



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2021 – 07:46 PM EST

PDB ID : 1P84
Title : HDBT inhibited Yeast Cytochrome bc1 Complex
Authors : Palsdottir, H.; Lojero, C.G.; Trumpower, B.L.; Hunte, C.
Deposited on : 2003-05-06
Resolution : 2.50 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 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

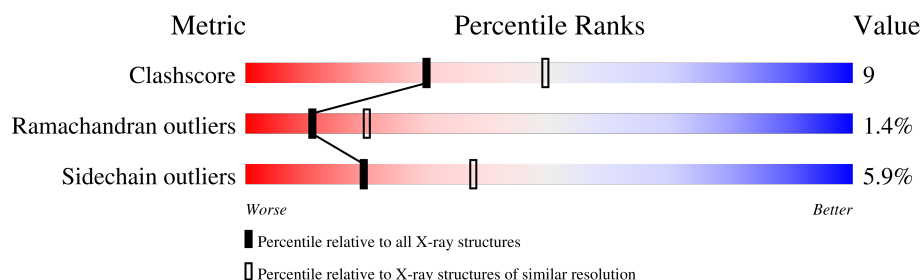
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)




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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	431	76% 22% .
2	B	352	63% 35% .
3	C	385	85% 14% .
4	D	246	83% 16% .
5	E	185	82% 17% .
6	F	74	78% 20% .
7	G	125	90% 10% .
8	H	93	85% 13% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	I	55	 85% 11% .
10	J	127	 69% 26% 5%
11	K	107	 60% 35% 6%

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 18069 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	0	0
			3344	2109	576	653	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	ASP	GLU	conflict	UNP P07256

- Molecule 2 is a protein called Ubiquinol-cytochrome C reductase complex core protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	352	Total	C	N	O	S	0	0	0
			2735	1747	453	534	1			

- Molecule 3 is a protein called cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	385	Total	C	N	O	S	0	0	0
			3089	2080	484	504	21			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	122	THR	ILE	conflict	UNP P00163

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	246	Total	C	N	O	S	0	0	0
			1941	1237	334	361	9			

- Molecule 5 is a protein called Ubiquinol-cytochrome C reductase iron-sulfur subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	185	Total	C	N	O	S	0	0	0
			1411	893	242	266	10			

- Molecule 6 is a protein called Ubiquinol-cytochrome C reductase complex 17 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	74	Total	C	N	O	S	0	0	0
			624	391	108	123	2			

- Molecule 7 is a protein called Ubiquinol-cytochrome C reductase complex 14 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	125	Total	C	N	O	S	0	0	0
			1012	648	172	190	2			

- Molecule 8 is a protein called Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	93	Total	C	N	O	S	98	0	0
			773	510	131	130	2			

- Molecule 9 is a protein called Ubiquinol-cytochrome C reductase complex 7.3 kDa protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	55	Total	C	N	O	0	0	0
			449	298	75	76			

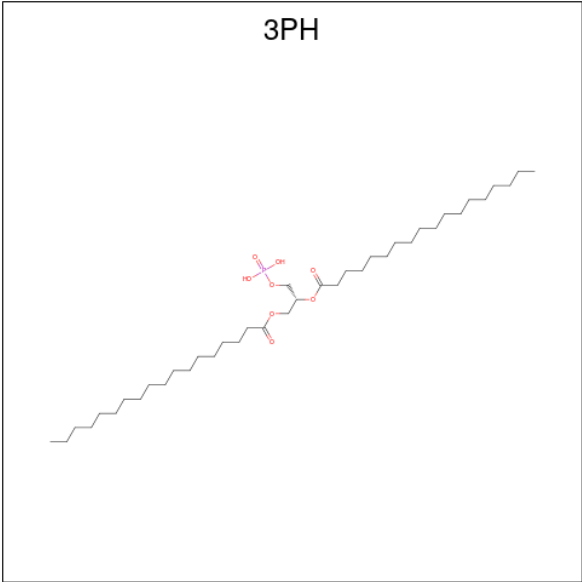
- Molecule 10 is a protein called Heavy Chain (Vh) Of Fv-Fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	127	Total	C	N	O	S	0	0	0
			1015	644	167	201	3			

- Molecule 11 is a protein called Light Chain (Vl) Of Fv-Fragment.

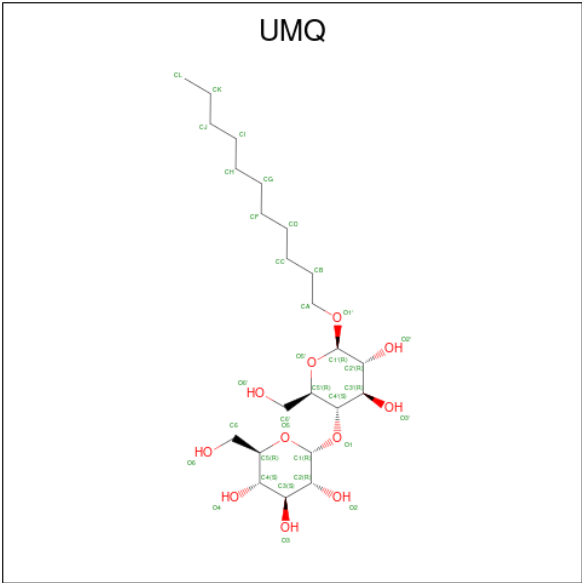
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	107	Total	C	N	O	S	0	0	0
			842	536	141	163	2			

- Molecule 12 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: C₃₉H₇₇O₈P).



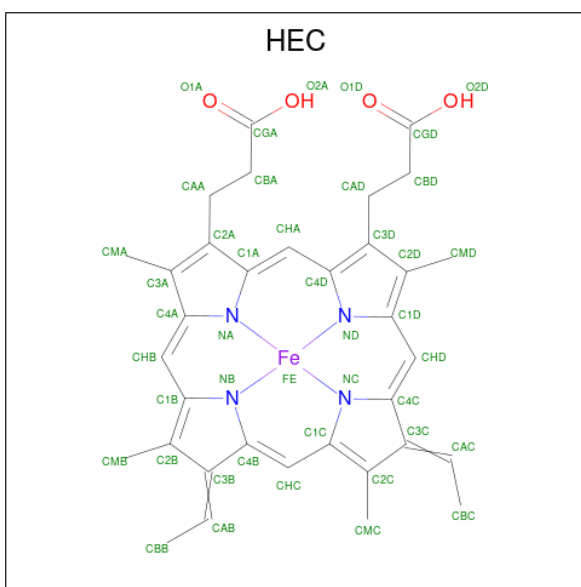
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	A	1	Total	C	O	P	0	0
			40	31	8	1		
12	D	1	Total	C	O	P	0	0
			38	29	8	1		

- Molecule 13 is UNDECYL-MALTOSIDE (three-letter code: UMQ) (formula: $C_{23}H_{44}O_{11}$).



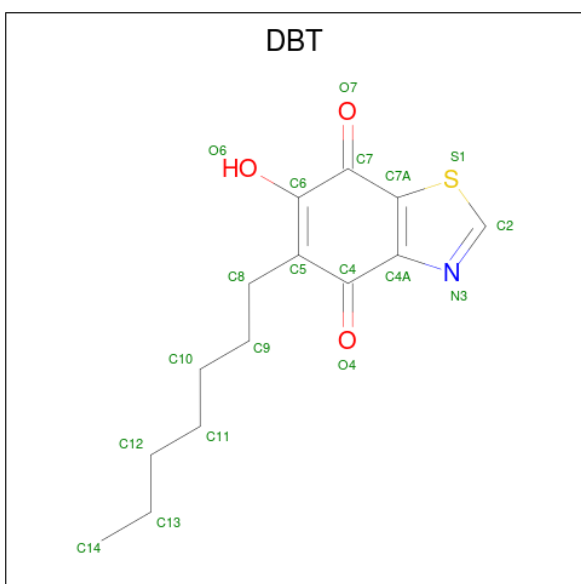
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	A	1	Total	C	O	0	0
			34	23	11		

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



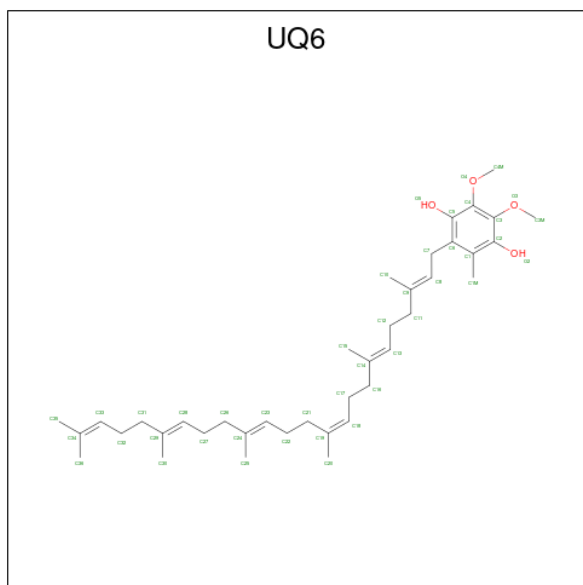
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
14	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
14	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 15 is 5-HEPTYL-6-HYDROXY-1,3-BENZOTHAZOLE-4,7-DIONE (three-letter code: DBT) (formula: $\text{C}_{14}\text{H}_{17}\text{NO}_3\text{S}$).



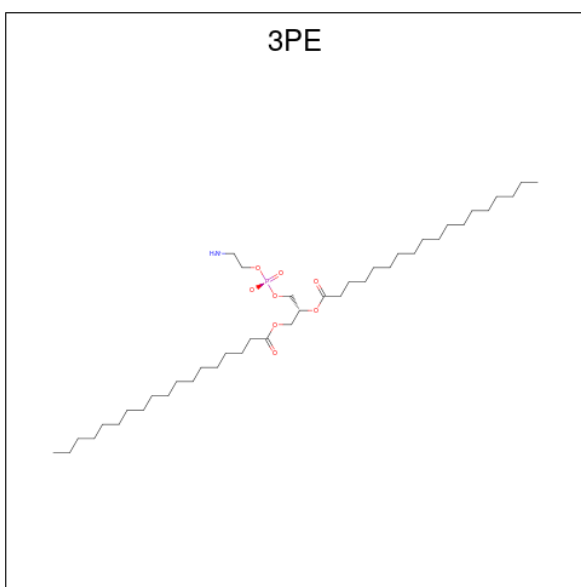
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	C	1	Total	C	N	O	S	0	0
			19	14	1	3	1		

- Molecule 16 is 5-(3,7,11,15,19,23-HEXAMETHYL-TETRACOSA-2,6,10,14,18,22-HEXAENYL)-2,3-DIMETHOXY-6-METHYL-BENZENE-1,4-DIOL (three-letter code: UQ6) (formula: C₃₉H₆₀O₄).



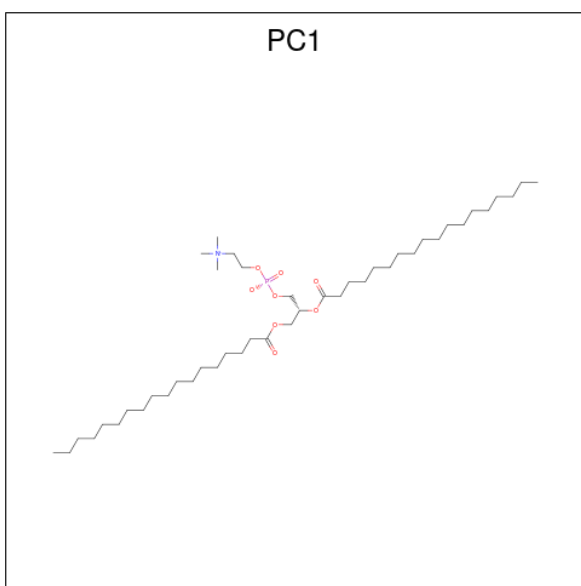
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	C	1	Total	C	O	0	0
			43	39	4		

- Molecule 17 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: 3PE) (formula: C₄₁H₈₂NO₈P).



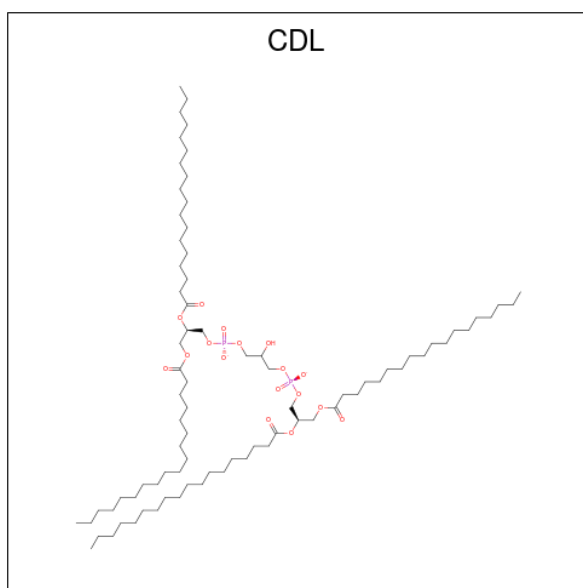
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	C	1	Total	C	N	O	P	0	0
			47	37	1	8	1		
17	C	1	Total	C	N	O	P	0	0
			40	30	1	8	1		

- Molecule 18 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



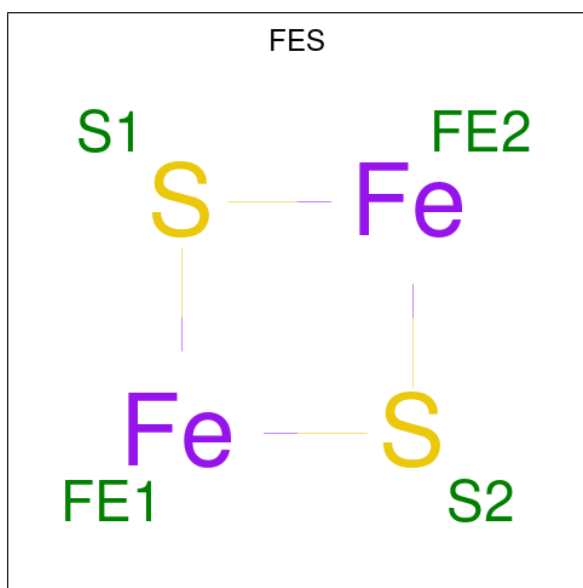
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	D	1	Total	C	N	O	P	0	0
			38	28	1	8	1		

- Molecule 19 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	D	1	Total	C	O	P	0	0
			76	57	17	2		

- Molecule 20 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

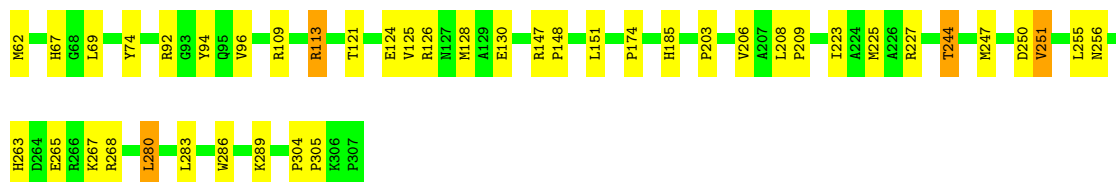
- Molecule 21 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	55	Total O 55 55	0	0
21	B	11	Total O 11 11	0	0
21	C	110	Total O 110 110	0	0
21	D	62	Total O 62 62	0	0
21	E	25	Total O 25 25	0	0
21	F	4	Total O 4 4	0	0
21	G	32	Total O 32 32	0	0
21	H	20	Total O 20 20	0	0
21	I	2	Total O 2 2	0	0
21	J	3	Total O 3 3	0	0
21	K	2	Total O 2 2	0	0



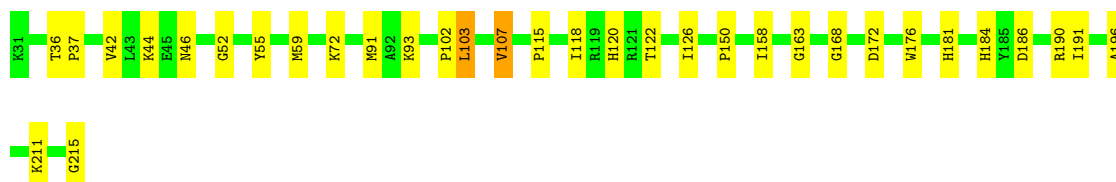
- Molecule 4: Cytochrome c1, heme protein

Chain D: 83% 16% .



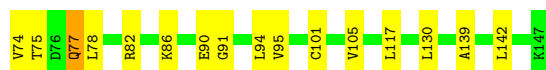
- Molecule 5: Ubiquinol-cytochrome C reductase iron-sulfur subunit

Chain E: 82% 17% .



- Molecule 6: Ubiquinol-cytochrome C reductase complex 17 kDa protein

Chain F: 78% 20% .



- Molecule 7: Ubiquinol-cytochrome C reductase complex 14 kDa protein

Chain G: 90% 10% .



- Molecule 8: Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C

Chain H: 85% 13% .



- Molecule 9: Ubiquinol-cytochrome C reductase complex 7.3 kDa protein

Chain I: 85% 11% .



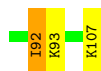
• Molecule 10: Heavy Chain (Vh) Of Fv-Fragment

Chain J: 69% 26% 5%



• Molecule 11: Light Chain (Vl) Of Fv-Fragment

Chain K: 60% 35% 6%



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	215.00Å 165.09Å 147.53Å 90.00° 117.33° 90.00°	Depositor
Resolution (Å)	25.00 – 2.50	Depositor
% Data completeness (in resolution range)	92.5 (25.00-2.50)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.228 , 0.252	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18069	wwPDB-VP
Average B, all atoms (Å ²)	71.0	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: UQ6, PC1, DBT, CDL, FES, 3PE, UMQ, HEC, 3PH

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	0.36	0/3405	0.59	0/4614
2	B	0.33	0/2781	0.59	0/3764
3	C	0.45	0/3191	0.64	1/4353 (0.0%)
4	D	0.37	0/2002	0.60	0/2726
5	E	0.35	0/1444	0.61	1/1957 (0.1%)
6	F	0.34	0/638	0.54	0/858
7	G	0.37	0/1032	0.64	0/1397
8	H	0.40	0/804	0.52	0/1088
9	I	0.41	0/462	0.50	0/622
10	J	0.35	0/1043	0.64	1/1422 (0.1%)
11	K	0.33	0/863	0.57	0/1172
All	All	0.37	0/17665	0.60	3/23973 (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
4	D	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	32	GLY	N-CA-C	6.55	129.48	113.10
3	C	346	VAL	N-CA-C	5.96	127.08	111.00
5	E	163	GLY	N-CA-C	5.45	126.73	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	94	TYR	Sidechain

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	3344	0	3321	70	0
2	B	2735	0	2774	83	0
3	C	3089	0	3125	34	0
4	D	1941	0	1862	26	0
5	E	1411	0	1386	24	0
6	F	624	0	581	11	0
7	G	1012	0	1026	9	0
8	H	773	0	736	12	0
9	I	449	0	445	6	0
10	J	1015	0	959	30	0
11	K	842	0	820	25	0
12	A	40	0	53	4	0
12	D	38	0	49	3	0
13	A	34	0	44	2	0
14	C	86	0	64	3	0
14	D	43	0	30	1	0
15	C	19	0	17	1	0
16	C	43	0	58	8	0
17	C	87	0	128	3	0
18	D	38	0	50	3	0
19	D	76	0	99	5	0
20	E	4	0	0	1	0
21	A	55	0	0	1	0
21	B	11	0	0	0	0
21	C	110	0	0	5	0
21	D	62	0	0	0	0
21	E	25	0	0	0	0
21	F	4	0	0	1	0
21	G	32	0	0	1	0
21	H	20	0	0	1	0
21	I	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	J	3	0	0	0	0
21	K	2	0	0	0	0
All	All	18069	0	17627	331	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 (331) 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)
16:C:706:UQ6:H1M1	16:C:706:UQ6:H103	1.31	1.10
6:F:77:GLN:H	6:F:77:GLN:HE21	1.01	0.98
17:C:710:3PE:H111	8:H:51:ARG:HD2	1.53	0.90
2:B:182:LYS:HB2	2:B:211:ALA:HB2	1.58	0.86
6:F:77:GLN:H	6:F:77:GLN:NE2	1.75	0.85
1:A:63:ASN:HB2	1:A:66:ASN:ND2	1.91	0.84
1:A:317:HIS:HE1	1:A:351:TRP:HE1	1.25	0.83
2:B:347:LYS:H	2:B:347:LYS:HD3	1.43	0.81
16:C:706:UQ6:H1M1	16:C:706:UQ6:C10	2.11	0.80
2:B:49:HIS:HD2	2:B:161:TYR:H	1.28	0.80
2:B:336:ILE:HG21	2:B:339:ASN:HB2	1.63	0.80
16:C:706:UQ6:H103	16:C:706:UQ6:C1M	2.10	0.79
2:B:300:ASN:O	2:B:304:ILE:HG12	1.84	0.77
2:B:146:LEU:HD23	2:B:286:THR:HG22	1.68	0.76
3:C:58:ILE:H	3:C:173:ASN:HD22	1.34	0.76
12:A:713:3PH:H12	21:A:775:HOH:O	1.85	0.75
2:B:305:VAL:HG21	2:B:368:LEU:HD22	1.69	0.74
19:D:731:CDL:HB22	7:G:85:HIS:NE2	2.03	0.74
19:D:731:CDL:H351	19:D:731:CDL:H151	1.69	0.74
6:F:77:GLN:HE21	6:F:77:GLN:N	1.83	0.72
11:K:32:PHE:HD2	11:K:92:ILE:HG22	1.54	0.72
2:B:30:THR:HG23	2:B:190:GLU:HB3	1.69	0.72
3:C:147:ILE:HD11	15:C:705:DBT:H92	1.72	0.72
2:B:336:ILE:HD12	2:B:336:ILE:H	1.55	0.71
2:B:49:HIS:CD2	2:B:161:TYR:H	2.07	0.70
2:B:254:GLU:HG2	2:B:276:LEU:HD23	1.74	0.70
3:C:176:ILE:N	21:C:809:HOH:O	2.25	0.69
1:A:73:TRP:CE3	1:A:76:ILE:HD11	2.27	0.69
1:A:63:ASN:HB2	1:A:66:ASN:HD21	1.56	0.68
2:B:336:ILE:CG2	2:B:339:ASN:HB2	2.23	0.68
7:G:77:ARG:HD3	7:G:88:LEU:HD11	1.76	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:GLY:H	1:A:61:ASN:ND2	1.92	0.67
6:F:78:LEU:HD13	6:F:142:LEU:HD22	1.74	0.67
1:A:99:ARG:HD3	1:A:174:LEU:HD12	1.74	0.67
3:C:27:ASN:HB2	19:D:731:CDL:OB3	1.95	0.67
3:C:58:ILE:H	3:C:173:ASN:ND2	1.91	0.67
3:C:208:ASN:HD22	3:C:210:LEU:H	1.40	0.67
14:C:701:HEC:HBC3	14:C:701:HEC:HHD	1.77	0.66
1:A:289:ASN:C	1:A:289:ASN:HD22	2.00	0.65
10:J:29:ILE:H	10:J:77:ASN:HD21	1.42	0.65
1:A:42:HIS:CD2	1:A:42:HIS:H	2.15	0.65
5:E:107:VAL:HG12	5:E:118:ILE:HB	1.77	0.64
6:F:91:GLY:O	6:F:95:VAL:HG13	1.98	0.64
6:F:74:VAL:HG12	6:F:75:THR:H	1.62	0.64
1:A:109:LEU:HG	1:A:110:PRO:HD2	1.80	0.64
2:B:40:ARG:HG3	2:B:155:LEU:HG	1.80	0.63
12:A:713:3PH:H282	3:C:230:LEU:HD13	1.81	0.63
2:B:65:LEU:O	2:B:69:ARG:HG2	1.99	0.63
2:B:110:TYR:HD2	2:B:205:LEU:HD23	1.64	0.62
11:K:37:GLN:HB2	11:K:47:LEU:HD11	1.81	0.62
3:C:132:TYR:OH	3:C:253:HIS:HD2	1.83	0.61
11:K:27:GLN:HG2	11:K:28:ASP:H	1.65	0.61
6:F:82:ARG:O	6:F:86:LYS:HG3	2.00	0.61
1:A:172:THR:HG23	1:A:173:PRO:HD2	1.83	0.61
11:K:29:ILE:HG22	11:K:92:ILE:HD12	1.81	0.61
5:E:115:PRO:HD2	5:E:158:ILE:HD11	1.83	0.61
11:K:2:ILE:HD12	11:K:2:ILE:H	1.65	0.61
2:B:264:LEU:HD12	2:B:317:ALA:HB2	1.82	0.61
4:D:113:ARG:HG2	4:D:151:LEU:O	2.00	0.61
11:K:29:ILE:HA	11:K:92:ILE:HG21	1.82	0.61
11:K:47:LEU:HA	11:K:58:VAL:HG11	1.84	0.60
10:J:61:ASN:HD22	10:J:63:SER:H	1.48	0.60
2:B:181:THR:HB	2:B:212:GLY:H	1.66	0.60
2:B:305:VAL:HG11	2:B:368:LEU:HB3	1.84	0.59
1:A:289:ASN:ND2	1:A:291:PHE:H	2.01	0.59
1:A:46:ALA:O	1:A:47:HIS:HB2	2.03	0.58
2:B:24:ALA:HB3	2:B:191:ASN:ND2	2.18	0.58
1:A:229:SER:HB3	1:A:232:THR:HB	1.85	0.58
10:J:6:GLU:H	10:J:114:GLN:HE21	1.49	0.58
3:C:4:ARG:HE	3:C:14:ASN:ND2	2.01	0.58
2:B:182:LYS:HD3	2:B:207:SER:HA	1.86	0.58
5:E:103:LEU:O	5:E:120:HIS:HB3	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:44:LYS:NZ	5:E:52:GLY:H	2.01	0.58
7:G:77:ARG:HD2	21:G:149:HOH:O	2.04	0.58
2:B:287:LEU:HD21	2:B:304:ILE:HG21	1.85	0.58
1:A:252:ARG:HD3	1:A:254:ASP:OD1	2.04	0.57
1:A:313:ASP:OD1	1:A:335:ARG:HD3	2.05	0.57
4:D:185:HIS:ND1	18:D:715:PC1:H142	2.19	0.57
1:A:258:LYS:HG2	1:A:335:ARG:HG3	1.87	0.57
10:J:99:SER:HB3	10:J:109:MET:HG2	1.87	0.56
10:J:61:ASN:ND2	10:J:63:SER:H	2.03	0.56
1:A:289:ASN:HD22	1:A:291:PHE:H	1.51	0.56
5:E:44:LYS:HB3	8:H:35:LYS:HA	1.87	0.56
11:K:38:GLN:O	11:K:84:ALA:HB1	2.05	0.56
5:E:191:ILE:HD13	5:E:196:ALA:HB3	1.88	0.56
10:J:36:ASN:OD1	10:J:51:TYR:HB3	2.05	0.56
1:A:306:ILE:HA	1:A:311:LEU:HD22	1.87	0.56
8:H:89:LEU:O	8:H:93:ASN:HB2	2.05	0.55
10:J:6:GLU:H	10:J:114:GLN:NE2	2.04	0.55
1:A:74:LYS:HG3	1:A:95:SER:HB3	1.88	0.55
3:C:214:GLY:O	3:C:218:ARG:HD2	2.06	0.55
1:A:73:TRP:CZ3	1:A:76:ILE:HD11	2.41	0.55
3:C:315:GLY:HA3	21:C:814:HOH:O	2.06	0.55
5:E:172:ASP:H	5:E:184:HIS:HD2	1.54	0.55
1:A:67:ASN:ND2	1:A:180:GLY:HA2	2.21	0.55
2:B:98:LEU:O	2:B:102:VAL:HG23	2.06	0.55
10:J:38:ILE:HA	10:J:49:VAL:HG23	1.89	0.55
3:C:323:LYS:CE	8:H:55:GLN:HE22	2.20	0.54
3:C:4:ARG:HE	3:C:14:ASN:HD21	1.55	0.54
3:C:44:ILE:HD12	16:C:706:UQ6:C20	2.37	0.54
11:K:34:ASN:HD22	11:K:49:TYR:HA	1.73	0.54
17:C:710:3PE:C11	8:H:51:ARG:HD2	2.33	0.54
9:I:52:VAL:O	9:I:56:ILE:HG12	2.07	0.54
2:B:36:HIS:HB2	2:B:184:ASN:OD1	2.08	0.53
3:C:173:ASN:O	21:C:809:HOH:O	2.19	0.53
5:E:55:TYR:O	5:E:59:MET:HG2	2.08	0.53
1:A:58:GLY:H	1:A:61:ASN:HD22	1.55	0.53
12:D:714:3PH:H2A2	12:D:714:3PH:H251	1.89	0.53
2:B:93:PHE:HD1	2:B:94:LEU:O	1.91	0.53
2:B:252:GLN:HG3	2:B:253:TYR:N	2.22	0.53
10:J:87:THR:HG22	10:J:88:THR:N	2.23	0.53
2:B:313:ASP:O	2:B:316:PRO:HD3	2.08	0.53
1:A:350:GLN:HE22	1:A:353:ARG:HH21	1.57	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:31:ASN:ND2	11:K:51:THR:HG21	2.24	0.53
3:C:208:ASN:HB2	3:C:209:PRO:HD2	1.91	0.53
3:C:25:SER:OG	7:G:79:HIS:HD2	1.92	0.52
2:B:110:TYR:CD2	2:B:205:LEU:HD23	2.44	0.52
4:D:247:MET:O	4:D:251:VAL:HG22	2.09	0.52
7:G:31:GLN:HA	7:G:31:GLN:NE2	2.24	0.52
5:E:93:LYS:HD3	5:E:215:GLY:HA3	1.91	0.52
1:A:68:GLY:HA3	1:A:185:LEU:HD11	1.92	0.52
1:A:217:GLU:HA	1:A:220:VAL:HG12	1.91	0.52
1:A:169:PHE:O	1:A:172:THR:HB	2.09	0.52
3:C:208:ASN:ND2	3:C:210:LEU:H	2.08	0.52
8:H:61:ILE:HB	8:H:62:PRO:HD3	1.92	0.52
1:A:77:PHE:CE1	1:A:124:PHE:HE1	2.28	0.51
1:A:265:VAL:HG21	1:A:426:LEU:HD12	1.93	0.51
1:A:172:THR:HG23	1:A:242:ALA:HA	1.91	0.51
3:C:77:ILE:O	3:C:81:LEU:HB2	2.11	0.51
2:B:315:SER:N	2:B:316:PRO:HD3	2.25	0.51
3:C:97:MET:HG2	14:C:702:HEC:HBC2	1.91	0.51
4:D:286:TRP:CE3	5:E:59:MET:HG3	2.45	0.51
1:A:156:HIS:HD2	1:A:159:ARG:HH21	1.57	0.51
2:B:115:LYS:HB2	2:B:118:GLU:HG3	1.92	0.51
1:A:172:THR:CG2	1:A:242:ALA:HA	2.40	0.51
4:D:147:ARG:HG2	4:D:148:PRO:O	2.10	0.51
5:E:103:LEU:HA	5:E:120:HIS:ND1	2.26	0.51
2:B:83:ASP:HB2	2:B:86:TYR:H	1.75	0.50
1:A:235:LYS:HB2	1:A:235:LYS:NZ	2.26	0.50
1:A:373:GLN:HG3	1:A:374:LEU:N	2.26	0.50
4:D:96:VAL:HB	4:D:251:VAL:HG13	1.94	0.50
4:D:263:HIS:NE2	4:D:267:LYS:HE3	2.26	0.50
11:K:4:LEU:HD23	11:K:88:CYS:SG	2.51	0.50
2:B:52:ASN:HD21	2:B:80:SER:C	2.15	0.50
2:B:347:LYS:HG2	2:B:348:LEU:N	2.27	0.50
3:C:175:THR:O	3:C:178:ARG:HG2	2.12	0.50
11:K:36:TYR:HE2	11:K:89:GLN:HG2	1.76	0.50
4:D:203:PRO:HG2	4:D:206:VAL:HG21	1.94	0.50
2:B:46:GLY:O	2:B:49:HIS:HB3	2.12	0.49
2:B:324:LYS:O	2:B:327:VAL:HG22	2.12	0.49
4:D:62:MET:HB3	4:D:67:HIS:NE2	2.27	0.49
6:F:90:GLU:HB3	21:F:149:HOH:O	2.12	0.49
6:F:101:CYS:O	6:F:105:VAL:HG23	2.13	0.49
10:J:37:TRP:CZ3	10:J:96:CYS:HB3	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:48:TRP:CZ2	10:J:50:GLY:HA2	2.48	0.49
2:B:182:LYS:HB2	2:B:211:ALA:CB	2.37	0.49
2:B:267:LEU:HD22	2:B:304:ILE:HD13	1.94	0.49
7:G:31:GLN:HA	7:G:31:GLN:HE21	1.77	0.49
10:J:99:SER:HA	10:J:108:ALA:O	2.13	0.48
11:K:6:GLN:HG2	11:K:23:CYS:SG	2.53	0.48
2:B:298:SER:OG	2:B:363:PRO:HD3	2.13	0.48
2:B:347:LYS:HD3	2:B:347:LYS:N	2.19	0.48
10:J:61:ASN:HD22	10:J:62:PRO:N	2.11	0.48
13:A:721:UMQ:O2'	9:I:18:VAL:HG22	2.14	0.48
2:B:62:ARG:HH21	2:B:62:ARG:HB2	1.77	0.48
2:B:197:LEU:O	2:B:201:VAL:HG23	2.13	0.48
2:B:26:THR:OG1	2:B:191:ASN:ND2	2.47	0.48
6:F:74:VAL:HG12	6:F:75:THR:N	2.28	0.48
1:A:127:GLN:C	1:A:129:ALA:H	2.17	0.48
4:D:125:VAL:HA	4:D:128:MET:HE3	1.96	0.48
5:E:168:GLY:HA2	5:E:176:TRP:CD1	2.48	0.48
2:B:58:ASN:OD1	2:B:63:SER:HA	2.14	0.48
5:E:172:ASP:H	5:E:184:HIS:CD2	2.31	0.48
1:A:179:ARG:HH21	1:A:179:ARG:HG2	1.78	0.47
5:E:181:HIS:HB2	20:E:704:FES:S1	2.54	0.47
10:J:54:ASN:HD22	10:J:54:ASN:H	1.62	0.47
1:A:67:ASN:HD22	1:A:181:THR:HG23	1.79	0.47
2:B:52:ASN:ND2	2:B:80:SER:OG	2.47	0.47
2:B:241:ILE:HA	2:B:352:ASN:O	2.15	0.47
1:A:77:PHE:HE1	1:A:124:PHE:HE1	1.60	0.47
1:A:117:LEU:HD11	1:A:219:LEU:HD12	1.96	0.47
3:C:379:TYR:CE1	3:C:383:VAL:HG21	2.50	0.47
1:A:349:LYS:HA	1:A:349:LYS:HD3	1.63	0.47
4:D:286:TRP:CD2	8:H:37:LEU:HD12	2.50	0.47
1:A:288:TYR:HB3	1:A:315:PHE:CE2	2.50	0.47
2:B:124:LEU:HB2	2:B:125:PRO:HD3	1.96	0.47
10:J:93:THR:HG22	10:J:117:THR:HG23	1.97	0.47
11:K:74:THR:HG22	11:K:75:ILE:N	2.29	0.47
11:K:52:SER:HB3	11:K:64:GLY:O	2.15	0.47
1:A:456:ARG:HH21	1:A:456:ARG:HG3	1.80	0.47
2:B:21:ALA:O	2:B:22:ARG:HB2	2.14	0.47
2:B:59:THR:HA	2:B:112:THR:HA	1.97	0.47
1:A:68:GLY:HA3	1:A:185:LEU:CD1	2.45	0.46
10:J:40:LEU:O	10:J:92:ALA:HB1	2.15	0.46
12:A:713:3PH:H3B2	12:D:714:3PH:H382	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:72:LYS:NZ	9:I:29:GLN:NE2	2.63	0.46
2:B:274:ALA:HB2	2:B:287:LEU:HD12	1.98	0.46
4:D:121:THR:OG1	4:D:124:GLU:HG3	2.15	0.46
11:K:2:ILE:HD12	11:K:2:ILE:N	2.29	0.46
11:K:14:SER:HB2	11:K:17:ASP:OD2	2.16	0.46
3:C:313:VAL:HG22	3:C:319:LYS:HE3	1.98	0.46
1:A:58:GLY:N	1:A:61:ASN:ND2	2.62	0.46
1:A:63:ASN:HB2	1:A:66:ASN:HD22	1.75	0.46
1:A:86:ALA:HB2	1:A:119:PHE:CZ	2.51	0.46
1:A:350:GLN:NE2	1:A:353:ARG:HD3	2.30	0.46
2:B:252:GLN:O	2:B:255:VAL:HG22	2.16	0.46
5:E:122:THR:O	5:E:126:ILE:HG13	2.17	0.46
1:A:67:ASN:ND2	1:A:181:THR:HG23	2.31	0.45
1:A:86:ALA:HB2	1:A:119:PHE:CE1	2.51	0.45
10:J:45:LYS:O	10:J:45:LYS:HG3	2.16	0.45
11:K:32:PHE:CD2	11:K:92:ILE:HG22	2.43	0.45
11:K:46:LEU:HD23	11:K:55:HIS:CD2	2.51	0.45
3:C:201:LEU:HD21	16:C:706:UQ6:H3M2	1.98	0.45
2:B:44:LYS:HB2	2:B:47:VAL:HG21	1.97	0.45
8:H:56:PHE:O	8:H:60:LEU:HB2	2.17	0.45
10:J:61:ASN:HD22	10:J:61:ASN:C	2.19	0.45
3:C:35:LEU:HD13	21:C:727:HOH:O	2.16	0.45
5:E:150:PRO:HB3	10:J:102:TYR:CE2	2.52	0.45
1:A:49:ALA:HA	1:A:212:GLY:HA3	1.98	0.45
2:B:313:ASP:HB3	2:B:344:LYS:O	2.16	0.45
11:K:50:TYR:O	11:K:51:THR:HG22	2.16	0.45
3:C:173:ASN:C	21:C:809:HOH:O	2.53	0.45
1:A:429:GLN:HE22	9:I:13:ARG:NH2	2.15	0.45
7:G:120:LEU:O	7:G:123:ILE:HG12	2.17	0.45
2:B:252:GLN:HB3	2:B:343:VAL:HG21	1.99	0.45
7:G:53:ASN:ND2	7:G:56:MET:H	2.15	0.45
2:B:69:ARG:O	2:B:73:LEU:HD23	2.17	0.44
19:D:731:CDL:HB22	7:G:85:HIS:HE2	1.82	0.44
10:J:14:PRO:O	10:J:15:SER:HB3	2.17	0.44
10:J:29:ILE:HG12	10:J:77:ASN:ND2	2.32	0.44
8:H:15:HIS:HB3	21:H:106:HOH:O	2.16	0.44
2:B:228:GLU:HA	2:B:353:TYR:O	2.17	0.44
10:J:49:VAL:CG1	10:J:68:LEU:HD23	2.47	0.44
1:A:317:HIS:HE1	1:A:351:TRP:NE1	2.05	0.44
1:A:121:ASN:ND2	1:A:125:ILE:HD12	2.33	0.44
5:E:191:ILE:CD1	5:E:196:ALA:HB3	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:29:SER:HA	2:B:191:ASN:HB3	2.00	0.44
1:A:142:LYS:HB2	1:A:142:LYS:NZ	2.33	0.44
2:B:155:LEU:H	2:B:155:LEU:HD12	1.82	0.44
2:B:155:LEU:HD12	2:B:155:LEU:N	2.32	0.44
14:C:701:HEC:HH C	14:C:701:HEC:HAB	1.83	0.44
4:D:203:PRO:HG2	4:D:206:VAL:CG2	2.48	0.44
1:A:29:VAL:HG11	1:A:400:LYS:HB3	1.99	0.44
1:A:58:GLY:N	1:A:61:ASN:HD22	2.15	0.44
1:A:289:ASN:C	1:A:289:ASN:ND2	2.70	0.44
4:D:304:PRO:HA	4:D:305:PRO:HD3	1.84	0.44
1:A:350:GLN:NE2	1:A:353:ARG:HH21	2.16	0.44
1:A:430:ASP:OD2	1:A:449:ARG:NH2	2.50	0.44
4:D:74:TYR:CE1	6:F:139:ALA:HA	2.53	0.44
2:B:141:SER:O	2:B:145:GLN:HG2	2.17	0.43
5:E:186:ASP:OD2	5:E:190:ARG:HD2	2.18	0.43
11:K:33:LEU:HD22	11:K:71:TYR:CG	2.53	0.43
1:A:69:VAL:HG13	1:A:70:SER:N	2.33	0.43
2:B:40:ARG:HB2	2:B:84:ARG:O	2.19	0.43
5:E:42:VAL:HG12	8:H:34:GLN:HG2	1.99	0.43
2:B:239:ALA:HB1	2:B:301:ILE:HD12	2.00	0.43
18:D:715:PC1:O12	18:D:715:PC1:H153	2.18	0.43
10:J:87:THR:HG22	10:J:88:THR:H	1.83	0.43
2:B:294:SER:HB3	2:B:358:ASP:HB3	2.01	0.43
10:J:38:ILE:O	10:J:38:ILE:HG13	2.19	0.43
12:A:713:3PH:H282	3:C:230:LEU:CD1	2.48	0.43
2:B:43:THR:HG22	2:B:175:PHE:HD1	1.82	0.43
1:A:179:ARG:H	1:A:179:ARG:HD2	1.83	0.43
2:B:193:VAL:HG23	2:B:196:ASP:HB2	2.01	0.43
3:C:110:ARG:NH2	3:C:205:GLY:O	2.52	0.43
5:E:72:LYS:HZ2	9:I:29:GLN:NE2	2.16	0.43
1:A:66:ASN:HD22	1:A:66:ASN:H	1.67	0.43
10:J:24:VAL:HG21	10:J:29:ILE:HD11	2.01	0.42
10:J:65:LYS:HA	10:J:68:LEU:HD11	2.00	0.42
2:B:250:LEU:HD21	2:B:336:ILE:HD13	2.01	0.42
4:D:255:LEU:HD23	4:D:255:LEU:HA	1.88	0.42
11:K:79:GLU:HA	11:K:80:PRO:HA	1.87	0.42
2:B:175:PHE:CE2	2:B:179:VAL:HG21	2.55	0.42
2:B:232:ARG:HB3	2:B:232:ARG:HH21	1.84	0.42
5:E:36:THR:HA	5:E:37:PRO:HD2	1.92	0.42
10:J:29:ILE:H	10:J:77:ASN:ND2	2.15	0.42
2:B:260:LEU:O	2:B:271:ILE:HD11	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:304:VAL:HG13	3:C:308:THR:HG23	2.02	0.42
1:A:172:THR:HG21	1:A:243:ALA:H	1.85	0.42
2:B:62:ARG:HH21	2:B:62:ARG:CB	2.33	0.42
2:B:64:ALA:O	2:B:68:VAL:HG23	2.19	0.42
11:K:4:LEU:CD2	11:K:88:CYS:SG	3.08	0.42
11:K:75:ILE:HG22	11:K:76:SER:N	2.35	0.42
2:B:150:THR:HG22	2:B:352:ASN:ND2	2.35	0.42
10:J:38:ILE:HD12	10:J:46:LEU:HD22	2.02	0.42
1:A:313:ASP:OD2	1:A:335:ARG:NH2	2.53	0.41
10:J:51:TYR:C	10:J:51:TYR:CD2	2.94	0.41
1:A:317:HIS:CE1	1:A:351:TRP:HE1	2.17	0.41
2:B:145:GLN:HA	2:B:145:GLN:NE2	2.36	0.41
3:C:157:VAL:O	3:C:160:ASP:HB2	2.20	0.41
4:D:265:GLU:OE2	4:D:268:ARG:NH2	2.53	0.41
2:B:40:ARG:CG	2:B:155:LEU:HG	2.49	0.41
2:B:230:ARG:HG2	2:B:230:ARG:HH21	1.85	0.41
8:H:51:ARG:HA	8:H:51:ARG:HD3	1.87	0.41
1:A:121:ASN:HD21	1:A:125:ILE:HD12	1.85	0.41
1:A:365:ARG:HD2	2:B:72:GLU:OE1	2.21	0.41
3:C:130:LEU:HD13	3:C:182:LEU:HB3	2.02	0.41
19:D:731:CDL:H112	19:D:731:CDL:HA4	1.56	0.41
1:A:91:LEU:HD23	1:A:106:VAL:HG11	2.02	0.41
13:A:721:UMQ:HJ1	13:A:721:UMQ:HG1	1.78	0.41
2:B:22:ARG:HH12	2:B:332:VAL:HB	1.85	0.41
2:B:24:ALA:HB3	2:B:191:ASN:HD21	1.86	0.41
17:C:710:3PE:H3A2	17:C:710:3PE:H372	1.84	0.41
4:D:223:ILE:HG12	4:D:225:MET:H	1.86	0.41
5:E:72:LYS:HZ3	9:I:29:GLN:HE22	1.67	0.41
2:B:255:VAL:HG12	2:B:321:THR:HG21	2.02	0.41
10:J:93:THR:HA	10:J:117:THR:HA	2.02	0.41
1:A:374:LEU:HD12	1:A:374:LEU:HA	1.86	0.41
3:C:182:LEU:HD12	3:C:182:LEU:HA	1.88	0.41
4:D:227:ARG:HH11	4:D:244:THR:HG21	1.86	0.41
1:A:37:VAL:HG13	1:A:207:VAL:HG22	2.03	0.41
2:B:175:PHE:CZ	2:B:179:VAL:HG21	2.56	0.41
2:B:227:GLU:HB2	2:B:352:ASN:OD1	2.21	0.41
2:B:238:VAL:HG13	2:B:356:VAL:HB	2.03	0.41
2:B:265:SER:OG	2:B:267:LEU:HD12	2.21	0.41
4:D:286:TRP:CD2	5:E:59:MET:HG3	2.55	0.41
1:A:344:ILE:HG21	1:A:448:ILE:HD12	2.03	0.41
3:C:206:SER:OG	16:C:706:UQ6:H3M1	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:92:ARG:HD2	4:D:250:ASP:OD2	2.20	0.41
4:D:289:LYS:HB2	8:H:37:LEU:HD13	2.03	0.41
11:K:36:TYR:OH	11:K:89:GLN:NE2	2.54	0.41
16:C:706:UQ6:H101	16:C:706:UQ6:H121	1.50	0.40
3:C:237:MET:HG2	12:D:714:3PH:H292	2.04	0.40
16:C:706:UQ6:H201	16:C:706:UQ6:H222	1.67	0.40
4:D:126:ARG:O	4:D:130:GLU:HG3	2.21	0.40
4:D:174:PRO:HG3	14:D:703:HEC:HMD3	2.04	0.40
18:D:715:PC1:O14	18:D:715:PC1:H121	2.21	0.40
2:B:137:CYS:SG	2:B:139:VAL:HG22	2.61	0.40
4:D:208:LEU:HA	4:D:209:PRO:HD3	1.93	0.40
2:B:37:GLY:HA3	2:B:179:VAL:HG11	2.04	0.40
4:D:280:LEU:HD12	4:D:280:LEU:HA	1.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	429/431 (100%)	391 (91%)	33 (8%)	5 (1%)	13	24
2	B	350/352 (99%)	304 (87%)	39 (11%)	7 (2%)	7	12
3	C	383/385 (100%)	368 (96%)	14 (4%)	1 (0%)	41	61
4	D	244/246 (99%)	233 (96%)	11 (4%)	0	100	100
5	E	183/185 (99%)	168 (92%)	12 (7%)	3 (2%)	9	17
6	F	72/74 (97%)	69 (96%)	3 (4%)	0	100	100
7	G	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
8	H	91/93 (98%)	78 (86%)	9 (10%)	4 (4%)	2	3
9	I	53/55 (96%)	49 (92%)	2 (4%)	2 (4%)	3	4
10	J	125/127 (98%)	114 (91%)	8 (6%)	3 (2%)	6	9

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	105/107 (98%)	88 (84%)	11 (10%)	6 (6%)	1	1
All	All	2158/2180 (99%)	1983 (92%)	144 (7%)	31 (1%)	11	20

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	152	ARG
2	B	335	PRO
3	C	223	SER
8	H	93	ASN
11	K	80	PRO
2	B	22	ARG
2	B	153	LYS
5	E	46	ASN
1	A	44	PRO
1	A	227	ASN
2	B	57	GLN
5	E	103	LEU
8	H	37	LEU
9	I	12	LYS
9	I	13	ARG
10	J	65	LYS
11	K	31	ASN
11	K	51	THR
1	A	228	LEU
5	E	102	PRO
8	H	38	GLN
11	K	78	LEU
2	B	333	SER
1	A	230	LEU
10	J	32	GLY
10	J	90	ASP
11	K	16	GLY
1	A	35	GLY
8	H	40	ILE
2	B	210	PRO
11	K	68	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	370/370 (100%)	343 (93%)	27 (7%)	14	27
2	B	301/301 (100%)	277 (92%)	24 (8%)	12	23
3	C	338/338 (100%)	316 (94%)	22 (6%)	17	33
4	D	204/204 (100%)	196 (96%)	8 (4%)	32	57
5	E	151/151 (100%)	148 (98%)	3 (2%)	55	79
6	F	67/67 (100%)	63 (94%)	4 (6%)	19	37
7	G	109/109 (100%)	105 (96%)	4 (4%)	34	60
8	H	77/77 (100%)	77 (100%)	0	100	100
9	I	45/45 (100%)	42 (93%)	3 (7%)	16	31
10	J	112/112 (100%)	104 (93%)	8 (7%)	14	28
11	K	93/93 (100%)	85 (91%)	8 (9%)	10	20
All	All	1867/1867 (100%)	1756 (94%)	111 (6%)	19	37

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	66	ASN
1	A	109	LEU
1	A	115	LYS
1	A	120	LEU
1	A	126	GLN
1	A	150	ASP
1	A	153	ASP
1	A	164	LEU
1	A	172	THR
1	A	173	PRO
1	A	179	ARG
1	A	183	GLU
1	A	227	ASN
1	A	239	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	241	LYS
1	A	252	ARG
1	A	261	ILE
1	A	289	ASN
1	A	306	ILE
1	A	330	PHE
1	A	336	ASN
1	A	343	LEU
1	A	361	THR
1	A	370	LEU
1	A	390	LEU
1	A	443	LEU
2	B	17	LEU
2	B	30	THR
2	B	31	LEU
2	B	40	ARG
2	B	43	THR
2	B	53	ARG
2	B	54	PHE
2	B	62	ARG
2	B	107	ASP
2	B	128	ARG
2	B	144	ASP
2	B	146	LEU
2	B	169	LEU
2	B	193	VAL
2	B	215	LEU
2	B	267	LEU
2	B	312	LYS
2	B	330	GLU
2	B	337	GLU
2	B	338	LEU
2	B	345	ASP
2	B	347	LYS
2	B	360	SER
2	B	362	LEU
3	C	5	LYS
3	C	35	LEU
3	C	38	LEU
3	C	79	ARG
3	C	81	LEU
3	C	89	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	99	LYS
3	C	101	LEU
3	C	182	LEU
3	C	184	TYR
3	C	185	LEU
3	C	218	ARG
3	C	223	SER
3	C	238	LEU
3	C	269	ILE
3	C	292	VAL
3	C	312	VAL
3	C	321	LEU
3	C	336	LEU
3	C	350	LEU
3	C	377	LEU
3	C	382	ARG
4	D	69	LEU
4	D	109	ARG
4	D	113	ARG
4	D	244	THR
4	D	251	VAL
4	D	256	ASN
4	D	280	LEU
4	D	283	LEU
5	E	91	MET
5	E	107	VAL
5	E	211	LYS
6	F	77	GLN
6	F	94	LEU
6	F	117	LEU
6	F	130	LEU
7	G	16	LEU
7	G	30	ASN
7	G	86	HIS
7	G	127	LYS
9	I	14	ASN
9	I	18	VAL
9	I	48	LEU
10	J	39	ARG
10	J	51	TYR
10	J	54	ASN
10	J	61	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	J	66	ASP
10	J	68	LEU
10	J	79	PHE
10	J	89	GLU
11	K	18	ARG
11	K	33	LEU
11	K	38	GLN
11	K	81	GLU
11	K	82	ASP
11	K	92	ILE
11	K	93	LYS
11	K	107	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	HIS
1	A	61	ASN
1	A	63	ASN
1	A	66	ASN
1	A	67	ASN
1	A	102	GLN
1	A	121	ASN
1	A	156	HIS
1	A	171	ASN
1	A	199	ASN
1	A	200	HIS
1	A	227	ASN
1	A	274	ASN
1	A	283	GLN
1	A	289	ASN
1	A	298	GLN
1	A	314	ASN
1	A	317	HIS
1	A	336	ASN
1	A	350	GLN
1	A	385	ASN
1	A	388	ASN
1	A	429	GLN
1	A	438	GLN
2	B	49	HIS
2	B	52	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	55	ASN
2	B	191	ASN
2	B	246	ASN
2	B	252	GLN
2	B	258	ASN
3	C	14	ASN
3	C	22	GLN
3	C	43	GLN
3	C	173	ASN
3	C	202	HIS
3	C	208	ASN
3	C	253	HIS
3	C	332	ASN
4	D	78	HIS
4	D	79	ASN
4	D	127	ASN
4	D	256	ASN
4	D	303	ASN
5	E	38	ASN
5	E	97	ASN
5	E	106	ASN
5	E	184	HIS
6	F	77	GLN
7	G	30	ASN
7	G	31	GLN
7	G	53	ASN
7	G	57	GLN
7	G	79	HIS
9	I	14	ASN
9	I	29	GLN
10	J	54	ASN
10	J	59	ASN
10	J	61	ASN
10	J	77	ASN
10	J	78	GLN
10	J	114	GLN
11	K	31	ASN
11	K	34	ASN
11	K	89	GLN
11	K	91	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

13 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	3PH	D	714	-	37,37,47	1.04	1 (2%)	41,42,52	1.58	9 (21%)
14	HEC	C	702	3	26,50,50	1.51	3 (11%)	18,82,82	1.71	6 (33%)
12	3PH	A	713	-	39,39,47	1.14	4 (10%)	43,44,52	1.60	5 (11%)
19	CDL	D	731	-	75,75,99	1.63	13 (17%)	81,87,111	1.47	12 (14%)
14	HEC	C	701	3	26,50,50	1.65	5 (19%)	18,82,82	1.61	4 (22%)
15	DBT	C	705	-	15,20,20	1.30	2 (13%)	16,27,27	1.29	2 (12%)
17	3PE	C	710	-	46,46,50	1.15	6 (13%)	49,51,55	1.27	3 (6%)
16	UQ6	C	706	-	43,43,43	3.20	18 (41%)	51,55,55	2.19	14 (27%)
14	HEC	D	703	4	26,50,50	1.67	2 (7%)	18,82,82	1.06	1 (5%)
13	UMQ	A	721	-	35,35,35	1.04	2 (5%)	46,46,46	1.73	8 (17%)
17	3PE	C	711	-	39,39,50	0.83	1 (2%)	42,44,55	1.03	2 (4%)
18	PC1	D	715	-	37,37,53	2.03	9 (24%)	43,45,61	1.52	7 (16%)
20	FES	E	704	5	0,4,4	0.00	-	-	-	-

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	3PH	D	714	-	-	8/39/39/49	-
14	HEC	C	702	3	-	0/6/54/54	-
12	3PH	A	713	-	-	19/41/41/49	-
19	CDL	D	731	-	-	40/86/86/110	-
14	HEC	C	701	3	-	0/6/54/54	-
15	DBT	C	705	-	-	2/7/27/27	0/2/2/2
17	3PE	C	710	-	-	20/50/50/54	-
16	UQ6	C	706	-	-	18/39/39/39	0/1/1/1
14	HEC	D	703	4	-	0/6/54/54	-
13	UMQ	A	721	-	-	6/20/60/60	0/2/2/2
17	3PE	C	711	-	-	15/43/43/54	-
18	PC1	D	715	-	-	19/41/41/57	-
20	FES	E	704	5	-	-	0/1/1/1

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	C	706	UQ6	C7-C6	10.82	1.63	1.51
16	C	706	UQ6	C5-C6	7.70	1.51	1.40
16	C	706	UQ6	C5-C4	7.30	1.51	1.39
18	D	715	PC1	O21-C21	7.24	1.54	1.34
18	D	715	PC1	O31-C31	6.21	1.51	1.33
14	D	703	HEC	C3B-C2B	-5.46	1.35	1.40
19	D	731	CDL	OA8-CA6	-5.10	1.33	1.45
14	D	703	HEC	C3C-C2C	-5.05	1.35	1.40
16	C	706	UQ6	O2-C2	-4.95	1.25	1.37
16	C	706	UQ6	C2-C3	4.87	1.47	1.39
14	C	701	HEC	C3C-C2C	-4.80	1.35	1.40
16	C	706	UQ6	O3-C3	4.78	1.47	1.38
14	C	702	HEC	C3C-C2C	-4.66	1.35	1.40
16	C	706	UQ6	C2-C1	4.10	1.48	1.40
16	C	706	UQ6	O5-C5	-4.07	1.27	1.37
14	C	702	HEC	C3B-C2B	-4.02	1.36	1.40
19	D	731	CDL	OA6-CA4	-4.02	1.36	1.46
13	A	721	UMQ	C3-C2	-3.99	1.42	1.52
14	C	701	HEC	C3B-C2B	-3.86	1.36	1.40
17	C	710	3PE	O21-C21	3.66	1.44	1.34
19	D	731	CDL	OA5-CA3	-3.65	1.30	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	C	706	UQ6	C33-C34	3.60	1.42	1.32
19	D	731	CDL	OB2-CB2	-3.46	1.31	1.44
12	D	714	3PH	O31-C3	-3.37	1.37	1.45
12	A	713	3PH	C1-C2	3.24	1.60	1.50
16	C	706	UQ6	C31-C29	3.09	1.57	1.51
16	C	706	UQ6	C28-C29	3.02	1.40	1.33
19	D	731	CDL	CB2-C1	3.02	1.61	1.51
19	D	731	CDL	CA3-CA4	-3.01	1.41	1.50
19	D	731	CDL	OA6-CA5	2.97	1.42	1.34
19	D	731	CDL	OA9-CA7	-2.93	1.13	1.22
15	C	705	DBT	C4A-C4	-2.90	1.46	1.50
18	D	715	PC1	P-O14	2.90	1.61	1.50
16	C	706	UQ6	C8-C9	2.90	1.39	1.33
16	C	706	UQ6	C23-C24	2.70	1.39	1.33
16	C	706	UQ6	C17-C18	-2.68	1.41	1.50
16	C	706	UQ6	C13-C14	2.66	1.39	1.33
14	C	701	HEC	CMC-C2C	2.64	1.57	1.51
18	D	715	PC1	O22-C21	2.62	1.30	1.22
15	C	705	DBT	C7A-C7	-2.56	1.43	1.50
19	D	731	CDL	O1-C1	2.47	1.50	1.43
17	C	710	3PE	O11-C1	-2.47	1.35	1.44
12	A	713	3PH	C3-C2	2.47	1.58	1.50
12	A	713	3PH	C32-C31	2.46	1.57	1.50
18	D	715	PC1	C32-C31	2.44	1.57	1.50
16	C	706	UQ6	C25-C24	2.38	1.56	1.50
17	C	710	3PE	P-O14	2.37	1.59	1.50
14	C	702	HEC	CBC-CAC	-2.37	1.40	1.49
16	C	706	UQ6	C15-C14	2.36	1.56	1.50
17	C	710	3PE	O31-C31	2.33	1.40	1.33
17	C	710	3PE	O32-C31	-2.33	1.15	1.22
19	D	731	CDL	CA2-C1	2.30	1.59	1.51
19	D	731	CDL	OB5-CB3	-2.26	1.36	1.44
18	D	715	PC1	C3-C2	2.25	1.57	1.50
18	D	715	PC1	O32-C31	2.25	1.29	1.22
19	D	731	CDL	OB8-CB7	2.20	1.39	1.33
16	C	706	UQ6	C11-C9	2.18	1.55	1.51
17	C	711	3PE	O21-C2	-2.15	1.41	1.46
14	C	701	HEC	CBC-CAC	-2.14	1.41	1.49
18	D	715	PC1	C1-C2	-2.08	1.44	1.50
12	A	713	3PH	P-O12	2.05	1.57	1.50
18	D	715	PC1	P-O13	2.04	1.67	1.59
13	A	721	UMQ	O5'-C5'	-2.01	1.39	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	C	701	HEC	CBB-CAB	-2.01	1.42	1.49
17	C	710	3PE	C1-C2	2.00	1.56	1.50
19	D	731	CDL	CB3-CB4	2.00	1.56	1.50

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	721	UMQ	CA-O1'-C1'	-8.02	100.54	113.84
16	C	706	UQ6	C3M-O3-C3	7.71	135.91	114.78
19	D	731	CDL	CB4-OB6-CB5	-6.23	102.45	117.79
16	C	706	UQ6	C17-C18-C19	5.37	140.59	127.66
12	A	713	3PH	P-O11-C1	5.34	133.00	118.30
16	C	706	UQ6	C4M-O4-C4	4.57	127.30	114.78
18	D	715	PC1	C3-C2-C1	-4.49	101.17	111.79
12	D	714	3PH	P-O11-C1	4.41	130.43	118.30
16	C	706	UQ6	C21-C19-C18	3.98	129.18	121.12
14	C	701	HEC	CMB-C2B-C3B	3.92	130.43	125.82
19	D	731	CDL	CA6-CA4-CA3	-3.91	102.55	111.79
17	C	710	3PE	C2-O21-C21	-3.89	108.21	117.79
18	D	715	PC1	C2-O21-C21	-3.78	108.48	117.79
12	A	713	3PH	O11-P-O12	3.66	116.75	106.47
16	C	706	UQ6	C1M-C1-C2	-3.66	114.30	120.50
19	D	731	CDL	CA4-OA6-CA5	-3.64	108.83	117.79
12	A	713	3PH	O13-P-O11	3.63	116.41	106.73
14	C	701	HEC	CMB-C2B-C1B	-3.58	122.95	128.46
12	D	714	3PH	O13-P-O11	3.57	116.24	106.73
14	C	702	HEC	CMC-C2C-C1C	-3.40	123.24	128.46
14	C	702	HEC	CMC-C2C-C3C	3.38	129.79	125.82
19	D	731	CDL	PA1-OA2-CA2	3.34	141.27	121.68
12	A	713	3PH	C3-C2-C1	-3.32	103.94	111.79
17	C	710	3PE	C3-C2-C1	3.31	119.61	111.79
12	D	714	3PH	C38-C37-C36	-3.30	97.66	114.42
19	D	731	CDL	PA1-OA5-CA3	-3.24	102.68	121.68
17	C	711	3PE	C2-O21-C21	-3.18	109.97	117.79
12	D	714	3PH	C3-C2-C1	-3.17	104.29	111.79
13	A	721	UMQ	O1'-CA-CB	3.13	120.54	109.56
16	C	706	UQ6	C6-C7-C8	3.06	117.01	112.17
12	A	713	3PH	O14-P-O11	-3.04	98.64	106.73
16	C	706	UQ6	C11-C12-C13	2.99	121.69	111.88
15	C	705	DBT	O7-C7-C7A	2.90	126.37	121.37
14	C	702	HEC	CMB-C2B-C1B	-2.85	124.08	128.46
18	D	715	PC1	C11-C12-N	2.80	125.13	115.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	714	3PH	O11-P-O12	2.78	114.28	106.47
16	C	706	UQ6	C2-C1-C6	2.76	121.74	118.75
19	D	731	CDL	CB6-CB4-CB3	-2.72	105.35	111.79
19	D	731	CDL	OB4-PB2-OB2	2.70	120.30	107.75
13	A	721	UMQ	C3'-C4'-C5'	-2.69	104.75	110.93
14	C	702	HEC	CMB-C2B-C3B	2.68	128.97	125.82
18	D	715	PC1	O21-C2-C1	2.65	118.01	108.40
15	C	705	DBT	C4-C4A-N3	2.65	124.17	119.94
14	D	703	HEC	CMD-C2D-C1D	-2.57	124.51	128.46
14	C	702	HEC	CBD-CAD-C3D	-2.54	107.81	112.49
14	C	701	HEC	CMD-C2D-C1D	-2.54	124.56	128.46
12	D	714	3PH	O14-P-O11	-2.51	100.06	106.73
13	A	721	UMQ	CD-CC-CB	-2.46	101.92	114.42
16	C	706	UQ6	C1M-C1-C6	2.44	123.96	120.42
13	A	721	UMQ	O1-C1-O5	-2.43	103.89	110.67
16	C	706	UQ6	C15-C14-C16	-2.42	111.21	115.27
19	D	731	CDL	PB2-OB2-CB2	2.41	135.79	121.68
17	C	710	3PE	C3E-C3D-C3C	-2.40	102.24	114.42
16	C	706	UQ6	C20-C19-C18	-2.38	117.57	123.68
18	D	715	PC1	C37-C36-C35	-2.36	102.46	114.42
18	D	715	PC1	C3-O31-C31	-2.32	108.54	117.12
16	C	706	UQ6	C36-C34-C35	-2.31	109.49	114.60
13	A	721	UMQ	O3'-C3'-C2'	-2.31	105.00	110.35
12	D	714	3PH	O31-C31-C32	-2.29	104.73	111.91
19	D	731	CDL	CB2-C1-CA2	-2.24	106.19	112.79
12	D	714	3PH	O31-C31-O32	2.22	129.19	123.59
14	C	702	HEC	CMA-C3A-C2A	2.19	129.06	124.94
12	D	714	3PH	O31-C3-C2	-2.18	102.08	108.43
14	C	701	HEC	CMC-C2C-C3C	-2.15	123.29	125.82
16	C	706	UQ6	C16-C14-C13	2.14	125.44	121.12
19	D	731	CDL	OA4-PA1-OA2	2.11	117.57	107.75
17	C	711	3PE	C29-C28-C27	-2.11	103.69	114.42
16	C	706	UQ6	C11-C9-C8	2.10	125.37	121.12
19	D	731	CDL	OA4-PA1-OA3	-2.09	101.91	112.24
19	D	731	CDL	OB4-PB2-OB3	-2.08	101.95	112.24
13	A	721	UMQ	C6'-C5'-C4'	-2.07	107.31	113.33
18	D	715	PC1	C23-C22-C21	2.06	121.10	113.62
13	A	721	UMQ	C1-O5-C5	-2.02	109.72	113.69

There are no chirality outliers.

All (147) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	C	706	UQ6	C18-C19-C21-C22
16	C	706	UQ6	C20-C19-C21-C22
16	C	706	UQ6	C19-C21-C22-C23
17	C	710	3PE	O13-C11-C12-N
17	C	711	3PE	C1-O11-P-O12
17	C	711	3PE	C1-O11-P-O13
17	C	711	3PE	C1-O11-P-O14
18	D	715	PC1	C1-O11-P-O12
18	D	715	PC1	C1-O11-P-O14
18	D	715	PC1	C12-C11-O13-P
18	D	715	PC1	C22-C21-O21-C2
19	D	731	CDL	CA2-OA2-PA1-OA4
19	D	731	CDL	CA2-OA2-PA1-OA5
19	D	731	CDL	OA5-CA3-CA4-OA6
19	D	731	CDL	OA7-CA5-OA6-CA4
19	D	731	CDL	C11-CA5-OA6-CA4
19	D	731	CDL	OB5-CB3-CB4-OB6
19	D	731	CDL	C51-CB5-OB6-CB4
19	D	731	CDL	OA9-CA7-OA8-CA6
19	D	731	CDL	C31-CA7-OA8-CA6
18	D	715	PC1	O22-C21-O21-C2
19	D	731	CDL	OB7-CB5-OB6-CB4
17	C	711	3PE	C25-C26-C27-C28
12	D	714	3PH	C22-C21-O21-C2
13	A	721	UMQ	O1'-CA-CB-CC
17	C	710	3PE	C37-C38-C39-C3A
12	D	714	3PH	O22-C21-O21-C2
16	C	706	UQ6	C4-C3-O3-C3M
16	C	706	UQ6	C12-C11-C9-C10
16	C	706	UQ6	C15-C14-C16-C17
16	C	706	UQ6	C30-C29-C31-C32
16	C	706	UQ6	C12-C11-C9-C8
16	C	706	UQ6	C13-C14-C16-C17
16	C	706	UQ6	C28-C29-C31-C32
16	C	706	UQ6	C24-C26-C27-C28
16	C	706	UQ6	C5-C4-O4-C4M
12	D	714	3PH	C31-C32-C33-C34
17	C	711	3PE	C21-C22-C23-C24
17	C	710	3PE	C31-C32-C33-C34
17	C	711	3PE	C31-C32-C33-C34
19	D	731	CDL	O1-C1-CB2-OB2
18	D	715	PC1	C1-O11-P-O13
19	D	731	CDL	CB2-OB2-PB2-OB5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	D	715	PC1	C31-C32-C33-C34
19	D	731	CDL	CA2-C1-CB2-OB2
12	A	713	3PH	O22-C21-O21-C2
12	A	713	3PH	C22-C21-O21-C2
12	A	713	3PH	C25-C26-C27-C28
17	C	711	3PE	C32-C33-C34-C35
19	D	731	CDL	C80-C81-C82-C83
18	D	715	PC1	C36-C37-C38-C39
12	A	713	3PH	C35-C36-C37-C38
15	C	705	DBT	C11-C10-C9-C8
17	C	711	3PE	C23-C24-C25-C26
17	C	710	3PE	C21-C22-C23-C24
19	D	731	CDL	C81-C82-C83-C84
13	A	721	UMQ	CF-CG-CH-CI
19	D	731	CDL	C35-C36-C37-C38
17	C	710	3PE	C33-C34-C35-C36
12	A	713	3PH	C34-C35-C36-C37
12	A	713	3PH	C37-C38-C39-C3A
17	C	711	3PE	C27-C28-C29-C2A
19	D	731	CDL	C71-C72-C73-C74
19	D	731	CDL	C74-C75-C76-C77
19	D	731	CDL	C78-C79-C80-C81
17	C	711	3PE	O13-C11-C12-N
18	D	715	PC1	C21-C22-C23-C24
16	C	706	UQ6	C2-C3-O3-C3M
19	D	731	CDL	C77-C78-C79-C80
17	C	710	3PE	C3B-C3C-C3D-C3E
17	C	710	3PE	C39-C3A-C3B-C3C
17	C	710	3PE	C3C-C3D-C3E-C3F
12	A	713	3PH	C29-C2A-C2B-C2C
17	C	710	3PE	C36-C37-C38-C39
12	A	713	3PH	C32-C33-C34-C35
19	D	731	CDL	C51-C52-C53-C54
12	D	714	3PH	C27-C28-C29-C2A
17	C	710	3PE	C2A-C2B-C2C-C2D
19	D	731	CDL	C12-C13-C14-C15
12	A	713	3PH	C27-C28-C29-C2A
19	D	731	CDL	C54-C55-C56-C57
16	C	706	UQ6	C3-C4-O4-C4M
15	C	705	DBT	C10-C11-C12-C13
17	C	710	3PE	O11-C1-C2-C3
17	C	711	3PE	O11-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	D	731	CDL	OA5-CA3-CA4-CA6
19	D	731	CDL	OB5-CB3-CB4-CB6
17	C	710	3PE	C3D-C3E-C3F-C3G
12	D	714	3PH	C25-C26-C27-C28
19	D	731	CDL	CA7-C31-C32-C33
19	D	731	CDL	C55-C56-C57-C58
12	D	714	3PH	C26-C27-C28-C29
12	A	713	3PH	C36-C37-C38-C39
12	A	713	3PH	C3A-C3B-C3C-C3D
12	D	714	3PH	C34-C35-C36-C37
18	D	715	PC1	C38-C39-C3A-C3B
12	A	713	3PH	C2C-C2D-C2E-C2F
17	C	711	3PE	C28-C29-C2A-C2B
19	D	731	CDL	C31-C32-C33-C34
18	D	715	PC1	O11-C1-C2-C3
12	A	713	3PH	C38-C39-C3A-C3B
12	D	714	3PH	C37-C38-C39-C3A
18	D	715	PC1	C33-C34-C35-C36
19	D	731	CDL	C14-C15-C16-C17
18	D	715	PC1	C24-C25-C26-C27
12	A	713	3PH	C24-C25-C26-C27
17	C	710	3PE	O11-C1-C2-O21
17	C	711	3PE	O11-C1-C2-O21
17	C	711	3PE	C33-C34-C35-C36
19	D	731	CDL	C83-C84-C85-C86
17	C	710	3PE	C3A-C3B-C3C-C3D
13	A	721	UMQ	CG-CH-CI-CJ
19	D	731	CDL	CB7-C71-C72-C73
19	D	731	CDL	CA2-OA2-PA1-OA3
19	D	731	CDL	CB2-OB2-PB2-OB3
12	A	713	3PH	O11-C1-C2-C3
16	C	706	UQ6	C9-C11-C12-C13
18	D	715	PC1	C25-C26-C27-C28
17	C	710	3PE	C12-C11-O13-P
18	D	715	PC1	O11-C1-C2-O21
18	D	715	PC1	O13-C11-C12-N
17	C	710	3PE	C27-C28-C29-C2A
17	C	710	3PE	C29-C2A-C2B-C2C
18	D	715	PC1	C35-C36-C37-C38
17	C	710	3PE	O31-C31-C32-C33
17	C	711	3PE	C2B-C2C-C2D-C2E
16	C	706	UQ6	C25-C24-C26-C27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	C	710	3PE	C11-O13-P-O11
18	D	715	PC1	C11-O13-P-O11
19	D	731	CDL	CB3-OB5-PB2-OB2
13	A	721	UMQ	CI-CJ-CK-CL
13	A	721	UMQ	C2'-C1'-O1'-CA
13	A	721	UMQ	O5'-C1'-O1'-CA
12	A	713	3PH	C2B-C2C-C2D-C2E
18	D	715	PC1	C26-C27-C28-C29
12	A	713	3PH	C28-C29-C2A-C2B
16	C	706	UQ6	C23-C24-C26-C27
19	D	731	CDL	OB9-CB7-OB8-CB6
12	A	713	3PH	O31-C31-C32-C33
19	D	731	CDL	C82-C83-C84-C85
19	D	731	CDL	C71-CB7-OB8-CB6
19	D	731	CDL	C12-C11-CA5-OA6
12	A	713	3PH	O32-C31-C32-C33
16	C	706	UQ6	C11-C12-C13-C14
17	C	710	3PE	C1-O11-P-O14
19	D	731	CDL	CA3-OA5-PA1-OA4
19	D	731	CDL	C12-C11-CA5-OA7

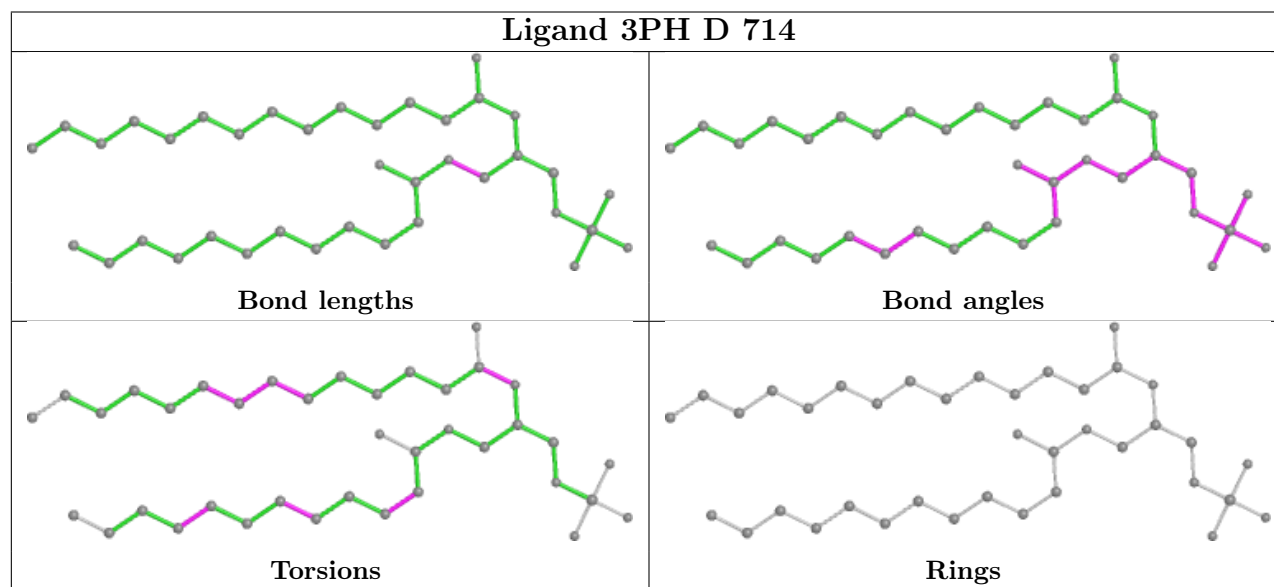
There are no ring outliers.

12 monomers are involved in 33 short contacts:

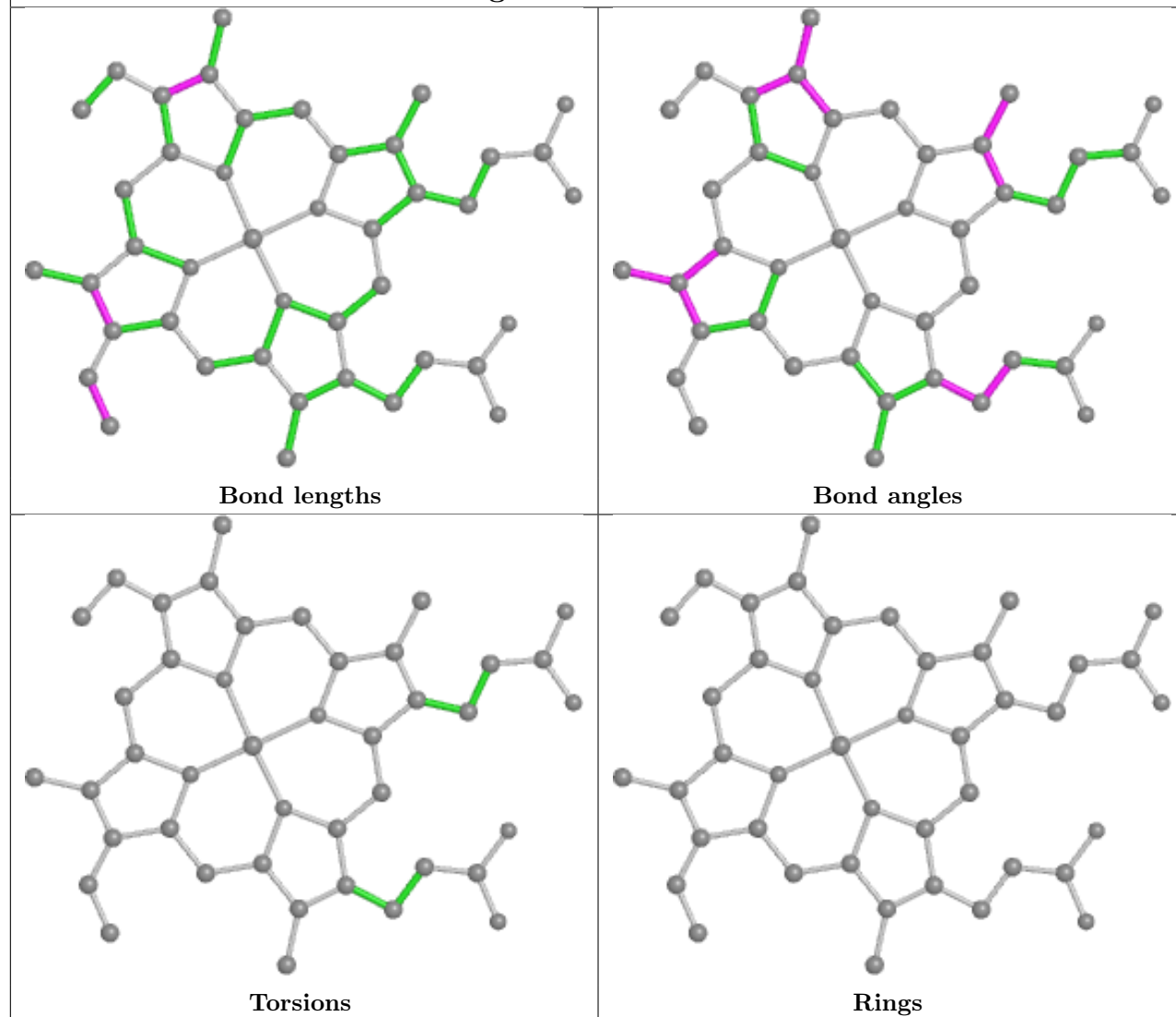
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	D	714	3PH	3	0
14	C	702	HEC	1	0
12	A	713	3PH	4	0
19	D	731	CDL	5	0
14	C	701	HEC	2	0
15	C	705	DBT	1	0
17	C	710	3PE	3	0
16	C	706	UQ6	8	0
14	D	703	HEC	1	0
13	A	721	UMQ	2	0
18	D	715	PC1	3	0
20	E	704	FES	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

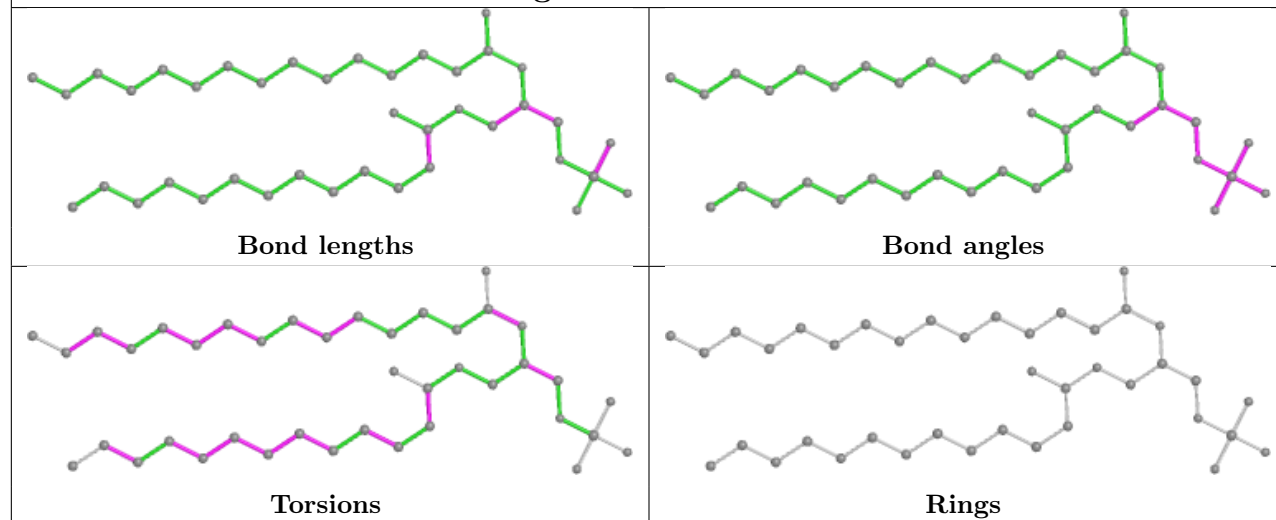
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

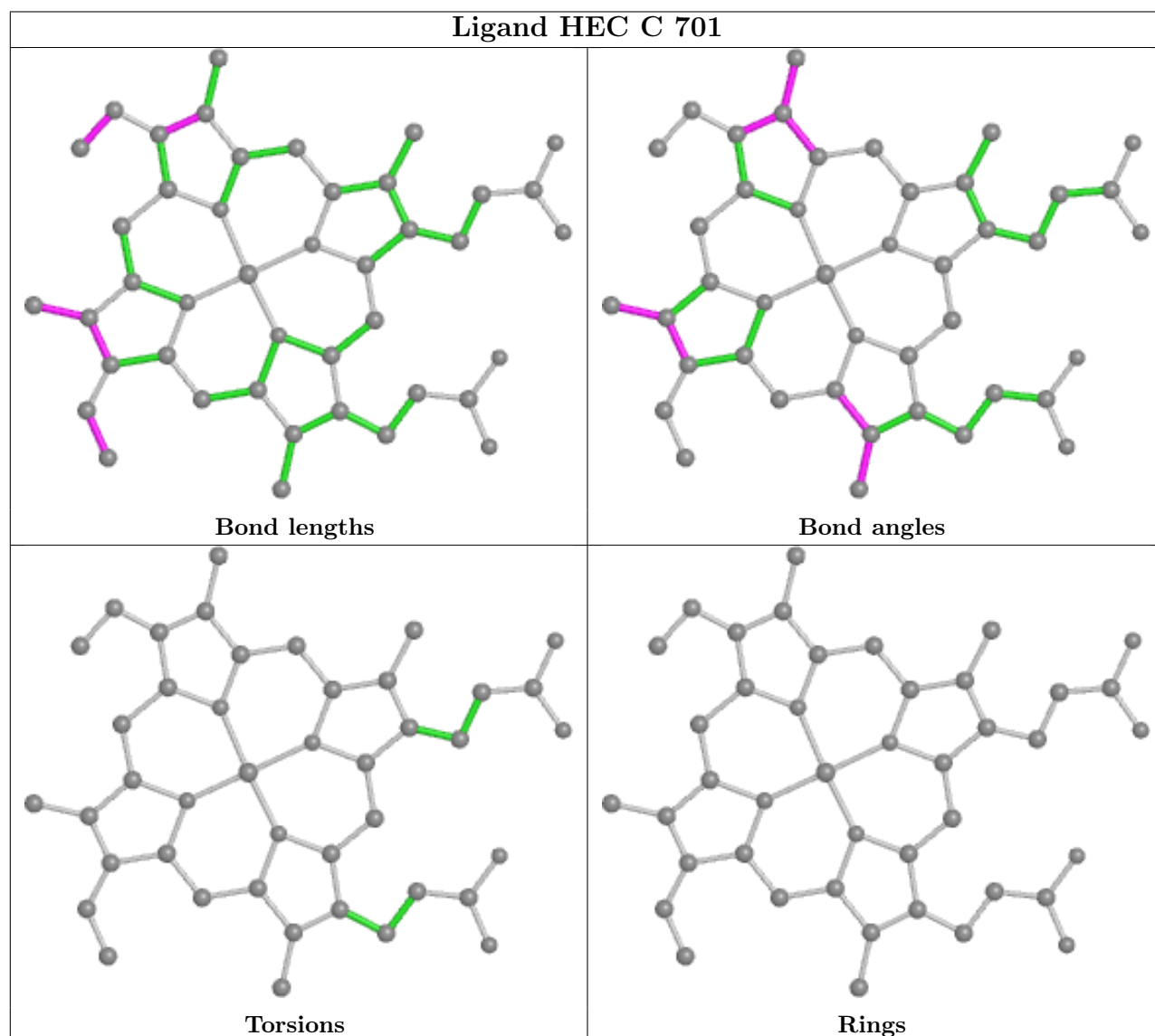
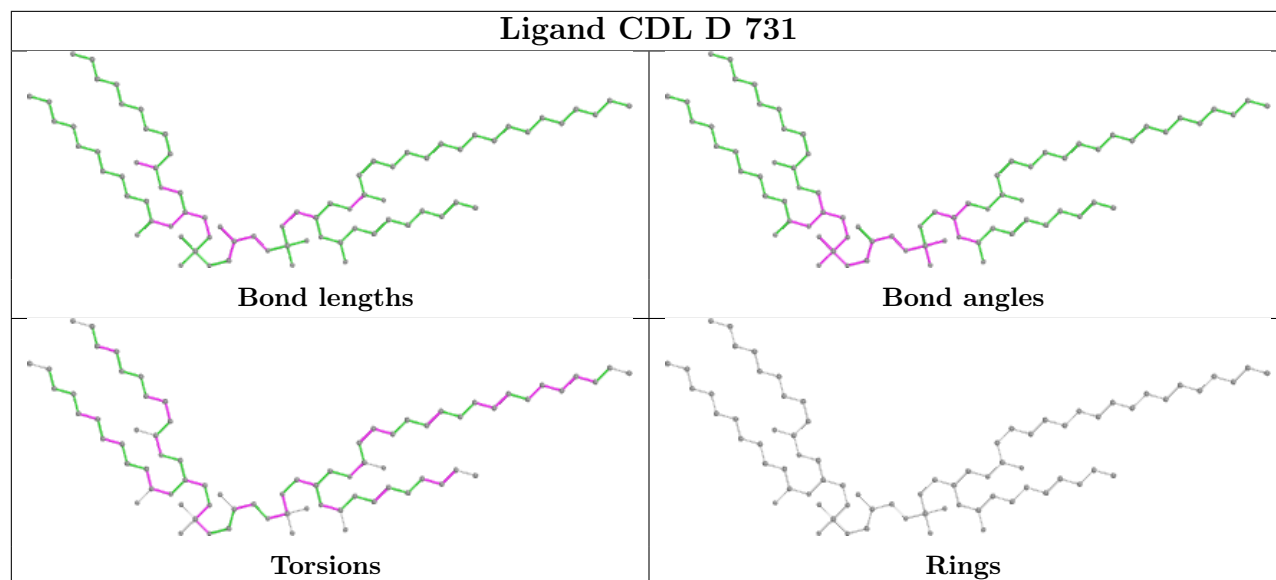


Ligand HEC C 702

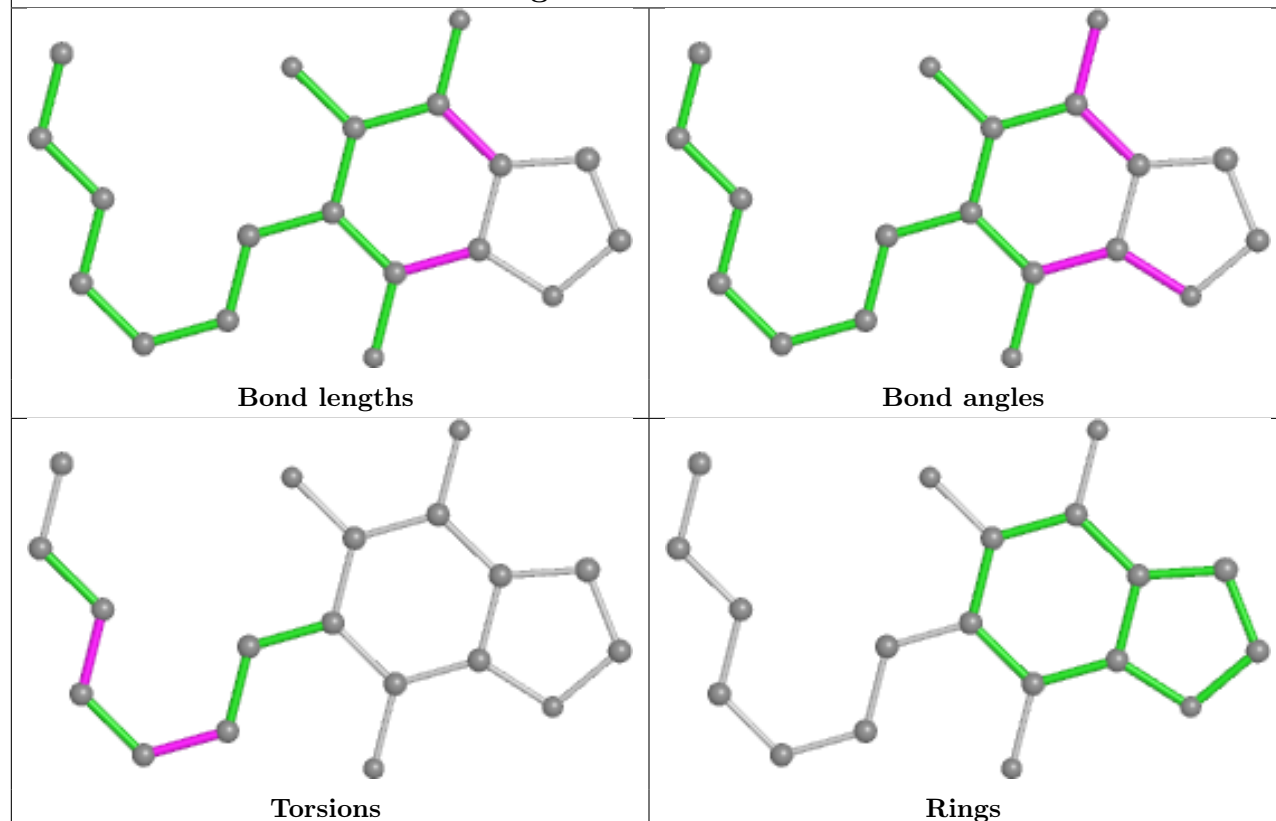


Ligand 3PH A 713

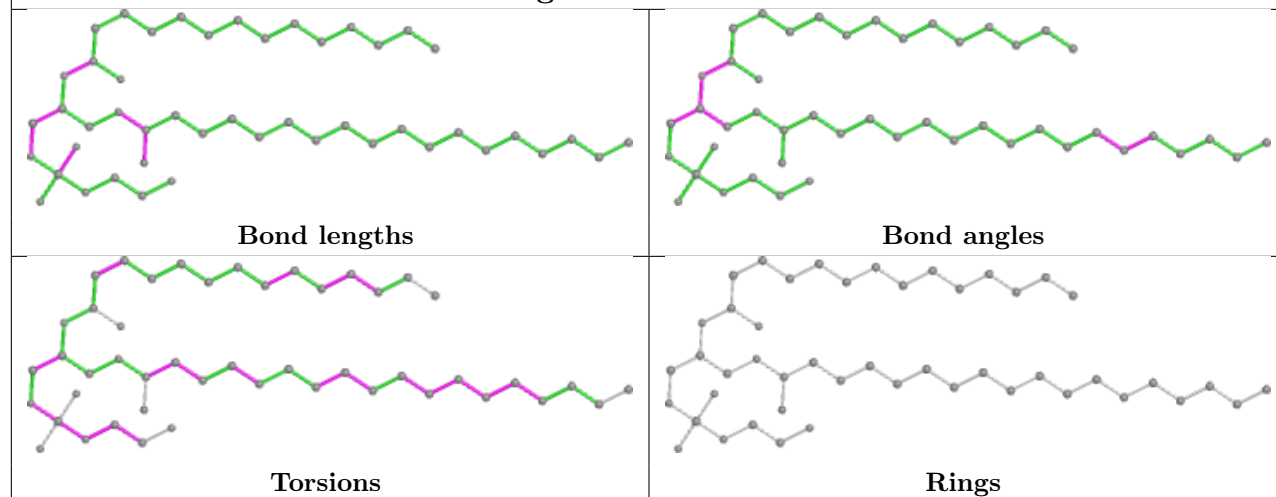




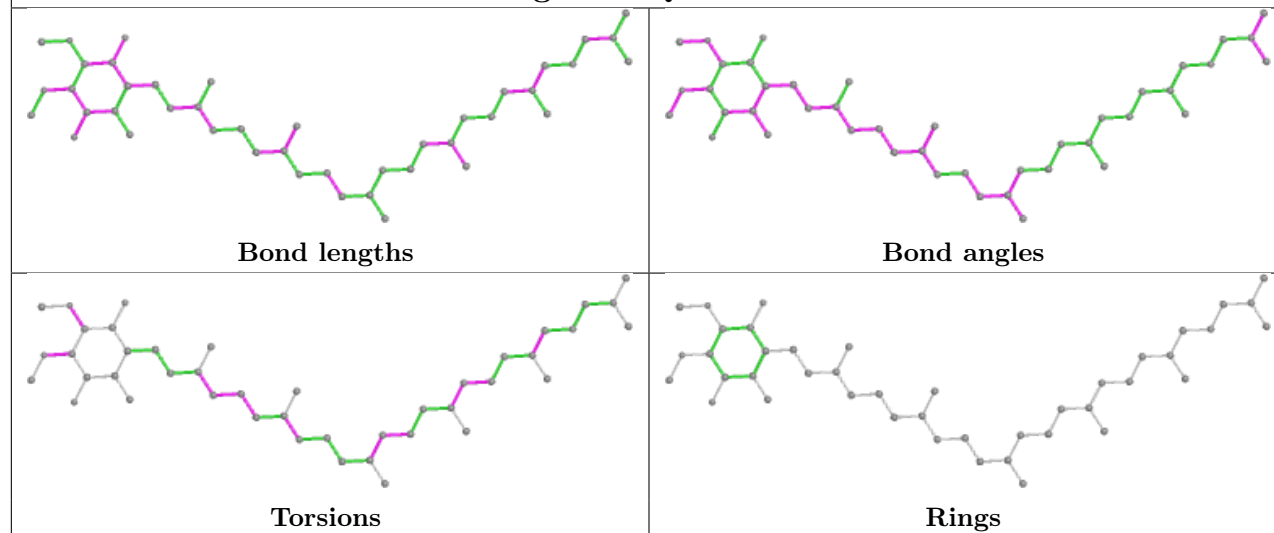
Ligand DBT C 705



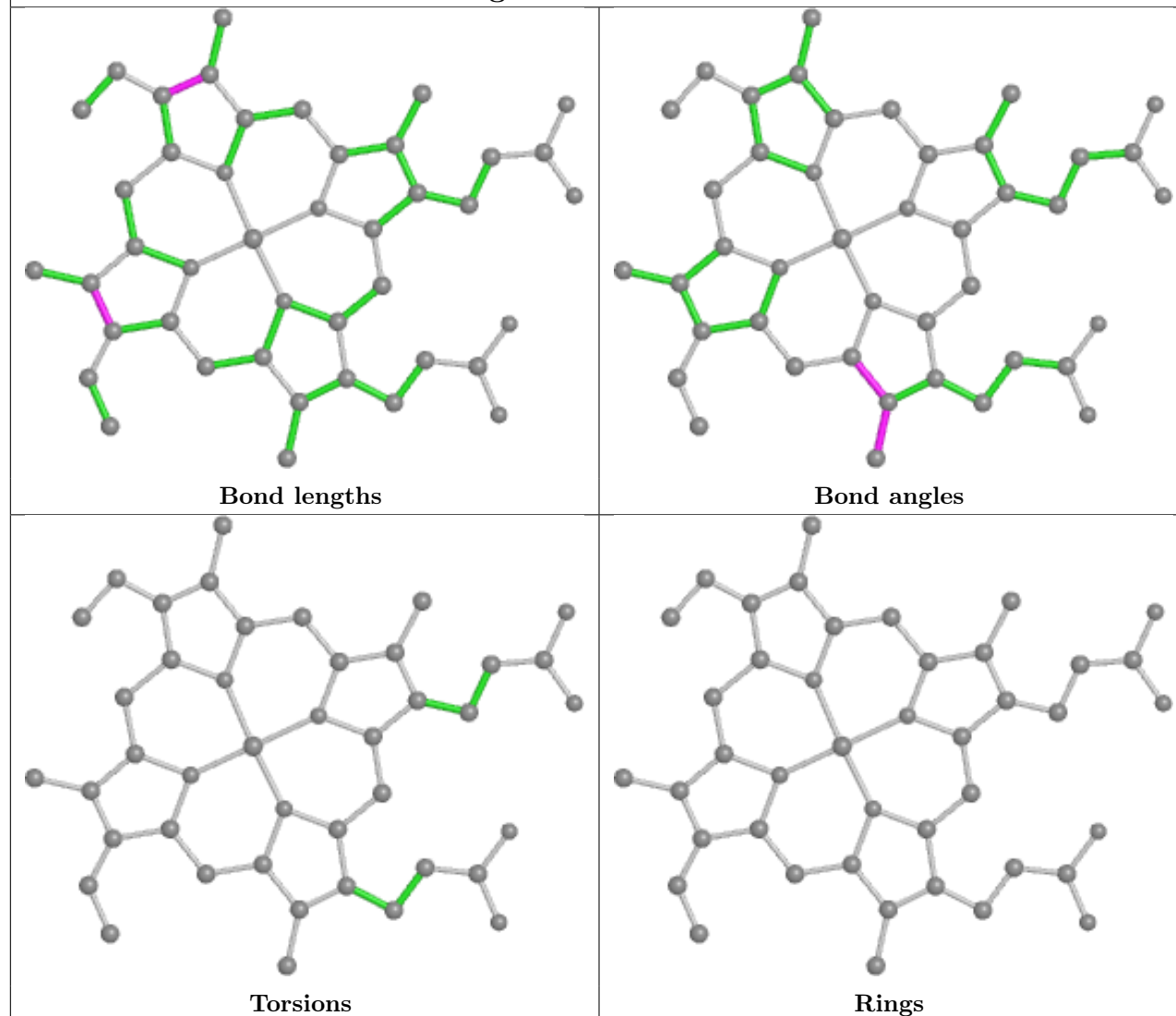
Ligand 3PE C 710

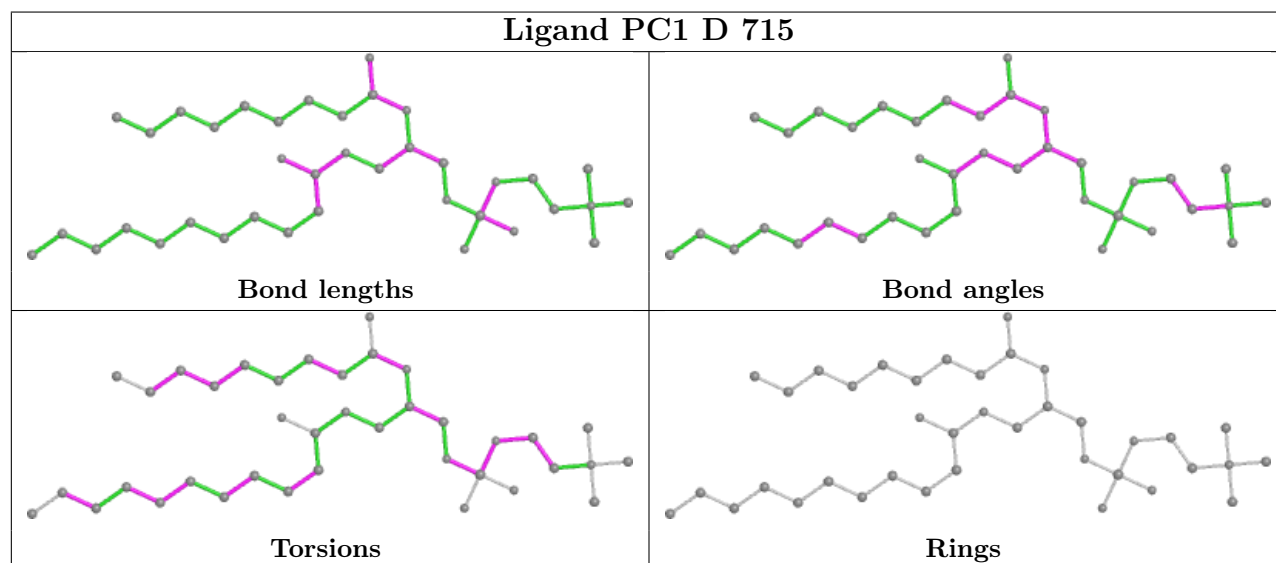
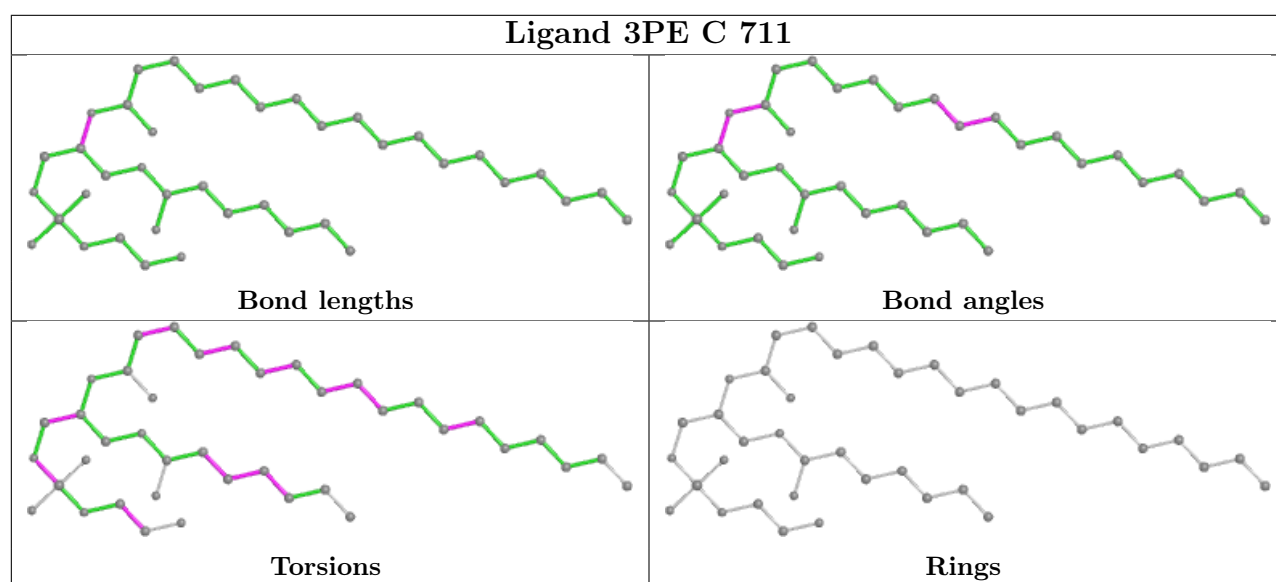
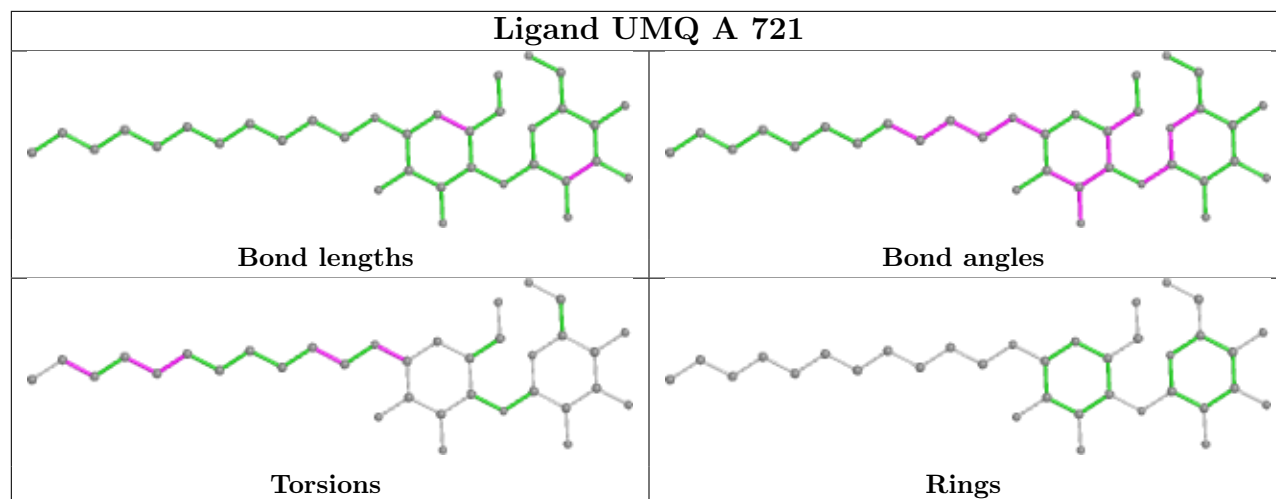


Ligand UQ6 C 706



Ligand HEC D 703





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.