



Full wwPDB EM Validation Report ⓘ

Jul 15, 2025 – 11:05 AM JST

PDB ID : 8X2J / pdb_00008x2j
EMDB ID : EMD-38012
Title : Cryo-EM structure of the photosynthetic alternative complex III with a quinone inhibitor HQNO from *Chloroflexus aurantiacus*
Authors : Xu, X.
Deposited on : 2023-11-09
Resolution : 2.70 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

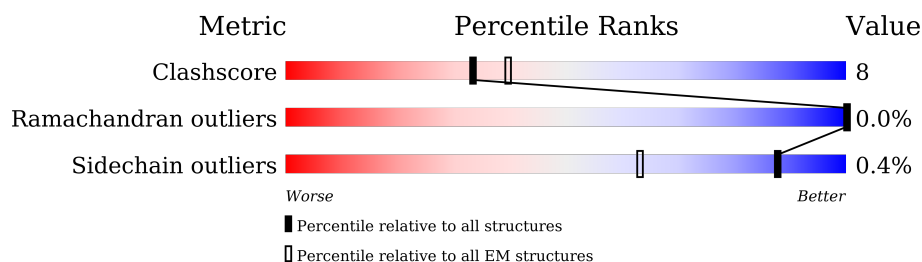
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	219	80% 19%
2	B	1029	72% 21% 8%
3	C	486	75% 17% 8%
4	D	179	77% 21% .
5	E	205	67% 13% 20%
6	F	411	83% 13% .
7	G	112	68% . 29%
8	I	37	78% 22%

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
11	F3S	B	1104	-	-	X	-

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 19918 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Cytochrome c7-like domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	218	Total	C	N	O	S	0	0
			1763	1129	306	313	15		

- Molecule 2 is a protein called Fe-S-cluster-containing hydrogenase components 1-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	951	Total	C	N	O	S	0	0
			7350	4622	1303	1395	30		

- Molecule 3 is a protein called Polysulphide reductase NrfD.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	449	Total	C	N	O	S	0	0
			3655	2476	576	586	17		

- Molecule 4 is a protein called Quinol:cytochrome c oxidoreductase membrane protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	175	Total	C	N	O	S	0	0
			1350	884	215	245	6		

- Molecule 5 is a protein called Cytochrome c domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	164	Total	C	N	O	S	0	0
			1292	819	220	246	7		

- Molecule 6 is a protein called Quinol:cytochrome c oxidoreductase quinone-binding subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	397	Total	C	N	O	S	0	0
			3128	2091	506	514	17		

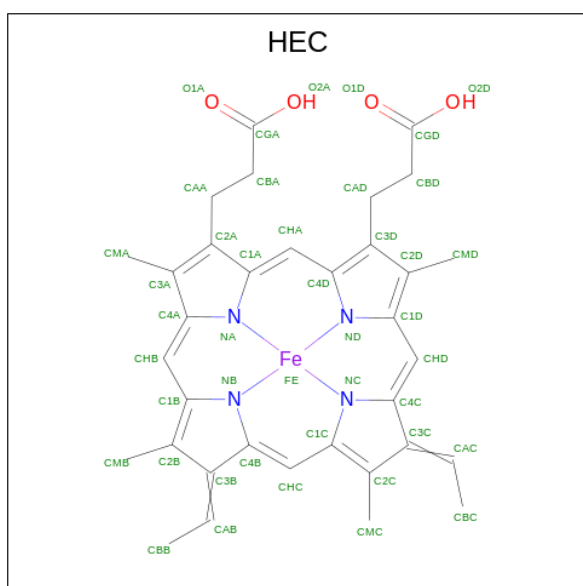
- Molecule 7 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	80	Total	C	N	O	S	0	0
			623	404	108	107	4		

- Molecule 8 is a protein called unknown.

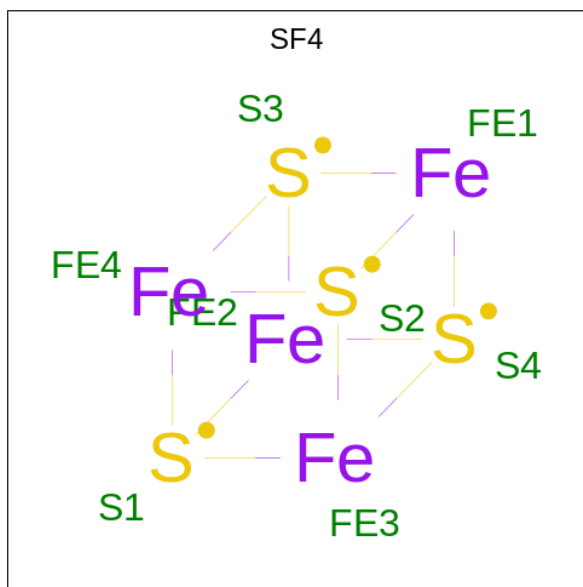
Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	37	Total	C	N	O	S	0	0
			305	212	42	48	3		

- Molecule 9 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



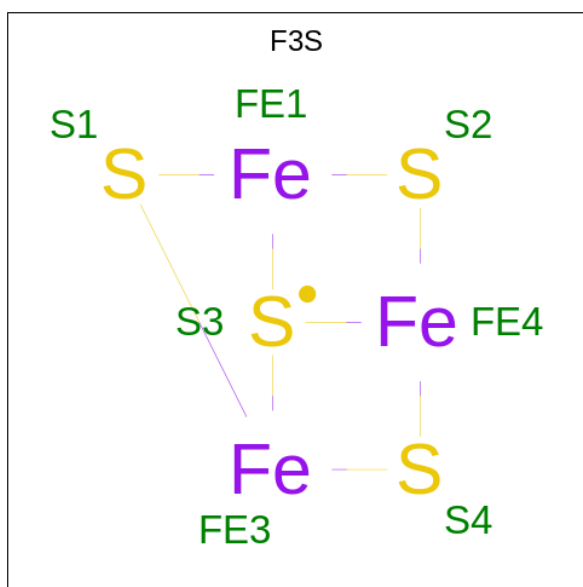
Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
9	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
9	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
9	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
9	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
9	E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 10 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



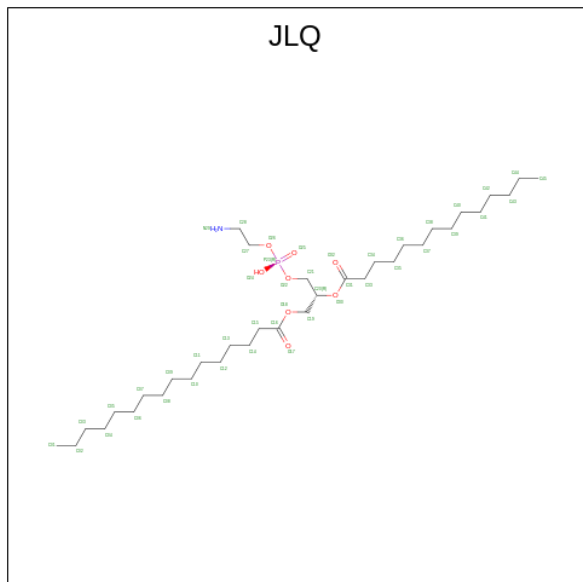
Mol	Chain	Residues	Atoms			AltConf
10	B	1	Total	Fe	S	0
			8	4	4	
10	B	1	Total	Fe	S	0
			8	4	4	
10	B	1	Total	Fe	S	0
			8	4	4	

- Molecule 11 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).



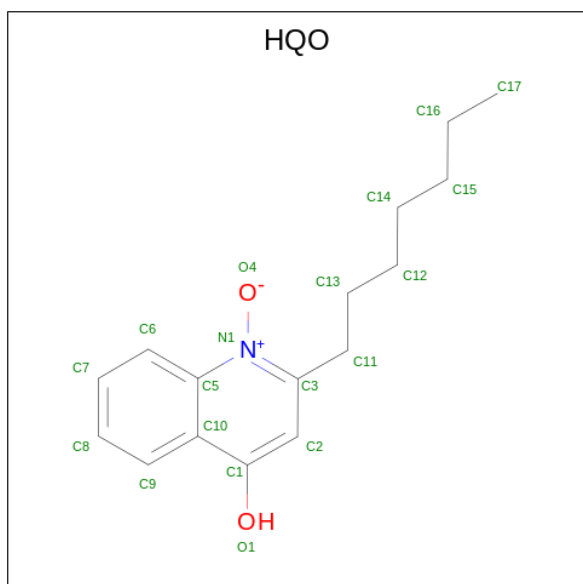
Mol	Chain	Residues	Atoms			AltConf
11	B	1	Total	Fe	S	0
			7	3	4	

- Molecule 12 is [(2 {R})-3-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-2-tetradecanoyloxy-propyl] hexadecanoate (CCD ID: JLQ) (formula: $C_{35}H_{70}NO_8P$).



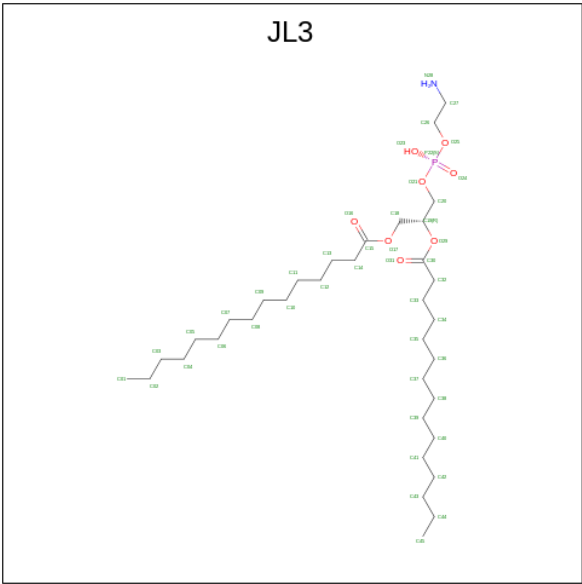
Mol	Chain	Residues	Atoms					AltConf
12	C	1	Total	C	N	O	P	0
			45	35	1	8	1	

- Molecule 13 is 2-HEPTYL-4-HYDROXY QUINOLINE N-OXIDE (CCD ID: HQO) (formula: $C_{16}H_{21}NO_2$).



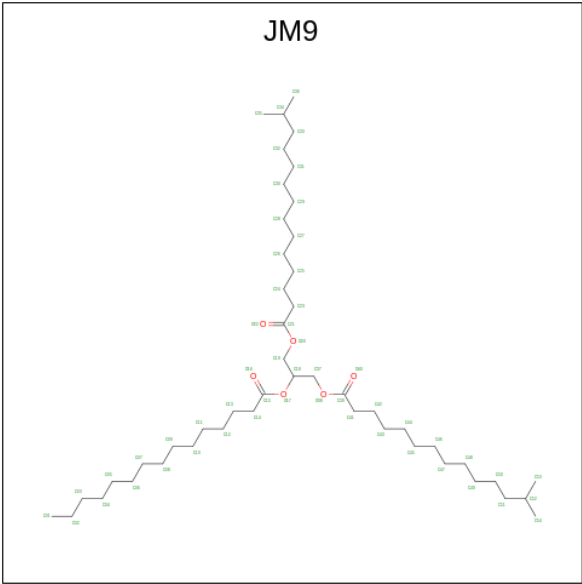
Mol	Chain	Residues	Atoms				AltConf
13	C	1	Total	C	N	O	0
			19	16	1	2	

- Molecule 14 is [(2 {R})-3-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-2-pentadecanoyloxy-propyl] pentadecanoate (CCD ID: JL3) (formula: C₃₅H₇₀NO₈P).



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

- Molecule 15 is 1,3-bis(13-methyltetradecanoyloxy)propan-2-yl pentadecanoate (CCD ID: JM9) (formula: C₄₈H₉₂O₆).

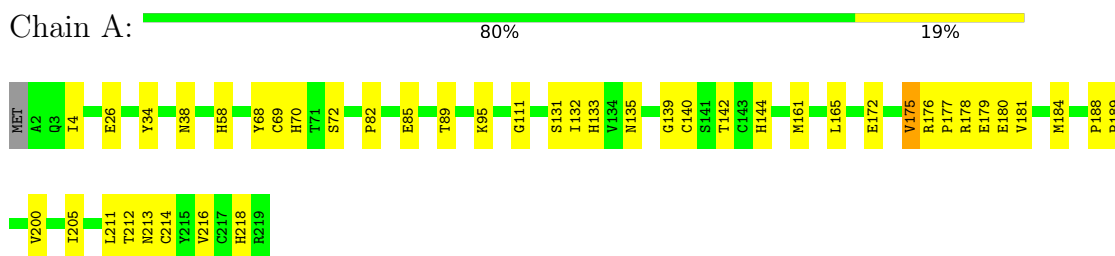


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
15	C	1	54	48	6	0

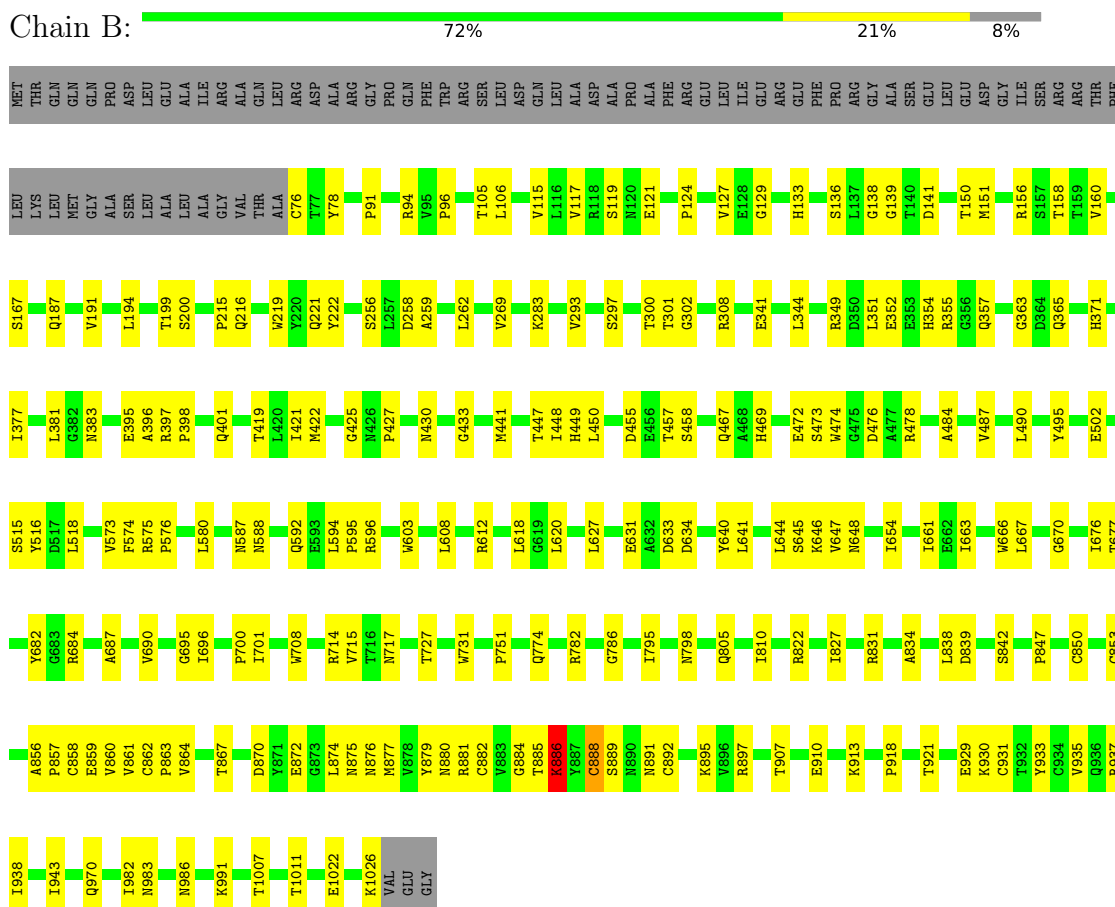
3 Residue-property plots [i](#)

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.


- Molecule 1: Cytochrome c7-like domain-containing protein

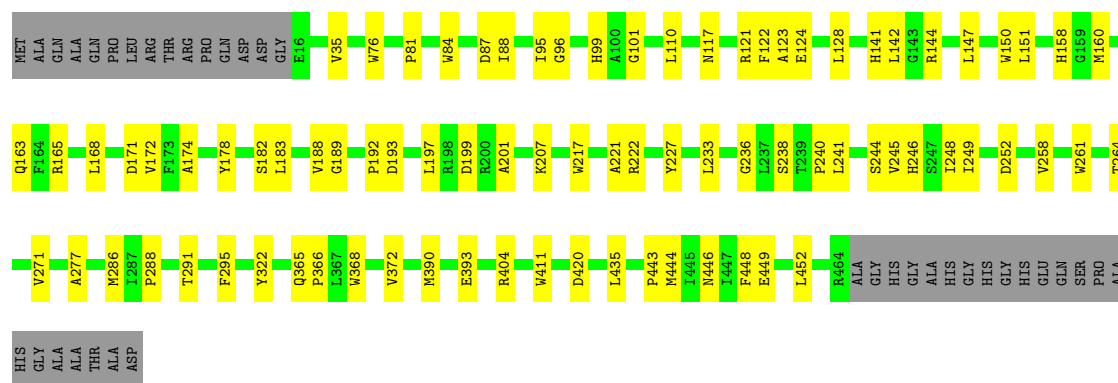


- Molecule 2: Fe-S-cluster-containing hydrogenase components 1-like protein




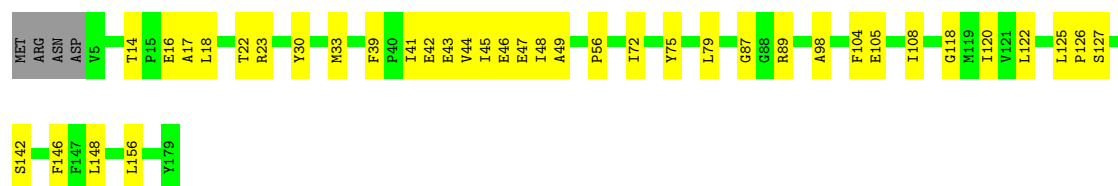
- Molecule 3: Polysulphide reductase NrfD

Chain C:  75% 17% 8%



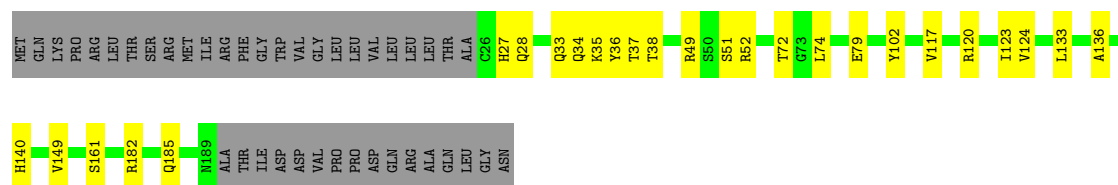
- Molecule 4: Quinol:cytochrome c oxidoreductase membrane protein

Chain D:  77% 21% 2%




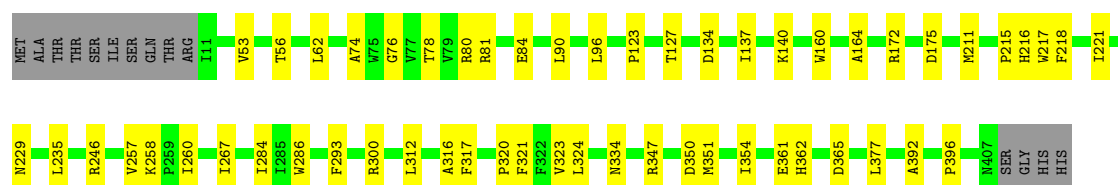
- Molecule 5: Cytochrome c domain-containing protein

Chain E:  67% 13% 20%



- Molecule 6: Quinol:cytochrome c oxidoreductase quinone-binding subunit 2

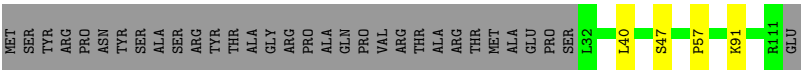
Chain F:  83% 13% 4%



- Molecule 7: Uncharacterized protein

Chain G:  68% 29%





● Molecule 8: unknown



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	160264	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: F3S, JM9, HQO, JL3, HEC, SF4, JLQ

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	0.28	0/1812	0.55	0/2472
2	B	0.29	0/7518	0.52	0/10249
3	C	0.26	0/3787	0.51	0/5179
4	D	0.36	0/1388	0.58	0/1895
5	E	0.19	0/1327	0.43	0/1803
6	F	0.25	0/3226	0.52	0/4408
7	G	0.19	0/635	0.49	0/865
8	I	0.22	0/318	0.48	0/436
All	All	0.27	0/20011	0.52	0/27307

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1763	0	1713	36	0
2	B	7350	0	7178	159	0
3	C	3655	0	3686	64	0
4	D	1350	0	1341	37	0
5	E	1292	0	1216	27	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	3128	0	3175	31	0
7	G	623	0	660	4	0
8	I	305	0	302	5	0
9	A	215	0	150	10	0
9	E	43	0	30	2	0
10	B	24	0	0	1	0
11	B	7	0	0	5	0
12	C	45	0	0	0	0
13	C	19	0	20	1	0
14	C	45	0	0	0	0
15	C	54	0	0	0	0
All	All	19918	0	19471	319	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 8.

All (319) 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)
2:B:888:CYS:SG	11:B:1104:F3S:FE1	1.42	1.09
4:D:156:LEU:HD12	4:D:156:LEU:O	1.65	0.95
3:C:171:ASP:OD1	3:C:248:ILE:HG22	1.80	0.81
5:E:124:VAL:O	5:E:124:VAL:HG13	1.82	0.80
2:B:620:LEU:HD13	2:B:647:VAL:HG21	1.66	0.78
4:D:120:ILE:HD12	4:D:125:LEU:HD23	1.66	0.77
4:D:45:ILE:HG23	4:D:49:ALA:HB3	1.69	0.75
2:B:297:SER:HB3	2:B:677:THR:HG21	1.70	0.74
1:A:216:VAL:HG13	9:A:302:HEC:HBA1	1.74	0.70
5:E:123:ILE:O	5:E:124:VAL:HG12	1.91	0.69
2:B:881:ARG:HH12	3:C:150:TRP:HB3	1.58	0.69
4:D:156:LEU:O	4:D:156:LEU:CD1	2.41	0.69
1:A:142:THR:HG23	1:A:176:ARG:HH21	1.57	0.68
2:B:133:HIS:HB3	2:B:136:SER:HB3	1.77	0.67
4:D:30:TYR:CE1	4:D:156:LEU:CD1	2.78	0.67
2:B:888:CYS:HG	11:B:1104:F3S:FE1	0.38	0.66
4:D:75:TYR:O	4:D:79:LEU:HB2	1.96	0.66
9:A:301:HEC:HHB	2:B:881:ARG:HD3	1.77	0.66
2:B:888:CYS:SG	11:B:1104:F3S:S1	2.95	0.64
2:B:618:LEU:HD22	2:B:717:ASN:HB2	1.79	0.64
2:B:870:ASP:HB2	2:B:874:LEU:H	1.63	0.64
2:B:119:SER:HB3	2:B:490:LEU:HD23	1.81	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:449:HIS:HD1	2:B:458:SER:HG	1.48	0.61
3:C:277:ALA:HB2	3:C:390:MET:HG2	1.83	0.61
1:A:211:LEU:HD21	9:A:302:HEC:HBD1	1.83	0.61
2:B:676:ILE:HD12	2:B:715:VAL:HG21	1.83	0.61
3:C:171:ASP:OD1	3:C:248:ILE:CG2	2.48	0.61
2:B:425:GLY:O	2:B:430:ASN:ND2	2.35	0.60
6:F:300:ARG:NH2	6:F:354:ILE:O	2.34	0.59
1:A:70:HIS:HE1	9:A:304:HEC:ND	2.01	0.59
2:B:94:ARG:NH1	5:E:52:ARG:O	2.35	0.59
4:D:30:TYR:CE1	4:D:156:LEU:HD12	2.38	0.59
2:B:862:CYS:O	3:C:163:GLN:NE2	2.34	0.59
2:B:78:TYR:O	5:E:28:GLN:NE2	2.35	0.58
6:F:80:ARG:HD2	6:F:396:PRO:HG3	1.85	0.58
2:B:573:VAL:HB	2:B:677:THR:HG22	1.84	0.58
2:B:805:GLN:HG3	2:B:810:ILE:HB	1.86	0.58
2:B:221:GLN:HG2	2:B:397:ARG:HH21	1.69	0.58
2:B:863:PRO:HB3	3:C:168:LEU:HB2	1.85	0.58
2:B:881:ARG:HE	3:C:160:MET:HE2	1.69	0.58
2:B:150:THR:OG1	2:B:588:ASN:ND2	2.37	0.57
5:E:49:ARG:O	5:E:52:ARG:NH2	2.37	0.57
1:A:140:CYS:HB2	1:A:184:MET:HE1	1.87	0.57
2:B:684:ARG:HE	2:B:687:ALA:HB2	1.70	0.57
3:C:221:ALA:HB1	4:D:45:ILE:HG12	1.86	0.57
1:A:135:ASN:O	1:A:178:ARG:NE	2.36	0.57
6:F:81:ARG:NH1	6:F:175:ASP:OD2	2.38	0.57
2:B:907:THR:HA	5:E:34:GLN:HG2	1.87	0.57
1:A:218:HIS:CE1	9:A:301:HEC:ND	2.73	0.56
2:B:885:THR:HG22	3:C:142:LEU:HD11	1.87	0.56
3:C:264:THR:HA	6:F:284:ILE:HD13	1.87	0.56
6:F:134:ASP:OD2	6:F:216:HIS:NE2	2.36	0.56
1:A:200:VAL:HG13	1:A:205:ILE:HB	1.87	0.56
6:F:320:PRO:O	6:F:324:LEU:HB2	2.06	0.56
4:D:120:ILE:O	4:D:126:PRO:HD3	2.06	0.56
4:D:118:GLY:O	4:D:122:LEU:HB2	2.06	0.56
6:F:229:ASN:ND2	6:F:351:MET:SD	2.79	0.56
1:A:69:CYS:HB3	1:A:82:PRO:HG3	1.88	0.56
2:B:352:GLU:HA	2:B:355:ARG:HE	1.71	0.56
4:D:22:THR:HG21	4:D:44:VAL:HG13	1.86	0.56
2:B:864:VAL:HB	2:B:881:ARG:CZ	2.36	0.56
3:C:121:ARG:NH2	3:C:446:ASN:OD1	2.38	0.55
5:E:124:VAL:O	5:E:124:VAL:CG1	2.53	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:94:ARG:NH2	2:B:121:GLU:OE1	2.39	0.55
2:B:441:MET:HE3	2:B:447:THR:HG21	1.88	0.55
4:D:46:GLU:HG3	4:D:47:GLU:OE1	2.06	0.55
2:B:427:PRO:HD2	2:B:457:THR:HG21	1.87	0.55
2:B:258:ASP:O	2:B:365:GLN:NE2	2.40	0.55
4:D:30:TYR:CE1	4:D:156:LEU:HD11	2.42	0.55
2:B:888:CYS:HB2	2:B:897:ARG:NE	2.22	0.55
3:C:35:VAL:HG11	3:C:444:MET:HE1	1.88	0.54
6:F:62:LEU:HD12	6:F:164:ALA:HB2	1.89	0.54
2:B:478:ARG:HA	2:B:484:ALA:H	1.72	0.54
3:C:249:ILE:O	3:C:252:ASP:OD1	2.23	0.54
3:C:217:TRP:HA	4:D:125:LEU:HD11	1.90	0.54
4:D:87:GLY:O	4:D:89:ARG:NH1	2.38	0.54
2:B:256:SER:HB2	2:B:293:VAL:HG12	1.89	0.54
1:A:139:GLY:HA3	1:A:176:ARG:CZ	2.38	0.54
3:C:449:GLU:HA	3:C:452:LEU:HB3	1.89	0.54
2:B:858:CYS:SG	2:B:875:ASN:ND2	2.80	0.54
2:B:913:LYS:HG2	5:E:34:GLN:HB3	1.90	0.54
2:B:676:ILE:CD1	2:B:715:VAL:HG21	2.38	0.53
2:B:850:CYS:SG	2:B:930:LYS:NZ	2.81	0.53
2:B:877:MET:SD	2:B:897:ARG:NH2	2.81	0.53
6:F:90:LEU:HD13	6:F:160:TRP:HB3	1.89	0.53
2:B:640:TYR:O	2:B:644:LEU:HG	2.09	0.53
5:E:136:ALA:O	5:E:182:ARG:NH2	2.38	0.53
2:B:654:ILE:HG12	2:B:715:VAL:HG22	1.90	0.53
6:F:96:LEU:HD13	6:F:377:LEU:HD11	1.90	0.53
2:B:381:LEU:HD23	2:B:383:ASN:HD21	1.73	0.53
3:C:221:ALA:HB3	4:D:48:ILE:HD11	1.91	0.53
2:B:575:ARG:HE	2:B:576:PRO:HD2	1.74	0.52
2:B:283:LYS:HG2	2:B:751:PRO:HG2	1.90	0.52
2:B:222:TYR:HA	2:B:401:GLN:HB3	1.92	0.52
2:B:262:LEU:HD12	2:B:301:THR:HA	1.90	0.52
2:B:986:ASN:O	2:B:991:LYS:NZ	2.42	0.52
2:B:117:VAL:HG22	2:B:127:VAL:HG22	1.91	0.52
4:D:156:LEU:HD12	4:D:156:LEU:C	2.34	0.52
2:B:774:GLN:NE2	6:F:286:TRP:O	2.43	0.52
5:E:149:VAL:HG11	9:E:301:HEC:HBD1	1.92	0.52
2:B:884:GLY:HA3	3:C:142:LEU:O	2.10	0.52
3:C:117:ASN:ND2	3:C:449:GLU:O	2.41	0.52
3:C:201:ALA:HB3	3:C:207:LYS:HD3	1.92	0.52
6:F:316:ALA:HB1	6:F:347:ARG:HH22	1.75	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:182:ARG:NH1	5:E:185:GLN:OE1	2.43	0.51
4:D:30:TYR:CD1	4:D:156:LEU:HD11	2.46	0.51
2:B:199:THR:HG22	2:B:395:GLU:HA	1.92	0.51
2:B:219:TRP:HB3	2:B:397:ARG:NH1	2.25	0.51
3:C:96:GLY:HA2	3:C:246:HIS:HE1	1.75	0.51
3:C:121:ARG:NH2	3:C:189:GLY:O	2.42	0.51
4:D:23:ARG:NH1	4:D:47:GLU:OE2	2.44	0.51
2:B:91:PRO:HB2	2:B:94:ARG:HB2	1.93	0.51
3:C:178:TYR:HB2	3:C:245:VAL:HG21	1.91	0.51
5:E:38:THR:O	5:E:51:SER:OG	2.29	0.51
2:B:888:CYS:SG	11:B:1104:F3S:S3	3.10	0.50
4:D:33:MET:HE3	4:D:148:LEU:HD11	1.93	0.50
2:B:645:SER:O	2:B:646:LYS:HB3	2.12	0.50
2:B:822:ARG:NH2	3:C:76:TRP:O	2.44	0.50
3:C:147:LEU:HD11	5:E:27:HIS:HE1	1.76	0.50
2:B:882:CYS:O	3:C:144:ARG:NH2	2.40	0.50
2:B:885:THR:HG22	3:C:142:LEU:CD1	2.42	0.50
2:B:921:THR:OG1	5:E:33:GLN:NE2	2.42	0.50
6:F:76:GLY:O	6:F:80:ARG:HB2	2.12	0.50
1:A:139:GLY:HA2	1:A:181:VAL:HG13	1.94	0.50
3:C:366:PRO:HB2	3:C:372:VAL:HG11	1.92	0.50
1:A:4:ILE:HD13	3:C:207:LYS:HB3	1.94	0.50
2:B:354:HIS:HB3	2:B:357:GLN:HB2	1.94	0.49
5:E:72:THR:HG23	5:E:74:LEU:H	1.77	0.49
1:A:144:HIS:CE1	9:A:303:HEC:ND	2.80	0.49
2:B:308:ARG:NH1	2:B:670:GLY:O	2.45	0.49
3:C:122:PHE:HB3	3:C:286:MET:HE1	1.94	0.49
3:C:258:VAL:HB	3:C:261:TRP:HB2	1.93	0.49
2:B:139:GLY:O	2:B:269:VAL:HG11	2.13	0.49
2:B:641:LEU:HD22	2:B:838:LEU:HD12	1.94	0.49
2:B:892:CYS:O	2:B:895:LYS:NZ	2.42	0.49
3:C:87:ASP:OD1	3:C:87:ASP:N	2.46	0.49
4:D:14:THR:HG23	4:D:17:ALA:H	1.76	0.49
1:A:132:ILE:HB	2:B:943:ILE:HG23	1.95	0.49
1:A:214:CYS:HB2	2:B:876:ASN:HD22	1.78	0.49
4:D:125:LEU:O	4:D:127:SER:N	2.38	0.49
2:B:918:PRO:HA	5:E:35:LYS:HD2	1.93	0.48
5:E:123:ILE:O	5:E:124:VAL:CG1	2.58	0.48
2:B:341:GLU:HA	2:B:344:LEU:HD12	1.96	0.48
2:B:455:ASP:OD1	2:B:684:ARG:NH2	2.47	0.48
2:B:515:SER:HA	2:B:518:LEU:HD12	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:595:PRO:HG3	2:B:727:THR:HG21	1.96	0.48
3:C:264:THR:HG23	6:F:221:ILE:H	1.78	0.48
6:F:172:ARG:HE	6:F:392:ALA:HB2	1.79	0.48
1:A:111:GLY:O	5:E:49:ARG:NH2	2.47	0.47
6:F:211:MET:HE3	6:F:218:PHE:HA	1.95	0.47
4:D:125:LEU:N	4:D:126:PRO:CD	2.78	0.47
6:F:81:ARG:NE	6:F:84:GLU:OE1	2.46	0.47
2:B:221:GLN:HG2	2:B:397:ARG:NH2	2.29	0.47
3:C:452:LEU:HB2	4:D:39:PHE:HB2	1.96	0.47
2:B:194:LEU:HB3	2:B:422:MET:HG3	1.97	0.47
3:C:192:PRO:HG2	3:C:448:PHE:CE1	2.49	0.47
2:B:618:LEU:HD22	2:B:717:ASN:CA	2.44	0.47
2:B:731:TRP:CD1	2:B:831:ARG:HH12	2.32	0.47
2:B:608:LEU:HD23	2:B:666:TRP:HB3	1.95	0.47
2:B:897:ARG:HA	2:B:930:LYS:HB3	1.95	0.47
3:C:238:SER:HA	3:C:241:LEU:HB3	1.96	0.47
2:B:857:PRO:HB2	2:B:891:ASN:O	2.14	0.47
3:C:174:ALA:HB1	3:C:245:VAL:HG22	1.95	0.47
2:B:592:GLN:HG3	2:B:603:TRP:HA	1.97	0.46
2:B:682:TYR:HB3	2:B:695:GLY:HA3	1.97	0.46
2:B:879:TYR:HE1	2:B:929:GLU:HA	1.80	0.46
6:F:246:ARG:NH2	6:F:334:ASN:OD1	2.47	0.46
2:B:618:LEU:HD22	2:B:717:ASN:N	2.30	0.46
3:C:124:GLU:OE2	3:C:182:SER:OG	2.33	0.46
2:B:618:LEU:HD22	2:B:717:ASN:CB	2.45	0.46
6:F:320:PRO:HA	6:F:323:VAL:HG22	1.97	0.46
2:B:877:MET:CE	2:B:882:CYS:HB2	2.46	0.46
7:G:40:LEU:HD13	8:I:21:THR:HG23	1.96	0.46
2:B:580:LEU:HD21	2:B:592:GLN:HE22	1.80	0.46
2:B:910:GLU:OE1	5:E:36:TYR:OH	2.32	0.46
3:C:171:ASP:HB3	13:C:502:HQQ:O4	2.16	0.46
3:C:233:LEU:HD11	4:D:56:PRO:HG3	1.97	0.46
3:C:165:ARG:HA	4:D:98:ALA:HB1	1.97	0.46
6:F:317:PHE:O	6:F:321:PHE:HB3	2.16	0.46
1:A:218:HIS:CG	2:B:880:ASN:HD21	2.33	0.46
2:B:199:THR:HB	2:B:478:ARG:HB2	1.98	0.46
2:B:648:ASN:HD21	2:B:731:TRP:HH2	1.64	0.46
4:D:18:LEU:HD22	4:D:146:PHE:HB3	1.98	0.46
2:B:396:ALA:O	2:B:398:PRO:HD3	2.16	0.46
2:B:870:ASP:HB3	2:B:872:GLU:H	1.81	0.46
2:B:661:ILE:HB	2:B:701:ILE:HG13	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:41:ILE:O	4:D:42:GLU:HB3	2.15	0.45
2:B:156:ARG:NH2	2:B:472:GLU:OE2	2.48	0.45
3:C:197:LEU:HD11	3:C:443:PRO:HD3	1.97	0.45
5:E:37:THR:HG22	5:E:38:THR:H	1.80	0.45
1:A:34:TYR:OH	2:B:76:CYS:O	2.32	0.45
1:A:72:SER:O	1:A:72:SER:OG	2.33	0.45
9:A:301:HEC:HMA1	2:B:881:ARG:HD2	1.98	0.45
2:B:377:ILE:O	2:B:381:LEU:HB2	2.16	0.45
2:B:654:ILE:HG12	2:B:715:VAL:HG13	1.99	0.45
2:B:633:ASP:OD1	2:B:633:ASP:N	2.49	0.45
2:B:867:THR:OG1	2:B:875:ASN:OD1	2.35	0.45
3:C:110:LEU:HD11	3:C:236:GLY:HA2	1.97	0.45
6:F:53:VAL:O	6:F:56:THR:OG1	2.26	0.45
1:A:165:LEU:HD22	1:A:212:THR:HG23	1.99	0.45
2:B:860:VAL:HG13	2:B:861:VAL:HG13	1.99	0.45
5:E:161:SER:HB2	9:E:301:HEC:HBD2	1.99	0.45
2:B:574:PHE:HB2	2:B:708:TRP:HA	1.98	0.45
1:A:72:SER:HB2	2:B:96:PRO:HD2	1.99	0.45
2:B:106:LEU:HD12	2:B:115:VAL:HG11	1.98	0.45
2:B:786:GLY:HA3	2:B:982:ILE:HD11	1.98	0.45
3:C:420:ASP:OD1	3:C:420:ASP:N	2.50	0.45
2:B:105:THR:HB	2:B:487:VAL:HG22	1.98	0.44
2:B:646:LYS:HD2	2:B:646:LYS:C	2.42	0.44
3:C:240:PRO:HB2	4:D:104:PHE:HZ	1.82	0.44
5:E:123:ILE:C	5:E:124:VAL:HG12	2.43	0.44
1:A:26:GLU:OE1	7:G:47:SER:OG	2.34	0.44
2:B:782:ARG:O	2:B:983:ASN:ND2	2.43	0.44
2:B:850:CYS:HB3	2:B:931:CYS:HB3	1.99	0.44
6:F:140:LYS:NZ	6:F:215:PRO:O	2.38	0.44
2:B:363:GLY:O	2:B:371:HIS:NE2	2.51	0.44
2:B:897:ARG:NH1	10:B:1103:SF4:S4	2.86	0.44
3:C:222:ARG:NH1	8:I:4:GLU:OE1	2.50	0.44
6:F:217:TRP:HD1	6:F:293:PHE:HA	1.83	0.44
1:A:38:ASN:HB2	7:G:57:PRO:HD2	2.00	0.44
2:B:587:ASN:HA	2:B:690:VAL:O	2.18	0.44
2:B:648:ASN:HB3	2:B:666:TRP:CE3	2.53	0.44
1:A:213:ASN:HB2	1:A:216:VAL:HG23	2.00	0.43
2:B:351:LEU:HD22	2:B:381:LEU:HD21	2.00	0.43
2:B:422:MET:HG2	2:B:427:PRO:HG2	1.99	0.43
2:B:300:THR:HB	2:B:795:ILE:HB	1.99	0.43
3:C:151:LEU:HB3	3:C:172:VAL:HG21	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:288:PRO:HA	3:C:291:THR:HG22	2.00	0.43
4:D:14:THR:OG1	4:D:16:GLU:OE1	2.35	0.43
2:B:450:LEU:HG	2:B:467:GLN:HB2	2.01	0.43
2:B:859:GLU:HA	2:B:867:THR:HG23	2.00	0.43
2:B:1022:GLU:HG3	2:B:1026:LYS:HE2	1.99	0.43
3:C:121:ARG:NH1	3:C:193:ASP:OD2	2.39	0.43
2:B:1022:GLU:HA	2:B:1026:LYS:HB2	1.99	0.43
1:A:132:ILE:HG23	1:A:133:HIS:HD2	1.83	0.43
2:B:631:GLU:HA	2:B:634:ASP:HB2	2.01	0.43
7:G:91:LYS:HA	7:G:91:LYS:HD2	1.85	0.43
1:A:176:ARG:O	1:A:177:PRO:C	2.60	0.43
2:B:937:ARG:NH1	2:B:970:GLN:OE1	2.44	0.43
3:C:99:HIS:CE1	3:C:271:VAL:HG13	2.54	0.43
6:F:123:PRO:O	6:F:127:THR:OG1	2.29	0.43
2:B:502:GLU:HG3	2:B:515:SER:HB2	2.01	0.43
2:B:612:ARG:NH2	2:B:839:ASP:OD2	2.49	0.43
2:B:933:TYR:OH	2:B:1011:THR:OG1	2.30	0.43
1:A:131:SER:O	1:A:135:ASN:ND2	2.45	0.42
2:B:422:MET:HE2	2:B:449:HIS:HD2	1.84	0.42
2:B:663:ILE:HA	2:B:696:ILE:HD12	1.99	0.42
2:B:596:ARG:NH2	2:B:682:TYR:OH	2.44	0.42
2:B:853:CYS:HB3	2:B:1007:THR:HB	2.00	0.42
1:A:95:LYS:HD2	1:A:95:LYS:HA	1.86	0.42
2:B:256:SER:HB3	2:B:259:ALA:HB3	2.00	0.42
1:A:161:MET:HG3	9:A:301:HEC:NC	2.33	0.42
2:B:293:VAL:HG21	2:B:302:GLY:HA2	2.01	0.42
2:B:474:TRP:CD1	2:B:516:TYR:HB2	2.55	0.42
3:C:128:LEU:HD11	3:C:183:LEU:HA	2.02	0.42
3:C:244:SER:OG	4:D:105:GLU:OE2	2.34	0.42
8:I:8:ASP:HB3	8:I:11:VAL:HG23	2.00	0.42
2:B:888:CYS:SG	11:B:1104:F3S:S2	3.17	0.42
3:C:241:LEU:HB2	4:D:108:ILE:HG21	2.00	0.42
6:F:74:ALA:O	6:F:78:THR:OG1	2.37	0.42
6:F:362:HIS:HB2	6:F:365:ASP:HB2	2.01	0.42
2:B:594:LEU:HD11	2:B:798:ASN:HB3	2.02	0.42
6:F:137:ILE:HG12	6:F:215:PRO:HB2	2.01	0.42
5:E:79:GLU:HG2	5:E:140:HIS:HB2	2.01	0.42
2:B:648:ASN:CG	2:B:667:LEU:H	2.27	0.42
2:B:895:LYS:HD2	3:C:81:PRO:HA	2.02	0.42
3:C:101:GLY:HA2	3:C:123:ALA:HB1	2.02	0.42
3:C:365:GLN:HA	3:C:368:TRP:HD1	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:3:PRO:HG2	8:I:6:SER:HB3	2.01	0.42
2:B:124:PRO:HG3	2:B:490:LEU:HB2	2.01	0.41
2:B:187:GLN:HG2	2:B:215:PRO:HD2	2.02	0.41
2:B:151:MET:O	2:B:156:ARG:NH1	2.44	0.41
2:B:349:ARG:HA	2:B:349:ARG:HD3	1.81	0.41
2:B:834:ALA:O	2:B:842:SER:OG	2.34	0.41
2:B:935:VAL:HA	2:B:938:ILE:HB	2.02	0.41
3:C:322:TYR:OH	3:C:393:GLU:OE1	2.33	0.41
3:C:435:LEU:HD23	3:C:435:LEU:HA	1.95	0.41
6:F:257:VAL:HA	6:F:260:ILE:HD12	2.02	0.41
2:B:421:ILE:HG13	2:B:448:ILE:HD13	2.02	0.41
2:B:433:GLY:HA3	2:B:700:PRO:HA	2.02	0.41
2:B:827:ILE:HD11	2:B:847:PRO:HB3	2.03	0.41
9:A:305:HEC:O1D	5:E:120:ARG:NH1	2.54	0.41
2:B:141:ASP:OD1	2:B:141:ASP:N	2.51	0.41
4:D:72:ILE:HD13	4:D:72:ILE:HA	1.96	0.41
1:A:58:HIS:CE1	9:A:305:HEC:NA	2.88	0.41
2:B:618:LEU:HB3	2:B:717:ASN:HB2	2.02	0.41
2:B:856:ALA:HB3	2:B:859:GLU:HB2	2.02	0.41
3:C:188:VAL:O	3:C:227:TYR:OH	2.34	0.41
3:C:404:ARG:HG2	3:C:411:TRP:CD2	2.56	0.41
2:B:160:VAL:O	2:B:167:SER:N	2.52	0.41
2:B:200:SER:OG	2:B:476:ASP:OD1	2.38	0.41
3:C:84:TRP:CG	3:C:88:ILE:HG13	2.56	0.41
3:C:199:ASP:OD2	4:D:142:SER:OG	2.36	0.41
6:F:235:LEU:HB3	6:F:267:ILE:HG12	2.03	0.41
1:A:161:MET:HB3	3:C:158:HIS:HA	2.03	0.41
2:B:158:THR:HA	2:B:495:TYR:HB3	2.03	0.41
1:A:68:TYR:HD2	5:E:102:TYR:HA	1.85	0.41
2:B:469:HIS:O	2:B:473:SER:HB3	2.21	0.41
2:B:627:LEU:HD21	2:B:644:LEU:HD12	2.03	0.41
3:C:95:ILE:HG21	3:C:249:ILE:HD13	2.03	0.41
5:E:133:LEU:O	5:E:185:GLN:NE2	2.48	0.41
8:I:10:GLU:HA	8:I:13:PRO:HG2	2.03	0.41
1:A:172:GLU:HA	1:A:175:VAL:HG22	2.03	0.40
2:B:191:VAL:HA	2:B:419:THR:HB	2.04	0.40
3:C:295:PHE:HE2	3:C:444:MET:HE2	1.86	0.40
6:F:312:LEU:HD11	6:F:350:ASP:HA	2.03	0.40
2:B:129:GLY:HA3	2:B:138:GLY:C	2.46	0.40
2:B:714:ARG:HD3	2:B:714:ARG:N	2.37	0.40
4:D:43:GLU:HA	4:D:46:GLU:OE2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:GLU:O	1:A:89:THR:OG1	2.37	0.40
2:B:646:LYS:HB3	2:B:646:LYS:HE3	1.88	0.40
4:D:22:THR:HG21	4:D:44:VAL:CG1	2.50	0.40
5:E:117:VAL:HG12	5:E:123:ILE:HG13	2.03	0.40
1:A:188:PRO:HA	1:A:189:PRO:HD3	1.92	0.40
2:B:187:GLN:HB3	2:B:216:GLN:HG3	2.04	0.40
4:D:45:ILE:C	4:D:47:GLU:N	2.79	0.40
1:A:211:LEU:HD23	1:A:211:LEU:HA	1.91	0.40
2:B:885:THR:O	2:B:886:LYS:C	2.65	0.40
6:F:258:LYS:HA	6:F:258:LYS:HD3	1.93	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 PDB entries followed by that with respect to all EM entries.

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	216/219 (99%)	206 (95%)	10 (5%)	0	100	100
2	B	949/1029 (92%)	892 (94%)	56 (6%)	1 (0%)	48	73
3	C	447/486 (92%)	432 (97%)	15 (3%)	0	100	100
4	D	173/179 (97%)	160 (92%)	13 (8%)	0	100	100
5	E	162/205 (79%)	155 (96%)	7 (4%)	0	100	100
6	F	395/411 (96%)	380 (96%)	15 (4%)	0	100	100
7	G	78/112 (70%)	75 (96%)	3 (4%)	0	100	100
8	I	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
All	All	2455/2678 (92%)	2334 (95%)	120 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	886	LYS

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 PDB entries followed by that with respect to all EM entries.

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	198/199 (100%)	195 (98%)	3 (2%)	60	83
2	B	768/830 (92%)	765 (100%)	3 (0%)	89	96
3	C	382/405 (94%)	381 (100%)	1 (0%)	91	97
4	D	143/147 (97%)	143 (100%)	0	100	100
5	E	135/171 (79%)	135 (100%)	0	100	100
6	F	318/330 (96%)	317 (100%)	1 (0%)	91	97
7	G	69/95 (73%)	69 (100%)	0	100	100
8	I	32/32 (100%)	32 (100%)	0	100	100
All	All	2045/2209 (93%)	2037 (100%)	8 (0%)	88	96

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	175	VAL
1	A	179	GLU
1	A	180	GLU
2	B	886	LYS
2	B	888	CYS
2	B	889	SER
3	C	141	HIS
6	F	361	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	ASN
1	A	155	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	82	GLN
2	B	383	ASN
2	B	588	ASN
2	B	693	ASN
2	B	769	ASN
2	B	880	ASN
3	C	141	HIS
3	C	246	HIS
5	E	147	ASN

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](#)

14 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	$\# Z > 2$
9	HEC	E	301	5	32,50,50	2.44	5 (15%)	24,82,82	1.38	4 (16%)
12	JLQ	C	501	-	44,44,44	0.99	4 (9%)	47,49,49	1.10	3 (6%)
9	HEC	A	303	1	32,50,50	2.41	5 (15%)	24,82,82	1.45	4 (16%)
9	HEC	A	304	1	32,50,50	2.38	5 (15%)	24,82,82	1.77	7 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	HEC	A	302	1	32,50,50	2.49	6 (18%)	24,82,82	1.79	7 (29%)
11	F3S	B	1104	2	0,9,9	-	-	-	-	-
14	JL3	C	503	-	44,44,44	0.96	3 (6%)	47,49,49	1.12	5 (10%)
10	SF4	B	1102	2	0,12,12	-	-	-	-	-
15	JM9	C	504	-	53,53,53	0.97	4 (7%)	58,58,58	0.89	3 (5%)
9	HEC	A	301	1	32,50,50	2.39	7 (21%)	24,82,82	1.89	7 (29%)
9	HEC	A	305	1	32,50,50	2.39	5 (15%)	24,82,82	1.46	4 (16%)
10	SF4	B	1101	2	0,12,12	-	-	-	-	-
10	SF4	B	1103	2	0,12,12	-	-	-	-	-
13	HQO	C	502	-	20,20,20	2.84	3 (15%)	18,26,26	1.25	2 (11%)

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
9	HEC	E	301	5	-	4/10/54/54	-
12	JLQ	C	501	-	-	33/48/48/48	-
9	HEC	A	303	1	-	2/10/54/54	-
9	HEC	A	304	1	-	2/10/54/54	-
9	HEC	A	302	1	-	4/10/54/54	-
11	F3S	B	1104	2	-	-	0/3/3/3
14	JL3	C	503	-	-	25/48/48/48	-
10	SF4	B	1102	2	-	-	0/6/5/5
15	JM9	C	504	-	-	28/56/56/56	-
9	HEC	A	301	1	-	0/10/54/54	-
9	HEC	A	305	1	-	0/10/54/54	-
10	SF4	B	1101	2	-	-	0/6/5/5
10	SF4	B	1103	2	-	-	0/6/5/5
13	HQO	C	502	-	-	3/7/7/7	0/2/2/2

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	502	HQO	O4-N1	-11.68	1.23	1.38
9	A	302	HEC	C2B-C3B	-8.25	1.32	1.40
9	A	303	HEC	C3C-C2C	-7.72	1.32	1.40
9	E	301	HEC	C2B-C3B	-7.43	1.33	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	305	HEC	C2B-C3B	-7.37	1.33	1.40
9	A	301	HEC	C2B-C3B	-7.37	1.33	1.40
9	A	304	HEC	C2B-C3B	-7.35	1.33	1.40
9	E	301	HEC	C3C-C2C	-7.32	1.33	1.40
9	A	303	HEC	C2B-C3B	-7.09	1.33	1.40
9	A	301	HEC	C3C-C2C	-7.02	1.33	1.40
9	A	305	HEC	C3C-C2C	-6.91	1.33	1.40
9	A	302	HEC	C3C-C2C	-6.79	1.33	1.40
9	A	304	HEC	C3C-C2C	-6.77	1.33	1.40
9	A	305	HEC	C3D-C2D	5.13	1.52	1.37
9	A	303	HEC	C3D-C2D	5.03	1.52	1.37
9	A	302	HEC	C3D-C2D	5.02	1.52	1.37
9	E	301	HEC	C3D-C2D	4.88	1.52	1.37
9	A	304	HEC	C3D-C2D	4.88	1.52	1.37
9	A	301	HEC	C3D-C2D	4.75	1.51	1.37
15	C	504	JM9	O20-C21	2.97	1.42	1.33
9	A	302	HEC	CAD-C3D	2.71	1.56	1.52
13	C	502	HQO	C1-C10	2.70	1.47	1.42
15	C	504	JM9	O17-C15	2.67	1.41	1.34
13	C	502	HQO	C10-C5	2.66	1.46	1.42
14	C	503	JL3	O29-C19	-2.62	1.40	1.46
12	C	501	JLQ	O30-C20	-2.48	1.40	1.46
15	C	504	JM9	O38-C39	2.46	1.40	1.33
12	C	501	JLQ	O30-C31	2.42	1.41	1.34
9	A	301	HEC	C1D-ND	2.38	1.41	1.36
14	C	503	JL3	O17-C15	2.34	1.40	1.33
12	C	501	JLQ	O18-C16	2.33	1.40	1.33
12	C	501	JLQ	O18-C19	-2.22	1.40	1.45
9	A	304	HEC	C1D-ND	2.20	1.40	1.36
15	C	504	JM9	O17-C18	-2.18	1.41	1.46
9	A	302	HEC	C4D-ND	2.15	1.40	1.36
9	A	301	HEC	C4D-ND	2.15	1.40	1.36
9	A	304	HEC	C4D-ND	2.14	1.40	1.36
9	E	301	HEC	C1D-ND	2.11	1.40	1.36
9	A	303	HEC	C1C-CHC	-2.10	1.35	1.41
9	A	305	HEC	C1D-ND	2.07	1.40	1.36
9	A	301	HEC	C2A-C3A	-2.07	1.31	1.37
14	C	503	JL3	O29-C30	2.06	1.40	1.34
9	A	301	HEC	C1C-CHC	-2.06	1.35	1.41
9	E	301	HEC	C4D-ND	2.05	1.40	1.36
9	A	302	HEC	C1D-ND	2.05	1.40	1.36
9	A	305	HEC	CAD-C3D	2.01	1.55	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	303	HEC	C1D-ND	2.01	1.40	1.36

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	501	JLQ	O30-C31-C33	5.28	122.88	111.50
14	C	503	JL3	O29-C30-C32	4.29	120.74	111.50
9	A	301	HEC	CMC-C2C-C1C	-4.18	122.05	128.46
9	A	301	HEC	CMC-C2C-C3C	4.12	130.66	125.82
15	C	504	JM9	O17-C15-C14	3.74	119.56	111.50
9	A	304	HEC	CMC-C2C-C1C	-3.69	122.79	128.46
9	A	302	HEC	CMC-C2C-C3C	3.46	129.89	125.82
9	A	302	HEC	CBD-CAD-C3D	3.46	118.52	112.62
9	A	302	HEC	CMC-C2C-C1C	-3.45	123.17	128.46
9	A	304	HEC	C1D-C2D-C3D	-3.40	104.63	107.00
9	A	304	HEC	CMC-C2C-C3C	3.32	129.73	125.82
9	A	305	HEC	C1D-C2D-C3D	-3.32	104.69	107.00
13	C	502	HQO	O1-C1-C10	3.20	120.31	116.31
9	A	301	HEC	CBA-CAA-C2A	-3.19	107.23	112.60
9	A	304	HEC	CBA-CAA-C2A	-3.09	107.40	112.60
9	A	301	HEC	C1D-C2D-C3D	-2.99	104.92	107.00
9	E	301	HEC	C1D-C2D-C3D	-2.90	104.97	107.00
9	A	303	HEC	C1D-C2D-C3D	-2.76	105.08	107.00
9	A	302	HEC	CMB-C2B-C1B	-2.74	124.26	128.46
15	C	504	JM9	O38-C39-C41	2.69	120.36	111.91
14	C	503	JL3	O17-C18-C19	-2.64	100.76	108.43
13	C	502	HQO	C2-C3-N1	2.63	121.83	118.94
9	A	303	HEC	CMC-C2C-C1C	-2.63	124.43	128.46
14	C	503	JL3	C19-O29-C30	-2.62	111.35	117.79
9	E	301	HEC	CMB-C2B-C1B	-2.60	124.47	128.46
12	C	501	JLQ	O18-C16-C15	2.59	120.04	111.91
9	A	304	HEC	CBD-CAD-C3D	-2.58	108.22	112.62
9	E	301	HEC	CMC-C2C-C1C	-2.56	124.53	128.46
9	A	301	HEC	CMB-C2B-C1B	-2.55	124.55	128.46
9	A	303	HEC	CMB-C2B-C1B	-2.54	124.56	128.46
14	C	503	JL3	O17-C15-C14	2.52	119.83	111.91
9	A	305	HEC	CMC-C2C-C1C	-2.50	124.62	128.46
15	C	504	JM9	O20-C21-C23	2.50	119.74	111.91
9	A	301	HEC	CMB-C2B-C3B	2.47	128.73	125.82
9	A	303	HEC	CMC-C2C-C3C	2.26	128.47	125.82
9	A	301	HEC	CBD-CAD-C3D	-2.24	108.79	112.62
9	A	305	HEC	CMC-C2C-C3C	2.23	128.45	125.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	C	503	JL3	O23-P22-O24	-2.23	101.21	112.24
9	A	302	HEC	CMB-C2B-C3B	2.21	128.42	125.82
9	A	302	HEC	CMA-C3A-C2A	2.21	129.10	124.94
12	C	501	JLQ	O24-P23-O25	-2.19	101.40	112.24
9	A	305	HEC	CMB-C2B-C1B	-2.18	125.12	128.46
9	A	304	HEC	CMB-C2B-C3B	2.17	128.37	125.82
9	A	304	HEC	CMB-C2B-C1B	-2.13	125.19	128.46
9	A	302	HEC	O1D-CGD-CBD	-2.09	116.36	123.08
9	E	301	HEC	CMC-C2C-C3C	2.00	128.17	125.82

There are no chirality outliers.

All (101) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	302	HEC	C2D-C3D-CAD-CBD
9	A	302	HEC	C4D-C3D-CAD-CBD
12	C	501	JLQ	C21-O22-P23-O24
12	C	501	JLQ	C21-O22-P23-O25
12	C	501	JLQ	C27-O26-P23-O25
12	C	501	JLQ	O32-C31-O30-C20
12	C	501	JLQ	C33-C31-O30-C20
13	C	502	HQO	C3-C11-C13-C12
14	C	503	JL3	C20-O21-P22-O24
14	C	503	JL3	C32-C30-O29-C19
15	C	504	JM9	O17-C18-C19-O20
15	C	504	JM9	O40-C39-O38-C37
14	C	503	JL3	O31-C30-O29-C19
14	C	503	JL3	C14-C15-O17-C18
15	C	504	JM9	C41-C39-O38-C37
14	C	503	JL3	O16-C15-O17-C18
12	C	501	JLQ	C15-C16-O18-C19
9	A	302	HEC	C2A-CAA-CBA-CGA
9	A	302	HEC	C3D-CAD-CBD-CGD
12	C	501	JLQ	C13-C14-C15-C16
12	C	501	JLQ	C31-C33-C34-C35
14	C	503	JL3	C30-C32-C33-C34
15	C	504	JM9	C49-C50-C51-C52
12	C	501	JLQ	O17-C16-O18-C19
12	C	501	JLQ	C21-O22-P23-O26
14	C	503	JL3	C20-O21-P22-O25
14	C	503	JL3	C26-O25-P22-O21
14	C	503	JL3	C08-C09-C10-C11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	C	504	JM9	C47-C48-C49-C50
15	C	504	JM9	C39-C41-C42-C43
12	C	501	JLQ	C08-C09-C10-C11
13	C	502	HQO	C12-C14-C15-C16
14	C	503	JL3	C32-C33-C34-C35
15	C	504	JM9	C29-C30-C31-C32
12	C	501	JLQ	C38-C39-C40-C41
14	C	503	JL3	O25-C26-C27-N28
12	C	501	JLQ	C34-C35-C36-C37
15	C	504	JM9	C48-C49-C50-C51
12	C	501	JLQ	C06-C07-C08-C09
15	C	504	JM9	C45-C46-C47-C48
12	C	501	JLQ	C07-C08-C09-C10
14	C	503	JL3	C40-C41-C42-C43
15	C	504	JM9	C43-C44-C45-C46
14	C	503	JL3	C05-C06-C07-C08
12	C	501	JLQ	C10-C11-C12-C13
12	C	501	JLQ	C36-C37-C38-C39
15	C	504	JM9	C09-C10-C11-C12
15	C	504	JM9	C11-C12-C13-C14
15	C	504	JM9	C05-C06-C07-C08
15	C	504	JM9	C41-C42-C43-C44
14	C	503	JL3	C03-C04-C05-C06
15	C	504	JM9	C25-C26-C27-C28
12	C	501	JLQ	C39-C40-C41-C42
12	C	501	JLQ	C01-C02-C03-C04
15	C	504	JM9	C02-C03-C04-C05
14	C	503	JL3	C07-C08-C09-C10
13	C	502	HQO	C14-C15-C16-C17
15	C	504	JM9	C37-C18-C19-O20
15	C	504	JM9	C27-C28-C29-C30
12	C	501	JLQ	C35-C36-C37-C38
14	C	503	JL3	C37-C38-C39-C40
14	C	503	JL3	O17-C18-C19-O29
14	C	503	JL3	C04-C05-C06-C07
15	C	504	JM9	C46-C47-C48-C49
14	C	503	JL3	C35-C36-C37-C38
12	C	501	JLQ	O18-C19-C20-C21
14	C	503	JL3	C26-O25-P22-O23
15	C	504	JM9	C10-C11-C12-C13
12	C	501	JLQ	C19-C20-C21-O22
12	C	501	JLQ	C42-C43-C44-C45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
12	C	501	JLQ	C11-C12-C13-C14
15	C	504	JM9	C06-C07-C08-C09
12	C	501	JLQ	O30-C20-C21-O22
12	C	501	JLQ	C09-C10-C11-C12
14	C	503	JL3	O17-C18-C19-C20
12	C	501	JLQ	O18-C19-C20-O30
15	C	504	JM9	C07-C08-C09-C10
14	C	503	JL3	C11-C12-C13-C14
12	C	501	JLQ	C27-O26-P23-O22
12	C	501	JLQ	C41-C42-C43-C44
14	C	503	JL3	C34-C35-C36-C37
12	C	501	JLQ	C40-C41-C42-C43
15	C	504	JM9	C19-C18-C37-O38
14	C	503	JL3	C33-C34-C35-C36
9	A	303	HEC	CAA-CBA-CGA-O1A
9	A	303	HEC	CAA-CBA-CGA-O2A
9	A	304	HEC	CAA-CBA-CGA-O1A
9	A	304	HEC	CAA-CBA-CGA-O2A
9	E	301	HEC	CAA-CBA-CGA-O2A
15	C	504	JM9	O16-C15-O17-C18
9	E	301	HEC	CAA-CBA-CGA-O1A
14	C	503	JL3	C10-C11-C12-C13
9	E	301	HEC	CAD-CBD-CGD-O2D
15	C	504	JM9	O38-C39-C41-C42
12	C	501	JLQ	C37-C38-C39-C40
9	E	301	HEC	CAD-CBD-CGD-O1D
15	C	504	JM9	C14-C15-O17-C18
15	C	504	JM9	C13-C14-C15-O17
12	C	501	JLQ	C14-C15-C16-O18
12	C	501	JLQ	O30-C31-C33-C34
15	C	504	JM9	O40-C39-C41-C42

There are no ring outliers.

9 monomers are involved in 19 short contacts:

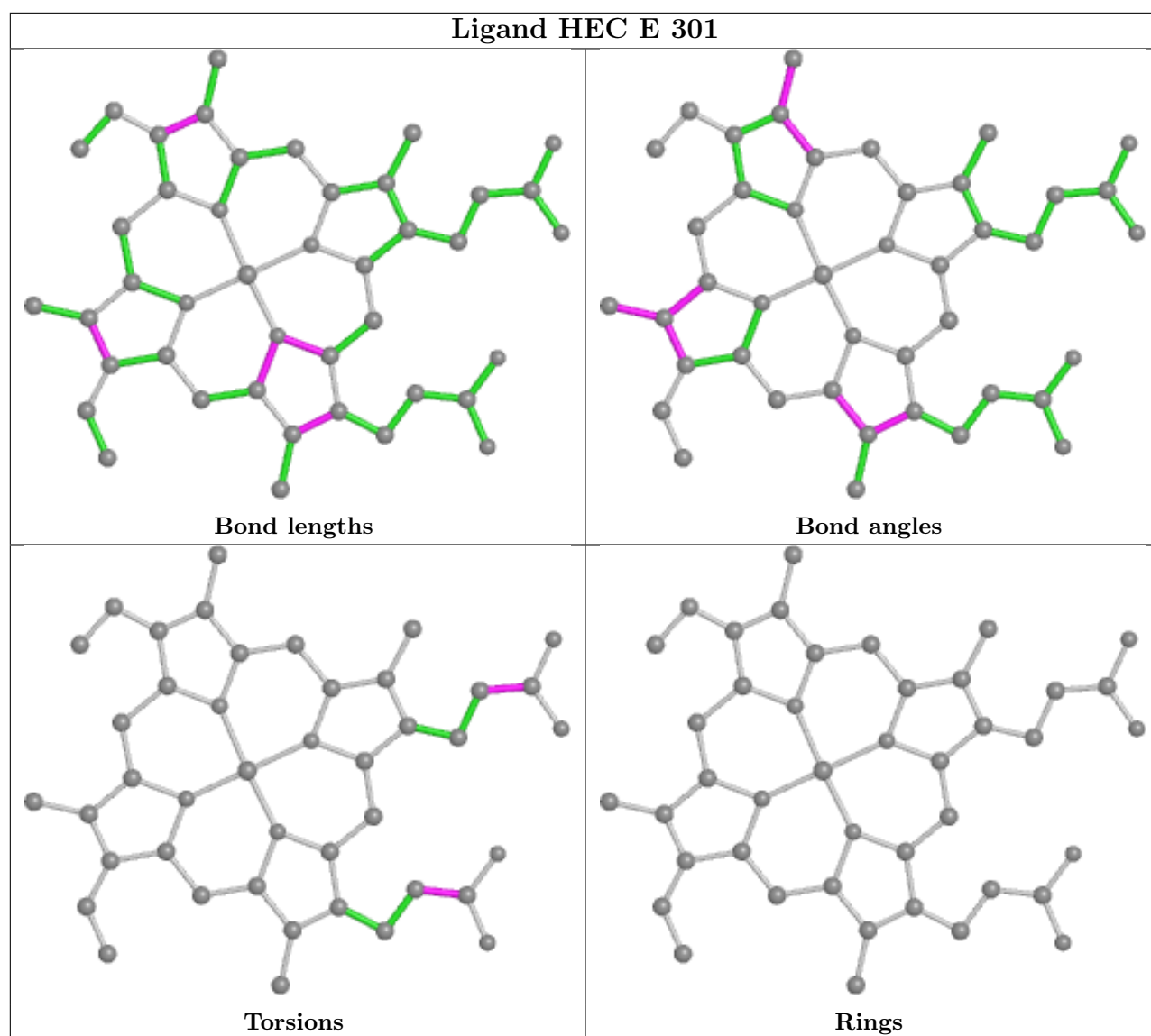
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	E	301	HEC	2	0
9	A	303	HEC	1	0
9	A	304	HEC	1	0
9	A	302	HEC	2	0
11	B	1104	F3S	5	0
9	A	301	HEC	4	0

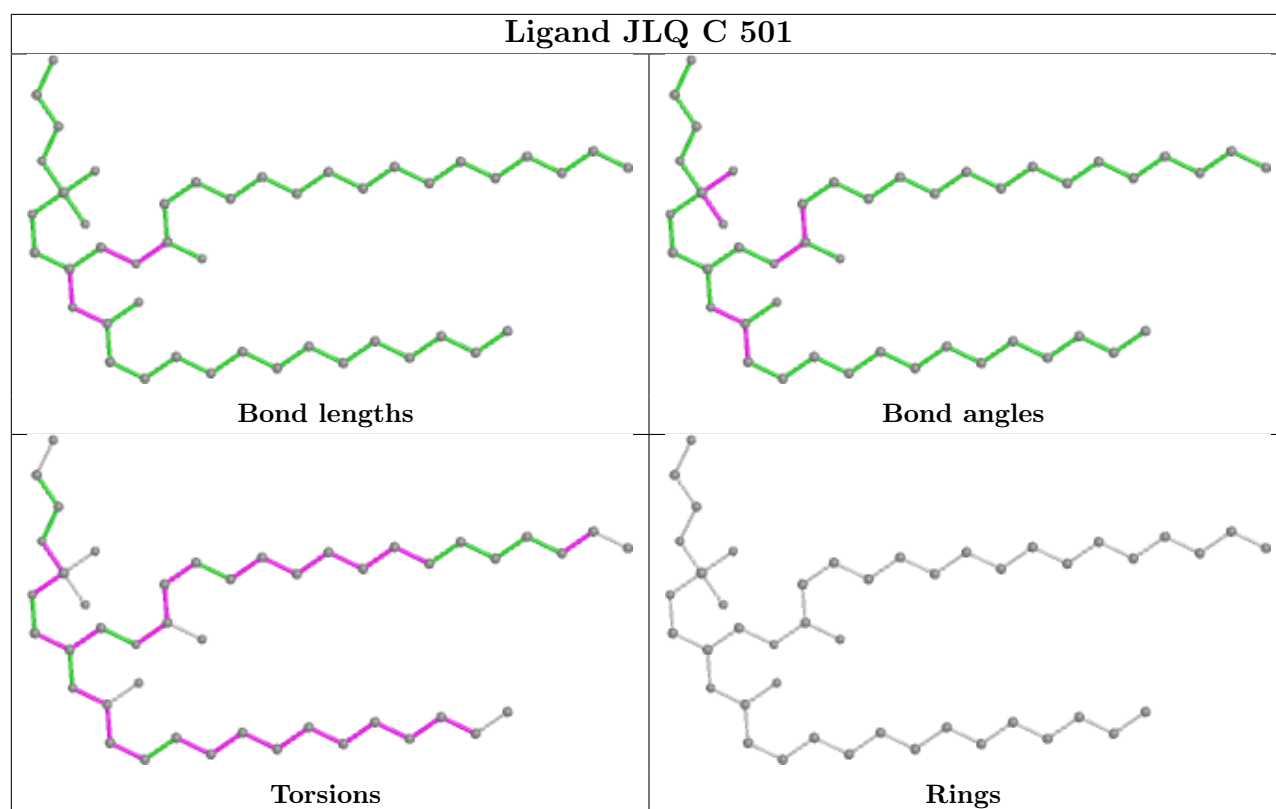
Continued on next page...

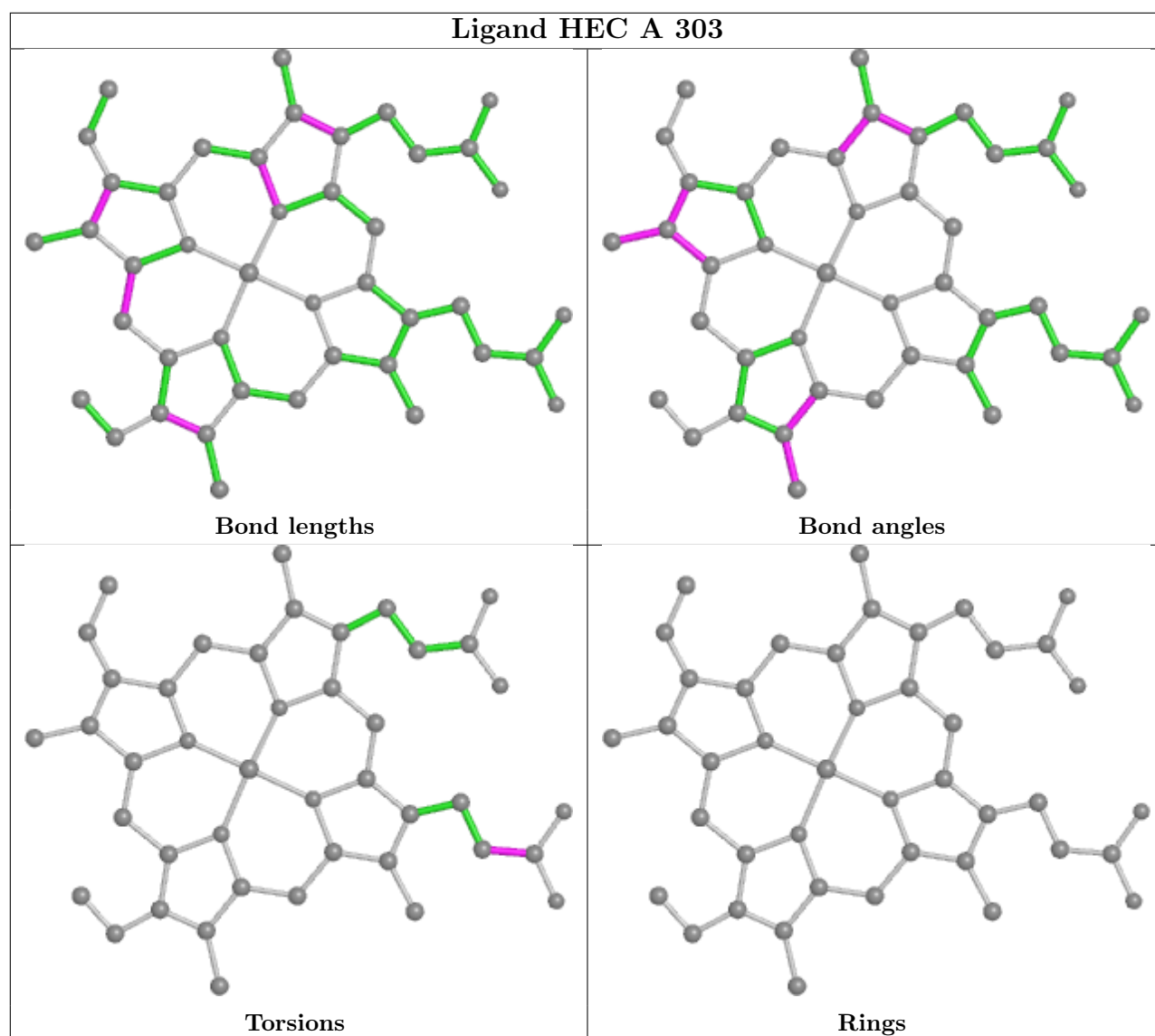
Continued from previous page...

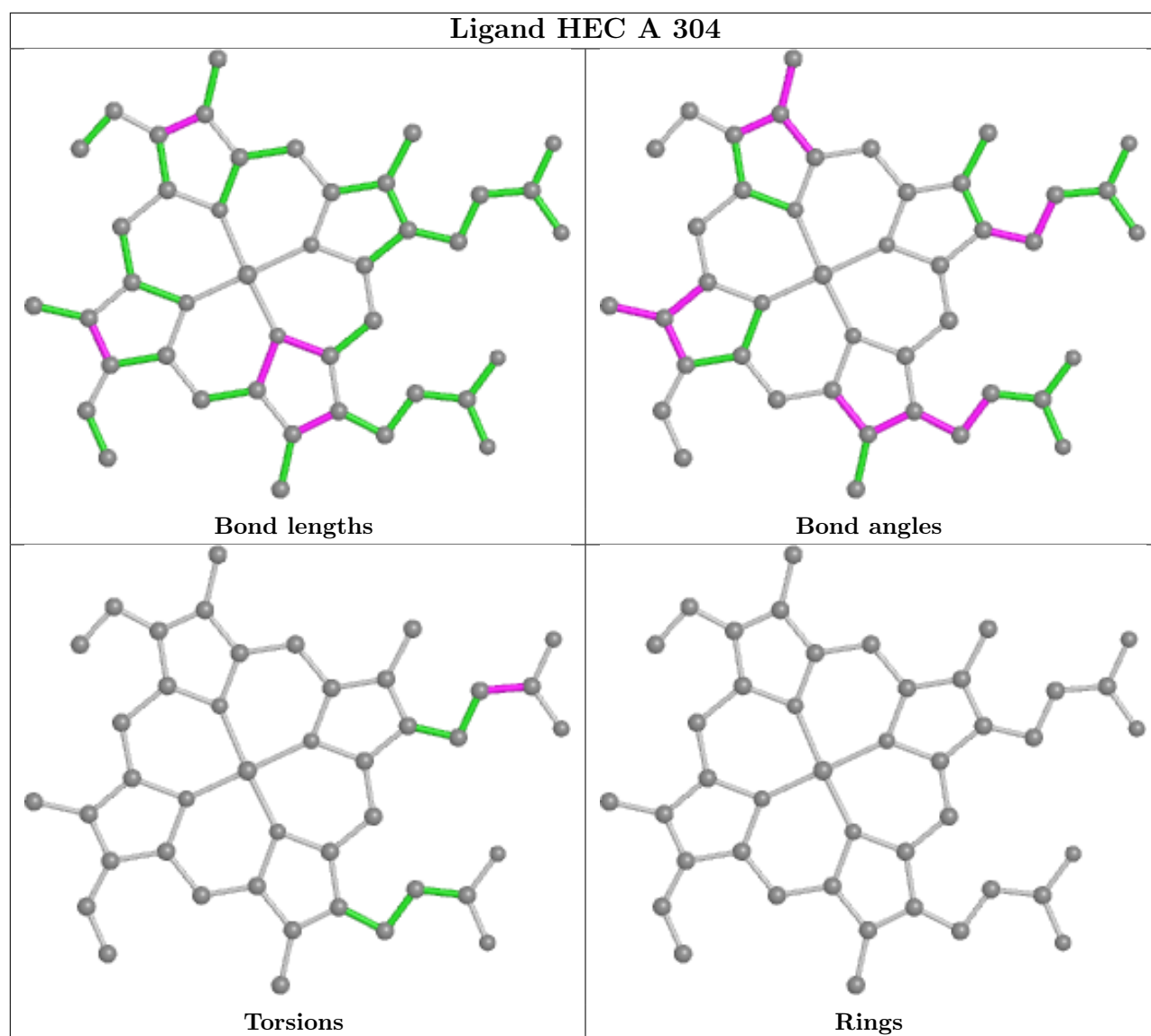
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	305	HEC	2	0
10	B	1103	SF4	1	0
13	C	502	HQO	1	0

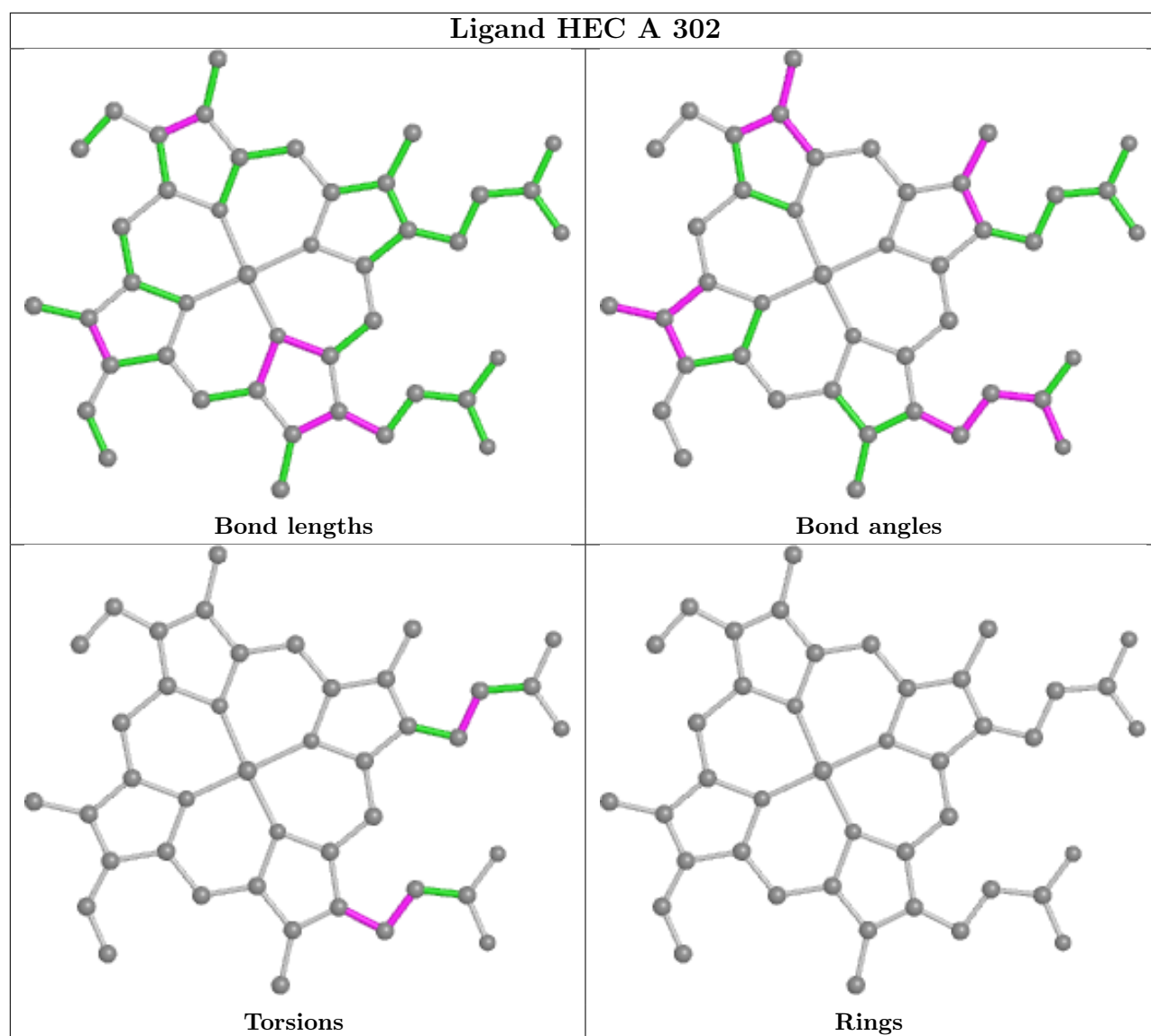
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

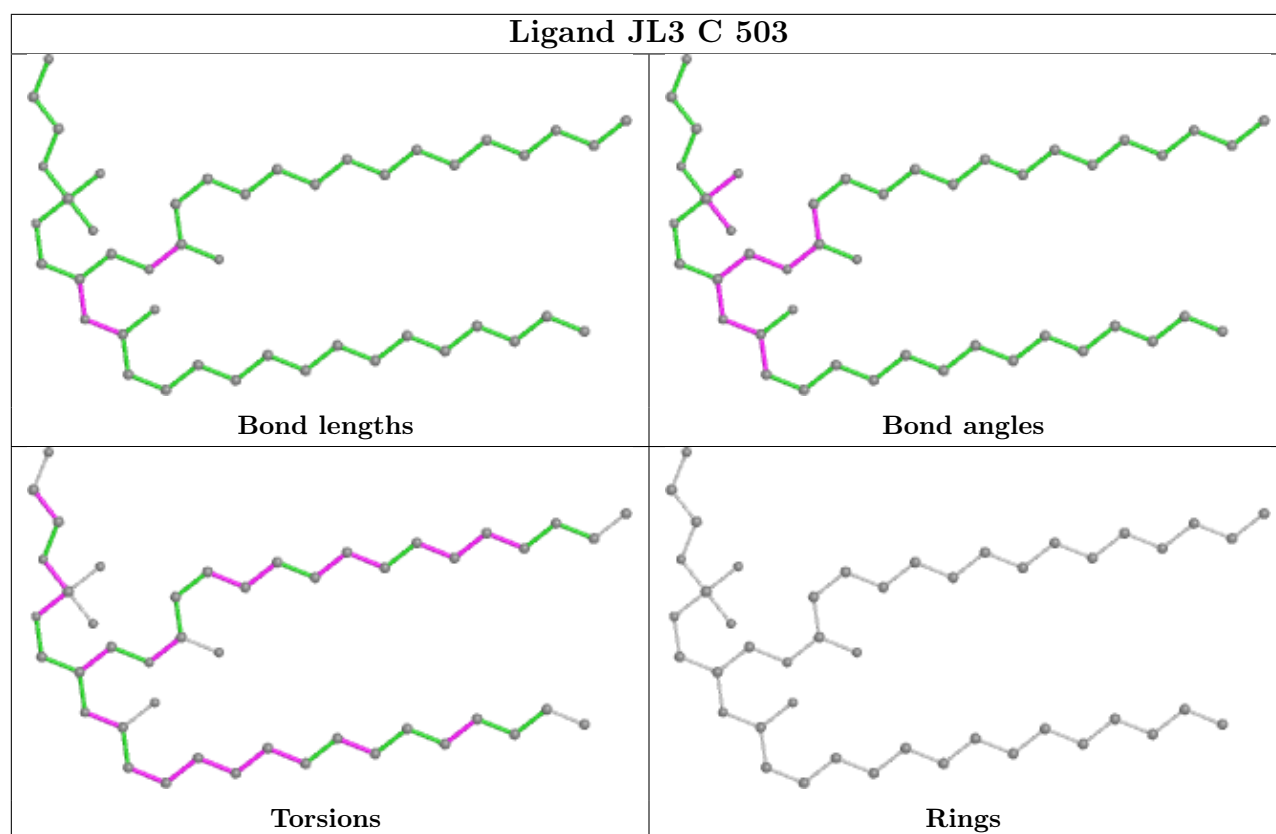


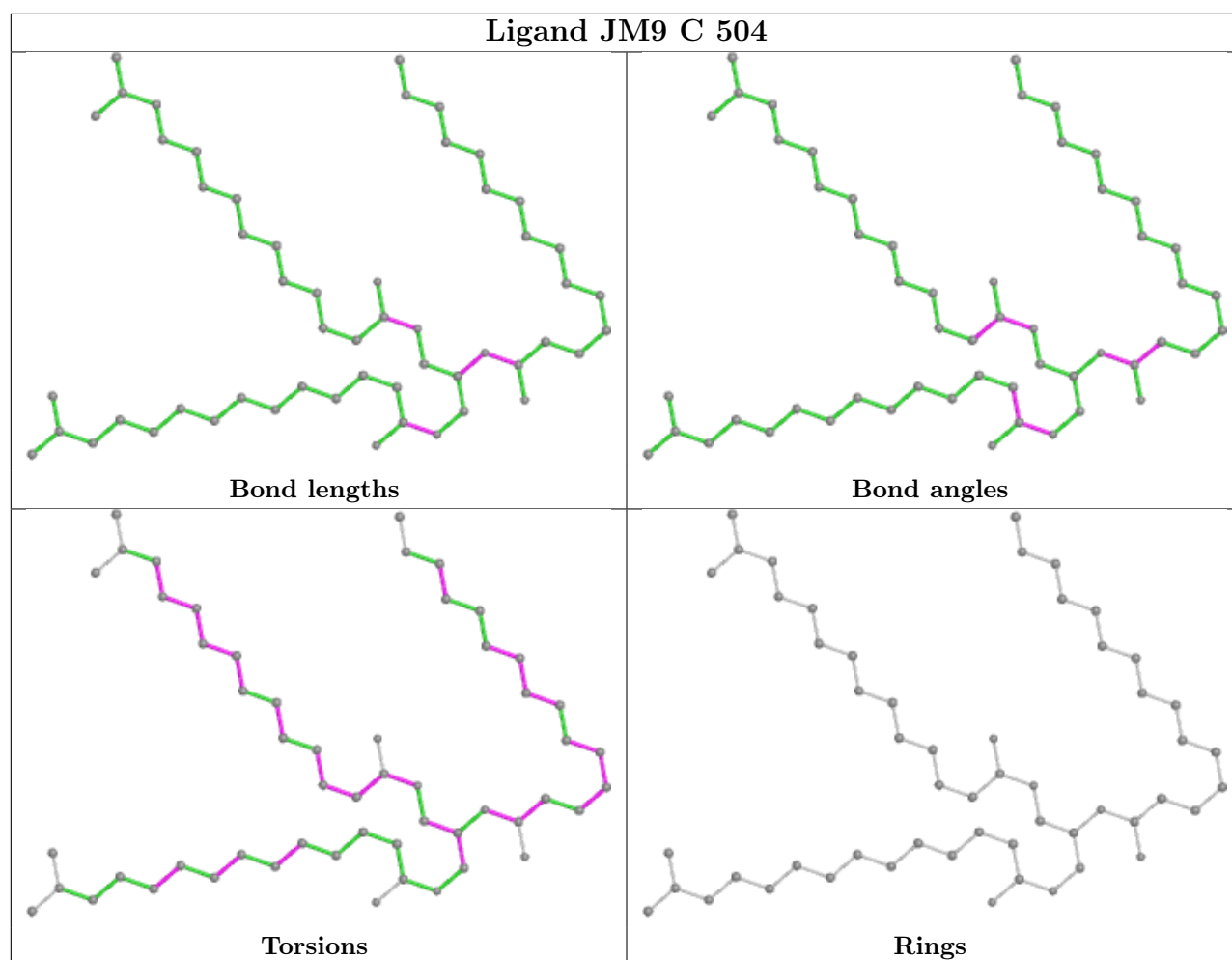


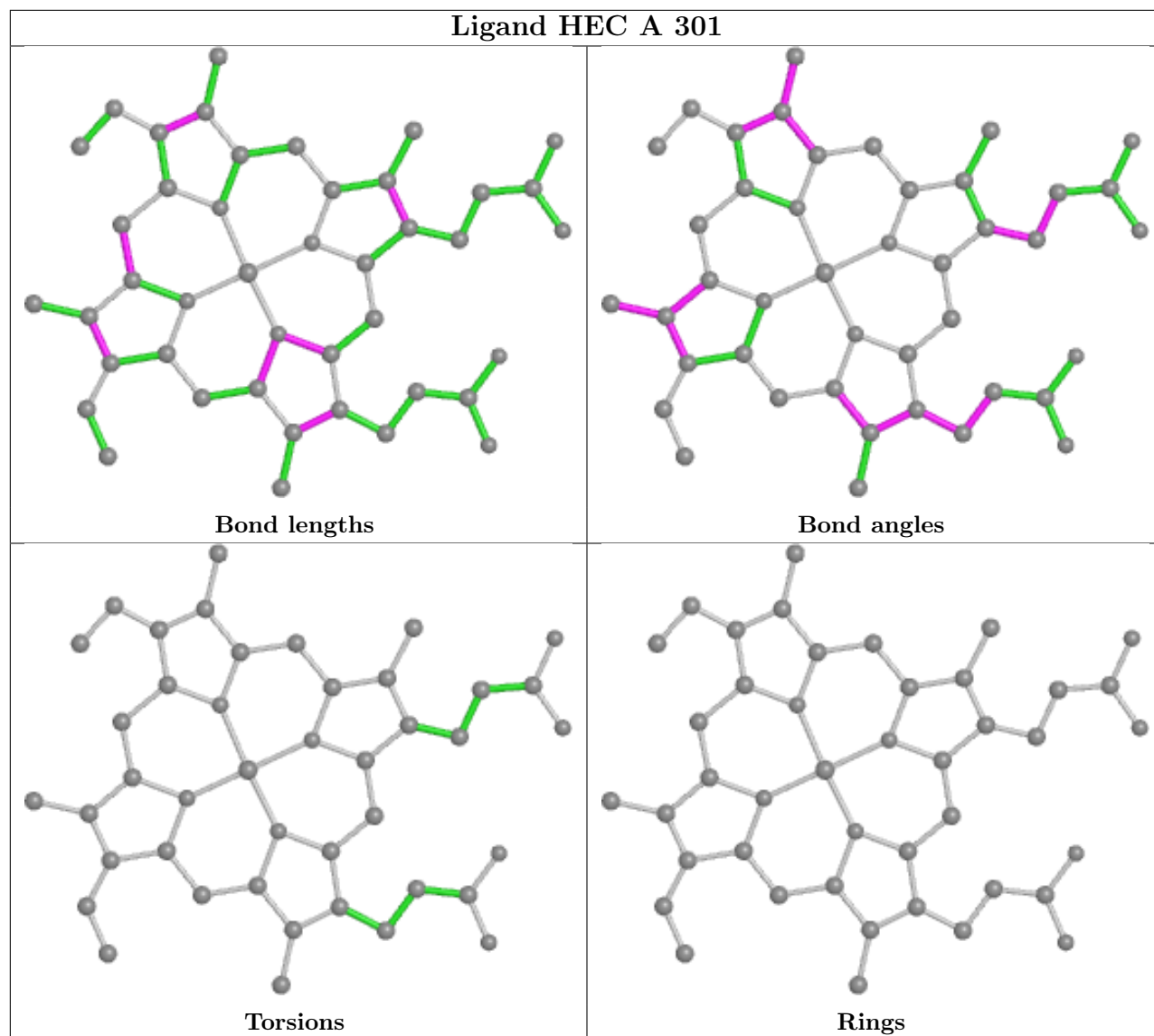


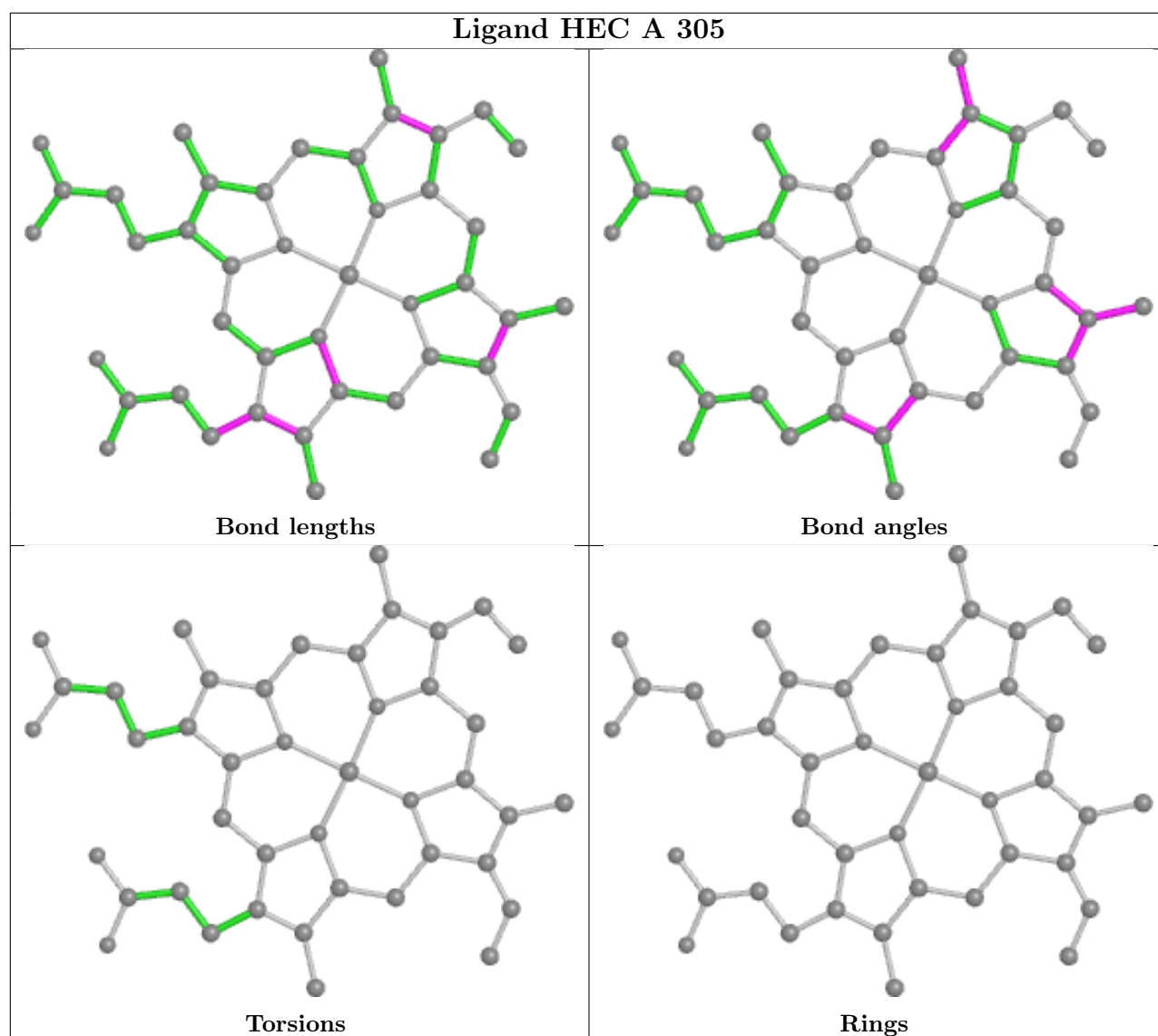


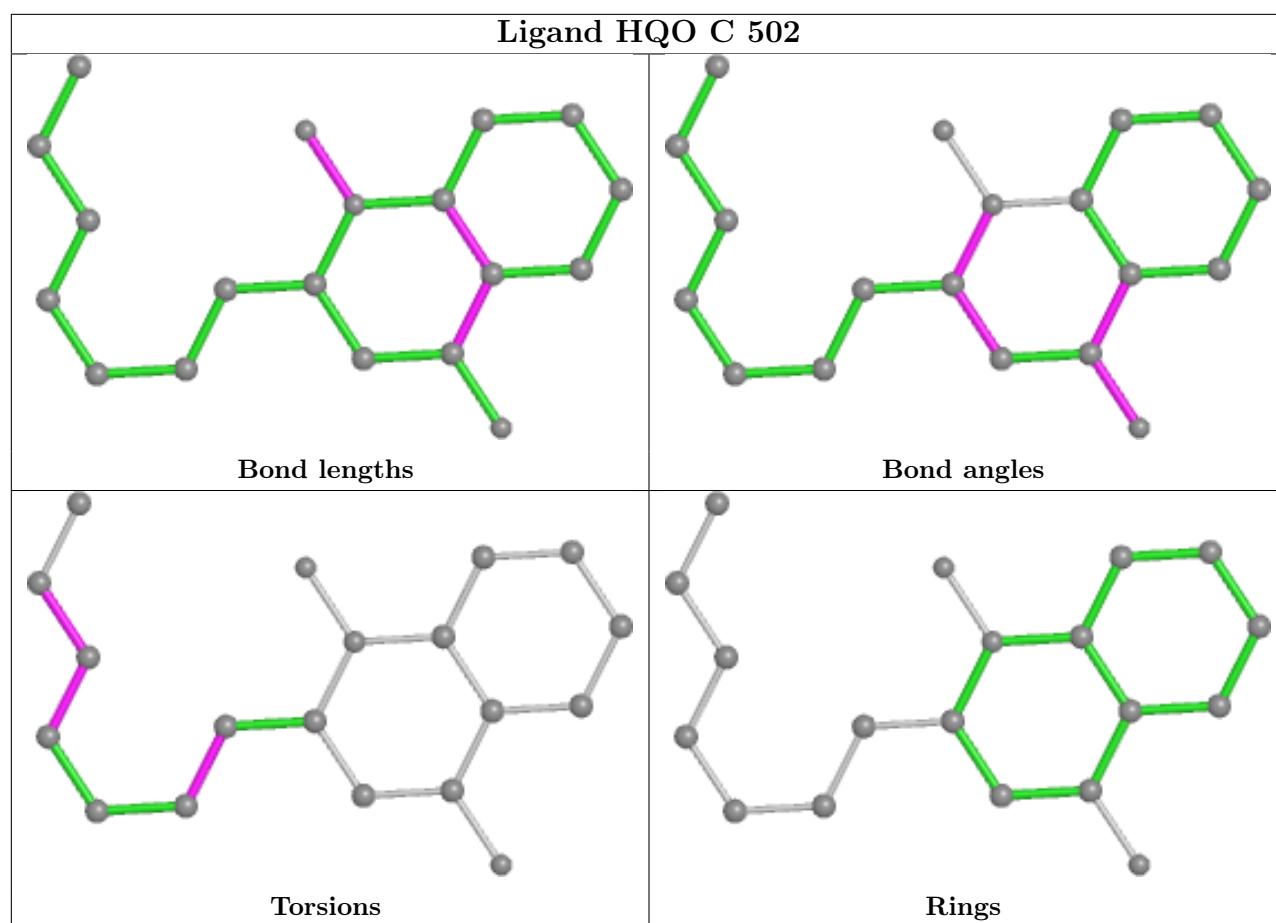












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.