



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 17, 2018 – 11:53 am GMT

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 : 1.7.3 (157068), CSD as539be (2018)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30686

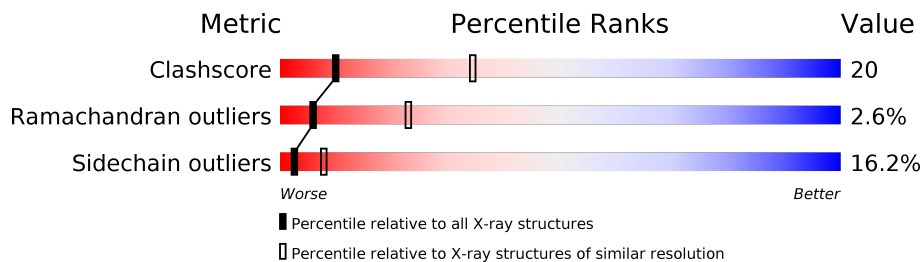
# 1 Overall quality at a glance

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	122078	1924 (2.90-2.90)
Ramachandran outliers	120005	1884 (2.90-2.90)
Sidechain outliers	119972	1886 (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. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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	-	-	-
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.

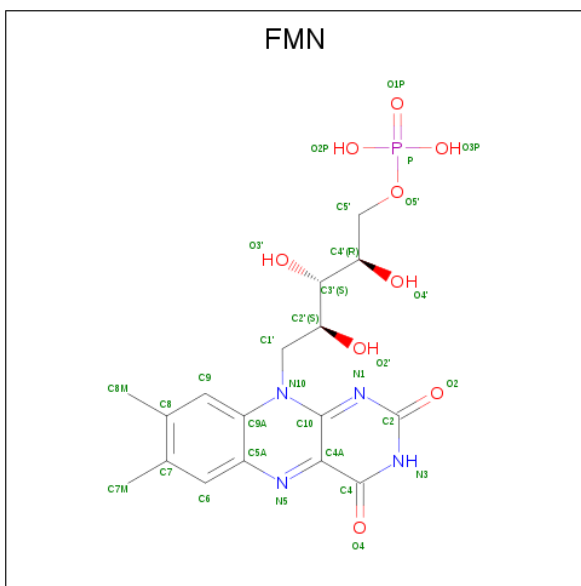
- Molecule 1 is a protein called L-LACTATE DEHYDROGENASE.

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

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).



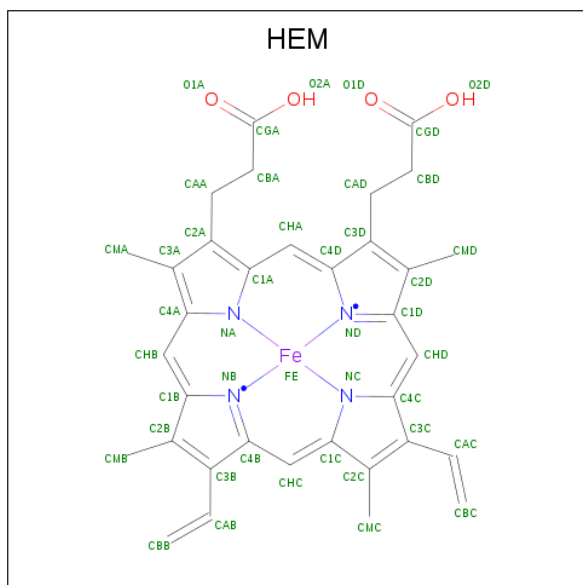
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
2	A	1	35	17	4	4	9	1	0	0

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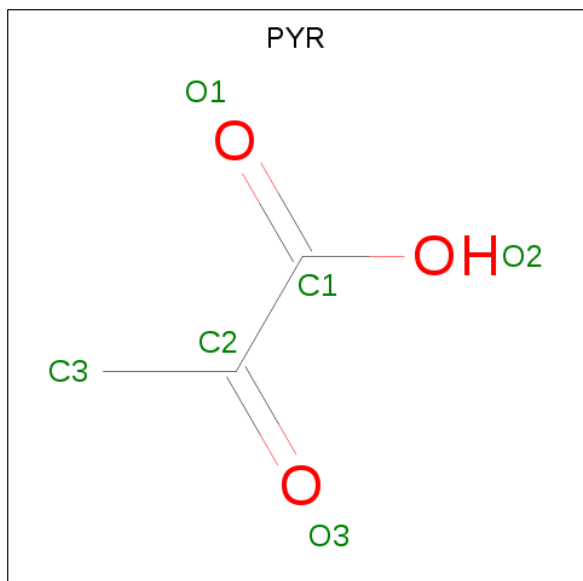
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			P
2	B	1	35	17	4	4	9	1	0	0

- 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	
			Total	C	Fe	H	N			O
3	A	1	47	34	1	4	4	4	0	0

- Molecule 4 is PYRUVIC ACID (three-letter code: PYR) (formula:  $C_3H_4O_3$ ).



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.

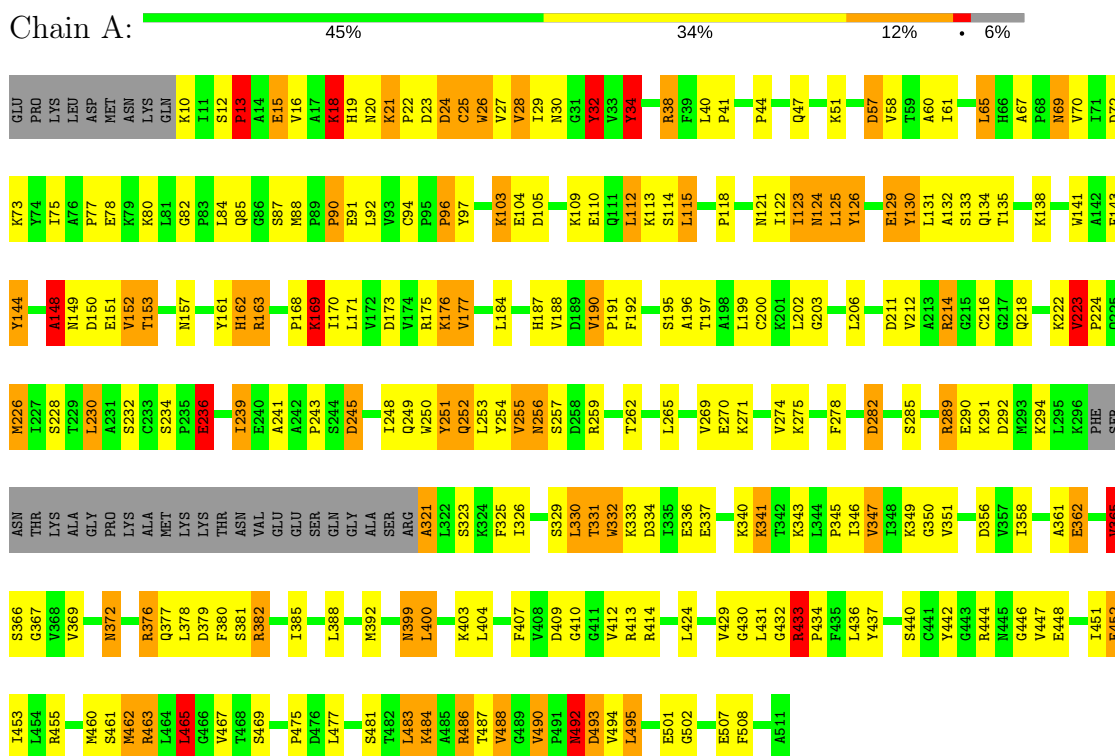
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	130	Total	H	O	0	0
			386	256	130		
5	B	11	Total	H	O	0	0
			33	22	11		

### 3 Residue-property plots

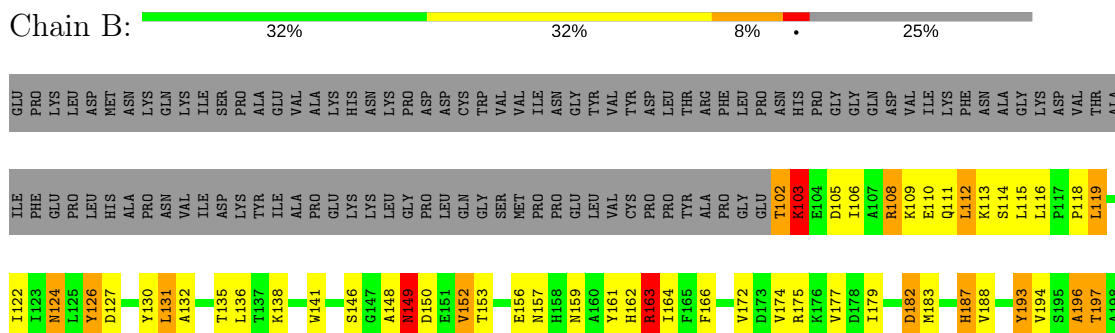
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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



L199	A276	K341	V412	L483
C200	L277	T342	R413	R486
K201	F278	K343	R414	T487
L202	V279	L344	G415	V488
G203	D282	P345	T416	G489
P205	A283	D417	D418	V490
L206	L286	V347	V418	F491
K210	G287	L348	L419	D492
D211	Q288	K349	K420	D493
V212	R289	A421	A421	V494
A213	E290	V351	V429	Y600
R214	M293	T354	G430	Y600
G215	K294	V357	L431	P603
G217	C216	L358	F435	T504
K222	L295	A361	L436	E507
V223	K296	G364	Y437	F508
P224	PHE	V365	A438	E509
Q225	SER	S366	M439	D610
L226	ASN	G367	S440	A511
T229	THR	Y442	C441	
L230	LYS	G443	Y442	
C233	ALA	R444	G443	
E236	GLY	V369	R444	
E237	PRO	L370	M445	
P243	LYS	S371	G446	
S244	ALA	N372	V447	
Q247	MET	R373	E448	
T248	LYS	G374	K449	
Q249	LYS	G375	A450	
W250	THR	R376	I451	
Y251	ASN	Q377	E452	
Q252	VAL	L378	I453	
L253	GLU	D379	L454	
Y254	GLU	F380	R455	
V255	SER	S381	D456	
R256	GLN	R382	E457	
S257	GLY	A383	I458	
D258	ALA	P384	E459	
R259	SER	I385	M460	
K260	ARG	E386	S461	
D263	ALA	V387	M462	
K267	LEU	L388	R463	
N268	SER	T391	L464	
E270	LYS	I394	L465	
K271	F325	K398	G466	
V274	I326	L400	V467	
K275	D327	K403	T468	
	P328	V406	S469	
	S329	F407	E472	
	L330	Y408	L473	
	W332	D409	L474	
	T331		K474	
	K339		L477	
	K340		L478	
			D479	
			L480	

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	164.50Å 164.50Å 114.00Å 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.	Xtrriage
Total number of atoms	8726	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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(°)	Ideal(°)
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:HH A	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%)	<b>5</b> <b>22</b>
1	B	378/511 (74%)	331 (88%)	38 (10%)	9 (2%)	<b>6</b> <b>25</b>
All	All	852/1022 (83%)	756 (89%)	74 (9%)	22 (3%)	<b>6</b> <b>23</b>

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	411/440 (93%)	344 (84%)	67 (16%)	<b>2</b> <b>7</b>
1	B	330/440 (75%)	277 (84%)	53 (16%)	<b>2</b> <b>8</b>
All	All	741/880 (84%)	621 (84%)	120 (16%)	<b>2</b> <b>8</b>

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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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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	$\# Z  > 2$
3	HEM	A	560	1	27,50,50	2.63	7 (25%)	17,82,82	2.66	6 (35%)
2	FMN	A	570	-	30,33,33	2.89	10 (33%)	38,50,50	3.83	17 (44%)
4	PYR	A	580	-	2,5,5	1.60	0	2,6,6	0.89	0
2	FMN	B	570	-	30,33,33	2.90	9 (30%)	38,50,50	3.15	15 (39%)
4	PYR	B	580	-	2,5,5	1.14	0	2,6,6	1.82	0

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
3	HEM	A	560	1	-	0/6/54/54	0/0/8/8
2	FMN	A	570	-	2/2/4/4	0/16/18/18	0/3/3/3
4	PYR	A	580	-	-	0/0/4/4	0/0/0/0
2	FMN	B	570	-	2/2/4/4	0/16/18/18	0/3/3/3
4	PYR	B	580	-	-	0/0/4/4	0/0/0/0

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	570	FMN	C1'-N10	-12.90	1.35	1.48
2	A	570	FMN	C1'-N10	-11.58	1.36	1.48
2	A	570	FMN	C2'-C3'	-5.29	1.43	1.53
3	A	560	HEM	C3C-CAC	-4.60	1.38	1.47
3	A	560	HEM	C3B-CAB	-4.44	1.39	1.47
3	A	560	HEM	C3B-C2B	-4.23	1.34	1.40
2	A	570	FMN	C6-C5A	-3.60	1.36	1.41
2	A	570	FMN	O2'-C2'	-3.60	1.35	1.43
3	A	560	HEM	C3C-C2C	-3.52	1.35	1.40
2	B	570	FMN	C6-C5A	-3.43	1.36	1.41
2	A	570	FMN	C4A-C10	-3.17	1.35	1.41
2	A	570	FMN	O4'-C4'	-2.89	1.37	1.43
2	B	570	FMN	C9A-C5A	-2.70	1.37	1.42
2	A	570	FMN	C9-C8	-2.29	1.31	1.37
2	A	570	FMN	C9-C9A	-2.20	1.36	1.40
2	B	570	FMN	C2'-C3'	-2.17	1.49	1.53
2	B	570	FMN	C2-N1	-2.14	1.33	1.38
2	A	570	FMN	C4'-C3'	-2.09	1.49	1.53
2	B	570	FMN	C8M-C8	2.15	1.55	1.51
3	A	560	HEM	CBC-CAC	2.32	1.44	1.29
3	A	560	HEM	CBB-CAB	2.45	1.45	1.29
2	A	570	FMN	C4A-N5	2.67	1.37	1.33
2	B	570	FMN	C4-C4A	2.89	1.46	1.41
2	B	570	FMN	C10-N1	2.93	1.37	1.33
2	B	570	FMN	C4A-N5	3.34	1.38	1.33
3	A	560	HEM	CAA-C2A	9.49	1.67	1.52

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	570	FMN	N3-C2-N1	-4.84	112.45	122.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	570	FMN	C9A-N10-C10	-4.24	116.12	121.77
2	B	570	FMN	N3-C2-N1	-3.87	114.44	122.37
2	B	570	FMN	C9A-N10-C10	-3.54	117.05	121.77
2	A	570	FMN	C8M-C8-C9	-3.41	111.95	120.36
2	A	570	FMN	O2'-C2'-C3'	-3.28	100.99	109.10
2	A	570	FMN	C7-C6-C5A	-2.98	116.72	121.17
2	B	570	FMN	O5'-P-O1P	-2.43	99.66	106.47
3	A	560	HEM	CMD-C2D-C1D	-2.14	125.18	128.46
2	B	570	FMN	C8M-C8-C9	-2.13	115.12	120.36
2	A	570	FMN	O5'-P-O1P	-2.07	100.66	106.47
3	A	560	HEM	C3B-C4B-NB	2.02	111.82	109.21
2	B	570	FMN	O4'-C4'-C5'	2.03	114.54	110.02
2	A	570	FMN	O4'-C4'-C5'	2.33	115.22	110.02
3	A	560	HEM	CBD-CAD-C3D	2.61	117.45	112.47
2	B	570	FMN	O3P-P-O2P	2.67	118.16	107.59
2	B	570	FMN	C8M-C8-C7	2.72	126.39	120.72
2	A	570	FMN	O3'-C3'-C4'	2.73	115.55	108.82
2	B	570	FMN	O5'-C5'-C4'	2.79	116.80	109.36
2	A	570	FMN	O4'-C4'-C3'	2.88	116.22	109.10
2	A	570	FMN	C8M-C8-C7	2.98	126.95	120.72
2	A	570	FMN	P-O5'-C5'	3.48	127.89	118.30
2	B	570	FMN	O2'-C2'-C1'	3.49	118.21	109.61
2	B	570	FMN	P-O5'-C5'	3.50	127.94	118.30
3	A	560	HEM	CBA-CAA-C2A	3.52	119.21	112.48
2	A	570	FMN	C1'-C2'-C3'	3.52	119.89	109.82
2	B	570	FMN	O4'-C4'-C3'	3.71	118.26	109.10
2	B	570	FMN	C4'-C3'-C2'	3.91	121.65	113.40
2	A	570	FMN	C5A-C9A-N10	4.10	120.84	117.71
2	B	570	FMN	C1'-N10-C9A	4.52	122.32	118.31
3	A	560	HEM	CAA-CBA-CGA	4.54	120.43	112.66
2	B	570	FMN	C5A-C9A-N10	4.59	121.22	117.71
2	A	570	FMN	O2'-C2'-C1'	4.79	121.43	109.61
2	A	570	FMN	C4'-C3'-C2'	5.54	125.08	113.40
2	A	570	FMN	C1'-N10-C10	6.75	125.20	118.46
3	A	560	HEM	CAA-C2A-C3A	7.24	149.67	129.00
2	B	570	FMN	C2-N1-C10	14.30	128.68	114.90
2	A	570	FMN	C2-N1-C10	16.84	131.12	114.90

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	570	FMN	C4'

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

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 17 short contacts:

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

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.