



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:16 PM UTC

PDB ID : 1KB9 / pdb_00001kb9
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

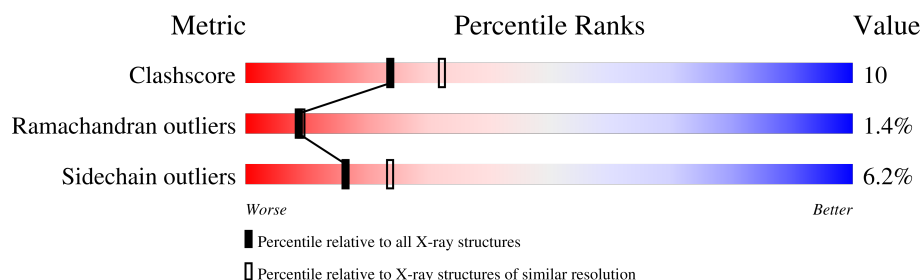
1 Overall quality at a glance

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	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (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 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	72% 25% .
2	B	352	63% 31% 6% .
3	C	385	81% 17% .
4	D	246	83% 15% .
5	E	185	75% 24% .
6	F	74	78% 18% .
7	G	125	81% 18% .
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
1	A	431	Total	C	N	O	S	0	0	0
			3343	2109	576	652	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
			2734	1747	453	533	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
			3088	2080	484	503	21			

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
4	D	246	Total	C	N	O	S	0	0	0
			1940	1237	334	360	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
			1410	893	242	265	10			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	125	Total	C	N	O	S	0	0	0
			1011	648	172	189	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
			772	510	131	129	2			

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

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

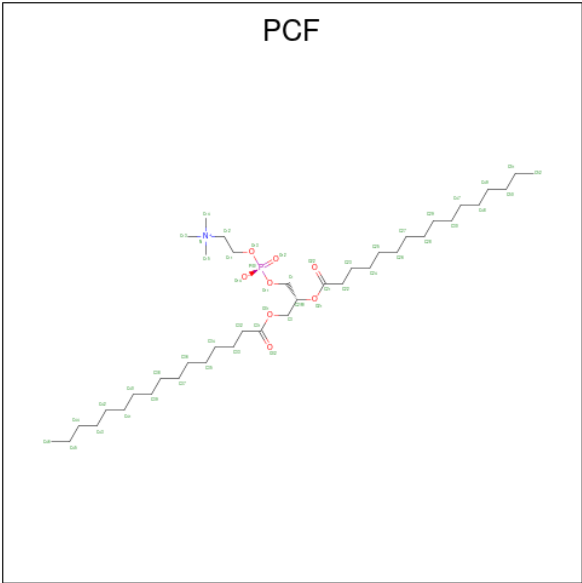
- Molecule 10 is a protein called HEAVY CHAIN (VH) OF FV-FRAGMENT.

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.

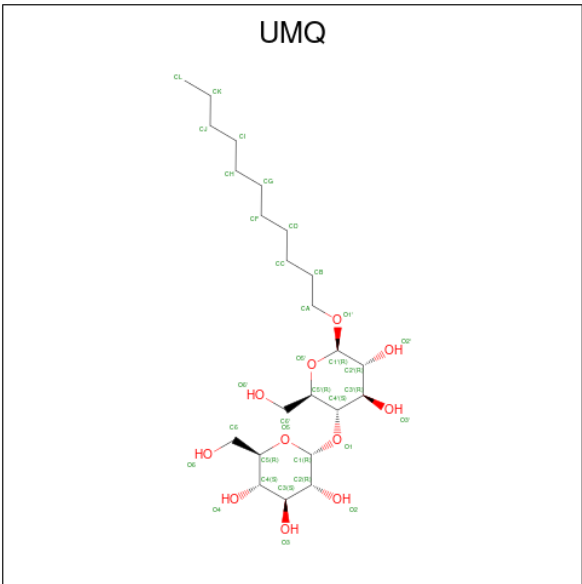
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	107	Total	C	N	O	S	0	0	0
			842	536	141	163	2			

- Molecule 12 is 1,2-DIACYL-SN-GLYCERO-3-PHOSHOCHOLINE (CCD ID: PCF) (formula: C₄₀H₈₀NO₈P).



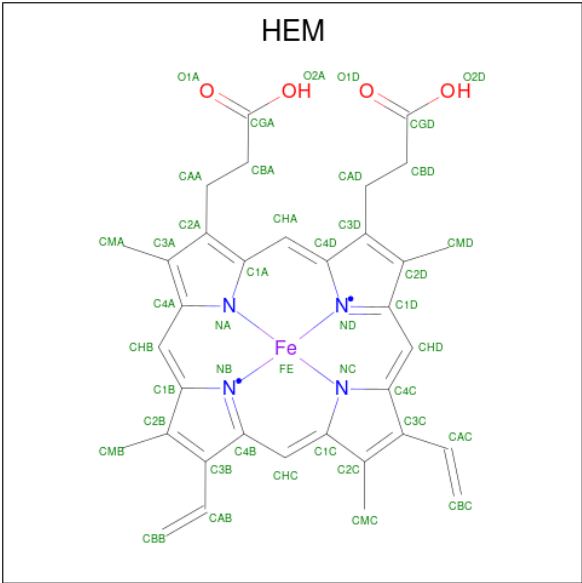
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	A	1	Total	C	N	O	P	0	0
			37	27	1	8	1		

- Molecule 13 is UNDECYL-MALTOSIDE (CCD ID: UMQ) (formula: C₂₃H₄₄O₁₁).



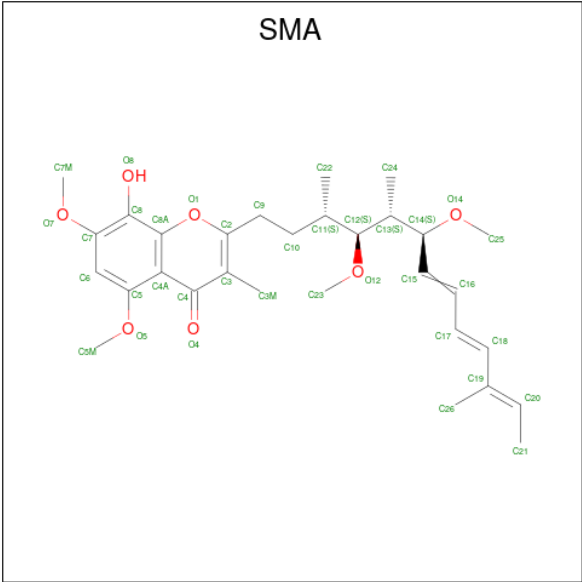
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	A	1	Total	C	O	0	0
			34	23	11		

- Molecule 14 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



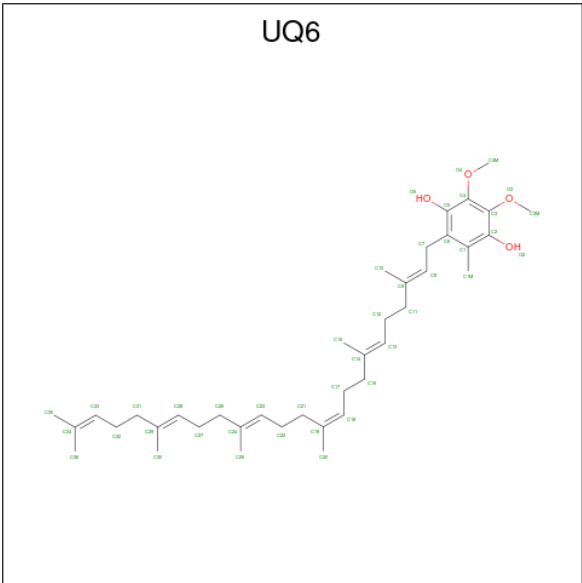
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
14	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
14	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 15 is STIGMATELLIN A (CCD ID: SMA) (formula: C₃₀H₄₂O₇).



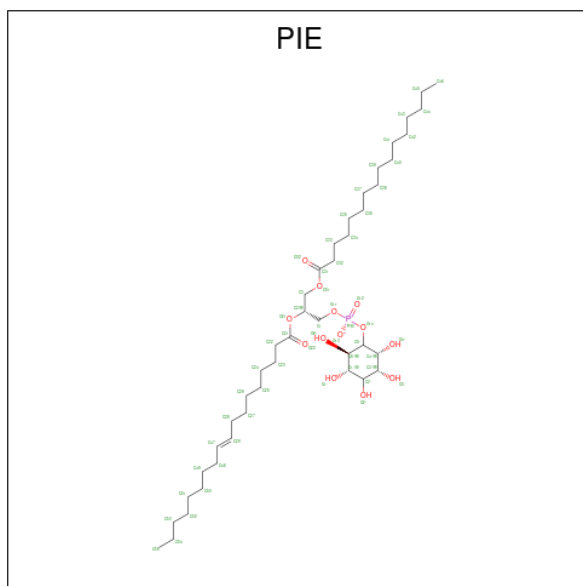
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	C	1	Total	C	O	0	0
			37	30	7		

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



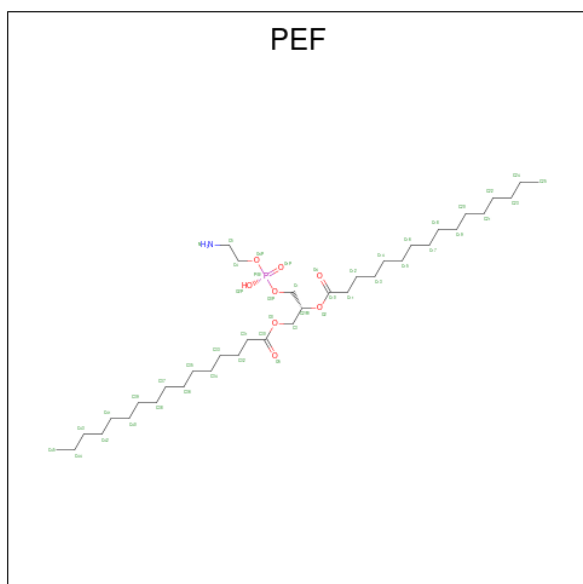
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	C	1	Total	C	O	0	0
			43	39	4		

- Molecule 17 is 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphoinositol (CCD ID: PIE) (formula:

$\text{C}_{43}\text{H}_{80}\text{O}_{13}\text{P}).$ 

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

- Molecule 18 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (CCD ID: PEF) (formula: $\text{C}_{37}\text{H}_{74}\text{NO}_8\text{P}$).



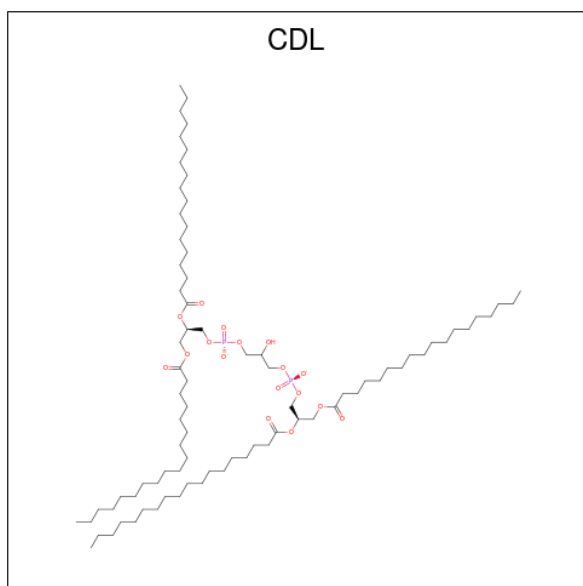
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	C	1	Total	C	N	O	P	0	0
			45	35	1	8	1		

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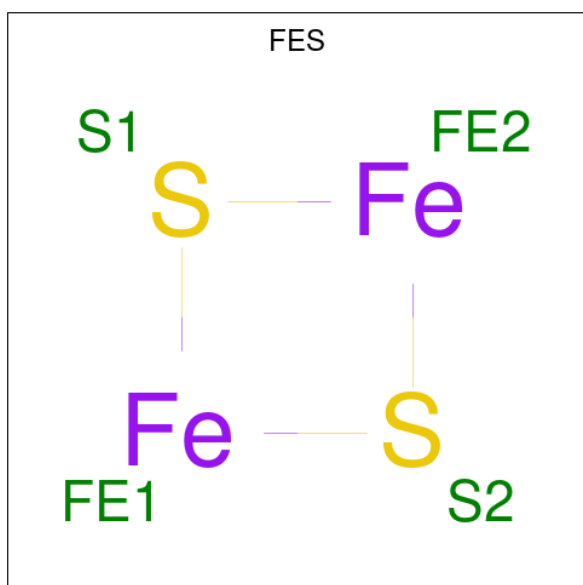
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	C	1	Total	C	N	O	P	0	0
			38	28	1	8	1		

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



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

- Molecule 20 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: 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.

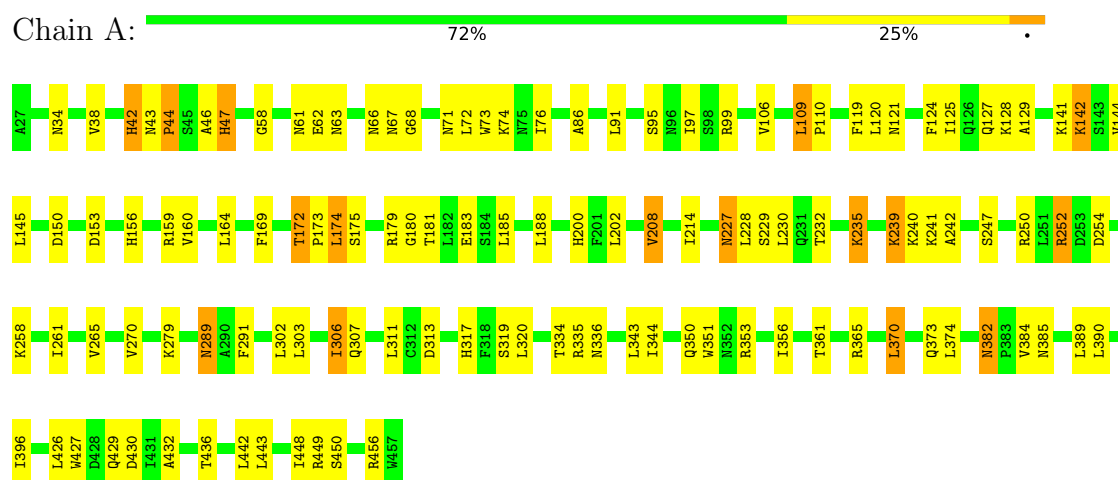
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	45	Total	O	0	0
			45	45		
21	B	9	Total	O	0	0
			9	9		
21	C	106	Total	O	0	0
			106	106		
21	D	67	Total	O	0	0
			67	67		
21	E	28	Total	O	0	0
			28	28		
21	F	7	Total	O	0	0
			7	7		
21	G	36	Total	O	0	0
			36	36		
21	H	14	Total	O	0	0
			14	14		
21	I	2	Total	O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

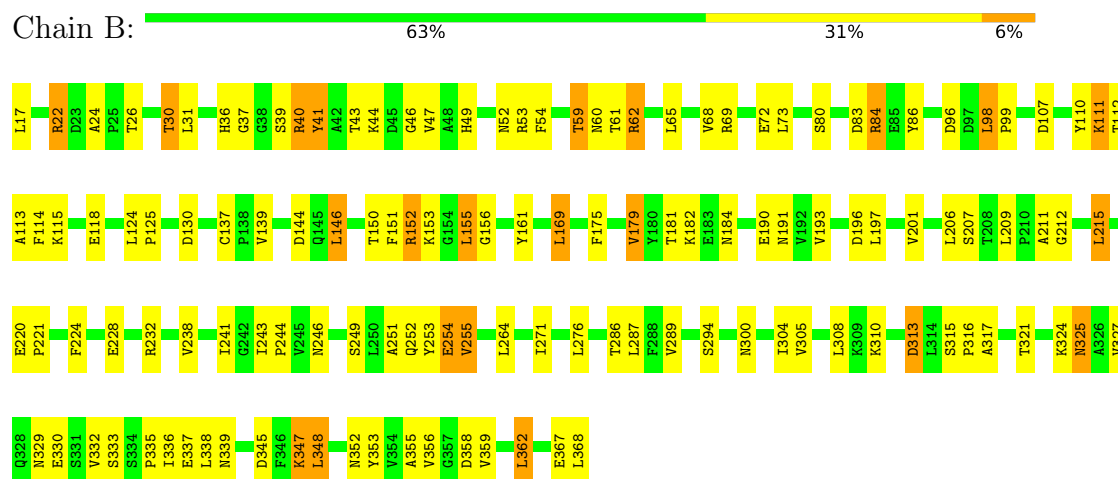
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

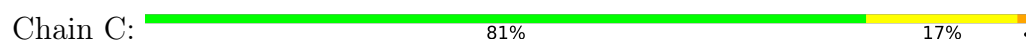
- Molecule 1: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX CORE PROTEIN I

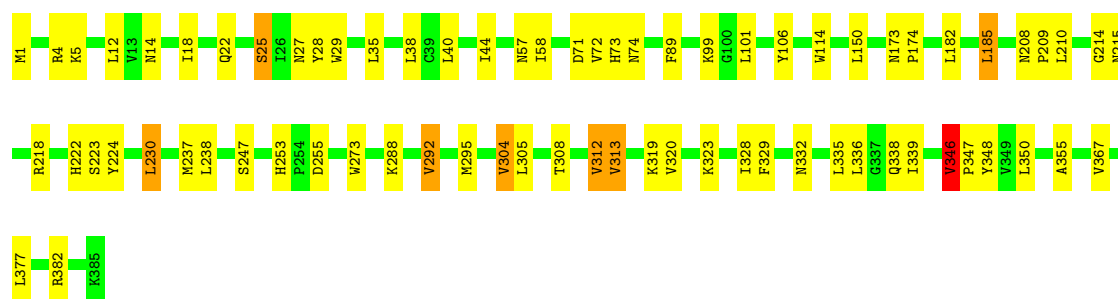


- Molecule 2: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX CORE PROTEIN 2



- Molecule 3: CYTOCHROME B





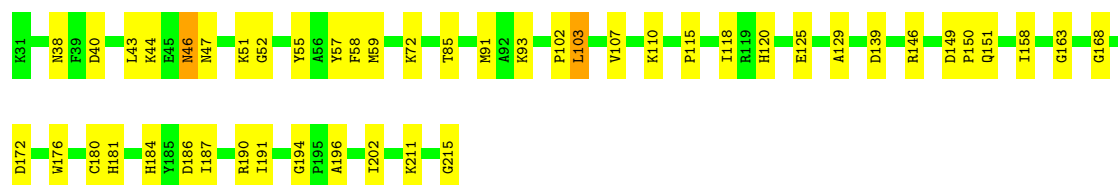
• Molecule 4: CYTOCHROME C1, HEME PROTEIN

Chain D: 83% 15% .



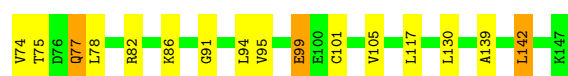
• Molecule 5: UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT

Chain E: 75% 24% .



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

Chain F: 78% 18% .



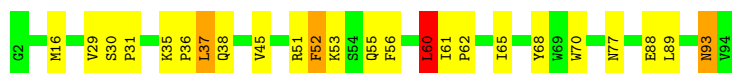
• Molecule 7: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 14 KD PROTEIN

Chain G: 81% 18% .

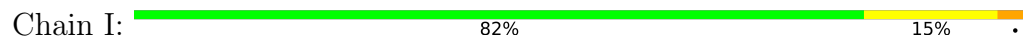


• Molecule 8: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX UBIQUINONE-BINDING PROTEIN QP-C

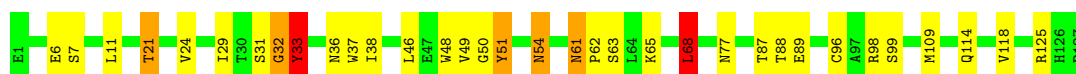
Chain H: 74% 22% . .



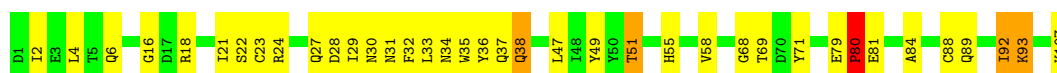
• Molecule 9: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 7.3 KD PROTEIN



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



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



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	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.	Xtriage
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, FES, PEF, PCF, UQ6, CDL, SMA, PIE, HEM

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	0.40	0/3404	0.90	5/4614 (0.1%)
2	B	0.37	0/2780	0.92	9/3764 (0.2%)
3	C	0.57	1/3190 (0.0%)	1.04	14/4353 (0.3%)
4	D	0.44	0/2001	0.99	6/2726 (0.2%)
5	E	0.43	0/1443	0.97	7/1957 (0.4%)
6	F	0.35	0/637	0.88	1/858 (0.1%)
7	G	0.43	0/1031	0.93	4/1397 (0.3%)
8	H	0.42	0/803	0.89	2/1088 (0.2%)
9	I	0.41	0/462	0.80	0/622
10	J	0.37	0/1043	0.89	6/1422 (0.4%)
11	K	0.37	0/863	0.82	0/1172
All	All	0.44	1/17657 (0.0%)	0.94	54/23973 (0.2%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	367	VAL	CA-CB	6.03	1.57	1.54

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	108	ASP	N-CA-C	7.91	121.88	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	179	VAL	N-CA-C	7.51	118.31	110.72
4	D	101	CYS	N-CA-C	7.48	119.07	111.07
3	C	346	VAL	N-CA-C	7.38	124.83	108.88
5	E	47	ASN	N-CA-C	-7.38	104.79	114.31
3	C	247	SER	CA-C-N	7.34	127.04	119.56
3	C	247	SER	C-N-CA	7.34	127.04	119.56
5	E	163	GLY	N-CA-C	6.81	124.71	115.32
4	D	83	GLU	N-CA-C	6.74	120.23	109.24
5	E	139	ASP	CA-C-N	6.71	128.22	119.84
5	E	139	ASP	C-N-CA	6.71	128.22	119.84
3	C	328	ILE	N-CA-C	-6.67	103.98	110.72
8	H	60	LEU	N-CA-C	6.43	117.95	111.07
2	B	359	VAL	N-CA-C	6.39	117.07	110.36
2	B	310	LYS	N-CA-C	-6.39	102.80	111.55
7	G	25	CYS	N-CA-C	6.25	119.03	111.40
3	C	273	TRP	N-CA-C	6.18	118.81	111.33
10	J	31	SER	N-CA-C	6.07	117.89	111.28
2	B	111	LYS	N-CA-C	6.06	120.69	109.24
2	B	84	ARG	N-CA-C	-6.01	105.43	112.89
1	A	427	TRP	N-CA-C	6.01	117.81	109.15
3	C	25	SER	N-CA-C	5.97	120.69	113.17
2	B	113	ALA	N-CA-C	5.93	118.50	111.33
3	C	346	VAL	CA-C-N	-5.92	112.48	119.05
3	C	346	VAL	C-N-CA	-5.92	112.48	119.05
10	J	32	GLY	N-CA-C	5.82	126.98	113.18
1	A	356	ILE	N-CA-C	5.77	121.34	109.34
3	C	320	VAL	N-CA-C	5.74	115.93	110.42
10	J	68	LEU	N-CA-C	5.70	117.42	110.41
10	J	36	ASN	N-CA-C	5.64	119.16	110.42
10	J	65	LYS	N-CA-C	5.61	118.92	111.75
2	B	155	LEU	N-CA-C	-5.56	106.27	113.16
3	C	185	LEU	N-CA-C	5.53	117.11	111.14
4	D	251	VAL	CB-CA-C	-5.42	104.82	112.14
7	G	87	LEU	N-CA-C	-5.40	101.32	109.85
3	C	348	TYR	N-CA-C	5.39	117.15	111.28
3	C	224	TYR	N-CA-C	5.39	117.59	111.02
8	H	53	LYS	N-CA-C	-5.38	106.56	113.23
1	A	334	THR	N-CA-C	5.38	117.43	108.99
6	F	142	LEU	N-CA-C	5.37	117.83	111.33
4	D	208	LEU	CA-C-N	5.37	123.58	119.66
4	D	208	LEU	C-N-CA	5.37	123.58	119.66
5	E	180	CYS	N-CA-C	5.36	116.80	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	44	LYS	N-CA-C	-5.32	101.49	109.95
5	E	194	GLY	CA-C-N	5.28	124.89	119.56
5	E	194	GLY	C-N-CA	5.28	124.89	119.56
1	A	382	ASN	CA-C-N	5.18	124.98	119.28
1	A	382	ASN	C-N-CA	5.18	124.98	119.28
3	C	215	ASN	N-CA-C	5.18	118.70	112.38
2	B	59	THR	N-CA-C	-5.15	102.39	110.17
10	J	33	TYR	N-CA-C	5.13	121.73	110.80
3	C	71	ASP	N-CA-C	5.08	119.61	113.41
7	G	51	GLU	N-CA-C	5.08	119.63	113.38
2	B	96	ASP	N-CA-C	5.06	118.95	112.87

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	3343	0	3321	76	0
2	B	2734	0	2774	81	0
3	C	3088	0	3125	42	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	23	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	C	37	0	40	7	0
16	C	43	0	58	10	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
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	353	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 (353) 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
2:B:347:LYS:H	2:B:347:LYS:HD3	1.37	0.88
1:A:317:HIS:HE1	1:A:351:TRP:HE1	1.25	0.85
3:C:237:MET:HE2	17:C:508:PIE:H291	1.58	0.84
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:H372	18:C:510:PEF:H181	1.71	0.73
2:B:182:LYS:HB2	2:B:211:ALA:HB2	1.71	0.72
3:C:218:ARG:HG3	8:H:16:MET:HE3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:115:PRO:HD2	5:E:158:ILE:HD11	1.69	0.72
16:C:506:UQ6:C1M	16:C:506:UQ6:H103	2.20	0.71
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
1:A:74:LYS:HG3	1:A:95:SER:HB3	1.71	0.71
16:C:506:UQ6:H103	16:C:506:UQ6:H1M2	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
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
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:O13	12:A:514:PCF:H152	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:HD22	10:J:54:ASN:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:44:ILE:HD12	16:C:506:UQ6:C20	2.31	0.59
1:A:289:ASN:C	1:A:289:ASN:HD22	2.10	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
5:E:58:PHE:HD2	5:E:59:MET:HE2	1.69	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
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
1:A:229:SER:HB3	1:A:232:THR:HB	1.86	0.56
2:B:44:LYS:HB2	2:B:47:VAL:HG21	1.87	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:58:GLY:H	1:A:61:ASN:HD22	1.54	0.55
1:A:270:VAL:HG21	1:A:396:ILE:HD13	1.88	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
2:B:252:GLN:O	2:B:255:VAL:HG22	2.07	0.55
3:C:295:MET:HE3	15:C:505:SMA:C23	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:127:GLN:C	1:A:129:ALA:H	2.16	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:HBC2	14:C:502:HEM:HMC2	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:H39	15:C:505:SMA:H21	1.91	0.52
4:D:203:PRO:HG2	4:D:206:VAL:HG21	1.91	0.52
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:HB2	1:A:142:LYS:NZ	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:4:LEU:HD23	11:K:88:CYS:SG	2.51	0.51
11:K:47:LEU:HA	11:K:58:VAL:HG11	1.93	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
10:J:51:TYR:C	10:J:51:TYR:CD2	2.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD12	11:K:2:ILE:H	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:68:GLY:HA3	1:A:185:LEU:CD1	2.41	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:373:GLN:HG3	1:A:374:LEU:N	2.26	0.49
12:A:514:PCF:H402	17:C:508:PIE:H382	1.93	0.49
3:C:27:ASN:HB2	19:C:511:CDL:OB3	2.11	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
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
10:J:61:ASN:HD22	10:J:61:ASN:C	2.20	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:H11	12:A:514:PCF:H153	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
16:C:506:UQ6:H103	16:C:506:UQ6:H1M3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:46:ALA:O	1:A:47:HIS:HB2	2.15	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
10:J:49:VAL:CG1	10:J:68:LEU:HD23	2.45	0.47
11:K:4:LEU:CD2	11:K:88:CYS:SG	3.02	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:39:SER:OG	2:B:84:ARG:HD3	2.16	0.46
2:B:197:LEU:O	2:B:201:VAL:HG23	2.15	0.46
2:B:355:ALA:HB1	2:B:362:LEU:HD23	1.98	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:HH21	1:A:179:ARG:HG2	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:111:ALA:HA	4:D:154:TYR:HA	1.97	0.46
4:D:121:THR:OG1	4:D:124:GLU:HG3	2.16	0.46
5:E:38:ASN:HD21	5:E:40:ASP:CG	2.23	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:HB3	2:B:232:ARG:HH21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:279:LYS:HG3	1:A:319:SER:HB3	1.98	0.45
2:B:252:GLN:HG3	2:B:253:TYR:N	2.31	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:37:GLY:HA3	2:B:179:VAL:HG11	1.99	0.45
2:B:155:LEU:N	2:B:155:LEU:HD12	2.31	0.45
4:D:304:PRO:HA	4:D:305:PRO:HD3	1.81	0.45
10:J:51:TYR:C	10:J:51:TYR:HD2	2.25	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
19:C:511:CDL:H112	19:C:511:CDL:HA4	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
3:C:295:MET:HE3	15:C:505:SMA:H33	1.98	0.45
3:C:27:ASN:OD1	3:C:29:TRP:HB2	2.17	0.44
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
1:A:200:HIS:C	1:A:202:LEU:H	2.25	0.44
10:J:6:GLU:H	10:J:114:GLN:HE21	1.66	0.44
12:A:514:PCF:H11	12:A:514:PCF:C15	2.48	0.44
2:B:254:GLU:HG2	2:B:276:LEU:HD23	1.98	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:ILE:C	1:A:306:ILE:HD12	2.43	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:36:HIS:HB2	2:B:184:ASN:OD1	2.19	0.43
2:B:251:ALA:O	2:B:255:VAL:HG13	2.18	0.43
3:C:332:ASN:HD21	3:C:355:ALA:HA	1.84	0.43
15:C:505:SMA:H36	15:C:505:SMA:H14	2.01	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
1:A:169:PHE:O	1:A:175:SER:HB3	2.18	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
1:A:247:SER:O	1:A:432:ALA:HA	2.19	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:HD12	3:C:230:LEU:HA	1.89	0.42
3:C:312:VAL:HG21	7:G:5:PHE:CE1	2.54	0.42
15:C:505:SMA:H36	15:C:505:SMA:C10	2.49	0.42
7:G:53:ASN:HD21	7:G:56:MET:H	1.68	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:H121	16:C:506:UQ6:H101	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:95:VAL:O	6:F:99:GLU:HB2	2.20	0.42
2:B:347:LYS:HD3	2:B:347:LYS:N	2.15	0.41
3:C:288:LYS:O	3:C:292:VAL:HG13	2.20	0.41
15:C:505:SMA:H39	15:C:505:SMA:C16	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:NZ	11:K:93:LYS:HB3	2.35	0.41
3:C:295:MET:HE3	15:C:505:SMA:H34	2.01	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
1:A:365:ARG:HH21	2:B:72:GLU:CD	2.28	0.41
2:B:59:THR:HA	2:B:112:THR:HA	2.02	0.41
2:B:347:LYS:HG2	2:B:348:LEU:H	1.84	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
1:A:250:ARG:NH1	1:A:442:LEU:O	2.54	0.41
1:A:370:LEU:O	1:A:374:LEU:HB2	2.21	0.41
19:C:511:CDL:H771	19:C:511:CDL:H802	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
4:D:256:ASN:C	4:D:256:ASN:HD22	2.29	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: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
2:B:241:ILE:HA	2:B:352:ASN:O	2.21	0.41
9:I:23:ALA:O	9:I:27:VAL:HG23	2.21	0.41
1:A:336:ASN:C	1:A:336:ASN:HD22	2.29	0.40
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:HD3	8:H:51:ARG:HA	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%)	14	17
2	B	350/352 (99%)	311 (89%)	31 (9%)	8 (2%)	5	4
3	C	383/385 (100%)	369 (96%)	12 (3%)	2 (0%)	24	31
4	D	244/246 (99%)	237 (97%)	7 (3%)	0	100	100
5	E	183/185 (99%)	171 (93%)	9 (5%)	3 (2%)	7	7
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%)	1	0
9	I	53/55 (96%)	50 (94%)	1 (2%)	2 (4%)	2	1
10	J	125/127 (98%)	111 (89%)	12 (10%)	2 (2%)	7	7
11	K	105/107 (98%)	89 (85%)	11 (10%)	5 (5%)	2	1
All	All	2158/2180 (99%)	2004 (93%)	123 (6%)	31 (1%)	9	9

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
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 ⓘ

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%)	12	16
2	B	301/301 (100%)	277 (92%)	24 (8%)	11	15
3	C	338/338 (100%)	318 (94%)	20 (6%)	18	26
4	D	204/204 (100%)	197 (97%)	7 (3%)	32	49
5	E	151/151 (100%)	146 (97%)	5 (3%)	33	50
6	F	67/67 (100%)	62 (92%)	5 (8%)	12	17
7	G	109/109 (100%)	102 (94%)	7 (6%)	16	23
8	H	77/77 (100%)	74 (96%)	3 (4%)	28	43
9	I	45/45 (100%)	43 (96%)	2 (4%)	25	38
10	J	112/112 (100%)	105 (94%)	7 (6%)	16	23
11	K	93/93 (100%)	86 (92%)	7 (8%)	12	17
All	All	1867/1867 (100%)	1752 (94%)	115 (6%)	16	24

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	42	HIS
1	A	47	HIS
1	A	109	LEU
1	A	120	LEU
1	A	142	LYS
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	183	GLU
1	A	208	VAL
1	A	227	ASN
1	A	235	LYS
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

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Mol	Chain	Res	Type
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	41	TYR
2	B	53	ARG
2	B	54	PHE
2	B	62	ARG
2	B	98	LEU
2	B	107	ASP
2	B	144	ASP
2	B	146	LEU
2	B	169	LEU
2	B	206	LEU
2	B	215	LEU
2	B	254	GLU
2	B	255	VAL
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	5	LYS
3	C	12	LEU
3	C	35	LEU
3	C	38	LEU
3	C	99	LYS
3	C	101	LEU
3	C	150	LEU
3	C	182	LEU
3	C	185	LEU
3	C	230	LEU
3	C	238	LEU
3	C	292	VAL
3	C	304	VAL

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Mol	Chain	Res	Type
3	C	305	LEU
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	268	ARG
4	D	280	LEU
4	D	283	LEU
5	E	46	ASN
5	E	51	LYS
5	E	91	MET
5	E	110	LYS
5	E	211	LYS
6	F	77	GLN
6	F	94	LEU
6	F	99	GLU
6	F	117	LEU
6	F	130	LEU
7	G	16	LEU
7	G	30	ASN
7	G	31	GLN
7	G	41	LEU
7	G	48	LEU
7	G	62	ARG
7	G	127	LYS
8	H	60	LEU
8	H	68	TYR
8	H	88	GLU
9	I	18	VAL
9	I	48	LEU
10	J	21	THR
10	J	51	TYR
10	J	54	ASN
10	J	61	ASN
10	J	68	LEU
10	J	89	GLU

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Mol	Chain	Res	Type
10	J	118	VAL
11	K	18	ARG
11	K	38	GLN
11	K	80	PRO
11	K	81	GLU
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 (71) 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	82	ASN
1	A	121	ASN
1	A	126	GLN
1	A	156	HIS
1	A	158	ASN
1	A	171	ASN
1	A	200	HIS
1	A	216	HIS
1	A	227	ASN
1	A	231	GLN
1	A	271	ASN
1	A	283	GLN
1	A	289	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
2	B	49	HIS
2	B	52	ASN
2	B	55	ASN
2	B	191	ASN
2	B	252	GLN
2	B	258	ASN

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Mol	Chain	Res	Type
2	B	325	ASN
3	C	14	ASN
3	C	22	GLN
3	C	43	GLN
3	C	57	ASN
3	C	173	ASN
3	C	177	GLN
3	C	208	ASN
3	C	253	HIS
3	C	332	ASN
4	D	78	HIS
4	D	79	ASN
4	D	127	ASN
5	E	38	ASN
5	E	97	ASN
5	E	106	ASN
5	E	124	HIS
5	E	151	GLN
5	E	184	HIS
6	F	77	GLN
7	G	31	GLN
7	G	53	ASN
7	G	79	HIS
7	G	91	ASN
7	G	97	GLN
9	I	14	ASN
9	I	29	GLN
9	I	42	ASN
10	J	54	ASN
10	J	59	ASN
10	J	61	ASN
10	J	77	ASN
10	J	78	GLN
10	J	114	GLN
10	J	126	HIS
11	K	31	ASN
11	K	34	ASN
11	K	55	HIS
11	K	89	GLN
11	K	90	HIS
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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	1.09	5 (6%)	81,87,111	1.15	5 (6%)
12	PCF	A	514	-	36,36,49	1.63	1 (2%)	42,44,57	1.29	2 (4%)
16	UQ6	C	506	-	43,43,43	2.49	14 (32%)	54,55,55	1.99	14 (25%)
18	PEF	C	513	-	37,37,46	0.72	0	40,42,51	0.98	1 (2%)
18	PEF	C	510	-	44,44,46	0.72	0	47,49,51	1.08	2 (4%)
13	UMQ	A	521	-	35,35,35	0.95	1 (2%)	46,46,46	1.45	7 (15%)
14	HEM	C	502	3	50,50,50	1.29	9 (18%)	67,82,82	0.70	0
20	FES	E	504	5	0,4,4	-	-	-	-	-
14	HEM	C	501	3	50,50,50	1.31	9 (18%)	67,82,82	1.08	3 (4%)
17	PIE	C	508	-	49,49,57	1.96	9 (18%)	58,61,69	1.40	9 (15%)
15	SMA	C	505	-	38,38,38	1.59	7 (18%)	47,52,52	2.05	11 (23%)
14	HEM	D	503	4	50,50,50	1.39	5 (10%)	67,82,82	0.97	3 (4%)

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	-	-	36/86/86/110	-
14	HEM	C	501	3	-	5/14/54/54	-
12	PCF	A	514	-	-	15/40/40/53	-
16	UQ6	C	506	-	-	14/39/39/39	0/1/1/1
18	PEF	C	513	-	-	13/41/41/50	-
18	PEF	C	510	-	-	23/48/48/50	-
13	UMQ	A	521	-	-	5/20/60/60	0/2/2/2
14	HEM	C	502	3	-	4/14/54/54	-
20	FES	E	504	5	-	-	0/1/1/1
15	SMA	C	505	-	2/2/5/10	21/34/34/34	0/2/2/2
17	PIE	C	508	-	-	16/44/68/76	0/1/1/1
14	HEM	D	503	4	-	6/14/54/54	-

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	C	508	PIE	P-O14	-9.20	1.31	1.59
12	A	514	PCF	O13-C11	-8.76	1.09	1.44
16	C	506	UQ6	C7-C6	6.62	1.59	1.51
16	C	506	UQ6	O5-C5	-5.66	1.23	1.36
16	C	506	UQ6	O2-C2	-5.45	1.24	1.36
14	D	503	HEM	CBB-CAB	4.80	1.53	1.30
16	C	506	UQ6	C2-C3	4.71	1.47	1.39
14	D	503	HEM	CBC-CAC	4.65	1.52	1.30
16	C	506	UQ6	C5-C4	4.41	1.46	1.39
17	C	508	PIE	C6'-C5'	4.25	1.63	1.52
17	C	508	PIE	C47-C29	4.25	1.55	1.31
16	C	506	UQ6	C5-C6	4.19	1.46	1.40
14	C	501	HEM	CMC-C2C	3.86	1.58	1.50
15	C	505	SMA	C4A-C8A	3.55	1.48	1.40
15	C	505	SMA	C20-C19	3.54	1.36	1.33
13	A	521	UMQ	C3-C2	-3.50	1.43	1.52
16	C	506	UQ6	C2-C1	3.47	1.46	1.40
14	C	502	HEM	FE-NB	3.38	2.05	1.94
17	C	508	PIE	C4'-C5'	3.36	1.61	1.52
15	C	505	SMA	C4A-C5	3.36	1.46	1.40
15	C	505	SMA	C13-C12	3.34	1.62	1.54
19	C	511	CDL	OB2-CB2	-3.26	1.32	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	C	511	CDL	OA8-CA6	-3.13	1.38	1.45
17	C	508	PIE	C6'-C1'	3.12	1.60	1.52
16	C	506	UQ6	C23-C24	2.94	1.39	1.33
16	C	506	UQ6	C28-C29	2.90	1.39	1.33
19	C	511	CDL	OA6-CA4	-2.88	1.39	1.46
14	C	501	HEM	CAB-C3B	-2.85	1.39	1.47
14	C	502	HEM	FE-NA	2.79	2.04	1.95
16	C	506	UQ6	C18-C19	2.77	1.39	1.33
14	C	501	HEM	CAC-C3C	-2.71	1.40	1.47
16	C	506	UQ6	C8-C9	2.68	1.39	1.33
14	C	502	HEM	FE-NC	2.66	2.03	1.95
16	C	506	UQ6	C33-C34	2.65	1.40	1.32
17	C	508	PIE	O31-C3	-2.64	1.39	1.45
14	D	503	HEM	FE-NA	2.63	2.03	1.95
16	C	506	UQ6	C13-C14	2.63	1.39	1.33
15	C	505	SMA	C6-C7	2.54	1.43	1.38
14	C	502	HEM	CBC-CAC	2.52	1.42	1.30
14	C	501	HEM	FE-ND	2.46	2.02	1.94
14	C	501	HEM	CBC-CAC	2.42	1.42	1.30
15	C	505	SMA	O12-C12	-2.42	1.36	1.42
14	C	502	HEM	CBB-CAB	2.40	1.41	1.30
14	C	501	HEM	CMB-C2B	2.39	1.55	1.50
14	D	503	HEM	FE-NB	2.29	2.02	1.94
19	C	511	CDL	O1-C1	2.29	1.50	1.43
14	C	502	HEM	CMB-C2B	2.19	1.55	1.50
17	C	508	PIE	P-O13	-2.15	1.45	1.55
19	C	511	CDL	CA2-C1	2.14	1.58	1.51
14	C	501	HEM	O2A-CGA	-2.13	1.23	1.30
15	C	505	SMA	O7-C7	2.11	1.40	1.37
16	C	506	UQ6	C21-C19	2.08	1.55	1.51
14	C	502	HEM	CAB-C3B	-2.08	1.41	1.47
14	C	501	HEM	CBB-CAB	2.08	1.40	1.30
17	C	508	PIE	O22-C21	-2.06	1.16	1.22
14	C	502	HEM	CMA-C3A	2.04	1.55	1.50
17	C	508	PIE	C1-C2	2.03	1.57	1.50
14	C	501	HEM	FE-NC	2.03	2.01	1.95
14	D	503	HEM	FE-NC	2.02	2.01	1.95
14	C	502	HEM	O2D-CGD	-2.02	1.24	1.30

All (57) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	C	506	UQ6	C3M-O3-C3	6.90	133.47	114.74
15	C	505	SMA	O14-C14-C15	6.49	129.90	111.05
15	C	505	SMA	C26-C19-C18	-6.42	108.28	118.09
12	A	514	PCF	C3-C2-C1	-5.71	98.47	111.78
13	A	521	UMQ	CA-O1'-C1'	-5.28	104.66	113.68
16	C	506	UQ6	C17-C18-C19	5.15	139.41	127.62
19	C	511	CDL	CB4-OB6-CB5	-4.94	105.98	117.80
15	C	505	SMA	O14-C14-C13	4.76	117.80	107.97
16	C	506	UQ6	C4M-O4-C4	4.61	127.26	114.74
17	C	508	PIE	C6'-C5'-C4'	-4.46	104.67	110.86
18	C	510	PEF	C2-O2-C10	-4.18	107.80	117.80
14	C	501	HEM	CMC-C2C-C1C	4.04	131.84	124.73
15	C	505	SMA	O12-C12-C13	4.01	113.88	107.97
18	C	513	PEF	C2-O2-C10	-3.90	108.45	117.80
17	C	508	PIE	C38-C37-C36	-3.60	96.18	114.37
17	C	508	PIE	C3-C2-C1	-3.56	103.48	111.78
14	D	503	HEM	CBB-CAB-C3B	-3.42	110.44	127.53
15	C	505	SMA	O7-C7-C8	3.36	118.05	114.53
19	C	511	CDL	CA6-CA4-CA3	-3.31	104.08	111.78
14	D	503	HEM	CBC-CAC-C3C	-3.19	111.60	127.53
16	C	506	UQ6	C1M-C1-C2	-3.02	115.49	120.52
13	A	521	UMQ	C3'-C4'-C5'	-3.01	104.26	110.93
19	C	511	CDL	CB6-CB4-CB3	-2.97	104.87	111.78
14	C	501	HEM	CMC-C2C-C3C	-2.90	121.41	128.43
15	C	505	SMA	C18-C19-C20	2.89	126.23	118.55
16	C	506	UQ6	C22-C23-C24	2.89	134.23	127.62
19	C	511	CDL	CA4-OA6-CA5	-2.87	110.92	117.80
16	C	506	UQ6	C27-C28-C29	2.82	134.07	127.62
16	C	506	UQ6	C21-C19-C18	2.69	127.20	121.17
14	D	503	HEM	CAC-C3C-C4C	-2.66	118.47	124.82
13	A	521	UMQ	O1'-C1'-C2'	2.61	112.24	108.27
13	A	521	UMQ	O1-C1-O5	-2.54	104.02	110.69
17	C	508	PIE	C39-C38-C37	2.48	126.88	114.37
14	C	501	HEM	CAC-C3C-C4C	2.47	130.71	124.82
17	C	508	PIE	O14-P-O12	-2.39	102.16	109.81
12	A	514	PCF	P-O13-C11	2.38	132.57	121.26
13	A	521	UMQ	O1'-CA-CB	2.35	117.35	109.37
16	C	506	UQ6	C30-C29-C31	-2.34	111.16	115.23
17	C	508	PIE	C2-O21-C21	-2.28	112.33	117.80
13	A	521	UMQ	C1'-C2'-C3'	-2.27	105.24	110.01
17	C	508	PIE	C48-C47-C29	-2.25	107.99	124.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	C	506	UQ6	C1M-C1-C6	2.24	123.66	120.43
15	C	505	SMA	O7-C7-C6	-2.24	120.22	124.08
18	C	510	PEF	C3-C2-C1	2.24	117.00	111.78
16	C	506	UQ6	C25-C24-C26	-2.20	111.41	115.23
15	C	505	SMA	C4A-C4-C3	-2.20	115.55	118.78
13	A	521	UMQ	C6'-C5'-C4'	-2.18	107.25	113.38
17	C	508	PIE	O31-C31-O32	2.18	129.07	123.63
17	C	508	PIE	O13-P-O12	-2.17	102.36	112.44
15	C	505	SMA	O1-C8A-C8	2.15	120.54	116.28
16	C	506	UQ6	C20-C19-C18	-2.10	118.22	123.63
15	C	505	SMA	C11-C12-C13	-2.09	108.70	114.29
16	C	506	UQ6	C6-C7-C8	2.09	115.63	112.06
16	C	506	UQ6	C11-C9-C8	2.05	125.77	121.17
19	C	511	CDL	CB6-OB8-CB7	-2.05	109.64	117.12
15	C	505	SMA	O1-C2-C9	2.03	114.42	110.12
16	C	506	UQ6	C36-C34-C35	-2.02	109.94	114.59

All (2) chirality outliers are listed below:

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

All (158) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	514	PCF	C11-O13-P-O11
12	A	514	PCF	C11-O13-P-O12
14	D	503	HEM	C2C-C3C-CAC-CBC
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	C13-C14-C15-C16
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
16	C	506	UQ6	C24-C26-C27-C28
17	C	508	PIE	C1-O11-P-O12
17	C	508	PIE	C1-O11-P-O13
17	C	508	PIE	C1-O11-P-O14
17	C	508	PIE	C4'-C5'-O14-P

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Mol	Chain	Res	Type	Atoms
18	C	510	PEF	O4P-C4-C5-N
18	C	513	PEF	O4P-C4-C5-N
18	C	513	PEF	C1-O3P-P-O4P
19	C	511	CDL	CA2-OA2-PA1-OA3
19	C	511	CDL	CA2-OA2-PA1-OA4
19	C	511	CDL	CA2-OA2-PA1-OA5
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	CB2-OB2-PB2-OB5
19	C	511	CDL	OB5-CB3-CB4-OB6
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
16	C	506	UQ6	C20-C19-C21-C22
18	C	510	PEF	C36-C37-C38-C39
13	A	521	UMQ	O1'-CA-CB-CC
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	C33-C34-C35-C36
16	C	506	UQ6	C18-C19-C21-C22
15	C	505	SMA	C17-C18-C19-C26
15	C	505	SMA	C17-C18-C19-C20
19	C	511	CDL	C77-C78-C79-C80
17	C	508	PIE	C22-C21-O21-C2
18	C	513	PEF	C14-C15-C16-C17
18	C	510	PEF	C30-C31-C32-C33
12	A	514	PCF	C21-C22-C23-C24
18	C	513	PEF	C10-C11-C12-C13
18	C	513	PEF	C30-C31-C32-C33
17	C	508	PIE	C36-C37-C38-C39
19	C	511	CDL	O1-C1-CB2-OB2
17	C	508	PIE	C31-C32-C33-C34
17	C	508	PIE	O22-C21-O21-C2
19	C	511	CDL	CA2-C1-CB2-OB2
13	A	521	UMQ	C2'-C1'-O1'-CA
16	C	506	UQ6	C19-C21-C22-C23
13	A	521	UMQ	O5'-C1'-O1'-CA

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Mol	Chain	Res	Type	Atoms
12	A	514	PCF	C22-C21-O21-C2
13	A	521	UMQ	CF-CG-CH-CI
18	C	510	PEF	C40-C41-C42-C43
19	C	511	CDL	C74-C75-C76-C77
12	A	514	PCF	O22-C21-O21-C2
12	A	514	PCF	C35-C36-C37-C38
18	C	513	PEF	C31-C32-C33-C34
15	C	505	SMA	C6-C5-O5-C5M
12	A	514	PCF	C36-C37-C38-C39
12	A	514	PCF	C38-C39-C40-C41
19	C	511	CDL	C78-C79-C80-C81
19	C	511	CDL	C83-C84-C85-C86
18	C	510	PEF	C16-C17-C18-C19
18	C	513	PEF	C20-C21-C22-C23
17	C	508	PIE	C32-C33-C34-C35
18	C	510	PEF	C38-C39-C40-C41
18	C	510	PEF	C35-C36-C37-C38
18	C	513	PEF	C16-C17-C18-C19
15	C	505	SMA	C4A-C5-O5-C5M
18	C	510	PEF	C41-C42-C43-C44
19	C	511	CDL	C71-C72-C73-C74
18	C	513	PEF	C12-C13-C14-C15
15	C	505	SMA	C24-C13-C14-O14
16	C	506	UQ6	C4-C3-O3-C3M
17	C	508	PIE	C37-C38-C39-C40
15	C	505	SMA	C12-C13-C14-C15
19	C	511	CDL	C80-C81-C82-C83
19	C	511	CDL	OA5-CA3-CA4-CA6
19	C	511	CDL	OB5-CB3-CB4-CB6
15	C	505	SMA	C22-C11-C12-O12
18	C	510	PEF	C12-C13-C14-C15
18	C	510	PEF	C18-C19-C20-C21
12	A	514	PCF	C33-C34-C35-C36
19	C	511	CDL	C81-C82-C83-C84
18	C	510	PEF	C42-C43-C44-C45
13	A	521	UMQ	CI-CJ-CK-CL
19	C	511	CDL	C12-C13-C14-C15
17	C	508	PIE	C26-C27-C28-C29
12	A	514	PCF	O11-C1-C2-C3
19	C	511	CDL	C31-C32-C33-C34
18	C	510	PEF	C15-C16-C17-C18
12	A	514	PCF	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
17	C	508	PIE	C25-C26-C27-C28
18	C	513	PEF	O3P-C1-C2-C3
14	D	503	HEM	C2B-C3B-CAB-CBB
19	C	511	CDL	C17-C18-C19-C20
15	C	505	SMA	C11-C12-C13-C14
19	C	511	CDL	C52-C53-C54-C55
18	C	510	PEF	O3P-C1-C2-O2
18	C	513	PEF	O3P-C1-C2-O2
14	D	503	HEM	C4C-C3C-CAC-CBC
18	C	510	PEF	C5-C4-O4P-P
18	C	510	PEF	C17-C18-C19-C20
15	C	505	SMA	C24-C13-C14-C15
16	C	506	UQ6	C2-C3-O3-C3M
15	C	505	SMA	C9-C10-C11-C12
18	C	510	PEF	O3P-C1-C2-C3
17	C	508	PIE	C29-C47-C48-C49
12	A	514	PCF	C32-C33-C34-C35
18	C	510	PEF	C39-C40-C41-C42
18	C	513	PEF	C18-C19-C20-C21
12	A	514	PCF	C11-O13-P-O14
18	C	513	PEF	C1-O3P-P-O1P
19	C	511	CDL	CB2-OB2-PB2-OB3
12	A	514	PCF	C34-C35-C36-C37
19	C	511	CDL	C55-C56-C57-C58
17	C	508	PIE	C22-C23-C24-C25
18	C	510	PEF	C34-C35-C36-C37
18	C	510	PEF	C19-C20-C21-C22
16	C	506	UQ6	C3-C4-O4-C4M
14	D	503	HEM	CAA-CBA-CGA-O2A
15	C	505	SMA	C12-C13-C14-O14
17	C	508	PIE	C39-C40-C41-C42
18	C	510	PEF	C11-C12-C13-C14
14	D	503	HEM	CAA-CBA-CGA-O1A
19	C	511	CDL	C76-C77-C78-C79
14	C	502	HEM	CAA-CBA-CGA-O1A
12	A	514	PCF	C37-C38-C39-C40
14	C	501	HEM	C3D-CAD-CBD-CGD
16	C	506	UQ6	C9-C11-C12-C13
14	C	502	HEM	CAA-CBA-CGA-O2A
19	C	511	CDL	C54-C55-C56-C57
14	C	502	HEM	CAD-CBD-CGD-O2D
14	C	501	HEM	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
17	C	508	PIE	C47-C48-C49-C50
14	C	501	HEM	CAA-CBA-CGA-O2A
15	C	505	SMA	C10-C11-C12-O12
14	C	501	HEM	CAA-CBA-CGA-O1A
16	C	506	UQ6	C26-C27-C28-C29
16	C	506	UQ6	C5-C4-O4-C4M
14	C	501	HEM	CAD-CBD-CGD-O1D
14	D	503	HEM	C4B-C3B-CAB-CBB
19	C	511	CDL	C11-C12-C13-C14
14	C	502	HEM	CAD-CBD-CGD-O1D
18	C	510	PEF	O2-C10-C11-C12
18	C	510	PEF	O3-C30-C31-C32
19	C	511	CDL	C12-C11-CA5-OA6
18	C	510	PEF	O4-C10-C11-C12
19	C	511	CDL	C32-C31-CA7-OA8
19	C	511	CDL	CA7-C31-C32-C33

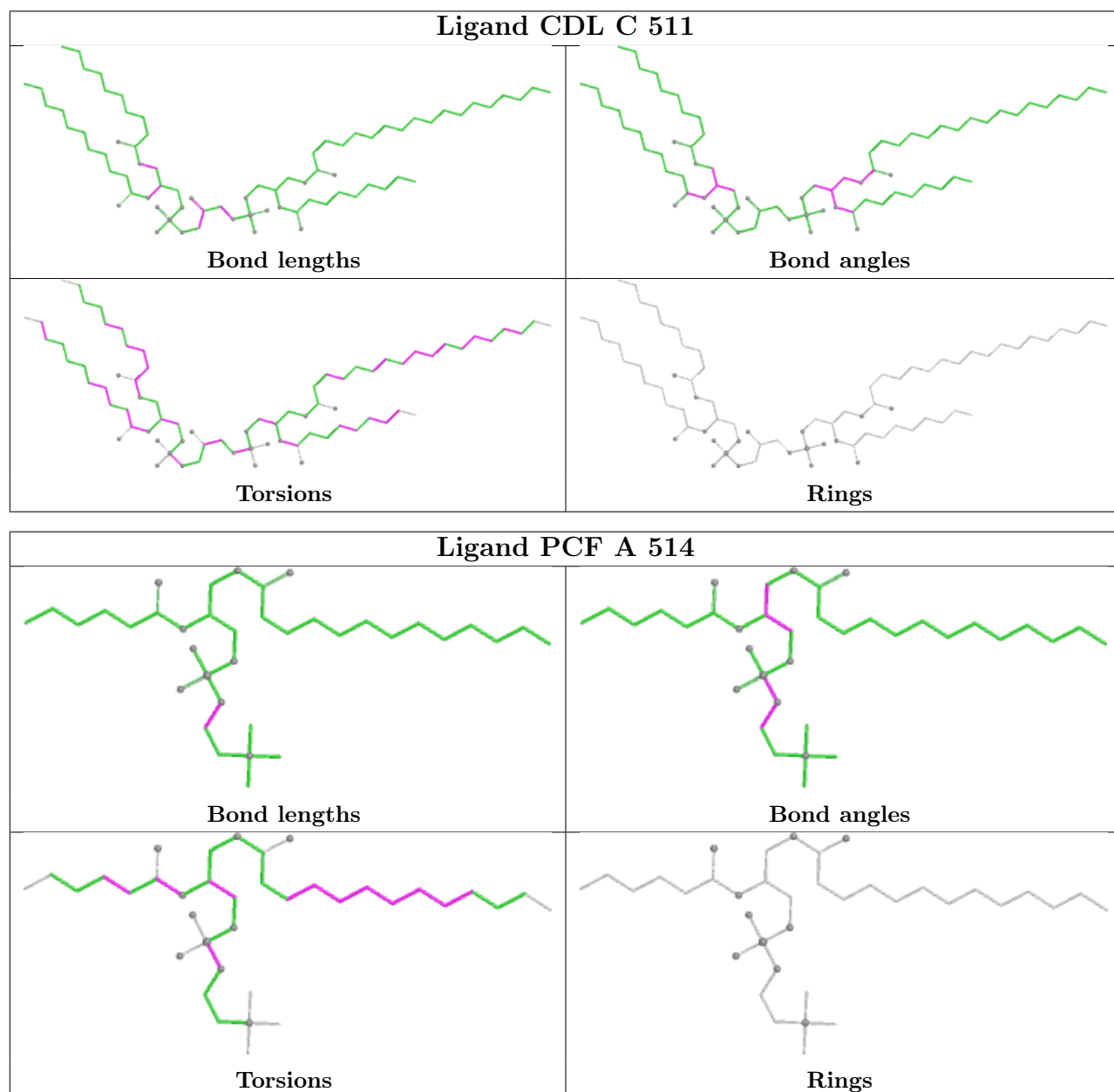
There are no ring outliers.

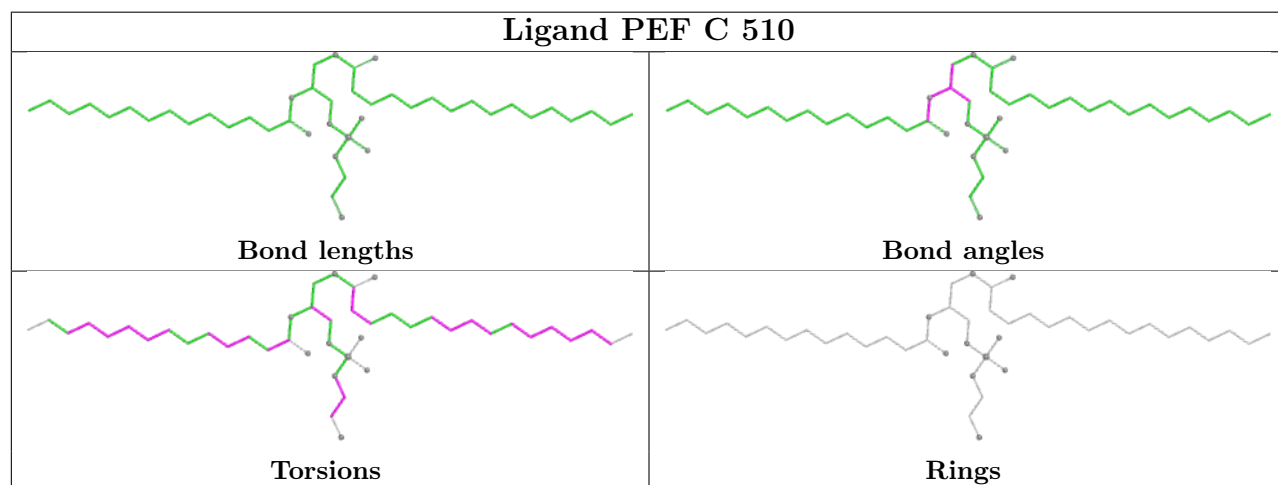
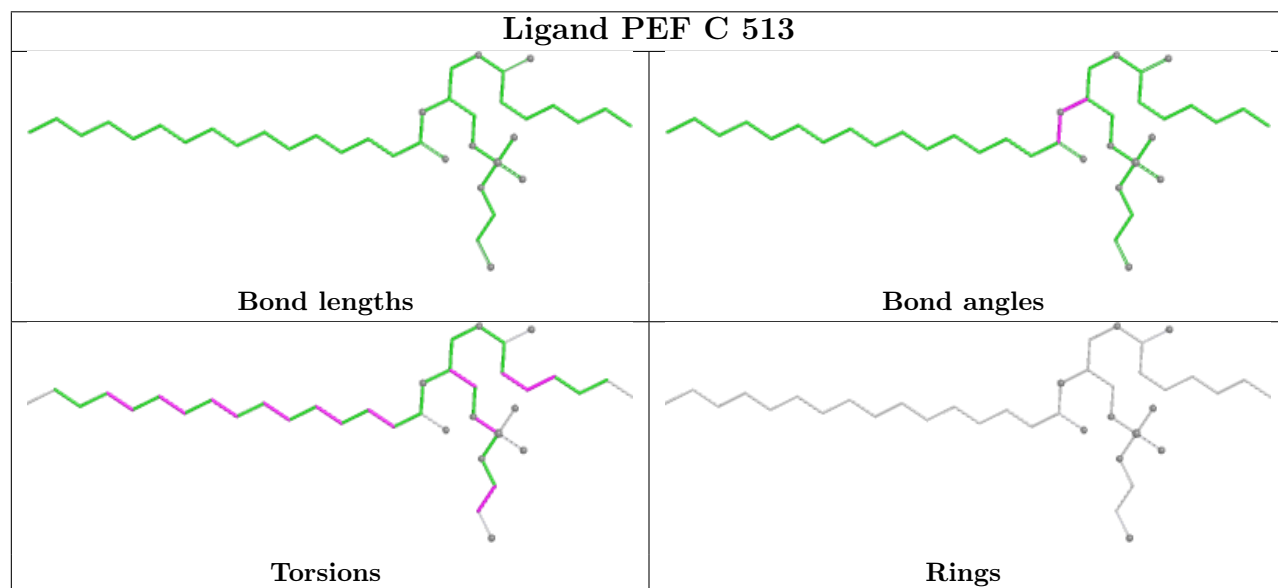
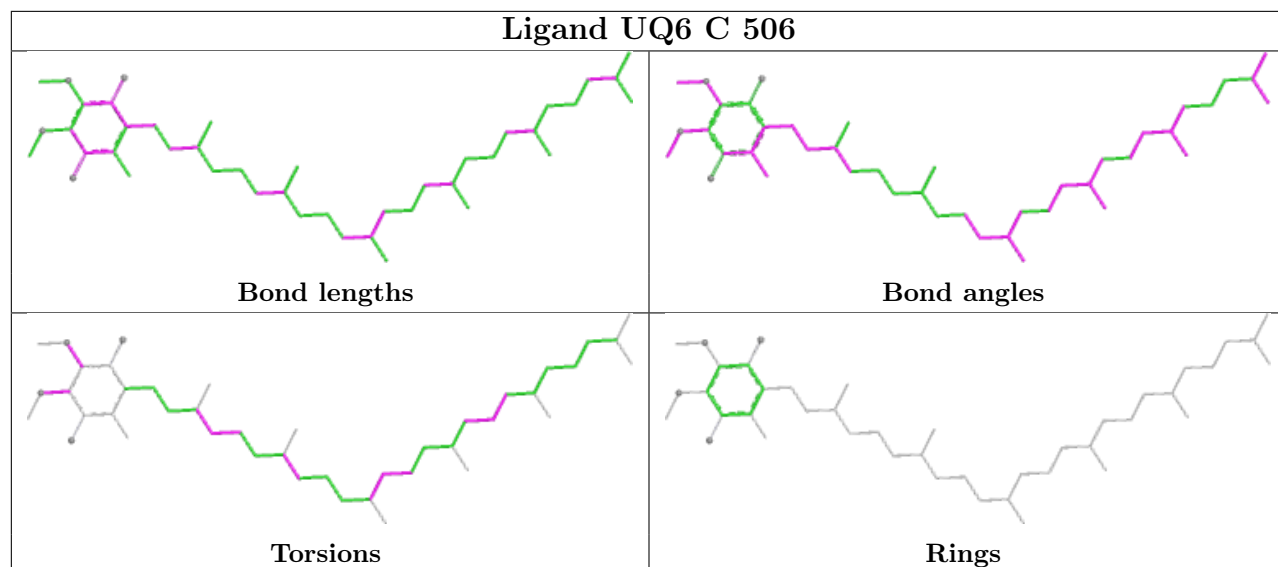
10 monomers are involved in 41 short contacts:

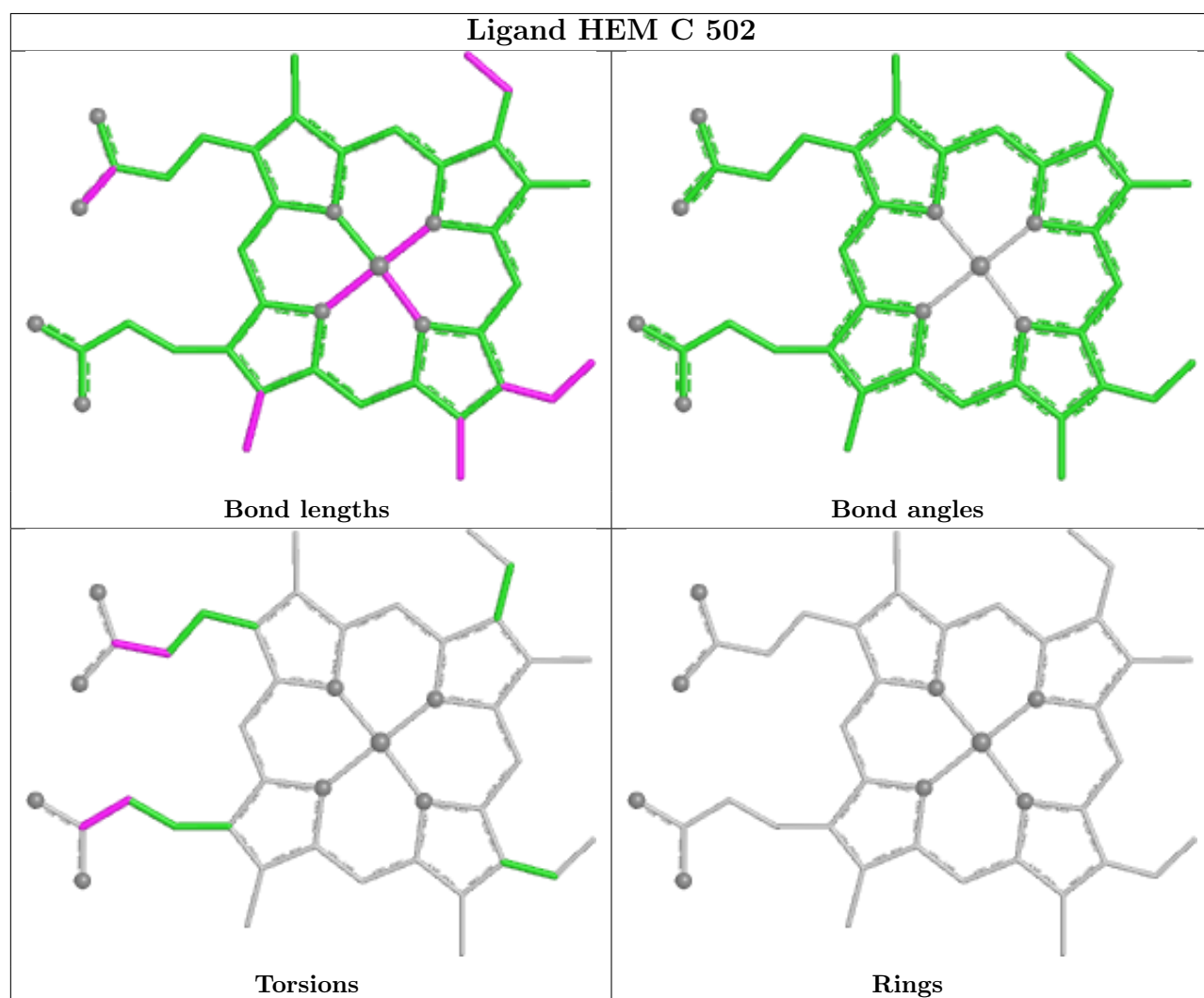
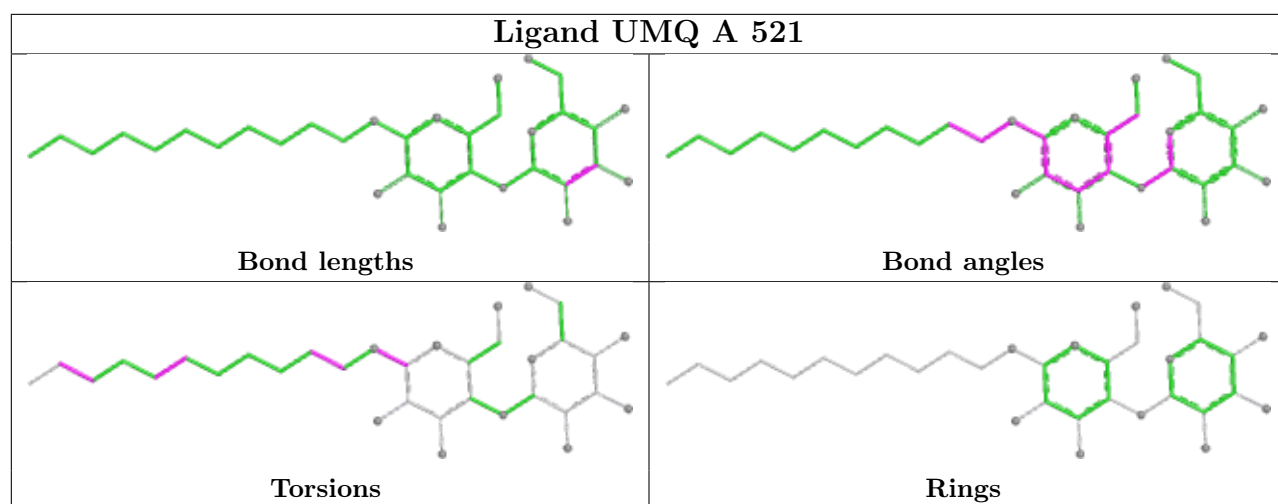
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	C	511	CDL	5	0
12	A	514	PCF	9	0
16	C	506	UQ6	10	0
18	C	510	PEF	3	0
13	A	521	UMQ	4	0
14	C	502	HEM	1	0
20	E	504	FES	1	0
14	C	501	HEM	3	0
17	C	508	PIE	2	0
15	C	505	SMA	7	0

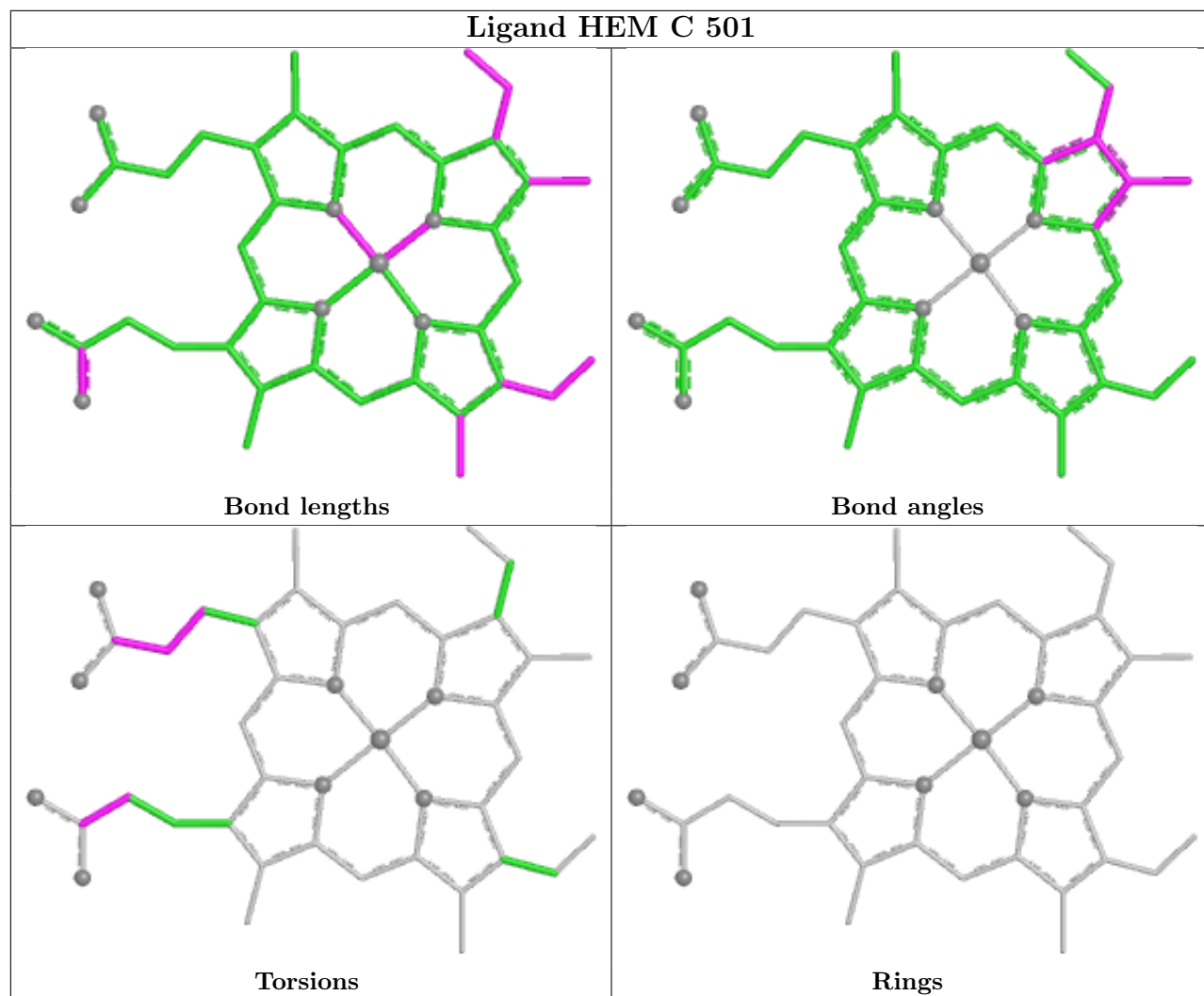
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

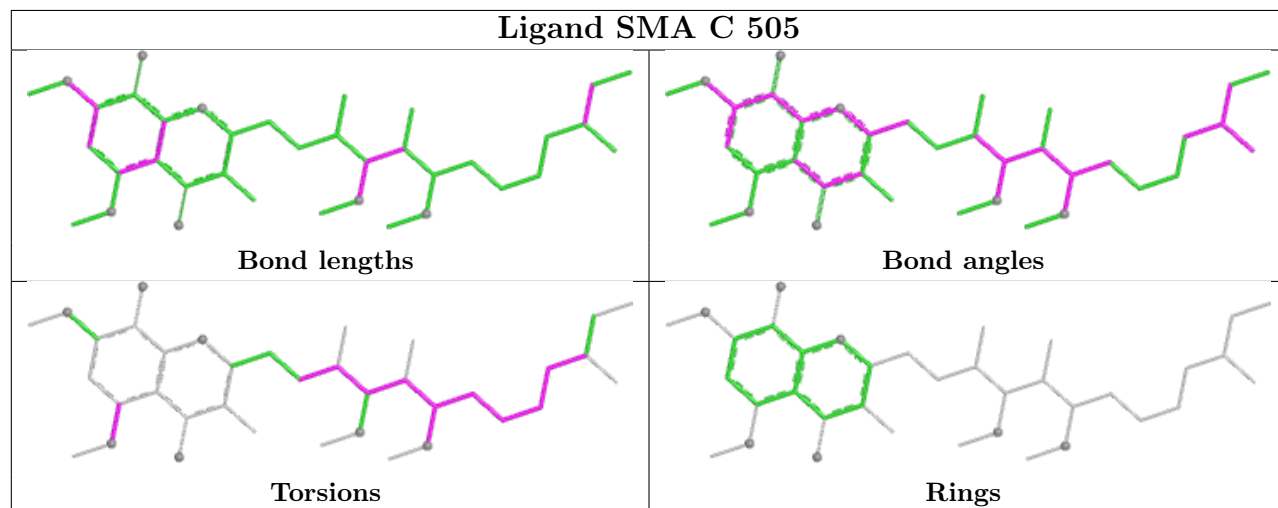
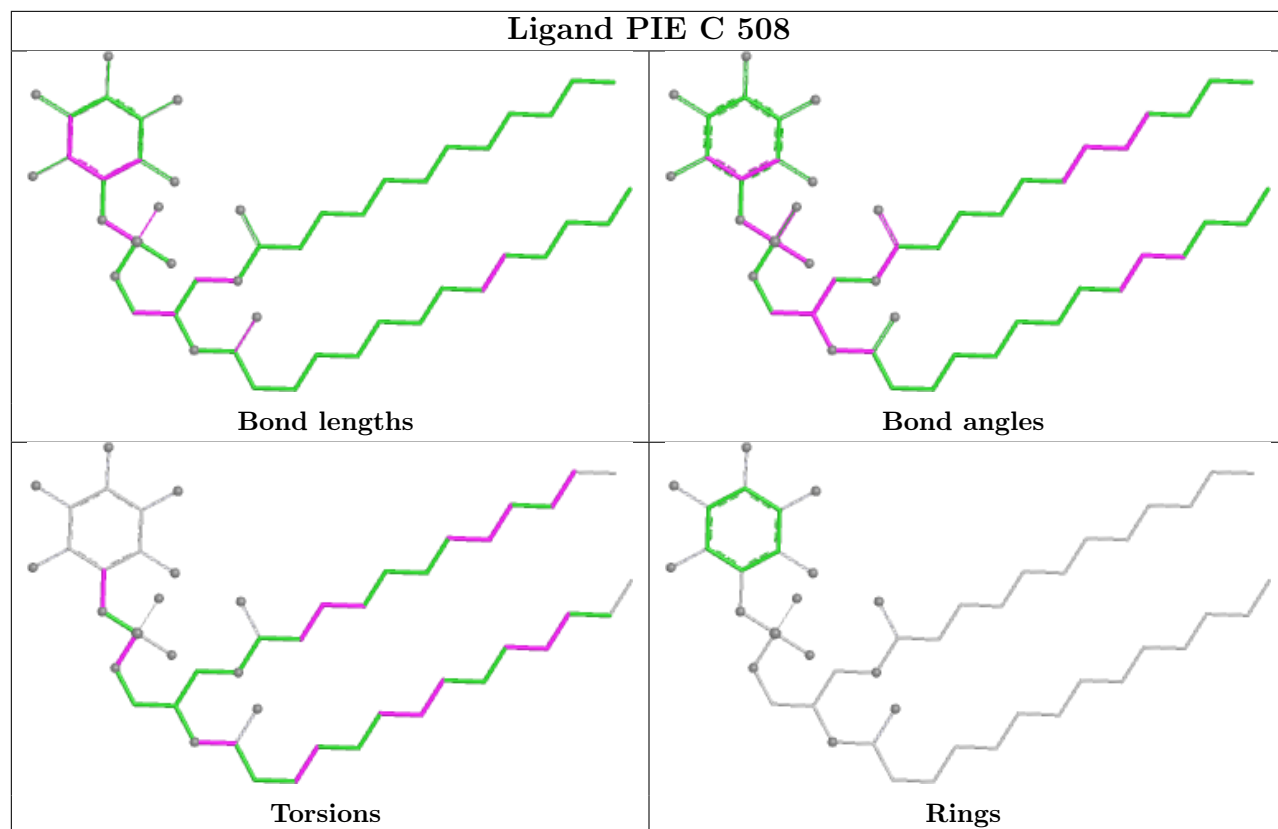
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

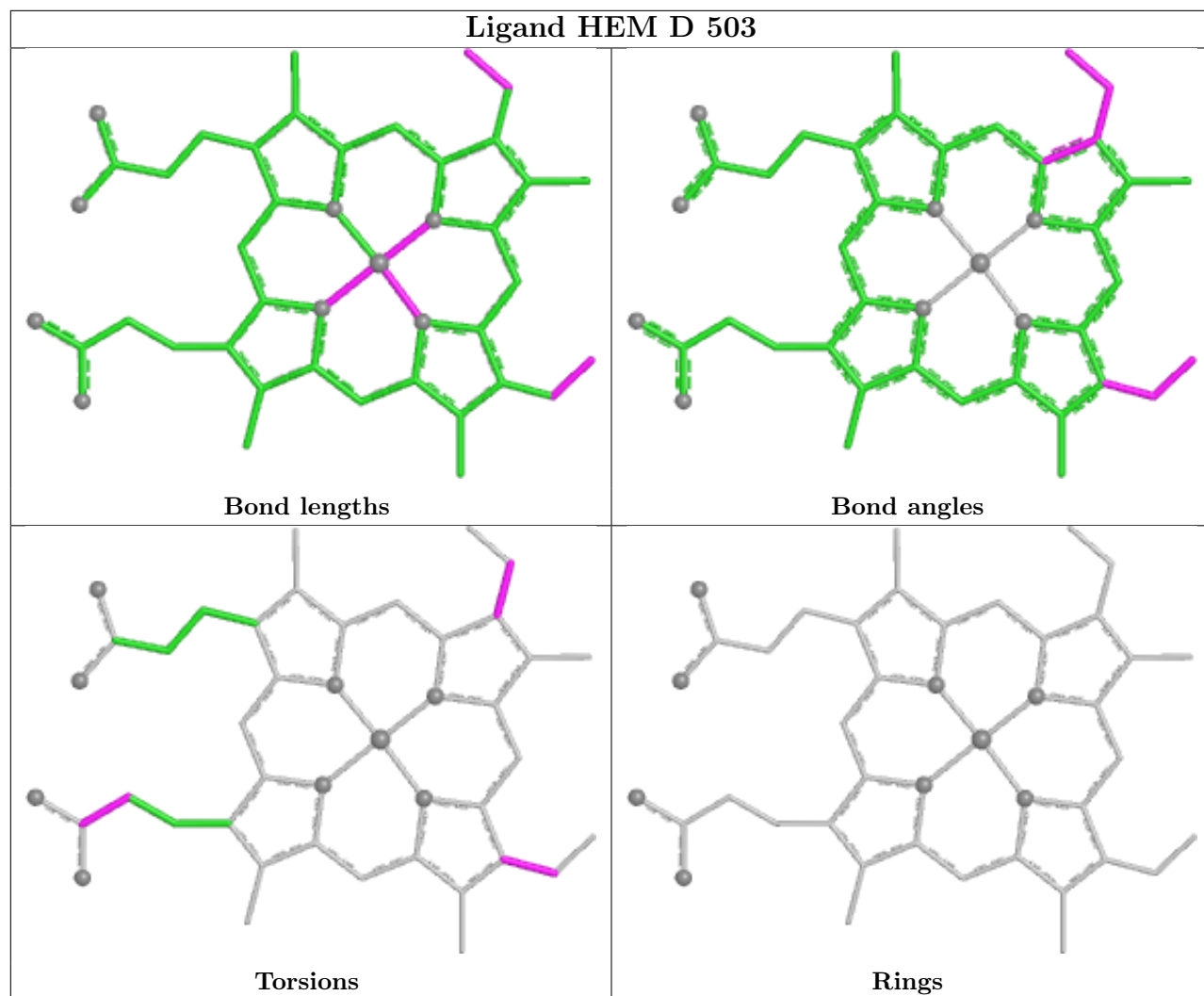












5.7 Other polymers [i](#)

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.