7	G	42	ARG	7.7
7	T	42	ARG	7.5
9	I	37	PHE	7.5
10	J	1	PHE	7.5
6	S	98	HIS	7.4
8	U	44	THR	7.3
5	R	109	VAL	7.2
9	V	2	THR	7.2
7	T	1	ALA	7.2
7	G	1	ALA	7.1
7	G	4	ALA	6.8

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Mol	Chain	Res	Type	RSRZ
6	F	2	SER	6.8
13	M	43	SER	6.7
7	T	5	LYS	6.6
7	G	2	SER	6.6
7	T	3	ALA	6.5
11	X	6	ALA	6.5
7	T	2	SER	6.5
8	H	46	LYS	6.4
8	U	45	ALA	6.3
9	V	3	ALA	6.2
7	T	36	TRP	6.2
10	J	58	LYS	6.1
6	S	2	SER	5.9
8	H	45	ALA	5.9
7	G	5	LYS	5.9
8	H	8	ILE	5.8
7	T	84	LYS	5.8
6	F	94	HIS	5.8
9	V	37	PHE	5.8
6	S	93	PRO	5.7
10	W	57	HIS	5.7
8	H	47	GLY	5.6
12	Y	47	LYS	5.5
7	T	39	SER	5.4
5	E	5	HIS	5.4
2	O	226	MET	5.4
8	H	44	THR	5.4
2	O	113	TYR	5.3
4	Q	33	LEU	5.2
8	U	46	LYS	5.2
2	O	90	ILE	5.1
10	W	1	PHE	5.0
9	V	4	LEU	5.0
7	T	4	ALA	5.0
8	U	48	GLY	5.0
11	X	13	TYR	5.0
2	O	59	GLN	4.9
4	Q	58	GLU	4.8
7	G	6	GLY	4.8
9	V	5	ALA	4.8
7	G	8	HIS	4.7
4	Q	35	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
8	U	10	ASN	4.6
3	P	3	HIS	4.6
8	H	48	GLY	4.5
4	Q	51	LEU	4.5
4	Q	39	ALA	4.4
13	Z	41	LYS	4.4
7	G	40	GLY	4.4
5	E	109	VAL	4.4
8	U	9	LYS	4.2
11	X	23	THR	4.1
13	Z	42	LYS	4.1
2	O	223	SER	4.0
10	W	52	TRP	3.9
2	O	91	ASN	3.9
7	G	39	SER	3.9
1	N	513	LEU	3.9
4	D	6	VAL	3.8
7	T	10	GLY	3.8
8	U	47	GLY	3.8
5	R	108	LYS	3.8
4	Q	147	LYS	3.8
9	I	34	PHE	3.7
9	V	33	THR	3.6
8	H	49	ASP	3.6
4	D	147	LYS	3.6
8	H	10	ASN	3.6
4	D	5	VAL	3.5
4	Q	46	ALA	3.5
7	G	36	TRP	3.4
6	S	95	GLN	3.4
10	W	55	PHE	3.4
2	B	59	GLN	3.4
11	X	7	PRO	3.4
4	Q	62	LEU	3.4
7	T	6	GLY	3.3
11	X	47	ARG	3.2
12	L	2	HIS	3.2
4	Q	73	ARG	3.1
8	U	49	ASP	3.1
13	M	40	TYR	3.1
7	G	84	LYS	3.1
7	T	41	HIS	3.1

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Mol	Chain	Res	Type	RSRZ
7	T	7	ASP	3.1
13	Z	39	ASN	3.1
7	G	45	PRO	3.0
12	L	47	LYS	3.0
8	H	43	MET	3.0
8	U	50	VAL	3.0
3	P	37	PHE	3.0
9	V	53	ASN	3.0
11	X	48	VAL	3.0
10	J	57	HIS	3.0
8	H	9	LYS	3.0
2	B	113	TYR	3.0
6	F	3	GLY	2.9
9	I	25	PHE	2.9
8	U	42	ALA	2.9
8	U	52	VAL	2.9
4	D	8	SER	2.9
10	J	56	PRO	2.9
4	Q	48	TRP	2.8
10	W	48	TYR	2.8
9	V	36	LYS	2.8
4	Q	97	ILE	2.8
3	C	37	PHE	2.8
4	Q	10	ASP	2.7
9	I	36	LYS	2.7
5	R	79	LYS	2.7
9	V	19	PHE	2.7
4	Q	140	TYR	2.7
9	I	29	LEU	2.7
5	E	7	THR	2.7
11	X	46	GLY	2.6
4	Q	9	GLU	2.6
10	J	2	GLU	2.6
7	T	40	GLY	2.6
9	I	26	MET	2.6
13	Z	40	TYR	2.6
10	J	52	TRP	2.6
5	R	93	LEU	2.5
10	W	56	PRO	2.5
7	T	43	GLU	2.5
13	Z	32	TRP	2.5
2	O	217	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	N	246	LEU	2.5
3	C	38	ASN	2.5
3	P	38	ASN	2.5
8	H	55	TRP	2.5
4	D	4	SER	2.5
9	V	7	PRO	2.5
2	B	90	ILE	2.4
5	R	96	LEU	2.4
7	G	37	LEU	2.4
9	V	25	PHE	2.4
4	Q	136	ALA	2.4
7	G	43	GLU	2.4
8	U	11	TYR	2.4
4	Q	52	SER	2.4
7	G	41	HIS	2.4
4	Q	142	LYS	2.3
8	H	39	CYS	2.3
8	H	52	VAL	2.3
9	I	18	ARG	2.3
13	M	42	LYS	2.3
11	X	18	LEU	2.3
4	Q	102	TYR	2.3
11	X	17	VAL	2.3
1	A	381	LEU	2.3
4	Q	59	LEU	2.3
4	D	7	LYS	2.3
9	I	19	PHE	2.2
2	B	87	MET	2.2
10	W	2	GLU	2.2
3	C	3	HIS	2.2
7	G	9	GLY	2.2
9	I	53	ASN	2.2
9	V	26	MET	2.2
13	Z	35	TYR	2.2
1	N	243	VAL	2.2
5	R	48	ILE	2.2
5	R	89	LEU	2.2
7	T	33	LEU	2.2
8	U	43	MET	2.2
11	X	36	ILE	2.2
9	V	65	LYS	2.2
5	R	52	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	385	ALA	2.2
7	G	7	ASP	2.2
1	A	193	VAL	2.1
2	B	60	GLU	2.1
9	V	52	ARG	2.1
9	V	34	PHE	2.1
13	M	39	ASN	2.1
5	R	86	ILE	2.1
1	A	513	LEU	2.1
9	I	4	LEU	2.1
9	V	18	ARG	2.1
10	J	4	ARG	2.1
7	G	12	GLY	2.1
7	T	9	GLY	2.1
2	O	224	ALA	2.1
9	V	8	GLN	2.1
8	H	85	ILE	2.1
4	D	11	TYR	2.0
2	B	65	TRP	2.0
2	O	65	TRP	2.0
5	E	81	ILE	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	0.30	0.58	98,99,100,100	0
7	TPO	T	11	11/12	0.45	0.38	71,81,100,100	0
7	TPO	G	11	11/12	0.56	0.34	71,79,100,100	0
9	SAC	I	1	9/10	0.73	0.31	91,93,94,96	0
1	FME	A	1	10/11	0.83	0.16	41,45,67,71	0
1	FME	N	1	10/11	0.86	0.18	44,49,68,69	0
2	FME	B	1	10/11	0.94	0.14	20,27,36,41	0
2	FME	O	1	10/11	0.96	0.14	32,33,40,42	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	PEK	P	4265	53/53	0.48	0.34	44,70,100,100	0
23	PEK	T	3263	53/53	0.55	0.45	44,91,100,100	0
23	PEK	C	3265	53/53	0.56	0.29	43,72,100,100	0
21	CHD	W	4060	29/29	0.58	0.57	84,98,100,100	0
25	PSC	O	4230	52/52	0.58	0.37	46,79,100,100	0
22	CDL	G	3269	100/100	0.59	0.33	48,87,100,100	0
21	CHD	J	3060	29/29	0.62	0.41	83,96,100,100	0
22	CDL	T	4269	100/100	0.62	0.31	45,85,100,100	0
25	PSC	E	3230	52/52	0.63	0.37	49,83,100,100	0
18	TGL	N	4522	63/63	0.63	0.33	38,63,76,84	0
19	PGV	N	4524	51/51	0.64	0.33	35,68,100,100	0
23	PEK	G	4263	53/53	0.65	0.37	44,87,100,100	0
19	PGV	C	3268	51/51	0.66	0.35	56,84,99,100	0
18	TGL	Q	4523	63/63	0.67	0.24	50,69,84,87	0
18	TGL	A	3522	63/63	0.68	0.32	31,61,76,79	0
22	CDL	P	4270	100/100	0.68	0.39	36,88,99,100	0
19	PGV	A	3524	51/51	0.68	0.30	29,69,99,100	0
18	TGL	N	4521	63/63	0.70	0.30	42,72,80,83	0
18	TGL	A	3523	63/63	0.72	0.26	49,66,83,87	0
22	CDL	C	3270	100/100	0.73	0.40	37,87,99,100	0
21	CHD	P	4271	29/29	0.74	0.36	79,91,95,97	0
21	CHD	C	3271	29/29	0.74	0.33	80,93,96,98	0
19	PGV	P	4268	51/51	0.74	0.29	62,83,98,100	0
18	TGL	A	3521	63/63	0.75	0.31	45,70,80,84	0
27	DMU	Z	4526	33/33	0.85	0.24	36,54,68,70	0
24	UNX	P	4262	1/1	0.87	0.36	28,28,28,28	0
27	DMU	M	3526	33/33	0.88	0.14	28,45,64,67	0
24	UNX	C	3262	1/1	0.91	0.30	33,33,33,33	0
21	CHD	P	4525	29/29	0.94	0.12	21,27,30,31	0
15	MG	N	4518	1/1	0.94	0.12	27,27,27,27	0
16	NA	N	4519	1/1	0.94	0.06	30,30,30,30	0
23	PEK	P	4264	53/53	0.94	0.14	25,42,70,71	0

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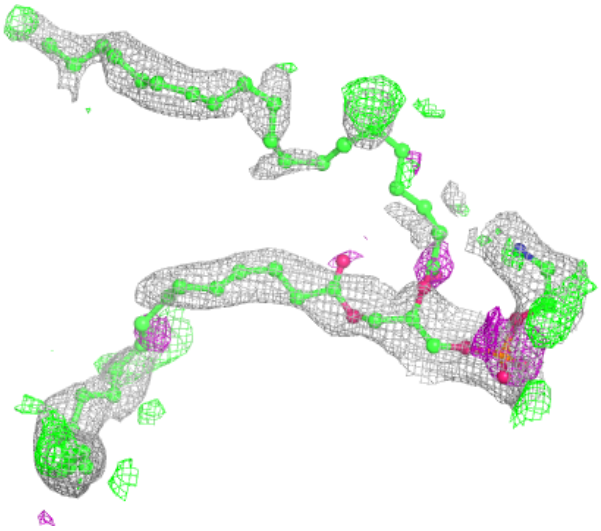
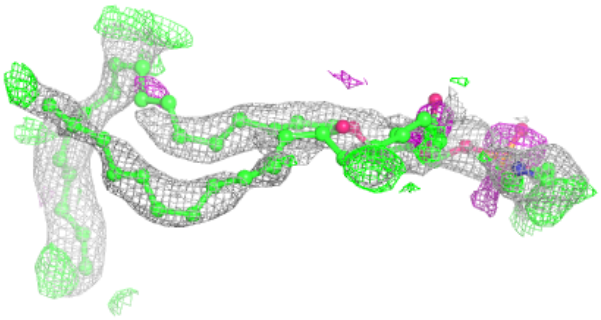
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	PEK	C	3264	53/53	0.95	0.12	21,41,70,72	0
19	PGV	P	4267	51/51	0.96	0.12	20,29,57,59	0
19	PGV	C	3267	51/51	0.96	0.12	20,30,54,59	0
21	CHD	C	3525	29/29	0.96	0.13	18,25,28,32	0
19	PGV	N	4266	51/51	0.97	0.11	19,30,48,53	0
20	CUA	O	228	2/2	0.97	0.08	24,24,24,27	0
21	CHD	B	4085	29/29	0.97	0.08	18,22,29,33	0
19	PGV	A	3266	51/51	0.97	0.11	17,27,49,51	0
16	NA	A	3519	1/1	0.97	0.09	25,25,25,25	0
17	HEA	N	515	60/60	0.98	0.15	17,23,33,35	0
21	CHD	O	3085	29/29	0.98	0.08	18,22,26,30	0
17	HEA	N	516	60/60	0.98	0.13	15,19,29,30	0
15	MG	A	3518	1/1	0.99	0.12	17,17,17,17	0
14	CU	N	517	1/1	0.99	0.10	19,19,19,19	0
17	HEA	A	515	60/60	0.99	0.16	13,19,30,33	0
26	ZN	F	99	1/1	0.99	0.07	25,25,25,25	0
26	ZN	S	99	1/1	0.99	0.07	28,28,28,28	0
17	HEA	A	516	60/60	0.99	0.13	12,17,25,27	0
20	CUA	B	228	2/2	0.99	0.08	16,16,16,18	0
14	CU	A	517	1/1	1.00	0.09	16,16,16,16	0

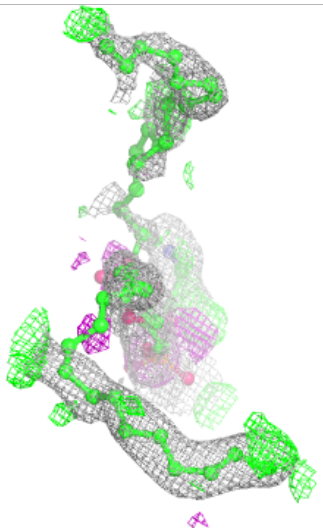
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PEK P 4265:

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

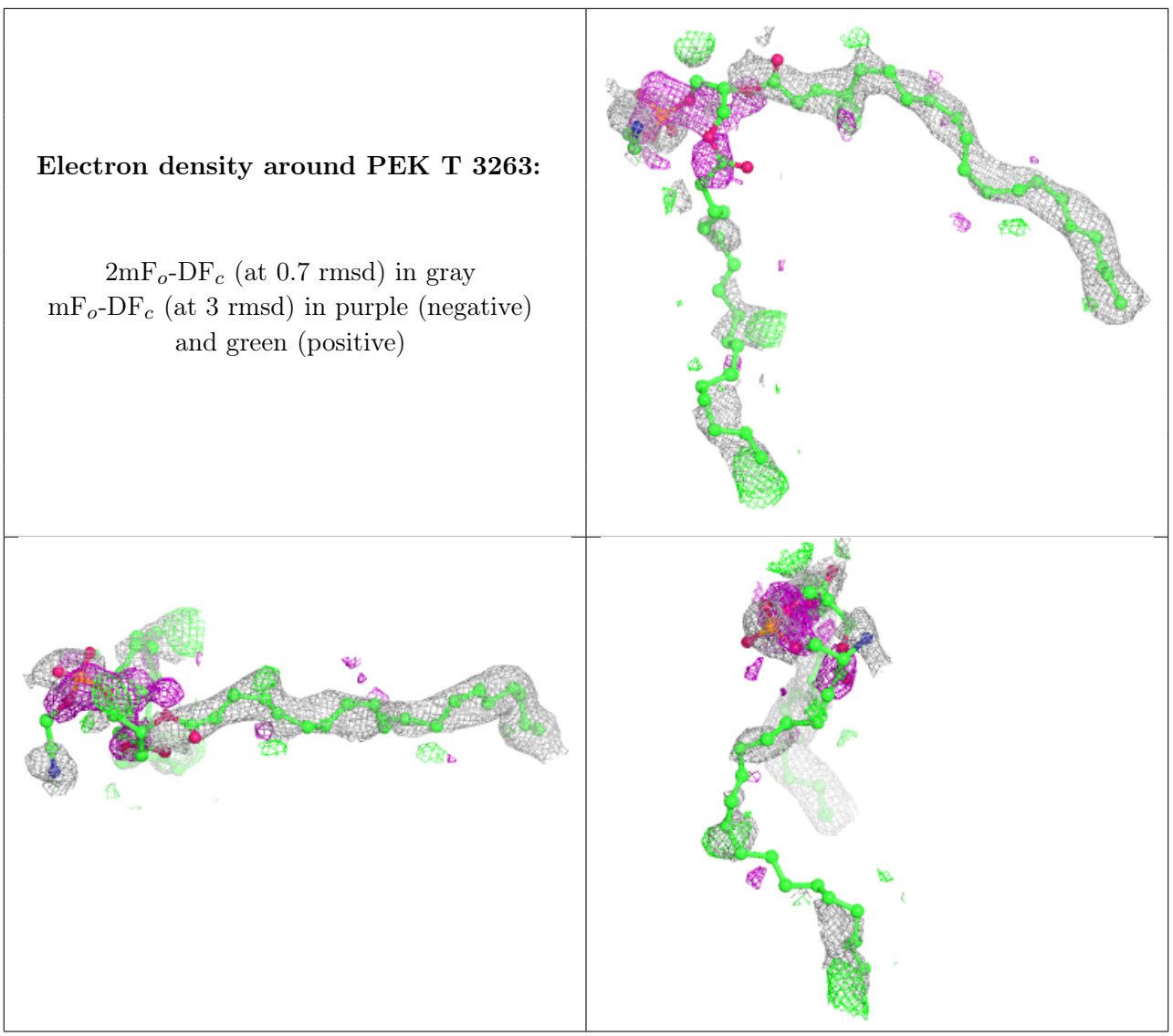






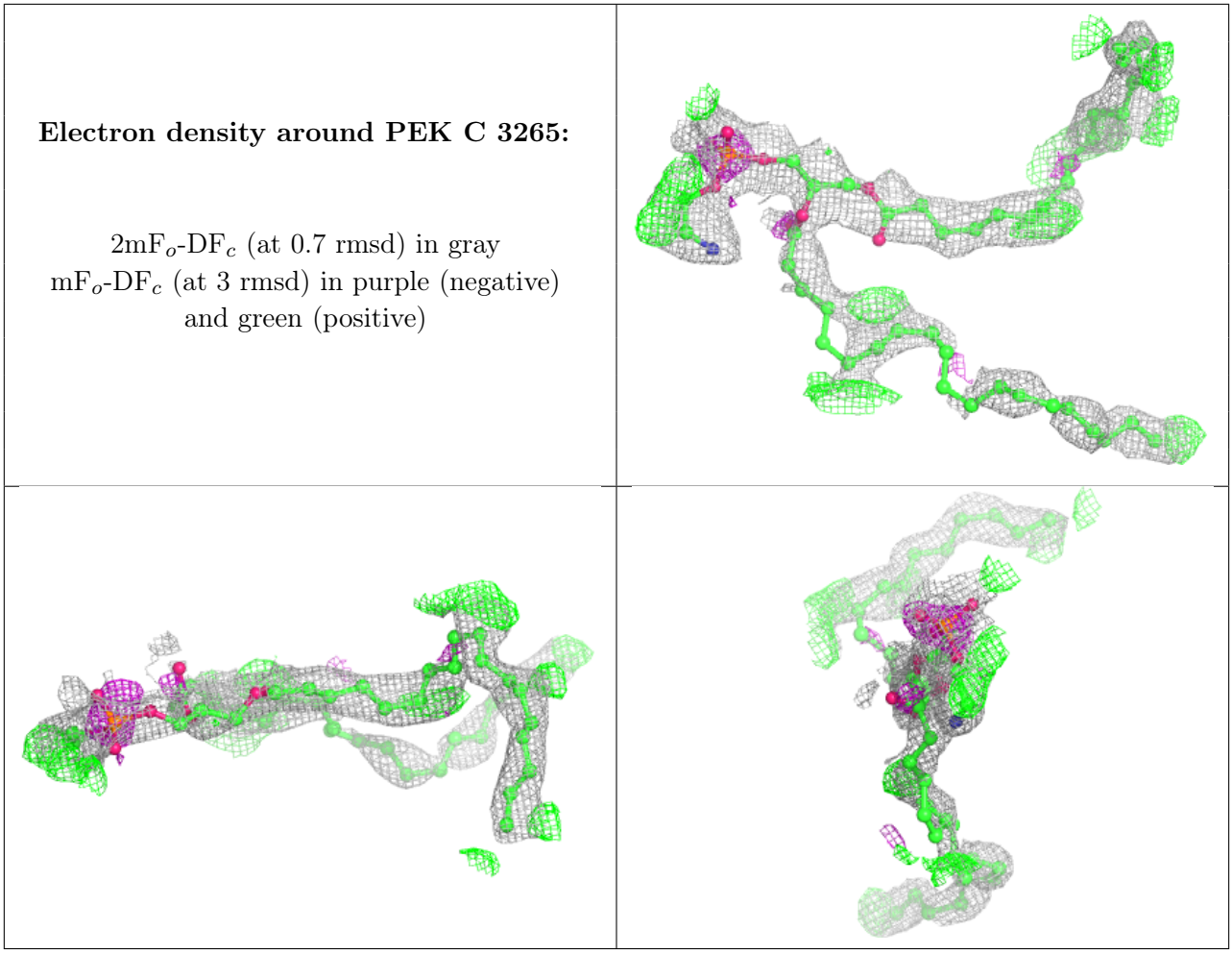
Electron density around PEK T 3263:

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



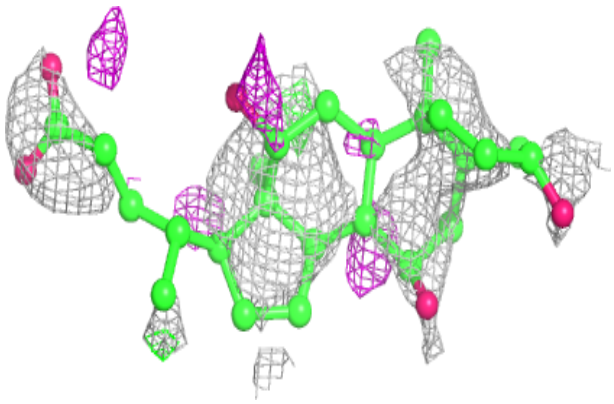
Electron density around PEK C 3265:

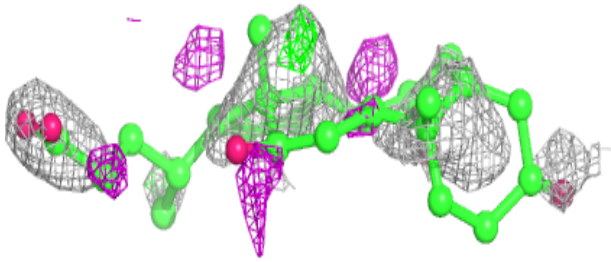
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

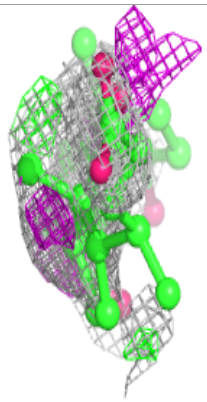


Electron density around CHD W 4060:

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

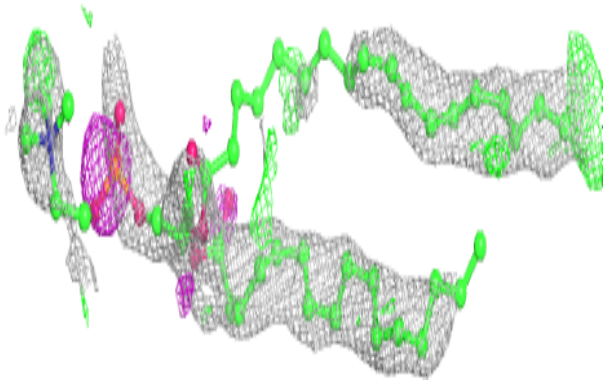


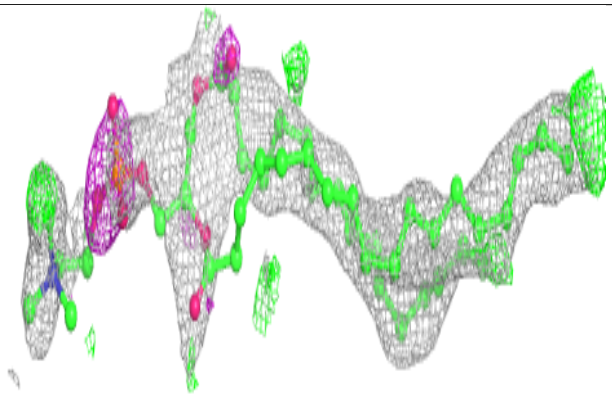


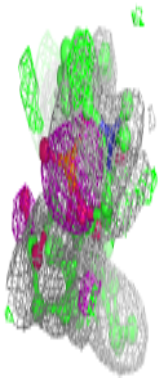


Electron density around PSC O 4230:

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

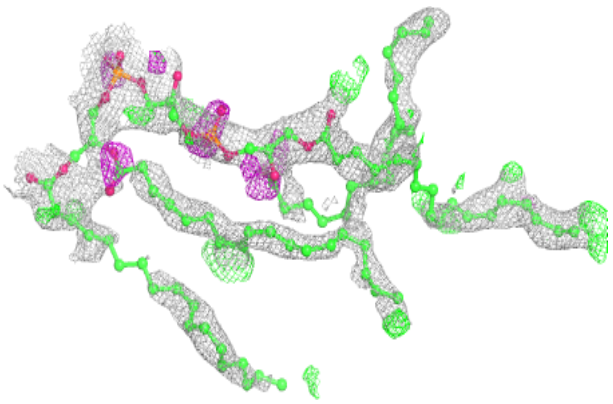


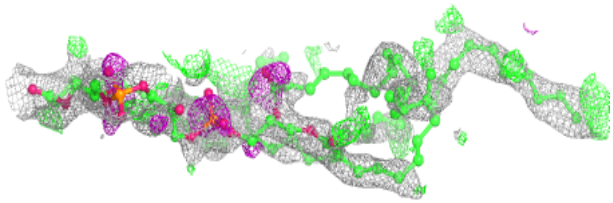


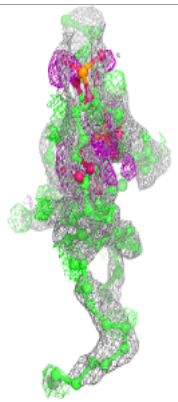


Electron density around CDL G 3269:

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

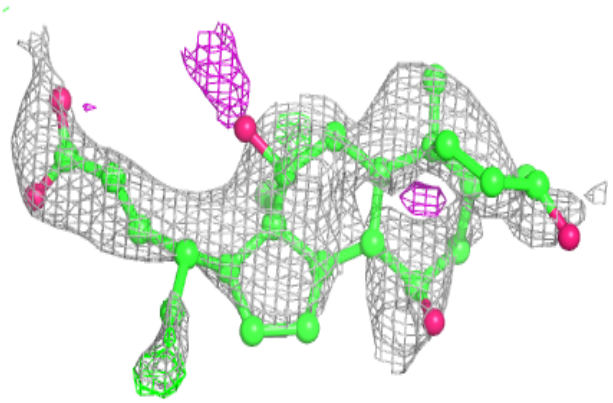


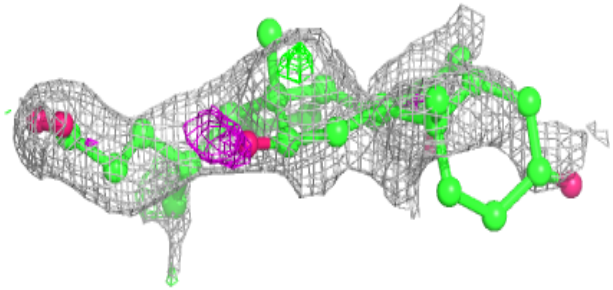


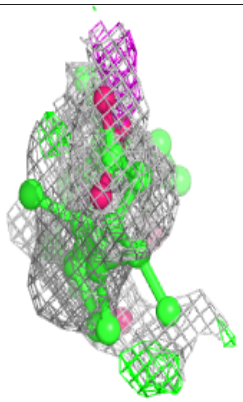


Electron density around CHD J 3060:

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

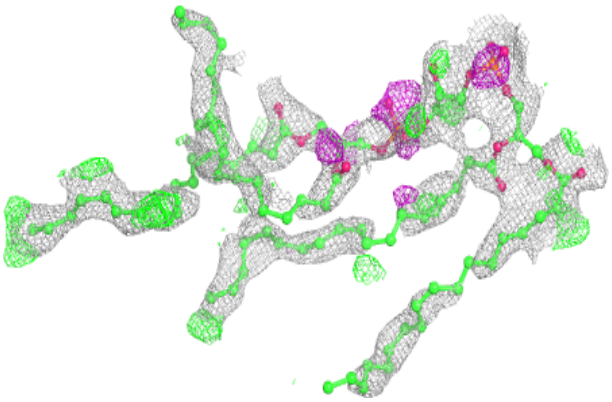


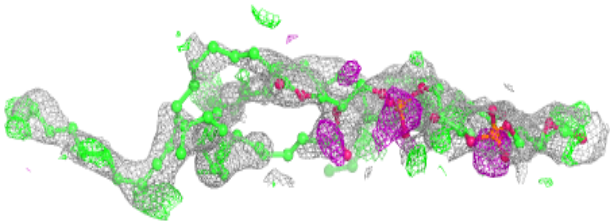


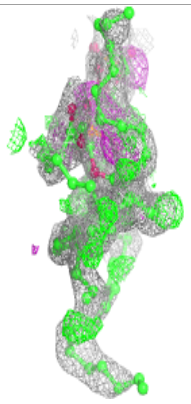


Electron density around CDL T 4269:

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

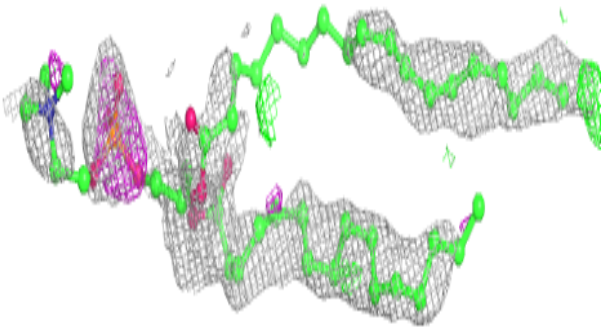


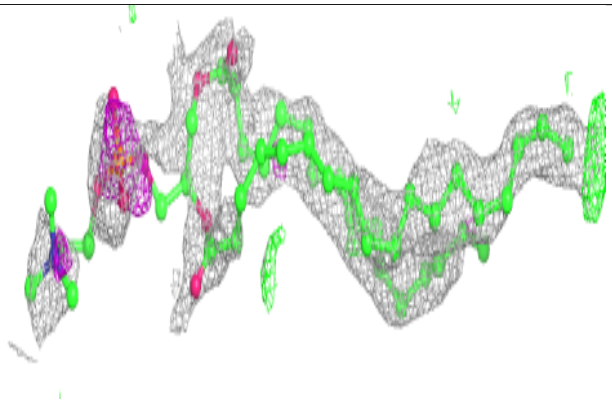


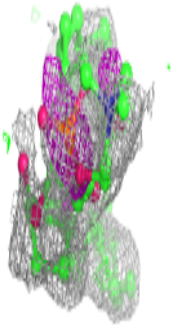


Electron density around PSC E 3230:

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

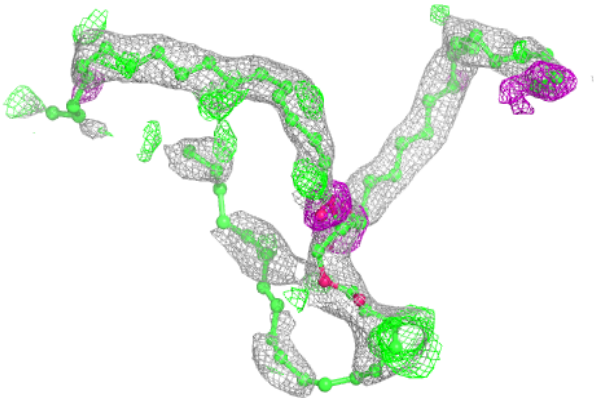


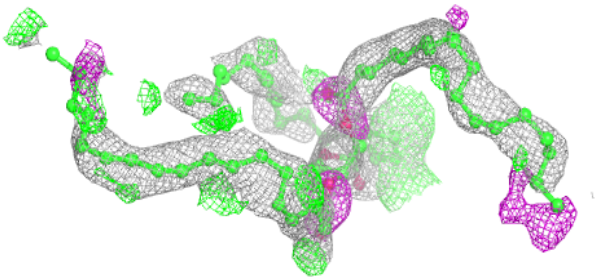


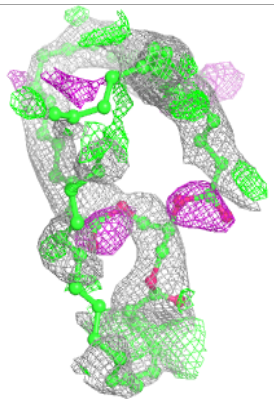


Electron density around TGL N 4522:

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

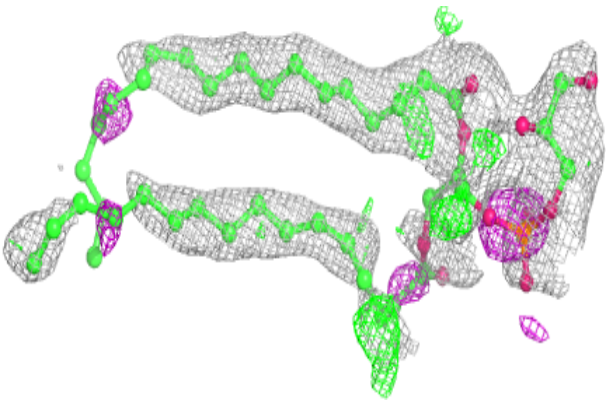


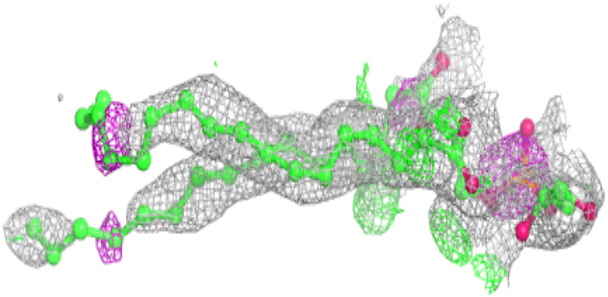


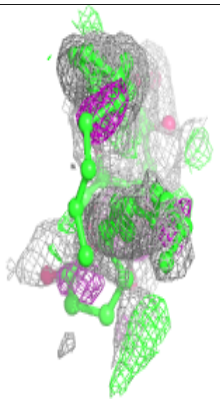


Electron density around PGV N 4524:

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

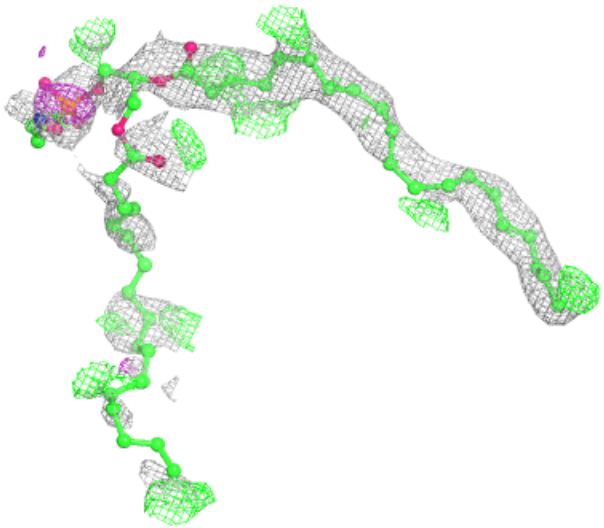


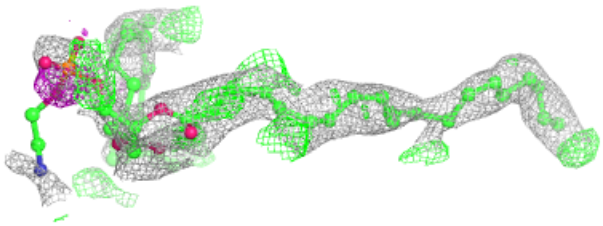


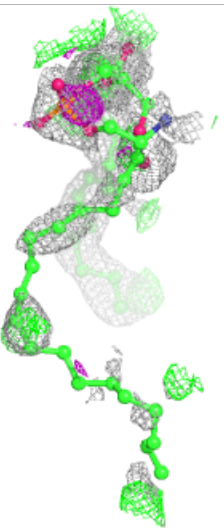


Electron density around PEK G 4263:

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

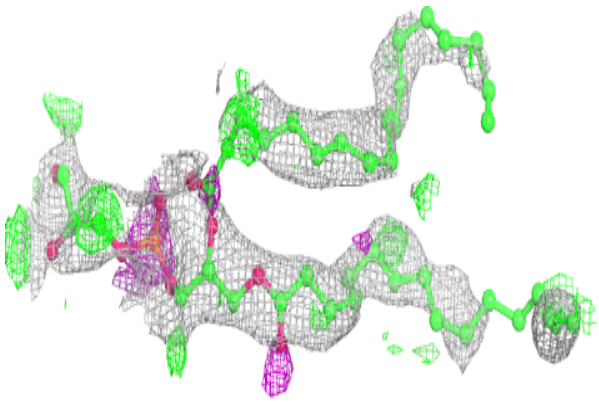


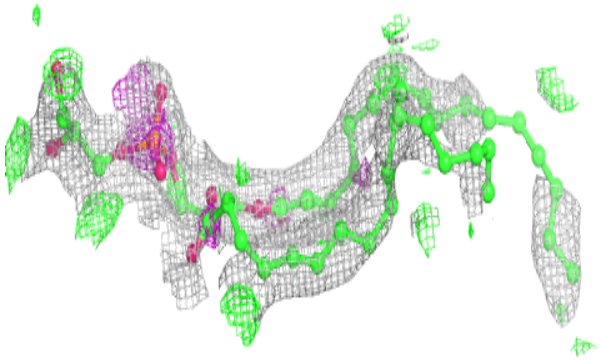


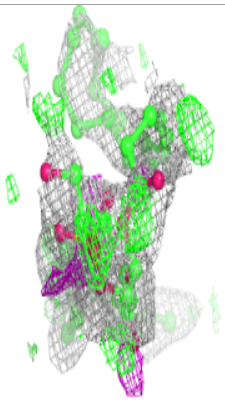


Electron density around PGV C 3268:

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

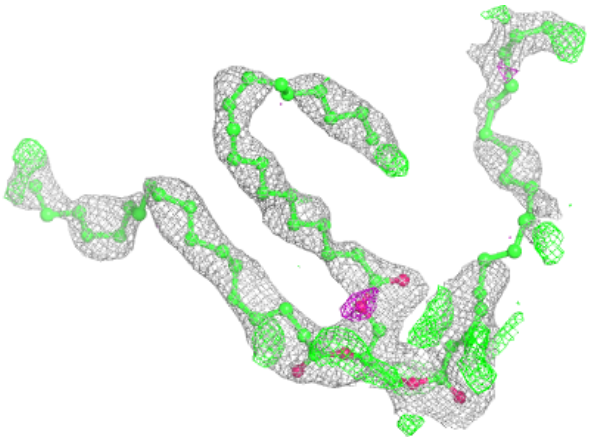


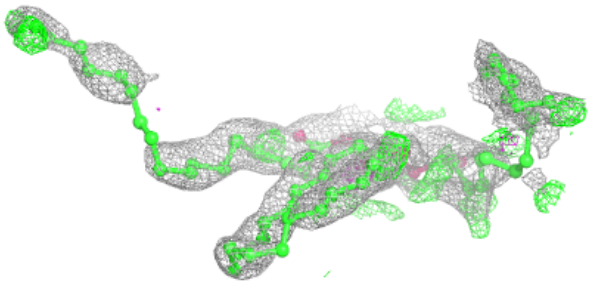


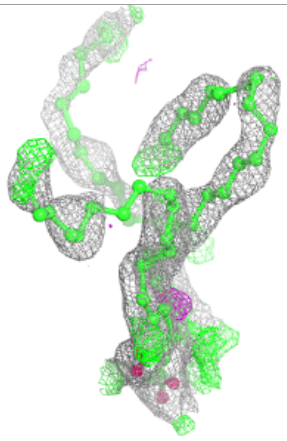


Electron density around TGL Q 4523:

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

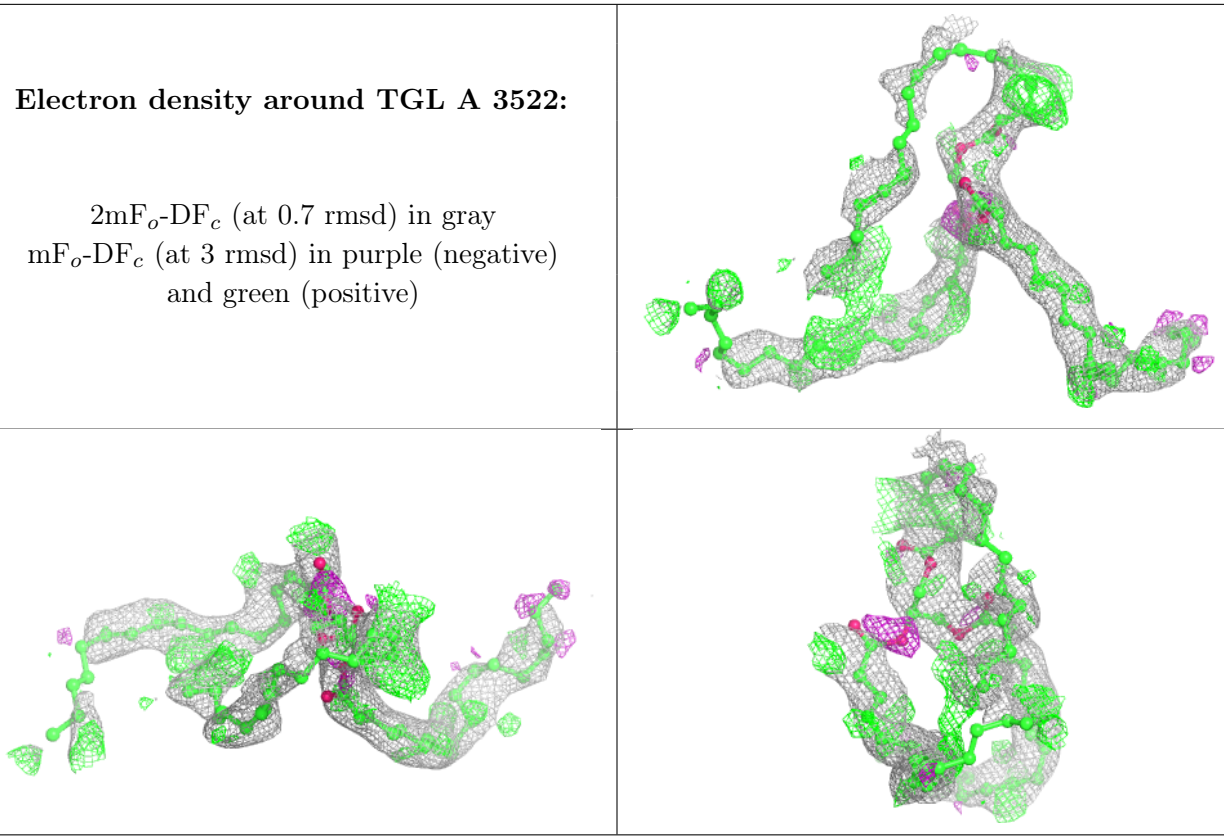






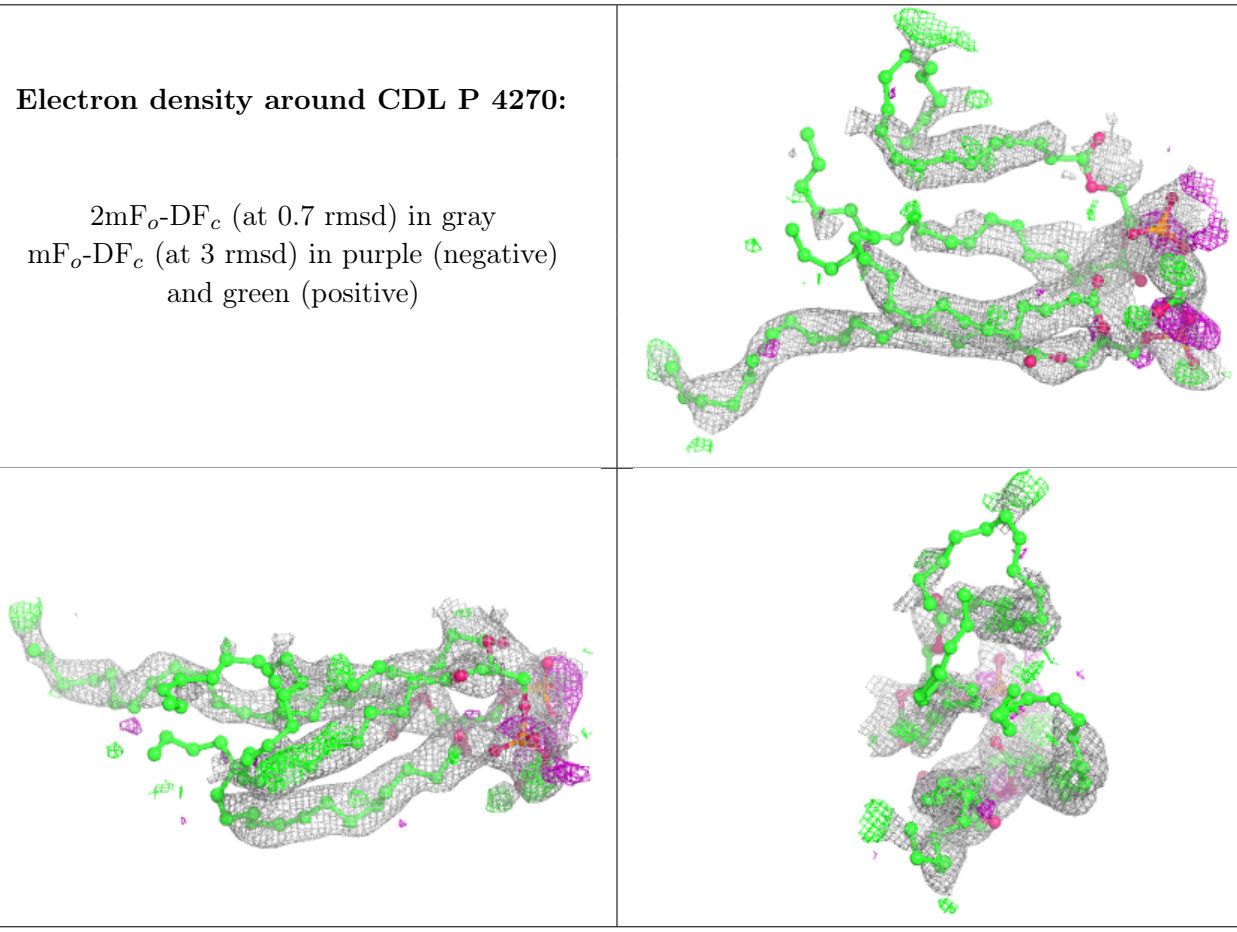
Electron density around TGL A 3522:

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



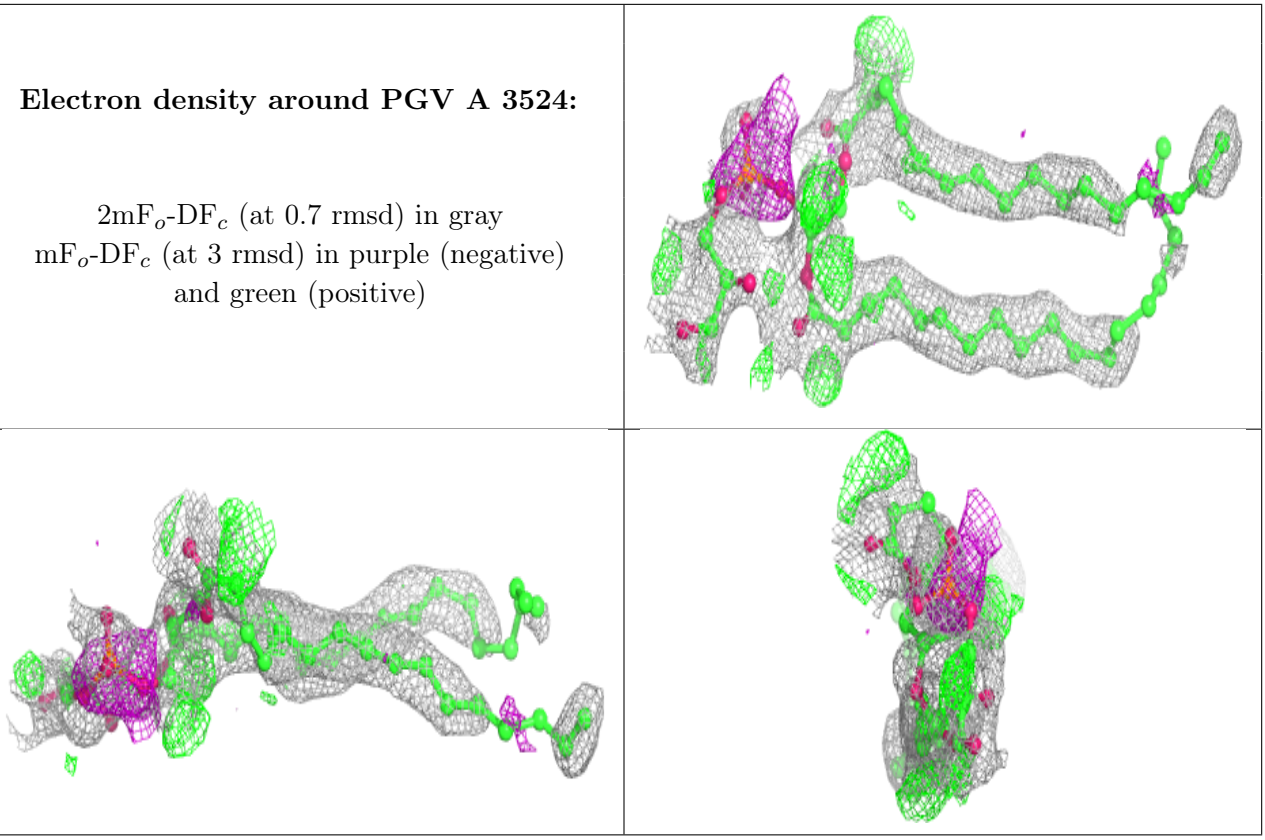
Electron density around CDL P 4270:

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



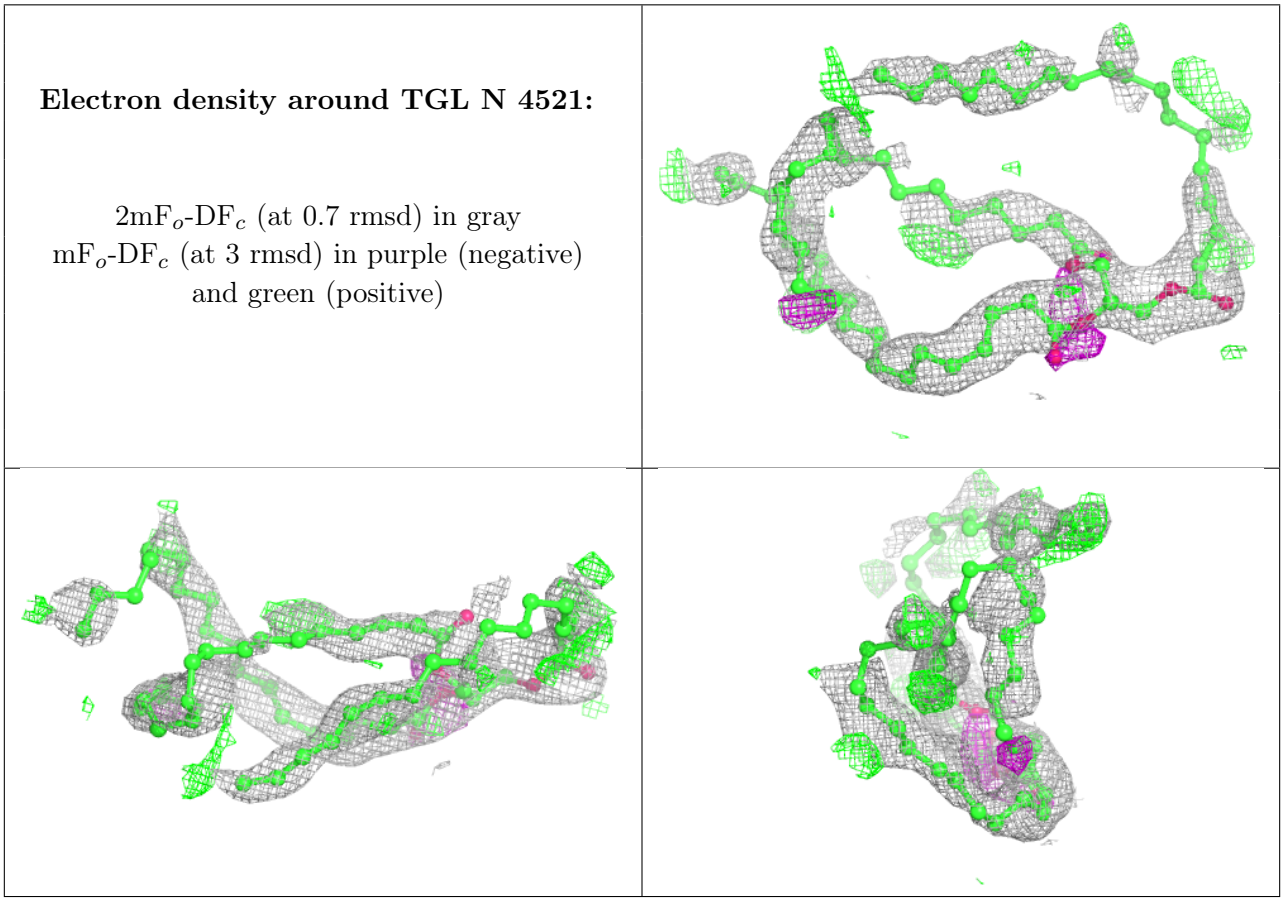
Electron density around PGV A 3524:

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



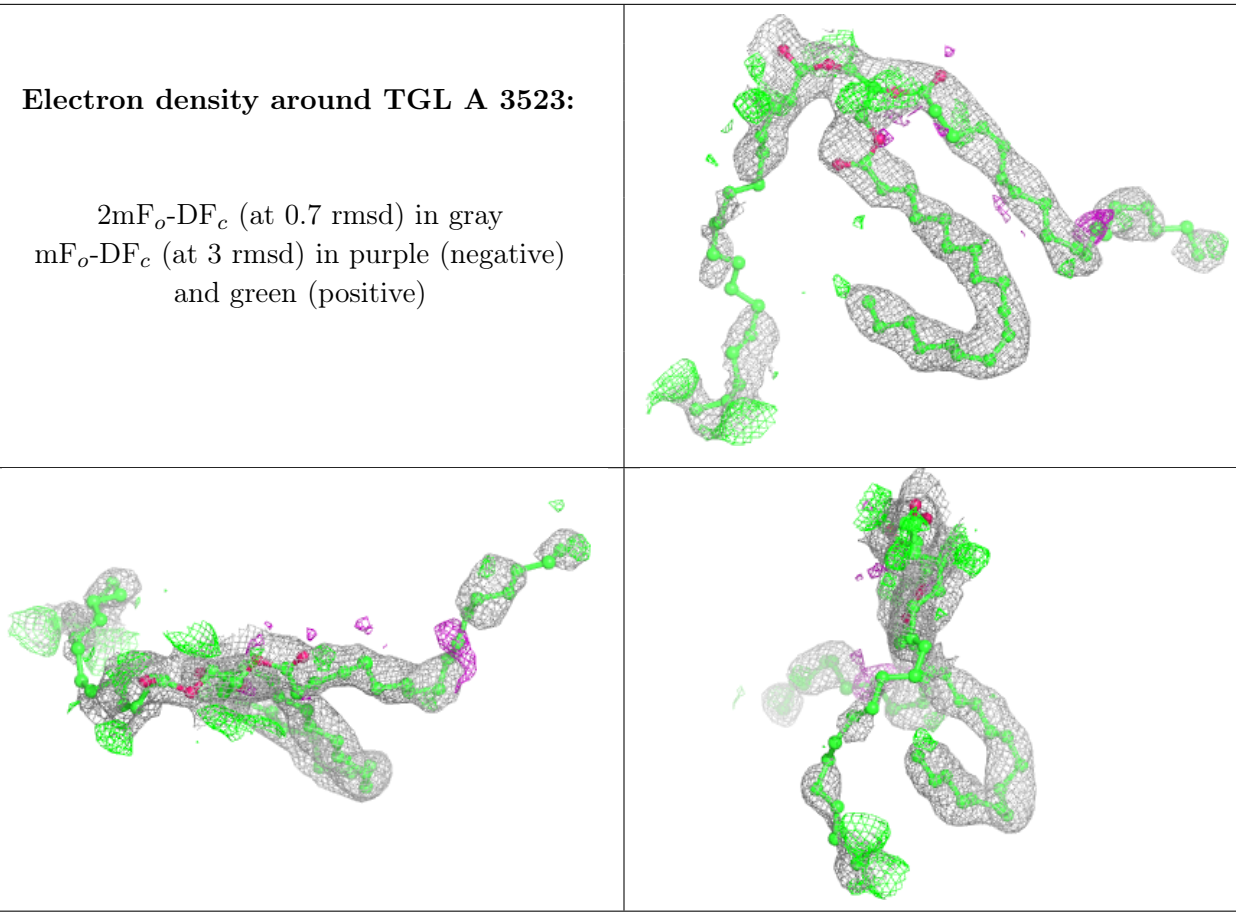
Electron density around TGL N 4521:

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



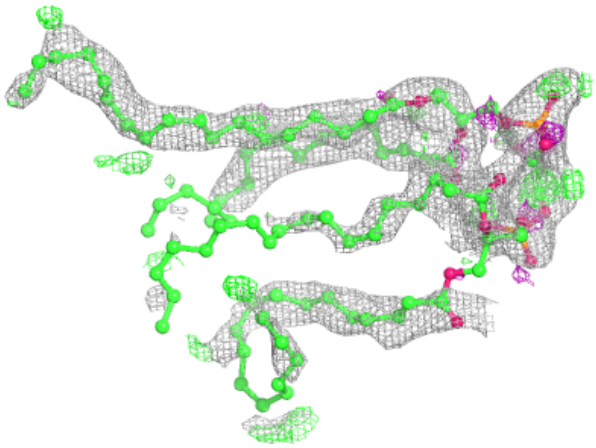
Electron density around TGL A 3523:

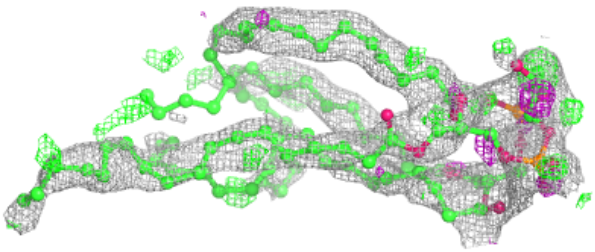
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

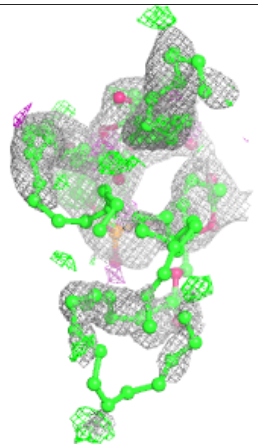


Electron density around CDL C 3270:

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

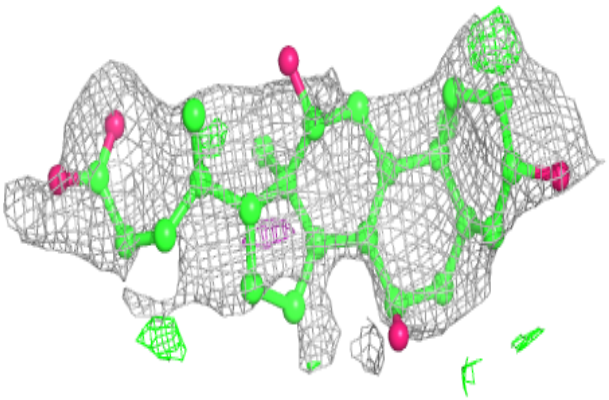


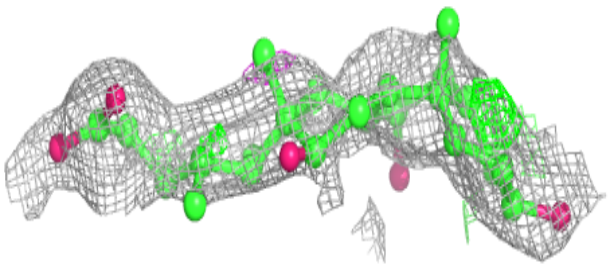


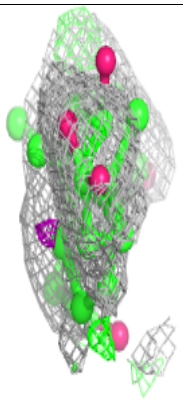


Electron density around CHD P 4271:

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

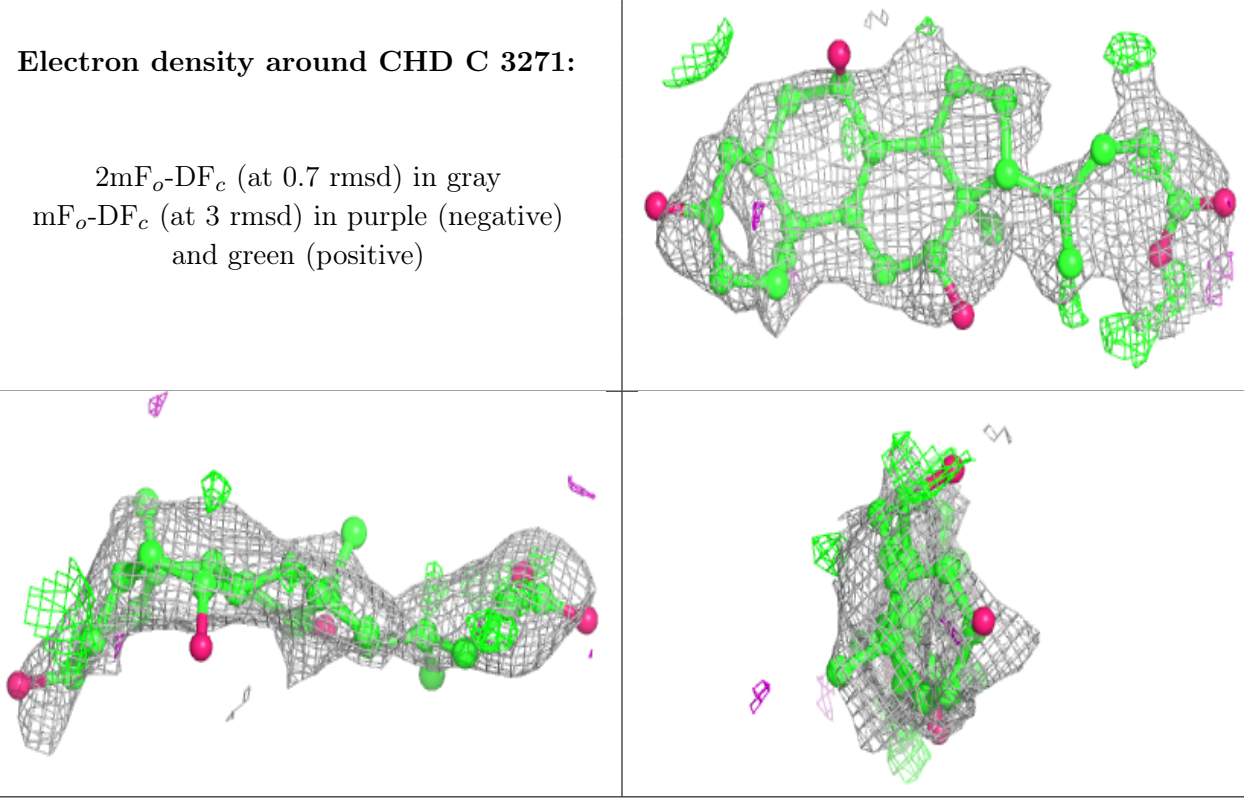






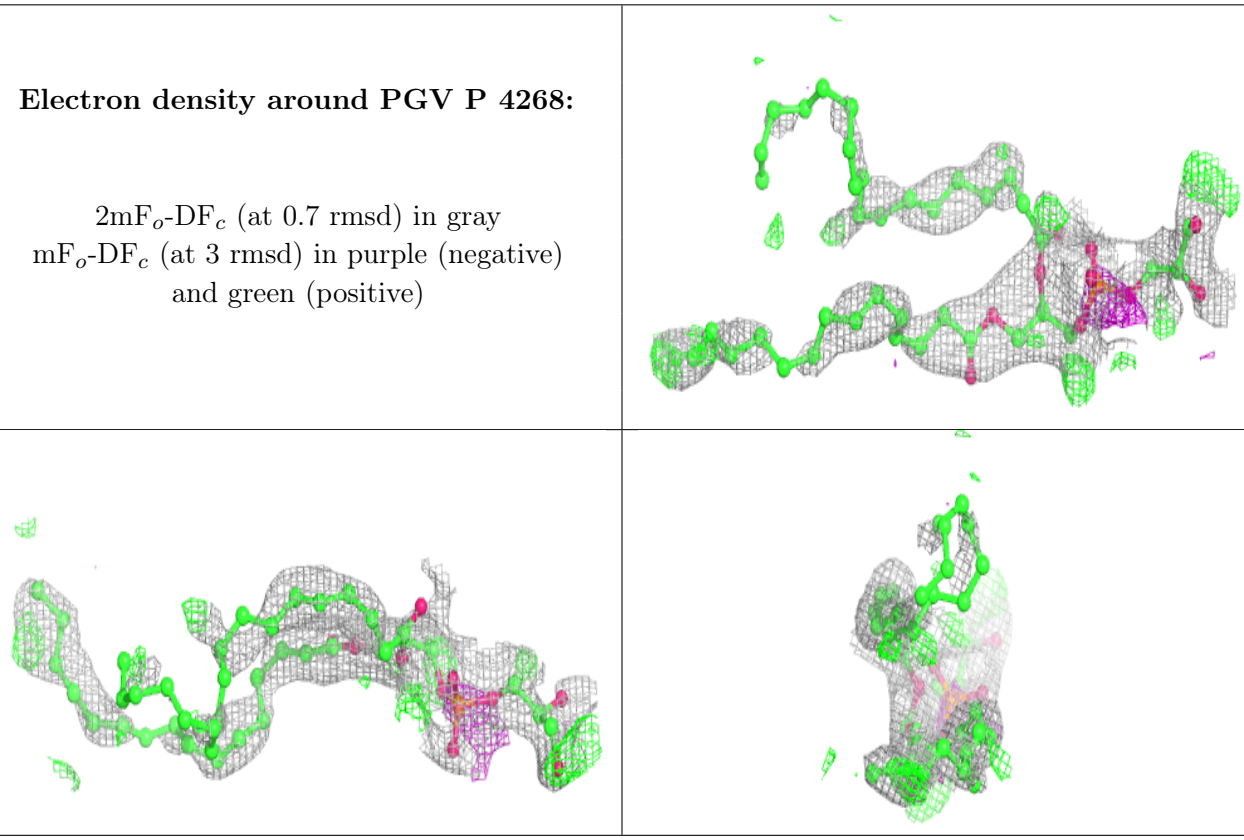
Electron density around CHD C 3271:

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



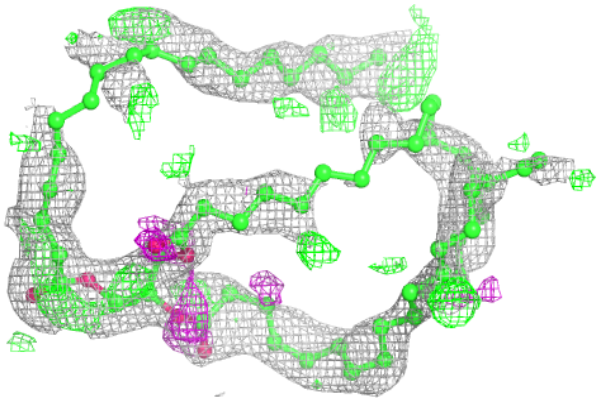
Electron density around PGV P 4268:

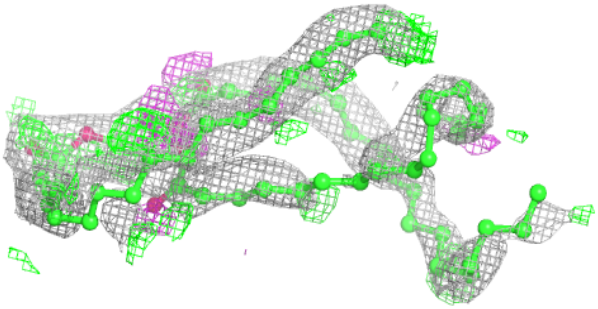
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

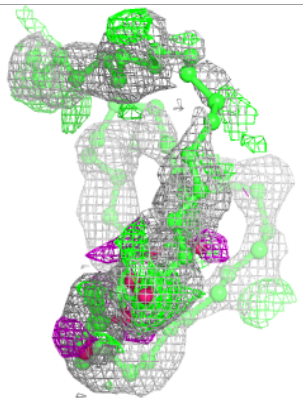


Electron density around TGL A 3521:

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

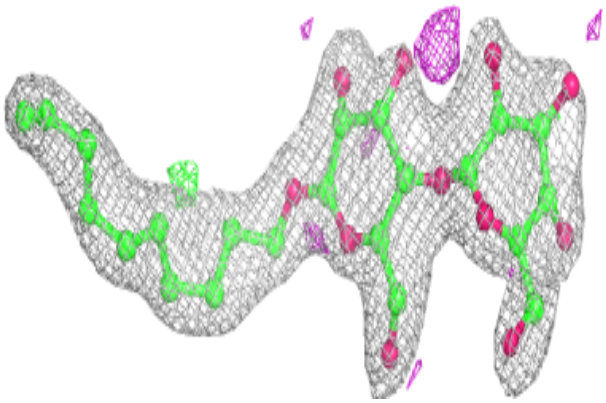


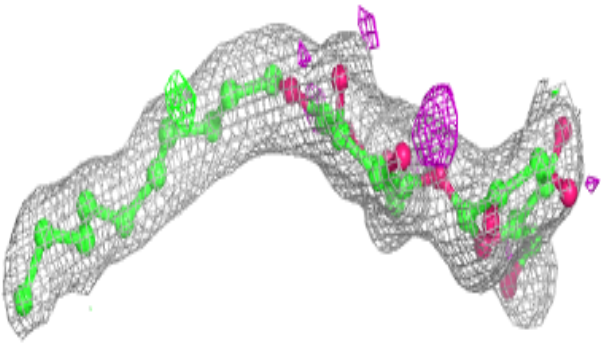


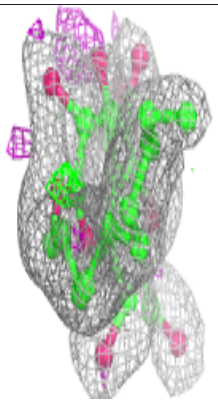


Electron density around DMU Z 4526:

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

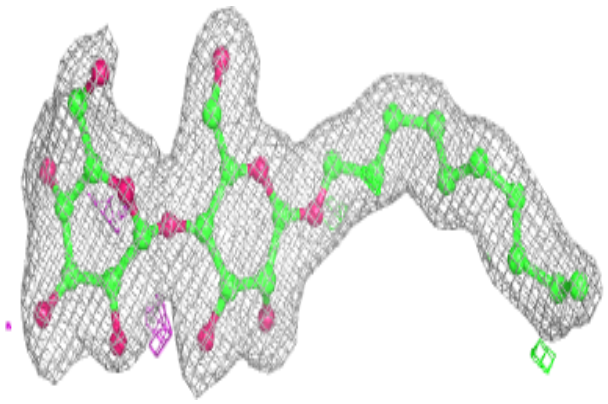


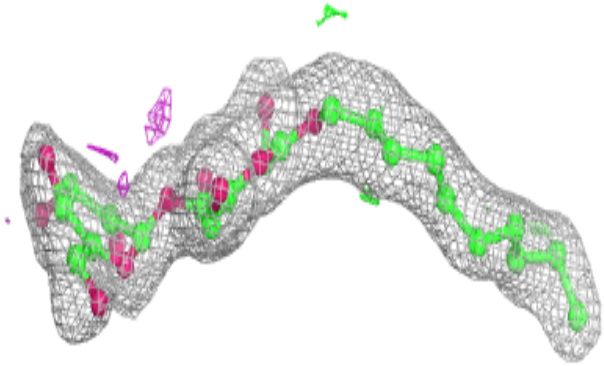


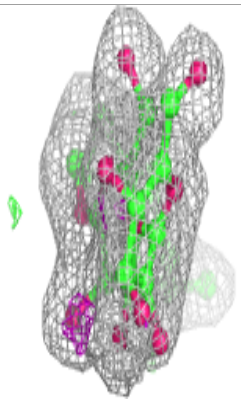


Electron density around DMU M 3526:

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

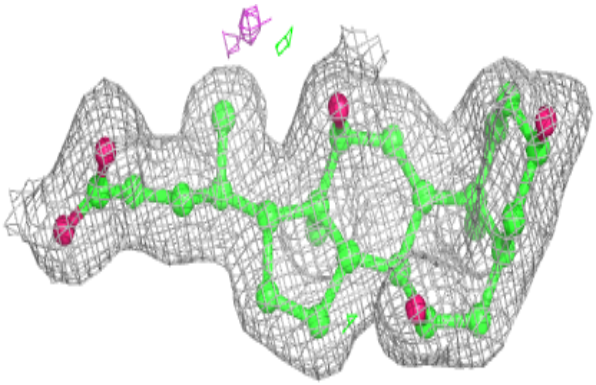


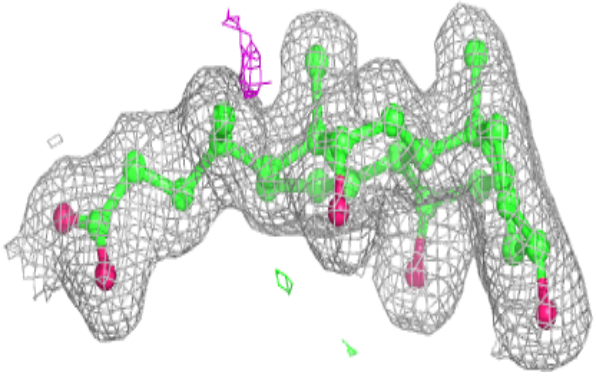


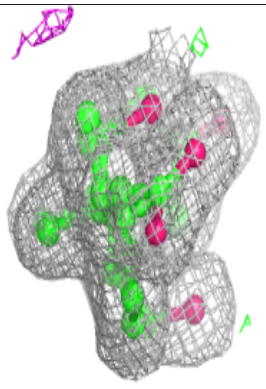


Electron density around CHD P 4525:

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

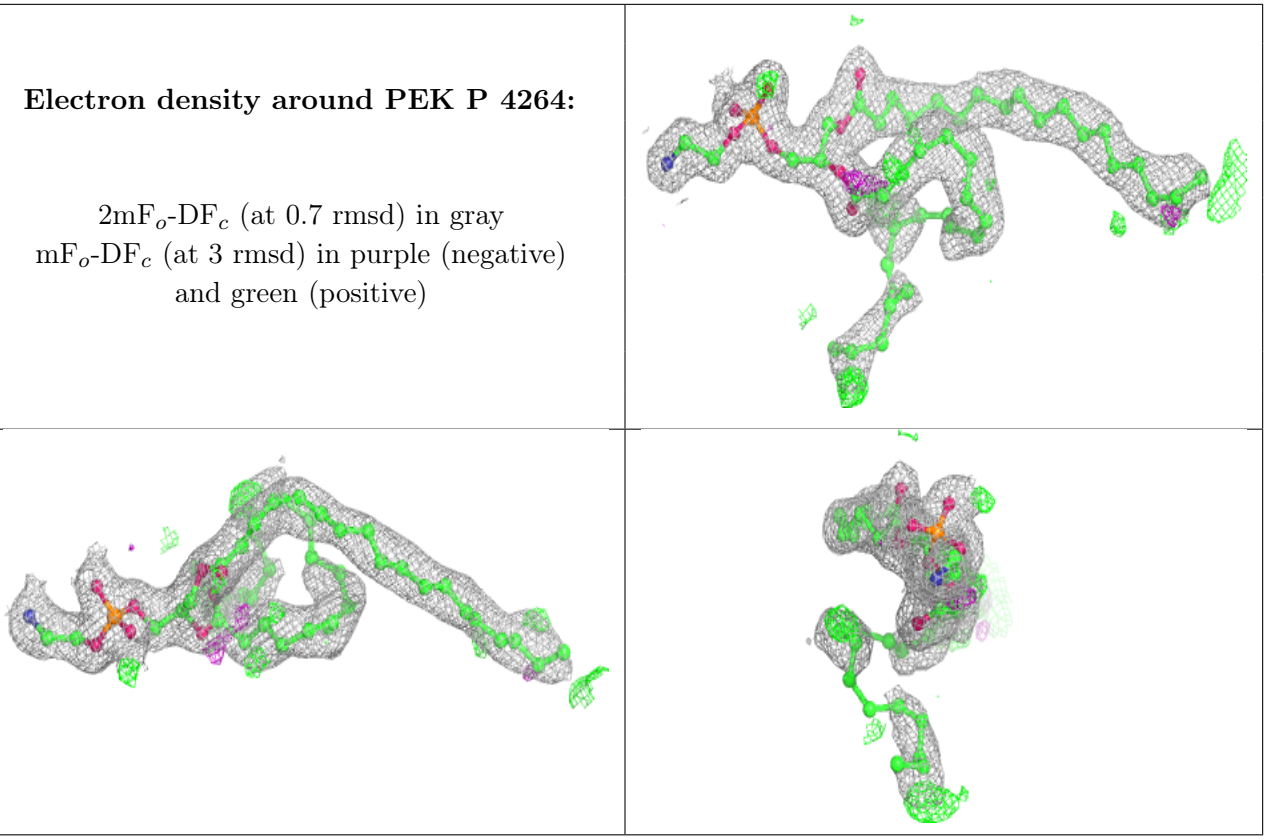






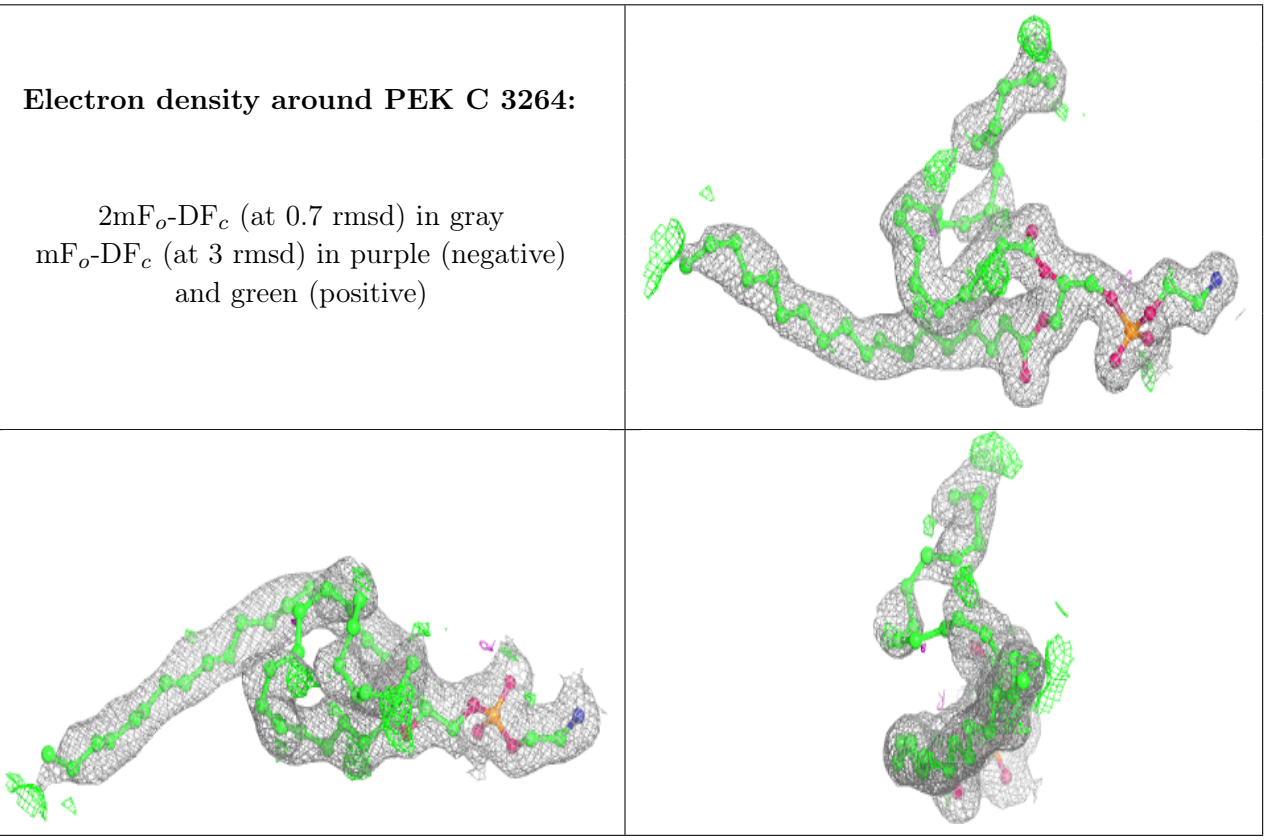
Electron density around PEK P 4264:

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



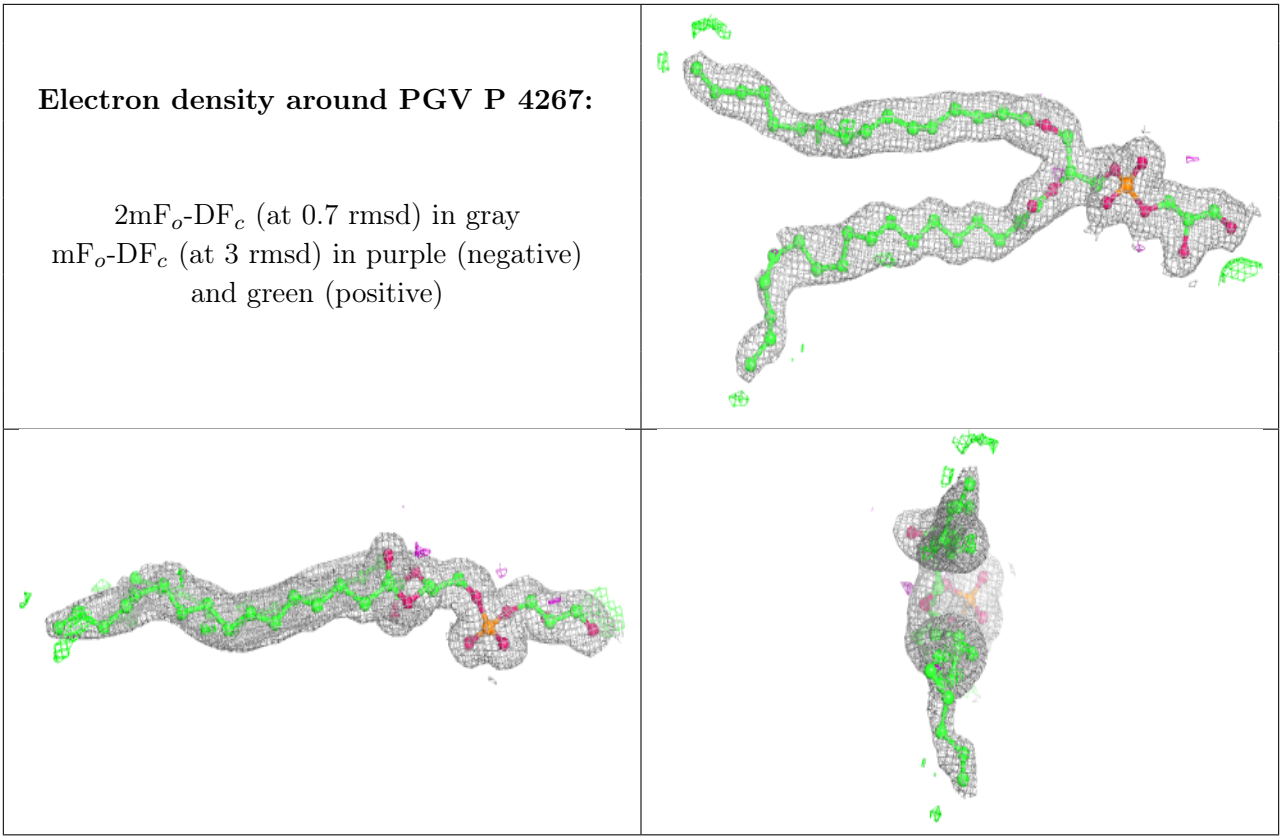
Electron density around PEK C 3264:

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



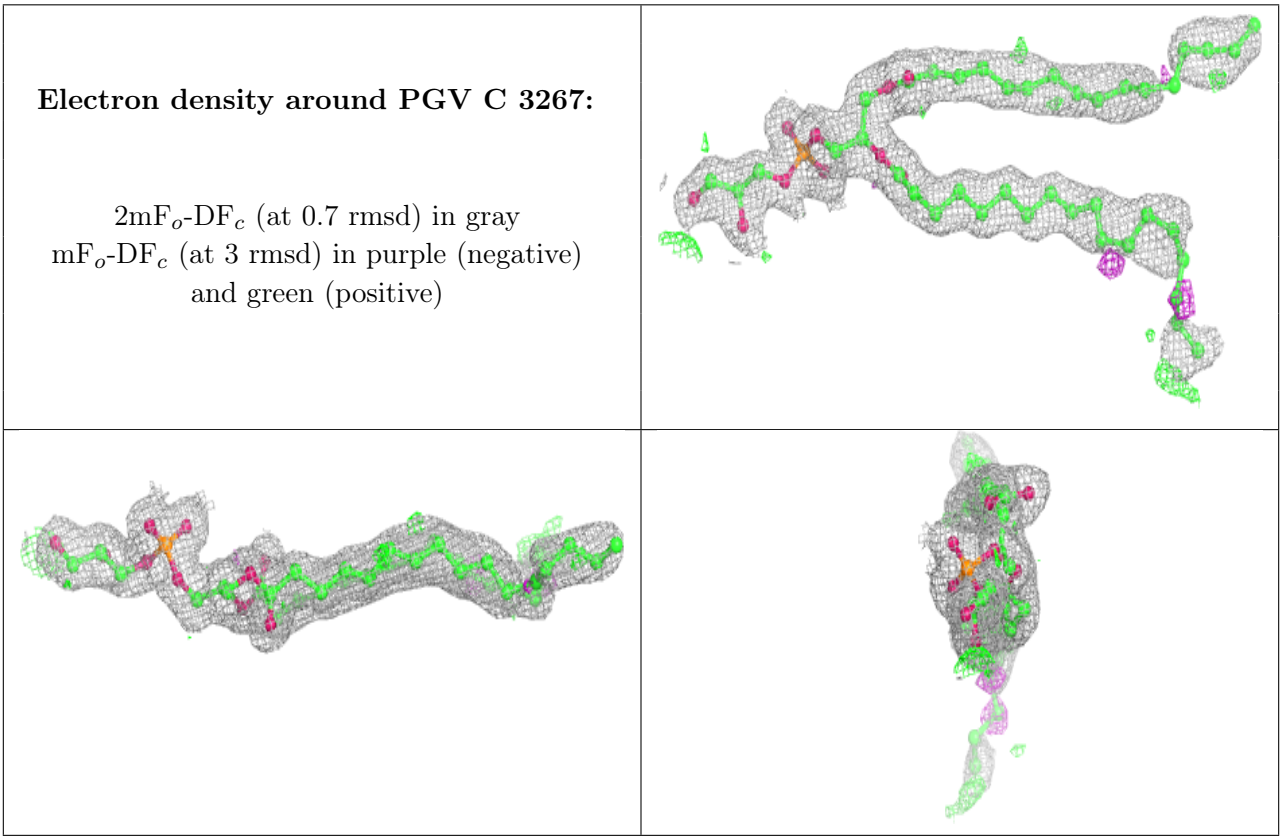
Electron density around PGV P 4267:

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



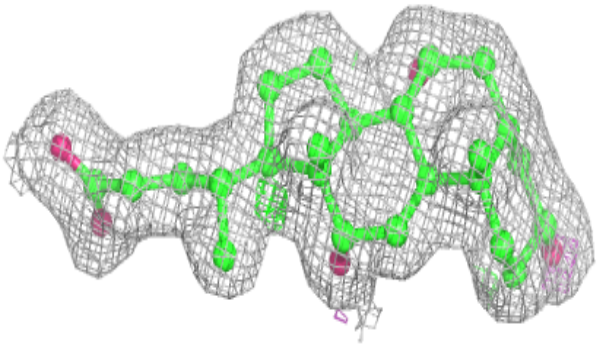
Electron density around PGV C 3267:

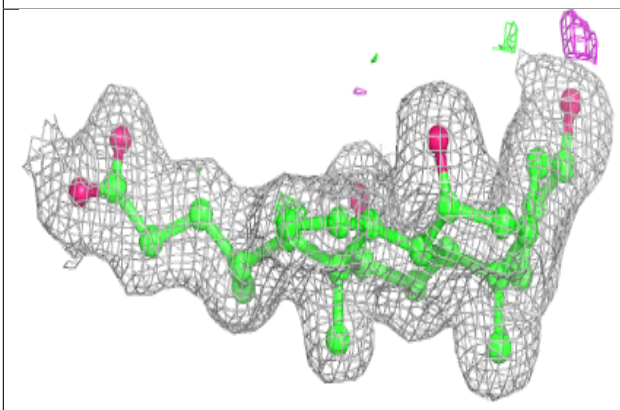
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

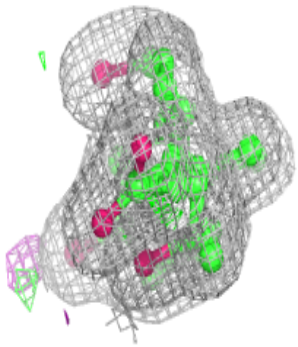


Electron density around CHD C 3525:

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

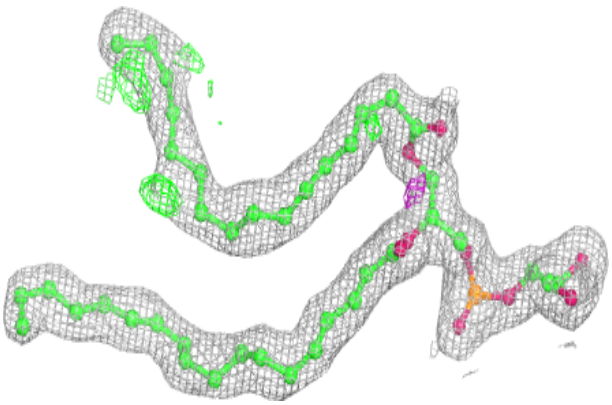


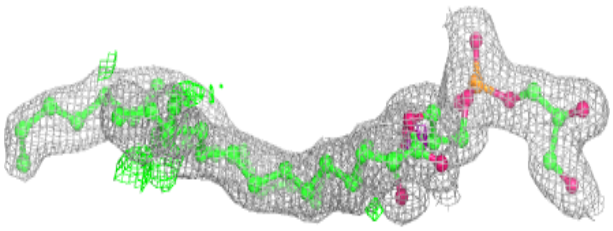


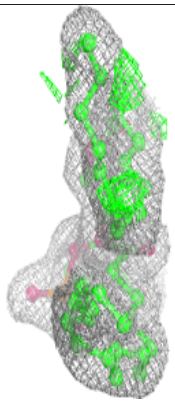


Electron density around PGV N 4266:

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

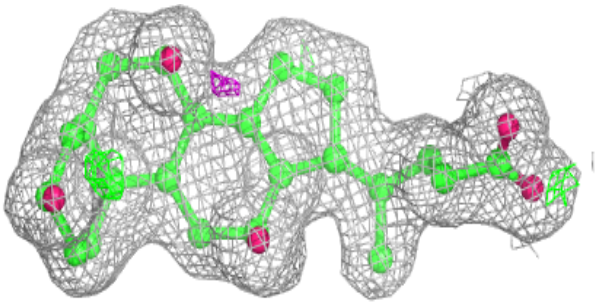


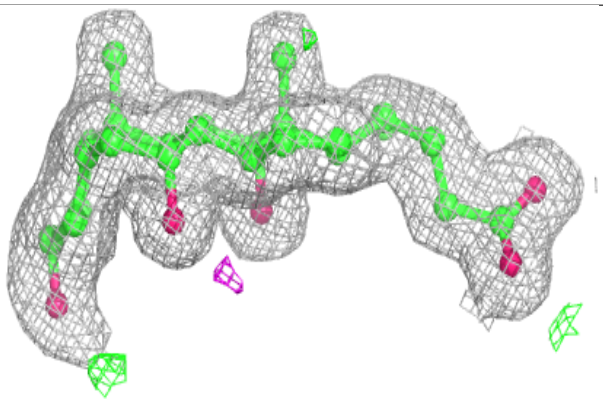


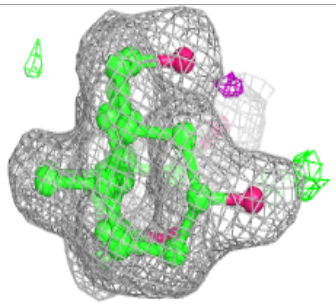


Electron density around CHD B 4085:

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

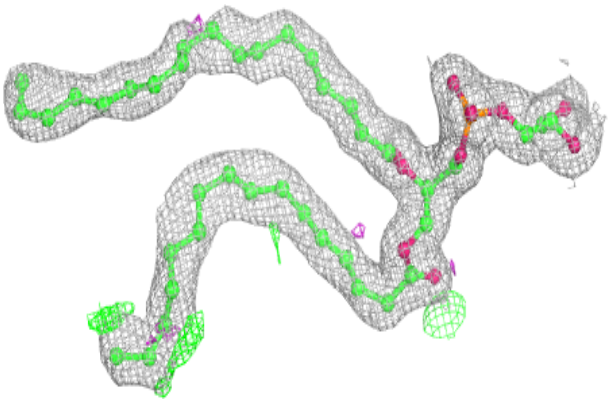


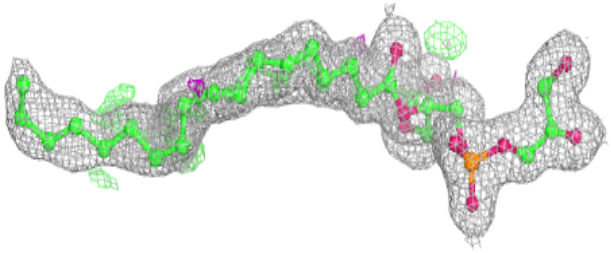


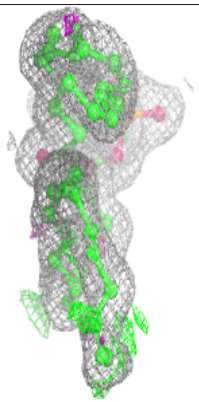


Electron density around PGV A 3266:

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

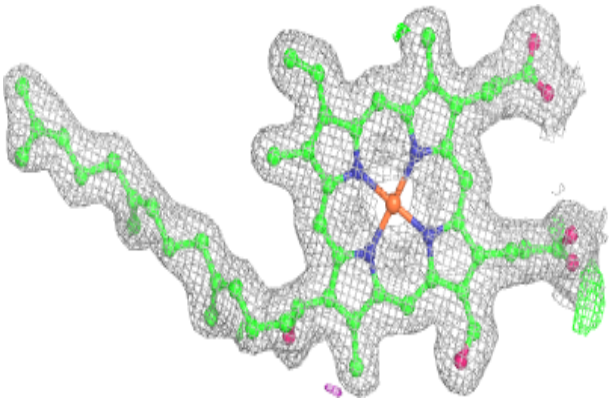


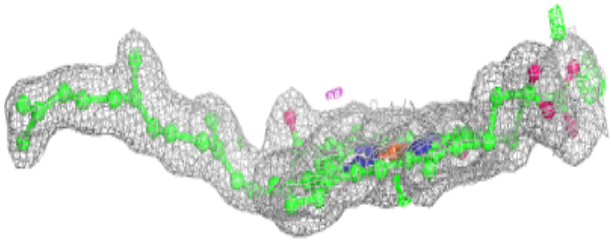


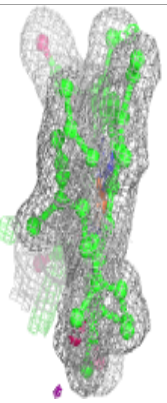


Electron density around HEA N 515:

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

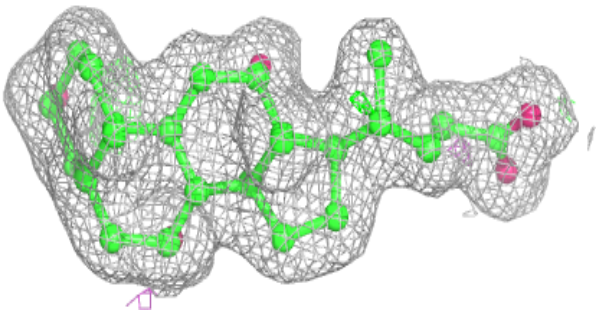


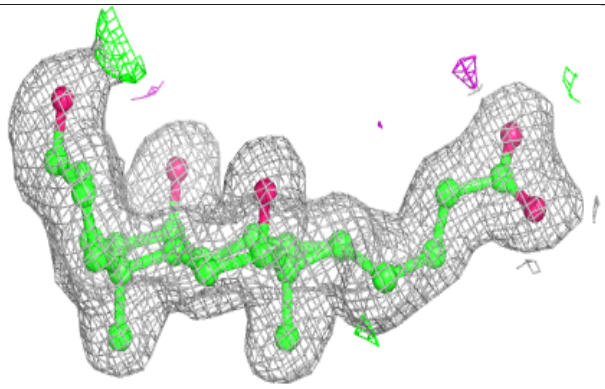


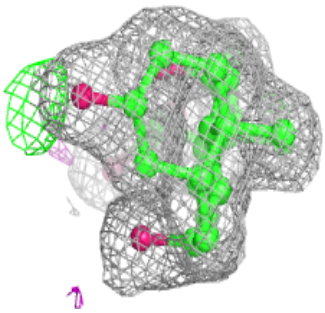


Electron density around CHD O 3085:

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

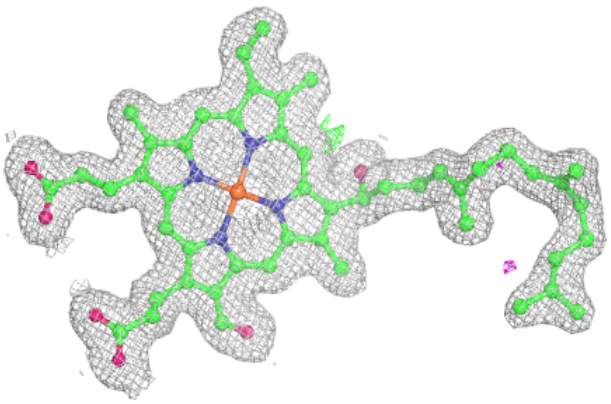


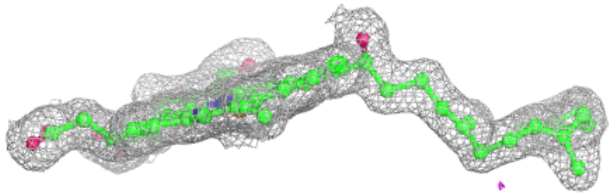


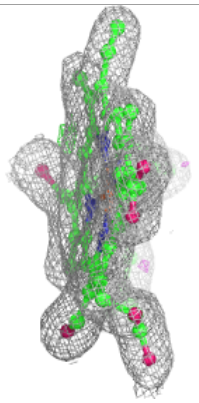


Electron density around HEA N 516:

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

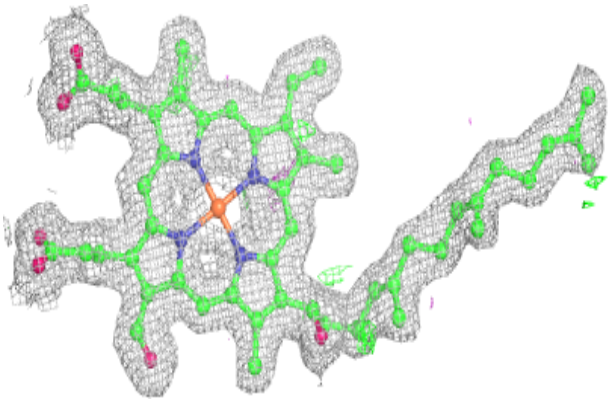


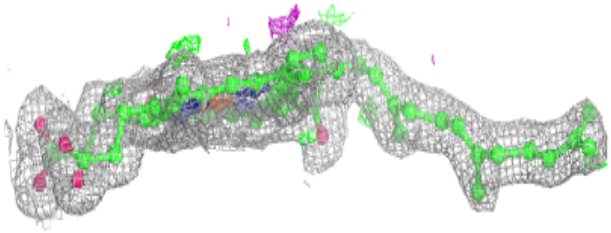


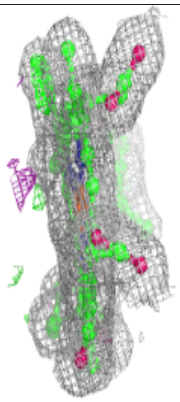


Electron density around HEA A 515:

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

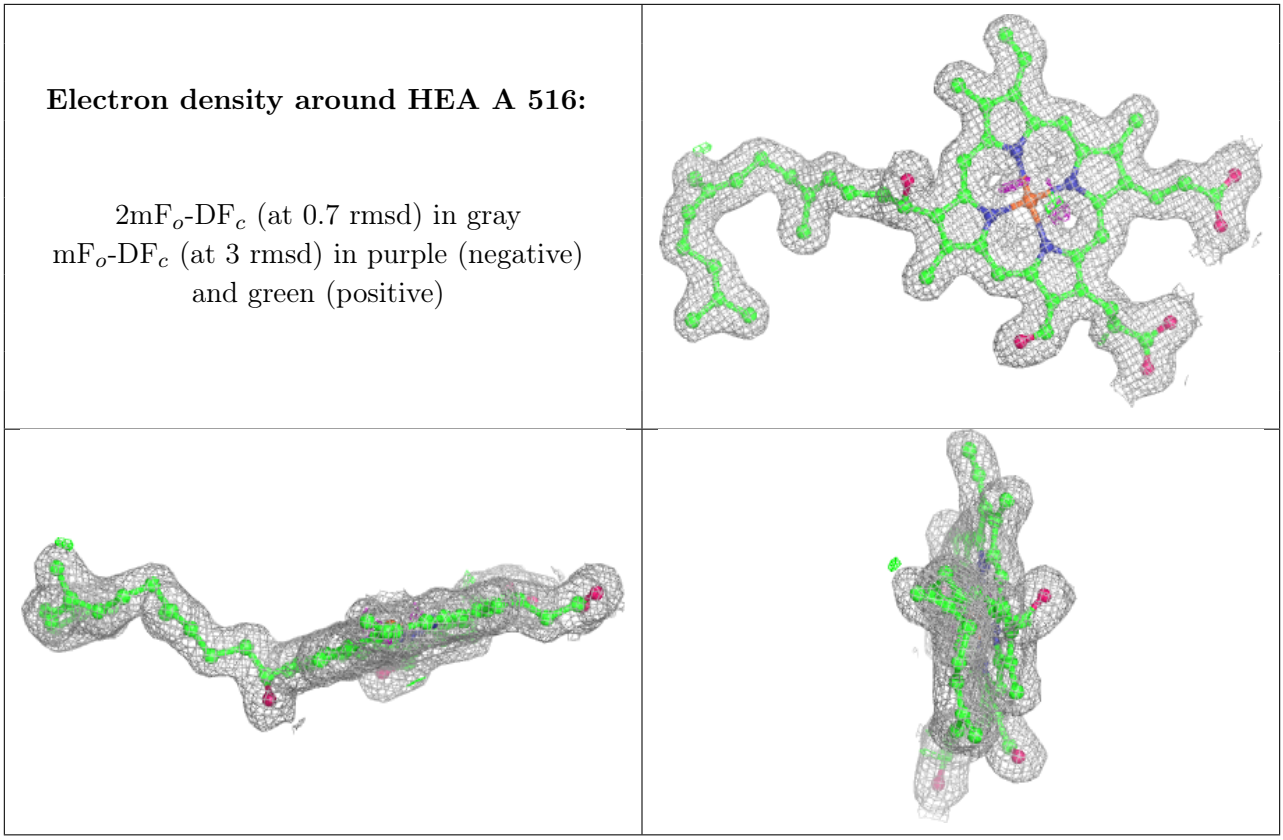






Electron density around HEA A 516:

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



6.5 Other polymers (i)

There are no such residues in this entry.