



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 08:10 PM EDT

PDB ID : 2FYU / pdb_00002fyu
Title : Crystal structure of bovine heart mitochondrial bc1 with jg144 inhibitor
Authors : Xia, D.; Esser, L.
Deposited on : 2006-02-08
Resolution : 2.26 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)	:	2.50

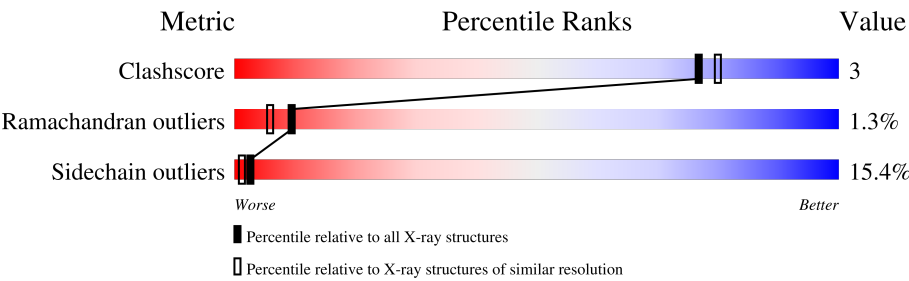
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 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	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)

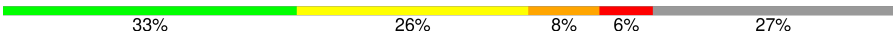
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	446	79% 18% .
2	B	439	75% 18% ..
3	C	379	76% 20% ..
4	D	241	71% 25% .
5	E	196	72% 26% ..
6	F	110	82% 10% ...
7	G	81	73% 12% 6% 7%
8	H	78	53% 26% 18%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	I	78	 33% 26% 8% 6% 27%
10	J	62	 63% 32% • •
11	K	56	 55% 34% • • 5%

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 16900 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
1	A	446	Total	C	N	O	S	0	0	0
			3458	2161	609	668	20			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	423	Total	C	N	O	S	0	0	0
			3172	1993	562	610	7			

- Molecule 3 is a protein called Cytochrome b.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	241	Total	C	N	O	S	0	0	0
			1918	1225	330	348	15			

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

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

- Molecule 6 is a protein called Hypothetical protein LOC616871.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	106	Total	C	N	O	S	0	0	0
			916	579	166	169	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	64	Total	C	N	O	S	0	0	0
			524	316	96	107	5			

- Molecule 9 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial.

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

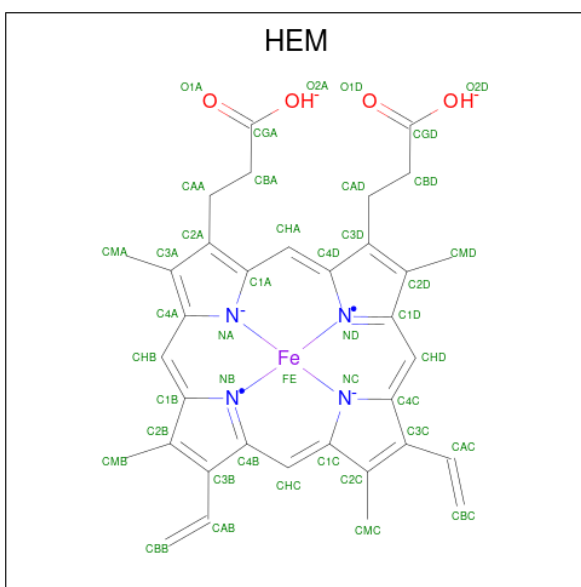
- Molecule 10 is a protein called Ubiquinol-cytochrome c reductase complex 7.2 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	60	Total	C	N	O	S	0	0	0
			495	324	86	85				

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

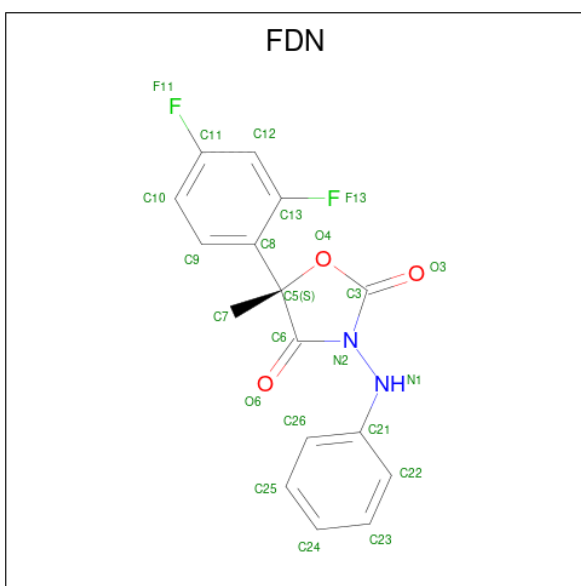
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	53	Total	C	N	O	S	0	0	0
			438	293	78	66	1			

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



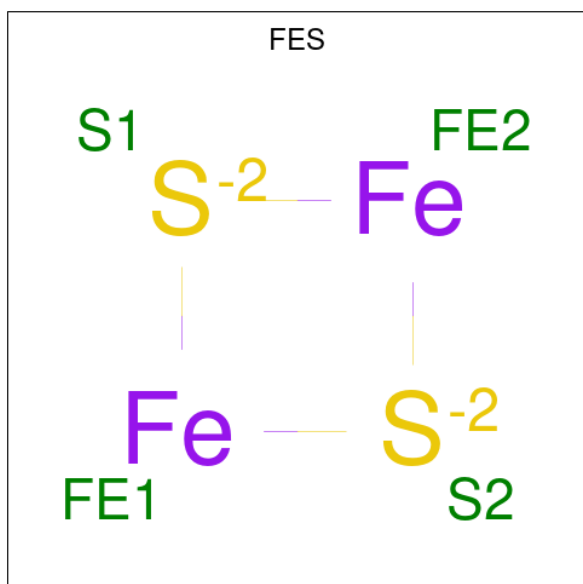
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
12	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
12	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 13 is (5S)-3-ANILINO-5-(2,4-DIFLUOROPHENYL)-5-METHYL-1,3-OXAZOLIDINE-2,4-DIONE (CCD ID: FDN) (formula: $C_{16}H_{12}F_2N_2O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	C	1	Total	C	F	N	O	0	0
			23	16	2	2	3		

- Molecule 14 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	38	Total	O	0	0
			38	38		
15	B	53	Total	O	0	0
			53	53		
15	C	84	Total	O	0	0
			84	84		
15	D	34	Total	O	0	0
			34	34		
15	F	27	Total	O	0	0
			27	27		
15	G	13	Total	O	0	0
			13	13		
15	H	2	Total	O	0	0
			2	2		
15	I	6	Total	O	0	0
			6	6		

Continued on next page...

Continued from previous page...

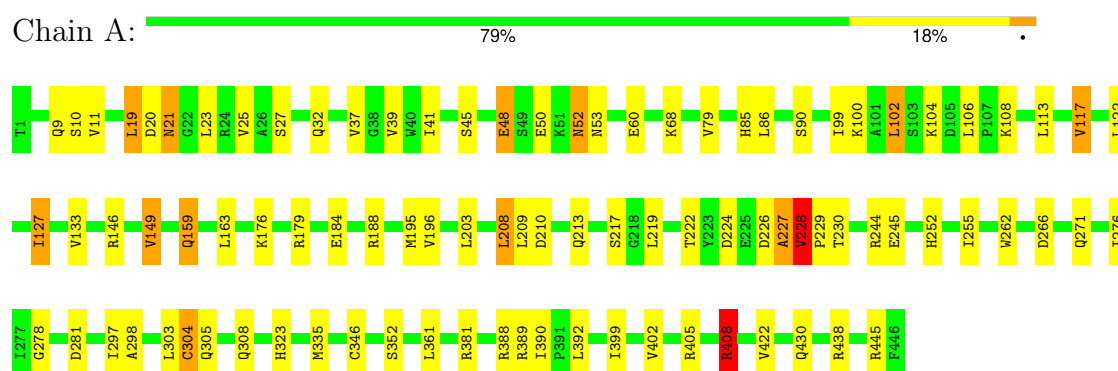
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	J	7	Total	O	0	0
			7	7		
15	K	3	Total	O	0	0
			3	3		

3 Residue-property plots

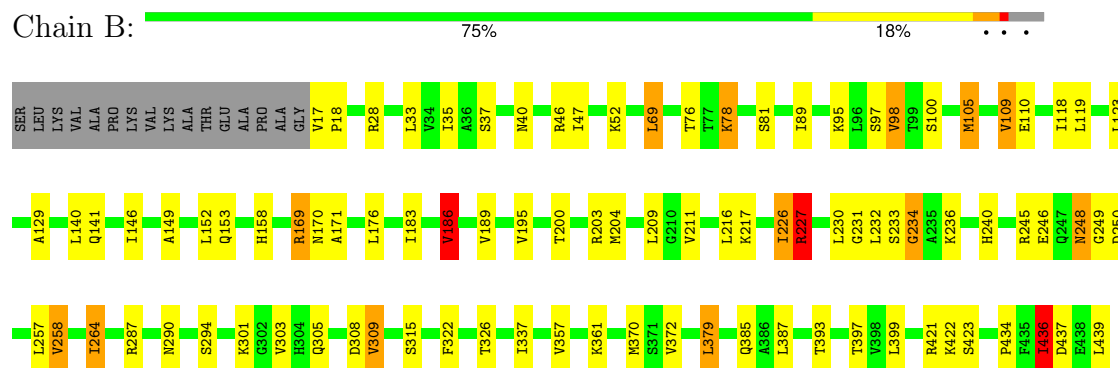
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

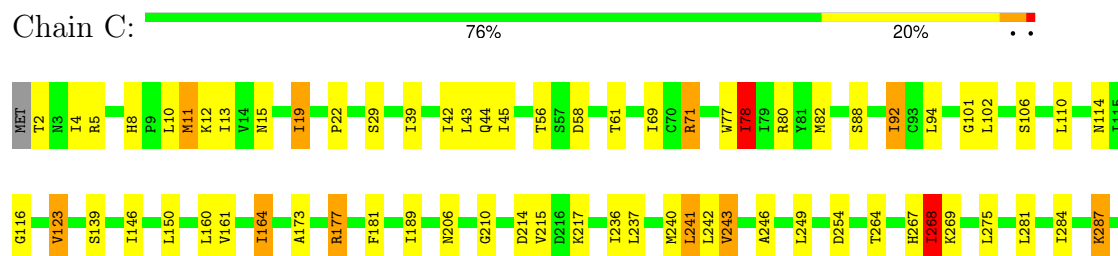
- Molecule 1: Ubiquinol-cytochrome-c reductase complex core protein I, mitochondrial



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



- Molecule 3: Cytochrome b





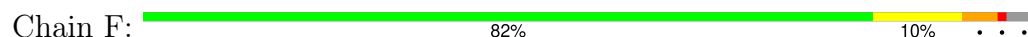
- Molecule 4: Cytochrome c1, heme protein, mitochondrial



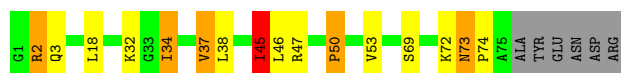
- Molecule 5: Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial



- Molecule 6: Hypothetical protein LOC616871



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

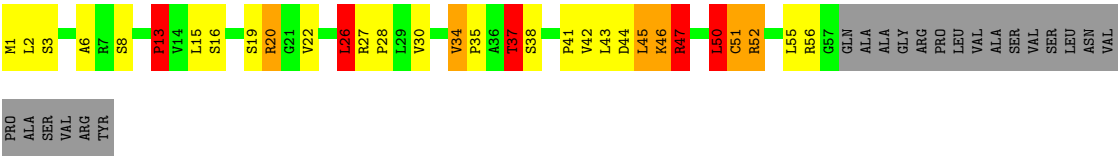


- Molecule 8: Ubiquinol-cytochrome c reductase complex 11 kDa protein



- Molecule 9: Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial

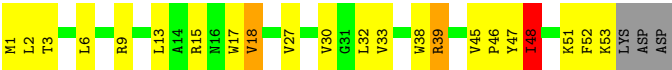




● Molecule 10: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein



● Molecule 11: Ubiquinol-cytochrome c reductase complex 6.4 kDa protein



4 Data and refinement statistics

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	154.26 Å 154.26 Å 590.19 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.26	Depositor
% Data completeness (in resolution range)	96.9 (40.00-2.26)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.248 , 0.283	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16900	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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: HEM, FES, FDN

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	1.11	11/3531 (0.3%)	1.42	6/4792 (0.1%)
2	B	1.18	11/3232 (0.3%)	1.42	7/4386 (0.2%)
3	C	1.24	16/3100 (0.5%)	1.52	3/4242 (0.1%)
4	D	1.25	10/1977 (0.5%)	1.47	13/2684 (0.5%)
5	E	1.31	16/1553 (1.0%)	1.39	2/2100 (0.1%)
6	F	1.24	5/935 (0.5%)	1.49	2/1253 (0.2%)
7	G	1.39	2/649 (0.3%)	1.47	4/878 (0.5%)
8	H	1.13	3/529 (0.6%)	1.56	0/708
9	I	1.45	3/411 (0.7%)	1.40	3/558 (0.5%)
10	J	1.19	2/508 (0.4%)	1.56	2/686 (0.3%)
11	K	1.41	6/454 (1.3%)	1.52	5/621 (0.8%)
All	All	1.22	85/16879 (0.5%)	1.46	47/22908 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	12
2	B	0	14
3	C	0	7
4	D	0	9
5	E	0	6
6	F	0	2
8	H	0	1
9	I	0	13
10	J	0	3
11	K	0	4
All	All	0	71

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	105	MET	SD-CE	-13.08	1.46	1.79
11	K	18	VAL	CA-CB	9.32	1.60	1.53
7	G	34	ILE	CA-CB	8.79	1.59	1.53
1	A	127	ILE	CA-CB	8.67	1.65	1.54
6	F	59	VAL	CA-CB	8.59	1.64	1.54
4	D	86	LYS	CA-C	8.56	1.56	1.52
6	F	47	ILE	CA-CB	7.92	1.63	1.54
3	C	92	ILE	CA-CB	7.81	1.64	1.54
7	G	37	VAL	CA-CB	7.72	1.64	1.54
4	D	137	PRO	CA-C	7.70	1.56	1.51
4	D	7	PRO	CA-C	7.64	1.56	1.51
2	B	226	ILE	CA-CB	7.50	1.63	1.54
11	K	48	ILE	CA-CB	7.11	1.64	1.54
5	E	136	ILE	CA-CB	7.08	1.62	1.53
6	F	16	ILE	CA-CB	6.86	1.63	1.54
5	E	171	ILE	CA-CB	6.72	1.61	1.54
11	K	45	VAL	CA-CB	6.69	1.62	1.54
2	B	186	VAL	CA-CB	6.67	1.62	1.53
3	C	146	ILE	CA-CB	6.64	1.62	1.54
3	C	123	VAL	CA-CB	6.57	1.63	1.54
2	B	146	ILE	CA-CB	6.57	1.62	1.54
3	C	348	ILE	CA-CB	6.53	1.61	1.54
4	D	168	VAL	CA-CB	6.43	1.63	1.54
6	F	37	ILE	CA-CB	6.29	1.61	1.54
3	C	284	ILE	CA-CB	6.29	1.61	1.54
5	E	103	LYS	CE-NZ	6.25	1.68	1.49
6	F	62	ILE	CA-CB	6.23	1.61	1.54
1	A	99	ILE	CA-CB	6.02	1.61	1.54
3	C	39	ILE	CA-CB	6.00	1.61	1.54
9	I	34	VAL	CA-CB	6.00	1.61	1.54
3	C	4	ILE	CA-CB	5.95	1.61	1.54
11	K	45	VAL	CA-C	5.94	1.57	1.53
2	B	195	VAL	CA-CB	5.83	1.61	1.54
4	D	52	VAL	CA-CB	5.83	1.61	1.54
1	A	276	ILE	CA-CB	5.82	1.61	1.54
5	E	45	VAL	CA-CB	5.81	1.61	1.54
5	E	106	ILE	CA-CB	5.80	1.61	1.54
10	J	42	ILE	CA-CB	5.78	1.61	1.54
4	D	229	VAL	CA-CB	5.70	1.61	1.54
3	C	215	VAL	CA-CB	5.68	1.61	1.54
4	D	26	ILE	CA-CB	5.68	1.61	1.54
8	H	31	VAL	CA-CB	5.65	1.61	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	55	VAL	CA-CB	5.58	1.60	1.54
5	E	68	VAL	CA-CB	5.57	1.62	1.54
5	E	145	VAL	CA-CB	5.56	1.59	1.53
3	C	268	ILE	CA-CB	5.55	1.62	1.54
9	I	42	VAL	CA-CB	5.55	1.61	1.53
11	K	27	VAL	CA-CB	5.51	1.60	1.54
4	D	239	PRO	CA-C	5.47	1.55	1.52
5	E	194	ILE	CA-CB	5.45	1.60	1.54
4	D	141	VAL	CA-CB	5.42	1.60	1.53
5	E	195	VAL	CA-CB	5.41	1.60	1.54
2	B	436	ILE	CA-CB	5.37	1.61	1.54
1	A	196	VAL	CA-CB	5.34	1.61	1.54
2	B	89	ILE	CA-CB	5.34	1.60	1.54
3	C	164	ILE	CA-CB	5.33	1.61	1.54
5	E	112	VAL	CA-CB	5.28	1.60	1.54
5	E	114	VAL	CA-CB	5.26	1.61	1.54
3	C	350	ILE	CA-CB	5.25	1.61	1.54
5	E	81	ILE	CA-CB	5.25	1.60	1.54
3	C	372	ILE	CA-CB	5.22	1.60	1.54
1	A	390	ILE	CA-CB	5.22	1.60	1.54
5	E	59	VAL	CA-CB	5.22	1.60	1.54
5	E	39	VAL	CA-CB	5.20	1.60	1.54
2	B	337	ILE	CA-CB	5.17	1.60	1.54
1	A	228	VAL	CA-CB	5.17	1.60	1.54
2	B	303	VAL	CA-CB	5.17	1.61	1.54
5	E	182	VAL	CA-CB	5.17	1.60	1.54
3	C	236	ILE	CA-CB	5.17	1.60	1.54
3	C	13	ILE	CA-CB	5.15	1.60	1.54
1	A	25	VAL	CA-CB	5.14	1.60	1.54
4	D	219	VAL	CA-CB	5.13	1.60	1.54
2	B	372	VAL	CA-CB	5.12	1.60	1.54
9	I	30	VAL	CA-CB	5.12	1.60	1.54
1	A	41	ILE	CA-CB	5.11	1.60	1.54
3	C	189	ILE	CA-CB	5.10	1.60	1.54
1	A	11	VAL	CA-CB	5.09	1.60	1.54
1	A	133	VAL	CA-CB	5.09	1.60	1.54
8	H	69	VAL	CA-CB	5.08	1.61	1.54
11	K	18	VAL	CA-C	5.08	1.56	1.52
2	B	183	ILE	CA-CB	5.07	1.60	1.53
1	A	422	VAL	CA-CB	5.05	1.60	1.54
3	C	69	ILE	CA-CB	5.04	1.60	1.54
10	J	46	ILE	CA-CB	5.03	1.61	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	44	VAL	CA-CB	5.01	1.61	1.54

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	34	ILE	N-CA-CB	9.33	116.38	110.50
10	J	47	ASN	N-CA-C	7.76	122.82	111.02
7	G	50	PRO	N-CA-C	7.52	119.87	110.70
6	F	59	VAL	N-CA-CB	6.67	118.35	110.55
1	A	149	VAL	N-CA-C	6.66	117.42	110.62
2	B	234	GLY	N-CA-C	6.59	120.46	110.18
4	D	239	PRO	CA-C-O	-6.35	115.71	120.73
3	C	243	VAL	N-CA-C	6.32	117.10	110.72
1	A	159	GLN	N-CA-C	6.31	124.24	110.80
4	D	7	PRO	CA-C-O	-6.21	116.43	120.90
5	E	54	VAL	N-CA-CB	6.11	117.70	110.55
1	A	149	VAL	N-CA-CB	6.09	118.83	110.54
11	K	17	TRP	CA-C-N	6.09	124.08	120.24
11	K	17	TRP	C-N-CA	6.09	124.08	120.24
11	K	18	VAL	N-CA-CB	6.06	114.32	110.50
6	F	59	VAL	N-CA-C	5.87	116.06	110.42
2	B	98	VAL	CB-CA-C	5.81	118.55	110.99
4	D	7	PRO	N-CA-C	5.74	115.98	110.47
1	A	266	ASP	N-CA-C	5.74	120.27	113.16
9	I	47	ARG	N-CA-C	5.68	122.91	110.80
4	D	7	PRO	O-C-N	5.66	123.91	121.31
1	A	195	MET	N-CA-C	5.58	118.57	109.24
4	D	137	PRO	N-CA-C	5.58	115.83	110.47
9	I	26	LEU	N-CA-C	5.55	120.36	111.81
4	D	86	LYS	N-CA-C	5.49	116.86	108.30
1	A	408	ARG	N-CA-C	5.45	118.15	111.82
4	D	137	PRO	O-C-N	5.45	123.82	121.31
4	D	239	PRO	O-C-N	5.45	123.71	121.15
3	C	78	ILE	N-CA-CB	5.42	117.91	110.54
2	B	227	ARG	N-CA-C	5.35	116.92	107.61
7	G	34	ILE	N-CA-C	5.34	120.36	112.61
9	I	37	THR	N-CA-C	5.34	117.70	111.02
2	B	158	HIS	N-CA-C	5.34	117.10	111.28
2	B	98	VAL	N-CA-C	5.28	115.68	107.28
10	J	24	ILE	N-CA-C	5.28	116.01	110.62
4	D	137	PRO	CA-C-O	-5.20	117.16	120.90
11	K	30	VAL	CA-C-N	5.14	125.65	119.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	30	VAL	C-N-CA	5.14	125.65	119.94
4	D	200	HIS	CA-C-N	5.08	127.33	120.38
4	D	200	HIS	C-N-CA	5.08	127.33	120.38
5	E	74	ILE	N-CA-C	5.06	115.19	108.11
7	G	45	ILE	N-CA-C	5.04	115.65	110.36
2	B	140	LEU	N-CA-C	5.03	118.57	112.23
4	D	228	SER	CA-C-N	5.02	127.61	120.53
4	D	228	SER	C-N-CA	5.02	127.61	120.53
2	B	186	VAL	CB-CA-C	5.00	118.03	111.33
3	C	77	TRP	N-CA-C	5.00	116.42	111.07

There are no chirality outliers.

All (71) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	20	ASP	Peptide
1	A	227	ALA	Peptide
1	A	228	VAL	Peptide
1	A	229	PRO	Peptide
1	A	244	ARG	Sidechain
1	A	278	GLY	Mainchain
1	A	281	ASP	Sidechain
1	A	303	LEU	Peptide
1	A	389	ARG	Sidechain
1	A	402	VAL	Mainchain
1	A	408	ARG	Sidechain
1	A	48	GLU	Mainchain
2	B	149	ALA	Mainchain
2	B	169	ARG	Peptide
2	B	17	VAL	Peptide
2	B	170	ASN	Peptide
2	B	171	ALA	Mainchain
2	B	18	PRO	Peptide
2	B	226	ILE	Peptide
2	B	227	ARG	Peptide
2	B	231	GLY	Peptide
2	B	234	GLY	Peptide
2	B	245	ARG	Sidechain
2	B	249	GLY	Peptide
2	B	322	PHE	Sidechain
2	B	434	PRO	Mainchain
3	C	139	SER	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
3	C	22	PRO	Mainchain
3	C	264	THR	Peptide
3	C	344	GLU	Peptide
3	C	346	PRO	Mainchain
3	C	5	ARG	Sidechain
3	C	71	ARG	Sidechain
4	D	145	GLU	Peptide
4	D	162	PRO	Mainchain
4	D	163	PRO	Peptide
4	D	33	TYR	Sidechain
4	D	53	GLY	Peptide
4	D	70	VAL	Peptide
4	D	73	GLY	Peptide
4	D	78	GLY	Peptide
4	D	91	PHE	Peptide
5	E	14	ARG	Sidechain
5	E	32	ARG	Sidechain
5	E	64	ALA	Mainchain
5	E	66	ALA	Peptide
5	E	70	ALA	Peptide
5	E	94	LYS	Peptide
6	F	20	TYR	Sidechain
6	F	73	GLN	Mainchain
8	H	52	GLU	Peptide
9	I	13	PRO	Mainchain
9	I	26	LEU	Peptide
9	I	34	VAL	Peptide
9	I	35	PRO	Peptide
9	I	37	THR	Peptide
9	I	43	LEU	Peptide
9	I	45	LEU	Peptide
9	I	46	LYS	Peptide
9	I	47	ARG	Mainchain
9	I	50	LEU	Mainchain,Peptide
9	I	52	ARG	Peptide
9	I	6	ALA	Peptide
10	J	2	ALA	Peptide
10	J	50	LYS	Peptide
10	J	51	LEU	Peptide
11	K	38	TRP	Mainchain,Peptide
11	K	46	PRO	Peptide
11	K	47	TYR	Peptide

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	3458	0	3356	18	0
2	B	3172	0	3152	24	0
3	C	3003	0	3065	26	0
4	D	1918	0	1870	15	0
5	E	1519	0	1503	9	0
6	F	916	0	909	3	0
7	G	628	0	636	5	0
8	H	524	0	504	2	0
9	I	406	0	437	5	0
10	J	495	0	493	2	0
11	K	438	0	447	2	0
12	C	86	0	60	3	0
12	D	43	0	30	3	0
13	C	23	0	12	1	0
14	E	4	0	0	0	0
15	A	38	0	0	0	0
15	B	53	0	0	1	0
15	C	84	0	0	0	0
15	D	34	0	0	0	0
15	F	27	0	0	0	0
15	G	13	0	0	0	0
15	H	2	0	0	0	0
15	I	6	0	0	0	0
15	J	7	0	0	0	0
15	K	3	0	0	0	0
All	All	16900	0	16474	96	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 3.

All (96) 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)
5:E:103:LYS:CE	5:E:103:LYS:NZ	1.68	1.53
2:B:385:GLN:HE22	2:B:393:THR:H	1.22	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:217:LYS:HE3	7:G:2:ARG:HH22	1.48	0.76
3:C:45:ILE:HA	12:C:381:HEM:HAB	1.73	0.70
2:B:248:ASN:HB3	2:B:250:ASP:HB2	1.79	0.65
4:D:211:MET:HA	4:D:211:MET:HE2	1.82	0.62
5:E:103:LYS:HE3	5:E:107:ASP:OD2	1.98	0.62
2:B:76:THR:HG23	2:B:81:SER:HA	1.81	0.62
2:B:308:ASP:OD1	9:I:28:PRO:HB2	2.01	0.61
1:A:255:ILE:HG21	1:A:335:MET:HE1	1.83	0.61
3:C:214:ASP:OD2	7:G:2:ARG:NH2	2.34	0.60
6:F:64:ARG:HH11	6:F:64:ARG:HB3	1.68	0.59
5:E:103:LYS:NZ	5:E:103:LYS:CD	2.63	0.58
1:A:48:GLU:HB2	1:A:52:ASN:HB3	1.85	0.58
2:B:385:GLN:HE22	2:B:393:THR:N	1.98	0.55
4:D:74:PRO:HB3	4:D:79:GLU:H	1.72	0.55
3:C:309:THR:HG21	3:C:367:PRO:O	2.07	0.54
1:A:19:LEU:HB3	1:A:21:ASN:HB2	1.89	0.54
15:B:482:HOH:O	9:I:15:LEU:HD12	2.08	0.53
3:C:349:THR:HA	3:C:352:GLN:HE21	1.73	0.53
5:E:156:TYR:HB2	5:E:165:TYR:HB2	1.90	0.53
4:D:118:ARG:HG3	4:D:194:ALA:HB1	1.91	0.53
2:B:357:VAL:HG12	2:B:361:LYS:HD2	1.92	0.52
2:B:169:ARG:HG3	2:B:240:HIS:HB2	1.93	0.51
3:C:275:LEU:HB2	3:C:336:THR:HG22	1.93	0.51
1:A:48:GLU:HG3	1:A:53:ASN:HA	1.93	0.50
6:F:37:ILE:HD12	6:F:43:VAL:HG21	1.93	0.50
2:B:258:VAL:HG12	2:B:423:SER:HB2	1.93	0.50
6:F:58:ARG:O	6:F:62:ILE:HG12	2.11	0.50
5:E:20:ASP:HB3	5:E:23:LYS:HB2	1.94	0.50
1:A:45:SER:HA	1:A:48:GLU:HG2	1.92	0.49
3:C:268:ILE:HG23	13:C:400:FDN:H25	1.94	0.49
4:D:37:CYS:SG	12:D:242:HEM:HAB	2.53	0.49
2:B:309:VAL:HG13	2:B:326:THR:HG22	1.95	0.49
7:G:50:PRO:HA	7:G:53:VAL:HG22	1.94	0.48
3:C:241:LEU:HD13	4:D:208:MET:HE1	1.94	0.48
2:B:69:LEU:HD13	2:B:105:MET:HE1	1.95	0.48
4:D:21:LEU:HD21	4:D:191:ARG:HG2	1.96	0.48
11:K:3:THR:HA	11:K:6:LEU:HD12	1.96	0.48
2:B:95:LYS:HB2	2:B:110:GLU:HG2	1.95	0.47
3:C:237:LEU:HD13	4:D:212:MET:HG2	1.95	0.47
4:D:171:PHE:HB3	4:D:174:GLY:HA2	1.97	0.47
1:A:146:ARG:HE	1:A:308:GLN:HE22	1.63	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:SER:O	9:I:13:PRO:HD2	2.16	0.46
3:C:150:LEU:HB2	3:C:161:VAL:HG22	1.97	0.46
2:B:37:SER:HB3	2:B:216:LEU:HD12	1.97	0.46
3:C:8:HIS:HD2	3:C:11:MET:H	1.64	0.46
3:C:287:LYS:HG2	5:E:141:HIS:HD2	1.81	0.46
3:C:206:ASN:HD21	3:C:210:GLY:HA2	1.81	0.45
1:A:308:GLN:HE21	1:A:323:HIS:CD2	2.35	0.45
1:A:102:LEU:HD23	1:A:104:LYS:HE3	1.99	0.45
2:B:385:GLN:NE2	2:B:393:THR:H	2.02	0.45
3:C:322:GLN:NE2	7:G:47:ARG:HH11	2.15	0.45
3:C:246:ALA:HB1	3:C:249:LEU:HB2	1.99	0.44
3:C:116:GLY:C	12:C:382:HEM:HBC2	2.42	0.44
3:C:287:LYS:HG3	5:E:177:PRO:HD3	1.99	0.44
10:J:33:ARG:HD3	11:K:48:ILE:HA	1.99	0.44
3:C:101:GLY:HA2	3:C:106:SER:HB2	1.99	0.44
1:A:39:VAL:HG11	1:A:117:VAL:HG21	2.00	0.43
3:C:78:ILE:HB	3:C:82:MET:HE3	1.99	0.43
3:C:58:ASP:HB3	3:C:61:THR:HG22	1.99	0.43
2:B:52:LYS:HB2	2:B:203:ARG:HB3	2.00	0.43
2:B:264:ILE:HG12	9:I:2:LEU:HD23	1.99	0.43
4:D:28:ARG:HD3	4:D:171:PHE:HE2	1.84	0.43
7:G:45:ILE:HD12	7:G:46:LEU:HG	2.01	0.43
1:A:85:HIS:CD2	2:B:370:MET:HE1	2.54	0.43
1:A:346:CYS:O	1:A:408:ARG:HB2	2.19	0.43
4:D:33:TYR:HA	4:D:37:CYS:SG	2.59	0.43
2:B:141:GLN:NE2	2:B:186:VAL:O	2.51	0.43
9:I:20:ARG:H	9:I:20:ARG:HG2	1.58	0.43
3:C:44:GLN:HG3	12:C:381:HEM:HBC2	2.00	0.43
2:B:200:THR:HB	2:B:227:ARG:HG2	2.00	0.43
2:B:78:LYS:HB2	2:B:129:ALA:HB1	2.00	0.42
3:C:287:LYS:HE2	5:E:177:PRO:HG3	2.02	0.42
3:C:15:ASN:HA	3:C:19:ILE:HG12	2.01	0.42
4:D:5:LEU:HB3	8:H:59:LEU:HD22	2.02	0.42
2:B:436:ILE:HA	2:B:439:LEU:HD12	2.01	0.42
1:A:21:ASN:HD21	1:A:217:SER:HA	1.85	0.42
5:E:2:HIS:HA	5:E:5:ILE:HD12	2.01	0.42
1:A:79:VAL:HG21	1:A:86:LEU:HD22	2.01	0.42
3:C:82:MET:HG2	3:C:240:MET:HE1	2.01	0.42
4:D:40:CYS:SG	12:D:242:HEM:HAC	2.60	0.42
4:D:37:CYS:SG	12:D:242:HEM:CAB	3.09	0.41
1:A:27:SER:HB3	1:A:208:LEU:HD12	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:109:VAL:HG22	2:B:119:LEU:HD12	2.02	0.41
1:A:60:GLU:OE2	2:B:287:ARG:NH2	2.53	0.41
1:A:361:LEU:HD23	1:A:399:ILE:HG12	2.02	0.41
4:D:110:PRO:HA	4:D:111:PRO:HD3	1.94	0.41
10:J:10:TYR:HA	10:J:14:PHE:HB2	2.03	0.41
1:A:252:HIS:CD2	1:A:323:HIS:HE1	2.39	0.41
1:A:298:ALA:HB1	1:A:304:CYS:HB2	2.03	0.41
2:B:209:LEU:HD13	2:B:379:LEU:HD12	2.02	0.41
4:D:168:VAL:HB	4:D:169:LEU:HD12	2.03	0.41
3:C:173:ALA:O	3:C:177:ARG:HB2	2.20	0.40
8:H:69:VAL:HG13	8:H:73:LEU:HD13	2.04	0.40
3:C:177:ARG:HG2	3:C:181:PHE:CE2	2.57	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	444/446 (100%)	427 (96%)	12 (3%)	5 (1%)	11	8
2	B	421/439 (96%)	396 (94%)	22 (5%)	3 (1%)	18	17
3	C	376/379 (99%)	356 (95%)	18 (5%)	2 (0%)	24	24
4	D	239/241 (99%)	215 (90%)	21 (9%)	3 (1%)	9	6
5	E	194/196 (99%)	183 (94%)	8 (4%)	3 (2%)	8	4
6	F	104/110 (94%)	102 (98%)	2 (2%)	0	100	100
7	G	73/81 (90%)	68 (93%)	3 (4%)	2 (3%)	4	2
8	H	62/78 (80%)	60 (97%)	2 (3%)	0	100	100
9	I	55/78 (70%)	36 (66%)	11 (20%)	8 (14%)	0	0
10	J	58/62 (94%)	51 (88%)	7 (12%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	51/56 (91%)	45 (88%)	4 (8%)	2 (4%)	2	1
All	All	2077/2166 (96%)	1939 (93%)	110 (5%)	28 (1%)	9	6

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	GLN
1	A	224	ASP
2	B	437	ASP
3	C	29	SER
5	E	67	ASP
5	E	73	LYS
7	G	73	ASN
9	I	3	SER
9	I	47	ARG
9	I	51	CYS
11	K	39	ARG
1	A	21	ASN
1	A	262	TRP
4	D	80	MET
5	E	72	SER
11	K	52	PHE
1	A	227	ALA
4	D	93	LYS
9	I	41	PRO
9	I	44	ASP
9	I	45	LEU
9	I	50	LEU
2	B	236	LYS
3	C	268	ILE
4	D	169	LEU
2	B	436	ILE
7	G	74	PRO
9	I	13	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%)	323 (87%)	47 (13%)	4	3
2	B	332/343 (97%)	290 (87%)	42 (13%)	4	3
3	C	326/327 (100%)	283 (87%)	43 (13%)	4	2
4	D	206/206 (100%)	169 (82%)	37 (18%)	2	0
5	E	168/168 (100%)	146 (87%)	22 (13%)	4	3
6	F	96/98 (98%)	86 (90%)	10 (10%)	7	5
7	G	66/71 (93%)	55 (83%)	11 (17%)	2	0
8	H	61/74 (82%)	42 (69%)	19 (31%)	0	0
9	I	44/60 (73%)	27 (61%)	17 (39%)	0	0
10	J	50/52 (96%)	38 (76%)	12 (24%)	1	0
11	K	43/46 (94%)	31 (72%)	12 (28%)	0	0
All	All	1762/1815 (97%)	1490 (85%)	272 (15%)	2	1

All (272) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	10	SER
1	A	19	LEU
1	A	23	LEU
1	A	32	GLN
1	A	37	VAL
1	A	50	GLU
1	A	52	ASN
1	A	68	LYS
1	A	90	SER
1	A	100	LYS
1	A	102	LEU
1	A	106	LEU
1	A	108	LYS
1	A	113	LEU
1	A	117	VAL
1	A	122	LEU
1	A	127	ILE
1	A	149	VAL
1	A	163	LEU
1	A	176	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	179	ARG
1	A	184	GLU
1	A	188	ARG
1	A	203	LEU
1	A	208	LEU
1	A	209	LEU
1	A	210	ASP
1	A	213	GLN
1	A	219	LEU
1	A	222	THR
1	A	226	ASP
1	A	228	VAL
1	A	230	THR
1	A	245	GLU
1	A	271	GLN
1	A	297	ILE
1	A	304	CYS
1	A	305	GLN
1	A	352	SER
1	A	381	ARG
1	A	388	ARG
1	A	392	LEU
1	A	405	ARG
1	A	430	GLN
1	A	438	ARG
1	A	445	ARG
2	B	28	ARG
2	B	33	LEU
2	B	35	ILE
2	B	40	ASN
2	B	46	ARG
2	B	47	ILE
2	B	69	LEU
2	B	78	LYS
2	B	97	SER
2	B	98	VAL
2	B	109	VAL
2	B	118	ILE
2	B	123	LEU
2	B	152	LEU
2	B	153	GLN
2	B	176	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	186	VAL
2	B	189	VAL
2	B	204	MET
2	B	211	VAL
2	B	217	LYS
2	B	227	ARG
2	B	230	LEU
2	B	232	LEU
2	B	233	SER
2	B	246	GLU
2	B	248	ASN
2	B	257	LEU
2	B	258	VAL
2	B	264	ILE
2	B	290	ASN
2	B	294	SER
2	B	301	LYS
2	B	305	GLN
2	B	309	VAL
2	B	315	SER
2	B	379	LEU
2	B	387	LEU
2	B	397	THR
2	B	399	LEU
2	B	421	ARG
2	B	422	LYS
3	C	2	THR
3	C	10	LEU
3	C	11	MET
3	C	12	LYS
3	C	19	ILE
3	C	42	ILE
3	C	43	LEU
3	C	56	THR
3	C	71	ARG
3	C	78	ILE
3	C	80	ARG
3	C	88	SER
3	C	92	ILE
3	C	94	LEU
3	C	102	LEU
3	C	110	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	114	ASN
3	C	123	VAL
3	C	160	LEU
3	C	164	ILE
3	C	177	ARG
3	C	241	LEU
3	C	242	LEU
3	C	243	VAL
3	C	254	ASP
3	C	267	HIS
3	C	268	ILE
3	C	269	LYS
3	C	281	LEU
3	C	287	LYS
3	C	292	LEU
3	C	294	LEU
3	C	309	THR
3	C	320	LEU
3	C	333	LEU
3	C	336	THR
3	C	350	ILE
3	C	357	LEU
3	C	361	LEU
3	C	363	LEU
3	C	365	LEU
3	C	375	LYS
3	C	379	TRP
4	D	2	ASP
4	D	5	LEU
4	D	13	SER
4	D	24	THR
4	D	35	GLN
4	D	37	CYS
4	D	40	CYS
4	D	60	GLU
4	D	62	LYS
4	D	66	GLU
4	D	67	GLU
4	D	68	VAL
4	D	69	GLU
4	D	76	GLU
4	D	86	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	89	ASP
4	D	93	LYS
4	D	99	GLU
4	D	106	ASN
4	D	113	LEU
4	D	116	ILE
4	D	118	ARG
4	D	144	ARG
4	D	164	ILE
4	D	167	GLU
4	D	168	VAL
4	D	170	GLU
4	D	171	PHE
4	D	179	MET
4	D	180	SER
4	D	181	GLN
4	D	184	LYS
4	D	203	ARG
4	D	214	LEU
4	D	223	LYS
4	D	226	LYS
4	D	241	LYS
5	E	4	ASP
5	E	12	ASP
5	E	21	SER
5	E	23	LYS
5	E	27	GLU
5	E	54	VAL
5	E	60	SER
5	E	62	MET
5	E	69	LEU
5	E	71	MET
5	E	77	LYS
5	E	85	LYS
5	E	94	LYS
5	E	103	LYS
5	E	104	LYS
5	E	113	GLU
5	E	116	GLN
5	E	128	LYS
5	E	129	LYS
5	E	131	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	184	SER
5	E	188	THR
6	F	10	SER
6	F	37	ILE
6	F	44	LYS
6	F	53	ASN
6	F	59	VAL
6	F	64	ARG
6	F	72	GLN
6	F	73	GLN
6	F	77	LYS
6	F	85	GLU
7	G	2	ARG
7	G	3	GLN
7	G	18	LEU
7	G	32	LYS
7	G	34	ILE
7	G	37	VAL
7	G	38	LEU
7	G	45	ILE
7	G	69	SER
7	G	72	LYS
7	G	73	ASN
8	H	18	THR
8	H	25	GLU
8	H	26	GLN
8	H	27	LEU
8	H	28	GLU
8	H	29	LYS
8	H	32	LYS
8	H	35	GLU
8	H	36	ARG
8	H	39	LEU
8	H	47	ARG
8	H	49	GLN
8	H	52	GLU
8	H	53	ASP
8	H	56	GLU
8	H	60	ASP
8	H	65	ARG
8	H	68	CYS
8	H	73	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	I	1	MET
9	I	8	SER
9	I	16	SER
9	I	19	SER
9	I	20	ARG
9	I	22	VAL
9	I	26	LEU
9	I	27	ARG
9	I	37	THR
9	I	38	SER
9	I	46	LYS
9	I	47	ARG
9	I	50	LEU
9	I	51	CYS
9	I	52	ARG
9	I	55	LEU
9	I	56	ARG
10	J	4	THR
10	J	5	LEU
10	J	17	THR
10	J	18	SER
10	J	24	ILE
10	J	37	GLN
10	J	44	GLU
10	J	48	GLU
10	J	54	HIS
10	J	55	ILE
10	J	58	LYS
10	J	60	GLU
11	K	1	MET
11	K	2	LEU
11	K	9	ARG
11	K	13	LEU
11	K	15	ARG
11	K	18	VAL
11	K	32	LEU
11	K	33	VAL
11	K	39	ARG
11	K	48	ILE
11	K	51	LYS
11	K	53	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	69	ASN
1	A	94	HIS
1	A	213	GLN
1	A	274	ASN
1	A	308	GLN
1	A	311	ASN
1	A	323	HIS
1	A	339	GLN
1	A	341	GLN
1	A	359	ASN
1	A	435	ASN
2	B	40	ASN
2	B	104	ASN
2	B	125	ASN
2	B	143	GLN
2	B	153	GLN
2	B	162	ASN
2	B	174	ASN
2	B	240	HIS
2	B	276	GLN
2	B	284	HIS
2	B	313	ASN
2	B	342	ASN
2	B	351	ASN
2	B	362	ASN
2	B	385	GLN
2	B	432	HIS
3	C	8	HIS
3	C	32	ASN
3	C	148	ASN
3	C	206	ASN
3	C	286	ASN
3	C	312	GLN
3	C	322	GLN
3	C	345	HIS
3	C	352	GLN
4	D	35	GLN
4	D	156	GLN
4	D	181	GLN
6	F	22	ASN
6	F	72	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	F	79	GLN
9	I	31	GLN
11	K	12	GLN
11	K	16	ASN
11	K	49	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](#)

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	D	242	4	50,50,50	1.84	12 (24%)	67,82,82	1.58	12 (17%)
13	FDN	C	400	-	24,25,25	2.47	10 (41%)	29,37,37	1.85	7 (24%)
14	FES	E	200	5	0,4,4	-	-	-	-	-
12	HEM	C	381	3	50,50,50	1.83	11 (22%)	67,82,82	1.61	15 (22%)
12	HEM	C	382	3	50,50,50	1.81	11 (22%)	67,82,82	1.61	15 (22%)

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	D	242	4	-	8/14/54/54	-
13	FDN	C	400	-	-	1/10/29/29	0/3/3/3
14	FES	E	200	5	-	-	0/1/1/1
12	HEM	C	381	3	-	7/14/54/54	-
12	HEM	C	382	3	-	8/14/54/54	-

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	400	FDN	O4-C3	5.66	1.44	1.35
12	D	242	HEM	CBC-CAC	5.42	1.56	1.30
12	D	242	HEM	CBB-CAB	5.27	1.55	1.30
12	C	382	HEM	CBB-CAB	5.12	1.55	1.30
12	C	382	HEM	CBC-CAC	4.97	1.54	1.30
12	C	381	HEM	CBC-CAC	4.81	1.53	1.30
12	C	381	HEM	CBB-CAB	4.73	1.53	1.30
12	C	381	HEM	CBD-CGD	-4.07	1.41	1.50
13	C	400	FDN	C3-N2	-4.06	1.34	1.43
12	C	382	HEM	CBD-CGD	-3.97	1.41	1.50
12	C	382	HEM	CHD-C4C	3.90	1.46	1.38
12	C	381	HEM	CHD-C4C	3.86	1.45	1.38
12	D	242	HEM	CHD-C4C	3.82	1.45	1.38
12	C	382	HEM	CBA-CGA	-3.58	1.42	1.50
12	C	381	HEM	CBA-CGA	-3.47	1.42	1.50
12	D	242	HEM	CBD-CGD	-3.37	1.42	1.50
13	C	400	FDN	N1-N2	-3.25	1.34	1.40
12	D	242	HEM	FE-NA	3.20	2.05	1.95
13	C	400	FDN	O4-C5	-3.19	1.43	1.47
12	D	242	HEM	CBA-CGA	-3.17	1.43	1.50
13	C	400	FDN	C8-C13	3.12	1.43	1.39
13	C	400	FDN	C21-N1	-3.11	1.36	1.41
13	C	400	FDN	C9-C8	2.95	1.43	1.39
13	C	400	FDN	C6-N2	-2.93	1.34	1.38
12	C	381	HEM	FE-NA	2.91	2.04	1.95
12	C	382	HEM	FE-ND	2.85	2.03	1.94
13	C	400	FDN	C12-C11	2.70	1.42	1.37
12	C	381	HEM	FE-NB	2.70	2.03	1.94
12	D	242	HEM	FE-NB	2.64	2.03	1.94
12	C	381	HEM	FE-ND	2.63	2.03	1.94
12	C	382	HEM	FE-NB	2.63	2.03	1.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	382	HEM	FE-NC	2.61	2.03	1.95
12	C	382	HEM	FE-NA	2.58	2.03	1.95
12	C	381	HEM	FE-NC	2.56	2.03	1.95
12	D	242	HEM	FE-ND	2.52	2.02	1.94
13	C	400	FDN	C12-C13	2.39	1.41	1.37
12	C	382	HEM	CAB-C3B	2.34	1.53	1.47
12	D	242	HEM	CAD-C3D	2.29	1.57	1.51
12	D	242	HEM	CAB-C3B	2.28	1.53	1.47
12	D	242	HEM	CAC-C3C	2.25	1.53	1.47
12	C	381	HEM	C4D-C3D	-2.17	1.41	1.45
12	D	242	HEM	FE-NC	2.16	2.02	1.95
12	C	382	HEM	C4A-C3A	2.02	1.47	1.43
12	C	381	HEM	C4A-C3A	2.01	1.47	1.43

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	400	FDN	C21-N1-N2	5.13	125.69	116.20
12	C	382	HEM	C4A-CHB-C1B	-3.92	117.03	126.25
13	C	400	FDN	C5-C6-N2	3.92	109.75	105.07
12	C	382	HEM	C2A-C1A-NA	-3.79	105.94	110.15
12	C	381	HEM	CBC-CAC-C3C	-3.68	109.14	127.53
12	C	381	HEM	CBB-CAB-C3B	-3.51	110.00	127.53
12	C	382	HEM	C4C-CHD-C1D	-3.50	118.58	126.02
12	D	242	HEM	C2A-C1A-NA	-3.47	106.31	110.15
12	D	242	HEM	CHD-C1D-ND	3.44	128.13	124.42
12	C	382	HEM	C4A-NA-C1A	3.25	111.11	105.82
13	C	400	FDN	F13-C13-C8	3.18	122.51	119.01
12	C	381	HEM	C1C-CHC-C4B	-3.07	119.50	126.02
12	C	381	HEM	C2A-C1A-NA	-3.03	106.79	110.15
12	C	382	HEM	C3A-C4A-NA	-3.02	105.31	110.14
12	D	242	HEM	CBC-CAC-C3C	-3.00	112.55	127.53
13	C	400	FDN	C13-C12-C11	3.00	119.86	116.67
12	C	382	HEM	CBB-CAB-C3B	-2.98	112.63	127.53
13	C	400	FDN	C12-C13-C8	-2.96	120.67	123.88
12	D	242	HEM	C4A-CHB-C1B	-2.92	119.38	126.25
12	D	242	HEM	C4A-NA-C1A	2.81	110.41	105.82
12	C	381	HEM	C4C-CHD-C1D	-2.80	120.07	126.02
12	C	381	HEM	C4A-CHB-C1B	-2.79	119.69	126.25
12	C	382	HEM	CHD-C1D-ND	2.75	127.38	124.42
12	D	242	HEM	CHB-C4A-NA	2.74	128.83	123.86
12	C	381	HEM	CHB-C4A-NA	2.73	128.82	123.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	242	HEM	C4C-CHD-C1D	-2.65	120.38	126.02
12	D	242	HEM	CHC-C1C-NC	2.65	127.34	124.45
12	D	242	HEM	C3A-C4A-NA	-2.65	105.89	110.14
12	C	382	HEM	O2D-CGD-CBD	2.62	122.28	114.00
12	C	382	HEM	CHA-C1A-NA	2.59	128.55	123.86
13	C	400	FDN	O3-C3-N2	2.55	128.68	119.95
12	C	381	HEM	C4A-NA-C1A	2.54	109.96	105.82
12	D	242	HEM	O2D-CGD-CBD	2.51	121.93	114.00
12	C	382	HEM	C1B-NB-C4B	2.42	108.08	105.21
12	D	242	HEM	CHA-C1A-NA	2.42	128.25	123.86
12	C	382	HEM	C1C-CHC-C4B	-2.41	120.90	126.02
12	C	381	HEM	CHB-C1B-NB	2.40	127.34	124.37
12	C	381	HEM	CHA-C1A-NA	2.36	128.14	123.86
12	C	382	HEM	CAD-C3D-C2D	-2.34	123.48	127.87
12	D	242	HEM	C1C-CHC-C4B	-2.28	121.16	126.02
12	C	381	HEM	C3A-C4A-NA	-2.28	106.48	110.14
12	C	382	HEM	CHC-C1C-NC	2.28	126.94	124.45
12	C	381	HEM	CMC-C2C-C1C	2.25	128.69	124.73
12	C	381	HEM	C2D-C1D-ND	-2.21	107.34	109.90
12	C	381	HEM	CHD-C4C-NC	2.17	126.82	124.45
12	C	382	HEM	CBC-CAC-C3C	-2.15	116.78	127.53
12	C	382	HEM	CAD-C3D-C4D	2.12	128.39	124.70
12	C	381	HEM	CHC-C4B-NB	2.11	126.69	124.42
13	C	400	FDN	C10-C11-C12	-2.09	120.48	123.23

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	C	381	HEM	C2B-C3B-CAB-CBB
12	C	381	HEM	C2C-C3C-CAC-CBC
12	C	381	HEM	C4C-C3C-CAC-CBC
12	C	382	HEM	C2B-C3B-CAB-CBB
12	C	382	HEM	C2C-C3C-CAC-CBC
12	D	242	HEM	C2C-C3C-CAC-CBC
12	D	242	HEM	C4C-C3C-CAC-CBC
12	C	381	HEM	C4B-C3B-CAB-CBB
12	C	382	HEM	C4B-C3B-CAB-CBB
12	D	242	HEM	C2B-C3B-CAB-CBB
12	C	382	HEM	C4C-C3C-CAC-CBC
12	D	242	HEM	CAA-CBA-CGA-O1A
12	D	242	HEM	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

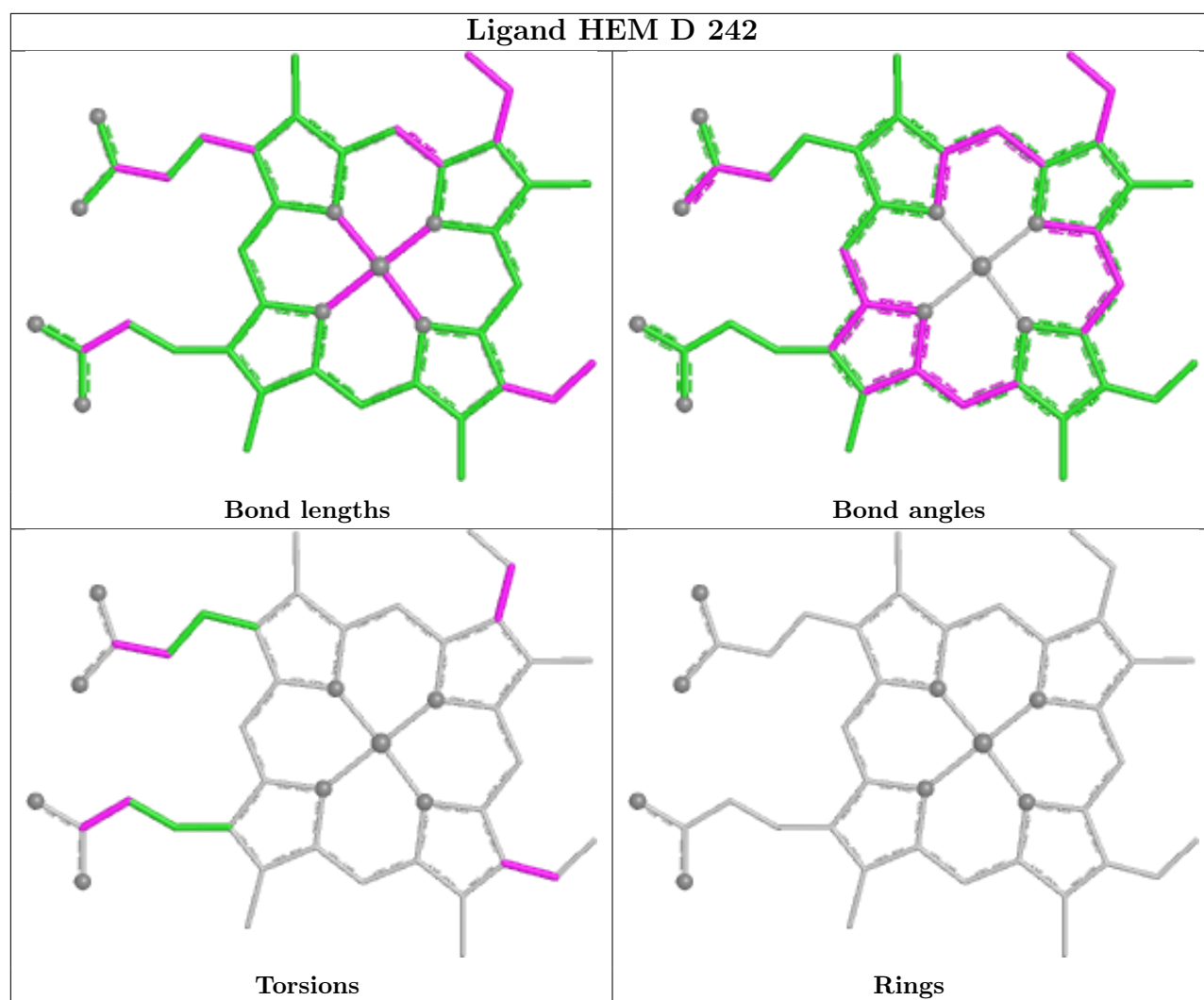
Mol	Chain	Res	Type	Atoms
12	C	382	HEM	CAA-CBA-CGA-O1A
12	C	381	HEM	CAD-CBD-CGD-O2D
12	D	242	HEM	CAA-CBA-CGA-O2A
12	D	242	HEM	CAD-CBD-CGD-O1D
12	C	382	HEM	CAA-CBA-CGA-O2A
12	C	381	HEM	CAD-CBD-CGD-O1D
12	C	381	HEM	C2A-CAA-CBA-CGA
12	C	382	HEM	CAD-CBD-CGD-O2D
13	C	400	FDN	O4-C5-C8-C9
12	D	242	HEM	C4B-C3B-CAB-CBB
12	C	382	HEM	CAD-CBD-CGD-O1D

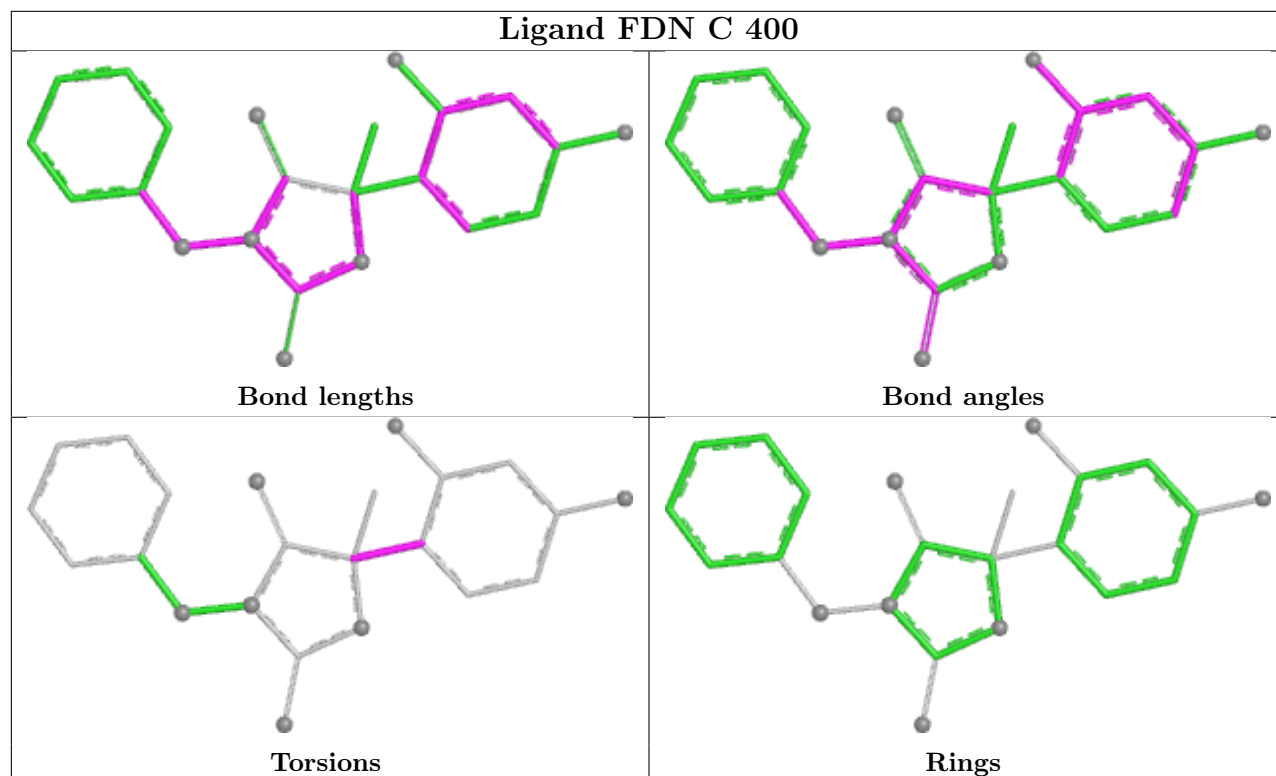
There are no ring outliers.

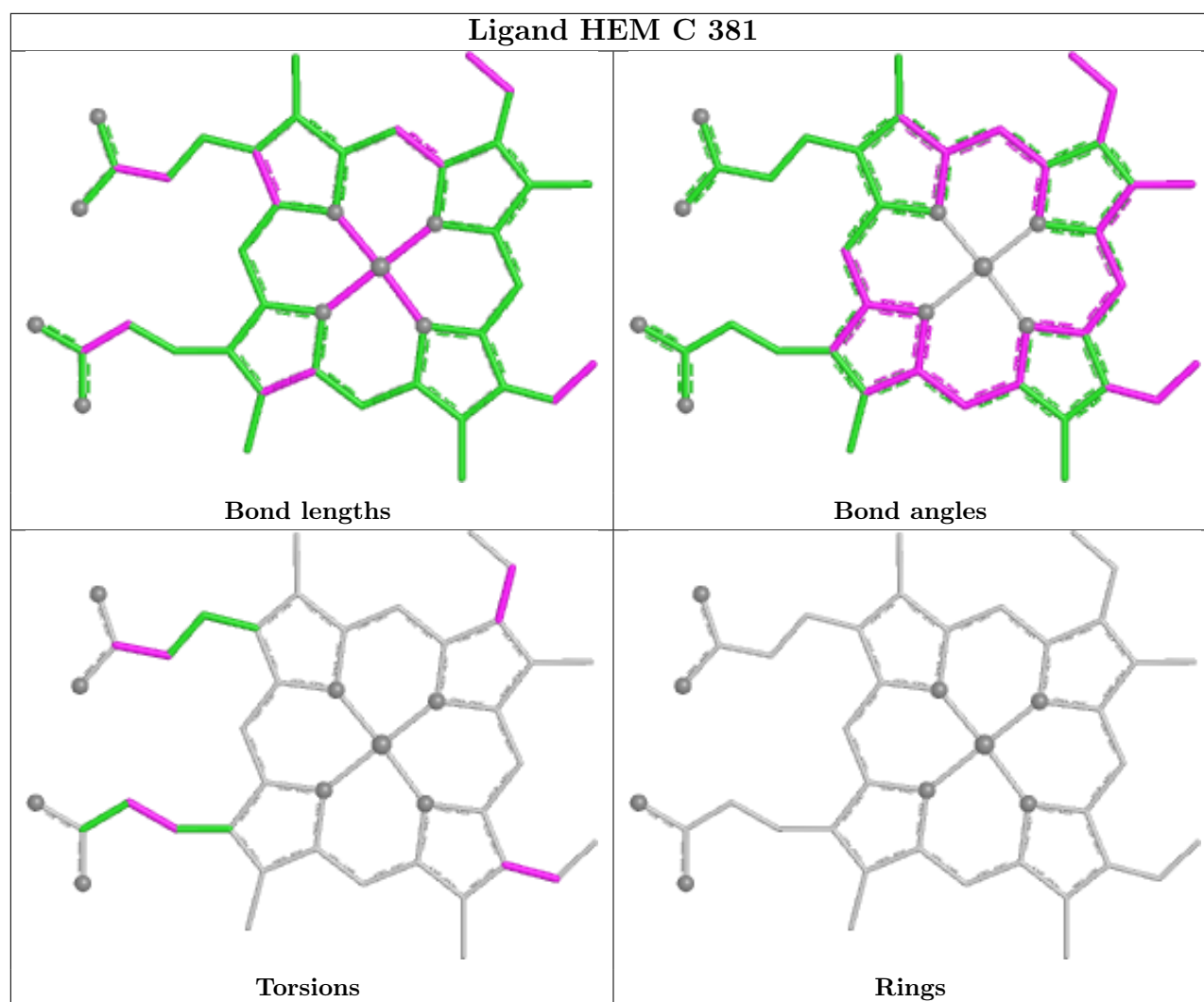
4 monomers are involved in 7 short contacts:

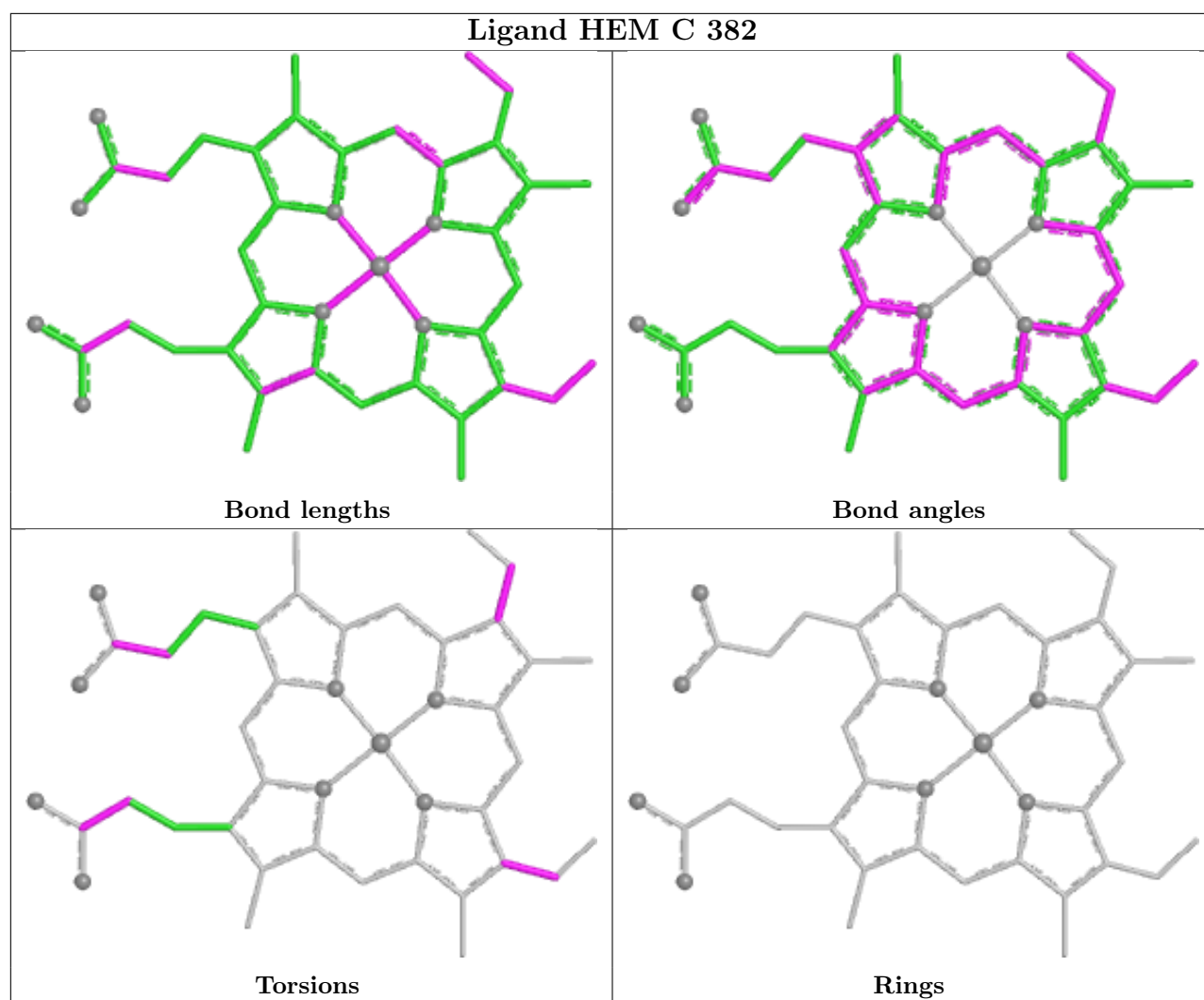
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	D	242	HEM	3	0
13	C	400	FDN	1	0
12	C	381	HEM	2	0
12	C	382	HEM	1	0

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.