Full wwPDB X-ray Structure Validation Report ⓘ

Aug 15, 2023 – 03:28 PM EDT

PDB ID	:	1SQB
Title	:	Crystal Structure Analysis of Bovine Bc1 with Azoxystrobin
Authors	:	Esser, L.; Quinn, B.; Li, Y.F.; Zhang, M.; Elberry, M.; Yu, L.; Yu, C.A.; Xia, D.
Deposited on	:	2004-03-18
Resolution	:	2.69 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:

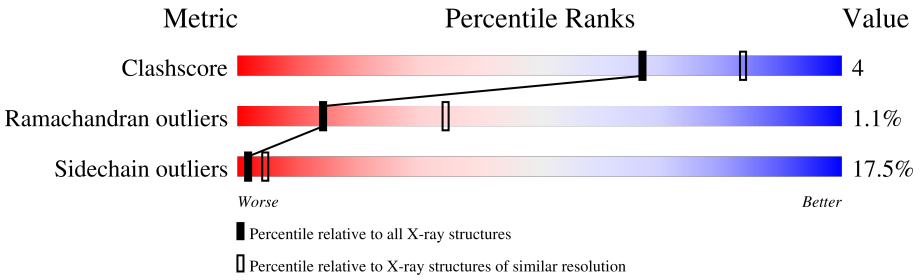
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	480	73% 18% • 7%
2	B	453	76% 16% • 6%
3	C	379	78% 19% •
4	D	241	75% 22% •
5	E	196	78% 21% •
6	F	110	78% 15% • 5%
7	G	81	68% 23% • 7%
8	H	78	51% 33% • 14%

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Mol	Chain	Length	Quality of chain
9	I	78	32% 29% 12% 27%
10	J	62	63% 32%
11	K	56	57% 36% 7%

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 16897 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, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	446	3458	2161	609	668	20	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	425	3181	1998	564	612	7	0	0	0

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	378	3003	2013	471	501	18	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	241	1919	1225	330	349	15	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	196	1519	957	263	291	8	0	0	0

- Molecule 6 is a protein called Ubiquinol-cytochrome C reductase complex 14 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	105	Total	C	N	O	S	0	0	0
			911	576	165	168	2			

- Molecule 7 is a protein called Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	75	Total	C	N	O	S	0	0	0
			628	410	118	99	1			

- Molecule 8 is a protein called Ubiquinol-cytochrome C reductase complex 11 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	67	Total	C	N	O	S	0	0	0
			548	332	99	112	5			

- Molecule 9 is a protein called Ubiquinol-cytochrome c reductase 8 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	57	Total	C	N	O	S	0	0	0
			406	253	77	74	2			

- Molecule 10 is a protein called Ubiquinol-cytochrome C reductase complex 7.2 kDa protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	61	Total	C	N	O	0	0	0
			502	329	87	86			

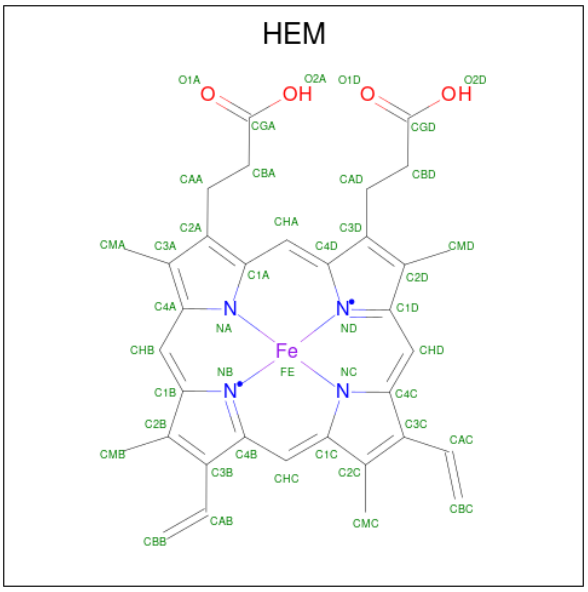
- Molecule 11 is a protein called Ubiquinol-cytochrome C reductase complex 6.4 kDa protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	K	52	Total	C	N	O	0	0	0
			425	282	77	66			

There is a discrepancy between the modelled and reference sequences:

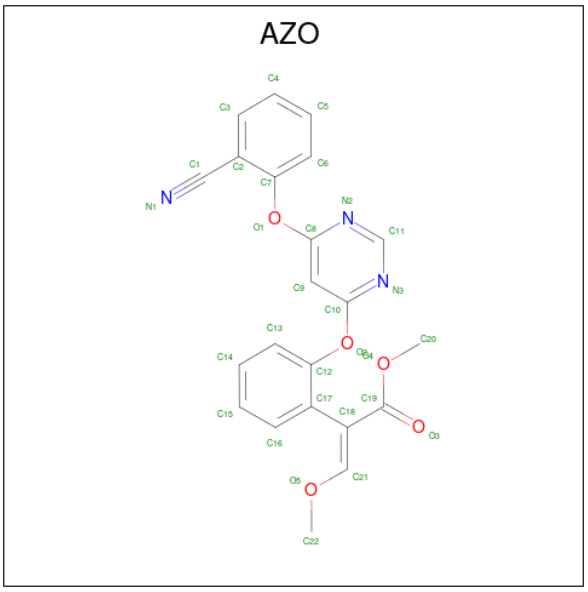
Chain	Residue	Modelled	Actual	Comment	Reference
K	34	TRP	SER	conflict	UNP P07552

- Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



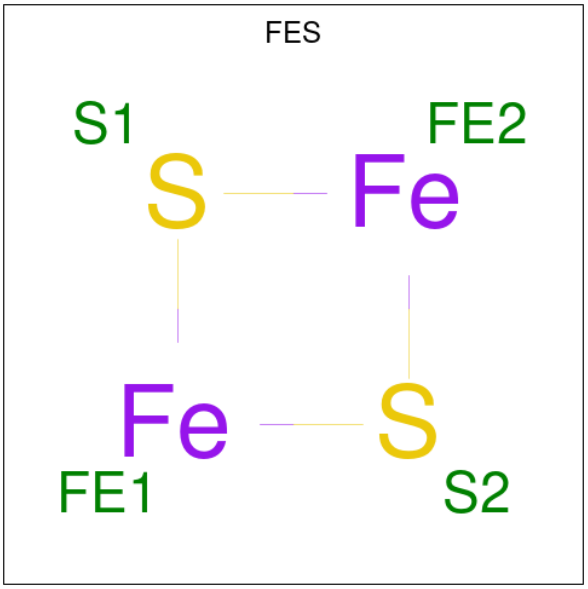
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 13 is METHYL (2Z)-2-(2-{[6-(2-CYANOPHENOXY)PYRIMIDIN-4-YL]OXY}PHENYL)-3-METHOXYACRYLATE (three-letter code: AZO) (formula: $C_{22}H_{17}N_3O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	C	1	Total C N O 30 22 3 5	0	0

- Molecule 14 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

- Molecule 15 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	47	Total O 47 47	0	0
15	B	82	Total O 82 82	0	0
15	C	37	Total O 37 37	0	0
15	D	19	Total O 19 19	0	0
15	E	2	Total O 2 2	0	0
15	F	21	Total O 21 21	0	0
15	G	20	Total O 20 20	0	0
15	H	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	I	3	Total O 3 3	0	0
15	K	2	Total O 2 2	0	0

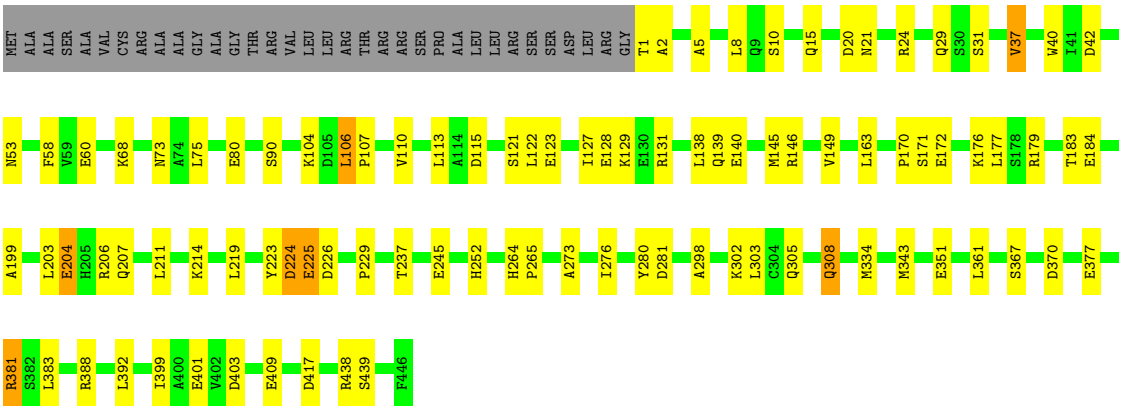
3 Residue-property plots (i)

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.

Note EDS was not executed.

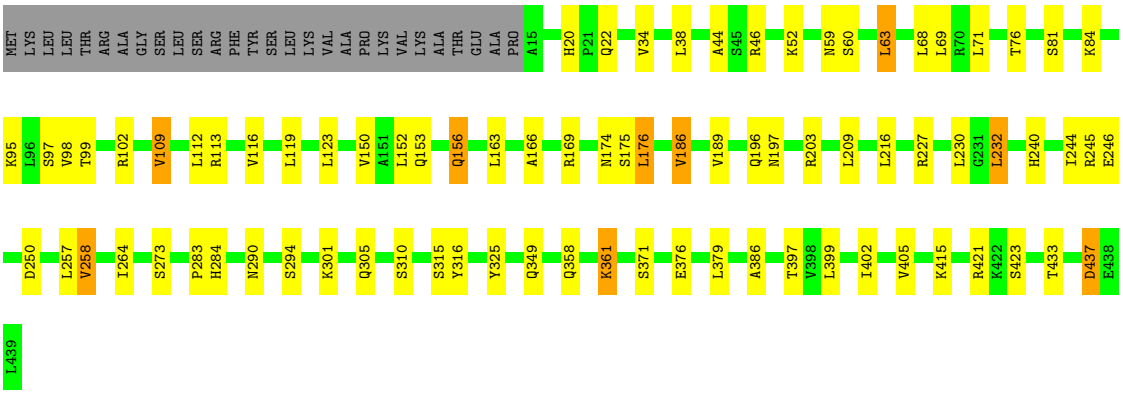
• Molecule 1: Ubiquinol-cytochrome C reductase complex core protein I, mitochondrial

Chain A:



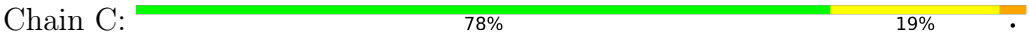
• Molecule 2: Ubiquinol-cytochrome C reductase complex core protein 2, mitochondrial

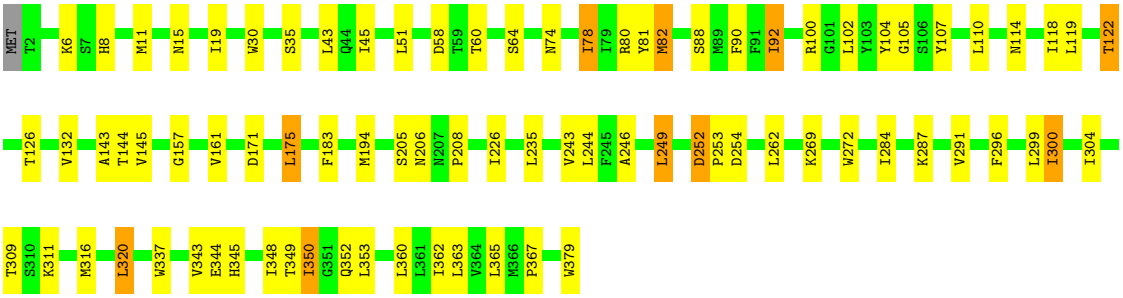
Chain B:



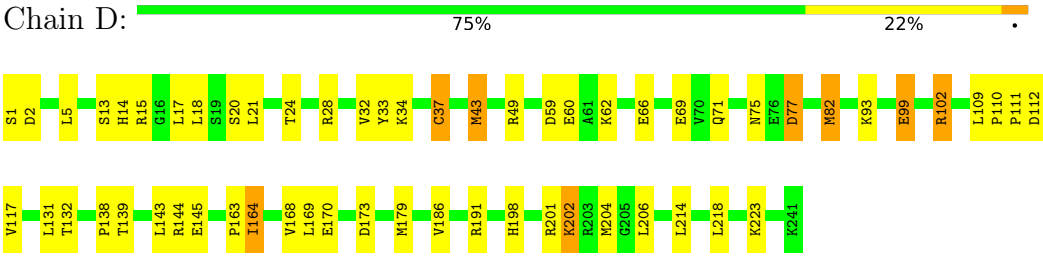
• Molecule 3: Cytochrome b

Chain C:

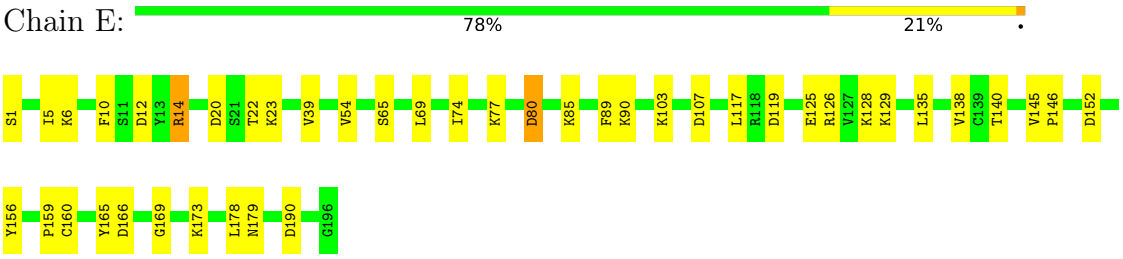




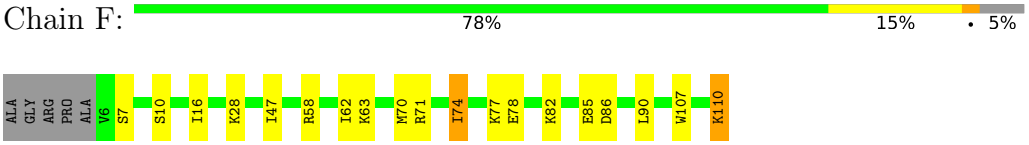
• Molecule 4: Cytochrome c1, heme protein, mitochondrial



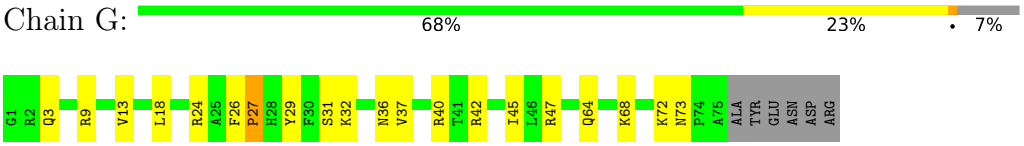
• Molecule 5: Ubiquinol-cytochrome c reductase iron-sulfur subunit



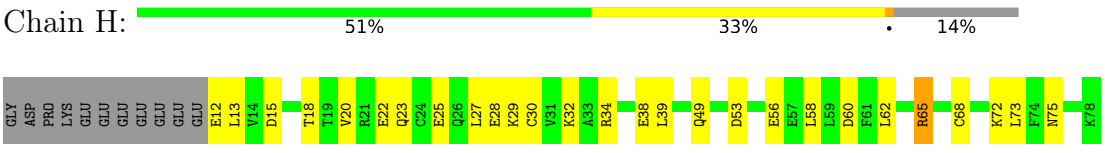
• Molecule 6: Ubiquinol-cytochrome C reductase complex 14 kDa protein



• Molecule 7: Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C

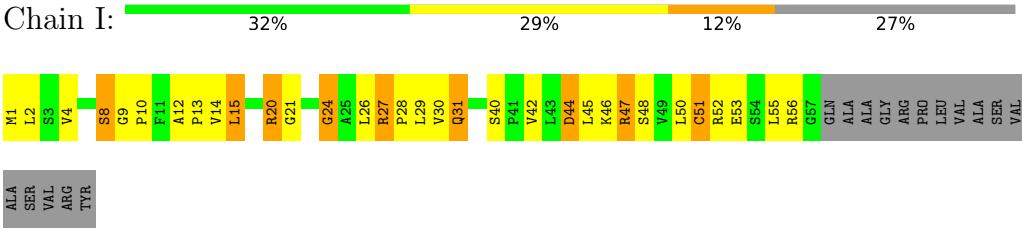


• Molecule 8: Ubiquinol-cytochrome C reductase complex 11 kDa protein



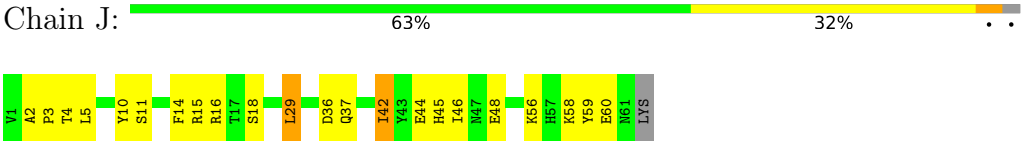
• Molecule 9: Ubiquinol-cytochrome c reductase 8 kDa protein

Chain I:



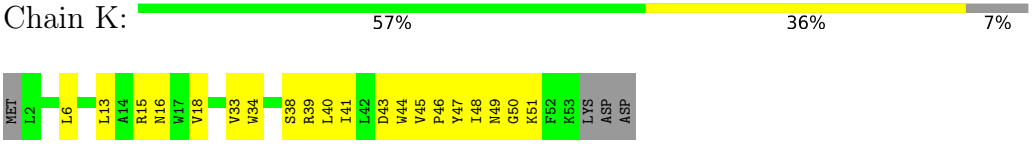
• Molecule 10: Ubiquinol-cytochrome C reductase complex 7.2 kDa protein

Chain J:



• Molecule 11: Ubiquinol-cytochrome C reductase complex 6.4 kDa protein

Chain K:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	153.55Å 153.55Å 596.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.69	Depositor
% Data completeness (in resolution range)	95.6 (40.00-2.69)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.241 , 0.288	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16897	wwPDB-VP
Average B, all atoms (Å^2)	13.0	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: AZO, FES, 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	0.79	0/3531	0.80	4/4792 (0.1%)
2	B	0.79	0/3241	0.80	0/4398
3	C	0.92	0/3100	0.77	3/4242 (0.1%)
4	D	0.87	0/1978	0.79	3/2684 (0.1%)
5	E	0.92	0/1553	0.79	4/2100 (0.2%)
6	F	0.87	0/930	0.82	1/1246 (0.1%)
7	G	1.01	0/649	0.78	0/878
8	H	0.78	0/553	0.88	1/741 (0.1%)
9	I	1.07	0/411	1.00	3/558 (0.5%)
10	J	0.96	0/515	0.76	0/696
11	K	1.00	0/439	0.79	0/600
All	All	0.87	0/16900	0.80	19/22935 (0.1%)

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
2	B	0	1

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	26	LEU	N-CA-C	5.97	127.11	111.00
6	F	86	ASP	CB-CG-OD2	5.69	123.42	118.30
3	C	252	ASP	CB-CG-OD1	5.65	123.38	118.30
4	D	2	ASP	CB-CG-OD1	5.48	123.23	118.30
1	A	224	ASP	CB-CG-OD1	5.39	123.16	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	417	ASP	CB-CG-OD2	5.34	123.11	118.30
4	D	112	ASP	CB-CG-OD2	5.31	123.08	118.30
5	E	107	ASP	CB-CG-OD2	5.27	123.04	118.30
5	E	80	ASP	CB-CG-OD2	5.22	123.00	118.30
3	C	320	LEU	CA-CB-CG	5.19	127.24	115.30
1	A	226	ASP	CB-CG-OD1	5.14	122.92	118.30
9	I	44	ASP	CB-CG-OD2	5.13	122.92	118.30
3	C	254	ASP	CB-CG-OD2	5.13	122.91	118.30
4	D	59	ASP	CB-CG-OD2	5.13	122.91	118.30
1	A	20	ASP	CB-CG-OD2	5.09	122.88	118.30
5	E	119	ASP	CB-CG-OD2	5.06	122.86	118.30
9	I	24	GLY	N-CA-C	5.04	125.71	113.10
5	E	152	ASP	CB-CG-OD2	5.04	122.84	118.30
8	H	60	ASP	CB-CG-OD2	5.03	122.82	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	174	ASN	Peptide

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	3458	0	3356	27	0
2	B	3181	0	3160	31	0
3	C	3003	0	3065	25	0
4	D	1919	0	1870	20	0
5	E	1519	0	1504	9	0
6	F	911	0	904	7	0
7	G	628	0	636	3	0
8	H	548	0	530	2	0
9	I	406	0	437	21	0
10	J	502	0	505	5	0
11	K	425	0	433	4	0
12	C	86	0	60	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	D	43	0	30	1	0
13	C	30	0	17	1	0
14	E	4	0	0	0	0
15	A	47	0	0	0	0
15	B	82	0	0	4	0
15	C	37	0	0	1	0
15	D	19	0	0	1	0
15	E	2	0	0	0	0
15	F	21	0	0	0	0
15	G	20	0	0	0	0
15	H	1	0	0	0	0
15	I	3	0	0	0	0
15	K	2	0	0	0	0
All	All	16897	0	16507	130	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 4.

All (130) 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:176:LEU:HD21	9:I:13:PRO:HD3	1.65	0.77
4:D:37:CYS:SG	12:D:242:HEM:HAB	2.24	0.77
6:F:28:LYS:HB3	6:F:74:ILE:HG12	1.68	0.76
2:B:310:SER:HB3	9:I:28:PRO:HD3	1.69	0.75
1:A:149:VAL:HG21	1:A:252:HIS:HB3	1.73	0.70
12:C:381:HEM:HMC2	12:C:381:HEM:HBC2	1.73	0.70
2:B:71:LEU:HD22	9:I:15:LEU:HD13	1.76	0.67
9:I:20:ARG:HG3	9:I:51:CYS:HA	1.78	0.65
2:B:166:ALA:HB2	2:B:244:ILE:HG13	1.78	0.65
3:C:119:LEU:HD22	12:C:381:HEM:HBB2	1.81	0.62
4:D:204:MET:HB2	15:D:676:HOH:O	1.98	0.62
3:C:126:THR:HG21	12:C:382:HEM:HBB2	1.81	0.62
1:A:303:LEU:HB3	1:A:334:MET:CE	2.30	0.61
2:B:258:VAL:HG12	2:B:423:SER:HB2	1.84	0.58
2:B:99:THR:HG22	15:B:579:HOH:O	2.03	0.57
4:D:117:VAL:HG21	4:D:191:ARG:HA	1.87	0.56
6:F:58:ARG:O	6:F:62:ILE:HG12	2.07	0.55
2:B:361:LYS:NZ	2:B:405:VAL:O	2.39	0.55
8:H:62:LEU:HD23	8:H:65:ARG:HH12	1.72	0.55
9:I:12:ALA:H	9:I:24:GLY:HA2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:76:THR:HG23	2:B:81:SER:HA	1.89	0.54
10:J:29:LEU:HG	11:K:34:TRP:HB2	1.89	0.54
15:B:732:HOH:O	9:I:21:GLY:HA3	2.08	0.54
10:J:10:TYR:HA	10:J:14:PHE:HB2	1.89	0.54
2:B:71:LEU:CD2	9:I:15:LEU:HD13	2.36	0.53
5:E:165:TYR:HB3	5:E:169:GLY:HA2	1.90	0.53
1:A:145:MET:O	1:A:149:VAL:HG23	2.08	0.52
2:B:150:VAL:HG13	9:I:47:ARG:HG2	1.92	0.52
4:D:218:LEU:HD22	5:E:39:VAL:HG13	1.90	0.52
2:B:71:LEU:HA	9:I:15:LEU:HD22	1.92	0.51
1:A:361:LEU:HD23	1:A:399:ILE:HG12	1.92	0.51
2:B:109:VAL:HG22	2:B:119:LEU:HD23	1.92	0.51
6:F:28:LYS:HB3	6:F:74:ILE:CG1	2.38	0.51
1:A:298:ALA:HA	1:A:303:LEU:HB2	1.92	0.51
6:F:47:ILE:HD13	6:F:90:LEU:HD21	1.92	0.51
9:I:46:LYS:HG2	9:I:47:ARG:N	2.26	0.50
3:C:78:ILE:O	3:C:82:MET:HB2	2.11	0.50
2:B:150:VAL:CG1	9:I:47:ARG:HG2	2.41	0.50
4:D:69:GLU:HB3	4:D:82:MET:HG2	1.94	0.50
4:D:43:MET:HG3	4:D:114:SER:HB3	1.93	0.50
1:A:303:LEU:HB3	1:A:334:MET:HE3	1.92	0.50
1:A:21:ASN:HD22	1:A:219:LEU:HB2	1.76	0.49
4:D:206:LEU:HD21	10:J:42:ILE:HG22	1.95	0.49
3:C:309:THR:HG21	3:C:367:PRO:O	2.12	0.49
1:A:281:ASP:OD2	9:I:47:ARG:HB2	2.12	0.49
3:C:300:ILE:HG12	3:C:362:ILE:HG21	1.94	0.48
11:K:33:VAL:HG22	11:K:41:ILE:HD13	1.95	0.48
2:B:34:VAL:HG11	2:B:386:ALA:HB1	1.96	0.47
2:B:102:ARG:HG2	15:B:567:HOH:O	2.15	0.47
2:B:264:ILE:HG12	9:I:2:LEU:HD23	1.96	0.47
2:B:68:LEU:HD23	2:B:186:VAL:HG22	1.97	0.47
2:B:169:ARG:HD2	2:B:240:HIS:HB2	1.97	0.47
6:F:82:LYS:HB2	6:F:85:GLU:HG2	1.96	0.47
2:B:325:TYR:HB3	9:I:28:PRO:HD2	1.96	0.46
5:E:156:TYR:HB2	5:E:165:TYR:HB2	1.95	0.46
3:C:349:THR:HA	3:C:352:GLN:HE21	1.81	0.46
4:D:28:ARG:O	4:D:32:VAL:HG23	2.16	0.46
9:I:4:VAL:HG12	9:I:10:PRO:HG2	1.97	0.46
2:B:156:GLN:HE21	2:B:156:GLN:H	1.62	0.45
2:B:52:LYS:HB2	2:B:203:ARG:HB3	1.97	0.45
6:F:107:TRP:HA	6:F:110:LYS:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:78:ILE:HD11	3:C:244:LEU:HD21	1.98	0.45
1:A:204:GLU:H	1:A:204:GLU:HG2	1.66	0.45
3:C:300:ILE:HD11	3:C:363:LEU:HD13	1.98	0.45
1:A:53:ASN:HD22	1:A:170:PRO:HD3	1.81	0.44
2:B:44:ALA:HA	2:B:112:LEU:HA	1.99	0.44
5:E:20:ASP:HB3	5:E:23:LYS:HB3	1.99	0.44
3:C:15:ASN:HA	3:C:19:ILE:HB	2.00	0.44
1:A:24:ARG:HD2	1:A:383:LEU:HD12	1.99	0.44
1:A:40:TRP:CZ2	1:A:377:GLU:HA	2.53	0.44
3:C:206:ASN:HB3	12:C:381:HEM:O1D	2.18	0.44
1:A:110:VAL:HG11	1:A:211:LEU:HB3	1.99	0.43
3:C:246:ALA:HB1	3:C:249:LEU:HB2	1.99	0.43
4:D:14:HIS:HB3	4:D:21:LEU:HA	1.99	0.43
4:D:18:LEU:HD22	4:D:206:LEU:HB2	2.00	0.43
4:D:163:PRO:HD2	4:D:164:ILE:HG13	1.99	0.43
3:C:132:VAL:HG12	3:C:175:LEU:HD23	2.00	0.43
1:A:146:ARG:HH12	1:A:308:GLN:HE22	1.65	0.43
3:C:81:TYR:HB2	3:C:243:VAL:HG13	2.00	0.43
4:D:138:PRO:HB3	8:H:58:LEU:HD13	2.00	0.43
1:A:273:ALA:HA	1:A:276:ILE:HD12	2.00	0.43
2:B:399:LEU:HA	2:B:402:ILE:HD12	2.00	0.43
4:D:99:GLU:HA	4:D:102:ARG:HG3	2.01	0.43
2:B:245:ARG:NH2	2:B:433:THR:O	2.45	0.43
1:A:146:ARG:HH22	1:A:308:GLN:HE22	1.66	0.43
3:C:118:ILE:O	3:C:122:THR:OG1	2.35	0.42
5:E:145:VAL:HA	5:E:146:PRO:HD3	1.91	0.42
2:B:59:ASN:O	2:B:63:LEU:HD13	2.19	0.42
10:J:2:ALA:HB3	10:J:3:PRO:HD3	2.01	0.42
1:A:106:LEU:N	1:A:107:PRO:HD2	2.34	0.42
1:A:149:VAL:HG21	1:A:252:HIS:CB	2.46	0.42
1:A:5:ALA:HA	1:A:8:LEU:HD12	2.01	0.42
2:B:99:THR:HB	9:I:14:VAL:HG13	2.01	0.42
4:D:75:ASN:HD21	4:D:77:ASP:HB2	1.83	0.42
7:G:24:ARG:HD2	7:G:27:PRO:HA	2.01	0.42
3:C:105:GLY:HA2	3:C:107:TYR:CE2	2.54	0.42
15:B:532:HOH:O	9:I:15:LEU:HD11	2.19	0.42
3:C:104:TYR:CD1	3:C:208:PRO:HA	2.54	0.42
3:C:337:TRP:CZ3	3:C:350:ILE:HD11	2.54	0.42
6:F:63:LYS:HE3	7:G:13:VAL:HG11	2.01	0.42
7:G:26:PHE:HB3	7:G:29:TYR:HB2	2.01	0.42
1:A:280:TYR:CG	1:A:281:ASP:N	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:ARG:HD2	9:I:56:ARG:HH12	1.85	0.42
4:D:110:PRO:HA	4:D:111:PRO:HD3	1.89	0.41
2:B:283:PRO:HD3	9:I:31:GLN:HG2	2.02	0.41
3:C:92:ILE:HG22	3:C:272:TRP:CZ2	2.55	0.41
4:D:131:LEU:HB3	4:D:164:ILE:HG12	2.00	0.41
3:C:8:HIS:HD2	3:C:11:MET:H	1.68	0.41
3:C:51:LEU:HD13	12:C:382:HEM:HBD1	2.03	0.41
1:A:37:VAL:HG13	1:A:199:ALA:HB2	2.01	0.41
1:A:264:HIS:HA	1:A:265:PRO:HD3	1.96	0.41
3:C:58:ASP:HB3	15:C:638:HOH:O	2.19	0.41
10:J:29:LEU:HD22	11:K:48:ILE:HG12	2.01	0.41
2:B:316:TYR:OH	9:I:10:PRO:HB3	2.20	0.41
4:D:198:HIS:HA	4:D:201:ARG:HH11	1.85	0.41
1:A:138:LEU:HB3	5:E:1:SER:H1	1.86	0.41
1:A:334:MET:HA	1:A:334:MET:HE2	2.02	0.41
2:B:325:TYR:HB3	9:I:28:PRO:CD	2.51	0.41
3:C:30:TRP:HB3	3:C:100:ARG:HG3	2.03	0.41
4:D:201:ARG:HG3	4:D:202:LYS:HZ3	1.86	0.41
5:E:146:PRO:HA	5:E:159:PRO:HD3	2.02	0.41
1:A:237:THR:OG1	5:E:14:ARG:NH2	2.53	0.41
2:B:150:VAL:O	2:B:153:GLN:HG2	2.20	0.41
3:C:143:ALA:N	13:C:383:AZO:H221	2.36	0.41
11:K:45:VAL:HA	11:K:46:PRO:HD3	1.91	0.41
1:A:80:GLU:HG3	2:B:284:HIS:HB2	2.02	0.40
5:E:10:PHE:HB2	5:E:14:ARG:HH11	1.85	0.40
3:C:78:ILE:HG13	4:D:204:MET:HE1	2.03	0.40
3:C:252:ASP:HA	3:C:253:PRO:HD3	1.96	0.40
4:D:33:TYR:HA	4:D:37:CYS:SG	2.62	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	444/480 (92%)	428 (96%)	13 (3%)	3 (1%)	22 46
2	B	423/453 (93%)	402 (95%)	18 (4%)	3 (1%)	22 46
3	C	376/379 (99%)	361 (96%)	13 (4%)	2 (0%)	29 54
4	D	239/241 (99%)	218 (91%)	19 (8%)	2 (1%)	19 43
5	E	194/196 (99%)	169 (87%)	23 (12%)	2 (1%)	15 37
6	F	103/110 (94%)	101 (98%)	2 (2%)	0	100 100
7	G	73/81 (90%)	69 (94%)	3 (4%)	1 (1%)	11 28
8	H	65/78 (83%)	63 (97%)	2 (3%)	0	100 100
9	I	55/78 (70%)	37 (67%)	11 (20%)	7 (13%)	0 0
10	J	59/62 (95%)	56 (95%)	2 (3%)	1 (2%)	9 23
11	K	50/56 (89%)	46 (92%)	3 (6%)	1 (2%)	7 19
All	All	2081/2214 (94%)	1950 (94%)	109 (5%)	22 (1%)	14 34

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	437	ASP
9	I	44	ASP
3	C	157	GLY
9	I	8	SER
9	I	29	LEU
9	I	53	GLU
10	J	56	LYS
1	A	2	ALA
1	A	225	GLU
4	D	144	ARG
4	D	145	GLU
5	E	65	SER
9	I	40	SER
11	K	50	GLY
1	A	229	PRO
2	B	176	LEU
2	B	232	LEU
9	I	9	GLY
5	E	5	ILE
9	I	27	ARG
7	G	27	PRO
3	C	345	HIS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	370/394 (94%)	312 (84%)	58 (16%)	2	6
2	B	332/355 (94%)	284 (86%)	48 (14%)	3	8
3	C	326/327 (100%)	278 (85%)	48 (15%)	3	7
4	D	206/206 (100%)	171 (83%)	35 (17%)	2	5
5	E	168/168 (100%)	141 (84%)	27 (16%)	2	6
6	F	96/98 (98%)	87 (91%)	9 (9%)	8	20
7	G	66/71 (93%)	51 (77%)	15 (23%)	1	2
8	H	64/74 (86%)	40 (62%)	24 (38%)	0	0
9	I	44/60 (73%)	29 (66%)	15 (34%)	0	0
10	J	51/52 (98%)	34 (67%)	17 (33%)	0	0
11	K	42/46 (91%)	29 (69%)	13 (31%)	0	0
All	All	1765/1851 (95%)	1456 (82%)	309 (18%)	2	4

All (309) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	THR
1	A	10	SER
1	A	15	GLN
1	A	29	GLN
1	A	31	SER
1	A	37	VAL
1	A	42	ASP
1	A	58	PHE
1	A	60	GLU
1	A	68	LYS
1	A	73	ASN
1	A	75	LEU
1	A	90	SER
1	A	104	LYS
1	A	106	LEU

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Mol	Chain	Res	Type
1	A	113	LEU
1	A	115	ASP
1	A	121	SER
1	A	122	LEU
1	A	123	GLU
1	A	127	ILE
1	A	128	GLU
1	A	129	LYS
1	A	131	ARG
1	A	139	GLN
1	A	140	GLU
1	A	163	LEU
1	A	171	SER
1	A	172	GLU
1	A	176	LYS
1	A	177	LEU
1	A	179	ARG
1	A	183	THR
1	A	184	GLU
1	A	203	LEU
1	A	204	GLU
1	A	206	ARG
1	A	207	GLN
1	A	214	LYS
1	A	223	TYR
1	A	224	ASP
1	A	225	GLU
1	A	245	GLU
1	A	302	LYS
1	A	305	GLN
1	A	308	GLN
1	A	343	MET
1	A	351	GLU
1	A	367	SER
1	A	370	ASP
1	A	381	ARG
1	A	388	ARG
1	A	392	LEU
1	A	401	GLU
1	A	403	ASP
1	A	409	GLU
1	A	438	ARG

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Mol	Chain	Res	Type
1	A	439	SER
2	B	20	HIS
2	B	22	GLN
2	B	38	LEU
2	B	46	ARG
2	B	60	SER
2	B	63	LEU
2	B	69	LEU
2	B	84	LYS
2	B	95	LYS
2	B	97	SER
2	B	98	VAL
2	B	109	VAL
2	B	113	ARG
2	B	116	VAL
2	B	123	LEU
2	B	152	LEU
2	B	156	GLN
2	B	163	LEU
2	B	175	SER
2	B	186	VAL
2	B	189	VAL
2	B	196	GLN
2	B	197	ASN
2	B	209	LEU
2	B	216	LEU
2	B	227	ARG
2	B	230	LEU
2	B	232	LEU
2	B	246	GLU
2	B	250	ASP
2	B	257	LEU
2	B	258	VAL
2	B	273	SER
2	B	290	ASN
2	B	294	SER
2	B	301	LYS
2	B	305	GLN
2	B	315	SER
2	B	349	GLN
2	B	358	GLN
2	B	361	LYS

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Mol	Chain	Res	Type
2	B	371	SER
2	B	376	GLU
2	B	379	LEU
2	B	397	THR
2	B	415	LYS
2	B	421	ARG
2	B	437	ASP
3	C	6	LYS
3	C	35	SER
3	C	43	LEU
3	C	45	ILE
3	C	60	THR
3	C	64	SER
3	C	74	ASN
3	C	78	ILE
3	C	80	ARG
3	C	82	MET
3	C	88	SER
3	C	90	PHE
3	C	92	ILE
3	C	102	LEU
3	C	110	LEU
3	C	114	ASN
3	C	122	THR
3	C	144	THR
3	C	145	VAL
3	C	161	VAL
3	C	171	ASP
3	C	175	LEU
3	C	183	PHE
3	C	194	MET
3	C	205	SER
3	C	226	ILE
3	C	235	LEU
3	C	249	LEU
3	C	262	LEU
3	C	269	LYS
3	C	284	ILE
3	C	287	LYS
3	C	291	VAL
3	C	296	PHE
3	C	299	LEU

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Mol	Chain	Res	Type
3	C	300	ILE
3	C	304	ILE
3	C	311	LYS
3	C	316	MET
3	C	320	LEU
3	C	343	VAL
3	C	344	GLU
3	C	348	ILE
3	C	350	ILE
3	C	353	LEU
3	C	360	LEU
3	C	365	LEU
3	C	379	TRP
4	D	1	SER
4	D	5	LEU
4	D	13	SER
4	D	15	ARG
4	D	17	LEU
4	D	20	SER
4	D	24	THR
4	D	34	LYS
4	D	37	CYS
4	D	43	MET
4	D	49	ARG
4	D	60	GLU
4	D	62	LYS
4	D	66	GLU
4	D	71	GLN
4	D	77	ASP
4	D	82	MET
4	D	93	LYS
4	D	99	GLU
4	D	102	ARG
4	D	109	LEU
4	D	116	ILE
4	D	132	THR
4	D	139	THR
4	D	143	LEU
4	D	164	ILE
4	D	168	VAL
4	D	169	LEU
4	D	170	GLU

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Mol	Chain	Res	Type
4	D	173	ASP
4	D	179	MET
4	D	186	VAL
4	D	202	LYS
4	D	214	LEU
4	D	223	LYS
5	E	6	LYS
5	E	12	ASP
5	E	14	ARG
5	E	22	THR
5	E	54	VAL
5	E	69	LEU
5	E	74	ILE
5	E	77	LYS
5	E	80	ASP
5	E	85	LYS
5	E	89	PHE
5	E	90	LYS
5	E	103	LYS
5	E	117	LEU
5	E	125	GLU
5	E	126	ARG
5	E	128	LYS
5	E	129	LYS
5	E	135	LEU
5	E	138	VAL
5	E	140	THR
5	E	160	CYS
5	E	166	ASP
5	E	173	LYS
5	E	178	LEU
5	E	179	ASN
5	E	190	ASP
6	F	7	SER
6	F	10	SER
6	F	16	ILE
6	F	70	MET
6	F	71	ARG
6	F	74	ILE
6	F	77	LYS
6	F	78	GLU
6	F	110	LYS

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Mol	Chain	Res	Type
7	G	3	GLN
7	G	9	ARG
7	G	18	LEU
7	G	31	SER
7	G	32	LYS
7	G	36	ASN
7	G	37	VAL
7	G	40	ARG
7	G	42	ARG
7	G	45	ILE
7	G	47	ARG
7	G	64	GLN
7	G	68	LYS
7	G	72	LYS
7	G	73	ASN
8	H	12	GLU
8	H	13	LEU
8	H	15	ASP
8	H	18	THR
8	H	20	VAL
8	H	22	GLU
8	H	23	GLN
8	H	25	GLU
8	H	27	LEU
8	H	28	GLU
8	H	29	LYS
8	H	30	CYS
8	H	32	LYS
8	H	34	ARG
8	H	38	GLU
8	H	39	LEU
8	H	49	GLN
8	H	53	ASP
8	H	56	GLU
8	H	65	ARG
8	H	68	CYS
8	H	72	LYS
8	H	73	LEU
8	H	75	ASN
9	I	1	MET
9	I	8	SER
9	I	15	LEU

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Mol	Chain	Res	Type
9	I	20	ARG
9	I	27	ARG
9	I	30	VAL
9	I	31	GLN
9	I	42	VAL
9	I	45	LEU
9	I	47	ARG
9	I	48	SER
9	I	50	LEU
9	I	51	CYS
9	I	52	ARG
9	I	55	LEU
10	J	4	THR
10	J	5	LEU
10	J	11	SER
10	J	15	ARG
10	J	16	ARG
10	J	18	SER
10	J	29	LEU
10	J	36	ASP
10	J	37	GLN
10	J	42	ILE
10	J	44	GLU
10	J	45	HIS
10	J	46	ILE
10	J	48	GLU
10	J	58	LYS
10	J	59	TYR
10	J	60	GLU
11	K	6	LEU
11	K	13	LEU
11	K	15	ARG
11	K	16	ASN
11	K	18	VAL
11	K	38	SER
11	K	39	ARG
11	K	40	LEU
11	K	43	ASP
11	K	44	TRP
11	K	47	TYR
11	K	49	ASN
11	K	51	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	52	ASN
1	A	53	ASN
1	A	73	ASN
1	A	279	HIS
2	B	104	ASN
2	B	158	HIS
2	B	162	ASN
2	B	170	ASN
2	B	276	GLN
2	B	277	HIS
2	B	342	ASN
2	B	349	GLN
3	C	8	HIS
3	C	44	GLN
3	C	74	ASN
3	C	114	ASN
3	C	341	GLN
3	C	352	GLN
4	D	31	GLN
4	D	105	ASN
4	D	106	ASN
4	D	181	GLN
5	E	164	HIS
5	E	179	ASN
7	G	3	GLN
8	H	26	GLN
11	K	12	GLN

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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	HEM	C	382	3	41,50,50	1.70	9 (21%)	45,82,82	1.59	9 (20%)
12	HEM	C	381	3	41,50,50	1.69	5 (12%)	45,82,82	1.66	10 (22%)
13	AZO	C	383	-	32,32,32	2.68	8 (25%)	42,42,42	2.90	11 (26%)
14	FES	E	200	5	0,4,4	-	-	-		
12	HEM	D	242	4	41,50,50	1.80	9 (21%)	45,82,82	1.79	9 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	HEM	C	382	3	-	8/12/54/54	-
12	HEM	C	381	3	-	6/12/54/54	-
13	AZO	C	383	-	-	1/23/23/23	0/3/3/3
14	FES	E	200	5	-	-	0/1/1/1
12	HEM	D	242	4	-	10/12/54/54	-

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	383	AZO	C21-C18	7.69	1.51	1.34
13	C	383	AZO	C18-C19	-5.65	1.33	1.48
13	C	383	AZO	O4-C19	5.36	1.45	1.33
13	C	383	AZO	C17-C12	5.26	1.50	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	383	AZO	C2-C7	5.08	1.51	1.40
12	D	242	HEM	CBB-CAB	5.07	1.55	1.30
12	C	382	HEM	CBB-CAB	5.05	1.55	1.30
12	C	381	HEM	CBB-CAB	5.00	1.55	1.30
12	C	381	HEM	CBD-CGD	-4.41	1.40	1.50
12	D	242	HEM	CBC-CAC	4.15	1.56	1.29
12	D	242	HEM	CBD-CGD	-4.02	1.41	1.50
12	C	381	HEM	CBC-CAC	3.91	1.55	1.29
12	C	382	HEM	CBC-CAC	3.83	1.54	1.29
12	C	381	HEM	CBA-CGA	-3.66	1.42	1.50
12	D	242	HEM	CBA-CGA	-3.62	1.42	1.50
12	C	382	HEM	CBA-CGA	-3.54	1.42	1.50
12	C	382	HEM	CBD-CGD	-3.44	1.42	1.50
13	C	383	AZO	C10-N3	3.14	1.37	1.32
12	C	381	HEM	C3C-CAC	3.09	1.54	1.47
13	C	383	AZO	C8-N2	3.00	1.37	1.32
12	D	242	HEM	CAA-C2A	2.96	1.56	1.52
13	C	383	AZO	O5-C21	2.87	1.40	1.34
12	D	242	HEM	C3C-CAC	2.77	1.53	1.47
12	C	382	HEM	C3C-CAC	2.73	1.53	1.47
12	D	242	HEM	C4D-C3D	-2.43	1.40	1.45
12	C	382	HEM	CAB-C3B	2.24	1.53	1.47
12	C	382	HEM	C3C-C2C	-2.21	1.37	1.40
12	D	242	HEM	CHB-C1B	2.18	1.40	1.35
12	C	382	HEM	CAA-C2A	2.16	1.55	1.52
12	D	242	HEM	C3C-C2C	-2.11	1.37	1.40
12	C	382	HEM	CHB-C1B	2.11	1.40	1.35

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	C	383	AZO	C11-N3-C10	9.55	121.67	114.48
13	C	383	AZO	C11-N2-C8	9.48	121.61	114.48
13	C	383	AZO	N2-C11-N3	-5.77	119.57	128.60
13	C	383	AZO	O4-C19-C18	5.16	119.58	112.01
12	C	381	HEM	C4C-CHD-C1D	-4.95	116.03	122.56
13	C	383	AZO	O5-C21-C18	-4.50	112.40	121.19
13	C	383	AZO	C22-O5-C21	-4.31	108.09	115.61
13	C	383	AZO	C9-C10-N3	-3.80	119.23	124.57
12	C	382	HEM	CHD-C1D-ND	3.69	128.44	124.43
13	C	383	AZO	C9-C8-N2	-3.53	119.61	124.57
12	D	242	HEM	CBA-CAA-C2A	3.52	118.62	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	D	242	HEM	C4B-CHC-C1C	-3.46	117.99	122.56
12	C	381	HEM	CHD-C1D-ND	3.41	128.13	124.43
12	D	242	HEM	CHB-C1B-NB	3.40	128.58	124.38
12	D	242	HEM	CBB-CAB-C3B	-3.32	111.12	127.62
13	C	383	AZO	C10-C9-C8	3.28	118.19	115.21
12	D	242	HEM	CHD-C1D-ND	3.25	127.96	124.43
12	C	381	HEM	CBB-CAB-C3B	-3.22	111.61	127.62
12	C	382	HEM	C4B-CHC-C1C	-3.11	118.46	122.56
12	D	242	HEM	C4C-CHD-C1D	-3.04	118.54	122.56
12	D	242	HEM	CMA-C3A-C4A	-3.03	123.81	128.46
12	C	382	HEM	CHB-C1B-NB	2.94	128.01	124.38
12	C	382	HEM	CBB-CAB-C3B	-2.66	114.41	127.62
12	C	382	HEM	O2D-CGD-CBD	2.63	122.48	114.03
12	C	382	HEM	C4C-CHD-C1D	-2.62	119.11	122.56
12	C	381	HEM	C4D-ND-C1D	2.57	107.73	105.07
13	C	383	AZO	C12-O2-C10	2.54	123.84	118.47
12	C	381	HEM	C1B-NB-C4B	2.52	107.68	105.07
13	C	383	AZO	O4-C19-O3	-2.44	118.82	123.53
12	C	381	HEM	C4B-CHC-C1C	-2.42	119.37	122.56
12	D	242	HEM	CHC-C4B-NB	2.38	127.02	124.43
12	D	242	HEM	CHA-C4D-ND	2.37	127.31	124.38
12	C	381	HEM	O2A-CGA-CBA	2.31	121.47	114.03
12	C	381	HEM	CMC-C2C-C3C	2.28	128.95	124.68
12	C	381	HEM	O2D-CGD-CBD	2.22	121.18	114.03
12	C	382	HEM	C4A-C3A-C2A	2.20	108.53	107.00
12	C	382	HEM	O2A-CGA-CBA	2.17	121.00	114.03
12	C	382	HEM	CHC-C4B-NB	2.15	126.77	124.43
12	C	381	HEM	CHB-C1B-NB	2.04	126.90	124.38

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	C	381	HEM	C2B-C3B-CAB-CBB
12	C	381	HEM	C4B-C3B-CAB-CBB
12	C	382	HEM	C2B-C3B-CAB-CBB
12	D	242	HEM	C1A-C2A-CAA-CBA
12	D	242	HEM	C3A-C2A-CAA-CBA
12	D	242	HEM	C2A-CAA-CBA-CGA
12	D	242	HEM	C2B-C3B-CAB-CBB
12	D	242	HEM	C4B-C3B-CAB-CBB
12	D	242	HEM	C3D-CAD-CBD-CGD

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Mol	Chain	Res	Type	Atoms
12	C	382	HEM	C2A-CAA-CBA-CGA
12	C	382	HEM	C4B-C3B-CAB-CBB
12	C	382	HEM	C3D-CAD-CBD-CGD
12	C	381	HEM	CAD-CBD-CGD-O1D
12	C	381	HEM	CAD-CBD-CGD-O2D
12	C	381	HEM	CAA-CBA-CGA-O1A
12	C	382	HEM	CAA-CBA-CGA-O1A
12	C	381	HEM	CAA-CBA-CGA-O2A
12	C	382	HEM	CAA-CBA-CGA-O2A
12	D	242	HEM	CAD-CBD-CGD-O1D
12	D	242	HEM	CAD-CBD-CGD-O2D
12	D	242	HEM	CAA-CBA-CGA-O1A
12	D	242	HEM	CAA-CBA-CGA-O2A
13	C	383	AZO	N1-C1-C2-C7
12	C	382	HEM	CAD-CBD-CGD-O1D
12	C	382	HEM	CAD-CBD-CGD-O2D

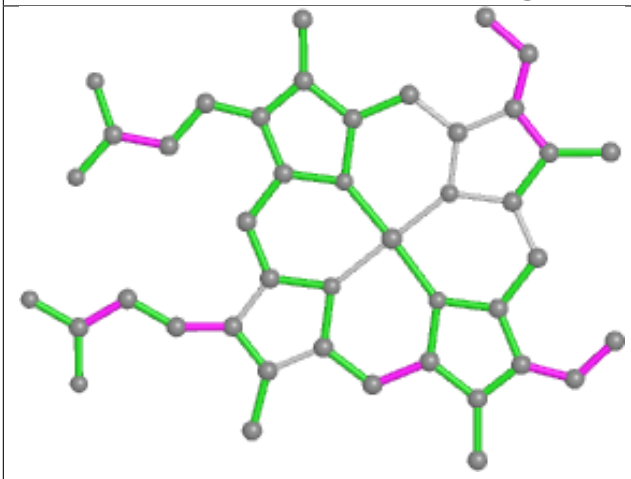
There are no ring outliers.

4 monomers are involved in 7 short contacts:

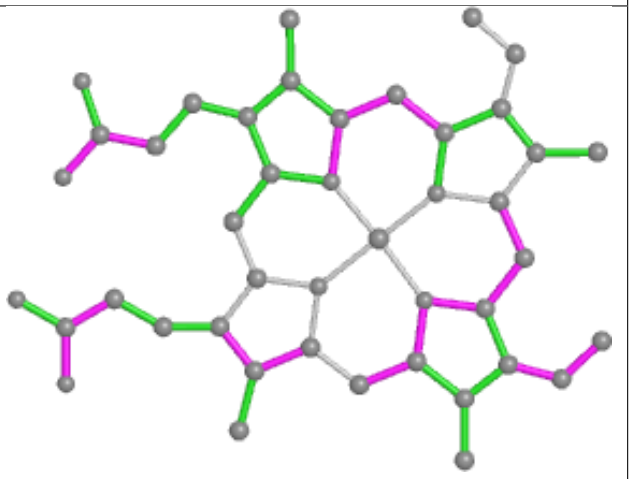
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	C	382	HEM	2	0
12	C	381	HEM	3	0
13	C	383	AZO	1	0
12	D	242	HEM	1	0

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 then 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.

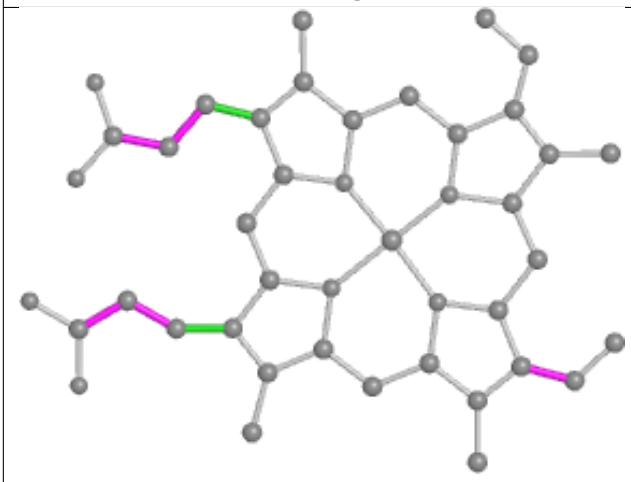
Ligand HEM C 382



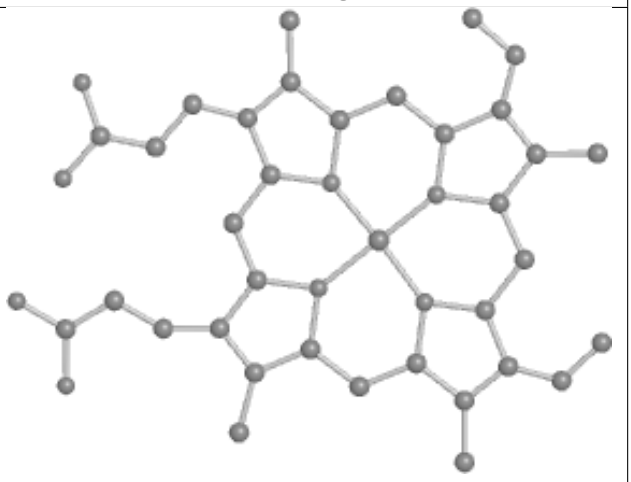
Bond lengths



Bond angles

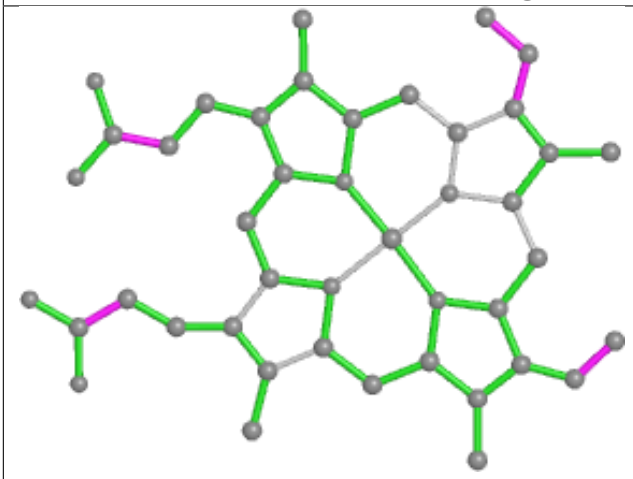


Torsions

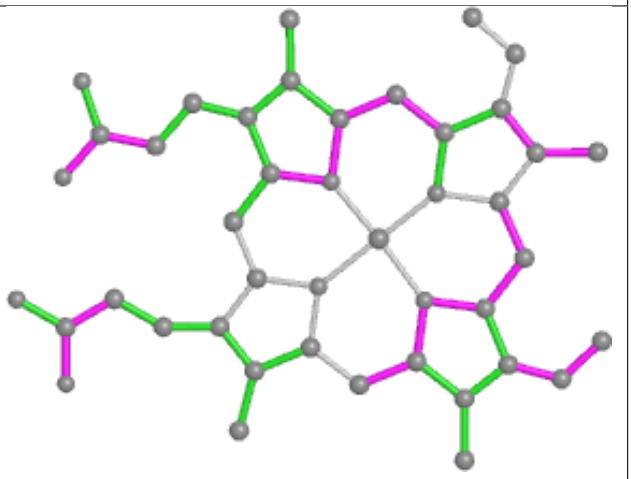


Rings

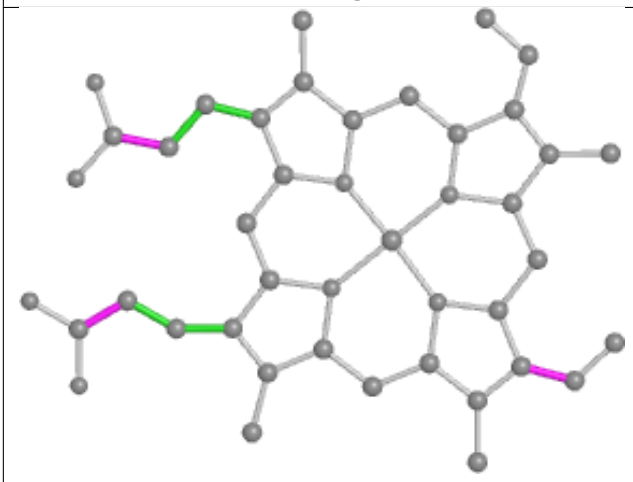
Ligand HEM C 381



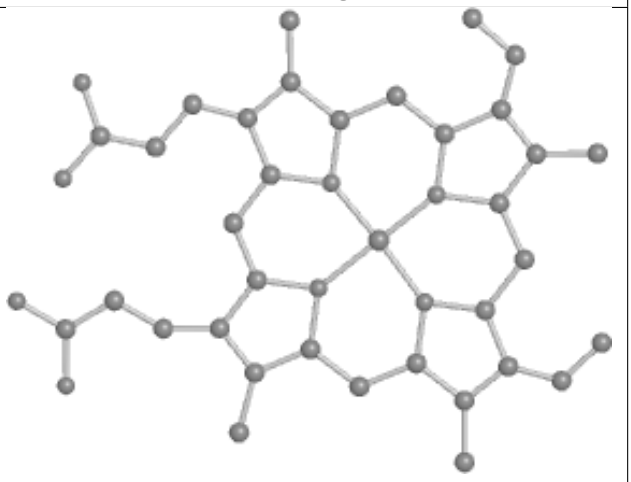
Bond lengths



Bond angles

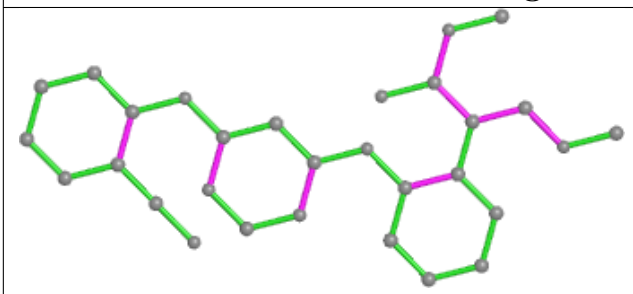


Torsions

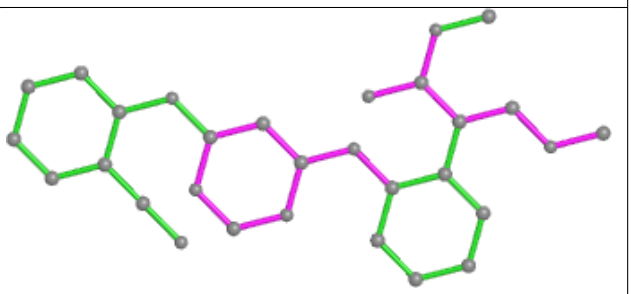


Rings

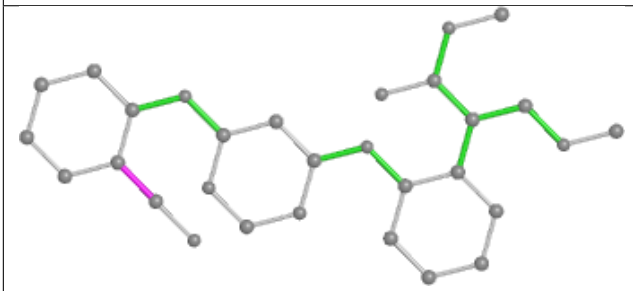
Ligand AZO C 383



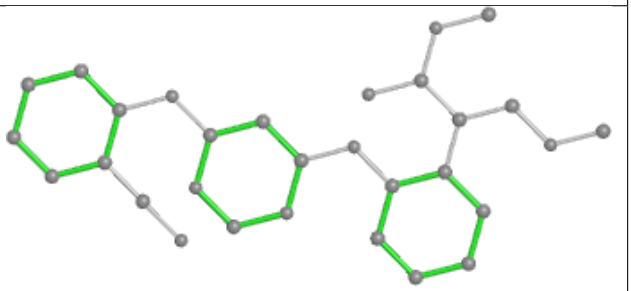
Bond lengths



Bond angles

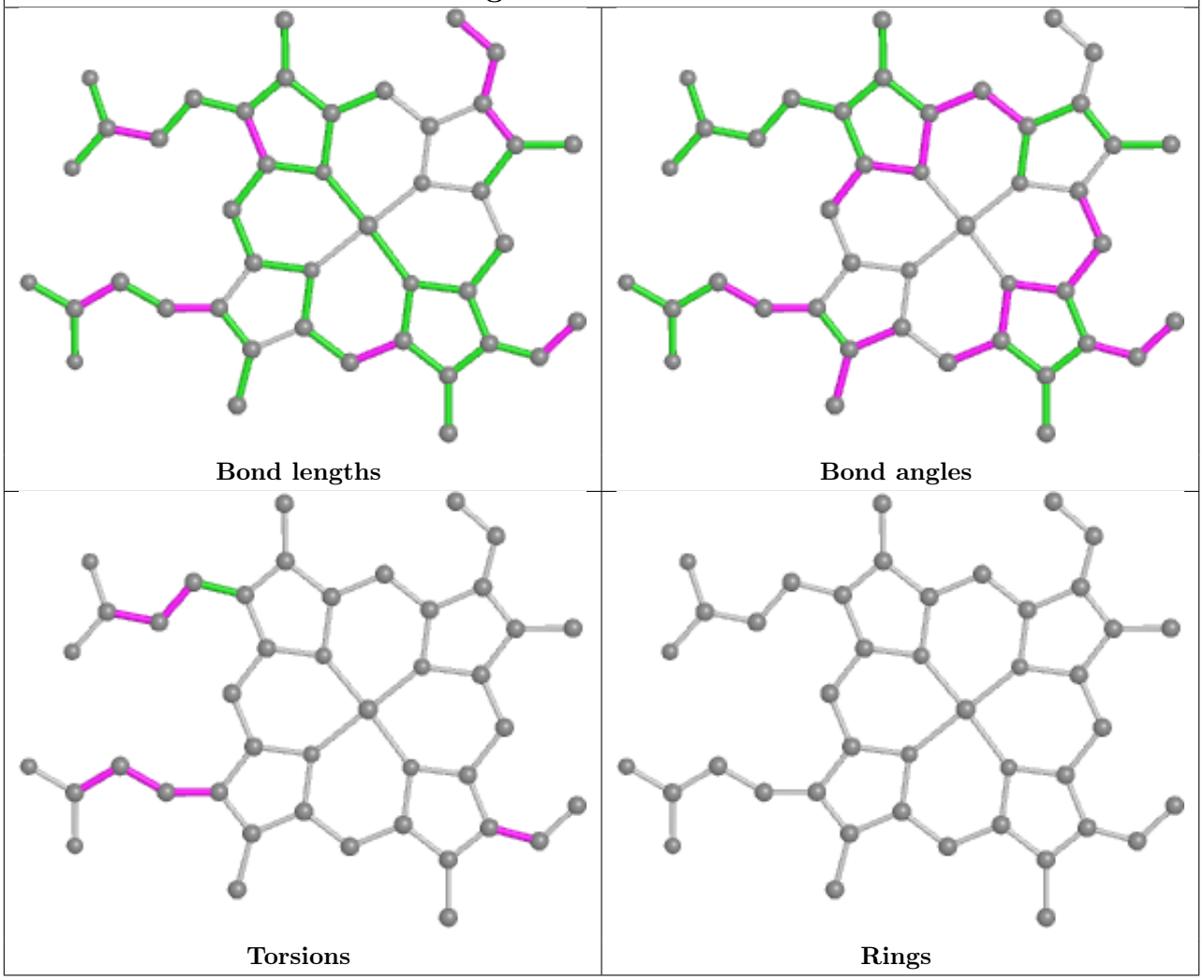


Torsions



Rings

Ligand HEM D 242



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.