



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 05:57 am BST

PDB ID : 1KB9
Title : YEAST CYTOCHROME BC1 COMPLEX
Authors : Lange, C.; Nett, J.H.; Trumpower, B.L.; Hunte, C.
Deposited on : 2001-11-05
Resolution : 2.30 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)
Xtrriage (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) : 2.11

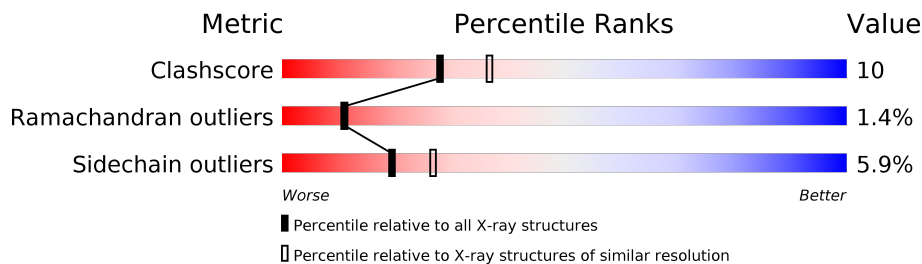
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)




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 on 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	72% 26% .
2	B	352	63% 32% .
3	C	385	84% 14% .
4	D	246	84% 15% .
5	E	185	79% 20% .
6	F	74	78% 20% .
7	G	125	86% 12% .
8	H	93	74% 22% .

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Mol	Chain	Length	Quality of chain
9	I	55	
10	J	127	
11	K	107	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	SMA	C	505	X	-	-	-

2 Entry composition i

There are 21 unique types of molecules in this entry. The entry contains 18040 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
			Total	C	N	O	S			
1	A	431	3343	2109	576	652	6	0	0	0

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
			Total	C	N	O	S			
2	B	352	2734	1747	453	533	1	0	0	0

- Molecule 3 is a protein called CYTOCHROME B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	385	3088	2080	484	503	21	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	270	VAL	ASP	CONFLICT	UNP P00163

- Molecule 4 is a protein called CYTOCHROME C1, HEME PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	246	1940	1237	334	360	9	0	0	0

- Molecule 5 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	185	1410	893	242	265	10	0	0	0

- Molecule 6 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 17 KD PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	74	623	391	108	122	2	0	0	0

- Molecule 7 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 14 KD PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	125	1011	648	172	189	2	0	0	0

- Molecule 8 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX UBIQUINONE-BINDING PROTEIN QP-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	93	772	510	131	129	2	98	0	0

- Molecule 9 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 7.3 KD PROTEIN.

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

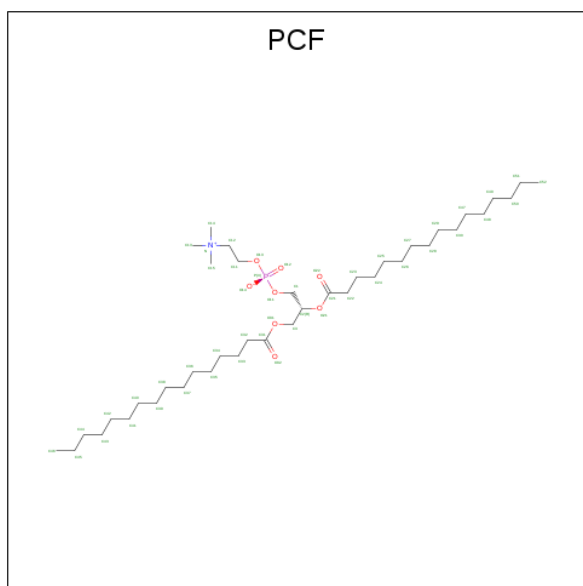
- Molecule 10 is a protein called HEAVY CHAIN (VH) OF FV-FRAGMENT.

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

- Molecule 11 is a protein called LIGHT CHAIN (VL) OF FV-FRAGMENT.

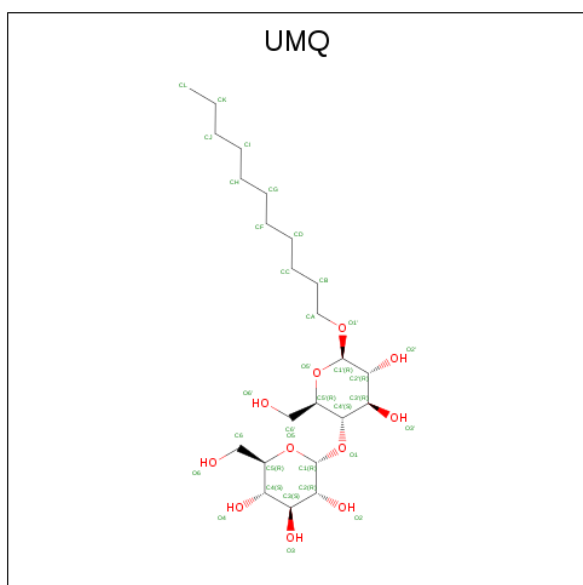
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	K	107	842	536	141	163	2	0	0	0

- Molecule 12 is 1,2-DIACYL-SN-GLYCERO-3-PHOSHOCHOLINE (three-letter code: PCF) (formula: $C_{40}H_{80}NO_8P$).



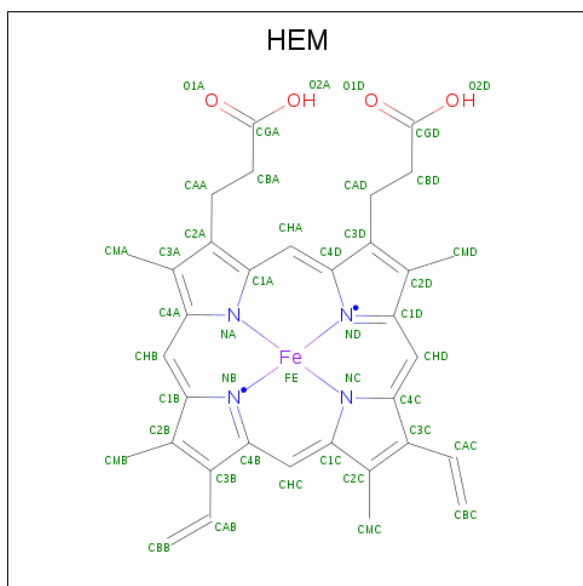
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
12	A	1	37	27	1	8	1	0	0

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



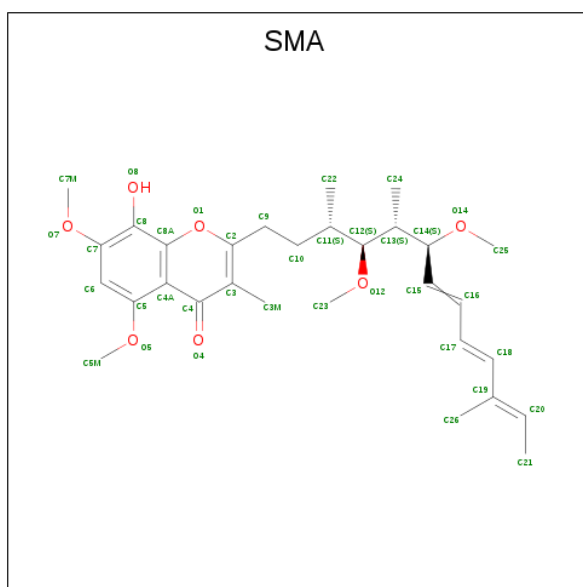
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	A	1	Total	C	O	0	0
			34	23	11		

- Molecule 14 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



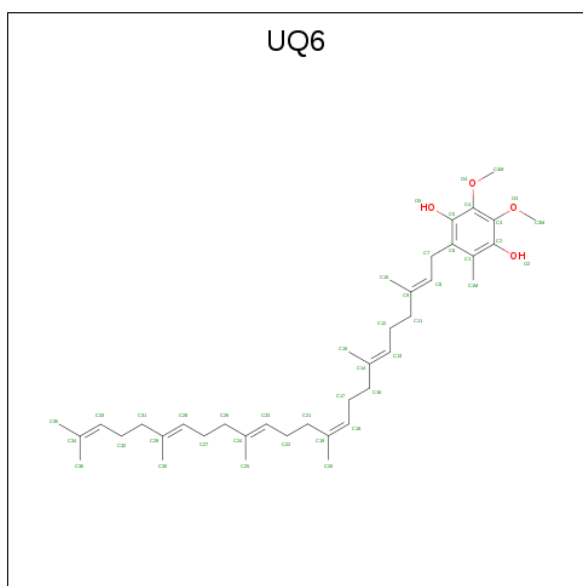
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
14	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
14	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 15 is STIGMATELLIN A (three-letter code: SMA) (formula: $C_{30}H_{42}O_7$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	C	1	Total	C O	0	0
			37	30 7		

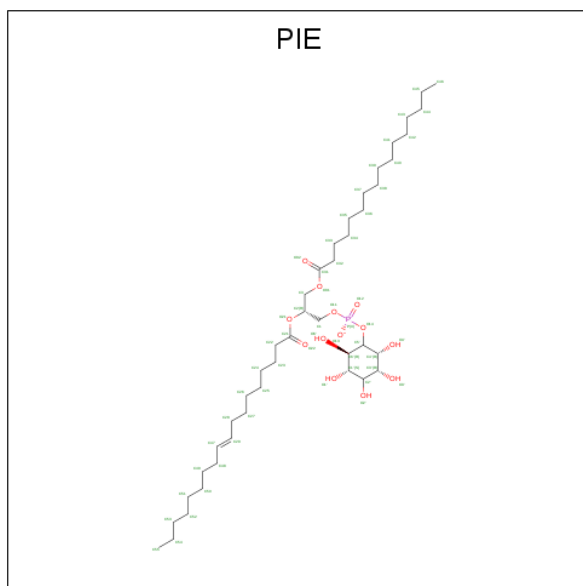
- Molecule 16 is 5-(3,7,11,15,19,23-HEXAMETHYL-TETRACOSA-2,6,10,14,18,22-HEX AENYL)-2,3-DIMETHOXY-6-METHYL-BENZENE-1,4-DIOL (three-letter code: UQ6) (formula: $C_{39}H_{60}O_4$).



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

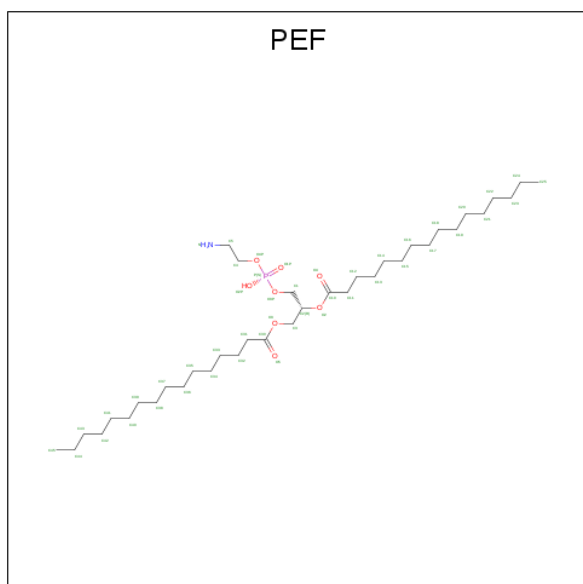
- Molecule 17 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOINOSITOL (three-letter code:

PIE) (formula: $C_{43}H_{80}O_{13}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
17	C	1	49	35	13	1	0	0

- Molecule 18 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (three-letter code: PEF) (formula: $C_{37}H_{74}NO_8P$).



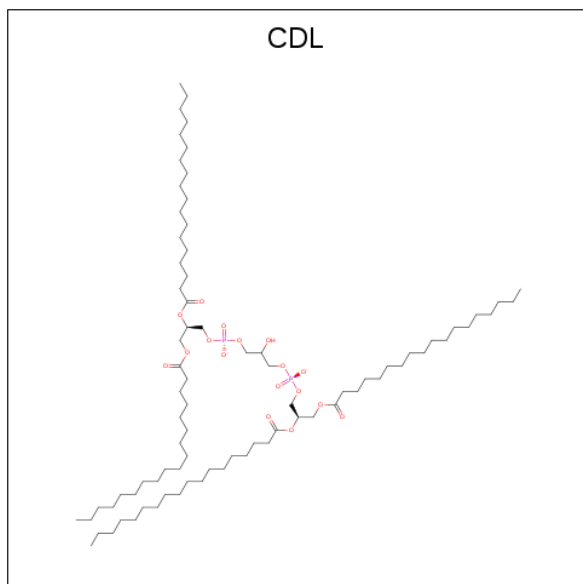
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
18	C	1	45	35	1	8	1	0	0

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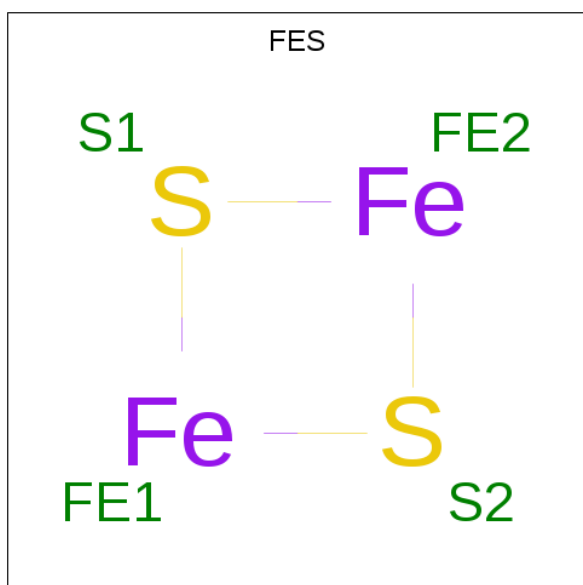
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
18	C	1	38	28	1	8	1	0	0

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



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

- 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.

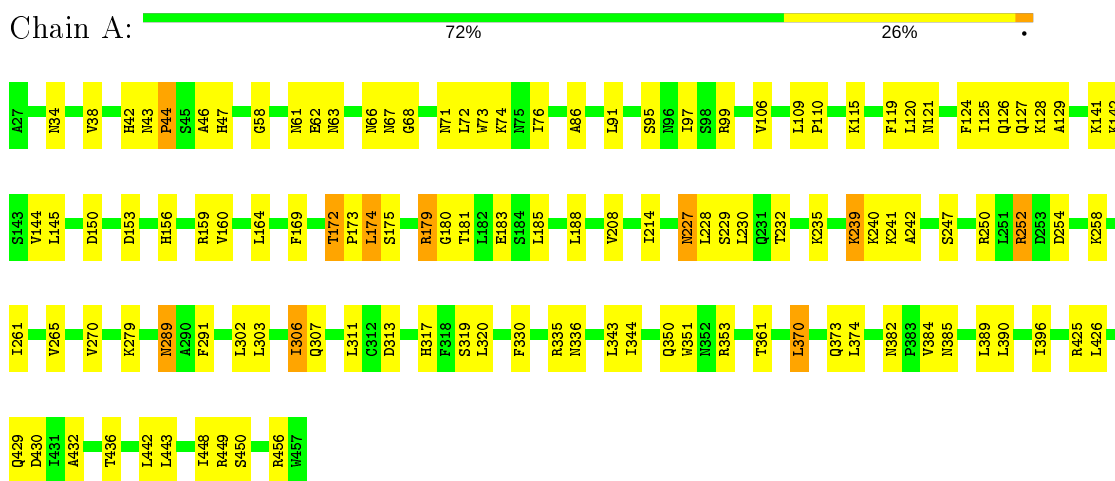
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	45	Total	O	0	0
			45	45		
21	B	9	Total	O	0	0
			9	9		
21	C	106	Total	O	0	0
			106	106		
21	D	67	Total	O	0	0
			67	67		
21	E	28	Total	O	0	0
			28	28		
21	F	7	Total	O	0	0
			7	7		
21	G	36	Total	O	0	0
			36	36		
21	H	14	Total	O	0	0
			14	14		
21	I	2	Total	O	0	0
			2	2		
21	J	5	Total	O	0	0
			5	5		
21	K	2	Total	O	0	0
			2	2		

3 Residue-property plots

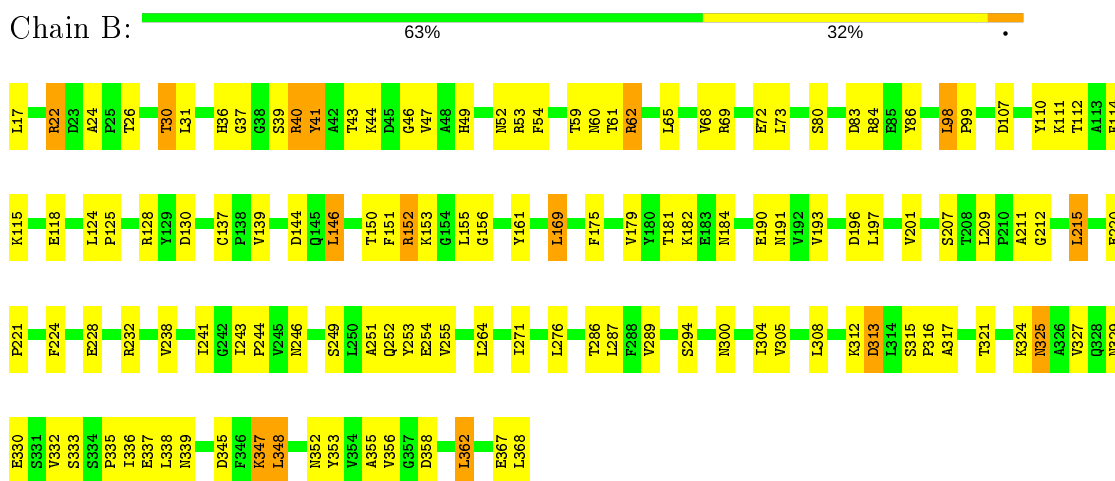
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

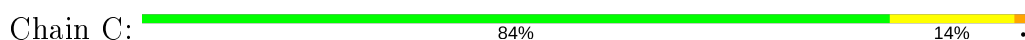
- Molecule 1: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX CORE PROTEIN I

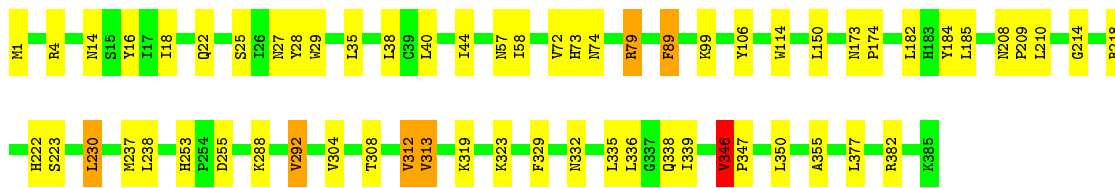


- Molecule 2: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX CORE PROTEIN 2

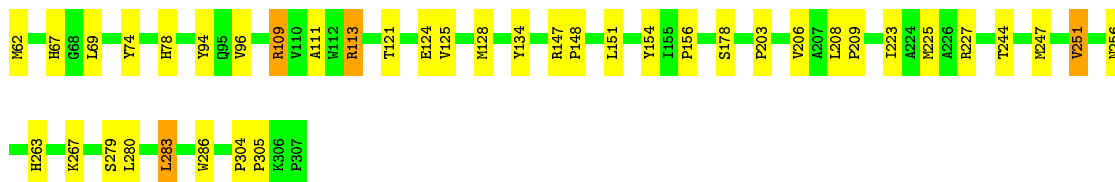
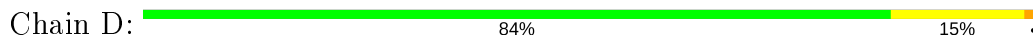


- Molecule 3: CYTOCHROME B

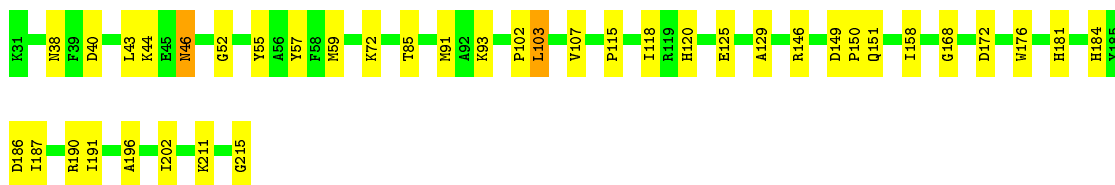




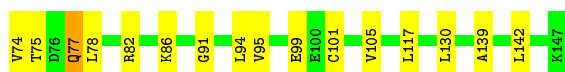
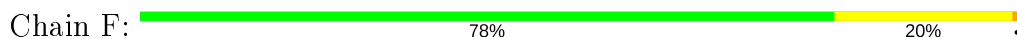
- Molecule 4: CYTOCHROME C1, HEME PROTEIN



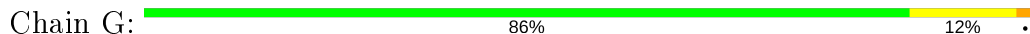
- Molecule 5: UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT



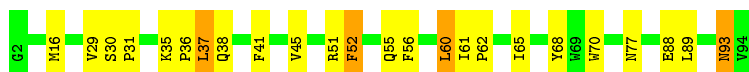
- Molecule 6: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 17 KD PROTEIN




- Molecule 7: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 14 KD PROTEIN



- Molecule 8: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX UBIQUINONE-BINDING PROTEIN QP-C



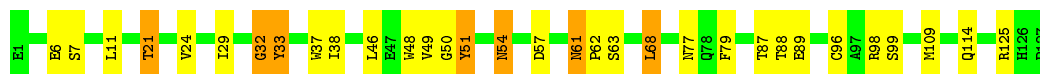
- Molecule 9: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 7.3 KD PROTEIN

Chain I:  80% 16% ..



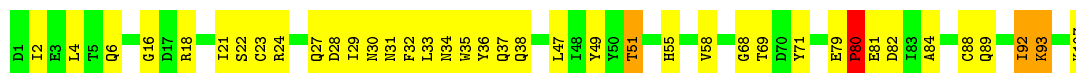
- Molecule 10: HEAVY CHAIN (VH) OF FV-FRAGMENT

Chain J:  75% 20% 6%



- Molecule 11: LIGHT CHAIN (VL) OF FV-FRAGMENT

Chain K:  64% 33% ..



4 Data and refinement statistics

Xtrriage (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	214.47Å 163.92Å 147.28Å 90.00° 117.50° 90.00°	Depositor
Resolution (Å)	14.96 – 2.30	Depositor
% Data completeness (in resolution range)	84.7 (14.96-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.218 , 0.249	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	18040	wwPDB-VP
Average B, all atoms (Å ²)	69.0	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: UMQ, CDL, PIE, FES, HEM, PEF, PCF, SMA, UQ6

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	0.34	0/3404	0.58	0/4614
2	B	0.31	0/2780	0.57	0/3764
3	C	0.45	0/3190	0.65	2/4353 (0.0%)
4	D	0.35	0/2001	0.60	0/2726
5	E	0.34	0/1443	0.61	0/1957
6	F	0.33	0/637	0.51	0/858
7	G	0.35	0/1031	0.62	1/1397 (0.1%)
8	H	0.39	0/803	0.52	0/1088
9	I	0.40	0/462	0.48	0/622
10	J	0.33	0/1043	0.61	1/1422 (0.1%)
11	K	0.31	0/863	0.53	0/1172
All	All	0.36	0/17657	0.59	4/23973 (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 (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	32	GLY	N-CA-C	5.55	126.98	113.10
3	C	79	ARG	NE-CZ-NH1	-5.46	117.57	120.30
7	G	71	ARG	NE-CZ-NH1	-5.33	117.63	120.30
3	C	346	VAL	N-CA-C	5.12	124.83	111.00

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 [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3343	0	3321	72	0
2	B	2734	0	2774	80	0
3	C	3088	0	3125	40	0
4	D	1940	0	1862	22	0
5	E	1410	0	1386	30	0
6	F	623	0	581	11	0
7	G	1011	0	1026	14	0
8	H	772	0	736	16	0
9	I	449	0	445	9	0
10	J	1015	0	959	25	0
11	K	842	0	820	24	0
12	A	37	0	48	9	0
13	A	34	0	44	4	0
14	C	86	0	60	4	0
14	D	43	0	30	0	0
15	C	37	0	40	4	0
16	C	43	0	58	11	0
17	C	49	0	58	2	0
18	C	83	0	118	3	0
19	C	76	0	99	5	0
20	E	4	0	0	1	0
21	A	45	0	0	0	0
21	B	9	0	0	0	0
21	C	106	0	0	1	0
21	D	67	0	0	1	0
21	E	28	0	0	0	0
21	F	7	0	0	0	0
21	G	36	0	0	2	0
21	H	14	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	I	2	0	0	0	0
21	J	5	0	0	0	0
21	K	2	0	0	0	0
All	All	18040	0	17590	348	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 10.

All (348) 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)
6:F:77:GLN:H	6:F:77:GLN:HE21	1.03	1.01
11:K:31:ASN:HD22	11:K:51:THR:HG21	1.31	0.95
16:C:506:UQ6:H103	16:C:506:UQ6:H1M1	1.51	0.92
2:B:347:LYS:HD3	2:B:347:LYS:H	1.37	0.88
1:A:317:HIS:HE1	1:A:351:TRP:HE1	1.25	0.85
3:C:253:HIS:HD2	3:C:255:ASP:H	1.26	0.83
1:A:99:ARG:HD3	1:A:174:LEU:HD12	1.59	0.83
7:G:31:GLN:HA	7:G:31:GLN:HE21	1.44	0.82
12:A:514:PCF:H141	13:A:521:UMQ:H62	1.63	0.80
6:F:77:GLN:H	6:F:77:GLN:NE2	1.77	0.79
3:C:22:GLN:HE22	16:C:506:UQ6:H3M3	1.49	0.78
6:F:78:LEU:HD13	6:F:142:LEU:HD22	1.68	0.76
7:G:77:ARG:HD3	7:G:88:LEU:HD11	1.67	0.75
18:C:510:PEF:H181	18:C:510:PEF:H372	1.71	0.73
2:B:182:LYS:HB2	2:B:211:ALA:HB2	1.71	0.72
5:E:115:PRO:HD2	5:E:158:ILE:HD11	1.69	0.72
1:A:63:ASN:HB2	1:A:66:ASN:ND2	2.05	0.71
2:B:336:ILE:HG21	2:B:339:ASN:HB2	1.73	0.71
2:B:30:THR:HG23	2:B:190:GLU:HB3	1.72	0.71
16:C:506:UQ6:H103	16:C:506:UQ6:C1M	2.20	0.71
1:A:74:LYS:HG3	1:A:95:SER:HB3	1.71	0.71
19:C:511:CDL:HB22	7:G:85:HIS:NE2	2.05	0.71
2:B:181:THR:HB	2:B:212:GLY:H	1.56	0.70
5:E:72:LYS:HZ3	9:I:29:GLN:HE22	1.38	0.70
3:C:58:ILE:H	3:C:173:ASN:HD22	1.38	0.70
2:B:336:ILE:HD12	2:B:336:ILE:H	1.57	0.69
5:E:72:LYS:NZ	9:I:29:GLN:HE22	1.89	0.69
3:C:44:ILE:HD12	16:C:506:UQ6:H202	1.75	0.69
7:G:77:ARG:HD2	21:G:155:HOH:O	1.93	0.67
11:K:32:PHE:HD2	11:K:92:ILE:HG22	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:300:ASN:O	2:B:304:ILE:HG12	1.94	0.67
10:J:29:ILE:H	10:J:77:ASN:HD21	1.41	0.67
4:D:62:MET:HB3	4:D:67:HIS:NE2	2.09	0.67
1:A:258:LYS:HG2	1:A:335:ARG:HG3	1.77	0.66
18:C:510:PEF:H42	8:H:51:ARG:HD2	1.78	0.65
10:J:61:ASN:HD22	10:J:63:SER:H	1.44	0.65
2:B:49:HIS:HD2	2:B:161:TYR:H	1.45	0.65
2:B:65:LEU:O	2:B:69:ARG:HG2	1.97	0.65
4:D:113:ARG:HG2	4:D:151:LEU:O	1.96	0.65
11:K:31:ASN:ND2	11:K:51:THR:HG21	2.09	0.65
2:B:287:LEU:HD21	2:B:304:ILE:HG21	1.77	0.64
11:K:6:GLN:HG2	11:K:23:CYS:SG	2.37	0.64
16:C:506:UQ6:H1M1	16:C:506:UQ6:C10	2.25	0.64
3:C:214:GLY:O	3:C:218:ARG:HD2	1.97	0.64
5:E:172:ASP:H	5:E:184:HIS:HD2	1.47	0.63
6:F:91:GLY:O	6:F:95:VAL:HG13	1.99	0.62
12:A:514:PCF:H152	12:A:514:PCF:O13	1.99	0.62
1:A:156:HIS:HD2	1:A:159:ARG:HH21	1.47	0.62
11:K:37:GLN:HB2	11:K:47:LEU:HD11	1.82	0.61
1:A:73:TRP:CE3	1:A:76:ILE:HD11	2.35	0.61
10:J:54:ASN:H	10:J:54:ASN:HD22	1.46	0.61
6:F:77:GLN:HE21	6:F:77:GLN:N	1.86	0.61
1:A:109:LEU:HG	1:A:110:PRO:HD2	1.82	0.60
1:A:42:HIS:CD2	1:A:42:HIS:H	2.19	0.60
5:E:44:LYS:NZ	5:E:52:GLY:H	2.00	0.60
11:K:27:GLN:HG2	11:K:28:ASP:H	1.67	0.60
3:C:44:ILE:HD12	16:C:506:UQ6:C20	2.31	0.59
2:B:241:ILE:HG12	2:B:287:LEU:HB3	1.83	0.59
11:K:29:ILE:HG22	11:K:92:ILE:HD12	1.85	0.59
5:E:172:ASP:H	5:E:184:HIS:CD2	2.20	0.59
2:B:336:ILE:CG2	2:B:339:ASN:HB2	2.33	0.59
2:B:115:LYS:HB2	2:B:118:GLU:HG3	1.85	0.58
2:B:24:ALA:HB3	2:B:191:ASN:ND2	2.18	0.58
4:D:96:VAL:HB	4:D:251:VAL:HG13	1.85	0.58
3:C:58:ILE:H	3:C:173:ASN:ND2	2.02	0.58
2:B:150:THR:HG22	2:B:352:ASN:ND2	2.19	0.58
1:A:68:GLY:HA3	1:A:185:LEU:HD11	1.86	0.57
1:A:252:ARG:HD3	1:A:254:ASP:OD1	2.04	0.57
3:C:25:SER:OG	7:G:79:HIS:HD2	1.87	0.57
3:C:1:MET:N	21:C:587:HOH:O	2.37	0.57
2:B:49:HIS:CD2	2:B:161:TYR:H	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:208:ASN:HD22	3:C:210:LEU:H	1.52	0.57
7:G:53:ASN:ND2	7:G:56:MET:H	2.03	0.56
2:B:44:LYS:HB2	2:B:47:VAL:HG21	1.87	0.56
1:A:229:SER:HB3	1:A:232:THR:HB	1.86	0.56
5:E:43:LEU:HD21	8:H:29:VAL:HG11	1.88	0.56
3:C:323:LYS:HE3	8:H:55:GLN:HE22	1.70	0.56
7:G:43:LEU:HD13	7:G:48:LEU:HD11	1.87	0.56
4:D:109:ARG:HG3	4:D:178:SER:CB	2.36	0.56
5:E:107:VAL:CG1	5:E:118:ILE:HB	2.36	0.56
1:A:313:ASP:OD1	1:A:335:ARG:HD3	2.05	0.55
1:A:270:VAL:HG21	1:A:396:ILE:HD13	1.88	0.55
1:A:58:GLY:H	1:A:61:ASN:HD22	1.54	0.55
6:F:74:VAL:HG12	6:F:75:THR:H	1.71	0.55
2:B:347:LYS:HG2	2:B:348:LEU:N	2.22	0.55
5:E:168:GLY:HA2	5:E:176:TRP:CD1	2.42	0.55
10:J:61:ASN:ND2	10:J:63:SER:H	2.05	0.55
5:E:72:LYS:NZ	9:I:29:GLN:NE2	2.54	0.55
10:J:29:ILE:HG12	10:J:77:ASN:ND2	2.21	0.55
1:A:289:ASN:HD22	1:A:289:ASN:C	2.10	0.55
2:B:252:GLN:O	2:B:255:VAL:HG22	2.07	0.55
1:A:67:ASN:HD22	1:A:181:THR:HG23	1.73	0.54
4:D:247:MET:O	4:D:251:VAL:HG22	2.08	0.54
1:A:317:HIS:CE1	1:A:351:TRP:HE1	2.15	0.54
13:A:521:UMQ:O2'	9:I:18:VAL:HG22	2.06	0.54
1:A:169:PHE:O	1:A:172:THR:HB	2.08	0.54
1:A:63:ASN:HB2	1:A:66:ASN:HD22	1.71	0.54
5:E:55:TYR:O	5:E:59:MET:HG2	2.08	0.54
1:A:124:PHE:HA	1:A:128:LYS:HD3	1.90	0.54
7:G:31:GLN:HA	7:G:31:GLN:NE2	2.20	0.54
2:B:238:VAL:HG13	2:B:356:VAL:HB	1.89	0.53
2:B:68:VAL:O	2:B:72:GLU:HG3	2.08	0.53
3:C:253:HIS:CD2	3:C:255:ASP:H	2.16	0.53
14:C:502:HEM:HMC2	14:C:502:HEM:HBC2	1.91	0.53
1:A:302:LEU:HB2	1:A:350:GLN:HG3	1.90	0.53
1:A:350:GLN:HE22	1:A:353:ARG:HH21	1.56	0.53
5:E:107:VAL:HG12	5:E:118:ILE:HB	1.91	0.53
10:J:87:THR:HG22	10:J:88:THR:N	2.24	0.53
1:A:265:VAL:HG21	1:A:426:LEU:HD12	1.91	0.52
1:A:344:ILE:HG21	1:A:448:ILE:HD12	1.91	0.52
15:C:505:SMA:H21	15:C:505:SMA:H39	1.91	0.52
4:D:203:PRO:HG2	4:D:206:VAL:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:38:ILE:HA	10:J:49:VAL:HG23	1.89	0.52
1:A:306:ILE:HA	1:A:311:LEU:HD22	1.90	0.52
12:A:514:PCF:H151	13:A:521:UMQ:H6'1	1.92	0.52
8:H:56:PHE:O	8:H:60:LEU:HB2	2.09	0.52
1:A:172:THR:HG23	1:A:173:PRO:HD2	1.91	0.52
3:C:57:ASN:HA	3:C:173:ASN:HD21	1.75	0.52
7:G:15:ILE:HG23	7:G:21:LEU:HB3	1.92	0.52
5:E:129:ALA:HB2	5:E:187:ILE:HG23	1.91	0.52
3:C:347:PRO:HG3	8:H:77:ASN:HB2	1.91	0.52
11:K:34:ASN:HD22	11:K:49:TYR:HA	1.75	0.52
2:B:246:ASN:HB2	2:B:249:SER:HB3	1.92	0.52
3:C:22:GLN:NE2	16:C:506:UQ6:H3M3	2.23	0.52
1:A:142:LYS:NZ	1:A:142:LYS:HB2	2.25	0.51
1:A:303:LEU:O	1:A:307:GLN:HG3	2.10	0.51
2:B:329:ASN:O	2:B:332:VAL:HG23	2.10	0.51
14:C:501:HEM:HBC2	14:C:501:HEM:HHD	1.93	0.51
11:K:47:LEU:HA	11:K:58:VAL:HG11	1.93	0.51
11:K:4:LEU:HD23	11:K:88:CYS:SG	2.51	0.51
2:B:315:SER:N	2:B:316:PRO:HD3	2.26	0.51
5:E:103:LEU:O	5:E:120:HIS:HB3	2.10	0.51
4:D:74:TYR:CE1	6:F:139:ALA:HA	2.46	0.51
6:F:82:ARG:O	6:F:86:LYS:HG3	2.10	0.51
10:J:99:SER:HB3	10:J:109:MET:HG2	1.91	0.51
11:K:32:PHE:CD2	11:K:92:ILE:HG22	2.43	0.51
2:B:110:TYR:HD1	2:B:209:LEU:HD23	1.76	0.51
2:B:264:LEU:HD12	2:B:317:ALA:HB2	1.92	0.51
4:D:286:TRP:CE3	5:E:59:MET:HG3	2.46	0.51
3:C:208:ASN:HB2	3:C:209:PRO:HD2	1.92	0.50
1:A:71:ASN:HA	1:A:97:ILE:HG13	1.94	0.50
8:H:89:LEU:O	8:H:93:ASN:HB2	2.11	0.50
11:K:2:ILE:H	11:K:2:ILE:HD12	1.76	0.50
5:E:125:GLU:HB3	5:E:187:ILE:HG12	1.92	0.50
9:I:5:SER:O	9:I:9:THR:HG23	2.12	0.50
1:A:235:LYS:HB2	1:A:235:LYS:NZ	2.26	0.50
1:A:289:ASN:ND2	1:A:291:PHE:H	2.10	0.50
1:A:68:GLY:HA3	1:A:185:LEU:CD1	2.41	0.50
1:A:373:GLN:HG3	1:A:374:LEU:N	2.26	0.49
3:C:27:ASN:HB2	19:C:511:CDL:OB3	2.11	0.49
12:A:514:PCF:H402	17:C:508:PIE:H382	1.93	0.49
2:B:69:ARG:O	2:B:73:LEU:HD23	2.12	0.49
11:K:55:HIS:O	11:K:58:VAL:HG22	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:GLN:NE2	1:A:353:ARG:HD3	2.27	0.49
2:B:137:CYS:SG	2:B:139:VAL:HG22	2.51	0.49
2:B:324:LYS:O	2:B:327:VAL:HG22	2.13	0.49
1:A:127:GLN:C	1:A:129:ALA:H	2.16	0.49
1:A:289:ASN:HD22	1:A:291:PHE:H	1.59	0.49
2:B:41:TYR:HB3	2:B:215:LEU:HD13	1.94	0.49
10:J:38:ILE:HD12	10:J:46:LEU:HD22	1.94	0.49
1:A:121:ASN:HD21	1:A:125:ILE:HD12	1.77	0.48
8:H:61:ILE:HB	8:H:62:PRO:HD3	1.95	0.48
3:C:329:PHE:HE2	18:C:510:PEF:H432	1.78	0.48
2:B:313:ASP:O	2:B:316:PRO:HD3	2.13	0.48
10:J:11:LEU:HD13	10:J:125:ARG:HD2	1.96	0.48
12:A:514:PCF:H153	12:A:514:PCF:H11	1.94	0.48
4:D:227:ARG:HH11	4:D:244:THR:HG21	1.78	0.48
2:B:52:ASN:ND2	2:B:80:SER:OG	2.46	0.48
1:A:67:ASN:ND2	1:A:180:GLY:HA2	2.28	0.48
2:B:294:SER:HB3	2:B:358:ASP:HB3	1.95	0.48
4:D:286:TRP:CD2	8:H:37:LEU:HD12	2.49	0.48
10:J:24:VAL:HG21	10:J:29:ILE:HD11	1.95	0.48
1:A:429:GLN:HE22	9:I:13:ARG:NH2	2.09	0.48
3:C:40:LEU:HD23	16:C:506:UQ6:H18	1.94	0.48
3:C:335:LEU:HD13	3:C:339:ILE:HG12	1.96	0.47
12:A:514:PCF:O13	12:A:514:PCF:C15	2.62	0.47
2:B:232:ARG:HB3	2:B:232:ARG:NH2	2.29	0.47
11:K:2:ILE:HD12	11:K:2:ILE:N	2.29	0.47
1:A:430:ASP:OD2	1:A:449:ARG:NH2	2.48	0.47
7:G:71:ARG:NH1	21:G:148:HOH:O	2.41	0.47
2:B:40:ARG:HB2	2:B:84:ARG:O	2.14	0.47
10:J:87:THR:HG22	10:J:88:THR:H	1.80	0.47
1:A:450:SER:HB3	12:A:514:PCF:H112	1.95	0.47
2:B:44:LYS:HB2	2:B:47:VAL:CG2	2.44	0.47
5:E:72:LYS:HZ2	9:I:29:GLN:NE2	2.12	0.47
6:F:101:CYS:O	6:F:105:VAL:HG23	2.14	0.47
11:K:4:LEU:CD2	11:K:88:CYS:SG	3.02	0.47
1:A:46:ALA:O	1:A:47:HIS:HB2	2.15	0.47
10:J:49:VAL:CG1	10:J:68:LEU:HD23	2.45	0.47
2:B:26:THR:OG1	2:B:191:ASN:ND2	2.48	0.47
1:A:121:ASN:ND2	1:A:125:ILE:HD12	2.29	0.46
2:B:151:PHE:O	2:B:156:GLY:HA3	2.14	0.46
2:B:252:GLN:HG3	2:B:253:TYR:N	2.31	0.46
2:B:197:LEU:O	2:B:201:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:355:ALA:HB1	2:B:362:LEU:HD23	1.98	0.46
2:B:39:SER:OG	2:B:84:ARG:HD3	2.16	0.46
10:J:51:TYR:CD2	10:J:51:TYR:C	2.89	0.46
1:A:72:LEU:HD13	1:A:144:VAL:HG21	1.98	0.46
2:B:182:LYS:HB2	2:B:211:ALA:CB	2.43	0.46
2:B:255:VAL:HG12	2:B:321:THR:HG21	1.96	0.46
4:D:134:TYR:OH	4:D:156:PRO:HD3	2.16	0.46
5:E:146:ARG:CZ	5:E:202:ILE:HD11	2.45	0.46
1:A:179:ARG:HG2	1:A:179:ARG:HH21	1.81	0.46
3:C:28:TYR:CE2	19:C:511:CDL:HA32	2.50	0.46
1:A:67:ASN:ND2	1:A:181:THR:HG23	2.31	0.46
4:D:121:THR:OG1	4:D:124:GLU:HG3	2.16	0.46
4:D:111:ALA:HA	4:D:154:TYR:HA	1.97	0.46
10:J:29:ILE:H	10:J:77:ASN:ND2	2.11	0.46
5:E:120:HIS:CD2	5:E:151:GLN:HG2	2.51	0.46
11:K:33:LEU:HD22	11:K:71:TYR:CG	2.51	0.46
2:B:317:ALA:O	2:B:321:THR:HG22	2.16	0.46
3:C:89:PHE:HE2	14:C:501:HEM:HBB2	1.81	0.46
2:B:232:ARG:HH21	2:B:232:ARG:HB3	1.80	0.45
2:B:308:LEU:HB2	2:B:348:LEU:HD22	1.98	0.45
3:C:4:ARG:HE	3:C:14:ASN:ND2	2.14	0.45
10:J:98:ARG:O	10:J:109:MET:HA	2.16	0.45
1:A:58:GLY:H	1:A:61:ASN:ND2	2.13	0.45
10:J:37:TRP:CZ3	10:J:96:CYS:HB3	2.52	0.45
11:K:51:THR:HG1	11:K:71:TYR:HD2	1.62	0.45
1:A:279:LYS:HG3	1:A:319:SER:HB3	1.98	0.45
2:B:321:THR:O	2:B:325:ASN:HB2	2.17	0.45
5:E:120:HIS:HD2	5:E:151:GLN:HG2	1.80	0.45
2:B:155:LEU:HD12	2:B:155:LEU:N	2.31	0.45
2:B:37:GLY:HA3	2:B:179:VAL:HG11	1.99	0.45
4:D:304:PRO:HA	4:D:305:PRO:HD3	1.81	0.45
5:E:93:LYS:HD3	5:E:215:GLY:HA3	1.98	0.45
10:J:48:TRP:CZ2	10:J:50:GLY:HA2	2.51	0.45
2:B:46:GLY:O	2:B:49:HIS:HB3	2.16	0.45
3:C:16:TYR:O	16:C:506:UQ6:H1M2	2.17	0.45
19:C:511:CDL:HA4	19:C:511:CDL:H112	1.49	0.45
4:D:147:ARG:HG2	4:D:148:PRO:O	2.16	0.45
1:A:160:VAL:CG2	1:A:436:THR:HG22	2.47	0.45
2:B:228:GLU:HA	2:B:353:TYR:O	2.17	0.45
10:J:61:ASN:HD22	10:J:61:ASN:C	2.20	0.45
3:C:27:ASN:OD1	3:C:29:TRP:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:33:LEU:HD23	11:K:35:TRP:HE1	1.82	0.44
1:A:172:THR:HG23	1:A:242:ALA:HA	1.99	0.44
12:A:514:PCF:C14	13:A:521:UMQ:H62	2.41	0.44
10:J:6:GLU:H	10:J:114:GLN:HE21	1.66	0.44
12:A:514:PCF:C15	12:A:514:PCF:H11	2.48	0.44
2:B:254:GLU:HG2	2:B:276:LEU:HD23	1.98	0.44
3:C:218:ARG:HG3	8:H:16:MET:CE	2.48	0.44
3:C:346:VAL:HG12	3:C:347:PRO:N	2.33	0.44
4:D:223:ILE:HG12	4:D:225:MET:H	1.82	0.44
5:E:44:LYS:HB3	8:H:35:LYS:HA	2.00	0.44
4:D:125:VAL:HA	4:D:128:MET:HE3	1.99	0.44
1:A:239:LYS:HB2	1:A:240:LYS:H	1.70	0.43
1:A:385:ASN:O	1:A:389:LEU:HG	2.17	0.43
2:B:61:THR:HG23	2:B:111:LYS:NZ	2.32	0.43
4:D:263:HIS:NE2	4:D:267:LYS:HE3	2.34	0.43
5:E:191:ILE:HD13	5:E:196:ALA:HB3	2.00	0.43
2:B:43:THR:HG22	2:B:175:PHE:HD1	1.82	0.43
4:D:78:HIS:HD2	21:D:517:HOH:O	2.01	0.43
10:J:61:ASN:HD22	10:J:62:PRO:N	2.15	0.43
2:B:24:ALA:HB3	2:B:191:ASN:HD21	1.84	0.43
2:B:305:VAL:HG11	2:B:368:LEU:HB3	2.00	0.43
3:C:18:ILE:HA	3:C:222:HIS:HB2	2.00	0.43
1:A:156:HIS:HD2	1:A:159:ARG:NH2	2.13	0.43
1:A:317:HIS:HE1	1:A:351:TRP:NE1	2.05	0.43
1:A:73:TRP:CZ3	1:A:76:ILE:HD11	2.53	0.43
2:B:62:ARG:HH21	2:B:62:ARG:HB2	1.83	0.43
4:D:227:ARG:NH1	4:D:244:THR:HG21	2.33	0.43
7:G:77:ARG:HD3	7:G:88:LEU:CD1	2.44	0.43
2:B:60:ASN:HB2	2:B:111:LYS:NZ	2.33	0.43
1:A:91:LEU:HD23	1:A:106:VAL:HG11	2.00	0.43
2:B:251:ALA:O	2:B:255:VAL:HG13	2.18	0.43
2:B:36:HIS:HB2	2:B:184:ASN:OD1	2.19	0.43
3:C:332:ASN:HD21	3:C:355:ALA:HA	1.84	0.43
15:C:505:SMA:H14	15:C:505:SMA:H36	2.01	0.43
1:A:169:PHE:O	1:A:175:SER:HB3	2.18	0.43
1:A:62:GLU:OE1	1:A:67:ASN:HA	2.19	0.43
1:A:74:LYS:HG3	1:A:95:SER:CB	2.44	0.43
3:C:73:HIS:O	3:C:74:ASN:HB2	2.18	0.43
7:G:120:LEU:O	7:G:123:ILE:HG12	2.19	0.43
2:B:220:GLU:HA	2:B:221:PRO:HD3	1.91	0.43
11:K:24:ARG:HA	11:K:69:THR:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:SER:O	1:A:432:ALA:HA	2.19	0.42
5:E:44:LYS:HZ2	5:E:52:GLY:H	1.66	0.42
2:B:146:LEU:HD23	2:B:286:THR:HG22	2.01	0.42
3:C:313:VAL:HG22	3:C:319:LYS:HE3	2.01	0.42
2:B:83:ASP:HB2	2:B:86:TYR:H	1.84	0.42
3:C:304:VAL:HG13	3:C:308:THR:HG23	2.00	0.42
1:A:74:LYS:HB2	1:A:97:ILE:HD11	2.02	0.42
6:F:74:VAL:HG12	6:F:75:THR:N	2.34	0.42
10:J:49:VAL:HG12	10:J:68:LEU:HD23	2.00	0.42
2:B:22:ARG:HH12	2:B:332:VAL:HB	1.84	0.42
3:C:106:TYR:HB3	3:C:114:TRP:CD2	2.55	0.42
5:E:149:ASP:HA	5:E:150:PRO:HD2	1.90	0.42
1:A:456:ARG:HH21	1:A:456:ARG:HG3	1.84	0.42
3:C:230:LEU:HA	3:C:230:LEU:HD12	1.89	0.42
3:C:312:VAL:HG21	7:G:5:PHE:CE1	2.54	0.42
15:C:505:SMA:C10	15:C:505:SMA:H36	2.49	0.42
7:G:53:ASN:HD21	7:G:56:MET:H	1.68	0.42
3:C:237:MET:CE	17:C:508:PIE:H291	2.49	0.42
10:J:7:SER:OG	10:J:21:THR:HG23	2.20	0.42
11:K:79:GLU:HA	11:K:80:PRO:HA	1.80	0.42
1:A:382:ASN:OD1	1:A:384:VAL:HG22	2.20	0.42
16:C:506:UQ6:H101	16:C:506:UQ6:H121	1.55	0.42
4:D:279:SER:O	4:D:283:LEU:HB2	2.20	0.42
5:E:186:ASP:OD2	5:E:190:ARG:HD2	2.20	0.42
6:F:95:VAL:O	6:F:99:GLU:HB2	2.20	0.42
2:B:347:LYS:N	2:B:347:LYS:HD3	2.15	0.41
3:C:288:LYS:O	3:C:292:VAL:HG13	2.20	0.41
15:C:505:SMA:C16	15:C:505:SMA:H39	2.49	0.41
1:A:350:GLN:NE2	1:A:353:ARG:HH21	2.19	0.41
2:B:182:LYS:HD3	2:B:207:SER:HA	2.01	0.41
11:K:93:LYS:HB3	11:K:93:LYS:NZ	2.35	0.41
8:H:35:LYS:HA	8:H:36:PRO:HD2	1.89	0.41
1:A:38:VAL:HA	1:A:208:VAL:HG13	2.01	0.41
2:B:347:LYS:HG2	2:B:348:LEU:H	1.84	0.41
2:B:59:THR:HA	2:B:112:THR:HA	2.02	0.41
14:C:501:HEM:HHD	14:C:501:HEM:CBC	2.49	0.41
1:A:43:ASN:HA	1:A:44:PRO:HD2	1.81	0.41
2:B:124:LEU:HB2	2:B:125:PRO:HD3	2.02	0.41
2:B:193:VAL:HG23	2:B:196:ASP:HB2	2.03	0.41
5:E:38:ASN:HD21	5:E:40:ASP:CG	2.23	0.41
1:A:370:LEU:O	1:A:374:LEU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ARG:NH1	1:A:442:LEU:O	2.54	0.41
19:C:511:CDL:H802	19:C:511:CDL:H771	1.85	0.41
5:E:181:HIS:HB2	20:E:504:FES:S1	2.61	0.41
2:B:98:LEU:N	2:B:99:PRO:HD2	2.35	0.41
1:A:214:ILE:O	1:A:214:ILE:HD12	2.21	0.41
3:C:173:ASN:HB3	3:C:174:PRO:HD3	2.03	0.41
3:C:338:GLN:HG3	8:H:70:TRP:CH2	2.55	0.41
11:K:21:ILE:HG22	11:K:22:SER:N	2.35	0.41
2:B:152:ARG:HD3	2:B:224:PHE:CD1	2.56	0.41
8:H:52:PHE:O	8:H:56:PHE:HB3	2.20	0.41
11:K:36:TYR:HE2	11:K:89:GLN:HG2	1.86	0.41
1:A:86:ALA:HB2	1:A:119:PHE:CZ	2.56	0.41
2:B:241:ILE:HA	2:B:352:ASN:O	2.21	0.41
2:B:238:VAL:HA	2:B:289:VAL:O	2.21	0.41
2:B:238:VAL:CG1	2:B:356:VAL:HB	2.51	0.41
9:I:23:ALA:O	9:I:27:VAL:HG23	2.21	0.41
2:B:271:ILE:HG21	2:B:287:LEU:HD11	2.03	0.40
16:C:506:UQ6:H171	16:C:506:UQ6:H151	1.92	0.40
8:H:61:ILE:O	8:H:65:ILE:HG13	2.22	0.40
4:D:208:LEU:HA	4:D:209:PRO:HD3	1.94	0.40
1:A:141:LYS:NZ	1:A:188:LEU:O	2.54	0.40
2:B:243:ILE:HA	2:B:244:PRO:HD3	1.87	0.40
5:E:57:TYR:HB3	9:I:7:TYR:OH	2.21	0.40
10:J:33:TYR:HB3	10:J:99:SER:O	2.20	0.40
10:J:51:TYR:HD2	10:J:51:TYR:C	2.25	0.40
2:B:49:HIS:HE1	2:B:130:ASP:OD1	2.05	0.40
2:B:114:PHE:O	2:B:169:LEU:HD11	2.21	0.40
3:C:72:VAL:HA	5:E:85:THR:HG22	2.03	0.40
8:H:30:SER:HA	8:H:31:PRO:HD3	1.95	0.40
8:H:51:ARG:HA	8:H:51:ARG:HD3	1.80	0.40
11:K:38:GLN:O	11:K:84:ALA:HB1	2.22	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	429/431 (100%)	397 (92%)	28 (6%)	4 (1%)	17	20
2	B	350/352 (99%)	311 (89%)	31 (9%)	8 (2%)	6	5
3	C	383/385 (100%)	369 (96%)	12 (3%)	2 (0%)	29	35
4	D	244/246 (99%)	237 (97%)	7 (3%)	0	100	100
5	E	183/185 (99%)	171 (93%)	9 (5%)	3 (2%)	9	9
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%)	79 (87%)	7 (8%)	5 (6%)	2	1
9	I	53/55 (96%)	50 (94%)	1 (2%)	2 (4%)	3	1
10	J	125/127 (98%)	111 (89%)	12 (10%)	2 (2%)	9	9
11	K	105/107 (98%)	89 (85%)	11 (10%)	5 (5%)	2	1
All	All	2158/2180 (99%)	2004 (93%)	123 (6%)	31 (1%)	11	11

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	335	PRO
3	C	223	SER
5	E	103	LEU
8	H	93	ASN
2	B	153	LYS
2	B	333	SER
5	E	46	ASN
8	H	37	LEU
9	I	13	ARG
10	J	33	TYR
11	K	30	ASN
11	K	51	THR
1	A	44	PRO
1	A	227	ASN
8	H	38	GLN
11	K	68	GLY
1	A	228	LEU
2	B	22	ARG
2	B	367	GLU
9	I	12	LYS

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Mol	Chain	Res	Type
11	K	80	PRO
1	A	230	LEU
2	B	152	ARG
2	B	348	LEU
3	C	346	VAL
11	K	16	GLY
2	B	313	ASP
5	E	102	PRO
8	H	52	PHE
10	J	32	GLY
8	H	45	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	370/370 (100%)	342 (92%)	28 (8%)	13	16
2	B	301/301 (100%)	278 (92%)	23 (8%)	13	16
3	C	338/338 (100%)	320 (95%)	18 (5%)	22	31
4	D	204/204 (100%)	197 (97%)	7 (3%)	37	51
5	E	151/151 (100%)	148 (98%)	3 (2%)	55	72
6	F	67/67 (100%)	63 (94%)	4 (6%)	19	26
7	G	109/109 (100%)	104 (95%)	5 (5%)	27	38
8	H	77/77 (100%)	73 (95%)	4 (5%)	23	32
9	I	45/45 (100%)	41 (91%)	4 (9%)	9	11
10	J	112/112 (100%)	104 (93%)	8 (7%)	14	19
11	K	93/93 (100%)	86 (92%)	7 (8%)	13	17
All	All	1867/1867 (100%)	1756 (94%)	111 (6%)	19	27

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

Mol	Chain	Res	Type
1	A	34	ASN
1	A	115	LYS
1	A	120	LEU
1	A	126	GLN
1	A	145	LEU
1	A	150	ASP
1	A	153	ASP
1	A	164	LEU
1	A	172	THR
1	A	174	LEU
1	A	179	ARG
1	A	183	GLU
1	A	227	ASN
1	A	239	LYS
1	A	241	LYS
1	A	252	ARG
1	A	261	ILE
1	A	289	ASN
1	A	306	ILE
1	A	320	LEU
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	425	ARG
1	A	443	LEU
2	B	17	LEU
2	B	30	THR
2	B	31	LEU
2	B	40	ARG
2	B	41	TYR
2	B	53	ARG
2	B	54	PHE
2	B	62	ARG
2	B	98	LEU
2	B	107	ASP
2	B	128	ARG
2	B	144	ASP
2	B	146	LEU
2	B	169	LEU
2	B	215	LEU

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Mol	Chain	Res	Type
2	B	312	LYS
2	B	325	ASN
2	B	330	GLU
2	B	337	GLU
2	B	338	LEU
2	B	345	ASP
2	B	347	LYS
2	B	362	LEU
3	C	35	LEU
3	C	38	LEU
3	C	79	ARG
3	C	89	PHE
3	C	99	LYS
3	C	150	LEU
3	C	182	LEU
3	C	184	TYR
3	C	185	LEU
3	C	230	LEU
3	C	238	LEU
3	C	292	VAL
3	C	312	VAL
3	C	313	VAL
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	251	VAL
4	D	256	ASN
4	D	280	LEU
4	D	283	LEU
5	E	46	ASN
5	E	91	MET
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	31	GLN

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Mol	Chain	Res	Type
7	G	48	LEU
7	G	86	HIS
7	G	127	LYS
8	H	41	PHE
8	H	60	LEU
8	H	68	TYR
8	H	88	GLU
9	I	13	ARG
9	I	14	ASN
9	I	18	VAL
9	I	48	LEU
10	J	21	THR
10	J	51	TYR
10	J	54	ASN
10	J	57	ASP
10	J	61	ASN
10	J	68	LEU
10	J	79	PHE
10	J	89	GLU
11	K	18	ARG
11	K	80	PRO
11	K	81	GLU
11	K	82	ASP
11	K	92	ILE
11	K	93	LYS
11	K	107	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) 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	121	ASN
1	A	126	GLN
1	A	156	HIS
1	A	171	ASN
1	A	199	ASN
1	A	200	HIS
1	A	289	ASN

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Mol	Chain	Res	Type
1	A	298	GLN
1	A	317	HIS
1	A	336	ASN
1	A	350	GLN
1	A	385	ASN
1	A	388	ASN
1	A	429	GLN
2	B	49	HIS
2	B	52	ASN
2	B	55	ASN
2	B	191	ASN
2	B	252	GLN
2	B	258	ASN
2	B	325	ASN
2	B	328	GLN
2	B	329	ASN
3	C	14	ASN
3	C	22	GLN
3	C	43	GLN
3	C	173	ASN
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
5	E	38	ASN
5	E	106	ASN
5	E	184	HIS
6	F	77	GLN
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

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Mol	Chain	Res	Type
10	J	114	GLN
11	K	31	ASN
11	K	34	ASN
11	K	89	GLN
11	K	90	HIS
11	K	91	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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
19	CDL	C	511	-	75,75,99	1.06	5 (6%)	81,87,111	1.13	5 (6%)
20	FES	E	504	5	0,4,4	0.00	-	-		
18	PEF	C	513	-	37,37,46	0.71	0	40,42,51	0.97	1 (2%)
12	PCF	A	514	-	36,36,49	1.59	1 (2%)	42,44,57	1.27	2 (4%)
13	UMQ	A	521	-	35,35,35	0.95	1 (2%)	46,46,46	1.45	7 (15%)
16	UQ6	C	506	-	43,43,43	2.46	14 (32%)	51,55,55	2.06	19 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	PEF	C	510	-	44,44,46	0.71	0	47,49,51	1.07	2 (4%)
14	HEM	C	501	3	27,50,50	1.76	5 (18%)	17,82,82	1.60	3 (17%)
15	SMA	C	505	-	35,38,38	1.70	8 (22%)	46,52,52	2.26	12 (26%)
14	HEM	C	502	3	27,50,50	1.45	5 (18%)	17,82,82	1.51	4 (23%)
14	HEM	D	503	4	27,50,50	1.66	6 (22%)	17,82,82	1.27	3 (17%)
17	PIE	C	508	-	49,49,57	2.15	9 (18%)	59,61,69	1.66	8 (13%)

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
19	CDL	C	511	-	-	38/86/86/110	-
20	FES	E	504	5	-	-	0/1/1/1
18	PEF	C	513	-	-	13/41/41/50	-
12	PCF	A	514	-	-	15/40/40/53	-
13	UMQ	A	521	-	-	5/20/60/60	0/2/2/2
16	UQ6	C	506	-	-	14/39/39/39	0/1/1/1
18	PEF	C	510	-	-	24/48/48/50	-
14	HEM	C	501	3	-	0/6/54/54	-
15	SMA	C	505	-	2/2/5/10	21/33/34/34	0/2/2/2
14	HEM	C	502	3	-	0/6/54/54	-
14	HEM	D	503	4	-	0/6/54/54	-
17	PIE	C	508	-	-	16/44/68/76	0/1/1/1

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	C	508	PIE	P-O14	-11.15	1.31	1.60
12	A	514	PCF	O13-C11	-8.51	1.09	1.44
16	C	506	UQ6	C7-C6	6.75	1.59	1.51
16	C	506	UQ6	O5-C5	-5.62	1.23	1.37
16	C	506	UQ6	O2-C2	-5.40	1.24	1.37
15	C	505	SMA	C4A-C8A	5.32	1.48	1.41
16	C	506	UQ6	C2-C3	4.70	1.47	1.39
16	C	506	UQ6	C5-C4	4.40	1.46	1.39
17	C	508	PIE	C6'-C5'	4.29	1.63	1.52
17	C	508	PIE	C47-C29	4.15	1.55	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	C	506	UQ6	C5-C6	4.01	1.46	1.40
14	C	501	HEM	C3B-CAB	-4.01	1.39	1.47
14	D	503	HEM	C3B-C2B	-3.84	1.35	1.40
14	C	501	HEM	C3C-CAC	-3.72	1.40	1.47
14	D	503	HEM	CBB-CAB	3.64	1.53	1.29
13	A	521	UMQ	C3-C2	-3.57	1.43	1.52
14	C	501	HEM	C3C-C2C	-3.55	1.35	1.40
14	D	503	HEM	C3C-C2C	-3.55	1.35	1.40
14	D	503	HEM	CBC-CAC	3.53	1.52	1.29
17	C	508	PIE	C4'-C5'	3.38	1.61	1.52
15	C	505	SMA	C13-C12	3.27	1.62	1.54
19	C	511	CDL	OB2-CB2	-3.26	1.32	1.44
17	C	508	PIE	C6'-C1'	3.19	1.60	1.52
16	C	506	UQ6	C2-C1	3.18	1.46	1.40
15	C	505	SMA	C20-C19	3.12	1.36	1.33
19	C	511	CDL	OA8-CA6	-3.06	1.38	1.45
14	C	501	HEM	CMC-C2C	2.99	1.58	1.51
14	C	502	HEM	C3B-CAB	-2.99	1.41	1.47
14	C	502	HEM	C3C-C2C	-2.98	1.36	1.40
14	C	501	HEM	C3B-C2B	-2.98	1.36	1.40
16	C	506	UQ6	C23-C24	2.85	1.39	1.33
16	C	506	UQ6	C28-C29	2.82	1.39	1.33
16	C	506	UQ6	C33-C34	2.80	1.40	1.32
14	C	502	HEM	C3C-CAC	-2.79	1.42	1.47
19	C	511	CDL	OA6-CA4	-2.70	1.39	1.46
16	C	506	UQ6	C18-C19	2.70	1.39	1.33
14	C	502	HEM	C3B-C2B	-2.69	1.36	1.40
16	C	506	UQ6	C8-C9	2.61	1.39	1.33
17	C	508	PIE	O31-C3	-2.58	1.39	1.45
16	C	506	UQ6	C13-C14	2.56	1.39	1.33
15	C	505	SMA	C6-C7	2.40	1.43	1.38
15	C	505	SMA	C3-C2	-2.34	1.36	1.39
15	C	505	SMA	O12-C12	-2.32	1.36	1.42
19	C	511	CDL	O1-C1	2.22	1.50	1.43
15	C	505	SMA	O7-C7	2.15	1.40	1.37
14	D	503	HEM	C3B-CAB	2.13	1.52	1.47
17	C	508	PIE	P-O13	-2.12	1.45	1.55
14	D	503	HEM	C3C-CAC	2.10	1.52	1.47
17	C	508	PIE	C1-C2	2.10	1.57	1.50
17	C	508	PIE	O22-C21	-2.08	1.16	1.22
16	C	506	UQ6	C21-C19	2.07	1.55	1.51
15	C	505	SMA	O1-C2	2.06	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	C	511	CDL	CA2-C1	2.02	1.58	1.51
14	C	502	HEM	CBC-CAC	2.00	1.42	1.29

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	C	508	PIE	P-O14-C5'	7.43	146.45	119.41
16	C	506	UQ6	C3M-O3-C3	6.82	133.47	114.78
15	C	505	SMA	C26-C19-C18	-6.21	108.28	118.08
15	C	505	SMA	O14-C14-C15	5.85	129.90	111.05
12	A	514	PCF	C3-C2-C1	-5.63	98.47	111.79
13	A	521	UMQ	CA-O1'-C1'	-5.54	104.66	113.84
15	C	505	SMA	C3-C4-C4A	-5.01	115.55	120.58
16	C	506	UQ6	C17-C18-C19	4.88	139.41	127.66
19	C	511	CDL	CB4-OB6-CB5	-4.80	105.98	117.79
15	C	505	SMA	O14-C14-C13	4.70	117.80	107.98
16	C	506	UQ6	C4M-O4-C4	4.56	127.26	114.78
15	C	505	SMA	C4-C3-C2	4.51	121.57	116.63
17	C	508	PIE	C6'-C5'-C4'	-4.28	104.67	110.85
18	C	510	PEF	C2-O2-C10	-4.06	107.80	117.79
14	C	501	HEM	CMD-C2D-C1D	-4.05	122.24	128.46
15	C	505	SMA	O12-C12-C13	4.01	113.88	107.97
18	C	513	PEF	C2-O2-C10	-3.79	108.45	117.79
17	C	508	PIE	C38-C37-C36	-3.59	96.18	114.42
15	C	505	SMA	O1-C8A-C8	3.52	120.54	116.12
17	C	508	PIE	C3-C2-C1	-3.51	103.48	111.79
15	C	505	SMA	O7-C7-C8	3.48	118.05	114.54
19	C	511	CDL	CA6-CA4-CA3	-3.26	104.08	111.79
14	C	501	HEM	CMB-C2B-C3B	3.21	130.69	124.68
14	C	502	HEM	CMC-C2C-C3C	3.15	130.56	124.68
14	D	503	HEM	CMD-C2D-C1D	-3.09	123.71	128.46
16	C	506	UQ6	C21-C19-C18	3.00	127.20	121.12
14	C	502	HEM	CMD-C2D-C1D	-2.99	123.88	128.46
14	C	502	HEM	CMB-C2B-C3B	2.97	130.23	124.68
16	C	506	UQ6	C1M-C1-C2	-2.96	115.49	120.50
14	C	501	HEM	CMD-C2D-C3D	2.95	130.51	124.94
19	C	511	CDL	CB6-CB4-CB3	-2.92	104.87	111.79
13	A	521	UMQ	C3'-C4'-C5'	-2.91	104.26	110.93
16	C	506	UQ6	C11-C12-C13	2.88	121.35	111.88
19	C	511	CDL	CA4-OA6-CA5	-2.79	110.92	117.79
16	C	506	UQ6	C22-C23-C24	2.73	134.23	127.66
16	C	506	UQ6	C27-C28-C29	2.66	134.07	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	521	UMQ	O1'-C1'-C2'	2.52	112.24	108.30
17	C	508	PIE	C39-C38-C37	2.45	126.88	114.42
16	C	506	UQ6	C30-C29-C31	-2.44	111.16	115.27
13	A	521	UMQ	O1-C1-O5	-2.38	104.02	110.67
15	C	505	SMA	C18-C19-C20	2.35	126.23	118.80
16	C	506	UQ6	C11-C9-C8	2.30	125.77	121.12
16	C	506	UQ6	C25-C24-C26	-2.30	111.41	115.27
13	A	521	UMQ	C1'-C2'-C3'	-2.28	105.24	110.00
15	C	505	SMA	O7-C7-C6	-2.27	120.22	124.12
16	C	506	UQ6	C1M-C1-C6	2.23	123.66	120.42
12	A	514	PCF	P-O13-C11	2.23	132.57	121.59
14	D	503	HEM	CMD-C2D-C3D	2.23	129.14	124.94
13	A	521	UMQ	O1'-CA-CB	2.22	117.35	109.56
17	C	508	PIE	C2-O21-C21	-2.22	112.33	117.79
18	C	510	PEF	C3-C2-C1	2.20	117.00	111.79
16	C	506	UQ6	C7-C6-C5	-2.19	117.93	120.82
16	C	506	UQ6	C6-C7-C8	2.19	115.63	112.17
17	C	508	PIE	C48-C47-C29	-2.18	107.99	124.73
16	C	506	UQ6	C16-C14-C13	2.18	125.52	121.12
17	C	508	PIE	O31-C31-O32	2.17	129.07	123.59
16	C	506	UQ6	C20-C19-C18	-2.13	118.22	123.68
14	C	502	HEM	CMD-C2D-C3D	2.12	128.95	124.94
15	C	505	SMA	O1-C2-C9	2.12	114.42	111.91
16	C	506	UQ6	C36-C34-C35	-2.11	109.94	114.60
14	D	503	HEM	CBD-CAD-C3D	2.10	116.35	112.48
15	C	505	SMA	C11-C12-C13	-2.09	108.70	114.29
13	A	521	UMQ	C6'-C5'-C4'	-2.09	107.25	113.33
16	C	506	UQ6	C15-C14-C16	-2.06	111.80	115.27
16	C	506	UQ6	C17-C16-C14	2.06	119.75	112.98
19	C	511	CDL	CB6-OB8-CB7	-2.02	109.64	117.12

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
15	C	505	SMA	C12
15	C	505	SMA	C14

All (146) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	C	511	CDL	CA2-OA2-PA1-OA3
19	C	511	CDL	CA2-OA2-PA1-OA4

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Mol	Chain	Res	Type	Atoms
19	C	511	CDL	OA5-CA3-CA4-OA6
19	C	511	CDL	OA7-CA5-OA6-CA4
19	C	511	CDL	C11-CA5-OA6-CA4
19	C	511	CDL	OB5-CB3-CB4-OB6
18	C	513	PEF	O4P-C4-C5-N
12	A	514	PCF	C11-O13-P-O12
16	C	506	UQ6	C24-C26-C27-C28
18	C	510	PEF	O4P-C4-C5-N
15	C	505	SMA	C11-C12-C13-C24
15	C	505	SMA	O12-C12-C13-C14
15	C	505	SMA	O12-C12-C13-C24
15	C	505	SMA	C15-C14-O14-C25
15	C	505	SMA	C14-C15-C16-C17
15	C	505	SMA	C15-C16-C17-C18
15	C	505	SMA	C16-C17-C18-C19
17	C	508	PIE	C1-O11-P-O12
17	C	508	PIE	C1-O11-P-O13
17	C	508	PIE	C4'-C5'-O14-P
19	C	511	CDL	OA9-CA7-OA8-CA6
19	C	511	CDL	OB7-CB5-OB6-CB4
19	C	511	CDL	C31-CA7-OA8-CA6
19	C	511	CDL	C51-CB5-OB6-CB4
15	C	505	SMA	C9-C10-C11-C22
15	C	505	SMA	C4A-C5-O5-C5M
16	C	506	UQ6	C20-C19-C21-C22
18	C	510	PEF	C36-C37-C38-C39
15	C	505	SMA	C6-C5-O5-C5M
13	A	521	UMQ	O1'-CA-CB-CC
19	C	511	CDL	C33-C34-C35-C36
16	C	506	UQ6	C12-C11-C9-C10
16	C	506	UQ6	C15-C14-C16-C17
16	C	506	UQ6	C12-C11-C9-C8
16	C	506	UQ6	C13-C14-C16-C17
19	C	511	CDL	C77-C78-C79-C80
18	C	513	PEF	C14-C15-C16-C17
17	C	508	PIE	C36-C37-C38-C39
16	C	506	UQ6	C18-C19-C21-C22
15	C	505	SMA	C17-C18-C19-C26
15	C	505	SMA	C17-C18-C19-C20
17	C	508	PIE	C22-C21-O21-C2
18	C	513	PEF	C10-C11-C12-C13
18	C	513	PEF	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
12	A	514	PCF	C21-C22-C23-C24
18	C	510	PEF	C30-C31-C32-C33
16	C	506	UQ6	C19-C21-C22-C23
19	C	511	CDL	O1-C1-CB2-OB2
17	C	508	PIE	C31-C32-C33-C34
19	C	511	CDL	CA2-OA2-PA1-OA5
19	C	511	CDL	CB2-OB2-PB2-OB5
12	A	514	PCF	C11-O13-P-O11
17	C	508	PIE	C1-O11-P-O14
19	C	511	CDL	CA2-C1-CB2-OB2
17	C	508	PIE	O22-C21-O21-C2
18	C	510	PEF	C40-C41-C42-C43
19	C	511	CDL	C74-C75-C76-C77
13	A	521	UMQ	CF-CG-CH-CI
18	C	513	PEF	C31-C32-C33-C34
13	A	521	UMQ	C2'-C1'-O1'-CA
12	A	514	PCF	C35-C36-C37-C38
12	A	514	PCF	C36-C37-C38-C39
12	A	514	PCF	C38-C39-C40-C41
18	C	510	PEF	C16-C17-C18-C19
17	C	508	PIE	C32-C33-C34-C35
12	A	514	PCF	O22-C21-O21-C2
12	A	514	PCF	C22-C21-O21-C2
19	C	511	CDL	C78-C79-C80-C81
18	C	510	PEF	C35-C36-C37-C38
13	A	521	UMQ	O5'-C1'-O1'-CA
18	C	513	PEF	C16-C17-C18-C19
18	C	510	PEF	C38-C39-C40-C41
19	C	511	CDL	C83-C84-C85-C86
18	C	513	PEF	C20-C21-C22-C23
19	C	511	CDL	C71-C72-C73-C74
18	C	510	PEF	C41-C42-C43-C44
15	C	505	SMA	C13-C14-C15-C16
18	C	513	PEF	C12-C13-C14-C15
18	C	510	PEF	C18-C19-C20-C21
17	C	508	PIE	C37-C38-C39-C40
19	C	511	CDL	C80-C81-C82-C83
15	C	505	SMA	C24-C13-C14-O14
16	C	506	UQ6	C4-C3-O3-C3M
15	C	505	SMA	C12-C13-C14-C15
19	C	511	CDL	CB3-OB5-PB2-OB2
12	A	514	PCF	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
19	C	511	CDL	OA5-CA3-CA4-CA6
19	C	511	CDL	OB5-CB3-CB4-CB6
18	C	510	PEF	C12-C13-C14-C15
19	C	511	CDL	C81-C82-C83-C84
18	C	510	PEF	C42-C43-C44-C45
13	A	521	UMQ	CI-CJ-CK-CL
15	C	505	SMA	C22-C11-C12-O12
19	C	511	CDL	C12-C13-C14-C15
17	C	508	PIE	C26-C27-C28-C29
19	C	511	CDL	C31-C32-C33-C34
12	A	514	PCF	O11-C1-C2-C3
18	C	510	PEF	C15-C16-C17-C18
18	C	513	PEF	C1-O3P-P-O4P
17	C	508	PIE	C25-C26-C27-C28
12	A	514	PCF	O11-C1-C2-O21
19	C	511	CDL	C17-C18-C19-C20
18	C	513	PEF	O3P-C1-C2-C3
19	C	511	CDL	C52-C53-C54-C55
18	C	510	PEF	C17-C18-C19-C20
15	C	505	SMA	C11-C12-C13-C14
18	C	513	PEF	O3P-C1-C2-O2
18	C	510	PEF	O3P-C1-C2-O2
15	C	505	SMA	C24-C13-C14-C15
16	C	506	UQ6	C2-C3-O3-C3M
19	C	511	CDL	CB2-OB2-PB2-OB3
18	C	513	PEF	C1-O3P-P-O1P
12	A	514	PCF	C11-O13-P-O14
18	C	510	PEF	C39-C40-C41-C42
18	C	510	PEF	O3P-C1-C2-C3
12	A	514	PCF	C32-C33-C34-C35
18	C	510	PEF	C5-C4-O4P-P
18	C	513	PEF	C18-C19-C20-C21
15	C	505	SMA	C9-C10-C11-C12
12	A	514	PCF	C34-C35-C36-C37
19	C	511	CDL	C55-C56-C57-C58
17	C	508	PIE	C22-C23-C24-C25
16	C	506	UQ6	C3-C4-O4-C4M
17	C	508	PIE	C29-C47-C48-C49
18	C	510	PEF	C34-C35-C36-C37
18	C	510	PEF	C19-C20-C21-C22
18	C	510	PEF	C4-O4P-P-O3P
17	C	508	PIE	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
18	C	510	PEF	C11-C12-C13-C14
19	C	511	CDL	C76-C77-C78-C79
15	C	505	SMA	C12-C13-C14-O14
12	A	514	PCF	C37-C38-C39-C40
16	C	506	UQ6	C9-C11-C12-C13
19	C	511	CDL	C54-C55-C56-C57
18	C	510	PEF	O2-C10-C11-C12
19	C	511	CDL	C11-C12-C13-C14
16	C	506	UQ6	C5-C4-O4-C4M
16	C	506	UQ6	C26-C27-C28-C29
17	C	508	PIE	C47-C48-C49-C50
18	C	510	PEF	O3-C30-C31-C32
15	C	505	SMA	C10-C11-C12-O12
18	C	510	PEF	O4-C10-C11-C12
19	C	511	CDL	C12-C11-CA5-OA6
19	C	511	CDL	CA7-C31-C32-C33
19	C	511	CDL	C12-C11-CA5-OA7
19	C	511	CDL	C32-C31-CA7-OA8

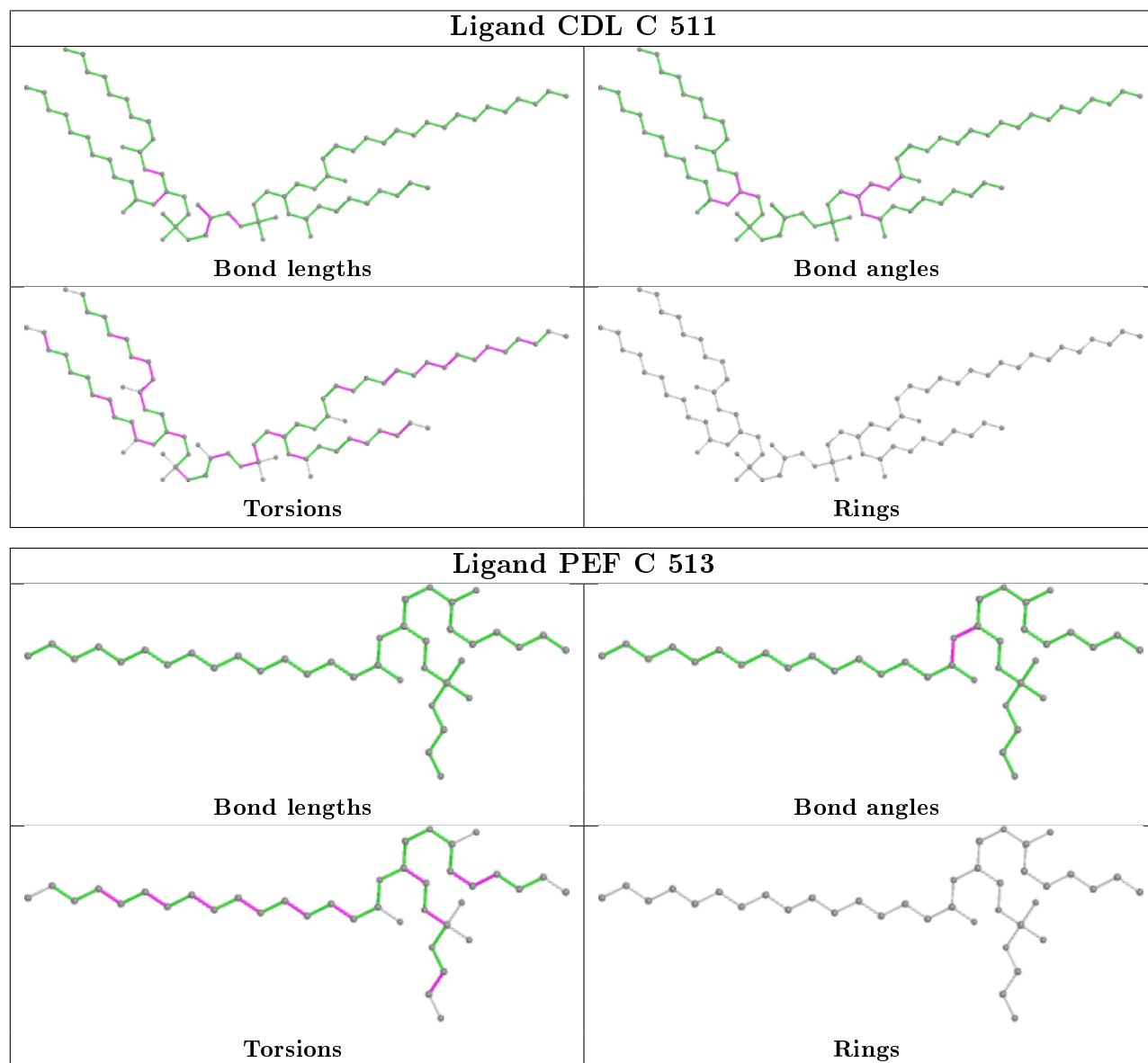
There are no ring outliers.

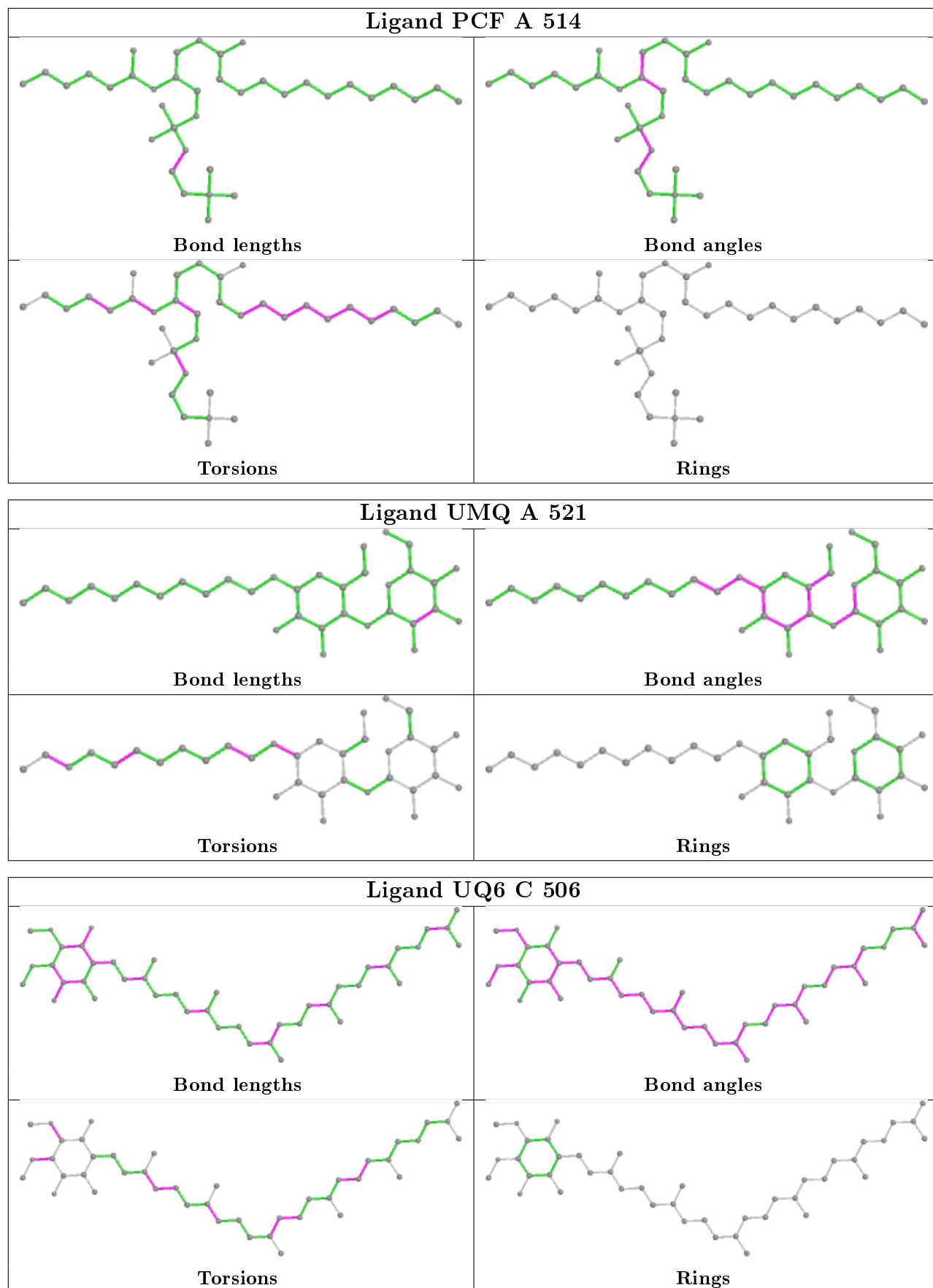
10 monomers are involved in 39 short contacts:

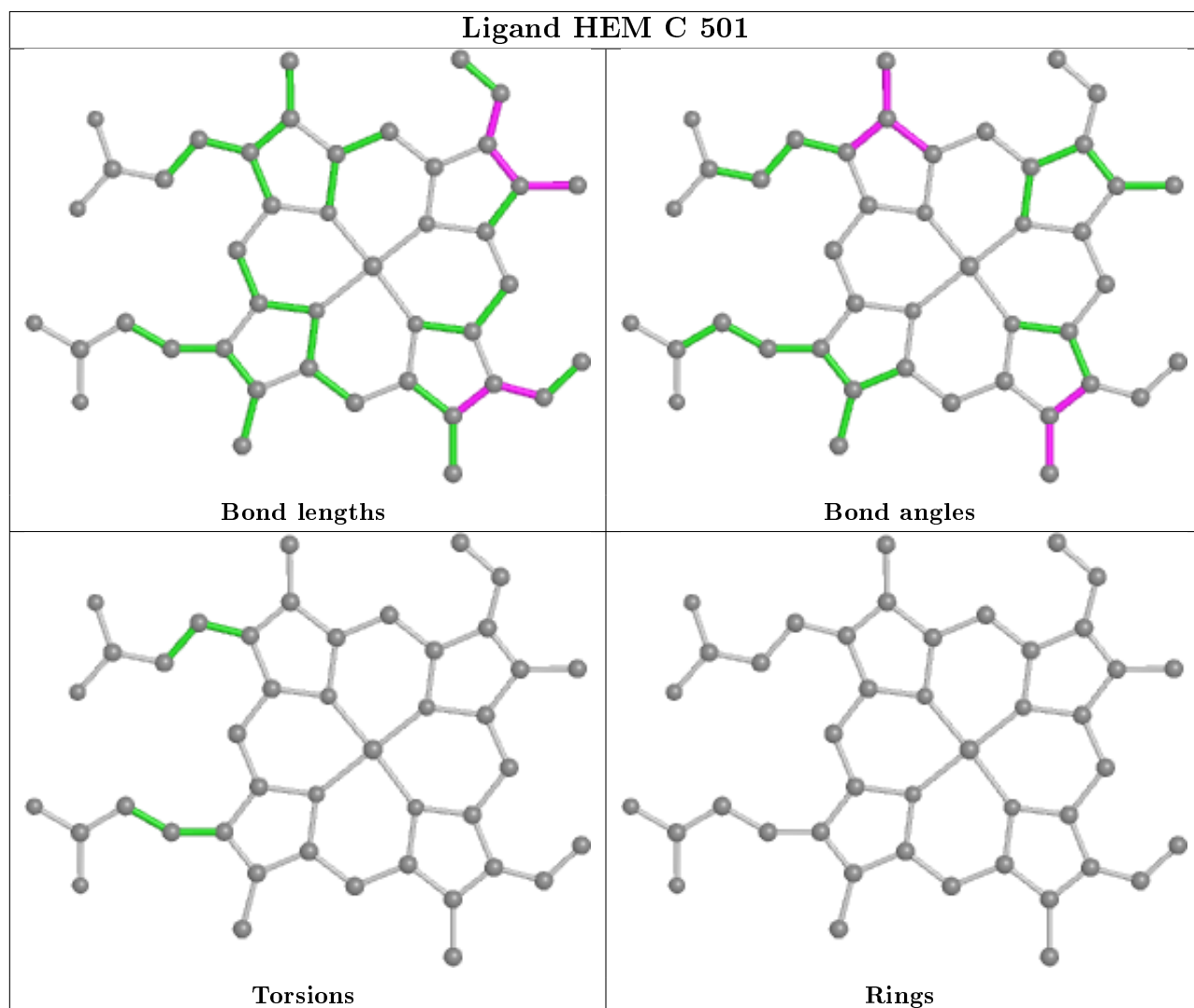
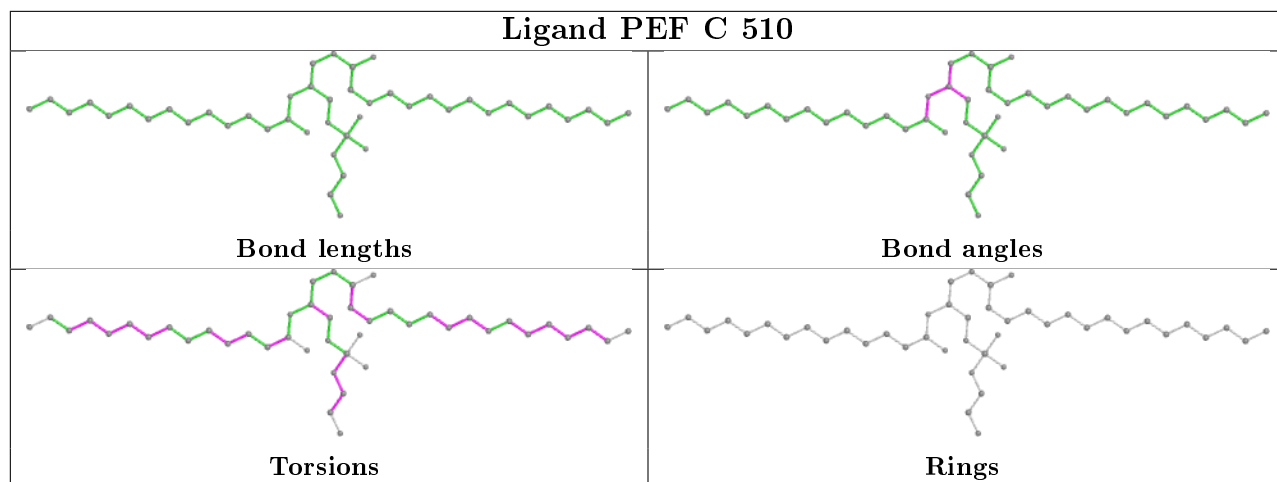
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	C	511	CDL	5	0
20	E	504	FES	1	0
12	A	514	PCF	9	0
13	A	521	UMQ	4	0
16	C	506	UQ6	11	0
18	C	510	PEF	3	0
14	C	501	HEM	3	0
15	C	505	SMA	4	0
14	C	502	HEM	1	0
17	C	508	PIE	2	0

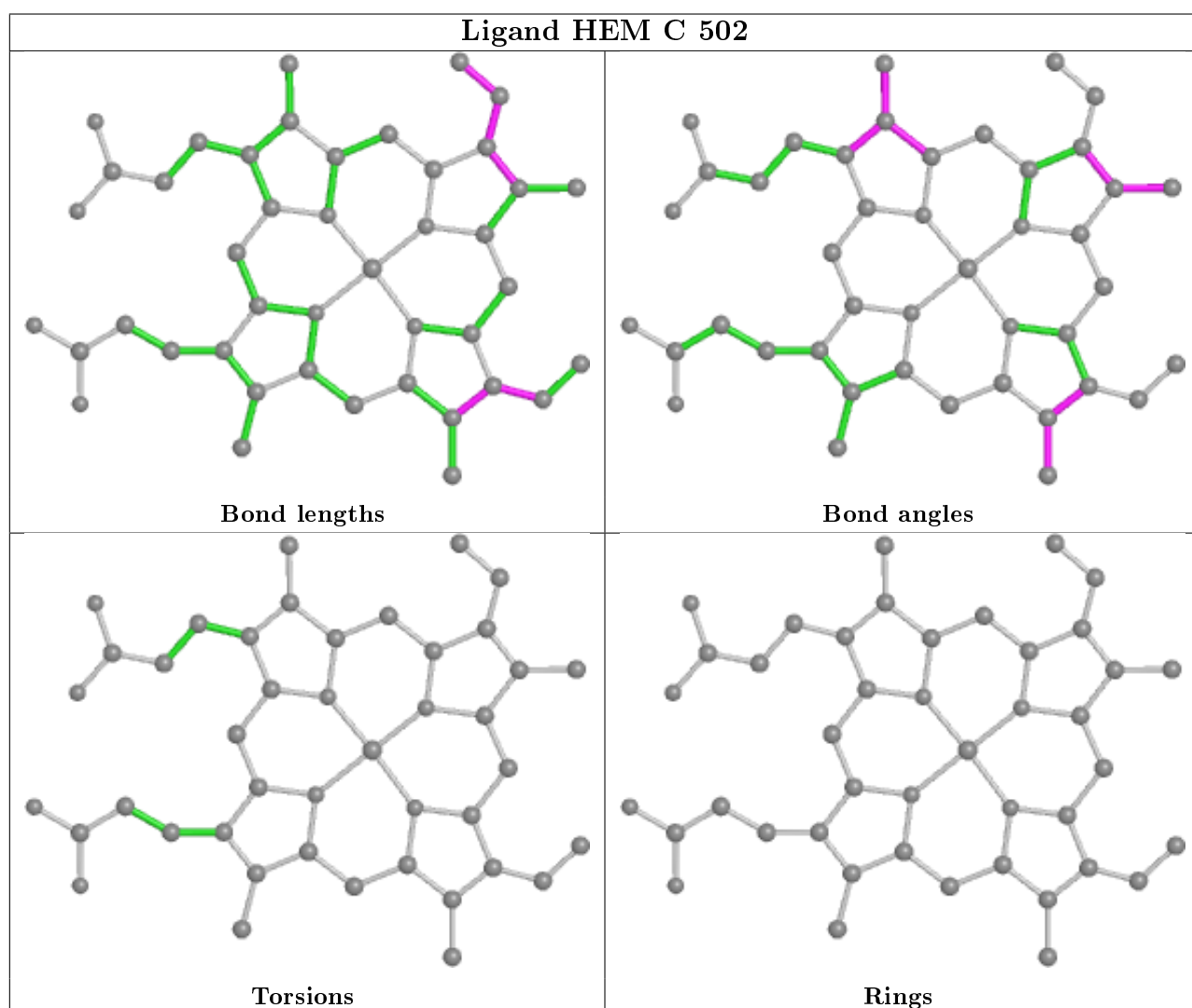
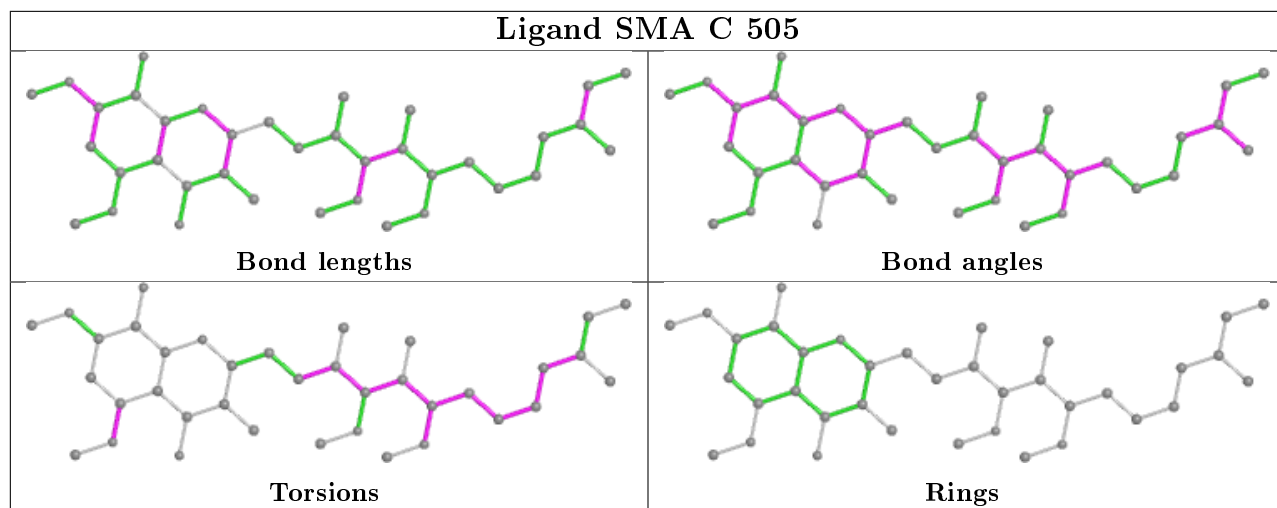
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

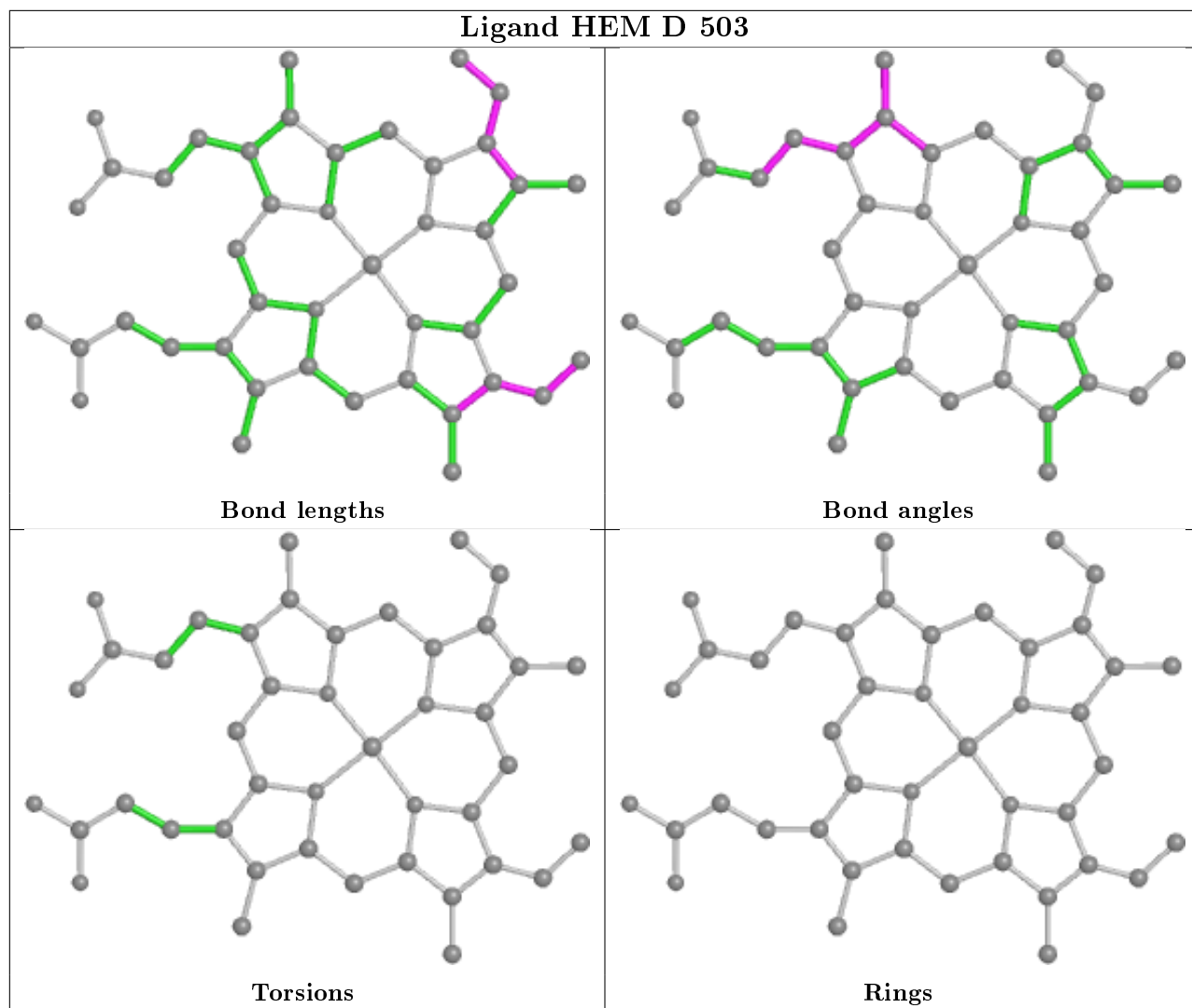
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents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

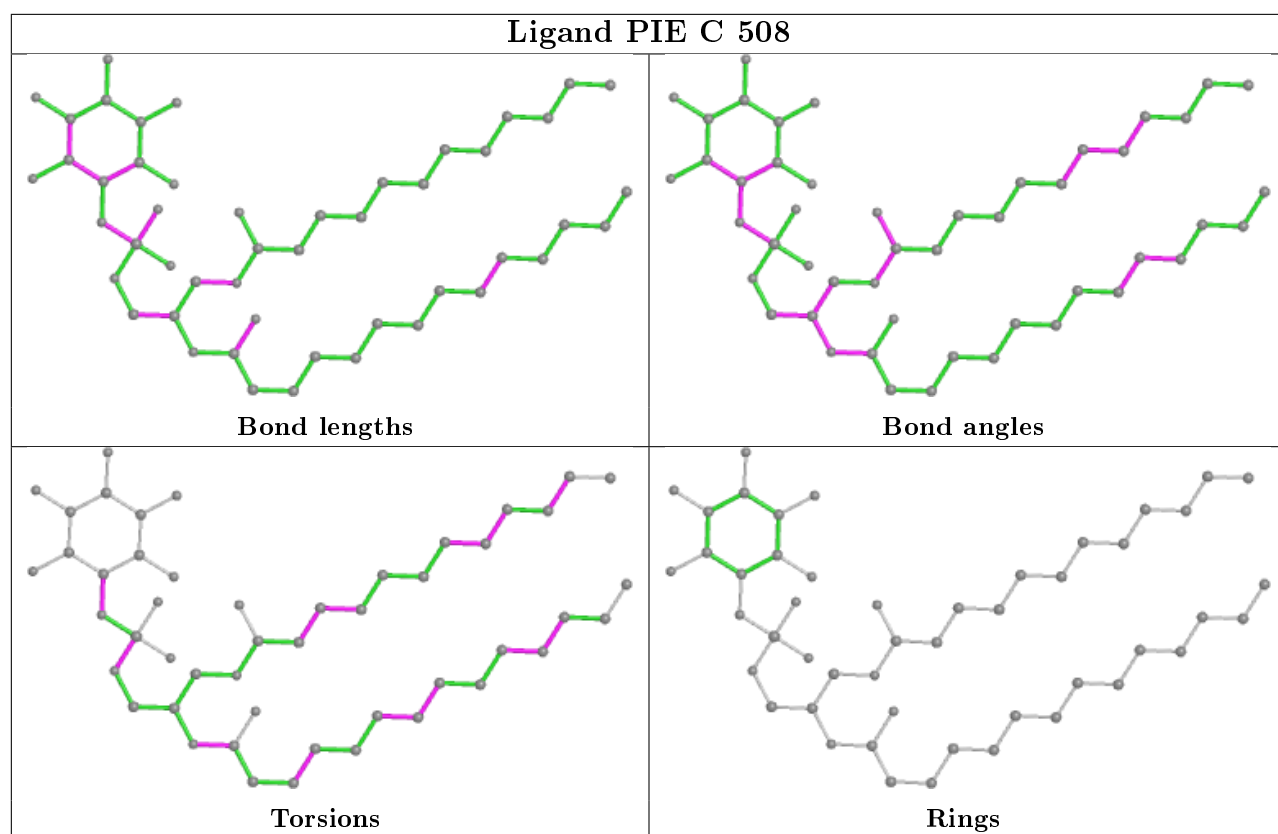












5.7 Other polymers [i](#)

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.