



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 09:09 am BST

PDB ID : 1LDC  
Title : X-RAY STRUCTURE OF TWO COMPLEXES OF THE Y143F FLAVO-CYTOCHROME B2 MUTANT CRYSTALLIZED IN THE PRESENCE OF LACTATE OR PHENYL-LACTATE  
Authors : Tegoni, M.; Cambillau, C.  
Deposited on : 1995-04-13  
Resolution : 2.90 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](mailto: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.

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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) : 2.11

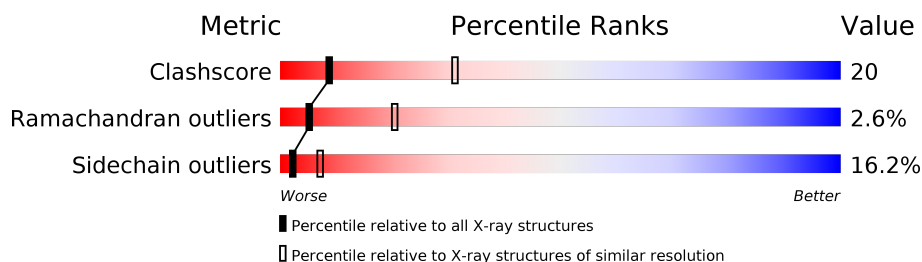
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	511	
1	B	511	

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
2	FMN	A	570	X	X	-	-
2	FMN	B	570	X	-	-	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8726 atoms, of which 1765 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 L-LACTATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	478	Total	C	H	N	O	S	0	0	0
			4530	2373	809	629	705	14			
1	B	382	Total	C	H	N	O	S	0	0	0
			3648	1893	666	507	571	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	PHE	TYR	ENGINEERED MUTATION	UNP P00175
B	143	PHE	TYR	ENGINEERED MUTATION	UNP P00175

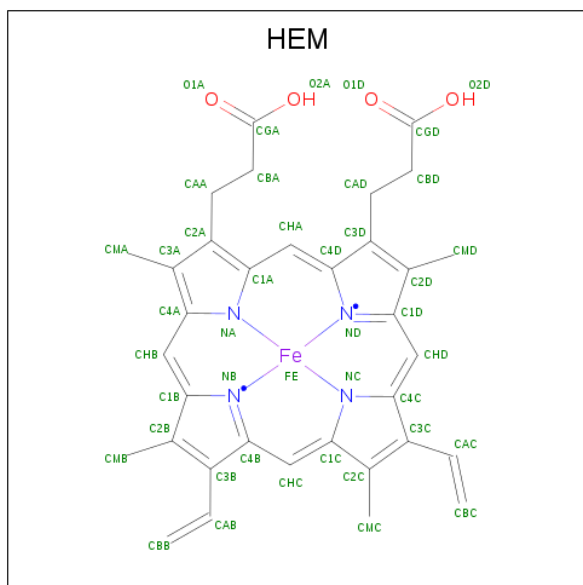
- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).



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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total	C	H	N	O	P	0	0
			35	17	4	4	9	1		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).

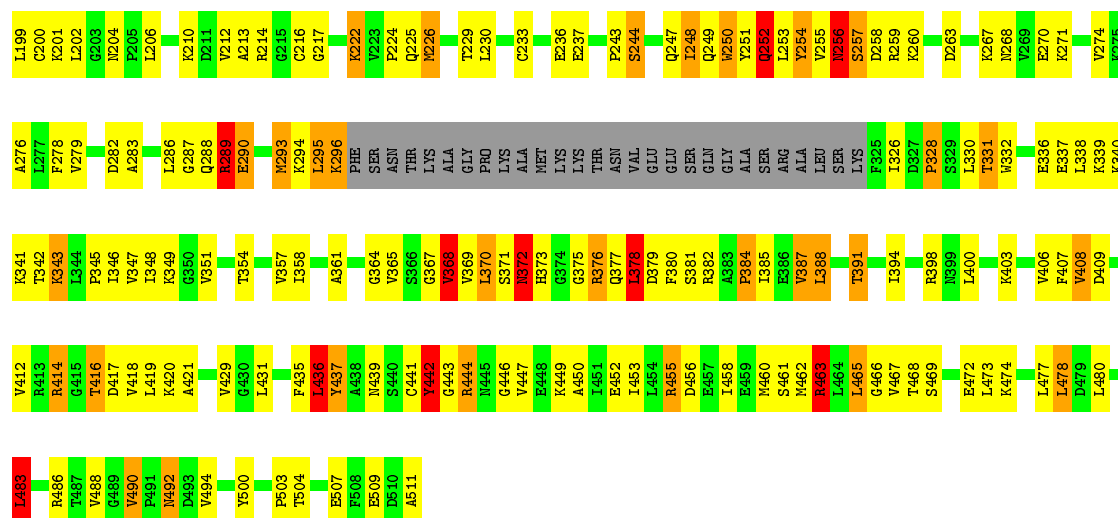


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	130	Total	H	O	0	0
			386	256	130		
5	B	11	Total	H	O	0	0
			33	22	11		





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 3 2 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	164.50 Å   164.50 Å   114.00 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	6.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.90)	Depositor
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.195 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8726	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	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: FMN, HEM, PYR

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	1.08	10/3794 (0.3%)	1.95	102/5140 (2.0%)
1	B	1.00	0/3030	1.95	80/4094 (2.0%)
All	All	1.05	10/6824 (0.1%)	1.95	182/9234 (2.0%)

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	6
1	B	0	2
All	All	0	8

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	103	LYS	CD-CE	8.02	1.71	1.51
1	A	32	TYR	CE1-CZ	6.87	1.47	1.38
1	A	32	TYR	CG-CD2	6.32	1.47	1.39
1	A	32	TYR	CE2-CZ	6.13	1.46	1.38
1	A	382	ARG	CZ-NH1	5.96	1.40	1.33
1	A	32	TYR	CG-CD1	5.75	1.46	1.39
1	A	475	PRO	CA-CB	-5.54	1.42	1.53
1	A	32	TYR	CD2-CE2	5.25	1.47	1.39
1	A	32	TYR	CA-CB	-5.07	1.42	1.53
1	A	501	GLU	CA-CB	-5.03	1.42	1.53

All (182) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	463	ARG	NE-CZ-NH2	-18.93	110.83	120.30
1	B	289	ARG	NE-CZ-NH1	18.50	129.55	120.30
1	A	382	ARG	NE-CZ-NH2	-15.38	112.61	120.30
1	A	413	ARG	NE-CZ-NH2	-15.36	112.62	120.30
1	A	492	ASN	CA-C-N	-13.15	88.26	117.20
1	A	486	ARG	NE-CZ-NH1	11.56	126.08	120.30
1	B	163	ARG	NE-CZ-NH1	11.49	126.04	120.30
1	B	379	ASP	CA-C-N	10.63	140.58	117.20
1	B	414	ARG	NE-CZ-NH1	10.30	125.45	120.30
1	B	289	ARG	NE-CZ-NH2	-9.87	115.36	120.30
1	A	214	ARG	NE-CZ-NH1	9.77	125.18	120.30
1	A	486	ARG	NE-CZ-NH2	-9.70	115.45	120.30
1	A	379	ASP	CA-C-N	9.57	138.26	117.20
1	A	32	TYR	CB-CG-CD2	-9.32	115.41	121.00
1	A	492	ASN	O-C-N	9.13	137.31	122.70
1	B	382	ARG	NE-CZ-NH2	-8.88	115.86	120.30
1	B	368	VAL	CA-CB-CG2	-8.82	97.67	110.90
1	A	289	ARG	NE-CZ-NH2	-8.68	115.96	120.30
1	B	332	TRP	CD1-CG-CD2	8.38	113.01	106.30
1	A	409	ASP	CB-CG-OD2	-8.18	110.94	118.30
1	B	126	TYR	CB-CG-CD1	-7.98	116.21	121.00
1	A	226	MET	CG-SD-CE	-7.98	87.44	100.20
1	B	376	ARG	NE-CZ-NH2	-7.87	116.36	120.30
1	B	250	TRP	CD1-CG-CD2	7.82	112.56	106.30
1	A	141	TRP	CD1-CG-CD2	7.67	112.44	106.30
1	B	382	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	A	26	TRP	CD1-CG-CD2	7.59	112.37	106.30
1	A	332	TRP	CD1-CG-CD2	7.52	112.32	106.30
1	A	251	TYR	CB-CG-CD1	-7.46	116.52	121.00
1	A	141	TRP	CE2-CD2-CG	-7.45	101.34	107.30
1	A	250	TRP	CD1-CG-CD2	7.44	112.25	106.30
1	A	413	ARG	NH1-CZ-NH2	7.44	127.58	119.40
1	B	416	THR	CA-CB-CG2	-7.34	102.12	112.40
1	B	463	ARG	CG-CD-NE	-7.28	96.52	111.80
1	B	254	TYR	CB-CG-CD2	-7.23	116.66	121.00
1	B	387	VAL	CG1-CB-CG2	-7.17	99.43	110.90
1	A	414	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	A	161	TYR	CB-CG-CD2	-7.04	116.77	121.00
1	B	332	TRP	CE2-CD2-CG	-7.03	101.68	107.30
1	B	112	LEU	CA-CB-CG	7.00	131.41	115.30
1	A	282	ASP	CB-CG-OD1	7.00	124.60	118.30
1	B	341	LYS	CA-CB-CG	7.00	128.80	113.40
1	B	473	LEU	CA-C-N	6.98	132.56	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	254	TYR	CB-CG-CD2	-6.97	116.82	121.00
1	A	250	TRP	CE2-CD2-CG	-6.92	101.77	107.30
1	A	188	VAL	CG1-CB-CG2	-6.91	99.85	110.90
1	B	414	ARG	NH1-CZ-NH2	-6.85	111.87	119.40
1	B	141	TRP	CE2-CD2-CG	-6.84	101.83	107.30
1	B	465	LEU	CB-CG-CD2	-6.83	99.39	111.00
1	B	226	MET	CG-SD-CE	-6.82	89.29	100.20
1	B	175	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	B	177	VAL	CG1-CB-CG2	-6.79	100.04	110.90
1	A	141	TRP	CG-CD2-CE3	6.79	140.01	133.90
1	A	223	VAL	N-CA-CB	-6.77	96.60	111.50
1	A	332	TRP	CE2-CD2-CG	-6.74	101.91	107.30
1	A	249	GLN	CA-CB-CG	-6.74	98.57	113.40
1	A	126	TYR	CB-CG-CD1	-6.73	116.96	121.00
1	A	477	LEU	CA-CB-CG	6.71	130.73	115.30
1	A	163	ARG	NE-CZ-NH2	-6.67	116.96	120.30
1	A	414	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	B	455	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	A	177	VAL	CG1-CB-CG2	-6.63	100.30	110.90
1	B	463	ARG	NH1-CZ-NH2	6.62	126.69	119.40
1	B	141	TRP	CG-CD2-CE3	6.62	139.85	133.90
1	A	26	TRP	CE2-CD2-CG	-6.58	102.04	107.30
1	B	163	ARG	CA-CB-CG	6.55	127.81	113.40
1	A	330	LEU	CA-CB-CG	6.53	130.32	115.30
1	B	398	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	A	223	VAL	CA-CB-CG2	-6.52	101.11	110.90
1	B	141	TRP	CD1-CG-CD2	6.50	111.50	106.30
1	B	473	LEU	O-C-N	-6.49	112.32	122.70
1	B	379	ASP	CA-C-O	-6.47	106.52	120.10
1	A	321	ALA	N-CA-C	-6.39	93.74	111.00
1	B	368	VAL	CA-CB-CG1	6.37	120.46	110.90
1	B	328	PRO	CA-N-CD	-6.36	102.60	111.50
1	A	152	VAL	CA-C-N	6.34	131.16	117.20
1	B	251	TYR	CB-CG-CD1	-6.34	117.20	121.00
1	B	511	ALA	N-CA-C	-6.31	93.97	111.00
1	A	253	LEU	CA-CB-CG	6.29	129.77	115.30
1	A	483	LEU	CB-CA-C	-6.28	98.27	110.20
1	B	341	LYS	N-CA-CB	-6.28	99.30	110.60
1	A	433	ARG	NE-CZ-NH2	6.26	123.43	120.30
1	B	250	TRP	CE2-CD2-CG	-6.22	102.32	107.30
1	A	130	TYR	CB-CG-CD1	-6.16	117.30	121.00
1	A	326	ILE	N-CA-C	-6.16	94.36	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	202	LEU	CB-CG-CD2	-6.16	100.53	111.00
1	B	379	ASP	O-C-N	-6.14	112.88	122.70
1	A	188	VAL	CA-CB-CG2	-6.12	101.72	110.90
1	A	214	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	A	184	LEU	CA-CB-CG	6.09	129.30	115.30
1	A	148	ALA	N-CA-CB	6.09	118.62	110.10
1	A	356	ASP	CB-CG-OD1	6.08	123.77	118.30
1	A	379	ASP	O-C-N	-6.04	113.03	122.70
1	A	112	LEU	CA-CB-CG	6.02	129.15	115.30
1	A	34	TYR	CB-CG-CD2	-5.99	117.40	121.00
1	A	188	VAL	CA-CB-CG1	5.96	119.84	110.90
1	B	274	VAL	CG1-CB-CG2	5.96	120.44	110.90
1	A	184	LEU	N-CA-CB	-5.95	98.50	110.40
1	A	78	GLU	CA-CB-CG	5.93	126.44	113.40
1	A	190	VAL	N-CA-CB	-5.92	98.46	111.50
1	B	141	TRP	CB-CG-CD1	-5.91	119.32	127.00
1	B	259	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	A	484	LYS	N-CA-CB	-5.90	99.98	110.60
1	A	382	ARG	NH1-CZ-NH2	5.86	125.84	119.40
1	A	123	ILE	CG1-CB-CG2	-5.83	98.58	111.40
1	A	38	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	A	347	VAL	CG1-CB-CG2	-5.82	101.59	110.90
1	A	493	ASP	CA-C-N	-5.78	104.48	117.20
1	A	141	TRP	CB-CG-CD1	-5.75	119.53	127.00
1	B	256	ASN	CB-CG-ND2	5.74	130.48	116.70
1	A	184	LEU	CB-CA-C	5.74	121.10	110.20
1	A	465	LEU	CA-CB-CG	5.74	128.49	115.30
1	B	444	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	B	279	VAL	CA-C-N	5.71	129.77	117.20
1	B	369	VAL	CB-CA-C	-5.70	100.57	111.40
1	B	504	THR	CA-CB-CG2	5.70	120.38	112.40
1	A	169	LYS	CB-CG-CD	-5.68	96.82	111.60
1	B	166	PHE	CB-CG-CD2	-5.66	116.84	120.80
1	A	24	ASP	CA-C-N	-5.65	104.77	117.20
1	B	293	MET	CG-SD-CE	5.65	109.23	100.20
1	A	350	GLY	CA-C-N	5.63	129.58	117.20
1	B	474	LYS	O-C-N	-5.62	110.42	121.10
1	A	488	VAL	N-CA-C	-5.60	95.88	111.00
1	A	148	ALA	CB-CA-C	-5.60	101.71	110.10
1	A	176	LYS	N-CA-C	-5.59	95.90	111.00
1	A	492	ASN	CA-CB-CG	5.59	125.69	113.40
1	A	28	VAL	CB-CA-C	-5.56	100.83	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	442	TYR	CB-CG-CD1	-5.55	117.67	121.00
1	A	372	ASN	OD1-CG-ND2	-5.54	109.15	121.90
1	B	256	ASN	OD1-CG-ND2	-5.54	109.16	121.90
1	B	364	GLY	CA-C-N	5.52	129.34	117.20
1	B	398	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	B	156	GLU	CA-CB-CG	5.49	125.48	113.40
1	B	490	VAL	CB-CA-C	5.48	121.82	111.40
1	A	245	ASP	CB-CA-C	-5.48	99.44	110.40
1	B	252	GLN	CA-C-N	-5.47	105.16	117.20
1	A	379	ASP	CA-C-O	-5.47	108.62	120.10
1	B	196	ALA	N-CA-C	5.46	125.75	111.00
1	A	173	ASP	CB-CG-OD1	5.46	123.21	118.30
1	B	152	VAL	CA-C-N	5.46	129.21	117.20
1	B	332	TRP	CG-CD1-NE1	-5.46	104.64	110.10
1	A	236	GLU	CA-CB-CG	5.45	125.39	113.40
1	B	450	ALA	CB-CA-C	-5.45	101.92	110.10
1	A	132	ALA	CB-CA-C	-5.45	101.93	110.10
1	A	173	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	B	436	LEU	CA-C-N	5.42	129.11	117.20
1	A	365	VAL	N-CA-CB	-5.41	99.59	111.50
1	A	262	THR	CA-CB-OG1	-5.39	97.68	109.00
1	A	188	VAL	N-CA-CB	-5.38	99.67	111.50
1	B	483	LEU	CA-CB-CG	5.35	127.61	115.30
1	B	296	LYS	CA-CB-CG	5.35	125.17	113.40
1	B	478	LEU	CA-CB-CG	5.35	127.60	115.30
1	A	341	LYS	CA-CB-CG	5.34	125.15	113.40
1	B	193	TYR	CB-CG-CD2	-5.33	117.80	121.00
1	B	124	ASN	CB-CG-ND2	5.31	129.44	116.70
1	A	211	ASP	CA-C-N	5.30	128.87	117.20
1	B	378	LEU	CB-CG-CD1	-5.30	101.99	111.00
1	A	144	TYR	CG-CD2-CE2	-5.29	117.07	121.30
1	A	169	LYS	CA-CB-CG	5.28	125.02	113.40
1	A	351	VAL	CA-CB-CG2	-5.27	102.99	110.90
1	A	493	ASP	CB-CG-OD1	5.26	123.04	118.30
1	A	153	THR	CA-CB-CG2	5.25	119.75	112.40
1	B	437	TYR	CB-CG-CD2	-5.24	117.86	121.00
1	A	290	GLU	O-C-N	-5.21	114.36	122.70
1	A	250	TRP	CG-CD2-CE3	5.18	138.56	133.90
1	B	465	LEU	CB-CG-CD1	5.18	119.81	111.00
1	B	372	ASN	CB-CG-ND2	5.17	129.10	116.70
1	A	289	ARG	CA-C-N	-5.16	105.84	117.20
1	B	102	THR	N-CA-CB	-5.15	100.51	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	463	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	B	112	LEU	N-CA-CB	-5.13	100.14	110.40
1	B	163	ARG	NH1-CZ-NH2	-5.12	113.77	119.40
1	A	157	ASN	CB-CG-ND2	5.11	128.96	116.70
1	A	290	GLU	CA-C-N	5.09	128.40	117.20
1	A	129	GLU	CB-CA-C	-5.05	100.30	110.40
1	A	18	LYS	CA-CB-CG	5.05	124.50	113.40
1	B	130	TYR	CB-CG-CD2	-5.04	117.97	121.00
1	B	271	LYS	CA-CB-CG	5.04	124.49	113.40
1	A	362	GLU	CA-C-N	5.04	128.28	117.20
1	A	376	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	A	57	ASP	N-CA-C	-5.01	97.47	111.00
1	A	365	VAL	CB-CA-C	5.00	120.91	111.40

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	148	ALA	Peptide
1	A	32	TYR	Sidechain
1	A	34	TYR	Sidechain
1	A	433	ARG	Sidechain
1	A	492	ASN	Mainchain
1	A	502	GLY	Peptide
1	B	442	TYR	Sidechain
1	B	500	TYR	Sidechain

## 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	3721	809	3783	146	0
1	B	2982	666	3044	139	0
2	A	31	4	16	3	0
2	B	31	4	19	4	0
3	A	43	4	30	8	0
4	A	6	0	3	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	6	0	3	1	0
5	A	130	256	0	13	0
5	B	11	22	0	0	0
All	All	6961	1765	6898	281	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 20.

All (281) 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)
1:A:289:ARG:HH21	1:A:376:ARG:NH2	1.38	1.22
1:A:289:ARG:NH2	1:A:376:ARG:NH2	2.06	1.04
1:A:488:VAL:HG22	1:B:490:VAL:HG11	1.51	0.93
1:A:289:ARG:NH2	1:A:376:ARG:HH22	1.69	0.88
1:B:148:ALA:C	1:B:149:ASN:HD22	1.76	0.87
1:A:143:PHE:O	1:A:376:ARG:NH2	2.10	0.84
1:A:58:VAL:HA	1:A:94:CYS:SG	2.18	0.83
1:B:163:ARG:NH2	1:B:486:ARG:HG3	1.95	0.82
1:A:197:THR:HG21	1:A:436:LEU:HD21	1.61	0.81
1:A:77:PRO:HA	1:A:80:LYS:HD2	1.63	0.80
1:A:109:LYS:HA	1:A:112:LEU:HD12	1.63	0.80
3:A:560:HEM:HHA	3:A:560:HEM:HBA2	1.63	0.79
1:B:217:GLY:HA3	1:B:247:GLN:NE2	2.00	0.76
1:A:433:ARG:HD2	5:A:627:HOH:O	1.85	0.76
1:A:289:ARG:HH21	1:A:376:ARG:HH22	1.27	0.75
1:A:490:VAL:HG22	1:A:492:ASN:ND2	2.03	0.74
1:B:373:HIS:O	1:B:376:ARG:HG3	1.88	0.73
1:A:228:SER:HA	1:A:252:GLN:HE21	1.52	0.73
1:A:488:VAL:HG22	1:B:490:VAL:CG1	2.20	0.71
1:A:256:ASN:HD22	1:A:257:SER:N	1.86	0.71
1:B:276:ALA:HB2	1:B:345:PRO:HG2	1.74	0.69
1:A:70:VAL:HB	3:A:560:HEM:HMB1	1.75	0.69
1:A:465:LEU:HD23	1:B:378:LEU:HD11	1.75	0.69
1:B:201:LYS:HE3	1:B:233:CYS:SG	2.33	0.68
1:A:256:ASN:HD22	1:A:257:SER:H	1.41	0.68
1:B:400:LEU:HA	1:B:403:LYS:HD3	1.75	0.67
1:B:349:LYS:NZ	2:B:570:FMN:H2'	2.11	0.65
1:A:148:ALA:N	1:A:376:ARG:HA	2.11	0.65
1:A:197:THR:CG2	1:A:436:LEU:HD21	2.27	0.65
1:A:400:LEU:O	1:A:403:LYS:HG2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:560:HEM:HHA	3:A:560:HEM:CBA	2.22	0.65
1:A:196:ALA:HB2	1:A:226:MET:HG2	1.79	0.64
1:B:201:LYS:HE3	1:B:233:CYS:HG	1.62	0.64
1:A:133:SER:O	5:A:609:HOH:O	2.15	0.64
1:B:182:ASP:HA	1:B:187:HIS:HA	1.80	0.64
1:A:144:TYR:O	1:A:433:ARG:HD3	1.98	0.63
1:A:508:PHE:CZ	1:B:131:LEU:HD12	2.33	0.63
1:B:229:THR:OG1	1:B:253:LEU:HA	2.00	0.62
1:B:132:ALA:HB2	1:B:437:TYR:HB3	1.81	0.62
1:A:385:ILE:HD11	1:A:424:LEU:HD12	1.82	0.61
1:A:461:SER:O	1:A:465:LEU:HB2	1.99	0.61
1:B:276:ALA:CB	1:B:345:PRO:HG2	2.30	0.61
3:A:560:HEM:CHA	3:A:560:HEM:HBA2	2.30	0.61
1:B:252:GLN:HA	1:B:278:PHE:O	2.01	0.61
1:B:478:LEU:HD13	1:B:480:LEU:HD21	1.83	0.61
1:B:152:VAL:HG21	1:B:380:PHE:CE2	2.36	0.60
1:A:21:LYS:HB3	1:A:24:ASP:O	2.01	0.60
1:A:124:ASN:ND2	1:A:126:TYR:HB2	2.16	0.59
1:A:40:LEU:HG	1:A:47:GLN:HB2	1.83	0.59
1:A:251:TYR:HB2	1:A:274:VAL:HG21	1.84	0.59
1:B:286:LEU:HG	1:B:289:ARG:NH2	2.17	0.59
1:A:196:ALA:HB1	1:A:228:SER:HB2	1.84	0.59
1:B:286:LEU:HD21	4:B:580:PYR:H33	1.86	0.58
1:B:196:ALA:HB2	1:B:226:MET:HG2	1.86	0.58
1:A:22:PRO:HB3	1:A:51:LYS:HD2	1.85	0.58
1:B:431:LEU:HB2	1:B:435:PHE:CE2	2.38	0.58
1:B:270:GLU:OE2	1:B:343:LYS:HB3	2.04	0.58
1:A:218:GLN:HE22	1:A:444:ARG:HD2	1.67	0.58
1:A:349:LYS:HA	1:A:369:VAL:HB	1.85	0.58
1:A:32:TYR:CE1	1:A:82:GLY:HA2	2.38	0.58
1:A:214:ARG:HD2	1:A:444:ARG:HD3	1.85	0.58
1:B:103:LYS:O	1:B:106:ILE:HG12	2.03	0.58
1:A:392:MET:HG3	1:A:424:LEU:O	2.04	0.58
1:B:183:MET:CE	1:B:250:TRP:HH2	2.16	0.58
1:B:349:LYS:HZ1	2:B:570:FMN:H2'	1.68	0.58
1:A:412:VAL:HG21	1:A:429:VAL:CG1	2.34	0.57
1:B:212:VAL:HG12	1:B:216:CYS:SG	2.44	0.57
1:A:218:GLN:HE22	1:A:444:ARG:HH11	1.52	0.57
1:B:122:ILE:HG23	1:B:127:ASP:HB2	1.87	0.56
1:A:144:TYR:OH	1:A:202:LEU:HB2	2.04	0.56
1:A:148:ALA:H	1:A:376:ARG:HA	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:ASN:HD22	1:B:126:TYR:HB2	1.70	0.56
1:A:430:GLY:O	5:A:612:HOH:O	2.17	0.56
1:B:256:ASN:HD22	1:B:257:SER:N	2.04	0.56
1:B:289:ARG:HH11	1:B:376:ARG:HB2	1.70	0.56
1:B:174:VAL:O	1:B:463:ARG:HD2	2.06	0.56
1:A:462:MET:HG2	1:A:467:VAL:HG23	1.88	0.56
1:A:65:LEU:HD21	1:A:202:LEU:HD21	1.87	0.55
1:A:75:ILE:O	1:A:80:LYS:HE3	2.06	0.55
1:A:199:LEU:HD21	3:A:560:HEM:HAA1	1.89	0.55
1:B:109:LYS:O	1:B:113:LYS:HB3	2.07	0.55
1:B:196:ALA:HB2	1:B:226:MET:HE3	1.89	0.55
1:B:161:TYR:CE1	1:B:385:ILE:HD13	2.41	0.55
1:B:212:VAL:HG13	1:B:447:VAL:HG11	1.89	0.55
1:A:113:LYS:O	1:A:115:LEU:N	2.40	0.55
1:A:110:GLU:HB2	1:A:113:LYS:HE3	1.88	0.55
1:B:492:ASN:HD21	1:B:494:VAL:HG22	1.72	0.55
1:A:358:ILE:O	1:A:362:GLU:HG3	2.07	0.54
1:A:442:TYR:HB2	1:A:446:GLY:HA3	1.90	0.54
1:B:194:VAL:HG11	1:B:212:VAL:HG11	1.89	0.54
1:A:110:GLU:HA	1:A:113:LYS:HG2	1.90	0.54
1:A:105:ASP:O	1:A:109:LYS:HG3	2.07	0.54
1:A:163:ARG:NH1	1:A:486:ARG:HA	2.23	0.54
1:A:125:LEU:HG	1:A:434:PRO:HB3	1.90	0.54
1:B:442:TYR:HB2	1:B:446:GLY:HA3	1.90	0.54
1:B:469:SER:O	1:B:472:GLU:HB2	2.07	0.53
1:A:431:LEU:HD23	1:A:434:PRO:HG2	1.89	0.53
1:A:75:ILE:HD11	3:A:560:HEM:HAB	1.88	0.53
1:A:162:HIS:HE1	5:A:652:HOH:O	1.90	0.53
1:A:270:GLU:HB3	1:A:343:LYS:NZ	2.23	0.53
1:B:244:SER:HB2	1:B:247:GLN:H	1.74	0.53
2:A:570:FMN:O4'	2:A:570:FMN:H1'2	2.09	0.53
1:A:248:ILE:HG23	1:A:275:LYS:HD3	1.91	0.53
1:B:388:LEU:HD12	1:B:408:VAL:HG21	1.91	0.53
1:B:108:ARG:HG3	1:B:135:THR:HA	1.90	0.52
1:A:214:ARG:HA	1:A:243:PRO:HD3	1.90	0.52
1:A:113:LYS:C	1:A:115:LEU:H	2.12	0.52
1:B:387:VAL:O	1:B:391:THR:HG23	2.09	0.51
1:A:347:VAL:HA	1:A:367:GLY:O	2.10	0.51
1:B:452:GLU:HG2	1:B:455:ARG:NH2	2.25	0.51
1:B:109:LYS:HD2	1:B:112:LEU:HD23	1.93	0.51
1:B:293:MET:O	1:B:295:LEU:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:VAL:HB	1:A:57:ASP:HA	1.93	0.51
1:B:449:LYS:HE2	1:B:453:ILE:HD11	1.92	0.51
1:B:289:ARG:HD2	1:B:376:ARG:HB3	1.93	0.50
1:B:337:GLU:HA	1:B:340:LYS:HD2	1.92	0.50
1:B:372:ASN:ND2	1:B:375:GLY:H	2.09	0.50
1:A:447:VAL:O	1:A:451:ILE:HG13	2.11	0.50
1:A:88:MET:SD	1:A:92:LEU:HD13	2.52	0.50
1:B:108:ARG:O	1:B:112:LEU:HB3	2.11	0.50
1:B:431:LEU:HB2	1:B:435:PHE:HE2	1.76	0.50
1:B:465:LEU:HD22	1:B:477:LEU:HD23	1.92	0.50
1:B:163:ARG:HH22	1:B:486:ARG:HG3	1.72	0.49
1:A:270:GLU:OE2	1:A:343:LYS:HG3	2.12	0.49
1:B:462:MET:HG2	1:B:467:VAL:HG23	1.94	0.49
1:A:122:ILE:HG22	1:A:453:ILE:HD11	1.93	0.49
1:B:255:VAL:HG21	1:B:330:LEU:HD21	1.94	0.49
1:B:196:ALA:CB	1:B:226:MET:HE3	2.43	0.49
1:B:339:LYS:HG2	1:B:346:ILE:HD12	1.95	0.49
1:B:467:VAL:HG11	1:B:477:LEU:HD21	1.95	0.49
1:A:171:LEU:O	1:B:331:THR:HA	2.12	0.49
1:A:187:HIS:HE1	5:A:602:HOH:O	1.95	0.49
1:B:256:ASN:ND2	1:B:258:ASP:H	2.09	0.49
1:B:361:ALA:CB	1:B:400:LEU:HD13	2.43	0.49
1:A:199:LEU:HA	1:A:232:SER:OG	2.14	0.48
1:A:452:GLU:HG3	1:A:455:ARG:NH2	2.29	0.48
1:A:331:THR:O	1:A:334:ASP:HB2	2.12	0.48
1:A:197:THR:CG2	1:A:200:CYS:SG	3.02	0.47
1:B:102:THR:HG21	1:B:138:LYS:NZ	2.29	0.47
1:B:179:ILE:HD11	1:B:455:ARG:HG2	1.96	0.47
1:A:153:THR:HG21	1:A:381:SER:HB3	1.97	0.47
1:A:321:ALA:N	5:A:718:HOH:O	2.47	0.47
1:A:345:PRO:HB3	1:A:366:SER:OG	2.14	0.47
1:B:283:ALA:O	1:B:326:ILE:HG21	2.14	0.47
1:B:124:ASN:ND2	1:B:126:TYR:HB2	2.29	0.47
1:B:213:ALA:HB2	1:B:225:GLN:HE22	1.79	0.47
1:A:112:LEU:HG	1:A:135:THR:HB	1.97	0.47
1:A:256:ASN:O	1:A:259:ARG:HD3	2.14	0.47
1:B:194:VAL:HG21	1:B:216:CYS:SG	2.54	0.47
1:B:183:MET:SD	1:B:188:VAL:HG21	2.55	0.47
1:B:226:MET:HE1	1:B:349:LYS:HD3	1.97	0.47
1:A:337:GLU:HB3	1:A:341:LYS:NZ	2.30	0.47
1:A:69:ASN:HD22	1:A:73:LYS:HD3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:GLU:O	1:A:18:LYS:HB3	2.15	0.46
1:A:214:ARG:NH1	5:A:651:HOH:O	2.48	0.46
1:A:234:SER:HB2	1:A:236:GLU:HG2	1.98	0.46
1:A:508:PHE:CE1	1:B:116:LEU:HD23	2.51	0.46
1:A:163:ARG:NH1	1:B:488:VAL:O	2.49	0.46
1:B:441:CYS:HB3	1:B:442:TYR:CD1	2.50	0.46
1:B:163:ARG:HB3	1:B:483:LEU:HA	1.97	0.46
1:B:164:ILE:HB	1:B:420:LYS:HD3	1.97	0.46
1:B:456:ASP:O	1:B:460:MET:HG3	2.16	0.46
1:B:108:ARG:HG2	1:B:135:THR:O	2.16	0.46
1:A:60:ALA:HB1	1:A:96:PRO:HG3	1.97	0.46
1:A:169:LYS:HE3	5:A:850:HOH:O	2.16	0.45
1:B:222:LYS:N	1:B:222:LYS:HD2	2.31	0.45
1:B:370:LEU:HD22	1:B:406:VAL:CG1	2.45	0.45
1:A:488:VAL:CG2	1:B:490:VAL:HG11	2.36	0.45
1:B:157:ASN:OD1	1:B:384:PRO:HD2	2.17	0.45
1:B:193:TYR:HE2	1:B:407:PHE:HD2	1.63	0.45
1:B:439:ASN:O	1:B:443:GLY:N	2.50	0.45
1:A:197:THR:HG21	1:A:436:LEU:CD2	2.40	0.45
1:B:256:ASN:HD22	1:B:257:SER:H	1.63	0.45
1:B:256:ASN:HD22	1:B:258:ASP:H	1.64	0.45
1:A:58:VAL:HG23	1:A:94:CYS:SG	2.56	0.45
1:B:339:LYS:HA	1:B:346:ILE:HD11	1.99	0.45
1:B:347:VAL:HG13	1:B:367:GLY:C	2.37	0.45
1:B:478:LEU:CD1	1:B:480:LEU:HD21	2.46	0.45
1:A:216:CYS:O	1:A:222:LYS:HA	2.17	0.45
1:A:214:ARG:NH1	1:A:241:ALA:HB1	2.32	0.45
1:B:419:LEU:HD13	1:B:465:LEU:HD12	1.99	0.45
1:B:385:ILE:HD11	1:B:421:ALA:HA	1.99	0.45
1:A:192:PHE:HA	1:A:429:VAL:O	2.17	0.45
1:A:29:ILE:HB	1:A:34:TYR:HE2	1.81	0.45
1:B:351:VAL:HG11	1:B:357:VAL:CG2	2.47	0.45
1:B:149:ASN:O	1:B:150:ASP:HB2	2.17	0.44
1:B:183:MET:HB3	1:B:183:MET:HE2	1.85	0.44
1:B:288:GLN:HG3	1:B:293:MET:SD	2.56	0.44
1:A:130:TYR:O	1:A:134:GLN:HG2	2.18	0.44
1:A:15:GLU:O	1:A:19:HIS:CE1	2.70	0.44
1:A:255:VAL:HG21	1:A:330:LEU:HD23	1.99	0.44
1:B:199:LEU:O	1:B:201:LYS:N	2.50	0.44
1:A:77:PRO:HA	1:A:80:LYS:CD	2.41	0.44
1:A:143:PHE:CD1	1:A:289:ARG:NH2	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:VAL:HG21	1:B:458:ILE:HD11	2.00	0.44
1:B:109:LYS:HD2	1:B:112:LEU:CD2	2.48	0.44
1:B:210:LYS:O	1:B:214:ARG:HG3	2.17	0.44
1:B:348:ILE:HD12	1:B:365:VAL:HG21	1.99	0.44
1:A:123:ILE:HG21	1:B:290:GLU:HG2	1.99	0.44
1:A:252:GLN:HA	1:A:278:PHE:O	2.17	0.44
1:A:361:ALA:HB1	1:A:400:LEU:HD22	2.00	0.44
1:B:412:VAL:HG13	1:B:417:ASP:HB2	1.99	0.44
1:A:32:TYR:HB3	1:A:34:TYR:OH	2.18	0.43
1:B:197:THR:HG21	1:B:436:LEU:HG	1.99	0.43
1:A:170:ILE:HD11	1:B:282:ASP:HA	1.99	0.43
1:B:111:GLN:O	1:B:115:LEU:HB2	2.18	0.43
1:B:149:ASN:HB3	1:B:290:GLU:OE2	2.17	0.43
1:B:243:PRO:HD2	1:B:247:GLN:HE22	1.83	0.43
2:B:570:FMN:H9	2:B:570:FMN:H1'2	1.63	0.43
1:A:176:LYS:HA	5:A:640:HOH:O	2.18	0.43
1:A:110:GLU:O	1:A:113:LYS:HG2	2.19	0.43
1:A:333:LYS:HD2	1:A:333:LYS:HA	1.74	0.43
3:A:560:HEM:O1A	4:A:580:PYR:O2	2.37	0.43
1:A:21:LYS:O	1:A:25:CYS:HB2	2.18	0.43
1:B:174:VAL:HB	1:B:463:ARG:HG3	2.01	0.43
2:B:570:FMN:O4'	2:B:570:FMN:H9	2.19	0.43
1:A:380:PHE:HE1	5:A:721:HOH:O	2.01	0.43
1:B:354:THR:OG1	1:B:391:THR:HG22	2.19	0.43
1:A:278:PHE:HA	1:A:347:VAL:O	2.19	0.43
1:B:230:LEU:HD12	1:B:230:LEU:N	2.34	0.43
1:A:187:HIS:CE1	5:A:602:HOH:O	2.69	0.42
1:A:330:LEU:HD22	1:A:334:ASP:HB3	2.00	0.42
1:A:361:ALA:HB2	1:A:404:LEU:HD22	2.01	0.42
1:B:492:ASN:ND2	1:B:494:VAL:HG22	2.33	0.42
1:A:129:GLU:HG2	1:A:437:TYR:CD2	2.54	0.42
1:B:230:LEU:HD13	1:B:254:TYR:CD2	2.54	0.42
1:B:289:ARG:NH1	1:B:377:GLN:HE21	2.17	0.42
1:B:462:MET:HG2	1:B:467:VAL:CG2	2.50	0.42
1:A:175:ARG:HH11	1:A:175:ARG:HB2	1.84	0.42
1:B:174:VAL:CG2	1:B:463:ARG:HG3	2.49	0.42
1:A:285:SER:O	1:A:377:GLN:NE2	2.53	0.42
1:B:230:LEU:CD1	1:B:254:TYR:HD2	2.33	0.42
1:B:439:ASN:OD1	1:B:443:GLY:HA2	2.19	0.42
1:A:138:LYS:HD2	5:A:701:HOH:O	2.20	0.42
1:A:12:SER:HA	1:A:13:PRO:HD3	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:VAL:O	1:A:274:VAL:HG22	2.18	0.42
1:A:346:ILE:HB	1:A:365:VAL:HG22	2.02	0.42
1:A:376:ARG:NH1	4:A:580:PYR:O3	2.53	0.42
1:A:432:GLY:HA3	2:A:570:FMN:H4'	2.01	0.42
1:B:106:ILE:O	1:B:110:GLU:HG2	2.20	0.42
1:A:223:VAL:HA	1:A:224:PRO:HD3	1.95	0.42
1:A:177:VAL:HG23	1:A:463:ARG:NH1	2.35	0.41
1:A:330:LEU:HD22	1:A:334:ASP:CB	2.49	0.41
1:A:282:ASP:O	1:A:377:GLN:HG2	2.20	0.41
1:B:201:LYS:HA	1:B:204:ASN:O	2.21	0.41
1:A:337:GLU:OE1	1:A:340:LYS:HE2	2.20	0.41
2:A:570:FMN:O4'	2:A:570:FMN:H9	2.19	0.41
1:B:153:THR:HG21	1:B:381:SER:HB3	2.02	0.41
1:B:357:VAL:HG13	1:B:368:VAL:HG11	2.02	0.41
1:B:358:ILE:HD11	1:B:394:ILE:HG21	2.01	0.41
1:A:487:THR:O	1:B:490:VAL:HG12	2.20	0.41
1:B:164:ILE:HG23	1:B:480:LEU:HD23	2.02	0.41
1:B:224:PRO:HA	1:B:248:ILE:O	2.20	0.41
1:A:16:VAL:HA	1:A:26:TRP:CE3	2.55	0.41
1:A:196:ALA:N	1:A:226:MET:HE2	2.35	0.41
1:B:148:ALA:C	1:B:149:ASN:ND2	2.59	0.41
1:B:400:LEU:O	1:B:403:LYS:HB2	2.21	0.41
1:A:151:GLU:OE1	1:A:291:LYS:NZ	2.54	0.41
1:A:239:ILE:HD11	1:A:274:VAL:HG12	2.03	0.41
1:A:332:TRP:O	1:A:336:GLU:HG3	2.20	0.41
1:A:61:ILE:HG23	1:A:97:TYR:HB2	2.03	0.41
1:B:214:ARG:HA	1:B:243:PRO:CD	2.50	0.41
1:B:336:GLU:O	1:B:339:LYS:HB2	2.20	0.41
1:A:118:PRO:HA	5:A:680:HOH:O	2.20	0.41
1:A:255:VAL:HG21	1:A:330:LEU:CD2	2.50	0.41
1:B:217:GLY:HA3	1:B:247:GLN:HE21	1.82	0.41
1:B:172:VAL:HG11	1:B:466:GLY:O	2.20	0.41
1:A:369:VAL:HG22	1:A:407:PHE:HB2	2.03	0.41
1:A:67:ALA:HA	1:A:232:SER:O	2.21	0.41
1:B:210:LYS:HD3	1:B:237:GLU:HB3	2.03	0.41
1:A:230:LEU:HD12	3:A:560:HEM:HMA2	2.03	0.41
1:A:382:ARG:HH21	1:A:484:LYS:NZ	2.19	0.41
1:A:168:PRO:HB3	1:A:465:LEU:HA	2.04	0.41
1:A:144:TYR:CD1	1:A:436:LEU:HD13	2.56	0.40
1:A:447:VAL:HG12	1:A:451:ILE:HD11	2.03	0.40
1:B:371:SER:HB2	1:B:409:ASP:OD1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:486:ARG:HH11	1:B:486:ARG:HD2	1.74	0.40
1:A:203:GLY:HA3	1:A:440:SER:OG	2.21	0.40
1:A:495:LEU:HD21	1:B:503:PRO:HB2	2.03	0.40
1:B:153:THR:OG1	1:B:381:SER:N	2.55	0.40
1:B:159:ASN:O	1:B:162:HIS:HB2	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	474/511 (93%)	425 (90%)	36 (8%)	13 (3%)	5	19
1	B	378/511 (74%)	331 (88%)	38 (10%)	9 (2%)	6	22
All	All	852/1022 (83%)	756 (89%)	74 (9%)	22 (3%)	5	20

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	PRO
1	A	104	GLU
1	A	114	SER
1	B	146	SER
1	B	149	ASN
1	A	69	ASN
1	A	399	ASN
1	A	493	ASP
1	B	103	LYS
1	B	200	CYS
1	B	287	GLY
1	B	290	GLU
1	B	294	LYS

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Mol	Chain	Res	Type
1	A	85	GLN
1	B	119	LEU
1	A	18	LYS
1	B	114	SER
1	A	13	PRO
1	A	23	ASP
1	A	149	ASN
1	A	150	ASP
1	A	410	GLY

### 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	411/440 (93%)	344 (84%)	67 (16%)	2	7
1	B	330/440 (75%)	277 (84%)	53 (16%)	2	7
All	All	741/880 (84%)	621 (84%)	120 (16%)	2	7

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LYS
1	A	13	PRO
1	A	15	GLU
1	A	20	ASN
1	A	21	LYS
1	A	25	CYS
1	A	27	VAL
1	A	30	ASN
1	A	32	TYR
1	A	38	ARG
1	A	41	PRO
1	A	44	PRO
1	A	65	LEU
1	A	72	ASP

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Mol	Chain	Res	Type
1	A	84	LEU
1	A	87	SER
1	A	90	PRO
1	A	91	GLU
1	A	96	PRO
1	A	103	LYS
1	A	115	LEU
1	A	121	ASN
1	A	124	ASN
1	A	125	LEU
1	A	131	LEU
1	A	152	VAL
1	A	162	HIS
1	A	169	LYS
1	A	190	VAL
1	A	191	PRO
1	A	195	SER
1	A	206	LEU
1	A	212	VAL
1	A	223	VAL
1	A	230	LEU
1	A	236	GLU
1	A	239	ILE
1	A	245	ASP
1	A	252	GLN
1	A	255	VAL
1	A	256	ASN
1	A	265	LEU
1	A	271	LYS
1	A	292	ASP
1	A	294	LYS
1	A	323	SER
1	A	325	PHE
1	A	329	SER
1	A	331	THR
1	A	365	VAL
1	A	372	ASN
1	A	378	LEU
1	A	388	LEU
1	A	399	ASN
1	A	400	LEU
1	A	448	GLU

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Mol	Chain	Res	Type
1	A	452	GLU
1	A	460	MET
1	A	462	MET
1	A	465	LEU
1	A	469	SER
1	A	481	SER
1	A	483	LEU
1	A	490	VAL
1	A	494	VAL
1	A	495	LEU
1	A	507	GLU
1	B	103	LYS
1	B	105	ASP
1	B	108	ARG
1	B	118	PRO
1	B	119	LEU
1	B	131	LEU
1	B	136	LEU
1	B	149	ASN
1	B	163	ARG
1	B	182	ASP
1	B	187	HIS
1	B	197	THR
1	B	206	LEU
1	B	222	LYS
1	B	236	GLU
1	B	244	SER
1	B	248	ILE
1	B	249	GLN
1	B	252	GLN
1	B	256	ASN
1	B	257	SER
1	B	260	LYS
1	B	263	ASP
1	B	267	LYS
1	B	268	ASN
1	B	289	ARG
1	B	295	LEU
1	B	296	LYS
1	B	328	PRO
1	B	331	THR
1	B	338	LEU

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Mol	Chain	Res	Type
1	B	342	THR
1	B	343	LYS
1	B	368	VAL
1	B	370	LEU
1	B	372	ASN
1	B	378	LEU
1	B	384	PRO
1	B	388	LEU
1	B	391	THR
1	B	408	VAL
1	B	414	ARG
1	B	416	THR
1	B	429	VAL
1	B	436	LEU
1	B	444	ARG
1	B	461	SER
1	B	463	ARG
1	B	468	THR
1	B	483	LEU
1	B	492	ASN
1	B	507	GLU
1	B	509	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	ASN
1	A	134	GLN
1	A	157	ASN
1	A	162	HIS
1	A	218	GLN
1	A	249	GLN
1	A	252	GLN
1	A	256	ASN
1	A	372	ASN
1	A	377	GLN
1	A	492	ASN
1	A	497	ASN
1	B	124	ASN
1	B	149	ASN
1	B	218	GLN
1	B	247	GLN

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Mol	Chain	Res	Type
1	B	256	ASN
1	B	372	ASN
1	B	397	GLN
1	B	492	ASN
1	B	497	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 carbohydrates 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	$\# Z  > 2$
4	PYR	B	580	-	2,5,5	1.17	0	2,6,6	1.81	0
2	FMN	B	570	-	31,33,33	2.87	10 (32%)	40,50,50	3.03	16 (40%)
2	FMN	A	570	-	31,33,33	2.88	10 (32%)	40,50,50	3.34	19 (47%)
4	PYR	A	580	-	2,5,5	1.64	1 (50%)	2,6,6	0.89	0
3	HEM	A	560	1	27,50,50	2.83	7 (25%)	17,82,82	2.76	6 (35%)

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
4	PYR	B	580	-	-	0/0/4/4	-
2	FMN	B	570	-	2/2/4/4	7/18/18/18	0/3/3/3
2	FMN	A	570	-	2/2/4/4	16/18/18/18	0/3/3/3
4	PYR	A	580	-	-	0/0/4/4	-
3	HEM	A	560	1	-	0/6/54/54	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	570	FMN	C1'-N10	-12.75	1.35	1.48
2	A	570	FMN	C1'-N10	-11.43	1.36	1.48
3	A	560	HEM	CAA-C2A	10.82	1.67	1.52
2	A	570	FMN	C2'-C3'	-5.50	1.43	1.53
3	A	560	HEM	C3C-CAC	-4.55	1.38	1.47
3	A	560	HEM	C3B-CAB	-4.41	1.39	1.47
3	A	560	HEM	C3B-C2B	-4.22	1.34	1.40
2	A	570	FMN	O2'-C2'	-3.69	1.35	1.43
2	A	570	FMN	C6-C5A	-3.64	1.36	1.41
3	A	560	HEM	C3C-C2C	-3.51	1.35	1.40
2	B	570	FMN	C6-C5A	-3.47	1.36	1.41
2	B	570	FMN	C4A-N5	3.40	1.38	1.33
2	B	570	FMN	C4-N3	3.17	1.38	1.33
2	B	570	FMN	C10-N1	3.04	1.37	1.33
2	A	570	FMN	O4'-C4'	-2.97	1.37	1.43
2	A	570	FMN	C4A-C10	-2.92	1.35	1.38
2	B	570	FMN	C9A-C5A	-2.76	1.37	1.42
2	A	570	FMN	C4A-N5	2.71	1.37	1.33
2	B	570	FMN	C4-C4A	2.69	1.46	1.41
3	A	560	HEM	CBB-CAB	2.48	1.45	1.29
2	A	570	FMN	C9-C8	-2.35	1.31	1.37
3	A	560	HEM	CBC-CAC	2.34	1.44	1.29
2	A	570	FMN	C9-C9A	-2.33	1.36	1.40
2	B	570	FMN	C2'-C3'	-2.26	1.49	1.53
2	A	570	FMN	C4'-C3'	-2.17	1.49	1.53
2	B	570	FMN	C2-N1	-2.14	1.33	1.38
2	B	570	FMN	C8M-C8	2.12	1.55	1.51
4	A	580	PYR	C3-C2	2.03	1.55	1.49

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	570	FMN	C4-N3-C2	11.80	125.11	115.14
2	A	570	FMN	C4-N3-C2	9.80	123.41	115.14
3	A	560	HEM	CAA-C2A-C3A	7.80	149.67	127.25
2	A	570	FMN	C1'-N10-C10	7.59	125.20	118.41
2	B	570	FMN	C4A-C4-N3	-6.76	114.18	123.43
2	A	570	FMN	C4-C4A-C10	6.22	124.07	119.95
2	A	570	FMN	C4'-C3'-C2'	5.64	125.08	113.36
2	A	570	FMN	C4A-C4-N3	-5.21	116.31	123.43
2	B	570	FMN	C1'-N10-C9A	5.12	122.32	118.29
2	A	570	FMN	O2'-C2'-C1'	4.92	121.43	109.59
2	B	570	FMN	C5A-C9A-N10	4.83	121.22	117.72
3	A	560	HEM	CAA-CBA-CGA	4.62	120.43	112.67
2	A	570	FMN	C9A-N10-C10	-4.42	116.12	121.91
2	A	570	FMN	C5A-C9A-N10	4.32	120.84	117.72
2	B	570	FMN	C4'-C3'-C2'	3.98	121.65	113.36
2	B	570	FMN	O4'-C4'-C3'	3.77	118.26	109.10
2	A	570	FMN	C4-C4A-N5	-3.76	114.30	118.60
2	B	570	FMN	C9A-N10-C10	-3.71	117.05	121.91
3	A	560	HEM	CBA-CAA-C2A	3.64	119.21	112.49
2	A	570	FMN	C1'-C2'-C3'	3.62	119.89	109.79
2	B	570	FMN	O2'-C2'-C1'	3.58	118.21	109.59
2	A	570	FMN	C8M-C8-C9	-3.51	111.95	120.34
2	B	570	FMN	P-O5'-C5'	3.50	127.94	118.30
2	A	570	FMN	P-O5'-C5'	3.48	127.89	118.30
2	A	570	FMN	O2'-C2'-C3'	-3.34	100.99	109.10
2	A	570	FMN	C7-C6-C5A	-3.18	116.72	121.22
2	A	570	FMN	C8M-C8-C7	3.03	126.95	120.74
2	A	570	FMN	O4'-C4'-C3'	2.93	116.22	109.10
2	A	570	FMN	O3'-C3'-C4'	2.79	115.55	108.81
2	B	570	FMN	O5'-C5'-C4'	2.79	116.80	109.36
2	B	570	FMN	C8M-C8-C7	2.76	126.39	120.74
2	B	570	FMN	O3P-P-O2P	2.75	118.16	107.64
3	A	560	HEM	CBD-CAD-C3D	2.70	117.45	112.48
2	B	570	FMN	O5'-P-O1P	-2.43	99.66	106.47
2	A	570	FMN	O4'-C4'-C5'	2.36	115.22	109.92
2	B	570	FMN	C4-C4A-C10	2.20	121.41	119.95
2	B	570	FMN	C8M-C8-C9	-2.18	115.12	120.34
3	A	560	HEM	CMD-C2D-C1D	-2.14	125.18	128.46
2	A	570	FMN	O5'-P-O1P	-2.07	100.66	106.47
2	B	570	FMN	O4'-C4'-C5'	2.06	114.54	109.92
3	A	560	HEM	C3B-C4B-NB	2.02	111.82	109.21

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	570	FMN	C4'
2	B	570	FMN	C2'
2	A	570	FMN	C4'
2	A	570	FMN	C2'

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	570	FMN	C2'-C1'-N10-C9A
2	B	570	FMN	N10-C1'-C2'-O2'
2	B	570	FMN	C3'-C4'-C5'-O5'
2	B	570	FMN	O4'-C4'-C5'-O5'
2	A	570	FMN	C2'-C1'-N10-C9A
2	A	570	FMN	N10-C1'-C2'-O2'
2	A	570	FMN	C1'-C2'-C3'-O3'
2	A	570	FMN	C1'-C2'-C3'-C4'
2	A	570	FMN	O2'-C2'-C3'-O3'
2	A	570	FMN	O2'-C2'-C3'-C4'
2	A	570	FMN	C2'-C3'-C4'-O4'
2	A	570	FMN	O3'-C3'-C4'-O4'
2	A	570	FMN	O3'-C3'-C4'-C5'
2	A	570	FMN	O4'-C4'-C5'-O5'
2	A	570	FMN	C5'-O5'-P-O1P
2	A	570	FMN	C5'-O5'-P-O3P
2	A	570	FMN	C2'-C3'-C4'-C5'
2	B	570	FMN	O3'-C3'-C4'-O4'
2	A	570	FMN	C4'-C5'-O5'-P
2	A	570	FMN	C3'-C4'-C5'-O5'
2	B	570	FMN	C4'-C5'-O5'-P
2	B	570	FMN	C2'-C3'-C4'-O4'
2	A	570	FMN	C5'-O5'-P-O2P

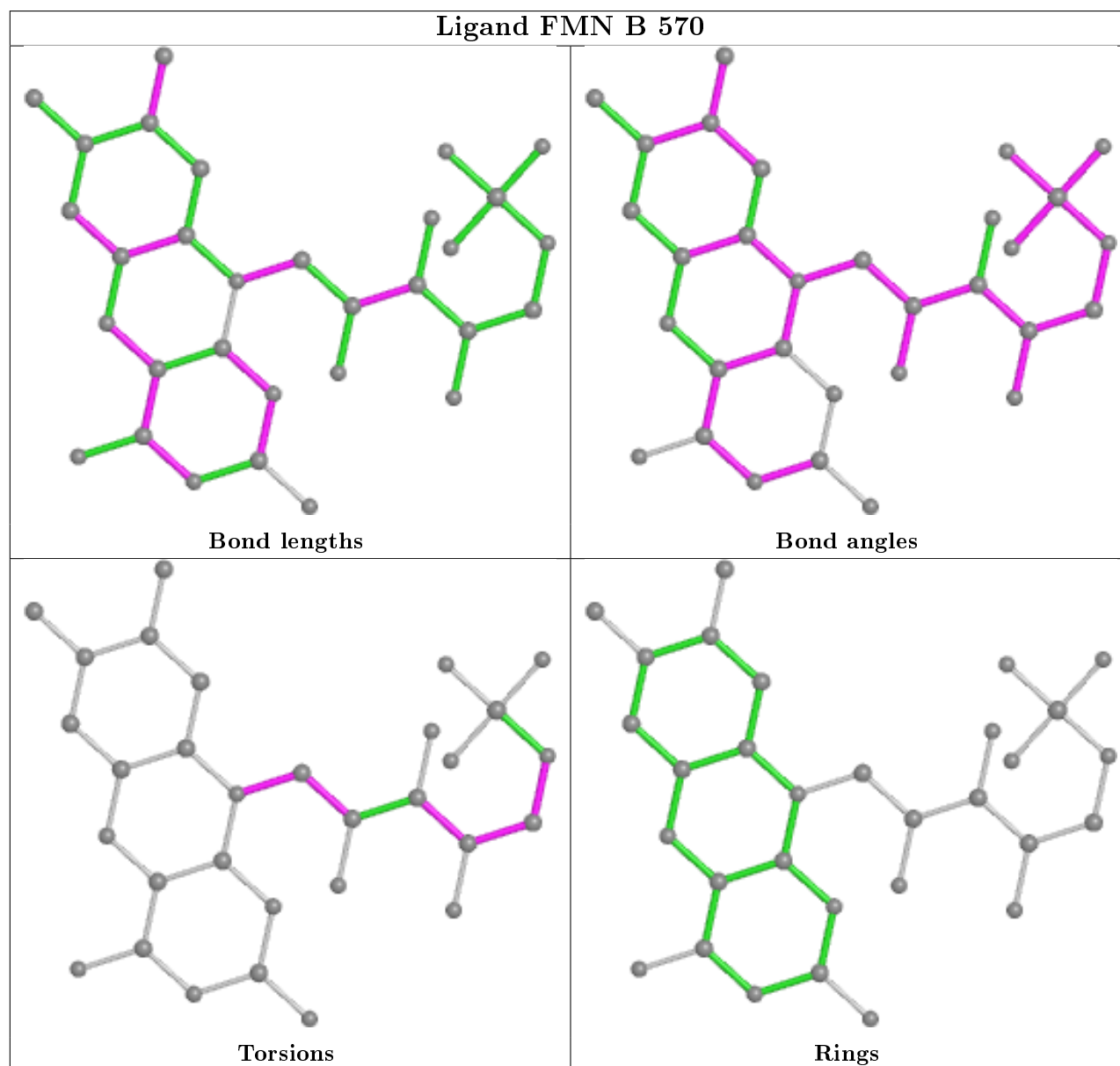
There are no ring outliers.

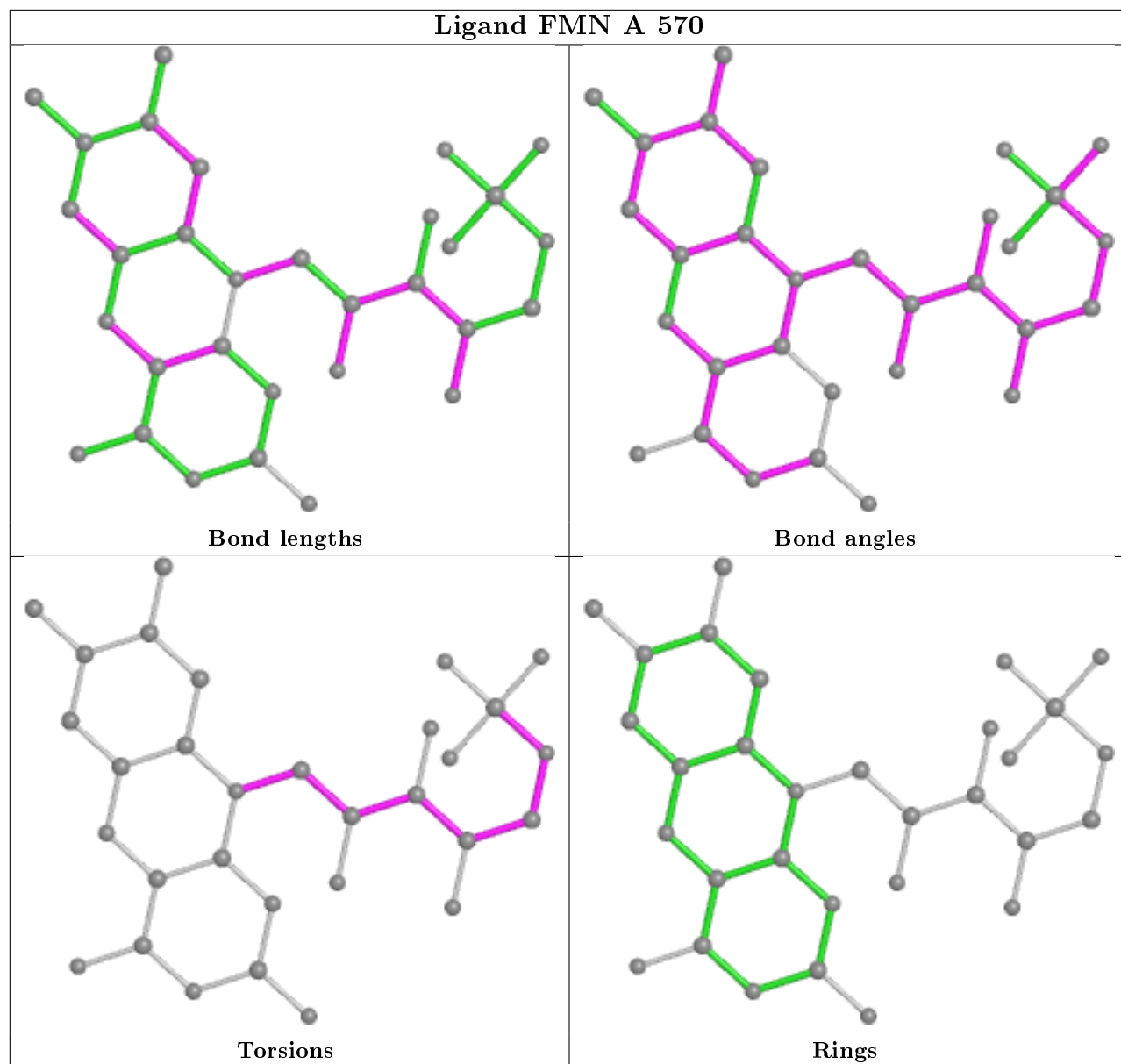
5 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	580	PYR	1	0
2	B	570	FMN	4	0
2	A	570	FMN	3	0
4	A	580	PYR	2	0
3	A	560	HEM	8	0

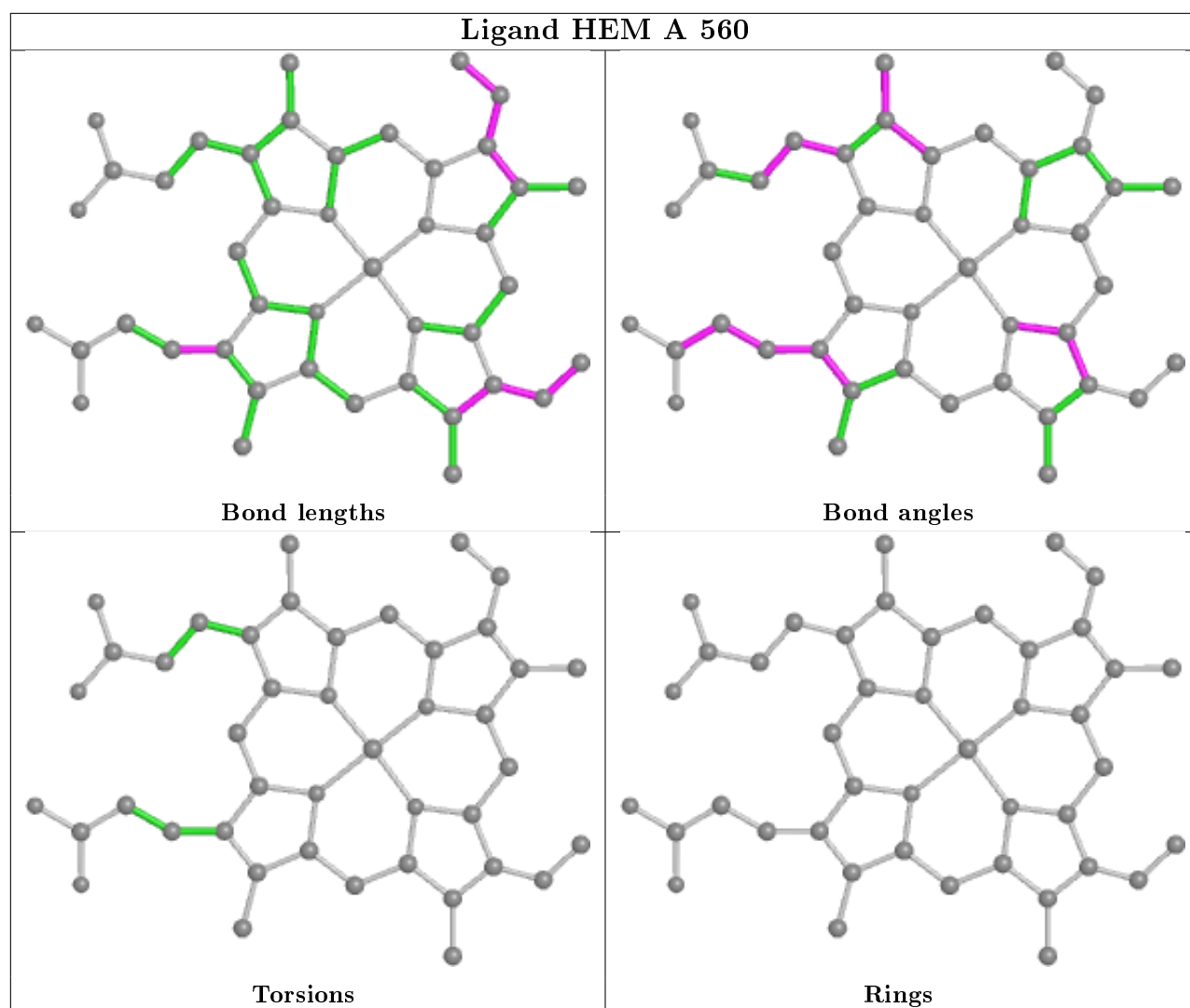
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.