



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2021 – 08:40 PM EST

PDB ID : 1SQP  
Title : Crystal Structure Analysis of Bovine Bcl with Myxothiazol  
Authors : Esser, L.; Quinn, B.; Li, Y.F.; Zhang, M.; Elberry, M.; Yu, L.; Yu, C.A.; Xia, D.  
Deposited on : 2004-03-19  
Resolution : 2.70 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](mailto: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.

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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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.17.1

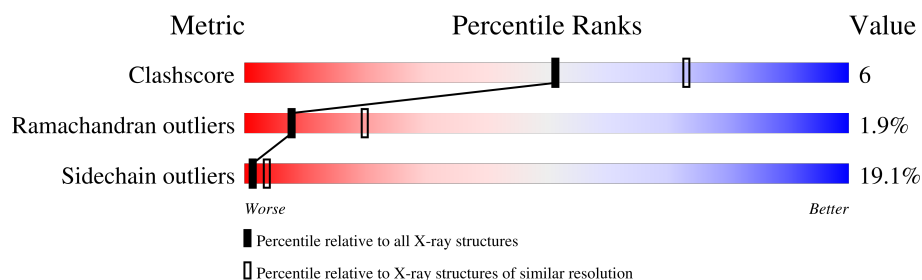
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	480	71% 20% • 7%
2	B	453	73% 16% • • 7%
3	C	379	72% 26% • •
4	D	241	68% 26% 6% •
5	E	196	70% 27% •
6	F	110	82% 13% • 5%
7	G	81	67% 25% • 7%
8	H	78	55% 29% • 14%

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Mol	Chain	Length	Quality of chain
9	I	78	
10	J	62	
11	K	56	

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
12	CDL	A	447	X	-	-	-
12	CDL	D	242	X	-	-	-
12	CDL	G	82	X	-	-	-

## 2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 17274 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 Ubiquinol-cytochrome-c reductase complex core protein I, mitochondrial precursor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	0	0
			3458	2161	609	668	20			

- Molecule 2 is a protein called Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial precursor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	423	Total	C	N	O	S	0	0	0
			3172	1993	562	610	7			

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	378	Total	C	N	O	S	0	0	0
			3003	2013	471	501	18			

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	241	Total	C	N	O	S	0	0	0
			1919	1225	330	349	15			

- Molecule 5 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial precursor (EC 1.10.2.2) (Rieske iron-sulfur protein) (RISP) [Contains: Ubiquinol-cytochrome c reductase 8 kDa protein (Complex III subunit IX)].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	196	Total	C	N	O	S	0	0	0
			1519	957	263	291	8			

- Molecule 6 is a protein called sub6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	105	Total	C	N	O	S	0	0	0
			911	576	165	168	2			

- Molecule 7 is a protein called Ubiquinol-cytochrome c reductase complex ubiquinone-binding protein QP-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	75	Total	C	N	O	S	0	0	0
			628	410	118	99	1			

- Molecule 8 is a protein called Ubiquinol-cytochrome c reductase complex 11 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	67	Total	C	N	O	S	0	0	0
			548	332	99	112	5			

- Molecule 9 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial precursor (EC 1.10.2.2) (Rieske iron-sulfur protein) (RISP) [Contains: Ubiquinol-cytochrome c reductase 8 kDa protein (Complex III subunit IX)].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	57	Total	C	N	O	S	0	0	0
			406	253	77	74	2			

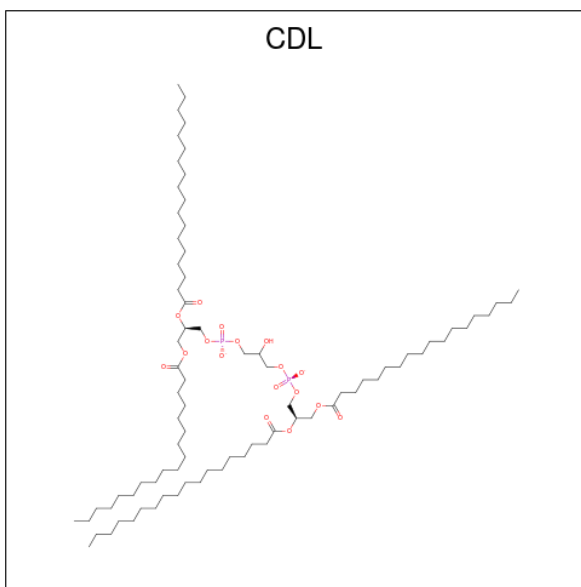
- Molecule 10 is a protein called Ubiquinol-cytochrome c reductase complex 7.2 kDa protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	61	Total	C	N	O	0	0	0
			502	329	87	86			

- Molecule 11 is a protein called Ubiquinol-cytochrome c reductase complex 6.4 kDa protein.

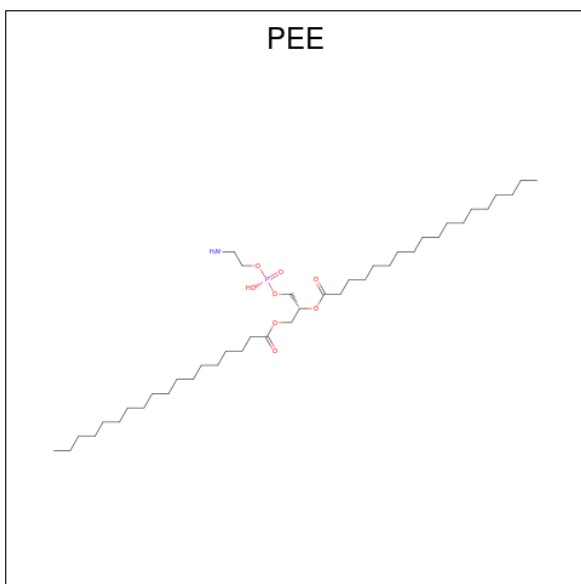
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	53	Total	C	N	O	S	0	0	0
			436	292	78	65	1			

- Molecule 12 is CARDIOLIPIN (three-letter code: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>).



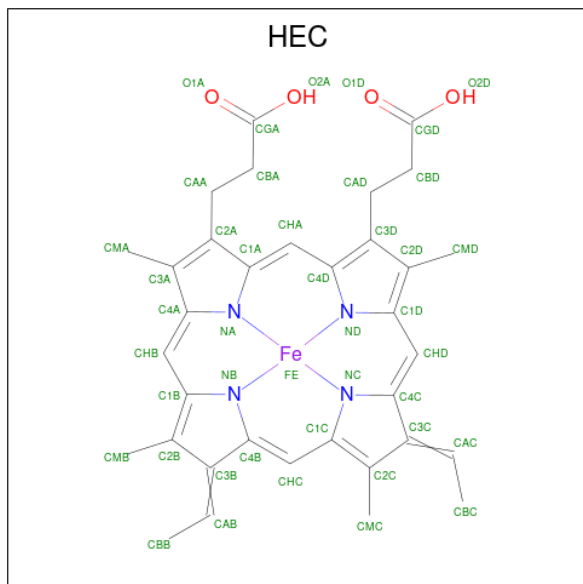
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	A	1	Total	C	O	P	0	0
			64	45	17	2		
12	D	1	Total	C	O	P	0	0
			64	45	17	2		
12	G	1	Total	C	O	P	0	0
			64	45	17	2		

- Molecule 13 is 1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula:  $C_{41}H_{83}NO_8P$ ).



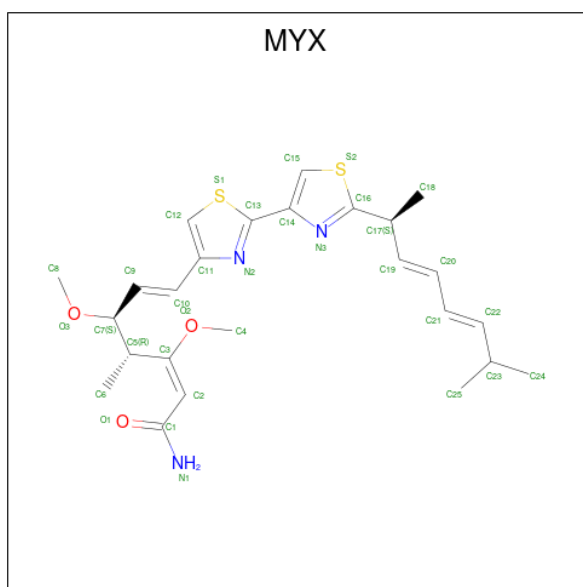
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	A	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
13	C	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
13	E	1	Total	C	N	O	P	0	0
			49	39	1	8	1		

- Molecule 14 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



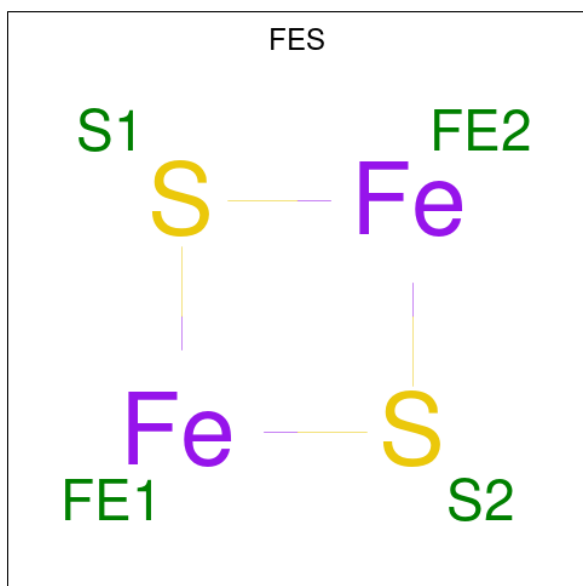
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
14	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
14	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 15 is (2Z,6E)-7-{2'-[(2E,4E)-1,6-DIMETHYLHEPTA-2,4-DIENYL]-2,4'-BI-1,3-THIAZOL-4-YL}-3,5-DIMETHOXY-4-METHYLHEPTA-2,6-DIENAMID E (three-letter code: MYX) (formula:  $C_{25}H_{33}N_3O_3S_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	C	1	Total	C	N	O	S	0	0
			33	25	3	3	2		

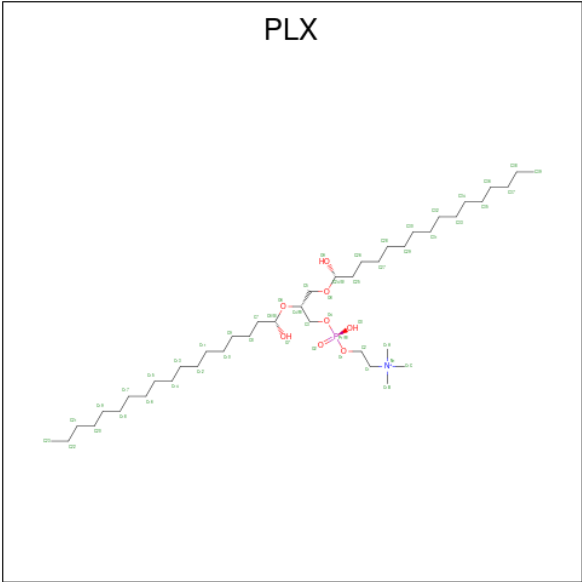
- Molecule 16 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	E	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 17 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (three-letter code: PLX) (formula:  $\text{C}_{42}\text{H}_{89}\text{NO}_8\text{P}$ ).





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

• Molecule 18 is water.

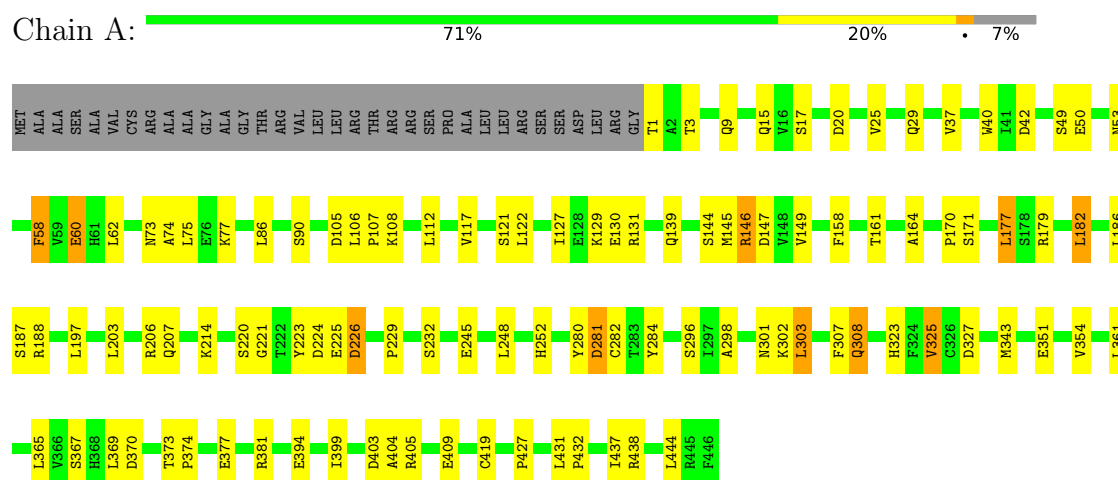
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	51	Total	O	0	0
			51	51		
18	B	84	Total	O	0	0
			84	84		
18	C	36	Total	O	0	0
			36	36		
18	D	11	Total	O	0	0
			11	11		
18	E	2	Total	O	0	0
			2	2		
18	F	15	Total	O	0	0
			15	15		
18	G	11	Total	O	0	0
			11	11		
18	I	2	Total	O	0	0
			2	2		
18	K	3	Total	O	0	0
			3	3		

### 3 Residue-property plots

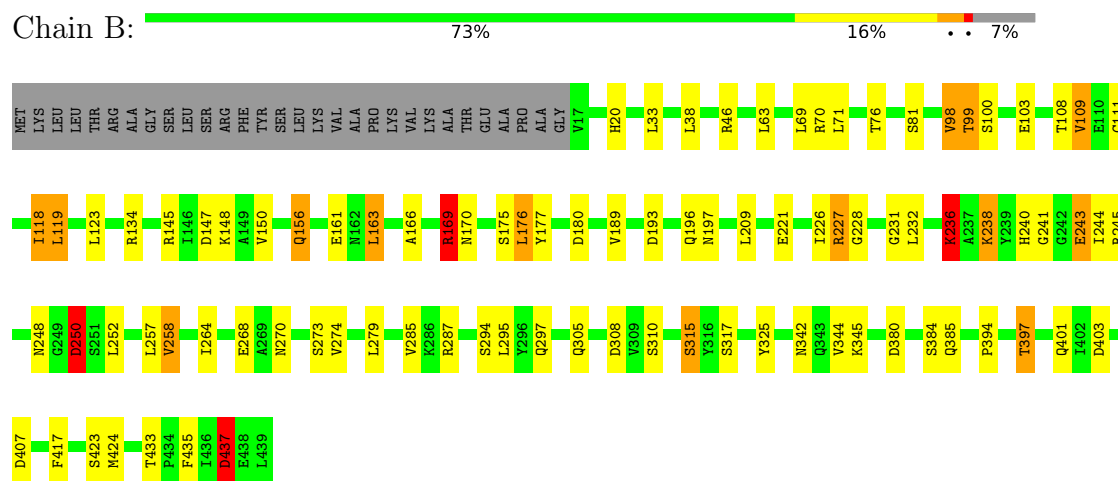
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

- Molecule 1: Ubiquinol-cytochrome-c reductase complex core protein I, mitochondrial precursor

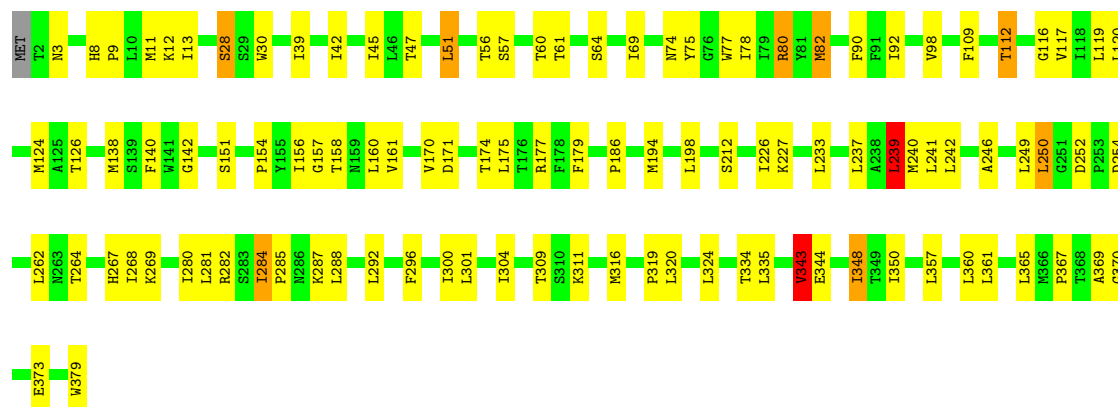


- Molecule 2: Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial precursor



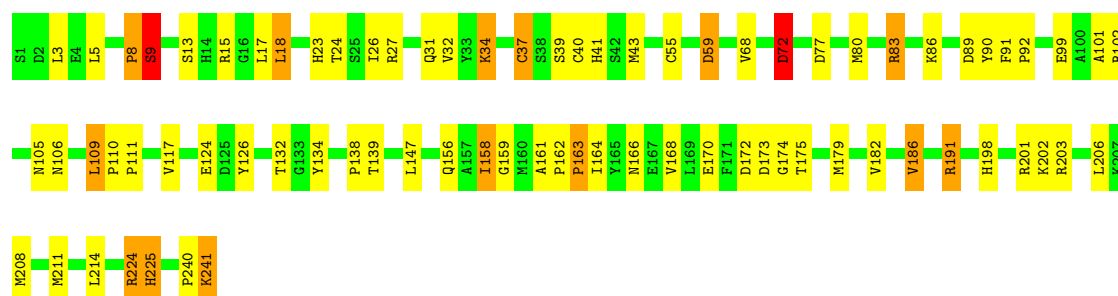
- Molecule 3: Cytochrome b





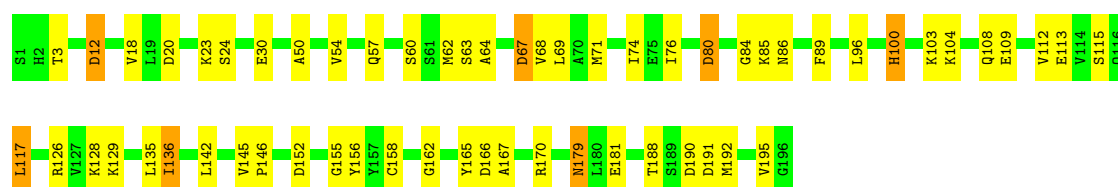
- Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain D: 68% 26% 6% .



- Molecule 5: Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial precursor (EC 1.10.2.2) (Rieske iron-sulfur protein) (RISP) [Contains: Ubiquinol-cytochrome c reductase 8 kDa protein (Complex III subunit IX)]

Chain E: 70% 27% .



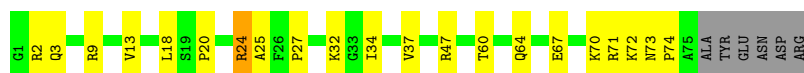
- Molecule 6: sub6

Chain F: 82% 13% 5%



- Molecule 7: Ubiquinol-cytochrome c reductase complex ubiquinone-binding protein QP-C

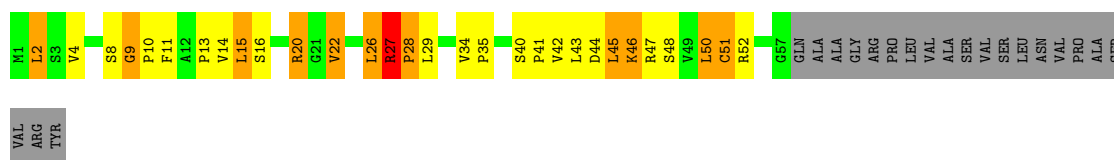
Chain G: 67% 25% 7%



- Molecule 8: Ubiquinol-cytochrome c reductase complex 11 kDa protein



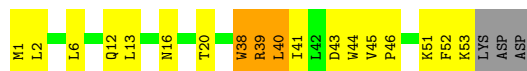
- Molecule 9: Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial precursor (EC 1.10.2.2) (Rieske iron-sulfur protein) (RISP) [Contains: Ubiquinol-cytochrome c reductase 8 kDa protein (Complex III subunit IX)]



- Molecule 10: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein



- Molecule 11: Ubiquinol-cytochrome c reductase complex 6.4 kDa protein



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	153.70Å 153.70Å 596.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.70	Depositor
% Data completeness (in resolution range)	94.1 (40.00-2.70)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.263 , 0.314	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17274	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FES, PLX, CDL, HEC, MYX, PEE

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	0.90	0/3531	0.84	5/4792 (0.1%)
2	B	0.99	0/3232	0.88	8/4386 (0.2%)
3	C	1.01	0/3100	0.82	3/4242 (0.1%)
4	D	0.97	0/1978	0.86	5/2684 (0.2%)
5	E	1.01	0/1553	0.82	6/2100 (0.3%)
6	F	0.99	0/930	0.88	0/1246
7	G	1.15	0/649	0.78	0/878
8	H	0.90	0/553	0.88	0/741
9	I	1.31	0/411	1.15	2/558 (0.4%)
10	J	1.06	0/515	0.85	0/696
11	K	1.13	0/452	0.82	0/618
All	All	0.99	0/16904	0.86	29/22941 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
6	F	0	1
All	All	0	3

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	172	ASP	CB-CG-OD2	6.79	124.41	118.30
1	A	327	ASP	CB-CG-OD2	6.56	124.20	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	308	ASP	CB-CG-OD2	6.40	124.06	118.30
2	B	147	ASP	CB-CG-OD2	6.28	123.95	118.30
3	C	320	LEU	CA-CB-CG	5.78	128.59	115.30
3	C	239	LEU	CA-CB-CG	5.71	128.43	115.30
9	I	44	ASP	CB-CG-OD2	5.51	123.26	118.30
2	B	193	ASP	CB-CG-OD2	5.51	123.25	118.30
4	D	109	LEU	CA-CB-CG	5.50	127.95	115.30
2	B	403	ASP	CB-CG-OD2	5.42	123.18	118.30
3	C	252	ASP	CB-CG-OD2	5.36	123.12	118.30
5	E	152	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	224	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	226	ASP	CB-CG-OD2	5.30	123.07	118.30
9	I	45	LEU	CA-CB-CG	5.29	127.47	115.30
2	B	163	LEU	CA-CB-CG	5.28	127.44	115.30
5	E	166	ASP	CB-CG-OD2	5.28	123.05	118.30
2	B	180	ASP	CB-CG-OD2	5.27	123.05	118.30
5	E	190	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	20	ASP	CB-CG-OD2	5.25	123.03	118.30
5	E	80	ASP	CB-CG-OD2	5.16	122.95	118.30
4	D	89	ASP	CB-CG-OD2	5.15	122.93	118.30
4	D	72	ASP	CB-CG-OD2	5.13	122.92	118.30
2	B	380	ASP	CB-CG-OD2	5.12	122.91	118.30
5	E	67	ASP	CB-CG-OD2	5.10	122.89	118.30
5	E	191	ASP	CB-CG-OD2	5.10	122.89	118.30
4	D	59	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	105	ASP	CB-CG-OD2	5.04	122.83	118.30
2	B	437	ASP	CB-CG-OD2	5.02	122.82	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	303	LEU	Peptide
2	B	169	ARG	Mainchain
6	F	99	ARG	Mainchain

## 5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3458	0	3356	32	0
2	B	3172	0	3152	44	0
3	C	3003	0	3065	39	0
4	D	1919	0	1869	31	0
5	E	1519	0	1504	12	0
6	F	911	0	902	3	0
7	G	628	0	636	8	0
8	H	548	0	530	3	0
9	I	406	0	437	27	0
10	J	502	0	505	3	0
11	K	436	0	445	11	0
12	A	64	0	72	1	0
12	D	64	0	72	0	0
12	G	64	0	72	2	0
13	A	49	0	75	1	0
13	C	49	0	75	0	0
13	E	49	0	75	3	0
14	C	86	0	64	10	0
14	D	43	0	31	8	0
15	C	33	0	33	1	0
16	E	4	0	0	0	0
17	J	52	0	88	4	0
18	A	51	0	0	0	0
18	B	84	0	0	2	0
18	C	36	0	0	0	0
18	D	11	0	0	0	0
18	E	2	0	0	1	0
18	F	15	0	0	0	0
18	G	11	0	0	1	0
18	I	2	0	0	0	0
18	K	3	0	0	0	0
All	All	17274	0	17058	189	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 6.

All (189) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:40:CYS:SG	14:D:243:HEC:HAC	1.33	1.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:11:MET:CE	3:C:11:MET:SD	2.02	1.48
11:K:38:TRP:HE3	11:K:41:ILE:CD1	1.25	1.48
11:K:38:TRP:CE3	11:K:41:ILE:CD1	2.04	1.41
4:D:40:CYS:SG	14:D:243:HEC:CAC	2.18	1.30
11:K:38:TRP:CE3	11:K:41:ILE:HD11	1.72	1.19
11:K:38:TRP:HE3	11:K:41:ILE:HD13	1.05	1.14
11:K:38:TRP:CZ3	11:K:41:ILE:HD11	2.15	0.81
11:K:38:TRP:CE3	11:K:41:ILE:HD12	2.16	0.78
11:K:38:TRP:CE3	11:K:41:ILE:HD13	1.97	0.78
9:I:4:VAL:HB	9:I:10:PRO:HG2	1.68	0.73
2:B:325:TYR:HB3	9:I:28:PRO:HD2	1.70	0.73
1:A:149:VAL:HG21	1:A:252:HIS:HB3	1.73	0.70
4:D:126:TYR:HE2	14:D:243:HEC:O2A	1.77	0.67
4:D:37:CYS:SG	14:D:243:HEC:C3B	2.82	0.67
2:B:310:SER:HB3	9:I:28:PRO:HD3	1.75	0.66
4:D:117:VAL:HG21	4:D:191:ARG:HA	1.76	0.66
4:D:163:PRO:HG2	14:D:243:HEC:HMC2	1.78	0.66
3:C:109:PHE:HB3	3:C:112:THR:HG23	1.78	0.65
9:I:9:GLY:HA2	9:I:26:LEU:O	2.01	0.61
2:B:248:ASN:HB3	2:B:250:ASP:HB2	1.83	0.60
4:D:72:ASP:HB2	4:D:83:ARG:HG2	1.85	0.59
4:D:159:GLY:HA3	14:D:243:HEC:HBD2	1.84	0.59
4:D:224:ARG:HD3	7:G:25:ALA:O	2.02	0.59
1:A:58:PHE:HB3	1:A:182:LEU:HD21	1.85	0.59
2:B:385:GLN:HG2	9:I:2:LEU:HD12	1.83	0.59
13:A:448:PEE:H14	17:J:63:PLX:H72	1.84	0.58
2:B:264:ILE:HD12	2:B:315:SER:HB3	1.84	0.58
9:I:34:VAL:HB	9:I:35:PRO:HD3	1.85	0.58
2:B:169:ARG:HD3	2:B:238:LYS:HB3	1.85	0.58
5:E:156:TYR:HB2	5:E:165:TYR:HB2	1.84	0.58
7:G:34:ILE:HA	7:G:37:VAL:HG22	1.85	0.57
4:D:23:HIS:HA	4:D:26:ILE:HD12	1.87	0.56
4:D:147:LEU:HB3	4:D:158:ILE:HA	1.87	0.56
5:E:170:ARG:HA	5:E:179:ASN:HB3	1.86	0.56
2:B:170:ASN:ND2	2:B:236:LYS:O	2.38	0.56
3:C:51:LEU:HD11	3:C:80:ARG:HA	1.88	0.56
5:E:20:ASP:HB3	5:E:23:LYS:HB2	1.87	0.56
3:C:142:GLY:HA2	15:C:383:MYX:H82	1.87	0.56
1:A:145:MET:O	1:A:149:VAL:HG23	2.06	0.55
2:B:394:PRO:HG2	2:B:397:THR:HG23	1.89	0.55
3:C:186:PRO:HG2	14:C:382:HEC:HMC3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:8:HIS:HD2	3:C:11:MET:HG3	1.70	0.55
2:B:99:THR:HG22	9:I:14:VAL:HG13	1.90	0.54
3:C:126:THR:HG21	14:C:382:HEC:HBB3	1.90	0.54
5:E:117:LEU:HD21	5:E:170:ARG:HB3	1.90	0.54
2:B:245:ARG:NH2	2:B:433:THR:O	2.40	0.54
9:I:46:LYS:HG2	9:I:47:ARG:N	2.23	0.54
3:C:309:THR:HG21	3:C:367:PRO:O	2.08	0.54
2:B:176:LEU:HD11	9:I:11:PHE:HB3	1.90	0.54
4:D:37:CYS:O	4:D:41:HIS:HB2	2.08	0.53
14:D:243:HEC:HMB1	14:D:243:HEC:HBB3	1.91	0.53
10:J:10:TYR:HA	10:J:14:PHE:HB2	1.91	0.53
3:C:369:ALA:O	3:C:373:GLU:HG3	2.08	0.53
1:A:351:GLU:H	11:K:12:GLN:NE2	2.07	0.53
2:B:279:LEU:HB3	2:B:295:LEU:HG	1.90	0.53
13:E:197:PEE:H62	17:J:63:PLX:H171	1.89	0.53
2:B:150:VAL:HG11	9:I:47:ARG:HD3	1.91	0.52
2:B:166:ALA:HB2	2:B:244:ILE:HG13	1.91	0.52
1:A:86:LEU:HD23	2:B:285:VAL:HG13	1.90	0.52
3:C:357:LEU:O	3:C:361:LEU:HB2	2.10	0.52
5:E:50:ALA:O	5:E:54:VAL:HG23	2.10	0.52
7:G:9:ARG:HD3	18:G:693:HOH:O	2.08	0.52
9:I:20:ARG:HE	9:I:51:CYS:HA	1.74	0.52
3:C:75:TYR:CD1	5:E:57:GLN:HG2	2.44	0.51
5:E:12:ASP:HB2	18:E:674:HOH:O	2.11	0.51
2:B:227:ARG:HH22	2:B:231:GLY:HA2	1.76	0.51
2:B:264:ILE:HG12	9:I:2:LEU:HD23	1.92	0.51
2:B:71:LEU:HD23	9:I:15:LEU:HG	1.93	0.50
2:B:384:SER:HB2	9:I:2:LEU:O	2.12	0.50
6:F:63:LYS:HD3	7:G:13:VAL:HG11	1.93	0.50
1:A:40:TRP:CZ2	1:A:377:GLU:HA	2.47	0.50
3:C:343:VAL:HG22	3:C:348:ILE:HG23	1.94	0.50
2:B:161:GLU:HG2	2:B:175:SER:OG	2.11	0.50
3:C:267:HIS:HD2	3:C:269:LYS:HB2	1.76	0.50
1:A:158:PHE:O	1:A:164:ALA:HB2	2.12	0.49
1:A:432:PRO:HB2	1:A:437:ILE:HG13	1.94	0.49
3:C:117:VAL:N	14:C:381:HEC:HBC2	2.27	0.49
1:A:146:ARG:HH12	1:A:308:GLN:HE22	1.60	0.49
1:A:131:ARG:NH2	1:A:177:LEU:O	2.45	0.49
1:A:373:THR:HB	1:A:374:PRO:HD3	1.94	0.48
4:D:134:TYR:CE2	4:D:162:PRO:HB3	2.47	0.48
7:G:24:ARG:HD2	7:G:27:PRO:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:150:VAL:CG1	9:I:47:ARG:HD3	2.44	0.48
2:B:156:GLN:HG2	9:I:27:ARG:HG3	1.95	0.48
4:D:138:PRO:HB3	8:H:58:LEU:HD13	1.96	0.48
4:D:161:ALA:O	4:D:163:PRO:HD3	2.13	0.48
1:A:62:LEU:HD13	1:A:122:LEU:HD23	1.95	0.48
1:A:431:LEU:HD12	1:A:432:PRO:HD2	1.96	0.48
2:B:76:THR:HG23	2:B:81:SER:HA	1.94	0.48
4:D:208:MET:HA	13:E:197:PEE:H48	1.96	0.48
10:J:37:GLN:HA	10:J:40:ASP:HB2	1.96	0.48
2:B:243:GLU:HA	2:B:424:MET:O	2.14	0.48
2:B:70:ARG:HG3	2:B:98:VAL:HG22	1.96	0.48
2:B:134:ARG:NH1	18:B:580:HOH:O	2.46	0.48
1:A:280:TYR:HB3	1:A:307:PHE:CE2	2.49	0.47
6:F:9:SER:O	6:F:13:LEU:HG	2.13	0.47
2:B:100:SER:O	9:I:13:PRO:HD2	2.13	0.47
1:A:75:LEU:HD12	1:A:112:LEU:HD22	1.97	0.47
3:C:119:LEU:HB3	14:C:381:HEC:HBB3	1.97	0.47
1:A:354:VAL:HG21	1:A:404:ALA:HA	1.96	0.47
3:C:28:SER:HB3	3:C:30:TRP:H	1.79	0.47
3:C:119:LEU:HD22	14:C:381:HEC:HBB3	1.96	0.47
3:C:309:THR:HG23	3:C:370:GLY:HA3	1.96	0.47
3:C:361:LEU:HA	3:C:365:LEU:HB2	1.95	0.47
10:J:8:ARG:O	10:J:12:LEU:HB2	2.14	0.46
2:B:108:THR:HG21	18:B:556:HOH:O	2.16	0.46
2:B:342:ASN:HD22	2:B:345:LYS:HD2	1.80	0.46
1:A:361:LEU:HD23	1:A:399:ILE:HG12	1.98	0.46
4:D:225:HIS:O	7:G:20:PRO:HB3	2.16	0.46
3:C:116:GLY:HA2	3:C:119:LEU:HD12	1.97	0.46
1:A:301:ASN:HB2	1:A:303:LEU:HG	1.98	0.46
1:A:325:VAL:HG21	9:I:43:LEU:HD12	1.97	0.46
5:E:84:GLY:H	5:E:100:HIS:HB3	1.81	0.46
3:C:179:PHE:HE1	14:C:382:HEC:HMD3	1.80	0.46
4:D:101:ALA:HB1	4:D:110:PRO:HD2	1.98	0.46
3:C:77:TRP:CZ3	4:D:201:ARG:HB3	2.51	0.45
12:G:82:CDL:HA61	12:G:82:CDL:H512	1.98	0.45
1:A:419:CYS:SG	1:A:438:ARG:NH1	2.89	0.45
4:D:32:VAL:O	4:D:37:CYS:SG	2.74	0.45
4:D:240:PRO:HB2	4:D:241:LYS:HD3	1.99	0.45
9:I:14:VAL:HB	9:I:22:VAL:HG23	1.99	0.45
2:B:344:VAL:HG11	2:B:417:PHE:CD2	2.52	0.45
2:B:325:TYR:HB3	9:I:28:PRO:CD	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:13:LEU:HA	6:F:16:ILE:HD12	1.98	0.45
12:A:447:CDL:H111	12:A:447:CDL:HB61	1.99	0.45
3:C:186:PRO:HG3	14:C:382:HEC:HBB3	1.99	0.45
3:C:324:LEU:HD12	3:C:369:ALA:HB2	1.99	0.45
4:D:32:VAL:HB	4:D:186:VAL:HG13	1.97	0.45
2:B:111:CYS:HB3	2:B:119:LEU:HD13	1.99	0.45
1:A:252:HIS:NE2	9:I:43:LEU:HG	2.32	0.44
4:D:40:CYS:SG	14:D:243:HEC:C3C	3.00	0.44
9:I:43:LEU:HA	9:I:46:LYS:HB3	1.98	0.44
11:K:39:ARG:HD3	11:K:39:ARG:H	1.82	0.44
1:A:298:ALA:HA	1:A:303:LEU:HB2	2.00	0.44
2:B:394:PRO:HG2	2:B:397:THR:CG2	2.47	0.44
1:A:248:LEU:O	1:A:427:PRO:HG3	2.17	0.44
4:D:110:PRO:HA	4:D:111:PRO:HD3	1.84	0.44
3:C:51:LEU:HD23	3:C:69:ILE:HD13	1.99	0.44
3:C:246:ALA:HB1	3:C:249:LEU:HB2	2.00	0.44
9:I:27:ARG:HA	9:I:28:PRO:HD2	1.98	0.43
1:A:53:ASN:HB3	1:A:170:PRO:HD2	2.01	0.43
3:C:179:PHE:CE1	14:C:382:HEC:HMD3	2.53	0.43
4:D:166:ASN:HB3	8:H:13:LEU:HD22	2.01	0.43
3:C:319:PRO:HB3	7:G:47:ARG:HH11	1.83	0.43
4:D:166:ASN:HD22	8:H:13:LEU:HD22	1.84	0.43
3:C:47:THR:HG21	3:C:82:MET:HB3	2.01	0.43
3:C:250:LEU:HD22	3:C:250:LEU:H	1.84	0.43
2:B:118:ILE:H	2:B:118:ILE:HG13	1.72	0.43
1:A:144:SER:HA	9:I:42:VAL:HG11	2.01	0.43
3:C:284:ILE:HA	3:C:285:PRO:HD3	1.93	0.43
3:C:98:VAL:HG22	14:C:381:HEC:HAC	2.01	0.42
12:G:82:CDL:H311	12:G:82:CDL:H121	2.00	0.42
2:B:103:GLU:OE1	2:B:317:SER:N	2.52	0.42
3:C:11:MET:CE	3:C:11:MET:CG	2.93	0.42
4:D:225:HIS:CD2	7:G:20:PRO:HB2	2.53	0.42
2:B:99:THR:HB	9:I:14:VAL:HG22	2.02	0.42
2:B:325:TYR:CB	9:I:28:PRO:HD2	2.44	0.42
3:C:239:LEU:HD13	3:C:240:MET:HG2	2.01	0.42
3:C:280:ILE:HG13	3:C:335:LEU:HD22	2.01	0.42
5:E:136:ILE:H	5:E:136:ILE:HG13	1.73	0.42
1:A:25:VAL:HG13	1:A:197:LEU:HD23	2.00	0.42
1:A:106:LEU:N	1:A:107:PRO:HD2	2.34	0.42
1:A:281:ASP:HB3	1:A:284:TYR:CE1	2.55	0.42
5:E:145:VAL:HA	5:E:146:PRO:HD3	1.95	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:20:ARG:HD2	9:I:48:SER:HB2	2.02	0.42
5:E:109:GLU:HG3	5:E:167:ALA:HB3	2.01	0.42
1:A:60:GLU:OE1	2:B:287:ARG:NH2	2.49	0.41
2:B:258:VAL:HG12	2:B:423:SER:HB2	2.01	0.41
3:C:301:LEU:HA	3:C:304:ILE:HD12	2.02	0.41
4:D:8:PRO:HB2	4:D:9:SER:H	1.69	0.41
5:E:136:ILE:HD12	5:E:181:GLU:HB3	2.01	0.41
1:A:158:PHE:HB3	1:A:161:THR:HG1	1.85	0.41
17:J:63:PLX:H1C2	17:J:63:PLX:H21	1.73	0.41
2:B:241:GLY:HA2	2:B:423:SER:OG	2.20	0.41
4:D:31:GLN:HA	4:D:34:LYS:HB3	2.01	0.41
1:A:158:PHE:HB3	1:A:161:THR:OG1	2.21	0.41
11:K:38:TRP:C	11:K:40:LEU:N	2.74	0.41
2:B:148:LYS:HG3	2:B:177:TYR:HB3	2.03	0.41
3:C:140:PHE:CE1	3:C:170:VAL:O	2.74	0.41
4:D:91:PHE:HA	4:D:92:PRO:HD3	1.97	0.41
4:D:147:LEU:HD13	4:D:158:ILE:HG13	2.01	0.41
11:K:45:VAL:HA	11:K:46:PRO:HD3	1.88	0.41
2:B:270:ASN:O	2:B:274:VAL:HG23	2.22	0.40
3:C:240:MET:SD	13:E:197:PEE:H17	2.61	0.40
3:C:116:GLY:O	14:C:381:HEC:HMC3	2.21	0.40
1:A:444:LEU:HD22	17:J:63:PLX:H52	2.04	0.40
2:B:109:VAL:HG22	2:B:119:LEU:HD23	2.04	0.40
2:B:156:GLN:H	2:B:156:GLN:NE2	2.20	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	444/480 (92%)	418 (94%)	20 (4%)	6 (1%)	<b>11</b> <b>28</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	421/453 (93%)	390 (93%)	27 (6%)	4 (1%)	15	37
3	C	376/379 (99%)	353 (94%)	19 (5%)	4 (1%)	14	34
4	D	239/241 (99%)	211 (88%)	21 (9%)	7 (3%)	4	10
5	E	194/196 (99%)	162 (84%)	29 (15%)	3 (2%)	10	26
6	F	103/110 (94%)	98 (95%)	5 (5%)	0	100	100
7	G	73/81 (90%)	66 (90%)	5 (7%)	2 (3%)	5	12
8	H	65/78 (83%)	58 (89%)	5 (8%)	2 (3%)	4	9
9	I	55/78 (70%)	31 (56%)	16 (29%)	8 (14%)	0	0
10	J	59/62 (95%)	50 (85%)	7 (12%)	2 (3%)	3	8
11	K	51/56 (91%)	43 (84%)	7 (14%)	1 (2%)	7	19
All	All	2080/2214 (94%)	1880 (90%)	161 (8%)	39 (2%)	8	20

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	250	ASP
3	C	154	PRO
4	D	8	PRO
7	G	73	ASN
9	I	29	LEU
10	J	56	LYS
11	K	52	PHE
1	A	50	GLU
1	A	220	SER
2	B	437	ASP
3	C	157	GLY
4	D	18	LEU
5	E	155	GLY
8	H	48	SER
9	I	8	SER
9	I	50	LEU
2	B	236	LYS
4	D	158	ILE
4	D	198	HIS
5	E	64	ALA
9	I	9	GLY
10	J	4	THR
1	A	74	ALA

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Mol	Chain	Res	Type
1	A	282	CYS
3	C	9	PRO
8	H	13	LEU
9	I	27	ARG
9	I	51	CYS
1	A	229	PRO
3	C	343	VAL
4	D	9	SER
4	D	163	PRO
9	I	41	PRO
4	D	174	GLY
2	B	228	GLY
9	I	40	SER
1	A	221	GLY
5	E	162	GLY
7	G	74	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	370/394 (94%)	315 (85%)	55 (15%)	3	7
2	B	332/355 (94%)	288 (87%)	44 (13%)	4	9
3	C	326/327 (100%)	262 (80%)	64 (20%)	1	3
4	D	206/206 (100%)	158 (77%)	48 (23%)	1	2
5	E	168/168 (100%)	130 (77%)	38 (23%)	1	2
6	F	96/99 (97%)	85 (88%)	11 (12%)	5	13
7	G	66/71 (93%)	55 (83%)	11 (17%)	2	5
8	H	64/74 (86%)	42 (66%)	22 (34%)	0	0
9	I	44/60 (73%)	32 (73%)	12 (27%)	0	1
10	J	51/52 (98%)	32 (63%)	19 (37%)	0	0
11	K	42/45 (93%)	29 (69%)	13 (31%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1765/1851 (95%)	1428 (81%)	337 (19%)	<b>1</b> <b>4</b>

All (337) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	THR
1	A	3	THR
1	A	9	GLN
1	A	15	GLN
1	A	17	SER
1	A	29	GLN
1	A	37	VAL
1	A	42	ASP
1	A	49	SER
1	A	58	PHE
1	A	60	GLU
1	A	73	ASN
1	A	77	LYS
1	A	90	SER
1	A	108	LYS
1	A	117	VAL
1	A	121	SER
1	A	127	ILE
1	A	129	LYS
1	A	130	GLU
1	A	139	GLN
1	A	146	ARG
1	A	147	ASP
1	A	171	SER
1	A	177	LEU
1	A	179	ARG
1	A	182	LEU
1	A	186	LEU
1	A	187	SER
1	A	188	ARG
1	A	203	LEU
1	A	206	ARG
1	A	207	GLN
1	A	214	LYS
1	A	223	TYR
1	A	225	GLU
1	A	226	ASP

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Mol	Chain	Res	Type
1	A	232	SER
1	A	245	GLU
1	A	281	ASP
1	A	296	SER
1	A	302	LYS
1	A	308	GLN
1	A	323	HIS
1	A	325	VAL
1	A	343	MET
1	A	365	LEU
1	A	367	SER
1	A	369	LEU
1	A	370	ASP
1	A	381	ARG
1	A	394	GLU
1	A	403	ASP
1	A	405	ARG
1	A	409	GLU
2	B	20	HIS
2	B	33	LEU
2	B	38	LEU
2	B	46	ARG
2	B	63	LEU
2	B	69	LEU
2	B	98	VAL
2	B	99	THR
2	B	109	VAL
2	B	118	ILE
2	B	119	LEU
2	B	123	LEU
2	B	145	ARG
2	B	156	GLN
2	B	163	LEU
2	B	169	ARG
2	B	176	LEU
2	B	189	VAL
2	B	196	GLN
2	B	197	ASN
2	B	209	LEU
2	B	221	GLU
2	B	226	ILE
2	B	227	ARG

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Mol	Chain	Res	Type
2	B	232	LEU
2	B	236	LYS
2	B	238	LYS
2	B	240	HIS
2	B	243	GLU
2	B	250	ASP
2	B	252	LEU
2	B	257	LEU
2	B	258	VAL
2	B	268	GLU
2	B	273	SER
2	B	294	SER
2	B	297	GLN
2	B	305	GLN
2	B	315	SER
2	B	397	THR
2	B	401	GLN
2	B	407	ASP
2	B	435	PHE
2	B	437	ASP
3	C	3	ASN
3	C	12	LYS
3	C	13	ILE
3	C	28	SER
3	C	39	ILE
3	C	42	ILE
3	C	45	ILE
3	C	51	LEU
3	C	56	THR
3	C	57	SER
3	C	60	THR
3	C	61	THR
3	C	64	SER
3	C	74	ASN
3	C	78	ILE
3	C	80	ARG
3	C	82	MET
3	C	90	PHE
3	C	92	ILE
3	C	112	THR
3	C	120	LEU
3	C	124	MET

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Mol	Chain	Res	Type
3	C	138	MET
3	C	151	SER
3	C	156	ILE
3	C	158	THR
3	C	160	LEU
3	C	161	VAL
3	C	171	ASP
3	C	174	THR
3	C	175	LEU
3	C	177	ARG
3	C	194	MET
3	C	198	LEU
3	C	212	SER
3	C	226	ILE
3	C	227	LYS
3	C	233	LEU
3	C	237	LEU
3	C	239	LEU
3	C	241	LEU
3	C	242	LEU
3	C	250	LEU
3	C	254	ASP
3	C	262	LEU
3	C	264	THR
3	C	268	ILE
3	C	281	LEU
3	C	282	ARG
3	C	284	ILE
3	C	287	LYS
3	C	288	LEU
3	C	292	LEU
3	C	296	PHE
3	C	300	ILE
3	C	311	LYS
3	C	316	MET
3	C	334	THR
3	C	343	VAL
3	C	344	GLU
3	C	348	ILE
3	C	350	ILE
3	C	360	LEU
3	C	379	TRP

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Mol	Chain	Res	Type
4	D	3	LEU
4	D	5	LEU
4	D	9	SER
4	D	13	SER
4	D	15	ARG
4	D	17	LEU
4	D	18	LEU
4	D	24	THR
4	D	27	ARG
4	D	34	LYS
4	D	37	CYS
4	D	39	SER
4	D	43	MET
4	D	55	CYS
4	D	59	ASP
4	D	68	VAL
4	D	72	ASP
4	D	77	ASP
4	D	80	MET
4	D	83	ARG
4	D	86	LYS
4	D	90	TYR
4	D	99	GLU
4	D	102	ARG
4	D	105	ASN
4	D	106	ASN
4	D	109	LEU
4	D	124	GLU
4	D	132	THR
4	D	139	THR
4	D	156	GLN
4	D	164	ILE
4	D	168	VAL
4	D	170	GLU
4	D	173	ASP
4	D	175	THR
4	D	179	MET
4	D	182	VAL
4	D	186	VAL
4	D	191	ARG
4	D	202	LYS
4	D	203	ARG

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Mol	Chain	Res	Type
4	D	206	LEU
4	D	211	MET
4	D	214	LEU
4	D	224	ARG
4	D	225	HIS
4	D	241	LYS
5	E	3	THR
5	E	12	ASP
5	E	18	VAL
5	E	24	SER
5	E	30	GLU
5	E	60	SER
5	E	62	MET
5	E	63	SER
5	E	67	ASP
5	E	68	VAL
5	E	69	LEU
5	E	71	MET
5	E	74	ILE
5	E	76	ILE
5	E	80	ASP
5	E	85	LYS
5	E	86	ASN
5	E	89	PHE
5	E	96	LEU
5	E	100	HIS
5	E	103	LYS
5	E	104	LYS
5	E	108	GLN
5	E	112	VAL
5	E	113	GLU
5	E	115	SER
5	E	117	LEU
5	E	126	ARG
5	E	128	LYS
5	E	129	LYS
5	E	135	LEU
5	E	136	ILE
5	E	142	LEU
5	E	158	CYS
5	E	179	ASN
5	E	188	THR

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Mol	Chain	Res	Type
5	E	192	MET
5	E	195	VAL
6	F	6	VAL
6	F	7	SER
6	F	18	LYS
6	F	71	ARG
6	F	73	GLN
6	F	77	LYS
6	F	81	THR
6	F	90	LEU
6	F	99	ARG
6	F	106	GLU
6	F	110	LYS
7	G	2	ARG
7	G	3	GLN
7	G	18	LEU
7	G	24	ARG
7	G	32	LYS
7	G	60	THR
7	G	64	GLN
7	G	67	GLU
7	G	70	LYS
7	G	71	ARG
7	G	72	LYS
8	H	13	LEU
8	H	18	THR
8	H	21	ARG
8	H	22	GLU
8	H	27	LEU
8	H	28	GLU
8	H	30	CYS
8	H	32	LYS
8	H	34	ARG
8	H	36	ARG
8	H	38	GLU
8	H	42	GLU
8	H	43	ARG
8	H	50	THR
8	H	55	THR
8	H	56	GLU
8	H	65	ARG
8	H	68	CYS

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Mol	Chain	Res	Type
8	H	71	HIS
8	H	72	LYS
8	H	77	LEU
8	H	78	LYS
9	I	2	LEU
9	I	15	LEU
9	I	16	SER
9	I	20	ARG
9	I	22	VAL
9	I	26	LEU
9	I	27	ARG
9	I	28	PRO
9	I	45	LEU
9	I	46	LYS
9	I	50	LEU
9	I	52	ARG
10	J	4	THR
10	J	8	ARG
10	J	9	LEU
10	J	12	LEU
10	J	15	ARG
10	J	16	ARG
10	J	25	VAL
10	J	30	PHE
10	J	36	ASP
10	J	37	GLN
10	J	42	ILE
10	J	44	GLU
10	J	45	HIS
10	J	48	GLU
10	J	53	LYS
10	J	56	LYS
10	J	58	LYS
10	J	59	TYR
10	J	60	GLU
11	K	1	MET
11	K	2	LEU
11	K	6	LEU
11	K	13	LEU
11	K	16	ASN
11	K	20	THR
11	K	38	TRP

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Mol	Chain	Res	Type
11	K	39	ARG
11	K	40	LEU
11	K	43	ASP
11	K	44	TRP
11	K	51	LYS
11	K	53	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	73	ASN
1	A	119	ASN
2	B	162	ASN
2	B	170	ASN
2	B	197	ASN
2	B	248	ASN
2	B	276	GLN
2	B	277	HIS
2	B	342	ASN
3	C	8	HIS
3	C	114	ASN
3	C	267	HIS
3	C	286	ASN
4	D	35	GLN
5	E	57	GLN
5	E	161	HIS
6	F	73	GLN
7	G	3	GLN
9	I	31	GLN
11	K	12	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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



## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
12	CDL	D	242	-	63,63,99	1.71	9 (14%)	69,75,111	1.59	7 (10%)
12	CDL	A	447	-	63,63,99	1.68	8 (12%)	69,75,111	1.62	8 (11%)
15	MYX	C	383	-	29,34,34	2.38	6 (20%)	21,45,45	1.59	3 (14%)
14	HEC	C	381	3	26,50,50	1.80	5 (19%)	18,82,82	1.35	3 (16%)
14	HEC	C	382	3	26,50,50	1.68	8 (30%)	18,82,82	1.21	2 (11%)
14	HEC	D	243	4	26,50,50	1.69	6 (23%)	18,82,82	1.37	3 (16%)
16	FES	E	198	5	0,4,4	0.00	-	-	-	-
13	PEE	E	197	-	48,48,50	1.33	4 (8%)	51,53,55	1.31	4 (7%)
13	PEE	C	380	-	48,48,50	1.32	4 (8%)	51,53,55	1.35	6 (11%)
17	PLX	J	63	-	51,51,51	0.79	2 (3%)	55,59,59	0.66	0
13	PEE	A	448	-	48,48,50	1.39	4 (8%)	51,53,55	1.44	5 (9%)
12	CDL	G	82	-	63,63,99	1.76	8 (12%)	69,75,111	1.72	10 (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
12	CDL	D	242	-	1/1/9/9	44/74/74/110	-
12	CDL	A	447	-	1/1/9/9	43/74/74/110	-
15	MYX	C	383	-	-	0/25/36/36	0/2/2/2
14	HEC	C	381	3	-	0/6/54/54	-
14	HEC	C	382	3	-	0/6/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	HEC	D	243	4	-	1/6/54/54	-
16	FES	E	198	5	-	-	0/1/1/1
13	PEE	E	197	-	-	24/52/52/54	-
13	PEE	C	380	-	-	26/52/52/54	-
17	PLX	J	63	-	-	33/55/55/55	-
13	PEE	A	448	-	-	31/52/52/54	-
12	CDL	G	82	-	1/1/9/9	43/74/74/110	-

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	383	MYX	C13-N2	9.04	1.44	1.31
15	C	383	MYX	O2-C3	6.05	1.47	1.35
12	G	82	CDL	PB2-OB3	5.70	1.71	1.50
12	D	242	CDL	PB2-OB3	5.52	1.70	1.50
12	A	447	CDL	PB2-OB3	5.43	1.70	1.50
13	A	448	PEE	P-O1P	5.40	1.70	1.50
12	A	447	CDL	PA1-OA3	5.22	1.69	1.50
14	C	381	HEC	C3B-C2B	-5.22	1.35	1.40
13	E	197	PEE	P-O1P	5.10	1.69	1.50
12	G	82	CDL	PA1-OA3	5.09	1.68	1.50
12	G	82	CDL	OA8-CA7	5.04	1.48	1.33
12	D	242	CDL	OA6-CA5	5.02	1.48	1.34
12	D	242	CDL	PA1-OA3	5.02	1.68	1.50
13	C	380	PEE	P-O1P	4.96	1.68	1.50
12	G	82	CDL	OA6-CA5	4.95	1.48	1.34
12	G	82	CDL	OB6-CB5	4.92	1.48	1.34
12	D	242	CDL	OA8-CA7	4.85	1.47	1.33
12	A	447	CDL	OA6-CA5	4.70	1.47	1.34
14	C	381	HEC	C3C-C2C	-4.67	1.35	1.40
13	C	380	PEE	O2-C10	4.53	1.47	1.34
13	A	448	PEE	O3-C30	4.52	1.46	1.33
12	A	447	CDL	OA8-CA7	4.37	1.46	1.33
12	A	447	CDL	OB8-CB7	4.18	1.45	1.33
13	C	380	PEE	O3-C30	4.17	1.45	1.33
12	D	242	CDL	OB6-CB5	4.15	1.46	1.34
13	E	197	PEE	O3-C30	4.15	1.45	1.33
13	A	448	PEE	O2-C10	4.14	1.46	1.34
13	E	197	PEE	O2-C10	4.13	1.46	1.34
12	D	242	CDL	OB8-CB7	4.06	1.45	1.33
12	A	447	CDL	OB6-CB5	3.77	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	82	CDL	OB8-CB7	3.66	1.44	1.33
14	D	243	HEC	C3C-C2C	-3.66	1.36	1.40
14	C	382	HEC	C3C-C2C	-3.55	1.37	1.40
14	C	382	HEC	C3B-C2B	-3.53	1.37	1.40
12	A	447	CDL	PA1-OA4	3.42	1.71	1.55
12	G	82	CDL	PA1-OA4	3.39	1.71	1.55
14	D	243	HEC	C3B-C2B	-3.30	1.37	1.40
12	G	82	CDL	PB2-OB4	3.28	1.70	1.55
12	D	242	CDL	PB2-OB4	3.17	1.70	1.55
12	D	242	CDL	PA1-OA4	3.17	1.70	1.55
13	E	197	PEE	P-O2P	3.10	1.69	1.55
14	D	243	HEC	C3B-C4B	3.04	1.48	1.43
15	C	383	MYX	C2-C1	2.96	1.53	1.47
13	A	448	PEE	P-O2P	2.96	1.69	1.55
15	C	383	MYX	C2-C3	2.91	1.39	1.33
15	C	383	MYX	C21-C20	2.90	1.52	1.44
12	A	447	CDL	PB2-OB4	2.90	1.68	1.55
17	J	63	PLX	O8-C24	2.85	1.45	1.40
13	C	380	PEE	P-O2P	2.75	1.68	1.55
14	D	243	HEC	C3C-C4C	2.64	1.47	1.43
14	C	382	HEC	C3B-C4B	2.60	1.47	1.43
14	C	382	HEC	C4A-C3A	2.53	1.48	1.42
14	C	381	HEC	C3C-C4C	2.48	1.47	1.43
14	C	381	HEC	C3B-C4B	2.45	1.47	1.43
14	D	243	HEC	CAD-C3D	2.41	1.55	1.52
14	C	382	HEC	C1B-NB	2.26	1.40	1.36
14	C	382	HEC	C3C-C4C	2.25	1.47	1.43
14	D	243	HEC	C4A-C3A	2.21	1.47	1.42
17	J	63	PLX	C7-C6	2.21	1.55	1.50
14	C	382	HEC	CAD-C3D	2.19	1.55	1.52
15	C	383	MYX	C13-S1	-2.14	1.70	1.73
14	C	381	HEC	CAD-C3D	2.10	1.55	1.52
12	D	242	CDL	C11-CA5	2.08	1.56	1.50
14	C	382	HEC	C1C-NC	2.05	1.40	1.36

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	447	CDL	OB6-CB5-OB7	-6.65	107.64	123.70
12	G	82	CDL	OB8-CB7-OB9	-6.47	107.25	123.59
12	G	82	CDL	OA6-CA5-OA7	-5.90	109.44	123.70
12	D	242	CDL	OB6-CB5-OB7	-5.84	109.60	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	242	CDL	OB8-CB7-OB9	-5.70	109.20	123.59
12	A	447	CDL	OA8-CA7-OA9	-5.48	109.76	123.59
13	A	448	PEE	O2-C10-O4	-5.34	110.80	123.70
12	A	447	CDL	OB8-CB7-OB9	-5.32	110.17	123.59
13	C	380	PEE	O3-C30-O5	-5.26	110.32	123.59
13	E	197	PEE	O3-C30-O5	-5.18	110.52	123.59
13	E	197	PEE	O2-C10-O4	-5.08	111.43	123.70
13	A	448	PEE	O3-C30-O5	-5.08	110.78	123.59
15	C	383	MYX	C4-O2-C3	4.67	124.33	116.52
12	G	82	CDL	OA7-CA5-C11	-4.65	105.58	123.73
12	G	82	CDL	OB6-CB5-OB7	-4.24	113.45	123.70
12	D	242	CDL	OB7-CB5-C51	-4.20	107.36	123.73
12	D	242	CDL	OA8-CA7-OA9	-4.07	113.33	123.59
13	A	448	PEE	O4-C10-C11	-4.00	108.12	123.73
12	G	82	CDL	OB9-CB7-C71	-3.96	108.29	123.73
13	C	380	PEE	O4-C10-C11	-3.94	108.34	123.73
12	G	82	CDL	OA8-CA7-OA9	-3.93	113.67	123.59
12	D	242	CDL	OA9-CA7-C31	-3.85	108.70	123.73
12	A	447	CDL	OA9-CA7-C31	-3.79	108.95	123.73
13	E	197	PEE	O4-C10-C11	-3.74	109.13	123.73
13	A	448	PEE	O5-C30-C31	-3.59	109.72	123.73
12	D	242	CDL	OA6-CA5-OA7	-3.58	115.05	123.70
12	A	447	CDL	OB9-CB7-C71	-3.58	109.78	123.73
12	G	82	CDL	OB7-CB5-C51	-3.53	109.97	123.73
12	D	242	CDL	OB9-CB7-C71	-3.52	110.01	123.73
12	A	447	CDL	OB7-CB5-C51	-3.39	110.49	123.73
12	G	82	CDL	OA9-CA7-C31	-3.35	110.66	123.73
15	C	383	MYX	O3-C7-C5	3.33	114.71	107.87
13	E	197	PEE	O5-C30-C31	-3.15	111.44	123.73
12	A	447	CDL	OA7-CA5-C11	-3.01	111.98	123.73
14	C	382	HEC	CBA-CAA-C2A	-2.96	107.02	112.48
13	C	380	PEE	O2-C10-O4	-2.92	116.64	123.70
14	D	243	HEC	CMB-C2B-C1B	-2.88	124.05	128.46
13	C	380	PEE	O2-C2-C1	2.86	118.75	108.40
14	D	243	HEC	CAA-CBA-CGA	-2.85	107.89	112.67
13	C	380	PEE	O5-C30-C31	-2.83	112.70	123.73
15	C	383	MYX	C23-C22-C21	-2.79	120.29	126.19
12	A	447	CDL	OA6-CA5-OA7	-2.76	117.02	123.70
14	D	243	HEC	CAD-CBD-CGD	-2.49	108.49	112.67
13	C	380	PEE	C2-O2-C10	2.49	123.91	117.79
14	C	381	HEC	CMD-C2D-C1D	-2.42	124.75	128.46
13	A	448	PEE	O3-C3-C2	2.37	115.33	108.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	C	382	HEC	CMB-C2B-C1B	-2.28	124.97	128.46
12	G	82	CDL	OA6-CA4-CA3	2.22	116.43	108.40
14	C	381	HEC	CMC-C2C-C1C	-2.19	125.09	128.46
12	G	82	CDL	OA6-CA5-C11	2.17	116.18	111.50
14	C	381	HEC	CBD-CAD-C3D	-2.03	108.74	112.49

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	A	447	CDL	CA4
12	D	242	CDL	CA4
12	G	82	CDL	CA4

All (245) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	447	CDL	CA3-OA5-PA1-OA2
12	A	447	CDL	CA3-OA5-PA1-OA3
12	A	447	CDL	CA3-OA5-PA1-OA4
12	A	447	CDL	CB3-OB5-PB2-OB3
12	A	447	CDL	OB6-CB4-CB6-OB8
12	A	447	CDL	OB7-CB5-OB6-CB4
12	D	242	CDL	O1-C1-CA2-OA2
12	D	242	CDL	CA2-OA2-PA1-OA4
12	D	242	CDL	CA2-OA2-PA1-OA5
12	D	242	CDL	CA3-OA5-PA1-OA4
12	D	242	CDL	C11-CA5-OA6-CA4
12	D	242	CDL	CB2-OB2-PB2-OB4
12	D	242	CDL	CB2-OB2-PB2-OB5
12	D	242	CDL	OB7-CB5-OB6-CB4
12	G	82	CDL	CA2-OA2-PA1-OA4
12	G	82	CDL	CA2-OA2-PA1-OA5
12	G	82	CDL	CA3-OA5-PA1-OA3
12	G	82	CDL	CB3-OB5-PB2-OB3
12	G	82	CDL	CB3-OB5-PB2-OB4
12	G	82	CDL	OB9-CB7-OB8-CB6
13	A	448	PEE	O4P-C4-C5-N
13	A	448	PEE	C1-O3P-P-O2P
13	A	448	PEE	C4-O4P-P-O1P
14	D	243	HEC	C2A-CAA-CBA-CGA
17	J	63	PLX	O7-C6-O6-C4
17	J	63	PLX	C3-O4-P1-O3

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Mol	Chain	Res	Type	Atoms
17	J	63	PLX	C25-C24-O8-C5
12	D	242	CDL	OB9-CB7-OB8-CB6
12	A	447	CDL	OB9-CB7-OB8-CB6
12	D	242	CDL	OA7-CA5-OA6-CA4
12	G	82	CDL	OA7-CA5-OA6-CA4
13	E	197	PEE	O4-C10-O2-C2
12	D	242	CDL	C71-CB7-OB8-CB6
12	G	82	CDL	C31-CA7-OA8-CA6
13	A	448	PEE	O4-C10-O2-C2
12	A	447	CDL	OA9-CA7-OA8-CA6
12	A	447	CDL	O1-C1-CB2-OB2
12	D	242	CDL	O1-C1-CB2-OB2
12	G	82	CDL	O1-C1-CB2-OB2
13	A	448	PEE	O5-C30-O3-C3
12	A	447	CDL	C11-CA5-OA6-CA4
13	C	380	PEE	C11-C10-O2-C2
13	C	380	PEE	O5-C30-O3-C3
13	E	197	PEE	O5-C30-O3-C3
12	G	82	CDL	C71-CB7-OB8-CB6
12	D	242	CDL	CA2-C1-CB2-OB2
12	A	447	CDL	C71-CB7-OB8-CB6
13	C	380	PEE	C30-C31-C32-C33
12	A	447	CDL	O1-C1-CA2-OA2
12	D	242	CDL	CA7-C31-C32-C33
12	A	447	CDL	CB5-C51-C52-C53
13	C	380	PEE	C10-C11-C12-C13
13	E	197	PEE	C10-C11-C12-C13
12	A	447	CDL	CB2-OB2-PB2-OB5
12	A	447	CDL	CB3-OB5-PB2-OB2
12	G	82	CDL	CA3-OA5-PA1-OA2
12	G	82	CDL	CB3-OB5-PB2-OB2
13	A	448	PEE	C1-O3P-P-O4P
13	A	448	PEE	C4-O4P-P-O3P
17	J	63	PLX	C3-O4-P1-O1
12	A	447	CDL	CA2-C1-CB2-OB2
12	D	242	CDL	CB2-C1-CA2-OA2
12	G	82	CDL	CA2-C1-CB2-OB2
17	J	63	PLX	O6-C6-C7-C8
12	D	242	CDL	C31-C32-C33-C34
13	C	380	PEE	C15-C16-C17-C18
13	C	380	PEE	C20-C21-C22-C23
17	J	63	PLX	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
12	A	447	CDL	C14-C15-C16-C17
13	C	380	PEE	C31-C32-C33-C34
17	J	63	PLX	C14-C15-C16-C17
12	D	242	CDL	C51-C52-C53-C54
17	J	63	PLX	C11-C10-C9-C8
12	A	447	CDL	C34-C35-C36-C37
12	G	82	CDL	C31-C32-C33-C34
13	C	380	PEE	C22-C23-C24-C25
12	A	447	CDL	C72-C73-C74-C75
13	A	448	PEE	C17-C18-C19-C20
13	E	197	PEE	C34-C35-C36-C37
12	D	242	CDL	C54-C55-C56-C57
13	C	380	PEE	C19-C20-C21-C22
13	E	197	PEE	C31-C32-C33-C34
13	E	197	PEE	C18-C19-C20-C21
17	J	63	PLX	C34-C35-C36-C37
12	A	447	CDL	C51-CB5-OB6-CB4
12	D	242	CDL	C34-C35-C36-C37
12	G	82	CDL	C12-C13-C14-C15
13	E	197	PEE	C38-C39-C40-C41
12	D	242	CDL	C13-C14-C15-C16
12	G	82	CDL	C74-C75-C76-C77
13	A	448	PEE	C40-C41-C42-C43
13	C	380	PEE	C18-C19-C20-C21
13	E	197	PEE	C22-C23-C24-C25
12	A	447	CDL	C53-C54-C55-C56
13	A	448	PEE	C15-C16-C17-C18
13	A	448	PEE	C39-C40-C41-C42
13	A	448	PEE	C21-C22-C23-C24
17	J	63	PLX	C31-C32-C33-C34
13	A	448	PEE	C10-C11-C12-C13
17	J	63	PLX	C33-C34-C35-C36
17	J	63	PLX	C35-C36-C37-C38
12	D	242	CDL	C33-C34-C35-C36
12	G	82	CDL	OA9-CA7-OA8-CA6
12	A	447	CDL	C32-C33-C34-C35
12	G	82	CDL	CB3-CB4-CB6-OB8
17	J	63	PLX	C15-C16-C17-C18
13	C	380	PEE	C17-C18-C19-C20
12	D	242	CDL	C51-CB5-OB6-CB4
13	A	448	PEE	C22-C23-C24-C25
12	D	242	CDL	C73-C74-C75-C76

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Mol	Chain	Res	Type	Atoms
13	C	380	PEE	C11-C12-C13-C14
12	G	82	CDL	C14-C15-C16-C17
13	A	448	PEE	C36-C37-C38-C39
13	A	448	PEE	C37-C38-C39-C40
12	G	82	CDL	OB7-CB5-OB6-CB4
12	G	82	CDL	C53-C54-C55-C56
12	D	242	CDL	OA9-CA7-OA8-CA6
12	A	447	CDL	C13-C14-C15-C16
13	E	197	PEE	C36-C37-C38-C39
17	J	63	PLX	C27-C28-C29-C30
12	A	447	CDL	C54-C55-C56-C57
12	G	82	CDL	C32-C33-C34-C35
13	C	380	PEE	C39-C40-C41-C42
13	E	197	PEE	C41-C42-C43-C44
17	J	63	PLX	C16-C17-C18-C19
13	E	197	PEE	C15-C16-C17-C18
12	G	82	CDL	C73-C74-C75-C76
13	C	380	PEE	C38-C39-C40-C41
12	G	82	CDL	C11-C12-C13-C14
13	E	197	PEE	C32-C33-C34-C35
12	G	82	CDL	C11-CA5-OA6-CA4
17	J	63	PLX	C12-C13-C14-C15
13	A	448	PEE	C12-C13-C14-C15
13	E	197	PEE	C16-C17-C18-C19
13	E	197	PEE	C13-C14-C15-C16
17	J	63	PLX	C9-C10-C11-C12
13	E	197	PEE	C21-C22-C23-C24
13	E	197	PEE	C35-C36-C37-C38
12	A	447	CDL	C51-C52-C53-C54
13	E	197	PEE	C42-C43-C44-C45
12	G	82	CDL	CA3-CA4-CA6-OA8
12	G	82	CDL	C35-C36-C37-C38
13	A	448	PEE	C18-C19-C20-C21
13	A	448	PEE	C20-C21-C22-C23
12	G	82	CDL	C15-C16-C17-C18
12	A	447	CDL	C75-C76-C77-C78
12	A	447	CDL	C74-C75-C76-C77
17	J	63	PLX	C7-C8-C9-C10
13	A	448	PEE	C24-C25-C26-C27
12	D	242	CDL	C55-C56-C57-C58
13	C	380	PEE	C37-C38-C39-C40
12	D	242	CDL	C71-C72-C73-C74

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Mol	Chain	Res	Type	Atoms
13	E	197	PEE	C24-C25-C26-C27
12	A	447	CDL	OB5-CB3-CB4-CB6
12	G	82	CDL	OA5-CA3-CA4-CA6
17	J	63	PLX	C20-C21-C22-C23
13	A	448	PEE	C42-C43-C44-C45
12	A	447	CDL	C52-C53-C54-C55
12	A	447	CDL	CB3-CB4-CB6-OB8
12	A	447	CDL	CA2-OA2-PA1-OA5
17	J	63	PLX	O7-C6-C7-C8
13	A	448	PEE	C35-C36-C37-C38
13	C	380	PEE	C16-C17-C18-C19
12	A	447	CDL	C1-CA2-OA2-PA1
17	J	63	PLX	C19-C20-C21-C22
17	J	63	PLX	C13-C14-C15-C16
12	D	242	CDL	CB5-C51-C52-C53
13	C	380	PEE	C41-C42-C43-C44
12	D	242	CDL	C11-C12-C13-C14
17	J	63	PLX	C25-C26-C27-C28
12	A	447	CDL	OB5-CB3-CB4-OB6
12	G	82	CDL	CB5-C51-C52-C53
12	D	242	CDL	OB6-CB4-CB6-OB8
12	G	82	CDL	OB6-CB4-CB6-OB8
13	C	380	PEE	C32-C33-C34-C35
13	A	448	PEE	C30-C31-C32-C33
12	D	242	CDL	CA3-OA5-PA1-OA2
13	C	380	PEE	C1-O3P-P-O4P
17	J	63	PLX	C29-C30-C31-C32
12	D	242	CDL	C1-CB2-OB2-PB2
13	C	380	PEE	C13-C14-C15-C16
12	A	447	CDL	CB2-OB2-PB2-OB3
12	A	447	CDL	CB2-OB2-PB2-OB4
12	A	447	CDL	CB3-OB5-PB2-OB4
12	D	242	CDL	CA2-OA2-PA1-OA3
12	D	242	CDL	CA3-OA5-PA1-OA3
12	D	242	CDL	CB2-OB2-PB2-OB3
12	G	82	CDL	CA2-OA2-PA1-OA3
13	A	448	PEE	C1-O3P-P-O1P
13	A	448	PEE	C4-O4P-P-O2P
13	C	380	PEE	C1-O3P-P-O1P
17	J	63	PLX	C3-O4-P1-O2
13	E	197	PEE	C11-C12-C13-C14
17	J	63	PLX	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
13	A	448	PEE	C16-C17-C18-C19
12	G	82	CDL	C52-C53-C54-C55
12	D	242	CDL	OA5-CA3-CA4-OA6
12	G	82	CDL	OA5-CA3-CA4-OA6
13	E	197	PEE	C37-C38-C39-C40
17	J	63	PLX	C6-C7-C8-C9
13	C	380	PEE	C40-C41-C42-C43
13	A	448	PEE	C31-C32-C33-C34
13	C	380	PEE	C14-C15-C16-C17
17	J	63	PLX	C10-C11-C12-C13
13	E	197	PEE	C4-O4P-P-O3P
17	J	63	PLX	C17-C18-C19-C20
12	G	82	CDL	CB2-C1-CA2-OA2
12	G	82	CDL	C13-C14-C15-C16
12	A	447	CDL	CB7-C71-C72-C73
12	D	242	CDL	CB7-C71-C72-C73
12	D	242	CDL	C14-C15-C16-C17
12	G	82	CDL	CA3-CA4-OA6-CA5
13	C	380	PEE	C1-C2-O2-C10
13	E	197	PEE	C30-C31-C32-C33
12	G	82	CDL	C1-CA2-OA2-PA1
17	J	63	PLX	O4-C3-C4-O6
12	A	447	CDL	CB2-C1-CA2-OA2
12	G	82	CDL	C71-C72-C73-C74
13	A	448	PEE	C23-C24-C25-C26
13	A	448	PEE	O3P-C1-C2-C3
12	G	82	CDL	O1-C1-CA2-OA2
12	D	242	CDL	CB3-CB4-CB6-OB8
17	J	63	PLX	C7-C6-O6-C4
12	D	242	CDL	C12-C13-C14-C15
12	D	242	CDL	OA5-CA3-CA4-CA6
12	G	82	CDL	C12-C11-CA5-OA6
13	A	448	PEE	O2-C10-C11-C12
17	J	63	PLX	C11-C12-C13-C14
13	C	380	PEE	C42-C43-C44-C45
12	D	242	CDL	C32-C31-CA7-OA9
13	A	448	PEE	C11-C10-O2-C2
12	D	242	CDL	C72-C71-CB7-OB9
12	G	82	CDL	C32-C31-CA7-OA9
13	C	380	PEE	O4-C10-C11-C12
12	D	242	CDL	CA3-CA4-CA6-OA8
12	D	242	CDL	C52-C51-CB5-OB7

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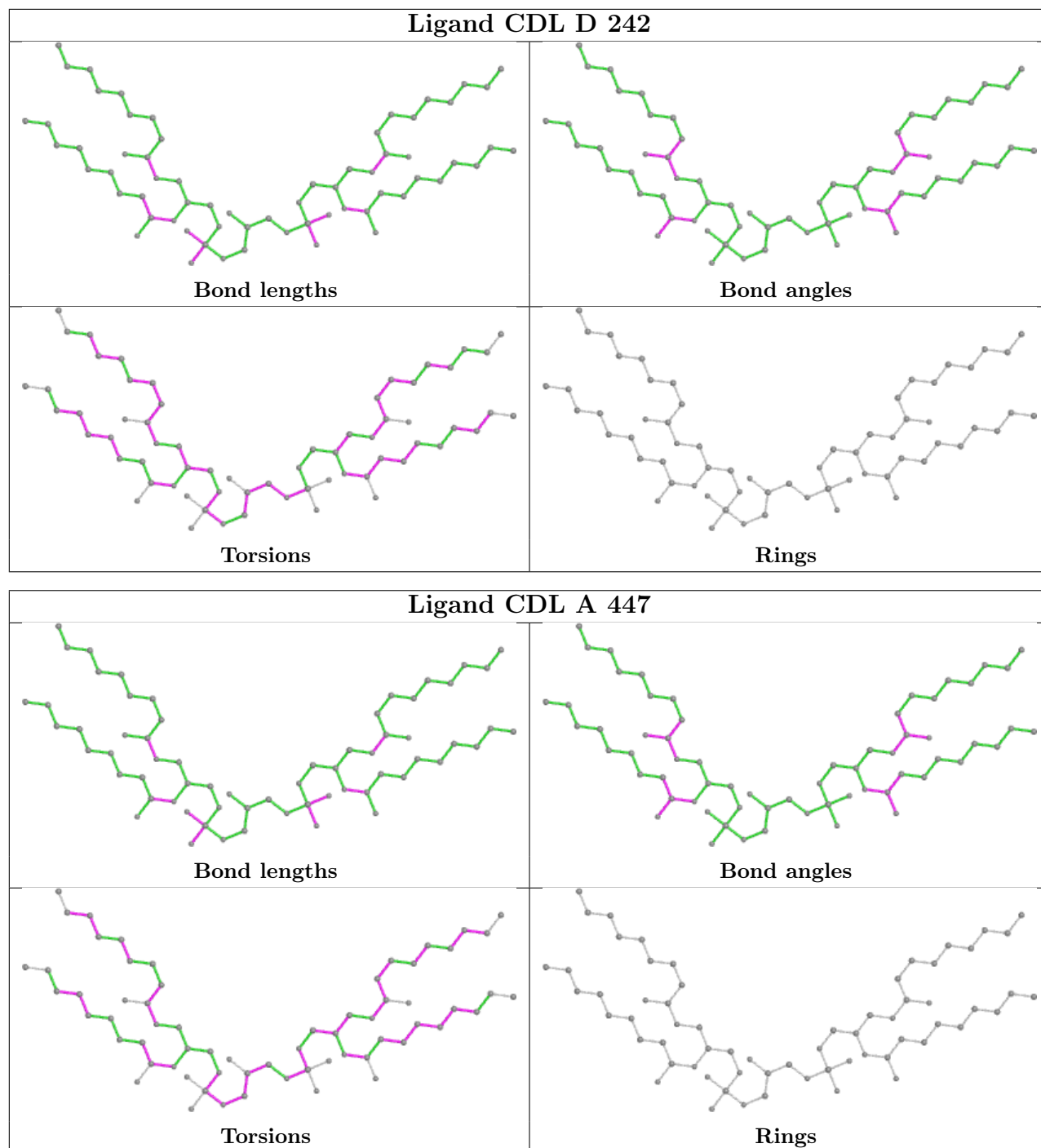
Mol	Chain	Res	Type	Atoms
12	A	447	CDL	CA2-OA2-PA1-OA4
13	E	197	PEE	C4-O4P-P-O1P
17	J	63	PLX	C2-C1-N1-C1C
13	E	197	PEE	C40-C41-C42-C43
12	A	447	CDL	C12-C11-CA5-OA7
12	A	447	CDL	C72-C71-CB7-OB9
12	A	447	CDL	C35-C36-C37-C38
12	G	82	CDL	C52-C51-CB5-OB7
12	A	447	CDL	C32-C31-CA7-OA9

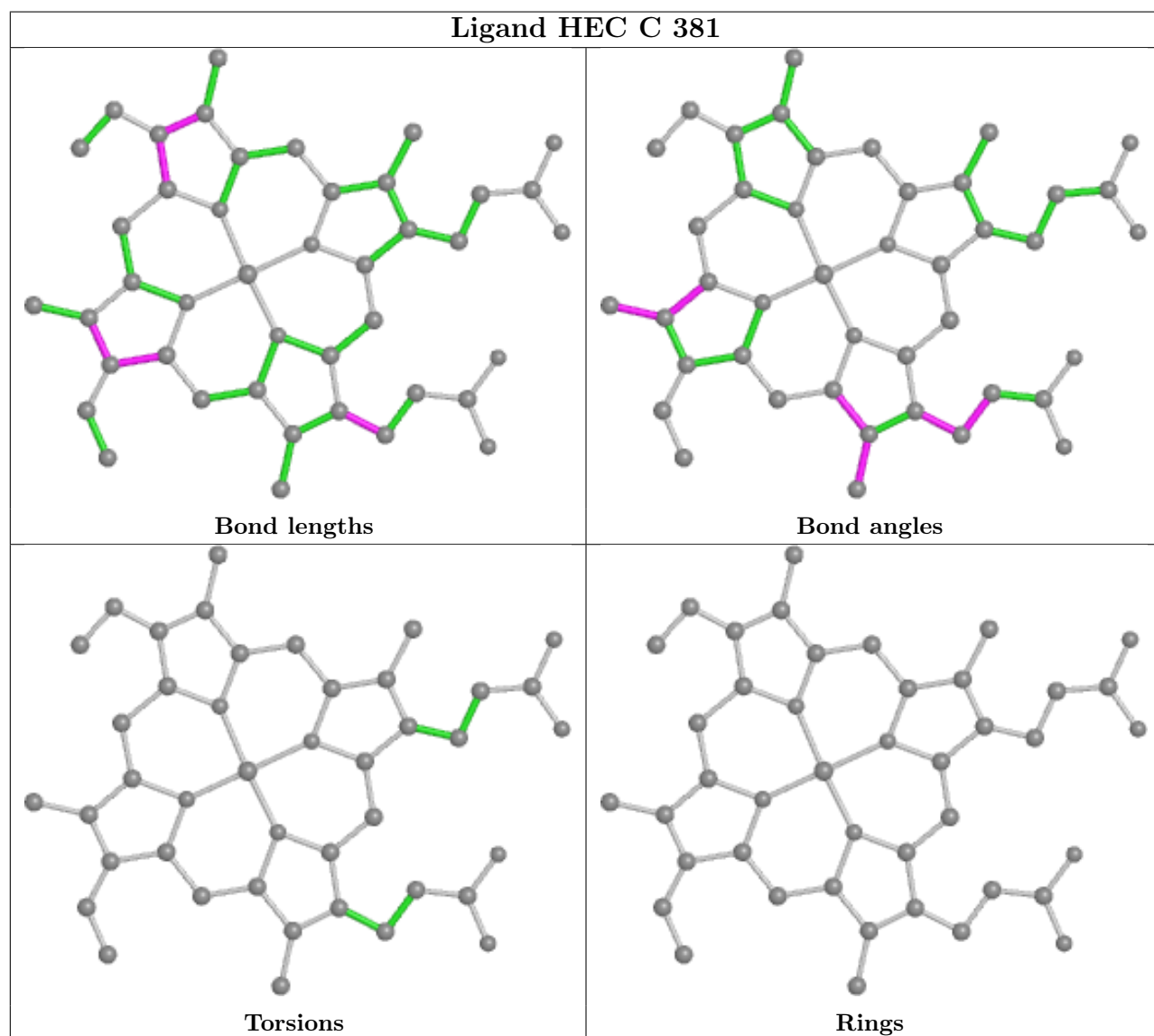
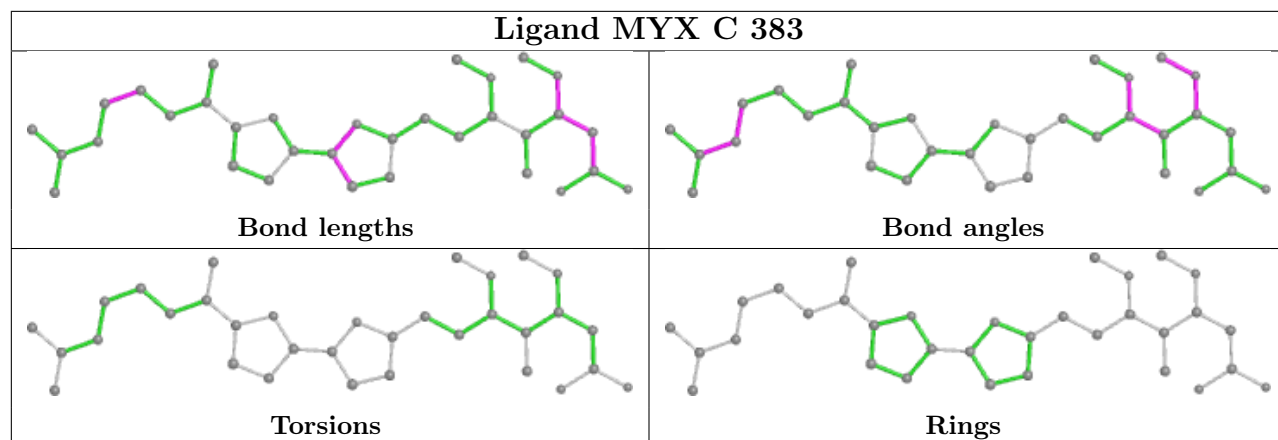
There are no ring outliers.

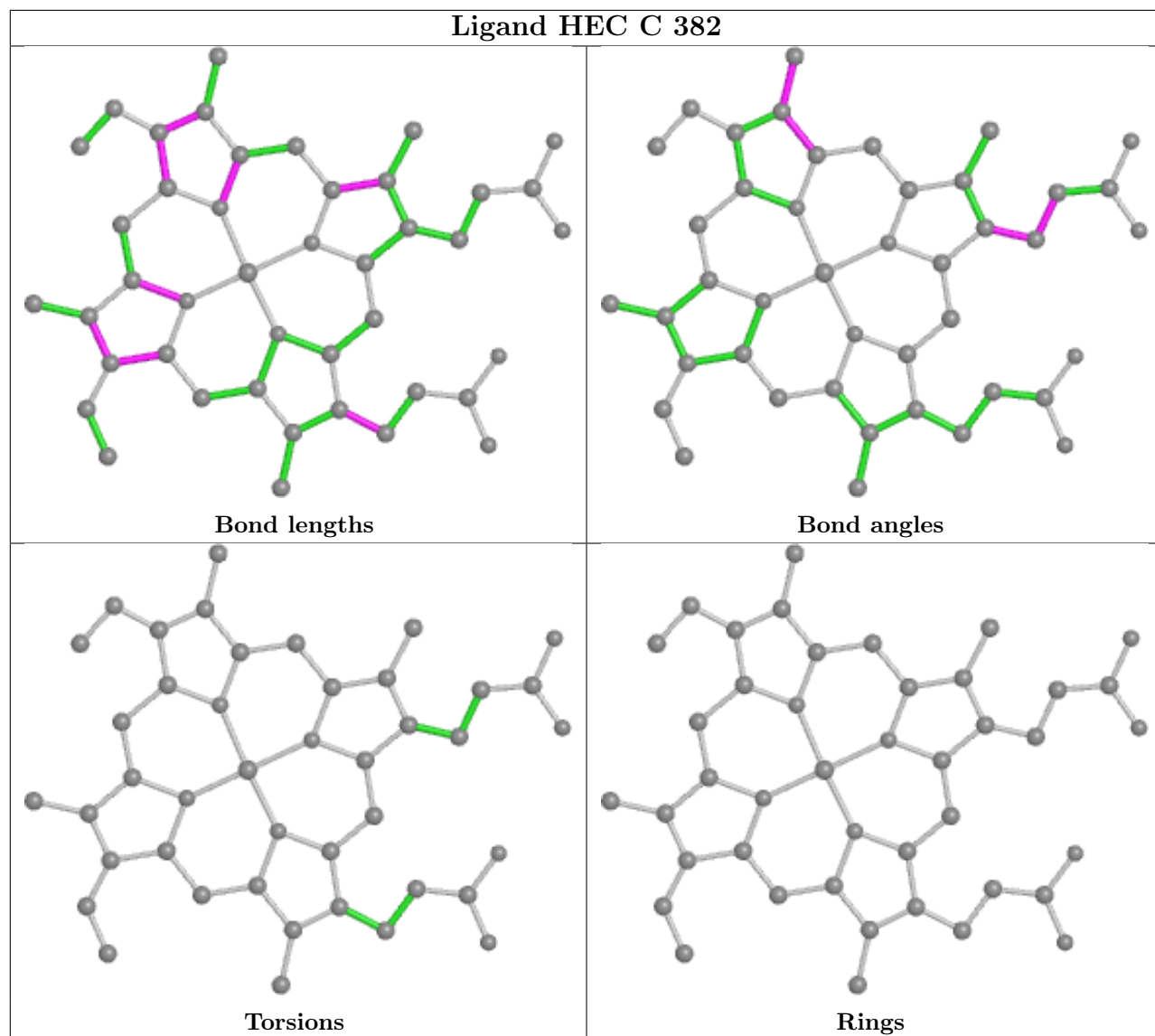
9 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	447	CDL	1	0
15	C	383	MYX	1	0
14	C	381	HEC	5	0
14	C	382	HEC	5	0
14	D	243	HEC	8	0
13	E	197	PEE	3	0
17	J	63	PLX	4	0
13	A	448	PEE	1	0
12	G	82	CDL	2	0

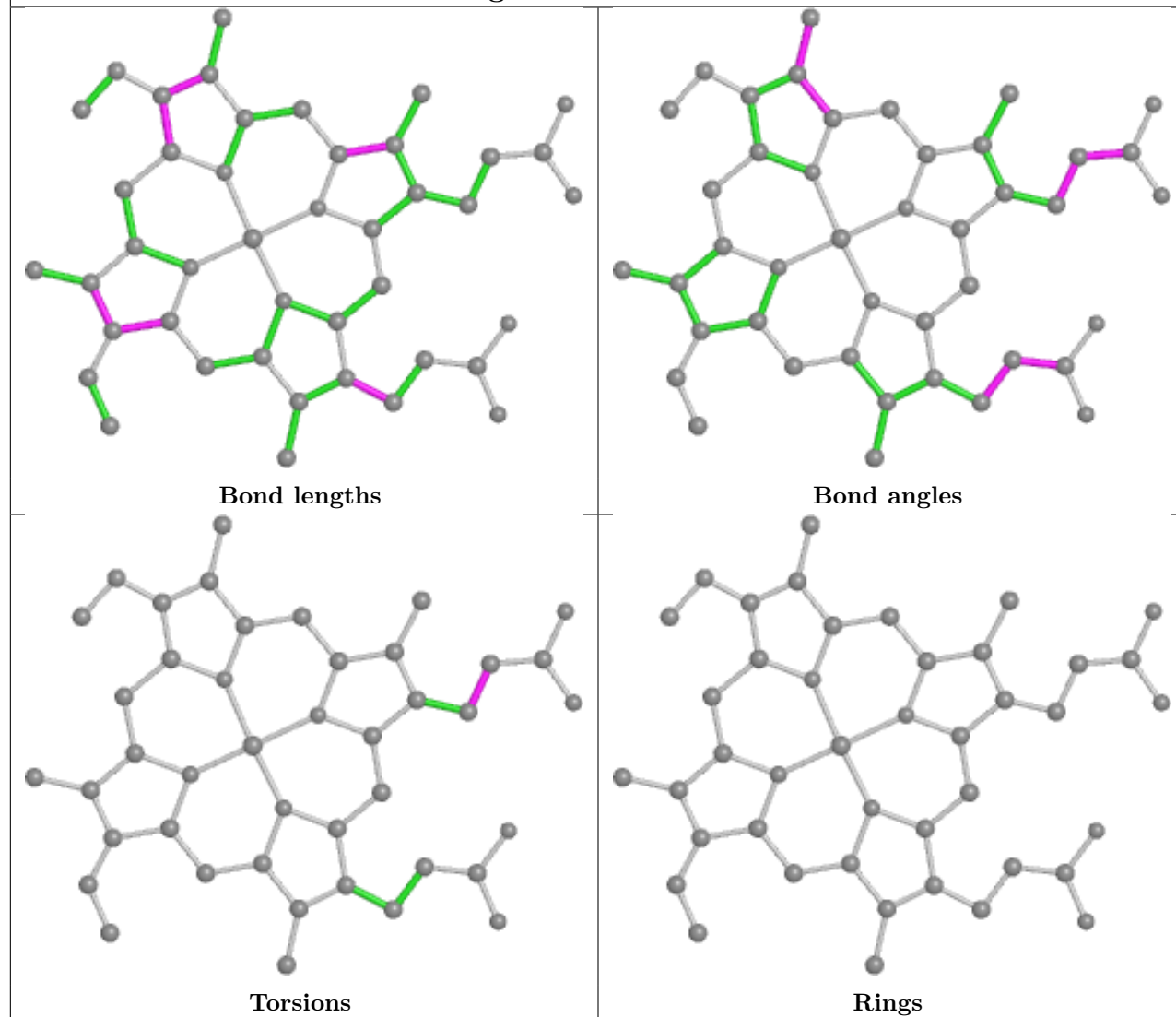
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



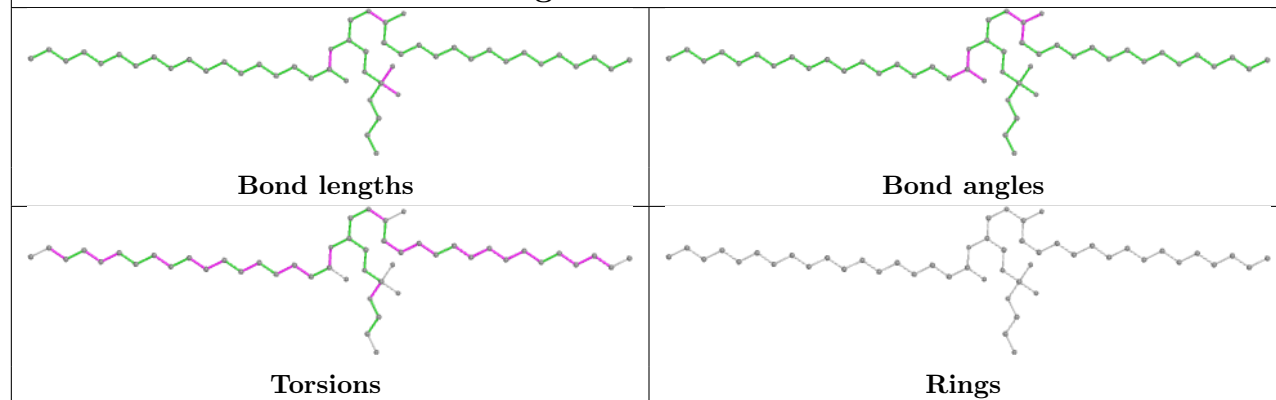


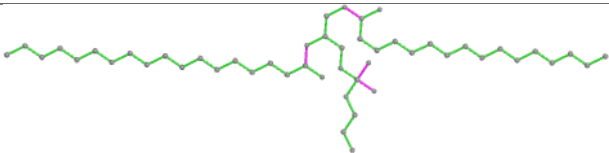
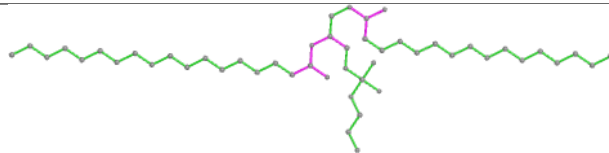
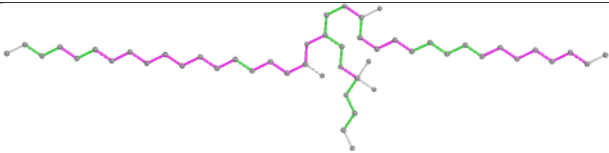
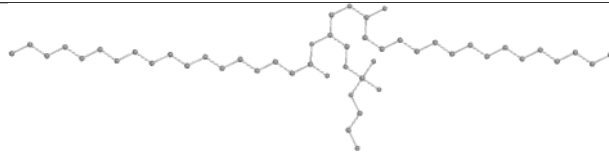


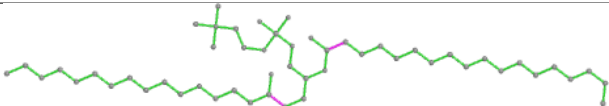
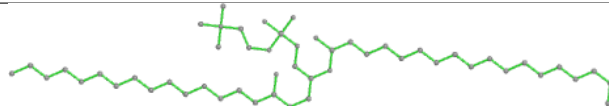
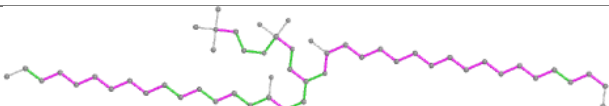
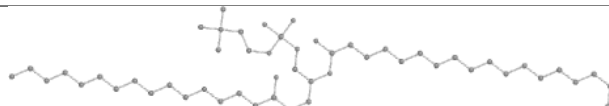
## Ligand HEC D 243

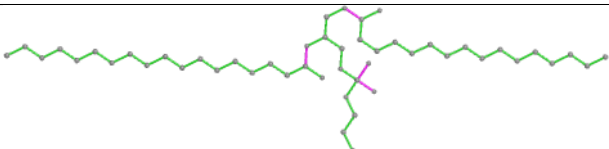
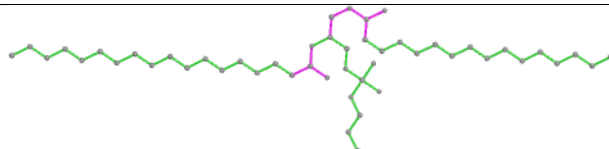
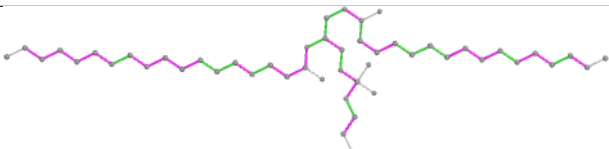
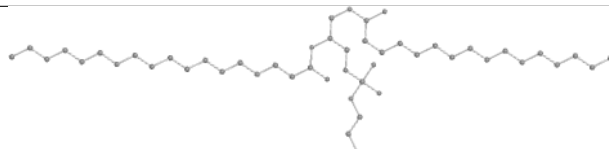


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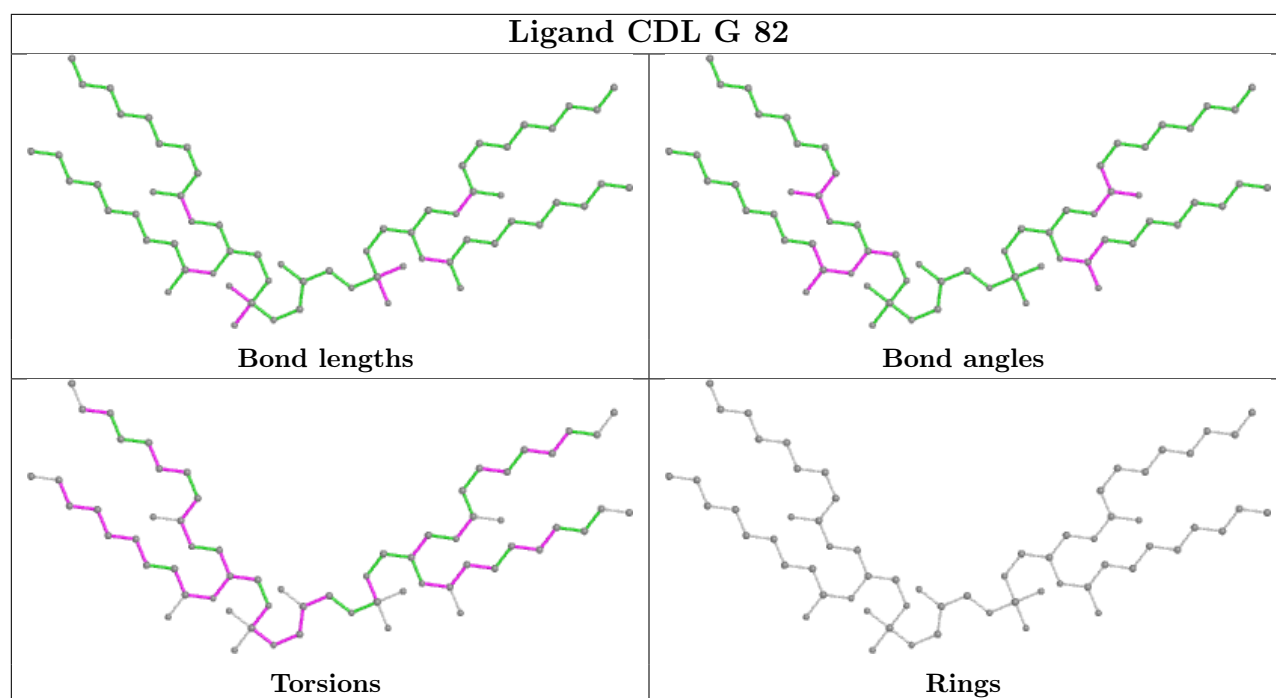


Ligand PEE C 380	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PLX J 63	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PEE A 448	
	
Bond lengths	Bond angles
	
Torsions	Rings





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.