



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:07 PM UTC

PDB ID : 2IBZ / pdb_00002ibz
Title : Yeast Cytochrome BC1 Complex with Stigmatellin
Authors : Hunte, C.
Deposited on : 2006-09-12
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

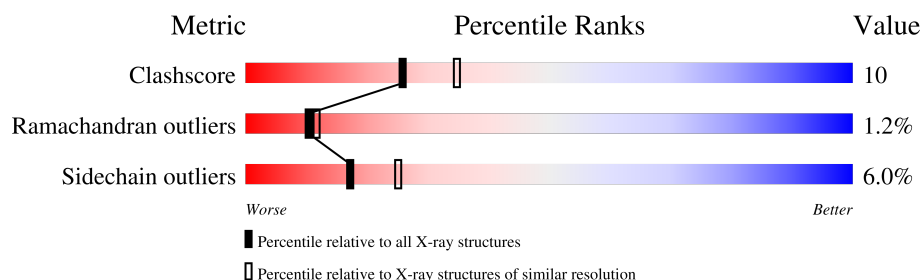
1 Overall quality at a glance

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% 26% .
2	B	352	68% 28% .
3	C	385	80% 18% .
4	D	248	81% 17% ..
5	E	185	73% 26% ..
6	H	74	77% 16% 7%
7	F	127	82% 15% ..
8	G	94	77% 19% ...

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Mol	Chain	Length	Quality of chain
9	I	66	71%11%17%
10	X	127	68%28%. .
11	Y	107	62%34%. .

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 17779 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 1.

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

- Molecule 3 is a protein called Cytochrome b.

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

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	245	Total	C	N	O	S	0	0	0
			1933	1232	333	359	9			

- Molecule 5 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit, mito-

chondrial precursor.

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	55	Total	C	N	O	0	0	0
			448	298	75	75			

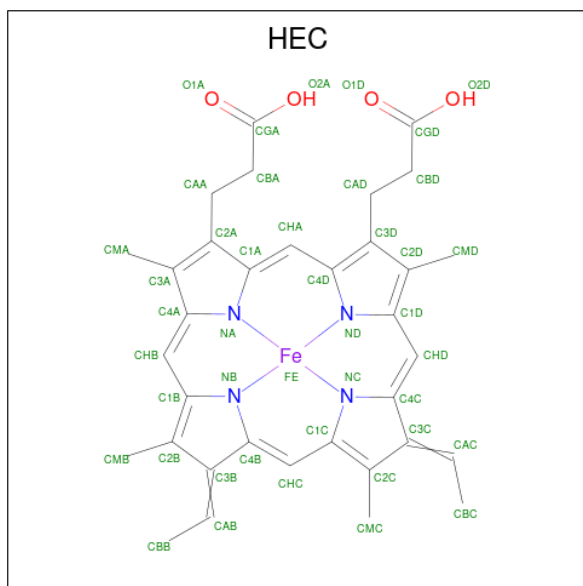
- Molecule 10 is a protein called Variable Heavy chain of antibody fragment.

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

- Molecule 11 is a protein called Variable Light chain of antibody fragment.

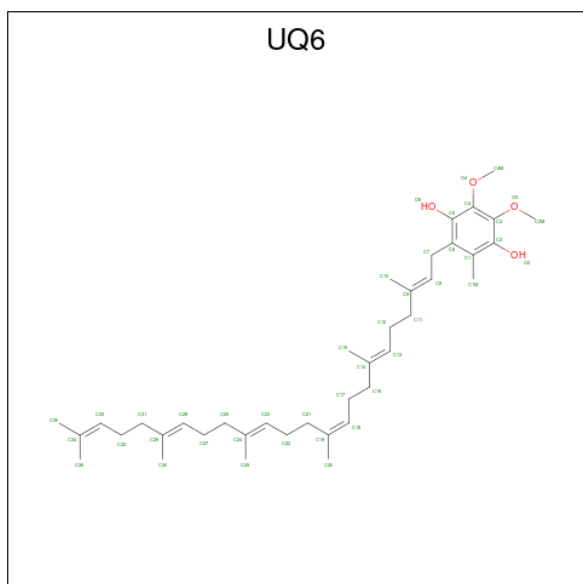
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	Y	107	Total	C	N	O	S	0	0	0
			842	536	141	163	2			

- Molecule 12 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



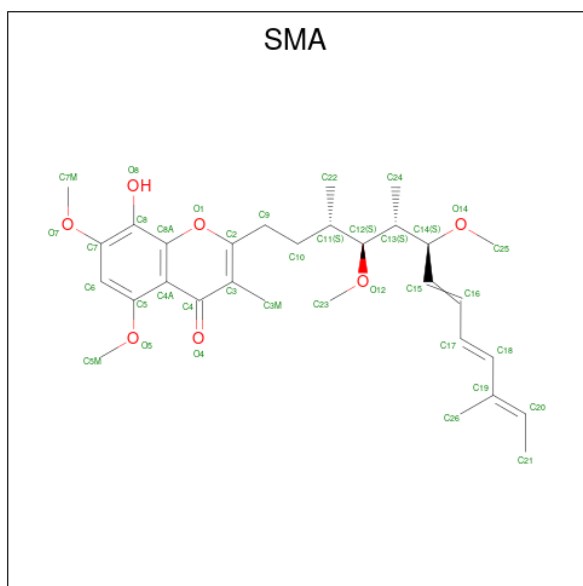
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
12	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
12	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 13 is 5-(3,7,11,15,19,23-HEXAMETHYL-TETRACOSA-2,6,10,14,18,22-HEXA ENYL)-2,3-DIMETHOXY-6-METHYL-BENZENE-1,4-DIOL (CCD ID: UQ6) (formula: $C_{39}H_{60}O_4$).



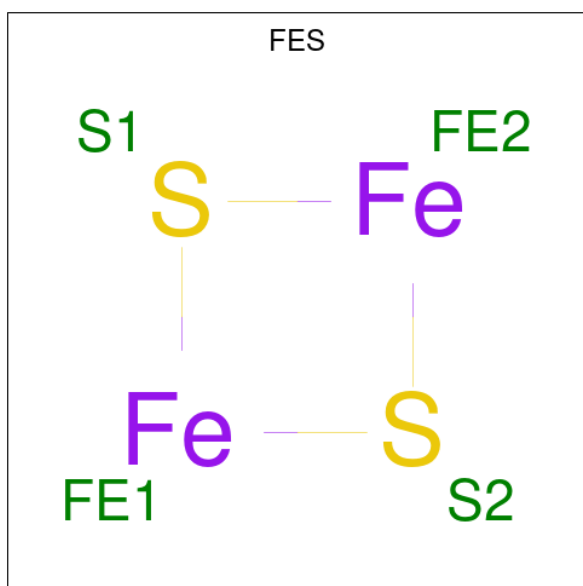
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	C	1	Total	C O	0	0
			43	39 4		

- Molecule 14 is STIGMATELLIN A (CCD ID: SMA) (formula: $C_{30}H_{42}O_7$).



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

- Molecule 15 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

- Molecule 16 is water.

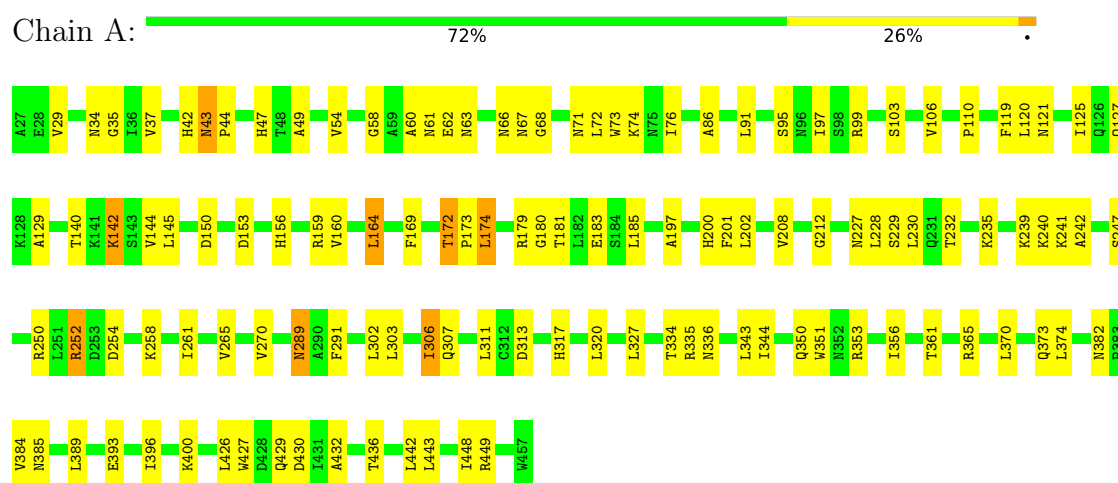
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	49	Total	O	0	0
			49	49		
16	B	11	Total	O	0	0
			11	11		
16	C	111	Total	O	0	0
			111	111		
16	D	68	Total	O	0	0
			68	68		
16	E	32	Total	O	0	0
			32	32		
16	H	6	Total	O	0	0
			6	6		
16	F	36	Total	O	0	0
			36	36		
16	G	19	Total	O	0	0
			19	19		
16	I	1	Total	O	0	0
			1	1		
16	X	5	Total	O	0	0
			5	5		
16	Y	2	Total	O	0	0
			2	2		

3 Residue-property plots

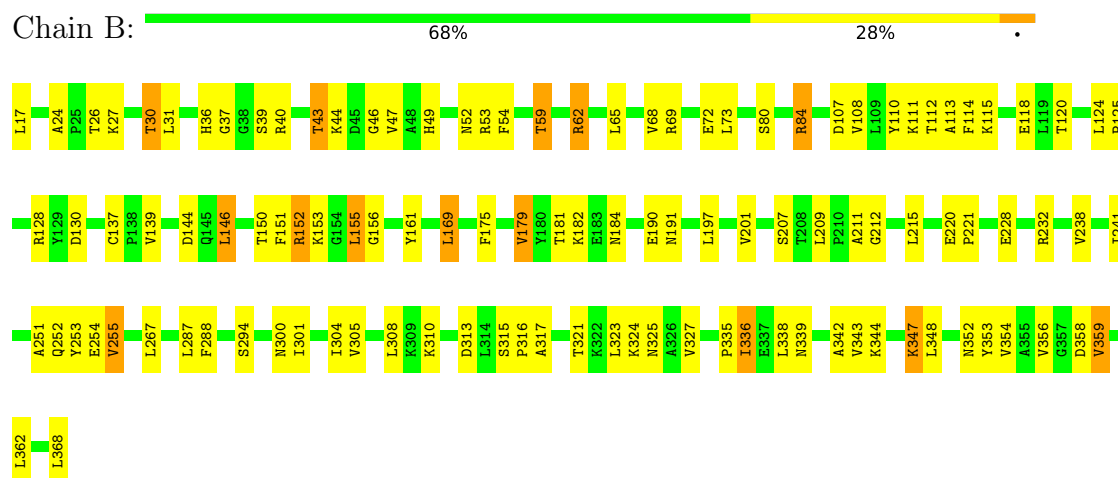
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

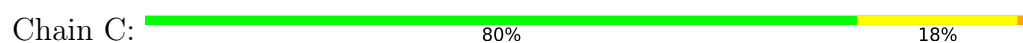
- Molecule 1: Ubiquinol-cytochrome-c reductase complex core protein 1

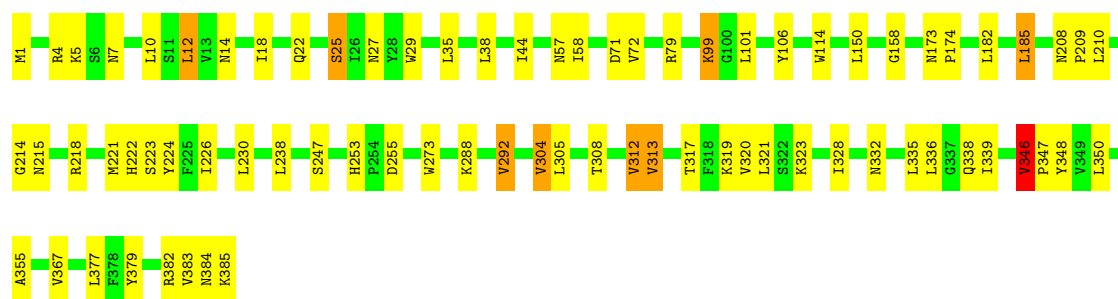


- Molecule 2: Ubiquinol-cytochrome-c reductase complex core protein 2



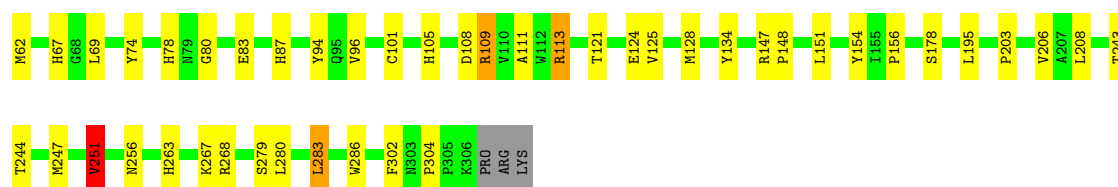
- Molecule 3: Cytochrome b





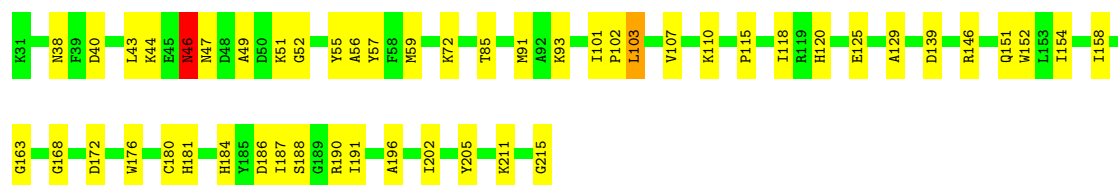
- Molecule 4: Cytochrome c1, heme protein, mitochondrial precursor

Chain D: 81% 17% ..



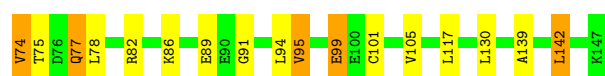
- Molecule 5: Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial precursor

Chain E: 73% 26% ..



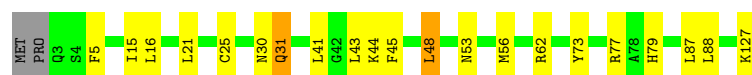
- Molecule 6: Ubiquinol-cytochrome c reductase complex 17 kDa protein

Chain H: 77% 16% 7%



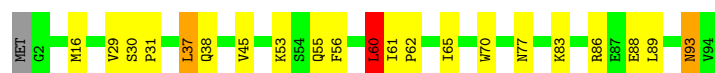
- Molecule 7: Ubiquinol-cytochrome c reductase complex 14 kDa protein

Chain F: 82% 15% ..



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

Chain G: 77% 19% ...



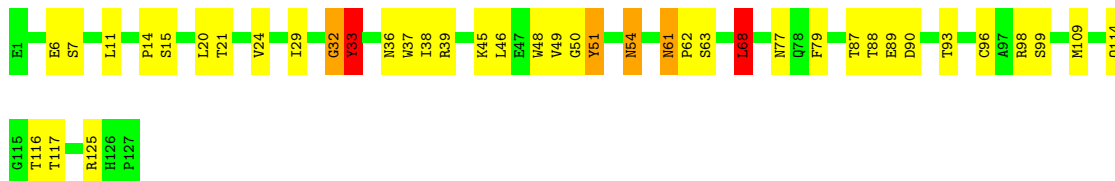
- Molecule 9: Ubiquinol-cytochrome c reductase complex 7.3 kDa protein

Chain I:  71% 11% 17%



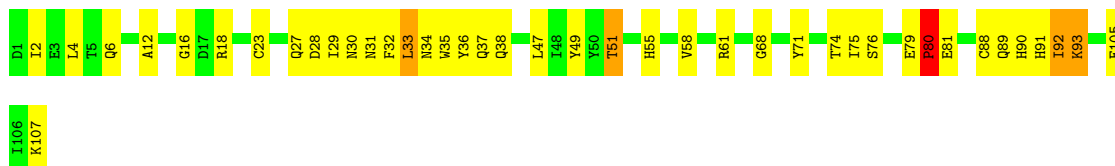
- Molecule 10: Variable Heavy chain of antibody fragment

Chain X:  68% 28%



- Molecule 11: Variable Light chain of antibody fragment

Chain Y:  62% 34%



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}	0.07	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.222 , 0.256	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17779	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: SMA, HEC, UQ6, FES

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	0.47	0/3405	0.94	5/4614 (0.1%)
2	B	0.41	0/2781	0.95	12/3764 (0.3%)
3	C	0.68	1/3191 (0.0%)	1.09	19/4353 (0.4%)
4	D	0.51	0/1993	1.03	10/2714 (0.4%)
5	E	0.50	0/1444	1.02	9/1957 (0.5%)
6	H	0.40	0/638	0.90	1/858 (0.1%)
7	F	0.51	0/1032	1.00	3/1397 (0.2%)
8	G	0.47	0/804	0.91	2/1088 (0.2%)
9	I	0.46	0/461	0.85	0/622
10	X	0.40	0/1043	0.91	4/1422 (0.3%)
11	Y	0.39	0/863	0.81	0/1172
All	All	0.50	1/17655 (0.0%)	0.98	65/23961 (0.3%)

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	6.57	1.57	1.54

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	108	ASP	N-CA-C	8.23	122.29	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	101	CYS	N-CA-C	7.74	119.35	111.07
3	C	247	SER	CA-C-N	7.52	127.23	119.56
3	C	247	SER	C-N-CA	7.52	127.23	119.56
3	C	346	VAL	N-CA-C	7.51	125.10	108.88
5	E	139	ASP	CA-C-N	7.38	129.07	119.84
5	E	139	ASP	C-N-CA	7.38	129.07	119.84
3	C	346	VAL	CA-C-N	-7.24	111.01	119.05
3	C	346	VAL	C-N-CA	-7.24	111.01	119.05
5	E	47	ASN	N-CA-C	-7.20	104.76	113.97
4	D	83	GLU	N-CA-C	7.18	120.94	109.24
5	E	163	GLY	N-CA-C	6.97	124.94	115.32
3	C	328	ILE	N-CA-C	-6.83	103.82	110.72
8	G	60	LEU	N-CA-C	6.70	118.24	111.07
3	C	273	TRP	N-CA-C	6.48	119.17	111.33
2	B	179	VAL	N-CA-C	6.43	119.13	111.09
2	B	359	VAL	N-CA-C	6.39	117.07	110.36
2	B	113	ALA	N-CA-C	6.36	119.02	111.33
3	C	320	VAL	N-CA-C	6.35	116.51	110.42
1	A	427	TRP	N-CA-C	6.28	118.19	109.15
2	B	84	ARG	N-CA-C	-6.25	105.14	112.89
7	F	25	CYS	N-CA-C	6.20	118.97	111.40
2	B	310	LYS	N-CA-C	-6.20	102.89	111.81
2	B	111	LYS	N-CA-C	6.19	120.95	109.56
3	C	348	TYR	N-CA-C	6.17	118.01	111.28
7	F	87	LEU	N-CA-C	-6.08	100.51	109.81
4	D	304	PRO	CA-C-N	6.01	125.95	119.76
4	D	304	PRO	C-N-CA	6.01	125.95	119.76
4	D	251	VAL	CB-CA-C	-5.95	104.11	112.14
3	C	25	SER	N-CA-C	5.91	120.62	113.17
10	X	36	ASN	N-CA-C	5.89	119.55	110.42
10	X	33	TYR	N-CA-C	5.87	123.30	110.80
1	A	356	ILE	N-CA-C	5.83	121.46	109.34
2	B	155	LEU	N-CA-C	-5.72	106.07	113.16
3	C	224	TYR	N-CA-C	5.69	117.96	111.02
1	A	334	THR	N-CA-C	5.62	117.82	108.99
3	C	185	LEU	N-CA-C	5.57	117.15	111.14
10	X	68	LEU	N-CA-C	5.47	117.14	110.41
7	F	44	LYS	N-CA-C	-5.45	101.28	109.95
6	H	142	LEU	N-CA-C	5.43	117.90	111.33
5	E	180	CYS	N-CA-C	5.38	116.83	111.07
3	C	215	ASN	N-CA-C	5.37	118.93	112.38
3	C	12	LEU	N-CA-C	-5.35	105.36	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	101	ILE	CA-C-N	5.35	126.53	119.84
5	E	101	ILE	C-N-CA	5.35	126.53	119.84
2	B	152	ARG	N-CA-C	5.33	122.15	110.80
3	C	317	THR	N-CA-C	5.32	117.77	111.33
1	A	43	ASN	CA-C-N	5.30	125.61	119.47
1	A	43	ASN	C-N-CA	5.30	125.61	119.47
3	C	71	ASP	N-CA-C	5.28	119.85	113.41
2	B	59	THR	N-CA-C	-5.20	102.32	110.17
8	G	53	LYS	N-CA-C	-5.19	106.79	113.23
10	X	32	GLY	N-CA-C	5.18	125.47	113.18
3	C	226	ILE	N-CA-C	-5.17	105.67	110.53
2	B	27	LYS	N-CA-C	5.16	119.43	113.18
3	C	79	ARG	NE-CZ-NH1	-5.10	116.40	121.50
5	E	152	TRP	N-CA-C	5.10	116.94	108.02
2	B	120	THR	N-CA-C	5.09	117.56	111.71
3	C	158	GLY	N-CA-C	5.07	118.77	112.64
5	E	188	SER	N-CA-C	-5.05	106.53	113.30
2	B	288	PHE	N-CA-C	5.04	116.62	108.41
4	D	87	HIS	N-CA-C	5.03	118.67	112.54
4	D	208	LEU	CA-C-N	5.01	123.32	119.66
4	D	208	LEU	C-N-CA	5.01	123.32	119.66
4	D	105	HIS	N-CA-C	5.00	117.13	109.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	94	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3344	0	3321	75	0
2	B	2735	0	2774	74	0
3	C	3089	0	3125	38	0
4	D	1933	0	1855	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1411	0	1386	30	0
6	H	624	0	581	11	0
7	F	1012	0	1026	13	0
8	G	773	0	736	13	0
9	I	448	0	445	6	0
10	X	1015	0	959	32	0
11	Y	842	0	820	29	0
12	C	86	0	64	2	0
12	D	43	0	30	1	0
13	C	43	0	58	7	0
14	C	37	0	41	0	0
15	E	4	0	0	1	0
16	A	49	0	0	1	0
16	B	11	0	0	0	0
16	C	111	0	0	1	0
16	D	68	0	0	2	0
16	E	32	0	0	0	0
16	F	36	0	0	1	0
16	G	19	0	0	0	0
16	H	6	0	0	0	0
16	I	1	0	0	0	0
16	X	5	0	0	1	0
16	Y	2	0	0	0	0
All	All	17779	0	17221	329	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 (329) 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:H:77:GLN:HE21	6:H:77:GLN:H	1.00	0.98
11:Y:31:ASN:HD22	11:Y:51:THR:HG21	1.36	0.90
5:E:72:LYS:HZ3	9:I:29:GLN:HE22	1.15	0.89
2:B:347:LYS:H	2:B:347:LYS:HD3	1.40	0.85
7:F:31:GLN:HA	7:F:31:GLN:HE21	1.41	0.85
1:A:99:ARG:HD3	1:A:174:LEU:HD12	1.59	0.85
3:C:253:HIS:HD2	3:C:255:ASP:H	1.28	0.82
6:H:77:GLN:H	6:H:77:GLN:NE2	1.75	0.82
3:C:7:ASN:HD22	3:C:10:LEU:H	1.28	0.81
1:A:317:HIS:HE1	1:A:351:TRP:HE1	1.28	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:182:LYS:HB2	2:B:211:ALA:HB2	1.61	0.81
1:A:63:ASN:HB2	1:A:66:ASN:ND2	1.97	0.80
7:F:77:ARG:HD3	7:F:88:LEU:HD11	1.65	0.79
3:C:44:ILE:HD12	13:C:506:UQ6:H202	1.64	0.79
12:C:401:HEC:HBC3	12:C:401:HEC:HHD	1.64	0.79
5:E:72:LYS:NZ	9:I:29:GLN:HE22	1.82	0.77
3:C:218:ARG:HG3	8:G:16:MET:HE3	1.68	0.75
6:H:78:LEU:HD13	6:H:142:LEU:HD22	1.67	0.75
3:C:58:ILE:H	3:C:173:ASN:HD22	1.34	0.74
5:E:115:PRO:HD2	5:E:158:ILE:HD11	1.69	0.72
1:A:74:LYS:HG3	1:A:95:SER:HB3	1.71	0.71
11:Y:31:ASN:ND2	11:Y:51:THR:HG21	2.05	0.71
1:A:156:HIS:HD2	1:A:159:ARG:HH21	1.38	0.71
7:F:77:ARG:HD2	16:F:154:HOH:O	1.91	0.71
4:D:62:MET:HB3	4:D:67:HIS:NE2	2.06	0.69
2:B:30:THR:HG23	2:B:190:GLU:HB3	1.75	0.69
6:H:91:GLY:O	6:H:95:VAL:HG13	1.91	0.69
10:X:54:ASN:HD22	10:X:54:ASN:H	1.41	0.69
11:Y:37:GLN:HB2	11:Y:47:LEU:HD11	1.76	0.68
6:H:74:VAL:HG12	6:H:75:THR:H	1.57	0.68
2:B:65:LEU:O	2:B:69:ARG:HG2	1.94	0.68
2:B:181:THR:HB	2:B:212:GLY:H	1.58	0.67
1:A:73:TRP:CE3	1:A:76:ILE:HD11	2.30	0.66
13:C:506:UQ6:C1M	13:C:506:UQ6:H103	2.24	0.66
2:B:300:ASN:O	2:B:304:ILE:HG12	1.96	0.66
3:C:214:GLY:O	3:C:218:ARG:HD2	1.95	0.66
2:B:336:ILE:HG21	2:B:339:ASN:HB2	1.79	0.65
1:A:258:LYS:HG2	1:A:335:ARG:HG3	1.78	0.65
2:B:49:HIS:HD2	2:B:161:TYR:H	1.45	0.65
6:H:77:GLN:HE21	6:H:77:GLN:N	1.84	0.65
4:D:113:ARG:HG2	4:D:151:LEU:O	1.97	0.63
3:C:253:HIS:CD2	3:C:255:ASP:H	2.15	0.63
2:B:44:LYS:HB2	2:B:47:VAL:HG21	1.81	0.63
1:A:350:GLN:HE22	1:A:353:ARG:HH21	1.46	0.62
3:C:58:ILE:H	3:C:173:ASN:ND2	1.98	0.62
5:E:107:VAL:HG12	5:E:118:ILE:HB	1.81	0.62
11:Y:32:PHE:HD2	11:Y:92:ILE:HG22	1.63	0.62
2:B:287:LEU:HD21	2:B:304:ILE:HG21	1.83	0.61
11:Y:27:GLN:HG2	11:Y:28:ASP:H	1.65	0.61
11:Y:4:LEU:HD23	11:Y:88:CYS:SG	2.41	0.61
10:X:61:ASN:HD22	10:X:63:SER:H	1.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:172:ASP:H	5:E:184:HIS:HD2	1.49	0.61
1:A:302:LEU:HB2	1:A:350:GLN:HG3	1.83	0.60
1:A:29:VAL:HG11	1:A:400:LYS:HB3	1.83	0.60
13:C:506:UQ6:H103	13:C:506:UQ6:H1M3	1.84	0.60
5:E:172:ASP:H	5:E:184:HIS:CD2	2.19	0.60
3:C:25:SER:OG	7:F:79:HIS:HD2	1.85	0.59
5:E:129:ALA:HB2	5:E:187:ILE:HG23	1.83	0.59
4:D:96:VAL:HB	4:D:251:VAL:HG13	1.84	0.59
2:B:241:ILE:HG12	2:B:287:LEU:HB3	1.84	0.59
5:E:44:LYS:NZ	5:E:52:GLY:H	2.00	0.59
11:Y:6:GLN:HG2	11:Y:23:CYS:SG	2.43	0.59
2:B:150:THR:HG22	2:B:352:ASN:ND2	2.18	0.59
1:A:63:ASN:HB2	1:A:66:ASN:HD22	1.66	0.58
3:C:57:ASN:HA	3:C:173:ASN:HD21	1.68	0.58
5:E:72:LYS:NZ	9:I:29:GLN:NE2	2.50	0.58
2:B:336:ILE:CG2	2:B:339:ASN:HB2	2.34	0.58
3:C:1:MET:N	16:C:581:HOH:O	2.36	0.58
2:B:49:HIS:CD2	2:B:161:TYR:H	2.22	0.58
4:D:109:ARG:HG3	4:D:178:SER:CB	2.34	0.57
2:B:40:ARG:HG3	2:B:155:LEU:HG	1.86	0.57
3:C:22:GLN:HE22	13:C:506:UQ6:H3M3	1.70	0.57
7:F:43:LEU:HD13	7:F:48:LEU:HD11	1.86	0.57
10:X:61:ASN:ND2	10:X:63:SER:H	2.03	0.57
11:Y:29:ILE:HG22	11:Y:92:ILE:HD12	1.86	0.57
1:A:265:VAL:HG21	1:A:426:LEU:HD12	1.87	0.57
1:A:289:ASN:C	1:A:289:ASN:HD22	2.12	0.57
3:C:347:PRO:HG3	8:G:77:ASN:HB2	1.86	0.57
1:A:67:ASN:HD22	1:A:181:THR:HG23	1.70	0.57
1:A:252:ARG:HD3	1:A:254:ASP:OD1	2.04	0.57
5:E:168:GLY:HA2	5:E:176:TRP:CD1	2.40	0.57
1:A:68:GLY:HA3	1:A:185:LEU:HD11	1.87	0.57
2:B:336:ILE:HD12	2:B:336:ILE:H	1.69	0.57
2:B:115:LYS:HB2	2:B:118:GLU:HG3	1.87	0.57
10:X:29:ILE:H	10:X:77:ASN:HD21	1.51	0.57
2:B:238:VAL:HG13	2:B:356:VAL:HB	1.86	0.56
5:E:55:TYR:O	5:E:59:MET:HG2	2.05	0.56
7:F:53:ASN:ND2	7:F:56:MET:H	2.02	0.56
3:C:323:LYS:HE3	8:G:55:GLN:HE22	1.69	0.56
3:C:208:ASN:HD22	3:C:210:LEU:H	1.53	0.56
1:A:313:ASP:OD1	1:A:335:ARG:HD3	2.05	0.56
1:A:303:LEU:O	1:A:307:GLN:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:44:ILE:HD12	13:C:506:UQ6:C20	2.36	0.55
2:B:347:LYS:HG2	2:B:348:LEU:N	2.21	0.55
5:E:107:VAL:CG1	5:E:118:ILE:HB	2.36	0.55
2:B:313:ASP:O	2:B:316:PRO:HD3	2.07	0.55
13:C:506:UQ6:H103	13:C:506:UQ6:H1M2	1.89	0.55
10:X:24:VAL:HG21	10:X:29:ILE:HD11	1.87	0.55
2:B:232:ARG:HB3	2:B:232:ARG:HH21	1.71	0.55
2:B:252:GLN:O	2:B:255:VAL:HG22	2.07	0.55
1:A:58:GLY:H	1:A:61:ASN:HD22	1.56	0.54
4:D:203:PRO:HG2	4:D:206:VAL:HG21	1.89	0.54
8:G:56:PHE:O	8:G:60:LEU:HB2	2.07	0.54
1:A:42:HIS:CD2	1:A:42:HIS:H	2.24	0.54
1:A:270:VAL:HG21	1:A:396:ILE:HD13	1.88	0.54
2:B:68:VAL:O	2:B:72:GLU:HG3	2.07	0.54
7:F:15:ILE:HG23	7:F:21:LEU:HB3	1.89	0.53
10:X:38:ILE:HA	10:X:49:VAL:HG23	1.89	0.53
4:D:247:MET:O	4:D:251:VAL:HG22	2.09	0.53
10:X:87:THR:HG22	10:X:88:THR:N	2.24	0.53
1:A:344:ILE:HG21	1:A:448:ILE:HD12	1.91	0.53
2:B:182:LYS:HB2	2:B:211:ALA:CB	2.37	0.53
1:A:47:HIS:O	1:A:110:PRO:HD3	2.09	0.53
2:B:52:ASN:ND2	2:B:80:SER:OG	2.42	0.53
1:A:169:PHE:O	1:A:172:THR:HB	2.09	0.52
1:A:156:HIS:HD2	1:A:159:ARG:NH2	2.03	0.52
10:X:51:TYR:C	10:X:51:TYR:CD2	2.88	0.52
2:B:255:VAL:HG12	2:B:321:THR:HG21	1.91	0.52
9:I:5:SER:O	9:I:9:THR:HG23	2.10	0.52
1:A:172:THR:HG23	1:A:242:ALA:HA	1.91	0.52
4:D:286:TRP:CE3	5:E:59:MET:HG3	2.45	0.52
1:A:68:GLY:HA3	1:A:185:LEU:CD1	2.39	0.52
1:A:172:THR:HG23	1:A:173:PRO:HD2	1.92	0.52
2:B:24:ALA:HB3	2:B:191:ASN:ND2	2.24	0.52
2:B:43:THR:HG22	2:B:175:PHE:HD1	1.73	0.52
1:A:67:ASN:ND2	1:A:180:GLY:HA2	2.25	0.51
10:X:49:VAL:HG12	10:X:68:LEU:HD23	1.92	0.51
1:A:317:HIS:CE1	1:A:351:TRP:HE1	2.17	0.51
1:A:430:ASP:OD2	1:A:449:ARG:NH2	2.44	0.51
11:Y:4:LEU:CD2	11:Y:88:CYS:SG	2.98	0.51
2:B:315:SER:N	2:B:316:PRO:HD3	2.25	0.51
10:X:61:ASN:HD22	10:X:61:ASN:C	2.18	0.51
4:D:121:THR:OG1	4:D:124:GLU:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:61:ASN:HD22	10:X:62:PRO:N	2.08	0.51
2:B:252:GLN:HB3	2:B:343:VAL:HG21	1.92	0.51
2:B:40:ARG:HB2	2:B:84:ARG:O	2.11	0.51
4:D:74:TYR:CE1	6:H:139:ALA:HA	2.46	0.51
1:A:142:LYS:HB2	1:A:142:LYS:NZ	2.26	0.51
5:E:38:ASN:HD21	5:E:40:ASP:CG	2.18	0.50
4:D:263:HIS:NE2	4:D:267:LYS:HE3	2.26	0.50
10:X:49:VAL:CG1	10:X:68:LEU:HD23	2.41	0.50
2:B:228:GLU:HA	2:B:353:TYR:O	2.12	0.50
10:X:48:TRP:CZ2	10:X:50:GLY:HA2	2.46	0.50
2:B:294:SER:HB3	2:B:358:ASP:HB3	1.94	0.50
10:X:99:SER:HB3	10:X:109:MET:HG2	1.94	0.50
2:B:232:ARG:HB3	2:B:232:ARG:NH2	2.27	0.49
10:X:32:GLY:O	10:X:54:ASN:HB3	2.11	0.49
11:Y:34:ASN:HD22	11:Y:49:TYR:HA	1.77	0.49
1:A:373:GLN:HG3	1:A:374:LEU:N	2.27	0.49
2:B:46:GLY:O	2:B:49:HIS:HB3	2.13	0.49
5:E:46:ASN:OD1	5:E:49:ALA:HA	2.12	0.49
2:B:44:LYS:HB2	2:B:47:VAL:CG2	2.40	0.49
4:D:147:ARG:HG2	4:D:148:PRO:O	2.12	0.49
8:G:61:ILE:HB	8:G:62:PRO:HD3	1.95	0.49
5:E:103:LEU:O	5:E:120:HIS:HB3	2.13	0.49
2:B:347:LYS:HD3	2:B:347:LYS:N	2.17	0.48
3:C:323:LYS:CE	8:G:55:GLN:HE22	2.26	0.48
10:X:6:GLU:H	10:X:114:GLN:HE21	1.62	0.48
1:A:49:ALA:HA	1:A:212:GLY:HA3	1.95	0.48
1:A:350:GLN:NE2	1:A:353:ARG:HD3	2.28	0.48
1:A:179:ARG:HH21	1:A:179:ARG:HG2	1.79	0.48
2:B:37:GLY:HA3	2:B:179:VAL:HG11	1.95	0.48
11:Y:2:ILE:N	11:Y:2:ILE:HD12	2.29	0.48
2:B:267:LEU:HD22	2:B:304:ILE:HD13	1.96	0.48
1:A:91:LEU:HD23	1:A:106:VAL:HG11	1.95	0.48
1:A:200:HIS:C	1:A:202:LEU:H	2.21	0.48
2:B:36:HIS:HB2	2:B:184:ASN:OD1	2.14	0.48
1:A:67:ASN:ND2	1:A:181:THR:HG23	2.29	0.48
1:A:235:LYS:HB2	1:A:235:LYS:NZ	2.29	0.48
2:B:110:TYR:HD1	2:B:209:LEU:HD23	1.79	0.48
11:Y:36:TYR:HE2	11:Y:89:GLN:HG2	1.79	0.48
5:E:93:LYS:HD3	5:E:215:GLY:HA3	1.95	0.47
1:A:71:ASN:HA	1:A:97:ILE:HG13	1.97	0.47
1:A:429:GLN:HE22	9:I:13:ARG:NH2	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:332:ASN:HD21	3:C:355:ALA:HA	1.79	0.47
7:F:31:GLN:HE21	7:F:31:GLN:CA	2.16	0.47
10:X:29:ILE:HG12	10:X:77:ASN:ND2	2.30	0.47
1:A:127:GLN:C	1:A:129:ALA:H	2.21	0.47
1:A:229:SER:HB3	1:A:232:THR:HB	1.96	0.47
1:A:306:ILE:HA	1:A:311:LEU:HD22	1.95	0.47
10:X:51:TYR:C	10:X:51:TYR:HD2	2.23	0.47
1:A:160:VAL:CG2	1:A:436:THR:HG22	2.45	0.47
2:B:43:THR:HG22	2:B:175:PHE:CD1	2.49	0.47
10:X:87:THR:HG22	10:X:88:THR:H	1.80	0.47
11:Y:47:LEU:HA	11:Y:58:VAL:HG11	1.97	0.47
5:E:186:ASP:OD2	5:E:190:ARG:HD2	2.15	0.47
1:A:289:ASN:ND2	1:A:291:PHE:H	2.14	0.46
2:B:313:ASP:HB3	2:B:344:LYS:O	2.15	0.46
1:A:72:LEU:HD13	1:A:144:VAL:HG21	1.97	0.46
1:A:365:ARG:HD2	2:B:72:GLU:OE1	2.15	0.46
3:C:4:ARG:HE	3:C:14:ASN:ND2	2.13	0.46
7:F:31:GLN:HA	7:F:31:GLN:NE2	2.18	0.46
10:X:37:TRP:CZ3	10:X:96:CYS:HB3	2.50	0.46
10:X:38:ILE:HD12	10:X:46:LEU:HD22	1.97	0.46
3:C:335:LEU:HD13	3:C:339:ILE:HG12	1.97	0.46
11:Y:33:LEU:HD22	11:Y:71:TYR:CG	2.51	0.46
1:A:62:GLU:OE1	1:A:67:ASN:HA	2.15	0.46
1:A:289:ASN:HD22	1:A:291:PHE:H	1.61	0.46
1:A:306:ILE:C	1:A:306:ILE:HD12	2.40	0.46
3:C:7:ASN:ND2	3:C:10:LEU:H	2.04	0.46
2:B:26:THR:OG1	2:B:191:ASN:ND2	2.48	0.46
2:B:69:ARG:O	2:B:73:LEU:HD23	2.15	0.46
5:E:43:LEU:HD21	8:G:29:VAL:HG11	1.98	0.46
11:Y:55:HIS:O	11:Y:58:VAL:HG22	2.15	0.46
3:C:208:ASN:HB2	3:C:209:PRO:HD2	1.97	0.46
5:E:125:GLU:HB3	5:E:187:ILE:HG12	1.96	0.46
11:Y:36:TYR:OH	11:Y:89:GLN:NE2	2.49	0.46
4:D:125:VAL:HA	4:D:128:MET:HE3	1.98	0.46
11:Y:33:LEU:HD23	11:Y:35:TRP:HE1	1.81	0.46
5:E:191:ILE:HD13	5:E:196:ALA:HB3	1.98	0.45
1:A:336:ASN:C	1:A:336:ASN:HD22	2.25	0.45
1:A:382:ASN:OD1	1:A:384:VAL:HG22	2.17	0.45
2:B:324:LYS:O	2:B:327:VAL:HG22	2.16	0.45
1:A:86:ALA:HB2	1:A:119:PHE:CZ	2.52	0.45
3:C:18:ILE:HA	3:C:222:HIS:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:ASN:O	1:A:389:LEU:HG	2.16	0.45
11:Y:2:ILE:HD12	11:Y:2:ILE:H	1.81	0.45
2:B:182:LYS:HD3	2:B:207:SER:HA	1.97	0.45
3:C:27:ASN:OD1	3:C:29:TRP:HB2	2.17	0.45
2:B:197:LEU:O	2:B:201:VAL:HG23	2.16	0.45
8:G:61:ILE:O	8:G:65:ILE:HG13	2.17	0.45
2:B:308:LEU:HB2	2:B:348:LEU:HD22	1.98	0.45
4:D:111:ALA:HA	4:D:154:TYR:HA	1.98	0.45
4:D:286:TRP:CD2	8:G:37:LEU:HD12	2.52	0.45
10:X:7:SER:OG	10:X:21:THR:HG23	2.17	0.45
10:X:11:LEU:HD13	10:X:125:ARG:HD2	1.98	0.45
2:B:59:THR:HA	2:B:112:THR:HA	1.99	0.45
10:X:14:PRO:O	10:X:15:SER:HB3	2.17	0.45
1:A:73:TRP:CZ3	1:A:76:ILE:HD11	2.52	0.44
2:B:347:LYS:HG2	2:B:348:LEU:H	1.81	0.44
11:Y:37:GLN:HB2	11:Y:47:LEU:CD1	2.44	0.44
1:A:74:LYS:HB2	1:A:97:ILE:HD11	2.00	0.44
8:G:89:LEU:O	8:G:93:ASN:HB2	2.17	0.44
7:F:53:ASN:HD21	7:F:56:MET:H	1.65	0.44
3:C:221:MET:HE1	13:C:506:UQ6:C3	2.48	0.44
4:D:243:THR:CB	6:H:77:GLN:HE22	2.30	0.44
1:A:365:ARG:HH21	2:B:72:GLU:CD	2.26	0.44
2:B:62:ARG:HH21	2:B:62:ARG:HB2	1.83	0.44
10:X:33:TYR:HB3	10:X:99:SER:O	2.18	0.44
6:H:101:CYS:O	6:H:105:VAL:HG23	2.17	0.44
10:X:49:VAL:HG12	10:X:68:LEU:CD2	2.47	0.44
3:C:312:VAL:HG21	7:F:5:PHE:CE1	2.52	0.44
4:D:78:HIS:HD2	16:D:324:HOH:O	2.01	0.44
11:Y:93:LYS:NZ	11:Y:93:LYS:HB3	2.33	0.44
1:A:250:ARG:NH1	1:A:442:LEU:O	2.51	0.43
1:A:350:GLN:NE2	1:A:353:ARG:HH21	2.12	0.43
11:Y:32:PHE:CD2	11:Y:92:ILE:HG22	2.48	0.43
2:B:305:VAL:HG11	2:B:368:LEU:HB3	2.00	0.43
10:X:93:THR:HA	10:X:117:THR:HA	1.99	0.43
2:B:49:HIS:HE1	2:B:130:ASP:OD1	2.02	0.43
4:D:286:TRP:CZ3	5:E:56:ALA:HA	2.54	0.43
10:X:98:ARG:O	10:X:109:MET:HA	2.19	0.43
11:Y:61:ARG:HB2	11:Y:76:SER:HB3	2.00	0.43
2:B:108:VAL:O	2:B:112:THR:HG23	2.19	0.43
2:B:305:VAL:HG21	2:B:368:LEU:HD22	2.01	0.43
1:A:54:VAL:HG13	1:A:103:SER:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:ARG:NH1	16:A:483:HOH:O	2.49	0.43
1:A:374:LEU:HD12	1:A:374:LEU:HA	1.87	0.43
5:E:146:ARG:CZ	5:E:202:ILE:HD11	2.49	0.43
1:A:197:ALA:O	1:A:201:PHE:HB2	2.19	0.43
3:C:106:TYR:HB3	3:C:114:TRP:CD2	2.54	0.43
5:E:154:ILE:HD12	5:E:205:TYR:CE2	2.54	0.43
4:D:286:TRP:CD2	5:E:59:MET:HG3	2.54	0.43
1:A:239:LYS:HB2	1:A:240:LYS:H	1.70	0.42
11:Y:34:ASN:ND2	11:Y:91:HIS:HE1	2.17	0.42
4:D:134:TYR:OH	4:D:156:PRO:HD3	2.19	0.42
4:D:279:SER:O	4:D:283:LEU:HB2	2.19	0.42
3:C:384:ASN:O	3:C:385:LYS:HB2	2.18	0.42
2:B:124:LEU:HB2	2:B:125:PRO:HD3	2.00	0.42
2:B:151:PHE:O	2:B:156:GLY:HA3	2.20	0.42
4:D:195:LEU:HD11	12:D:3:HEC:HMB2	2.01	0.42
4:D:256:ASN:C	4:D:256:ASN:HD22	2.27	0.42
11:Y:79:GLU:HA	11:Y:80:PRO:HA	1.78	0.42
2:B:39:SER:OG	2:B:84:ARG:HD3	2.20	0.42
2:B:155:LEU:N	2:B:155:LEU:HD12	2.34	0.42
3:C:346:VAL:HG12	3:C:347:PRO:N	2.35	0.42
2:B:220:GLU:HA	2:B:221:PRO:HD3	1.88	0.42
5:E:120:HIS:CD2	5:E:151:GLN:HG2	2.54	0.42
2:B:317:ALA:O	2:B:321:THR:HG22	2.20	0.42
4:D:302:PHE:HB2	7:F:73:TYR:CD1	2.54	0.42
1:A:60:ALA:O	1:A:173:PRO:HB3	2.20	0.42
2:B:321:THR:O	2:B:325:ASN:HB2	2.19	0.42
5:E:57:TYR:HB3	9:I:7:TYR:OH	2.20	0.42
7:F:45:PHE:O	7:F:48:LEU:HB2	2.20	0.42
3:C:379:TYR:CE1	3:C:383:VAL:HG21	2.55	0.41
6:H:95:VAL:O	6:H:99:GLU:HB2	2.20	0.41
10:X:20:LEU:HD22	10:X:116:THR:HG21	2.02	0.41
11:Y:12:ALA:HB2	11:Y:105:GLU:HB2	2.01	0.41
1:A:247:SER:O	1:A:432:ALA:HA	2.20	0.41
2:B:251:ALA:O	2:B:255:VAL:HG13	2.20	0.41
8:G:30:SER:HA	8:G:31:PRO:HD3	1.95	0.41
8:G:83:LYS:O	8:G:86:ARG:HG2	2.20	0.41
2:B:175:PHE:CZ	2:B:179:VAL:HG21	2.55	0.41
3:C:4:ARG:HE	3:C:14:ASN:HD21	1.66	0.41
4:D:113:ARG:NH1	16:D:369:HOH:O	2.53	0.41
6:H:82:ARG:O	6:H:86:LYS:HG3	2.21	0.41
11:Y:32:PHE:O	11:Y:90:HIS:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:GLY:H	1:A:61:ASN:ND2	2.17	0.41
1:A:121:ASN:ND2	1:A:125:ILE:HD12	2.36	0.41
4:D:80:GLY:O	4:D:267:LYS:NZ	2.51	0.41
4:D:109:ARG:HG3	4:D:178:SER:HB2	2.03	0.41
5:E:181:HIS:HB2	15:E:4:FES:S1	2.61	0.41
16:X:130:HOH:O	11:Y:49:TYR:HB2	2.20	0.41
3:C:338:GLN:HG3	8:G:70:TRP:CH2	2.55	0.41
3:C:304:VAL:HG13	3:C:308:THR:HG23	2.01	0.41
12:C:401:HEC:HHH	12:C:401:HEC:CBC	2.43	0.41
1:A:164:LEU:HD13	1:A:327:LEU:HD13	2.03	0.41
2:B:241:ILE:CG1	2:B:287:LEU:HB3	2.51	0.41
2:B:252:GLN:HG3	2:B:253:TYR:N	2.34	0.41
3:C:173:ASN:HB3	3:C:174:PRO:HD3	2.03	0.41
5:E:120:HIS:HD2	5:E:151:GLN:HG2	1.84	0.41
2:B:146:LEU:HD13	2:B:354:VAL:CG2	2.51	0.41
2:B:241:ILE:HA	2:B:352:ASN:O	2.21	0.41
3:C:313:VAL:HG22	3:C:319:LYS:HE3	2.03	0.41
11:Y:74:THR:HG22	11:Y:75:ILE:N	2.36	0.40
2:B:137:CYS:SG	2:B:139:VAL:HG22	2.60	0.40
3:C:99:LYS:C	3:C:99:LYS:HD2	2.46	0.40
1:A:72:LEU:HA	1:A:72:LEU:HD12	1.84	0.40
2:B:114:PHE:O	2:B:169:LEU:HD11	2.21	0.40
2:B:301:ILE:O	2:B:305:VAL:HG23	2.21	0.40
3:C:72:VAL:HA	5:E:85:THR:HG22	2.03	0.40
3:C:288:LYS:O	3:C:292:VAL:HG13	2.21	0.40
10:X:45:LYS:HG3	10:X:45:LYS:O	2.21	0.40
11:Y:33:LEU:HD23	11:Y:35:TRP:NE1	2.36	0.40
10:X:24:VAL:CG2	10:X:29:ILE:HD11	2.49	0.40
10:X:54:ASN:H	10:X:54:ASN:ND2	2.13	0.40
1:A:43:ASN:HA	1:A:44:PRO:HD2	1.88	0.40
1:A:74:LYS:HG3	1:A:95:SER:CB	2.47	0.40
1:A:76:ILE:HG23	1:A:140:THR:HG21	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/431 (100%)	400 (93%)	25 (6%)	4 (1%)	14	17
2	B	350/352 (99%)	308 (88%)	38 (11%)	4 (1%)	11	13
3	C	383/385 (100%)	368 (96%)	13 (3%)	2 (0%)	24	31
4	D	243/248 (98%)	236 (97%)	7 (3%)	0	100	100
5	E	183/185 (99%)	172 (94%)	8 (4%)	3 (2%)	7	7
6	H	72/74 (97%)	69 (96%)	3 (4%)	0	100	100
7	F	123/127 (97%)	121 (98%)	2 (2%)	0	100	100
8	G	91/94 (97%)	80 (88%)	7 (8%)	4 (4%)	2	1
9	I	53/66 (80%)	51 (96%)	0	2 (4%)	2	1
10	X	125/127 (98%)	114 (91%)	9 (7%)	2 (2%)	7	7
11	Y	105/107 (98%)	88 (84%)	12 (11%)	5 (5%)	2	1
All	All	2157/2196 (98%)	2007 (93%)	124 (6%)	26 (1%)	10	12

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	335	PRO
3	C	223	SER
5	E	103	LEU
8	G	93	ASN
10	X	33	TYR
2	B	152	ARG
2	B	153	LYS
5	E	46	ASN
11	Y	51	THR
1	A	227	ASN
8	G	37	LEU
8	G	38	GLN
9	I	13	ARG
11	Y	30	ASN
11	Y	68	GLY
1	A	228	LEU
9	I	12	LYS
1	A	230	LEU
2	B	342	ALA

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Mol	Chain	Res	Type
10	X	90	ASP
11	Y	16	GLY
3	C	346	VAL
5	E	102	PRO
1	A	35	GLY
8	G	45	VAL
11	Y	80	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	370/370 (100%)	347 (94%)	23 (6%)	16	24
2	B	301/301 (100%)	280 (93%)	21 (7%)	14	19
3	C	338/338 (100%)	317 (94%)	21 (6%)	16	24
4	D	203/206 (98%)	195 (96%)	8 (4%)	28	43
5	E	151/151 (100%)	146 (97%)	5 (3%)	33	50
6	H	67/67 (100%)	59 (88%)	8 (12%)	5	6
7	F	109/111 (98%)	102 (94%)	7 (6%)	16	23
8	G	77/78 (99%)	75 (97%)	2 (3%)	40	59
9	I	45/54 (83%)	43 (96%)	2 (4%)	25	38
10	X	112/112 (100%)	105 (94%)	7 (6%)	16	23
11	Y	93/93 (100%)	85 (91%)	8 (9%)	10	13
All	All	1866/1881 (99%)	1754 (94%)	112 (6%)	17	25

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	37	VAL
1	A	120	LEU
1	A	142	LYS

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Mol	Chain	Res	Type
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	241	LYS
1	A	252	ARG
1	A	261	ILE
1	A	289	ASN
1	A	306	ILE
1	A	320	LEU
1	A	343	LEU
1	A	361	THR
1	A	370	LEU
1	A	393	GLU
1	A	443	LEU
2	B	17	LEU
2	B	30	THR
2	B	31	LEU
2	B	43	THR
2	B	53	ARG
2	B	54	PHE
2	B	62	ARG
2	B	107	ASP
2	B	128	ARG
2	B	144	ASP
2	B	146	LEU
2	B	169	LEU
2	B	215	LEU
2	B	254	GLU
2	B	255	VAL
2	B	323	LEU
2	B	336	ILE
2	B	338	LEU
2	B	347	LYS
2	B	359	VAL
2	B	362	LEU
3	C	5	LYS
3	C	12	LEU

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Mol	Chain	Res	Type
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
3	C	305	LEU
3	C	312	VAL
3	C	313	VAL
3	C	321	LEU
3	C	336	LEU
3	C	350	LEU
3	C	377	LEU
3	C	382	ARG
4	D	69	LEU
4	D	109	ARG
4	D	113	ARG
4	D	244	THR
4	D	251	VAL
4	D	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	H	74	VAL
6	H	77	GLN
6	H	89	GLU
6	H	94	LEU
6	H	95	VAL
6	H	99	GLU
6	H	117	LEU
6	H	130	LEU
7	F	16	LEU
7	F	30	ASN

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Mol	Chain	Res	Type
7	F	31	GLN
7	F	41	LEU
7	F	48	LEU
7	F	62	ARG
7	F	127	LYS
8	G	60	LEU
8	G	88	GLU
9	I	18	VAL
9	I	48	LEU
10	X	39	ARG
10	X	51	TYR
10	X	54	ASN
10	X	61	ASN
10	X	68	LEU
10	X	79	PHE
10	X	89	GLU
11	Y	18	ARG
11	Y	33	LEU
11	Y	38	GLN
11	Y	80	PRO
11	Y	81	GLU
11	Y	92	ILE
11	Y	93	LYS
11	Y	107	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) 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	102	GLN
1	A	121	ASN
1	A	126	GLN
1	A	156	HIS
1	A	158	ASN
1	A	170	GLN
1	A	171	ASN
1	A	200	HIS

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Mol	Chain	Res	Type
1	A	216	HIS
1	A	227	ASN
1	A	231	GLN
1	A	271	ASN
1	A	289	ASN
1	A	317	HIS
1	A	336	ASN
1	A	350	GLN
1	A	376	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	103	ASN
2	B	170	GLN
2	B	191	ASN
2	B	252	GLN
3	C	7	ASN
3	C	14	ASN
3	C	22	GLN
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	151	GLN
5	E	184	HIS
6	H	77	GLN
6	H	111	GLN
7	F	31	GLN
7	F	53	ASN
7	F	57	GLN
7	F	79	HIS
7	F	91	ASN

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Mol	Chain	Res	Type
7	F	97	GLN
9	I	14	ASN
9	I	29	GLN
9	I	42	ASN
10	X	54	ASN
10	X	59	ASN
10	X	61	ASN
10	X	77	ASN
10	X	78	GLN
10	X	114	GLN
10	X	126	HIS
11	Y	31	ASN
11	Y	34	ASN
11	Y	55	HIS
11	Y	89	GLN
11	Y	90	HIS
11	Y	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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
15	FES	E	4	5	0,4,4	-	-	-		
12	HEC	C	401	3	46,50,50	1.33	5 (10%)	58,82,82	1.39	5 (8%)
13	UQ6	C	506	-	43,43,43	2.62	17 (39%)	54,55,55	2.07	16 (29%)
14	SMA	C	505	-	38,38,38	1.04	4 (10%)	47,52,52	0.92	3 (6%)
12	HEC	C	402	3	46,50,50	1.20	7 (15%)	58,82,82	0.86	0
12	HEC	D	3	4	46,50,50	1.41	2 (4%)	58,82,82	1.72	3 (5%)

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
15	FES	E	4	5	-	-	0/1/1/1
12	HEC	C	401	3	-	9/14/54/54	-
13	UQ6	C	506	-	-	10/39/39/39	0/1/1/1
14	SMA	C	505	-	-	3/34/34/34	0/2/2/2
12	HEC	C	402	3	-	6/14/54/54	-
12	HEC	D	3	4	-	6/14/54/54	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	506	UQ6	C7-C6	7.05	1.59	1.51
13	C	506	UQ6	O5-C5	-5.62	1.24	1.36
12	D	3	HEC	CAB-C3B	5.60	1.53	1.35
13	C	506	UQ6	O2-C2	-5.32	1.24	1.36
12	D	3	HEC	CAC-C3C	5.18	1.51	1.35
12	C	401	HEC	CMC-C2C	5.02	1.61	1.50
13	C	506	UQ6	C2-C3	4.89	1.47	1.39
13	C	506	UQ6	C5-C6	4.55	1.46	1.40
13	C	506	UQ6	C5-C4	4.53	1.46	1.39
13	C	506	UQ6	C2-C1	3.65	1.47	1.40
13	C	506	UQ6	C18-C19	3.34	1.40	1.33
14	C	505	SMA	O1-C2	3.24	1.40	1.36
13	C	506	UQ6	C23-C24	3.17	1.40	1.33
13	C	506	UQ6	C13-C14	3.13	1.40	1.33
13	C	506	UQ6	C8-C9	2.98	1.39	1.33
13	C	506	UQ6	C28-C29	2.96	1.39	1.33
12	C	401	HEC	CMB-C2B	2.89	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	506	UQ6	C33-C34	2.70	1.40	1.32
12	C	402	HEC	CAC-C3C	2.66	1.43	1.35
12	C	402	HEC	CMB-C2B	2.64	1.56	1.50
14	C	505	SMA	C20-C19	2.47	1.35	1.33
14	C	505	SMA	C4A-C5	2.45	1.45	1.40
12	C	402	HEC	CMA-C3A	2.38	1.55	1.50
12	C	402	HEC	CBB-CAB	-2.38	1.40	1.49
12	C	402	HEC	CAB-C3B	2.35	1.42	1.35
13	C	506	UQ6	C11-C9	2.31	1.56	1.51
13	C	506	UQ6	C21-C19	2.31	1.56	1.51
12	C	402	HEC	CBC-CAC	-2.30	1.41	1.49
12	C	401	HEC	O2A-CGA	-2.29	1.23	1.30
12	C	401	HEC	CBB-CAB	-2.28	1.41	1.49
12	C	402	HEC	O2D-CGD	-2.13	1.23	1.30
13	C	506	UQ6	O3-C3	2.13	1.42	1.38
13	C	506	UQ6	C31-C29	2.08	1.55	1.51
12	C	401	HEC	CBC-CAC	-2.07	1.41	1.49
14	C	505	SMA	C7-C8	2.05	1.43	1.40

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	3	HEC	CBB-CAB-C3B	-8.39	110.67	127.43
12	D	3	HEC	CBC-CAC-C3C	-8.10	111.24	127.43
13	C	506	UQ6	C3M-O3-C3	7.03	133.81	114.74
13	C	506	UQ6	C17-C18-C19	5.87	141.07	127.62
12	C	401	HEC	CBC-CAC-C3C	-5.82	115.81	127.43
12	C	401	HEC	CMC-C2C-C1C	5.19	133.32	125.42
13	C	506	UQ6	C4M-O4-C4	4.50	126.95	114.74
13	C	506	UQ6	C21-C19-C18	3.16	128.27	121.17
14	C	505	SMA	C9-C10-C11	-2.97	108.91	114.46
13	C	506	UQ6	C6-C7-C8	2.96	117.12	112.06
13	C	506	UQ6	C1M-C1-C2	-2.96	115.59	120.52
12	C	401	HEC	CMC-C2C-C3C	-2.83	119.89	126.55
13	C	506	UQ6	C27-C28-C29	2.78	134.00	127.62
13	C	506	UQ6	C22-C23-C24	2.70	133.81	127.62
14	C	505	SMA	C4A-C4-C3	-2.52	115.06	118.78
13	C	506	UQ6	C30-C29-C31	-2.39	111.08	115.23
12	C	401	HEC	CMD-C2D-C3D	2.37	130.65	125.62
13	C	506	UQ6	C20-C19-C18	-2.32	117.66	123.63
13	C	506	UQ6	C25-C24-C26	-2.24	111.33	115.23
14	C	505	SMA	O8-C8-C7	2.23	124.00	119.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	3	HEC	CMD-C2D-C3D	2.21	130.31	125.62
13	C	506	UQ6	C17-C16-C14	2.20	120.48	113.19
12	C	401	HEC	CMD-C2D-C1D	-2.18	122.10	125.42
13	C	506	UQ6	C15-C14-C16	-2.14	111.52	115.23
13	C	506	UQ6	C1M-C1-C6	2.13	123.50	120.43
13	C	506	UQ6	C11-C9-C8	2.12	125.94	121.17
13	C	506	UQ6	C16-C14-C13	2.07	125.82	121.17

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	C	401	HEC	C2B-C3B-CAB-CBB
12	C	401	HEC	C4B-C3B-CAB-CBB
12	C	401	HEC	C2C-C3C-CAC-CBC
12	C	401	HEC	C4C-C3C-CAC-CBC
12	C	402	HEC	C2C-C3C-CAC-CBC
12	C	402	HEC	C4C-C3C-CAC-CBC
12	D	3	HEC	C2B-C3B-CAB-CBB
12	D	3	HEC	C4B-C3B-CAB-CBB
12	D	3	HEC	C2C-C3C-CAC-CBC
12	D	3	HEC	C4C-C3C-CAC-CBC
13	C	506	UQ6	C24-C26-C27-C28
13	C	506	UQ6	C15-C14-C16-C17
13	C	506	UQ6	C20-C19-C21-C22
13	C	506	UQ6	C13-C14-C16-C17
13	C	506	UQ6	C18-C19-C21-C22
13	C	506	UQ6	C4-C3-O3-C3M
13	C	506	UQ6	C12-C11-C9-C10
13	C	506	UQ6	C12-C11-C9-C8
13	C	506	UQ6	C19-C21-C22-C23
13	C	506	UQ6	C2-C3-O3-C3M
14	C	505	SMA	C6-C5-O5-C5M
14	C	505	SMA	C4A-C5-O5-C5M
14	C	505	SMA	C9-C10-C11-C22
12	C	401	HEC	C3D-CAD-CBD-CGD
12	C	402	HEC	CAA-CBA-CGA-O1A
12	C	402	HEC	CAA-CBA-CGA-O2A
12	D	3	HEC	CAA-CBA-CGA-O2A
12	D	3	HEC	CAA-CBA-CGA-O1A
12	C	401	HEC	CAD-CBD-CGD-O2D
12	C	401	HEC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
12	C	401	HEC	CAA-CBA-CGA-O2A
12	C	402	HEC	CAD-CBD-CGD-O2D
12	C	402	HEC	CAD-CBD-CGD-O1D
12	C	401	HEC	CAD-CBD-CGD-O1D

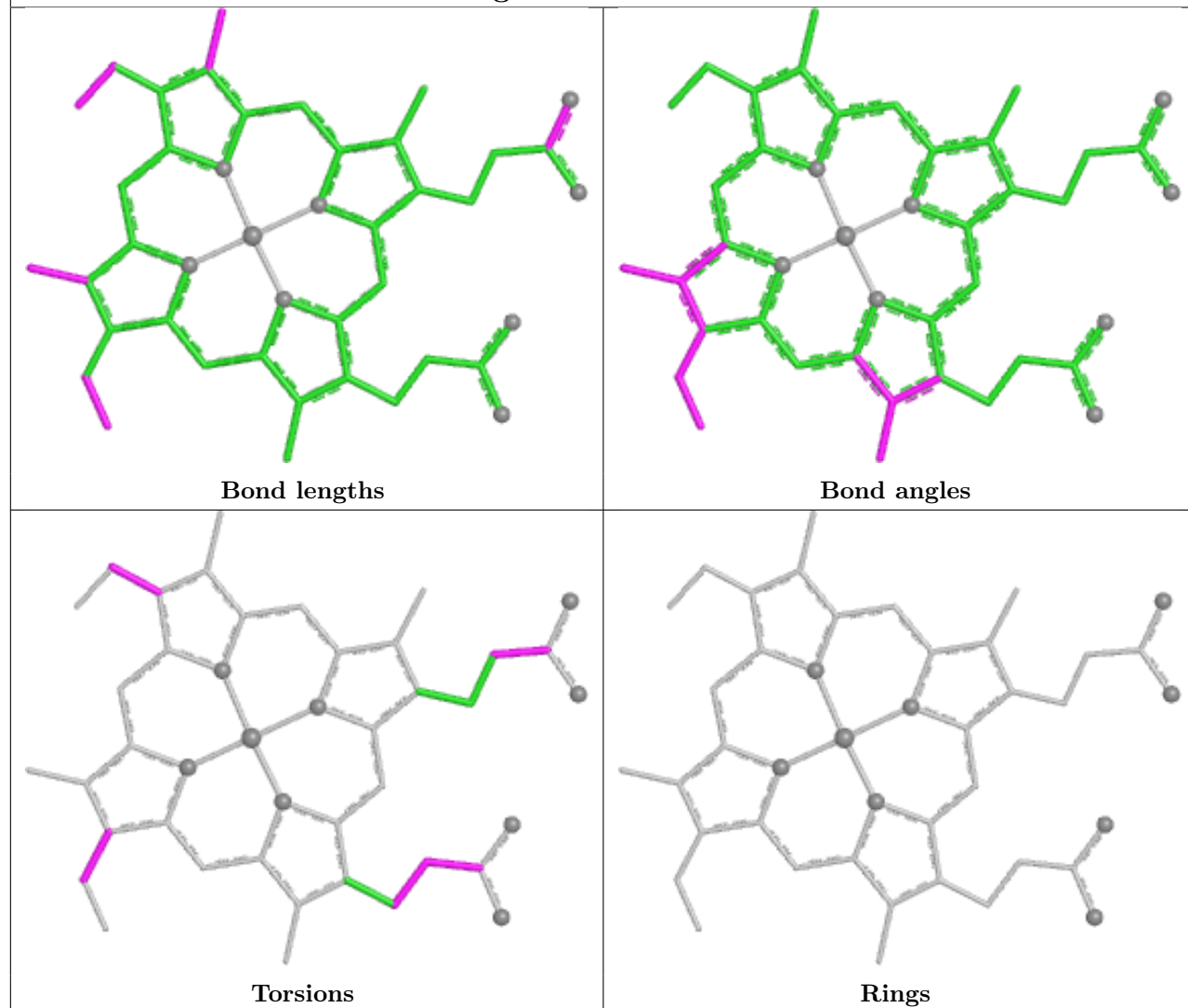
There are no ring outliers.

4 monomers are involved in 11 short contacts:

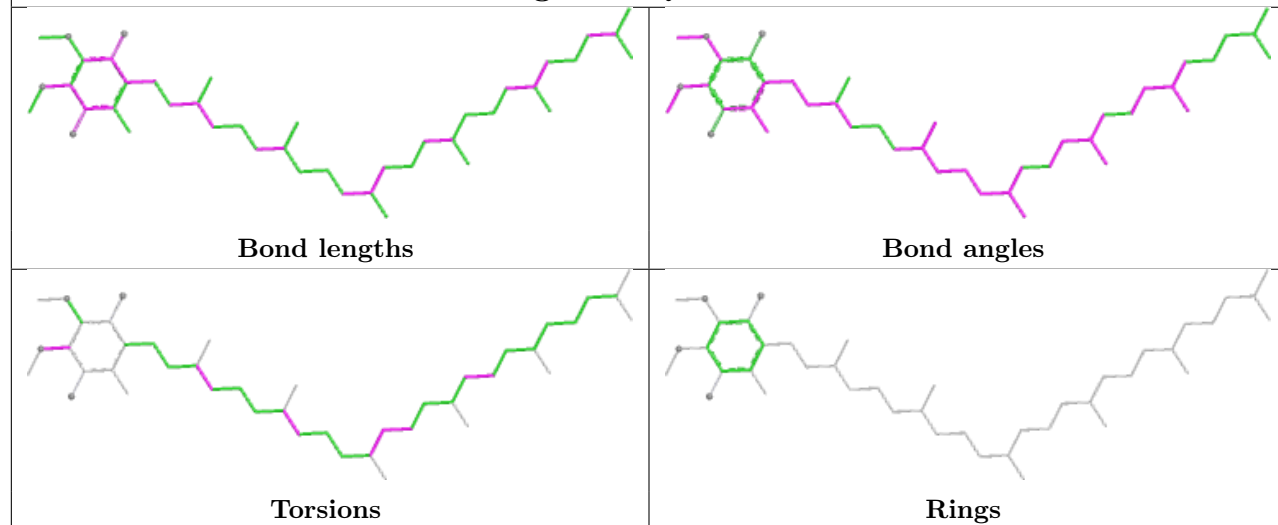
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	E	4	FES	1	0
12	C	401	HEC	2	0
13	C	506	UQ6	7	0
12	D	3	HEC	1	0

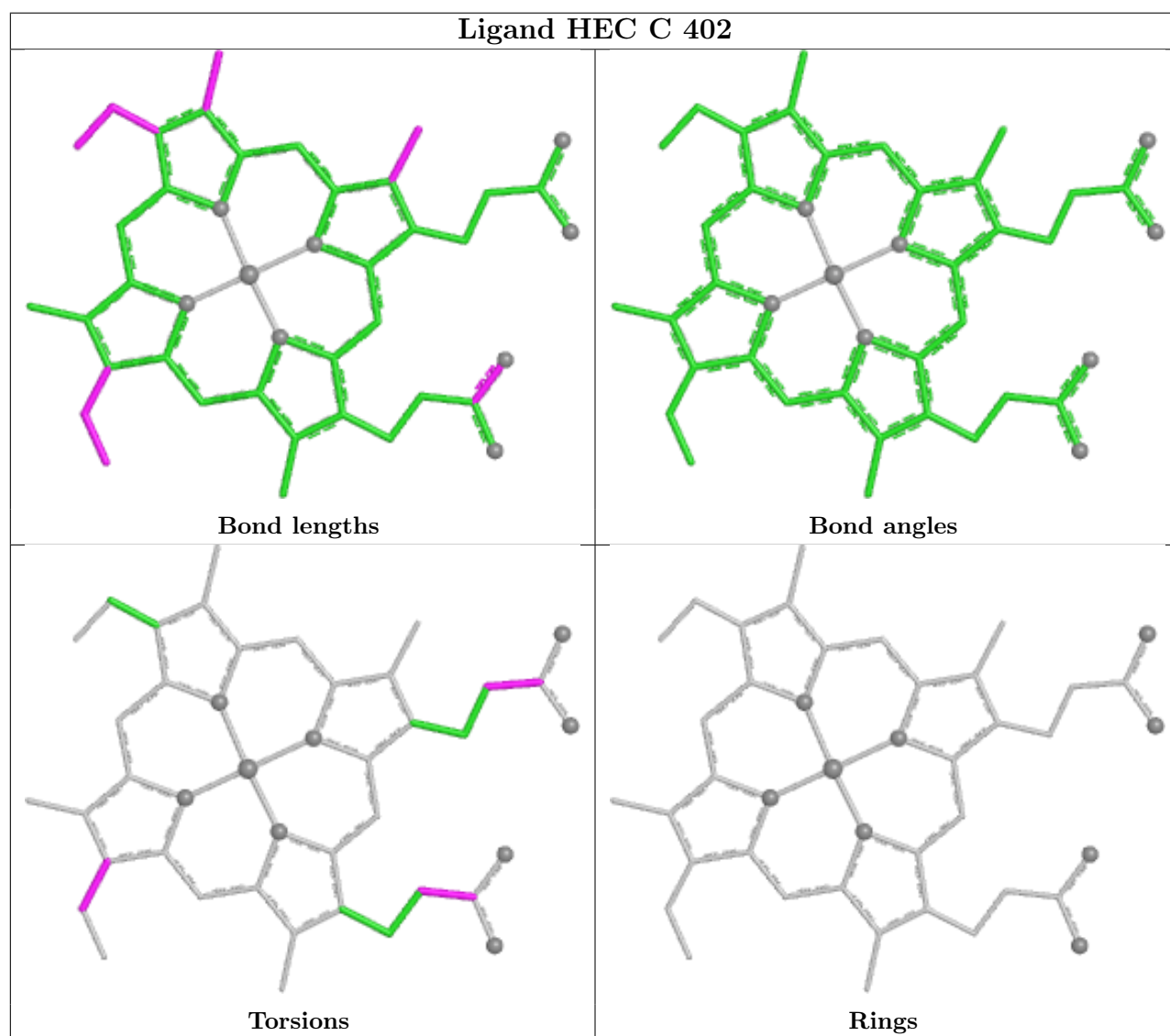
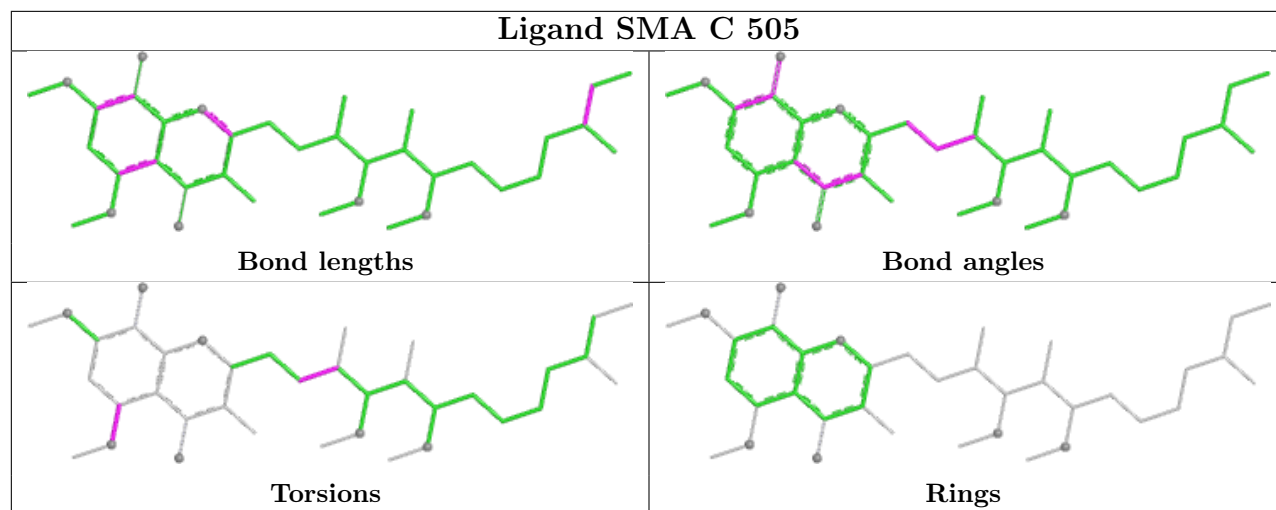
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

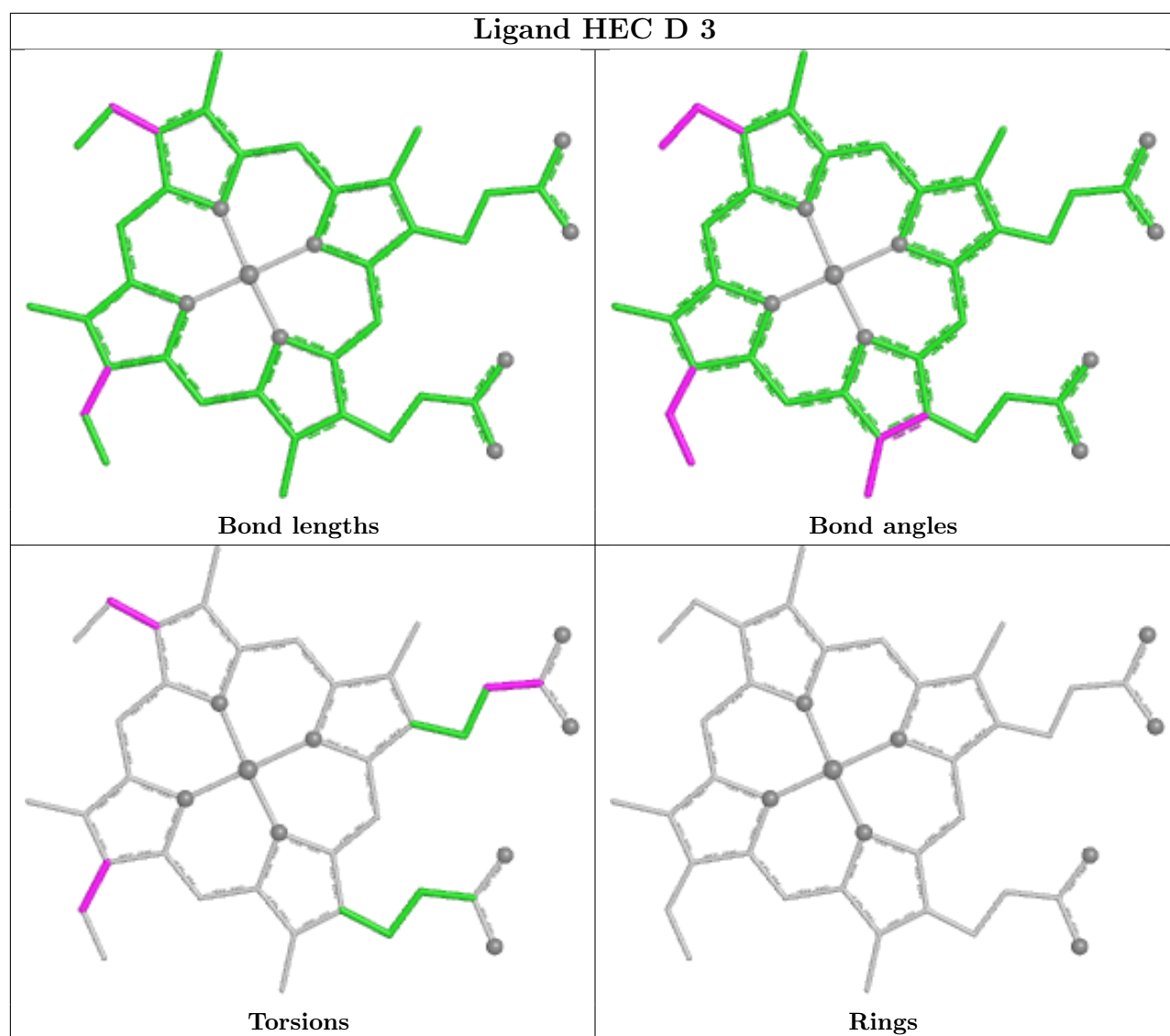
Ligand HEC C 401



Ligand UQ6 C 506







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.