



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 03:53 am BST

PDB ID : 1LCO
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 : 1995-03-30
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

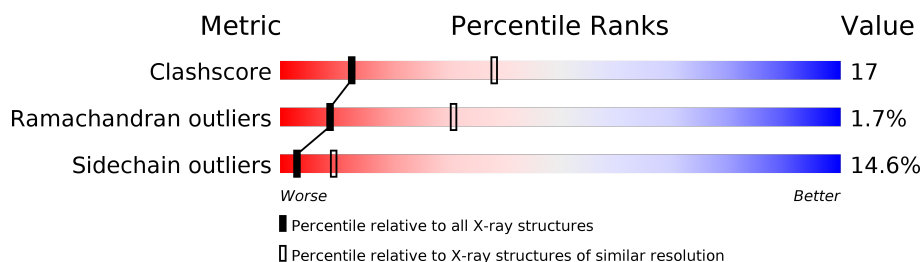
1 Overall quality at a glance

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 ≥ 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
3	FMN	A	570	X	-	-	-
3	FMN	B	570	X	-	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8915 atoms, of which 1840 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	480	Total	C	H	N	O	S	0	0	0
			4547	2384	811	631	707	14			
1	B	391	Total	C	H	N	O	S	0	0	0
			3732	1930	687	521	583	11			

There are 2 discrepancies between the modelled and reference sequences:

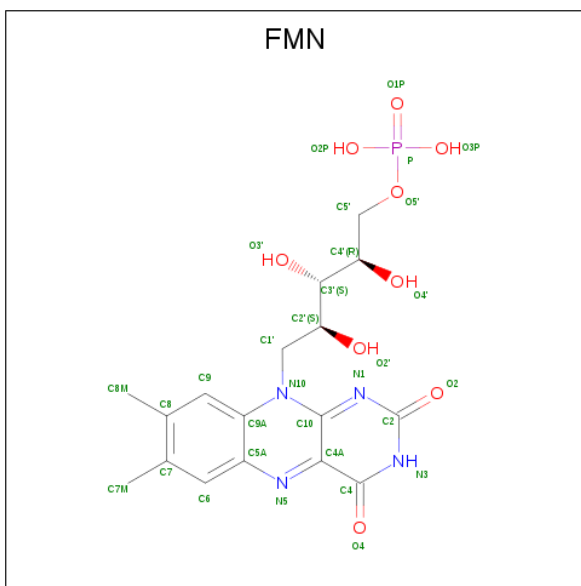
Chain	Residue	Modelled	Actual	Comment	Reference
A	143	PHE	TYR	CONFLICT	UNP P00175
B	143	PHE	TYR	CONFLICT	UNP P00175

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



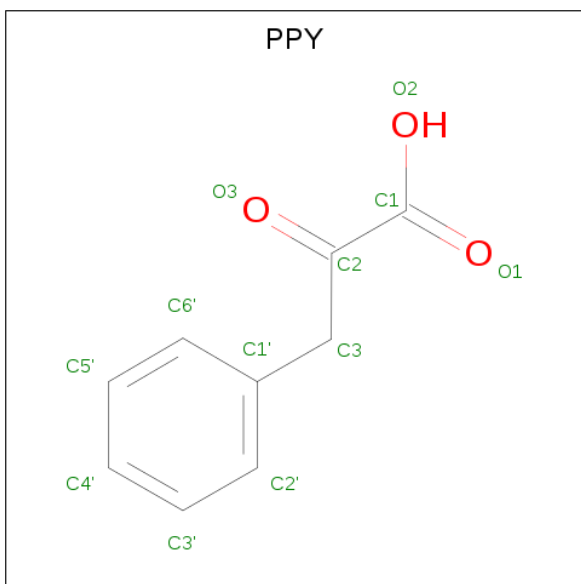
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Fe	H	N	O	0	0
			47	34	1	4	4	4		

- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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

- Molecule 4 is 3-PHENYLPYRUVIC ACID (three-letter code: PPY) (formula: $C_9H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			12	9	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			12	9	3		

- Molecule 5 is water.

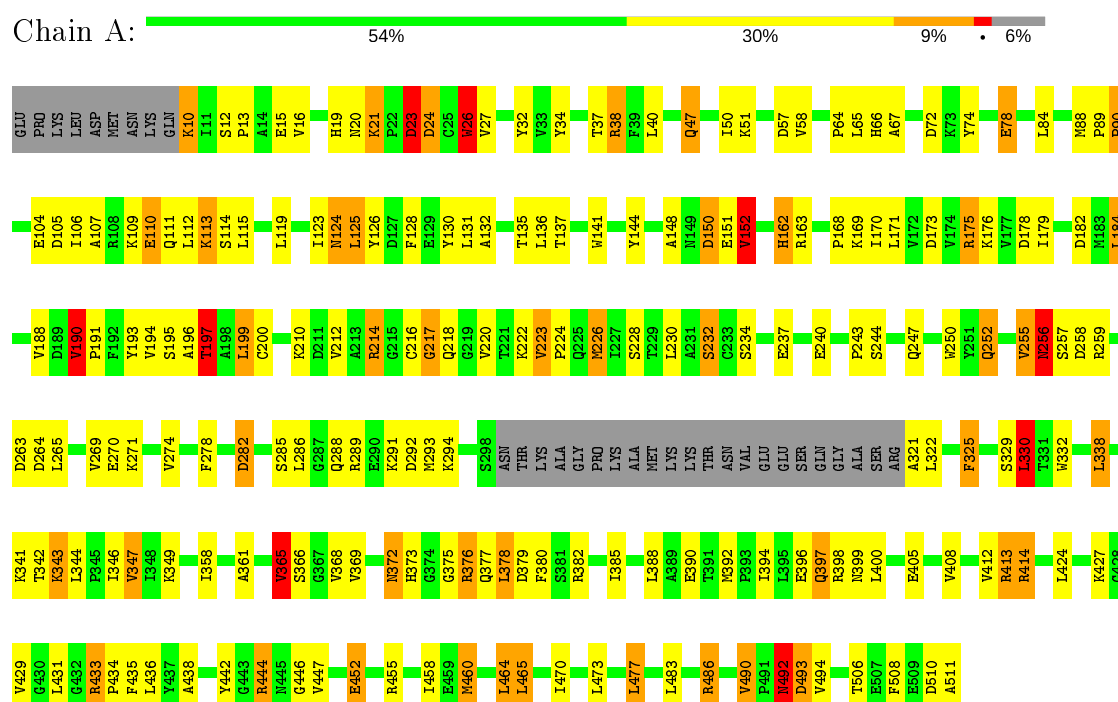
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	152	Total	H	O	0	0
			456	304	152		
5	B	13	Total	H	O	0	0
			39	26	13		

3 Residue-property plots

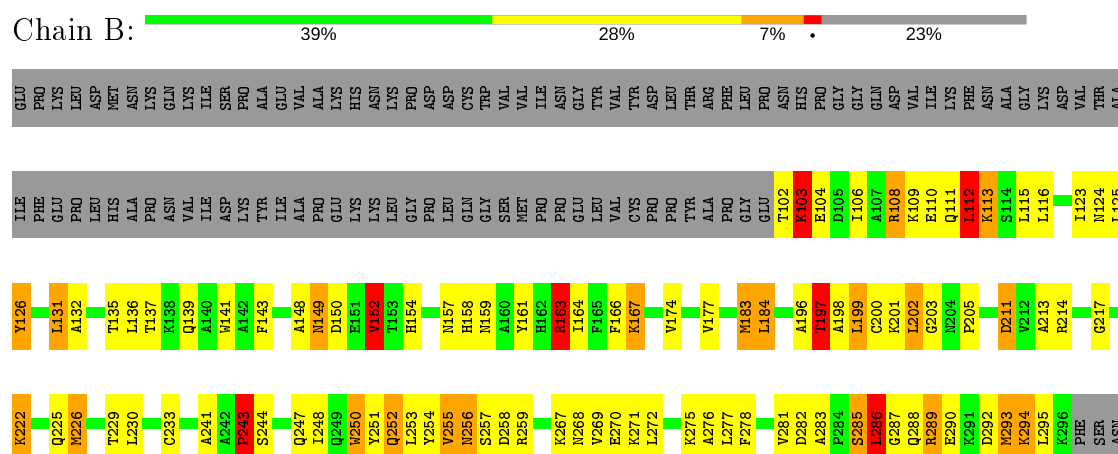
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

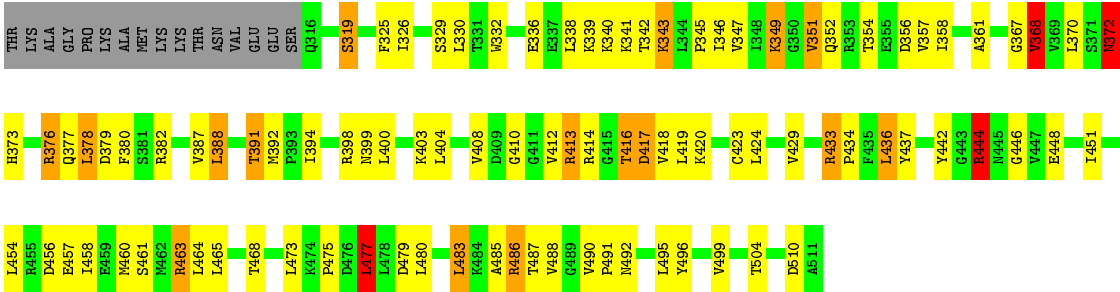
Note EDS was not executed.

• Molecule 1: L-LACTATE DEHYDROGENASE



• Molecule 1: L-LACTATE DEHYDROGENASE





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, α , β , γ	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}	0.13	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.186 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8915	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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, PPY

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	0.98	2/3810 (0.1%)	1.85	78/5161 (1.5%)
1	B	0.97	0/3093	1.86	71/4177 (1.7%)
All	All	0.98	2/6903 (0.0%)	1.86	149/9338 (1.6%)

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	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	413	ARG	CZ-NH1	5.40	1.40	1.33
1	A	382	ARG	CZ-NH1	5.07	1.39	1.33

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	414	ARG	NE-CZ-NH1	16.62	128.61	120.30
1	A	382	ARG	NE-CZ-NH2	-14.70	112.95	120.30
1	B	251	TYR	CB-CG-CD1	-13.46	112.93	121.00
1	B	289	ARG	NE-CZ-NH2	-13.10	113.75	120.30
1	A	492	ASN	CA-C-N	-12.82	89.00	117.20
1	A	413	ARG	NE-CZ-NH2	-11.39	114.61	120.30
1	B	163	ARG	NE-CZ-NH1	10.72	125.66	120.30
1	B	376	ARG	NE-CZ-NH1	10.61	125.61	120.30
1	A	379	ASP	CA-C-N	10.43	140.15	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	486	ARG	NE-CZ-NH1	10.30	125.45	120.30
1	B	376	ARG	NE-CZ-NH2	-10.15	115.22	120.30
1	A	226	MET	CG-SD-CE	-10.09	84.05	100.20
1	A	214	ARG	NE-CZ-NH1	10.02	125.31	120.30
1	A	414	ARG	NE-CZ-NH2	-9.64	115.48	120.30
1	A	193	TYR	CB-CG-CD2	9.46	126.67	121.00
1	B	382	ARG	NE-CZ-NH2	-9.29	115.65	120.30
1	A	193	TYR	CB-CG-CD1	-8.88	115.67	121.00
1	B	286	LEU	CA-CB-CG	8.74	135.41	115.30
1	B	382	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	B	259	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	B	379	ASP	CA-C-N	8.44	135.76	117.20
1	A	150	ASP	CA-CB-CG	8.42	131.93	113.40
1	B	496	TYR	CB-CG-CD2	-8.42	115.95	121.00
1	A	150	ASP	CB-CG-OD1	8.14	125.62	118.30
1	A	24	ASP	CA-C-N	-8.11	99.35	117.20
1	A	250	TRP	CD1-CG-CD2	7.82	112.56	106.30
1	B	444	ARG	NE-CZ-NH1	7.81	124.21	120.30
1	A	332	TRP	CD1-CG-CD2	7.67	112.43	106.30
1	A	379	ASP	CA-C-O	-7.67	104.00	120.10
1	B	226	MET	CG-SD-CE	-7.66	87.94	100.20
1	B	332	TRP	CD1-CG-CD2	7.62	112.40	106.30
1	A	141	TRP	CD1-CG-CD2	7.55	112.34	106.30
1	A	444	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	B	214	ARG	NE-CZ-NH1	7.49	124.04	120.30
1	B	141	TRP	CD1-CG-CD2	7.48	112.28	106.30
1	B	251	TYR	CB-CG-CD2	7.45	125.47	121.00
1	B	372	ASN	CB-CG-ND2	7.43	134.53	116.70
1	B	141	TRP	CE2-CD2-CG	-7.40	101.38	107.30
1	A	492	ASN	O-C-N	7.25	134.29	122.70
1	A	26	TRP	CD1-CG-CD2	7.23	112.09	106.30
1	B	141	TRP	CG-CD2-CE3	7.23	140.40	133.90
1	A	141	TRP	CE2-CD2-CG	-7.21	101.53	107.30
1	A	477	LEU	CA-CB-CG	7.13	131.71	115.30
1	A	332	TRP	CE2-CD2-CG	-7.01	101.69	107.30
1	A	465	LEU	CA-CB-CG	6.97	131.34	115.30
1	A	347	VAL	CG1-CB-CG2	-6.96	99.77	110.90
1	B	332	TRP	CE2-CD2-CG	-6.91	101.77	107.30
1	B	413	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	A	38	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	B	197	THR	N-CA-CB	-6.88	97.22	110.30
1	B	113	LYS	CA-C-N	-6.87	102.08	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	398	ARG	NE-CZ-NH2	-6.87	116.86	120.30
1	A	214	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	B	486	ARG	N-CA-C	-6.83	92.57	111.00
1	B	254	TYR	CA-C-N	6.81	132.18	117.20
1	B	496	TYR	CB-CG-CD1	6.79	125.08	121.00
1	A	188	VAL	CG1-CB-CG2	-6.79	100.03	110.90
1	B	444	ARG	CA-CB-CG	6.71	128.16	113.40
1	B	126	TYR	CB-CG-CD1	-6.60	117.04	121.00
1	A	190	VAL	N-CA-CB	-6.55	97.09	111.50
1	B	398	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	A	26	TRP	CE2-CD2-CG	-6.49	102.11	107.30
1	A	250	TRP	CE2-CD2-CG	-6.46	102.13	107.30
1	B	293	MET	CG-SD-CE	-6.43	89.92	100.20
1	A	433	ARG	NE-CZ-NH2	6.41	123.50	120.30
1	B	379	ASP	O-C-N	-6.38	112.49	122.70
1	B	141	TRP	CB-CG-CD1	-6.38	118.71	127.00
1	A	113	LYS	CA-C-N	-6.31	103.33	117.20
1	B	250	TRP	CD1-CG-CD2	6.30	111.34	106.30
1	B	289	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	B	183	MET	CG-SD-CE	-6.14	90.37	100.20
1	B	277	LEU	CA-CB-CG	6.10	129.32	115.30
1	A	110	GLU	CA-CB-CG	6.08	126.78	113.40
1	B	349	LYS	CG-CD-CE	-6.06	93.72	111.90
1	B	486	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	A	486	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	A	447	VAL	CG1-CB-CG2	-6.01	101.28	110.90
1	B	477	LEU	CA-CB-CG	6.01	129.11	115.30
1	A	289	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	B	463	ARG	N-CA-CB	-5.98	99.84	110.60
1	A	408	VAL	CG1-CB-CG2	-5.97	101.34	110.90
1	B	141	TRP	CG-CD1-NE1	-5.96	104.14	110.10
1	A	150	ASP	CB-CG-OD2	-5.94	112.95	118.30
1	A	223	VAL	N-CA-CB	-5.90	98.51	111.50
1	B	112	LEU	CA-CB-CG	5.88	128.82	115.30
1	B	487	THR	CA-C-N	5.86	130.09	117.20
1	B	410	GLY	CA-C-N	-5.85	104.50	116.20
1	A	141	TRP	CB-CG-CD1	-5.85	119.40	127.00
1	A	250	TRP	CG-CD1-NE1	-5.83	104.27	110.10
1	B	433	ARG	NE-CZ-NH2	5.79	123.19	120.30
1	A	382	ARG	NH1-CZ-NH2	5.74	125.71	119.40
1	A	74	TYR	CB-CG-CD2	-5.73	117.56	121.00
1	A	376	ARG	CD-NE-CZ	-5.73	115.58	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	ALA	CB-CA-C	-5.72	101.51	110.10
1	B	391	THR	OG1-CB-CG2	-5.71	96.86	110.00
1	A	38	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	A	264	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	B	243	PRO	CA-C-N	5.63	129.59	117.20
1	B	387	VAL	CG1-CB-CG2	-5.62	101.90	110.90
1	A	130	TYR	CB-CG-CD2	-5.62	117.63	121.00
1	A	78	GLU	CA-CB-CG	5.60	125.73	113.40
1	A	240	GLU	CA-CB-CG	5.59	125.71	113.40
1	B	341	LYS	CA-CB-CG	5.58	125.69	113.40
1	B	510	ASP	CA-C-N	-5.57	104.94	117.20
1	B	152	VAL	CA-C-N	5.57	129.45	117.20
1	A	282	ASP	CB-CG-OD1	5.57	123.31	118.30
1	A	126	TYR	CB-CG-CD1	-5.57	117.66	121.00
1	A	330	LEU	CA-CB-CG	5.55	128.06	115.30
1	B	444	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	B	483	LEU	CB-CG-CD1	-5.51	101.62	111.00
1	B	351	VAL	CA-CB-CG2	-5.51	102.63	110.90
1	A	325	PHE	CB-CG-CD2	-5.47	116.97	120.80
1	A	182	ASP	CB-CG-OD2	-5.46	113.38	118.30
1	B	377	GLN	CA-C-N	5.46	129.22	117.20
1	B	288	GLN	CA-CB-CG	5.46	125.41	113.40
1	B	250	TRP	CE2-CD2-CG	-5.43	102.96	107.30
1	A	217	GLY	O-C-N	-5.42	114.03	122.70
1	A	197	THR	N-CA-CB	-5.40	100.05	110.30
1	B	184	LEU	CA-CB-CG	5.33	127.57	115.30
1	B	154	HIS	CA-C-N	5.33	128.93	117.20
1	A	151	GLU	N-CA-C	5.32	125.37	111.00
1	A	47	GLN	CA-CB-CG	5.31	125.09	113.40
1	B	464	LEU	O-C-N	-5.31	114.20	122.70
1	A	397	GLN	CA-CB-CG	5.31	125.08	113.40
1	A	220	VAL	CA-CB-CG1	-5.29	102.96	110.90
1	B	159	ASN	CB-CG-ND2	5.28	129.38	116.70
1	A	176	LYS	N-CA-C	-5.27	96.77	111.00
1	A	256	ASN	CB-CG-ND2	5.25	129.31	116.70
1	A	378	LEU	CA-CB-CG	5.25	127.38	115.30
1	A	365	VAL	CG1-CB-CG2	5.20	119.21	110.90
1	A	493	ASP	N-CA-C	5.20	125.03	111.00
1	B	163	ARG	CA-CB-CG	5.18	124.80	113.40
1	A	124	ASN	CB-CG-ND2	5.18	129.12	116.70
1	A	382	ARG	CB-CG-CD	-5.15	98.22	111.60
1	A	141	TRP	CG-CD2-CE3	5.14	138.53	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	418	VAL	CG1-CB-CG2	-5.14	102.68	110.90
1	B	368	VAL	CA-CB-CG2	-5.13	103.20	110.90
1	A	34	TYR	CB-CG-CD2	-5.12	117.93	121.00
1	B	404	LEU	CB-CG-CD2	-5.09	102.34	111.00
1	A	396	GLU	CA-C-N	5.09	128.39	117.20
1	B	454	LEU	CB-CG-CD2	-5.07	102.38	111.00
1	A	433	ARG	NH1-CZ-NH2	-5.05	113.84	119.40
1	A	152	VAL	CA-C-N	5.04	128.29	117.20
1	B	108	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	B	352	GLN	O-C-N	-5.04	114.64	122.70
1	A	58	VAL	CG1-CB-CG2	5.02	118.93	110.90
1	A	398	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	B	417	ASP	CB-CG-OD1	5.01	122.81	118.30
1	A	130	TYR	CG-CD2-CE2	-5.00	117.30	121.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	150	ASP	Peptide
1	A	492	ASN	Mainchain

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	3736	811	3793	117	0
1	B	3045	687	3112	125	0
2	A	43	4	30	3	0
3	A	31	4	19	3	0
3	B	31	4	19	6	0
4	A	12	0	7	1	0
4	B	12	0	7	2	0
5	A	152	304	0	9	0
5	B	13	26	0	0	0
All	All	7075	1840	6987	230	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 17.

All (230) 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:B:143:PHE:HA	1:B:289:ARG:HH22	1.45	0.79
1:B:290:GLU:HA	1:B:293:MET:HG3	1.64	0.79
1:A:40:LEU:HG	1:A:47:GLN:HB2	1.67	0.76
1:B:197:THR:HG21	1:B:436:LEU:HG	1.67	0.75
1:A:291:LYS:HD2	5:A:754:HOH:O	1.87	0.73
1:A:465:LEU:HD23	1:B:378:LEU:HD11	1.72	0.72
1:B:351:VAL:HG11	1:B:357:VAL:HG23	1.72	0.71
1:B:199:LEU:HD11	4:B:580:PPY:H3'	1.73	0.70
1:B:108:ARG:O	1:B:112:LEU:HD23	1.92	0.70
1:A:431:LEU:HD23	1:A:434:PRO:HG2	1.73	0.69
1:B:163:ARG:NH2	1:B:486:ARG:HG3	2.08	0.68
1:A:13:PRO:HB2	5:A:764:HOH:O	1.94	0.67
1:A:16:VAL:HA	1:A:26:TRP:HE3	1.61	0.66
1:A:190:VAL:HG11	1:A:223:VAL:HG22	1.77	0.65
1:A:112:LEU:HG	1:A:135:THR:HB	1.78	0.65
1:B:197:THR:CG2	1:B:436:LEU:HG	2.27	0.64
1:B:269:VAL:HA	1:B:272:LEU:HD12	1.81	0.63
1:B:256:ASN:HD22	1:B:257:SER:N	1.95	0.63
1:A:361:ALA:HB1	1:A:400:LEU:HD22	1.81	0.63
1:A:132:ALA:HA	5:A:634:HOH:O	1.97	0.62
1:B:201:LYS:HE3	1:B:233:CYS:SG	2.40	0.61
1:B:461:SER:O	1:B:465:LEU:HD12	2.01	0.61
1:A:16:VAL:HA	1:A:26:TRP:CE3	2.35	0.61
1:B:157:ASN:HD21	1:B:372:ASN:HD21	1.48	0.61
1:B:388:LEU:HD22	1:B:392:MET:HG2	1.83	0.60
1:A:385:ILE:HD11	1:A:424:LEU:HD12	1.84	0.60
1:A:256:ASN:HD22	1:A:257:SER:N	2.00	0.60
1:B:143:PHE:HA	1:B:289:ARG:NH2	2.16	0.59
1:B:416:THR:O	1:B:420:LYS:HG3	2.02	0.59
1:B:442:TYR:HB2	1:B:446:GLY:HA3	1.84	0.59
3:A:570:FMN:O4'	3:A:570:FMN:H1'2	2.02	0.59
1:A:162:HIS:HE1	5:A:670:HOH:O	1.86	0.58
1:A:490:VAL:HG22	1:A:492:ASN:ND2	2.19	0.58
1:A:270:GLU:OE1	1:A:343:LYS:HG3	2.04	0.58
1:A:460:MET:HE3	1:B:286:LEU:O	2.03	0.58
1:A:508:PHE:CZ	1:B:131:LEU:HD12	2.39	0.58
1:A:218:GLN:NE2	1:A:444:ARG:HH11	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:TYR:O	1:A:433:ARG:HD3	2.04	0.57
1:B:217:GLY:HA3	1:B:247:GLN:NE2	2.20	0.57
1:B:124:ASN:HD22	1:B:126:TYR:H	1.53	0.57
1:B:400:LEU:HA	1:B:403:LYS:HD3	1.86	0.57
1:A:372:ASN:HD22	1:A:375:GLY:H	1.50	0.57
1:A:373:HIS:O	1:A:376:ARG:HG3	2.04	0.56
1:A:234:SER:OG	1:A:237:GLU:HG3	2.06	0.56
1:A:511:ALA:H	1:B:115:LEU:HD13	1.71	0.56
1:B:108:ARG:HG2	1:B:135:THR:O	2.06	0.55
1:B:256:ASN:HA	1:B:325:PHE:O	2.07	0.55
1:A:285:SER:HA	1:A:321:ALA:O	2.06	0.55
1:B:148:ALA:N	1:B:376:ARG:HA	2.21	0.55
1:B:354:THR:HA	1:B:391:THR:HG22	1.89	0.55
1:A:358:ILE:HD11	1:A:394:ILE:HG21	1.89	0.55
1:A:218:GLN:HE22	1:A:444:ARG:HH11	1.54	0.55
1:A:490:VAL:HG22	1:A:492:ASN:HD22	1.72	0.55
1:A:270:GLU:HB3	1:A:343:LYS:NZ	2.21	0.54
1:B:424:LEU:HD21	1:B:480:LEU:HD11	1.87	0.54
1:A:244:SER:O	1:A:247:GLN:HG2	2.07	0.54
1:B:152:VAL:HG21	1:B:380:PHE:CE2	2.43	0.54
1:A:152:VAL:HG21	1:A:380:PHE:CE2	2.43	0.53
1:A:173:ASP:OD1	1:B:329:SER:HA	2.08	0.53
1:B:347:VAL:HG13	1:B:367:GLY:C	2.29	0.53
1:A:168:PRO:HG3	1:B:378:LEU:HD12	1.90	0.53
1:A:40:LEU:HD11	1:A:51:LYS:HG3	1.90	0.53
1:B:211:ASP:O	1:B:444:ARG:HB3	2.08	0.53
1:A:460:MET:CE	1:B:285:SER:HB2	2.39	0.53
1:B:183:MET:CE	1:B:250:TRP:HH2	2.23	0.52
1:B:103:LYS:O	1:B:106:ILE:HG12	2.09	0.52
1:B:125:LEU:HG	1:B:434:PRO:HB3	1.92	0.52
2:A:560:HEM:HBD1	4:A:580:PPY:H4'	1.91	0.51
1:B:199:LEU:HB2	1:B:202:LEU:HD12	1.90	0.51
1:B:403:LYS:HD2	1:B:403:LYS:N	2.25	0.51
1:A:282:ASP:O	1:A:377:GLN:HG2	2.10	0.51
1:B:109:LYS:O	1:B:113:LYS:HB3	2.11	0.51
1:B:111:GLN:HB3	1:B:135:THR:HG22	1.93	0.51
1:B:276:ALA:HA	1:B:345:PRO:HD2	1.91	0.51
1:A:256:ASN:ND2	1:A:258:ASP:H	2.09	0.51
1:A:24:ASP:HA	1:A:37:THR:OG1	2.10	0.51
1:B:229:THR:OG1	1:B:253:LEU:HA	2.09	0.51
1:A:89:PRO:HD3	5:A:764:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:ARG:HG3	1:B:457:GLU:OE1	2.11	0.50
1:A:392:MET:HG3	1:A:424:LEU:O	2.12	0.49
1:A:125:LEU:HG	1:A:434:PRO:HB3	1.92	0.49
1:B:198:ALA:HB1	4:B:580:PPY:H2'	1.94	0.49
1:A:109:LYS:HA	1:A:112:LEU:HD12	1.93	0.49
1:A:170:ILE:HD11	1:B:282:ASP:HA	1.94	0.49
1:A:66:HIS:HA	2:A:560:HEM:O2A	2.13	0.49
1:A:197:THR:HG23	1:A:436:LEU:HD21	1.93	0.49
1:B:349:LYS:NZ	3:B:570:FMN:H2'	2.28	0.49
1:B:124:ASN:HD21	1:B:126:TYR:HB2	1.78	0.49
1:A:460:MET:HE2	1:B:285:SER:HB2	1.95	0.48
1:B:339:LYS:HA	1:B:346:ILE:HD11	1.95	0.48
1:B:354:THR:OG1	1:B:391:THR:HG22	2.12	0.48
1:B:357:VAL:HG22	1:B:368:VAL:HG11	1.95	0.48
1:A:196:ALA:HB1	1:A:228:SER:HB2	1.95	0.48
1:A:105:ASP:O	1:A:109:LYS:HG3	2.13	0.48
1:A:110:GLU:HA	1:A:113:LYS:HG3	1.96	0.48
1:A:196:ALA:HB2	1:A:226:MET:HE2	1.95	0.48
3:A:570:FMN:H1'2	3:A:570:FMN:H9	1.64	0.48
1:A:442:TYR:HB2	1:A:446:GLY:HA3	1.96	0.48
1:B:136:LEU:HD23	1:B:136:LEU:N	2.29	0.48
3:B:570:FMN:O4'	3:B:570:FMN:H9	2.14	0.48
1:B:166:PHE:CE2	1:B:416:THR:HG22	2.48	0.48
1:B:358:ILE:HD11	1:B:394:ILE:CG2	2.44	0.48
1:A:179:ILE:HD11	1:A:455:ARG:HG2	1.96	0.47
1:A:412:VAL:HG21	1:A:429:VAL:CG1	2.44	0.47
1:A:175:ARG:HH11	1:A:175:ARG:HB2	1.79	0.47
1:A:57:ASP:HB2	1:A:88:MET:HG3	1.96	0.47
1:A:113:LYS:O	1:A:115:LEU:N	2.45	0.47
1:A:197:THR:CG2	1:A:436:LEU:HD21	2.45	0.47
1:B:149:ASN:HB3	1:B:290:GLU:OE2	2.14	0.47
1:A:163:ARG:NH1	1:A:486:ARG:HA	2.29	0.47
1:A:460:MET:C	1:A:460:MET:SD	2.92	0.47
1:A:252:GLN:HA	1:A:278:PHE:O	2.14	0.47
1:B:213:ALA:CA	1:B:225:GLN:HE22	2.28	0.47
1:B:423:CYS:O	1:B:475:PRO:HG3	2.15	0.47
1:A:508:PHE:CE1	1:B:131:LEU:HD12	2.50	0.47
1:B:164:ILE:HB	1:B:420:LYS:HD3	1.97	0.47
1:A:508:PHE:CE2	1:B:116:LEU:HD23	2.50	0.46
1:B:124:ASN:HD22	1:B:126:TYR:N	2.13	0.46
1:B:256:ASN:HD22	1:B:257:SER:H	1.60	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:ALA:H	1:A:226:MET:HE1	1.80	0.46
1:A:452:GLU:HG3	1:A:455:ARG:NH2	2.31	0.46
1:B:278:PHE:HA	1:B:347:VAL:O	2.15	0.46
1:A:16:VAL:HG21	1:A:84:LEU:HD12	1.98	0.46
1:A:214:ARG:HA	1:A:243:PRO:HD3	1.97	0.46
1:A:171:LEU:HD21	1:B:281:VAL:HG11	1.97	0.46
1:A:107:ALA:HA	1:A:110:GLU:HG3	1.98	0.46
1:A:184:LEU:HD21	1:A:347:VAL:HG21	1.98	0.46
1:B:177:VAL:HG23	1:B:468:THR:HA	1.98	0.46
1:B:283:ALA:O	1:B:326:ILE:HG21	2.16	0.46
1:A:199:LEU:HD21	2:A:560:HEM:HAA2	1.97	0.45
1:B:109:LYS:NZ	1:B:112:LEU:HD11	2.31	0.45
1:B:252:GLN:HA	1:B:278:PHE:O	2.15	0.45
1:A:470:ILE:HA	1:A:473:LEU:HD12	1.96	0.45
1:A:288:GLN:HG3	1:A:293:MET:SD	2.57	0.45
1:A:270:GLU:HG2	1:A:344:LEU:HG	1.98	0.45
1:B:149:ASN:O	1:B:150:ASP:HB2	2.17	0.45
1:B:358:ILE:HD11	1:B:394:ILE:HG22	1.98	0.45
1:B:412:VAL:HG13	1:B:417:ASP:HB2	1.98	0.45
1:A:413:ARG:HD3	1:A:413:ARG:HA	1.84	0.45
1:B:166:PHE:HE2	1:B:416:THR:HG22	1.82	0.45
1:B:256:ASN:ND2	1:B:258:ASP:H	2.15	0.45
1:A:338:LEU:HD13	1:A:346:ILE:HD12	1.99	0.45
1:A:342:THR:HG21	1:A:346:ILE:HD11	1.98	0.45
1:A:508:PHE:HE2	1:B:116:LEU:HD23	1.82	0.45
1:A:67:ALA:HA	1:A:232:SER:O	2.17	0.45
1:B:109:LYS:HZ1	1:B:112:LEU:HD11	1.81	0.45
1:B:255:VAL:HG13	1:B:330:LEU:HD11	1.99	0.45
3:B:570:FMN:O4'	3:B:570:FMN:H1'2	2.17	0.45
1:A:10:LYS:HB3	5:A:761:HOH:O	2.17	0.45
1:A:107:ALA:O	1:A:110:GLU:HG3	2.17	0.45
1:A:255:VAL:HG11	1:A:330:LEU:HD21	1.99	0.45
1:B:256:ASN:HD22	1:B:258:ASP:H	1.64	0.45
1:B:419:LEU:HD21	1:B:458:ILE:HG23	1.98	0.45
1:B:361:ALA:CB	1:B:400:LEU:HD13	2.48	0.44
1:B:448:GLU:O	1:B:451:ILE:HB	2.17	0.44
1:B:495:LEU:O	1:B:499:VAL:HG22	2.18	0.44
1:A:21:LYS:HB3	1:A:23:ASP:O	2.18	0.44
1:A:286:LEU:HA	1:A:377:GLN:HE22	1.82	0.44
1:A:510:ASP:N	1:B:115:LEU:HD22	2.33	0.44
1:B:183:MET:HE1	1:B:250:TRP:HH2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:ALA:O	1:B:243:PRO:HD3	2.18	0.44
1:A:349:LYS:NZ	3:A:570:FMN:H2'	2.33	0.44
1:A:216:CYS:O	1:A:222:LYS:HA	2.18	0.44
1:A:349:LYS:HA	1:A:369:VAL:HB	2.00	0.44
1:B:330:LEU:HD23	1:B:330:LEU:HA	1.77	0.44
1:B:270:GLU:OE2	1:B:343:LYS:HB3	2.18	0.44
1:B:163:ARG:HD2	1:B:485:ALA:O	2.17	0.44
1:B:108:ARG:NH2	1:B:137:THR:HA	2.33	0.44
1:B:158:HIS:O	1:B:161:TYR:HB2	2.18	0.44
1:B:413:ARG:HH22	3:B:570:FMN:P	2.41	0.43
1:A:217:GLY:O	1:A:222:LYS:NZ	2.50	0.43
1:B:456:ASP:O	1:B:460:MET:HG3	2.18	0.43
3:B:570:FMN:H9	3:B:570:FMN:H1'2	1.55	0.43
1:A:123:ILE:HD12	1:B:294:LYS:HG2	2.00	0.43
1:B:166:PHE:HE2	1:B:416:THR:CG2	2.32	0.43
1:B:213:ALA:HA	1:B:225:GLN:HE22	1.83	0.43
1:B:203:GLY:O	1:B:205:PRO:HD3	2.18	0.43
1:B:199:LEU:HD23	1:B:230:LEU:O	2.19	0.43
1:B:400:LEU:O	1:B:403:LYS:HB2	2.19	0.43
1:B:106:ILE:O	1:B:110:GLU:HG2	2.17	0.43
1:B:388:LEU:HD22	1:B:392:MET:CG	2.49	0.43
1:A:136:LEU:N	5:A:634:HOH:O	2.52	0.43
1:B:148:ALA:H	1:B:376:ARG:HA	1.83	0.43
1:B:213:ALA:HA	1:B:225:GLN:NE2	2.34	0.43
1:B:174:VAL:O	1:B:463:ARG:HD3	2.17	0.43
1:B:465:LEU:HD23	1:B:477:LEU:HG	2.00	0.42
1:A:12:SER:HA	1:A:13:PRO:HD2	1.79	0.42
1:B:132:ALA:HB2	1:B:437:TYR:HB3	2.01	0.42
1:B:278:PHE:CD2	1:B:347:VAL:HB	2.54	0.42
1:B:108:ARG:HH21	1:B:137:THR:HA	1.83	0.42
1:B:268:ASN:O	1:B:271:LYS:HB3	2.20	0.42
1:B:433:ARG:HB3	1:B:437:TYR:CE2	2.54	0.42
1:A:270:GLU:HB3	1:A:343:LYS:HZ1	1.85	0.42
1:A:414:ARG:NH2	1:B:290:GLU:OE2	2.53	0.42
1:B:351:VAL:HG13	1:B:356:ASP:HB2	2.02	0.42
1:A:405:GLU:OE1	1:A:427:LYS:HG2	2.20	0.42
1:B:286:LEU:HD13	1:B:287:GLY:O	2.20	0.42
1:A:194:VAL:HG22	1:A:435:PHE:CD2	2.55	0.42
1:A:210:LYS:HE3	1:A:210:LYS:HB2	1.78	0.42
1:B:222:LYS:N	1:B:222:LYS:HD2	2.35	0.41
1:A:163:ARG:NH1	1:B:488:VAL:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:GLU:HB2	5:A:739:HOH:O	2.19	0.41
1:A:458:ILE:HD13	1:A:458:ILE:HG21	1.82	0.41
1:B:102:THR:HB	1:B:104:GLU:OE2	2.20	0.41
1:B:111:GLN:CB	1:B:135:THR:HG22	2.50	0.41
1:A:197:THR:HG22	1:A:200:CYS:SG	2.60	0.41
1:A:322:LEU:HB2	5:A:730:HOH:O	2.19	0.41
1:A:226:MET:HE1	1:A:349:LYS:HE3	2.03	0.41
1:A:269:VAL:O	1:A:274:VAL:HG22	2.21	0.41
1:A:144:TYR:CD1	1:A:436:LEU:HD13	2.56	0.41
1:A:128:PHE:CD1	1:A:438:ALA:HA	2.55	0.41
1:B:290:GLU:HA	1:B:293:MET:CG	2.43	0.41
1:B:336:GLU:O	1:B:339:LYS:HB2	2.21	0.41
1:A:294:LYS:HB2	1:A:294:LYS:NZ	2.36	0.41
1:B:196:ALA:HB2	1:B:226:MET:HE3	2.02	0.41
1:A:113:LYS:C	1:A:115:LEU:H	2.24	0.41
1:A:24:ASP:H	1:A:37:THR:HG23	1.86	0.41
1:A:372:ASN:ND2	1:A:375:GLY:H	2.19	0.41
1:A:40:LEU:HD12	1:A:50:ILE:HB	2.03	0.41
1:B:167:LYS:HD2	1:B:479:ASP:HB2	2.03	0.41
1:A:106:ILE:HA	1:A:106:ILE:HD13	1.93	0.40
1:A:223:VAL:HA	1:A:224:PRO:HD3	2.01	0.40
1:A:256:ASN:HD22	1:A:258:ASP:H	1.67	0.40
1:A:460:MET:HE1	1:B:285:SER:HB2	2.03	0.40
1:A:346:ILE:HB	1:A:365:VAL:HG22	2.03	0.40
1:B:123:ILE:HD13	1:B:123:ILE:HG21	1.81	0.40
1:A:13:PRO:O	1:A:16:VAL:HB	2.22	0.40
1:B:473:LEU:HD23	1:B:473:LEU:HA	1.89	0.40
1:A:465:LEU:CD1	1:A:477:LEU:HG	2.52	0.40
1:B:413:ARG:NH2	3:B:570:FMN:O1P	2.52	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	476/511 (93%)	428 (90%)	39 (8%)	9 (2%)	8	28
1	B	387/511 (76%)	348 (90%)	33 (8%)	6 (2%)	9	32
All	All	863/1022 (84%)	776 (90%)	72 (8%)	15 (2%)	9	31

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	149	ASN
1	A	104	GLU
1	A	114	SER
1	A	119	LEU
1	A	493	ASP
1	B	319	SER
1	B	103	LYS
1	A	65	LEU
1	A	90	PRO
1	A	199	LEU
1	B	340	LYS
1	A	23	ASP
1	A	464	LEU
1	B	399	ASN
1	B	200	CYS

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	412/440 (94%)	350 (85%)	62 (15%)	3	9
1	B	336/440 (76%)	289 (86%)	47 (14%)	3	10
All	All	748/880 (85%)	639 (85%)	109 (15%)	3	9

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LYS

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Mol	Chain	Res	Type
1	A	15	GLU
1	A	19	HIS
1	A	20	ASN
1	A	21	LYS
1	A	23	ASP
1	A	26	TRP
1	A	27	VAL
1	A	32	TYR
1	A	38	ARG
1	A	64	PRO
1	A	72	ASP
1	A	78	GLU
1	A	90	PRO
1	A	111	GLN
1	A	124	ASN
1	A	125	LEU
1	A	131	LEU
1	A	137	THR
1	A	152	VAL
1	A	162	HIS
1	A	169	LYS
1	A	175	ARG
1	A	178	ASP
1	A	184	LEU
1	A	190	VAL
1	A	191	PRO
1	A	195	SER
1	A	197	THR
1	A	212	VAL
1	A	230	LEU
1	A	232	SER
1	A	252	GLN
1	A	255	VAL
1	A	256	ASN
1	A	259	ARG
1	A	263	ASP
1	A	265	LEU
1	A	271	LYS
1	A	292	ASP
1	A	325	PHE
1	A	329	SER
1	A	330	LEU

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Mol	Chain	Res	Type
1	A	338	LEU
1	A	341	LYS
1	A	343	LYS
1	A	365	VAL
1	A	366	SER
1	A	368	VAL
1	A	372	ASN
1	A	378	LEU
1	A	388	LEU
1	A	397	GLN
1	A	399	ASN
1	A	452	GLU
1	A	460	MET
1	A	464	LEU
1	A	483	LEU
1	A	490	VAL
1	A	492	ASN
1	A	494	VAL
1	A	506	THR
1	B	103	LYS
1	B	112	LEU
1	B	131	LEU
1	B	139	GLN
1	B	152	VAL
1	B	163	ARG
1	B	167	LYS
1	B	184	LEU
1	B	197	THR
1	B	199	LEU
1	B	202	LEU
1	B	211	ASP
1	B	222	LYS
1	B	243	PRO
1	B	244	SER
1	B	248	ILE
1	B	252	GLN
1	B	255	VAL
1	B	256	ASN
1	B	267	LYS
1	B	275	LYS
1	B	285	SER
1	B	286	LEU

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Mol	Chain	Res	Type
1	B	292	ASP
1	B	294	LYS
1	B	295	LEU
1	B	319	SER
1	B	338	LEU
1	B	342	THR
1	B	343	LYS
1	B	368	VAL
1	B	370	LEU
1	B	372	ASN
1	B	373	HIS
1	B	378	LEU
1	B	388	LEU
1	B	408	VAL
1	B	416	THR
1	B	429	VAL
1	B	436	LEU
1	B	444	ARG
1	B	477	LEU
1	B	483	LEU
1	B	490	VAL
1	B	491	PRO
1	B	492	ASN
1	B	504	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	85	GLN
1	A	124	ASN
1	A	157	ASN
1	A	162	HIS
1	A	218	GLN
1	A	252	GLN
1	A	256	ASN
1	A	372	ASN
1	A	377	GLN
1	A	439	ASN
1	A	492	ASN
1	A	497	ASN
1	B	124	ASN

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Mol	Chain	Res	Type
1	B	218	GLN
1	B	225	GLN
1	B	247	GLN
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
2	HEM	A	560	1	27,50,50	1.77	6 (22%)	17,82,82	1.58	4 (23%)
3	FMN	B	570	-	31,33,33	2.94	9 (29%)	40,50,50	3.23	16 (40%)
4	PPY	B	580	-	9,12,12	1.63	1 (11%)	10,15,15	0.73	0
3	FMN	A	570	-	31,33,33	3.18	6 (19%)	40,50,50	3.40	22 (55%)
4	PPY	A	580	-	9,12,12	1.42	2 (22%)	10,15,15	1.58	2 (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
2	HEM	A	560	1	-	3/6/54/54	-
3	FMN	B	570	-	2/2/4/4	9/18/18/18	0/3/3/3
4	PPY	B	580	-	-	0/4/8/8	0/1/1/1
3	FMN	A	570	-	2/2/4/4	13/18/18/18	0/3/3/3
4	PPY	A	580	-	-	0/4/8/8	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	570	FMN	C1'-N10	-14.63	1.33	1.48
3	B	570	FMN	C1'-N10	-13.09	1.34	1.48
3	A	570	FMN	C10-N1	4.89	1.39	1.33
3	A	570	FMN	C2'-C3'	-4.78	1.44	1.53
3	B	570	FMN	C10-N1	4.44	1.39	1.33
2	A	560	HEM	C3C-CAC	-4.40	1.38	1.47
4	B	580	PPY	C3-C2	4.36	1.55	1.51
3	A	570	FMN	C6-C5A	-4.29	1.35	1.41
2	A	560	HEM	C3C-C2C	-3.69	1.35	1.40
2	A	560	HEM	C3B-CAB	-3.63	1.40	1.47
3	B	570	FMN	C2'-C3'	-3.56	1.46	1.53
3	B	570	FMN	C6-C5A	-3.52	1.36	1.41
4	A	580	PPY	C3-C2	3.49	1.55	1.51
2	A	560	HEM	C3B-C2B	-2.81	1.36	1.40
2	A	560	HEM	CBB-CAB	2.73	1.47	1.29
3	B	570	FMN	C4A-N5	2.69	1.37	1.33
3	B	570	FMN	C9-C9A	-2.68	1.35	1.40
3	B	570	FMN	C4-N3	2.67	1.37	1.33
2	A	560	HEM	CBC-CAC	2.45	1.45	1.29
3	B	570	FMN	C4-C4A	2.33	1.45	1.41
4	A	580	PPY	O3-C2	2.33	1.26	1.22
3	B	570	FMN	C9A-C5A	-2.32	1.37	1.42
3	A	570	FMN	C4-C4A	2.15	1.45	1.41
3	A	570	FMN	C9A-C5A	-2.13	1.38	1.42

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	570	FMN	C4-N3-C2	11.00	124.43	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	570	FMN	C4-N3-C2	9.96	123.55	115.14
3	A	570	FMN	C4-C4A-C10	7.72	125.06	119.95
3	B	570	FMN	C4A-C4-N3	-6.73	114.22	123.43
3	A	570	FMN	C4A-C4-N3	-5.94	115.31	123.43
3	B	570	FMN	C4-C4A-C10	5.93	123.87	119.95
3	B	570	FMN	C5A-C9A-N10	5.91	122.00	117.72
3	A	570	FMN	O4'-C4'-C5'	5.54	122.38	109.92
3	A	570	FMN	P-O5'-C5'	5.43	133.25	118.30
3	A	570	FMN	O2'-C2'-C1'	5.15	121.99	109.59
3	A	570	FMN	C4-C4A-N5	-4.90	112.99	118.60
3	B	570	FMN	C1'-N10-C10	4.49	122.43	118.41
3	B	570	FMN	C9A-N10-C10	-4.42	116.12	121.91
3	B	570	FMN	O2'-C2'-C1'	4.37	120.12	109.59
3	B	570	FMN	C4'-C3'-C2'	4.26	122.22	113.36
3	A	570	FMN	C9A-N10-C10	-4.05	116.61	121.91
3	A	570	FMN	O4'-C4'-C3'	4.02	118.89	109.10
3	B	570	FMN	C4-C4A-N5	-3.94	114.09	118.60
3	B	570	FMN	C1'-N10-C9A	3.92	121.38	118.29
4	A	580	PPY	C1'-C3-C2	-3.81	105.99	114.52
3	A	570	FMN	C7M-C7-C6	-3.73	111.41	120.34
3	A	570	FMN	C6-C5A-N5	-3.72	114.95	119.05
3	A	570	FMN	C1'-N10-C10	3.59	121.62	118.41
3	A	570	FMN	C7M-C7-C8	3.29	127.48	120.74
3	A	570	FMN	C5A-C9A-N10	3.21	120.05	117.72
3	B	570	FMN	C8M-C8-C7	2.99	126.87	120.74
3	B	570	FMN	C8M-C8-C9	-2.93	113.34	120.34
3	B	570	FMN	O4'-C4'-C3'	2.82	115.95	109.10
3	B	570	FMN	O5'-C5'-C4'	2.71	116.59	109.36
2	A	560	HEM	CAA-CBA-CGA	2.70	117.19	112.67
3	A	570	FMN	C8M-C8-C7	2.64	126.15	120.74
3	A	570	FMN	O3'-C3'-C4'	2.54	114.95	108.81
3	A	570	FMN	O3P-P-O5'	-2.47	100.16	106.73
3	B	570	FMN	O3P-P-O2P	2.37	116.70	107.64
2	A	560	HEM	CBA-CAA-C2A	2.36	116.84	112.49
3	B	570	FMN	O3P-P-O5'	-2.35	100.48	106.73
3	A	570	FMN	O3P-P-O2P	2.32	116.51	107.64
3	A	570	FMN	C4'-C3'-C2'	2.26	118.06	113.36
3	A	570	FMN	C8M-C8-C9	-2.21	115.05	120.34
2	A	560	HEM	C3B-C4B-NB	2.20	112.06	109.21
3	A	570	FMN	C1'-N10-C9A	2.15	119.98	118.29
4	A	580	PPY	O3-C2-C3	-2.08	117.46	120.75
2	A	560	HEM	CMD-C2D-C1D	-2.06	125.29	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	570	FMN	C6-C5A-C9A	2.03	121.71	119.05

All (4) chirality outliers are listed below:

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

All (25) torsion outliers are listed below:

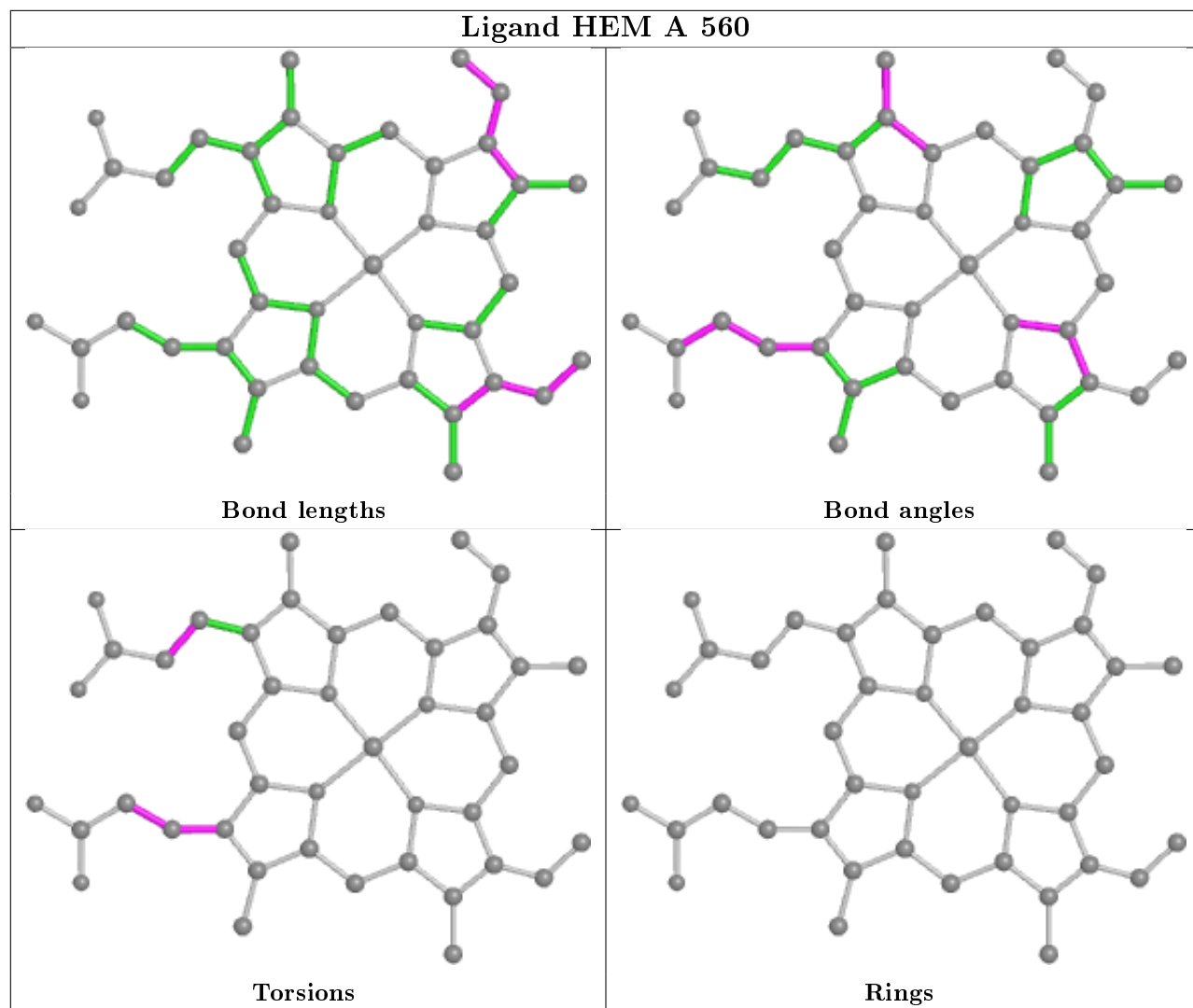
Mol	Chain	Res	Type	Atoms
2	A	560	HEM	C3A-C2A-CAA-CBA
3	B	570	FMN	C2'-C1'-N10-C9A
3	B	570	FMN	C2'-C1'-N10-C10
3	B	570	FMN	N10-C1'-C2'-O2'
3	B	570	FMN	C3'-C4'-C5'-O5'
3	B	570	FMN	O4'-C4'-C5'-O5'
3	A	570	FMN	C2'-C1'-N10-C9A
3	A	570	FMN	N10-C1'-C2'-O2'
3	A	570	FMN	C1'-C2'-C3'-O3'
3	A	570	FMN	O2'-C2'-C3'-O3'
3	A	570	FMN	C2'-C3'-C4'-O4'
3	A	570	FMN	O3'-C3'-C4'-O4'
3	A	570	FMN	O3'-C3'-C4'-C5'
3	A	570	FMN	O4'-C4'-C5'-O5'
3	A	570	FMN	C5'-O5'-P-O2P
3	A	570	FMN	C5'-O5'-P-O3P
3	B	570	FMN	O3'-C3'-C4'-O4'
3	B	570	FMN	C2'-C3'-C4'-O4'
3	A	570	FMN	C5'-O5'-P-O1P
3	B	570	FMN	C4'-C5'-O5'-P
3	A	570	FMN	C4'-C5'-O5'-P
3	A	570	FMN	O2'-C2'-C3'-C4'
2	A	560	HEM	C3D-CAD-CBD-CGD
3	B	570	FMN	O3'-C3'-C4'-C5'
2	A	560	HEM	C2A-CAA-CBA-CGA

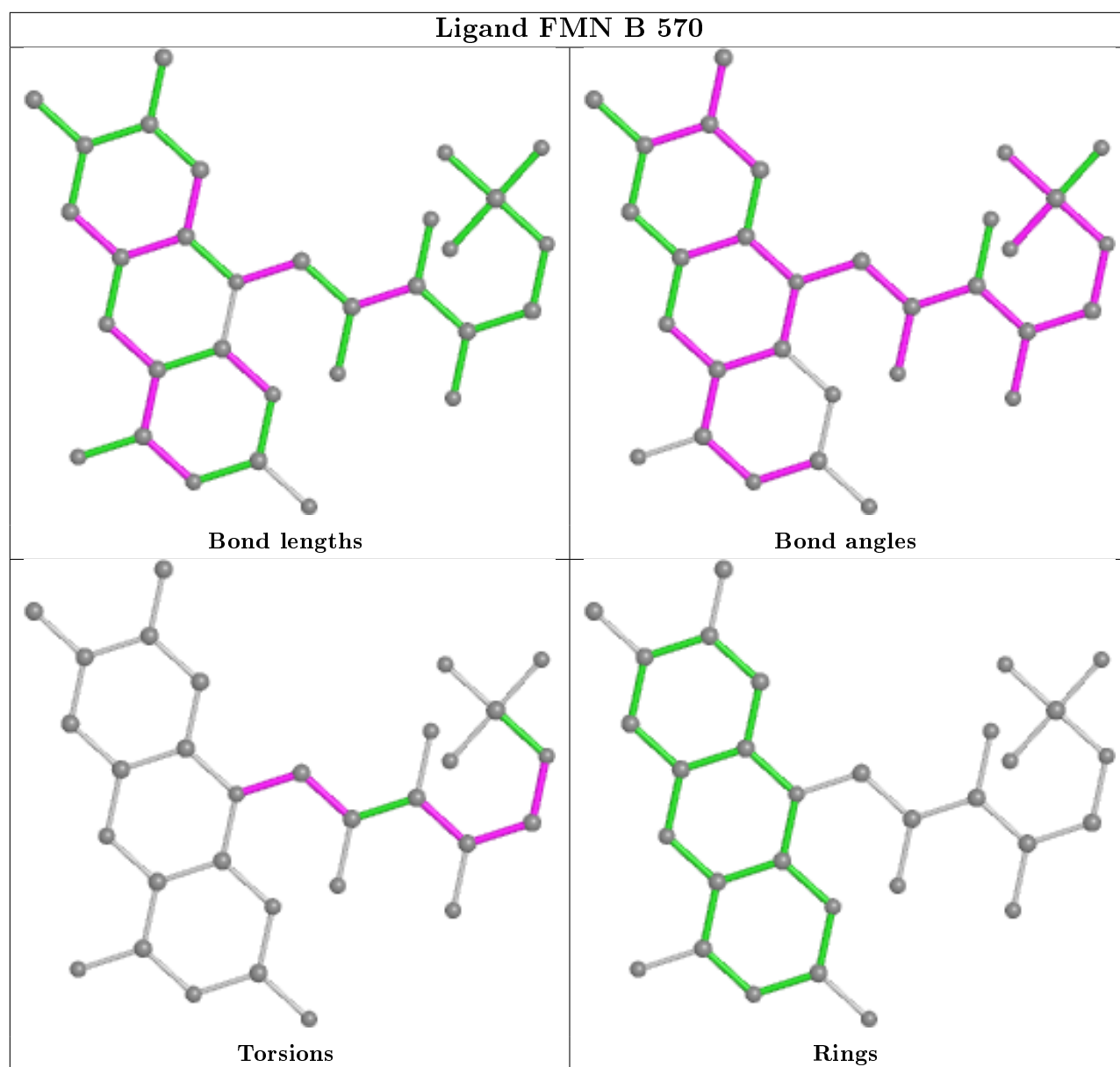
There are no ring outliers.

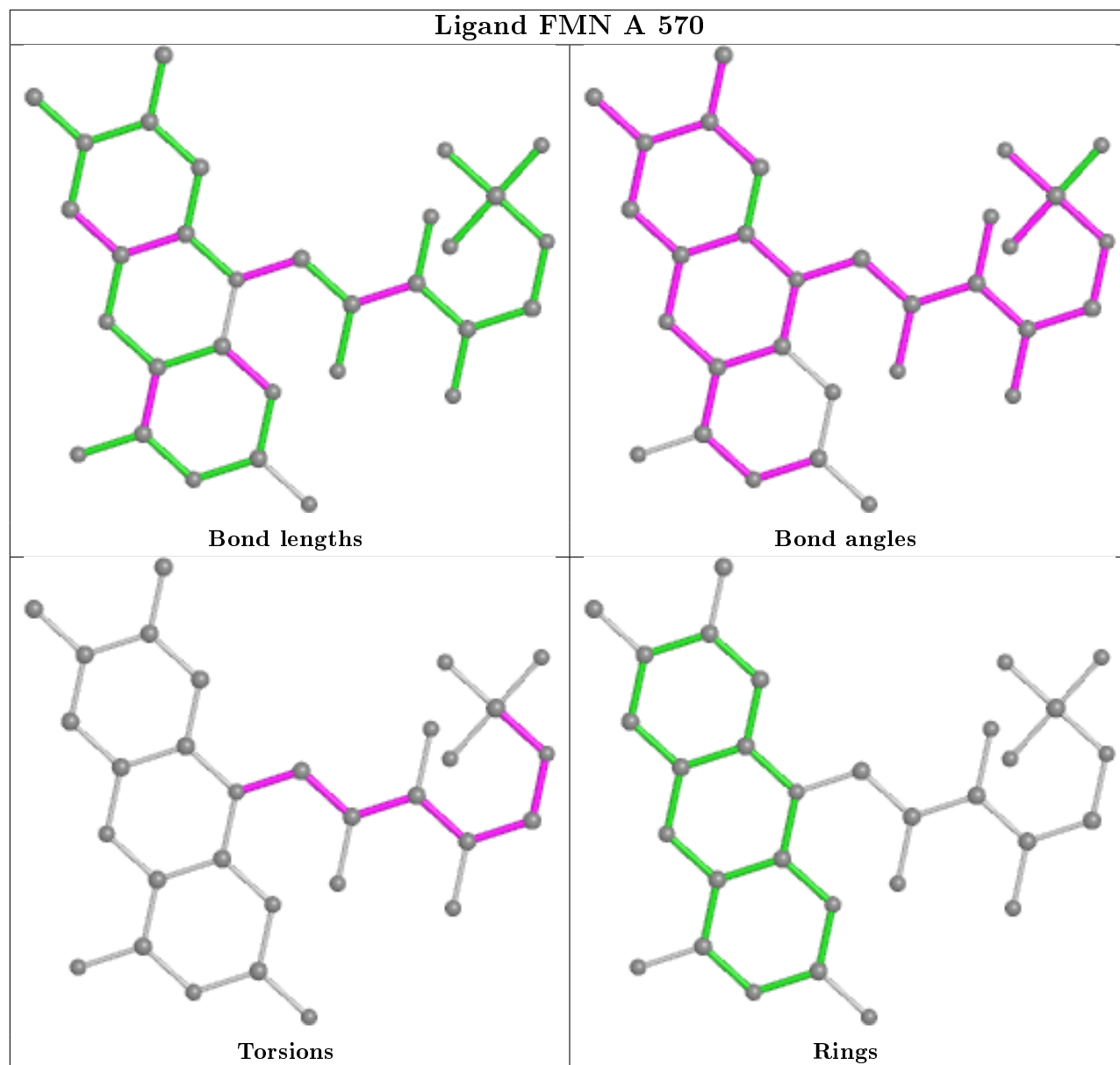
5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	560	HEM	3	0
3	B	570	FMN	6	0
4	B	580	PPY	2	0
3	A	570	FMN	3	0
4	A	580	PPY	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.