



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 23, 2018 – 05:10 PM EST

PDB ID : 1D4C  
Title : CRYSTAL STRUCTURE OF THE UNCOMPLEXED FORM OF THE FLAVOCYTOCHROME C FUMARATE REDUCTASE OF SHEWANELLA PUTREFACIENS STRAIN MR-1  
Authors : Leys, D.; Tsapin, A.S.; Meyer, T.E.; Cusanovich, M.A.; Van Beeumen, J.J.  
Deposited on : 1999-10-03  
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

<http://wwpdb.org/validation/2016/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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

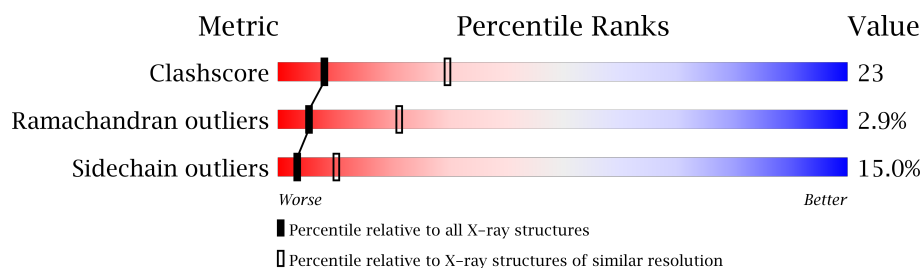
# 1 Overall quality at a glance

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	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (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	572	 51% 35% 12% .
1	B	572	 51% 35% 11% ..
1	C	572	 51% 33% 13% ..
1	D	572	 50% 37% 12% .

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	FAD	A	600	X	-	-	-
3	FAD	B	700	X	-	-	-
3	FAD	C	800	X	-	-	-
3	FAD	D	900	X	-	-	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 17470 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called FLAVOCYTOCHROME C FUMARATE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	570	Total	C	N	O	S	0	0	0
			4124	2562	736	807	19			
1	B	566	Total	C	N	O	S	0	0	0
			4093	2542	731	801	19			
1	C	568	Total	C	N	O	S	0	0	0
			4099	2546	733	801	19			
1	D	570	Total	C	N	O	S	0	0	0
			4113	2553	734	807	19			

- 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	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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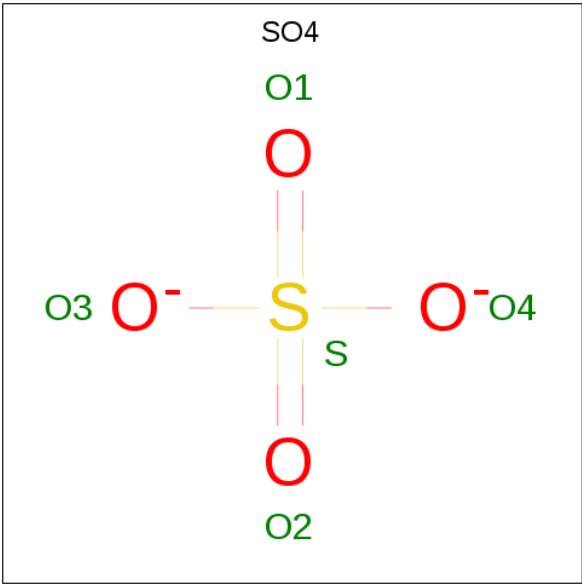
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0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

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0

- Molecule 5 is water.

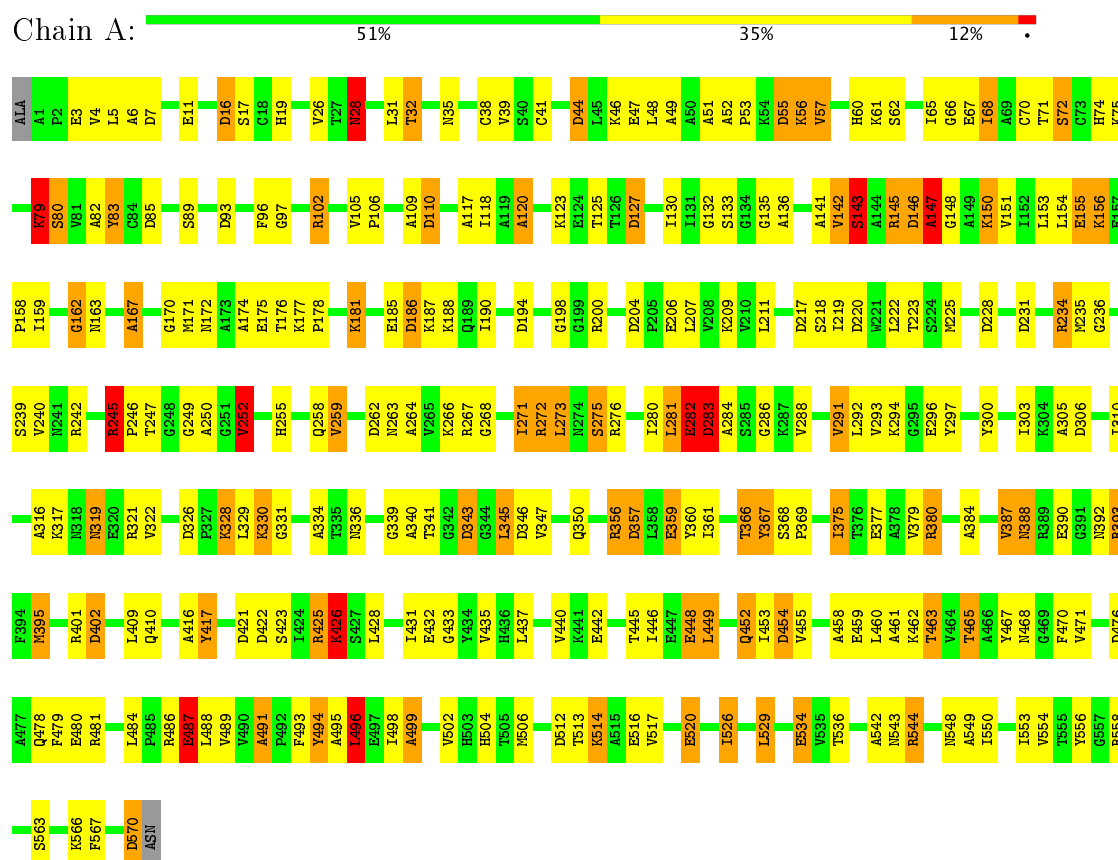
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	48	Total O 48 48	0	0
5	B	29	Total O 29 29	0	0
5	C	30	Total O 30 30	0	0
5	D	19	Total O 19 19	0	0

### 3 Residue-property plots

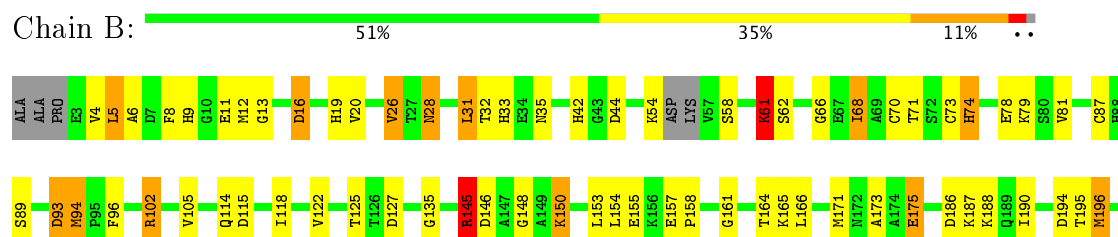
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

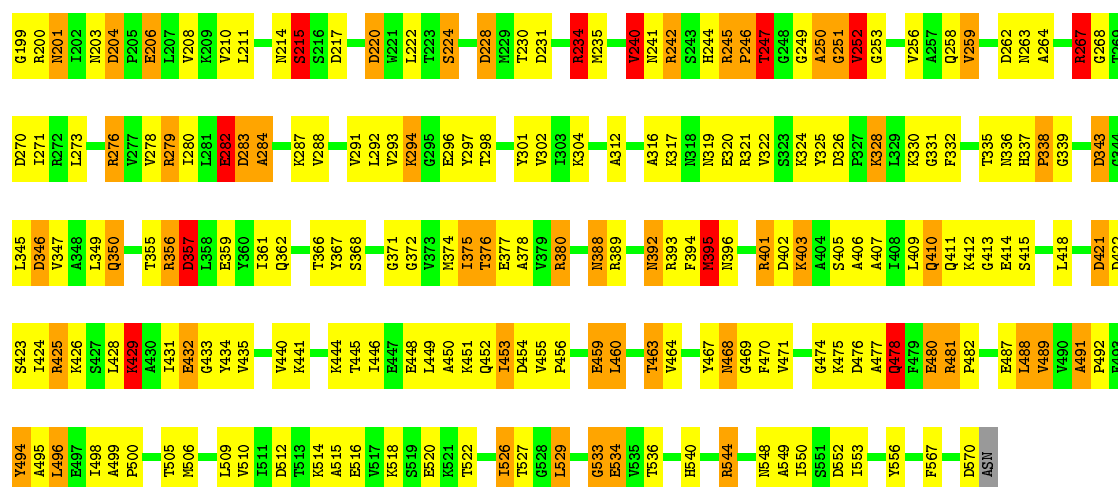
#### • Molecule 1: FLAVOCYTOCHROME C FUMARATE REDUCTASE



#### • Molecule 1: FLAVOCYTOCHROME C FUMARATE REDUCTASE

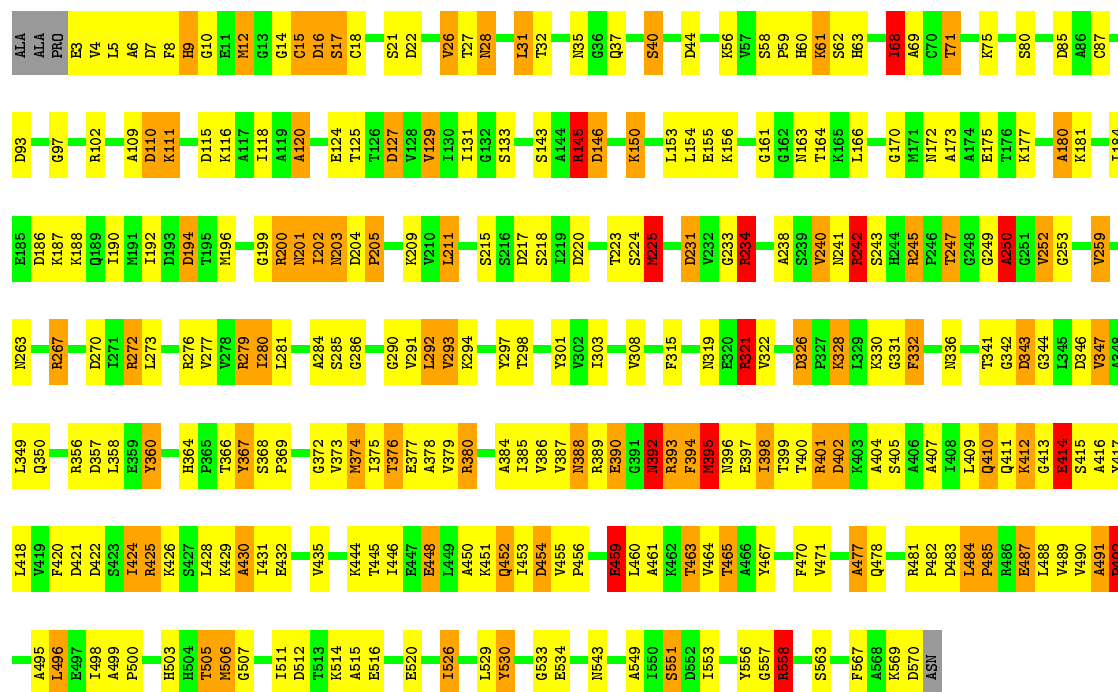






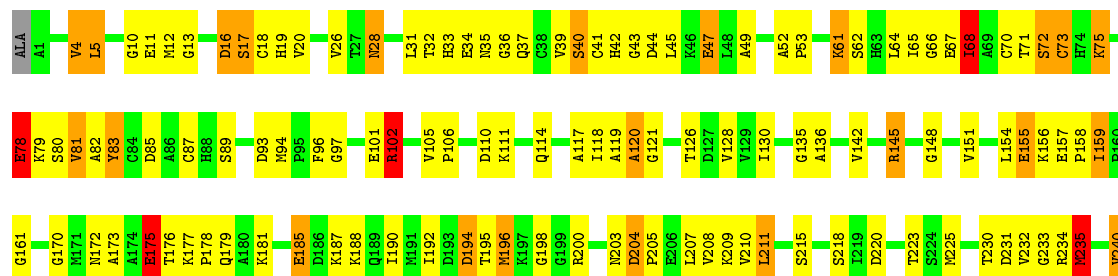
### • Molecule 1: FLAVOCYTOCHROME C FUMARATE REDUCTASE

Chain C: 51% 33% 13% ..



### • Molecule 1: FLAVOCYTOCHROME C FUMARATE REDUCTASE

Chain D: 50% 37% 12% .



S563	D476	S405	K328	I241
D570	A477	A406	L329	R242
ASN	Q478	L409	K330	S243
	F479	Q410	G331	H244
	E480	Q411		R245
	R481		N336	P246
	P482			T247
	D483	S415	A340	G248
	L484			G249
	P485	L418	I345	A250
	R486	V419	D346	G251
	E487	F420	V347	V252
	L488	D421	A348	
	V489	D422	L349	Q258
	V490	S423	Q350	V259
	A491	I424		L260
	P492	K425	T355	D261
	F493	R426	K356	D262
	Y494	S427	D357	
	A495	L428	I358	K267
	L496	K429	E359	G268
	E497	A430	Y360	T269
	I498	I431	I361	D270
	A499	E432		
	P500	G433	B364	L273
	A501	Y434	F365	
	V502		T366	V277
	M506	I439	Y367	V278
		V440	S368	R279
		K441	P369	I280
			A370	L281
		K444	G371	E282
	K514	T445	G372	D283
	A515	I446		A284
	E516	E447	I375	V288
	V517	E448	T376	
	K518	L449	E377	V291
	S519	A450	A378	L292
	E520	K451	V379	V293
		Q452	R380	
	P525	I453	G381	Y297
	I526	D454	N382	
		V455	G383	
	L529	P456	A384	Y300
		A457	I385	
		A458		T303
		E459	N388	
		L460	R389	A307
	N543	A461		
	R544	K462	N392	I310
	L545	T463	R393	
	G546	V464	F394	A316
	G547		N395	
	N548	Y467	N396	N319
	A549			E320
		N468	T400	R321
	D552	C469	R401	V322
	I553	F470	D402	
	V554	V471	K403	D326
				P327
	R558	K475	A404	

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.69Å 216.36Å 112.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90	Depositor
% Data completeness (in resolution range)	93.7 (15.00-2.90)	Depositor
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.210 , 0.300	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17470	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, SO4, FAD

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	0.76	0/4192	2.22	144/5683 (2.5%)
1	B	0.74	7/4159 (0.2%)	1.97	112/5637 (2.0%)
1	C	0.71	3/4166 (0.1%)	2.04	126/5649 (2.2%)
1	D	0.64	1/4179 (0.0%)	1.94	98/5665 (1.7%)
All	All	0.72	11/16696 (0.1%)	2.05	480/22634 (2.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
1	C	0	3
1	D	0	2
All	All	0	10

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	480	GLU	CD-OE1	9.81	1.36	1.25
1	C	459	GLU	CD-OE1	9.29	1.35	1.25
1	C	459	GLU	CD-OE2	8.55	1.35	1.25
1	B	476	ASP	CG-OD1	8.47	1.44	1.25
1	B	459	GLU	CD-OE2	7.25	1.33	1.25
1	B	475	LYS	C-O	6.75	1.36	1.23
1	C	477	ALA	C-O	6.54	1.35	1.23
1	B	469	GLY	N-CA	6.24	1.55	1.46
1	B	468	ASN	CG-OD1	5.73	1.36	1.24
1	B	251	GLY	N-CA	-5.35	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	468	ASN	CG-ND2	5.30	1.46	1.32

All (480) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	245	ARG	CD-NE-CZ	29.02	164.23	123.60
1	A	267	ARG	CD-NE-CZ	24.00	157.20	123.60
1	A	102	ARG	NE-CZ-NH2	23.33	131.97	120.30
1	D	401	ARG	CD-NE-CZ	21.85	154.19	123.60
1	D	242	ARG	NE-CZ-NH1	20.69	130.65	120.30
1	A	380	ARG	NE-CZ-NH2	20.37	130.49	120.30
1	A	558	ARG	NE-CZ-NH2	20.21	130.40	120.30
1	D	242	ARG	NE-CZ-NH2	-20.14	110.23	120.30
1	A	321	ARG	NE-CZ-NH1	20.03	130.31	120.30
1	A	200	ARG	NE-CZ-NH1	19.64	130.12	120.30
1	C	234	ARG	NE-CZ-NH1	19.24	129.92	120.30
1	B	356	ARG	CD-NE-CZ	19.17	150.43	123.60
1	C	267	ARG	CD-NE-CZ	18.93	150.10	123.60
1	A	272	ARG	NE-CZ-NH2	-18.02	111.29	120.30
1	B	276	ARG	NE-CZ-NH2	-17.51	111.54	120.30
1	B	401	ARG	NE-CZ-NH2	-17.43	111.58	120.30
1	C	234	ARG	NE-CZ-NH2	-17.00	111.80	120.30
1	B	145	ARG	CD-NE-CZ	16.74	147.04	123.60
1	A	267	ARG	NE-CZ-NH1	-15.98	112.31	120.30
1	D	401	ARG	NE-CZ-NH2	-15.82	112.39	120.30
1	A	558	ARG	CG-CD-NE	15.57	144.50	111.80
1	B	401	ARG	NE-CZ-NH1	15.23	127.92	120.30
1	A	242	ARG	NE-CZ-NH2	15.15	127.88	120.30
1	D	356	ARG	NE-CZ-NH2	14.97	127.79	120.30
1	A	380	ARG	NE-CZ-NH1	-14.79	112.91	120.30
1	C	401	ARG	NE-CZ-NH1	14.62	127.61	120.30
1	C	356	ARG	NE-CZ-NH1	-14.27	113.17	120.30
1	A	281	LEU	C-N-CA	14.13	157.03	121.70
1	C	401	ARG	NE-CZ-NH2	-13.94	113.33	120.30
1	A	102	ARG	NE-CZ-NH1	-13.90	113.35	120.30
1	B	246	PRO	C-N-CA	13.74	156.06	121.70
1	D	267	ARG	NE-CZ-NH1	-13.68	113.46	120.30
1	D	279	ARG	NE-CZ-NH2	13.48	127.04	120.30
1	D	185	GLU	CA-CB-CG	13.26	142.58	113.40
1	C	102	ARG	NE-CZ-NH1	13.16	126.88	120.30
1	C	328	LYS	CA-CB-CG	13.06	142.13	113.40
1	C	242	ARG	NE-CZ-NH1	-12.98	113.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	245	ARG	NE-CZ-NH2	-12.73	113.94	120.30
1	A	245	ARG	CB-CG-CD	12.62	144.42	111.60
1	C	146	ASP	CB-CG-OD1	12.48	129.54	118.30
1	A	321	ARG	NE-CZ-NH2	-12.40	114.10	120.30
1	C	401	ARG	CD-NE-CZ	12.31	140.83	123.60
1	C	357	ASP	CB-CG-OD2	12.16	129.24	118.30
1	B	356	ARG	NE-CZ-NH1	-12.06	114.27	120.30
1	D	401	ARG	NE-CZ-NH1	11.96	126.28	120.30
1	C	102	ARG	NE-CZ-NH2	-11.96	114.32	120.30
1	B	270	ASP	CB-CG-OD2	11.80	128.92	118.30
1	B	552	ASP	CB-CG-OD1	11.79	128.91	118.30
1	B	481	ARG	NE-CZ-NH2	-11.68	114.46	120.30
1	C	491	ALA	CA-C-O	-11.49	95.97	120.10
1	C	102	ARG	CD-NE-CZ	11.46	139.65	123.60
1	C	5	LEU	CA-CB-CG	11.38	141.46	115.30
1	A	481	ARG	CD-NE-CZ	11.04	139.06	123.60
1	A	200	ARG	CD-NE-CZ	10.91	138.87	123.60
1	B	234	ARG	NE-CZ-NH1	10.85	125.72	120.30
1	B	220	ASP	CB-CG-OD1	10.59	127.83	118.30
1	D	395	MET	CA-CB-CG	10.56	131.25	113.30
1	B	570	ASP	CB-CG-OD1	10.56	127.80	118.30
1	C	200	ARG	NE-CZ-NH2	-10.55	115.03	120.30
1	C	156	LYS	CA-CB-CG	10.52	136.55	113.40
1	D	486	ARG	NE-CZ-NH1	10.52	125.56	120.30
1	D	281	LEU	C-N-CA	10.52	147.99	121.70
1	B	217	ASP	CB-CG-OD1	10.46	127.72	118.30
1	B	570	ASP	CA-CB-CG	10.33	136.13	113.40
1	B	93	ASP	CB-CG-OD2	-10.33	109.00	118.30
1	A	267	ARG	CA-C-N	10.24	136.69	116.20
1	C	200	ARG	NE-CZ-NH1	10.24	125.42	120.30
1	C	61	LYS	CA-CB-CG	10.17	135.77	113.40
1	A	93	ASP	CB-CG-OD1	-10.10	109.21	118.30
1	D	242	ARG	CD-NE-CZ	10.09	137.72	123.60
1	A	276	ARG	NE-CZ-NH1	9.90	125.25	120.30
1	B	250	ALA	C-N-CA	9.83	142.93	122.30
1	A	217	ASP	CB-CG-OD2	-9.79	109.49	118.30
1	A	357	ASP	CB-CG-OD1	-9.71	109.56	118.30
1	A	393	ARG	CD-NE-CZ	9.64	137.09	123.60
1	C	279	ARG	NE-CZ-NH1	9.63	125.12	120.30
1	A	491	ALA	CA-C-O	-9.57	100.00	120.10
1	A	242	ARG	CD-NE-CZ	9.54	136.95	123.60
1	D	491	ALA	CA-C-O	-9.48	100.19	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	492	PRO	N-CA-CB	9.46	114.66	103.30
1	B	251	GLY	N-CA-C	9.46	136.75	113.10
1	A	200	ARG	NE-CZ-NH2	-9.37	115.62	120.30
1	A	267	ARG	NE-CZ-NH2	9.35	124.97	120.30
1	D	356	ARG	CD-NE-CZ	9.26	136.56	123.60
1	A	262	ASP	CB-CG-OD1	9.17	126.55	118.30
1	C	272	ARG	NE-CZ-NH2	-9.10	115.75	120.30
1	A	494	TYR	CB-CG-CD1	-9.07	115.56	121.00
1	A	425	ARG	NE-CZ-NH2	-9.03	115.78	120.30
1	B	267	ARG	CA-C-N	9.02	134.24	116.20
1	C	558	ARG	CG-CD-NE	8.95	130.59	111.80
1	A	356	ARG	NE-CZ-NH2	8.92	124.76	120.30
1	D	200	ARG	NE-CZ-NH1	8.88	124.74	120.30
1	D	492	PRO	CA-N-CD	-8.88	99.07	111.50
1	A	486	ARG	NE-CZ-NH2	-8.87	115.86	120.30
1	C	301	TYR	CA-CB-CG	8.87	130.25	113.40
1	B	492	PRO	N-CA-CB	8.84	113.91	103.30
1	C	85	ASP	CB-CG-OD2	-8.73	110.44	118.30
1	A	272	ARG	NH1-CZ-NH2	8.70	128.97	119.40
1	B	61	LYS	CA-CB-CG	8.70	132.55	113.40
1	D	67	GLU	OE1-CD-OE2	8.69	133.73	123.30
1	B	491	ALA	CA-C-O	-8.61	102.03	120.10
1	B	346	ASP	CB-CG-OD1	8.60	126.04	118.30
1	C	477	ALA	CA-C-O	-8.60	102.05	120.10
1	A	402	ASP	CB-CG-OD1	8.58	126.02	118.30
1	B	200	ARG	NE-CZ-NH1	-8.57	116.02	120.30
1	A	93	ASP	CB-CG-OD2	8.54	125.99	118.30
1	A	544	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	D	220	ASP	CB-CG-OD1	8.52	125.97	118.30
1	D	102	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	A	228	ASP	CB-CG-OD2	8.45	125.91	118.30
1	A	558	ARG	NE-CZ-NH1	-8.39	116.10	120.30
1	A	44	ASP	CB-CG-OD2	8.33	125.80	118.30
1	B	245	ARG	NE-CZ-NH1	-8.33	116.14	120.30
1	C	534	GLU	OE1-CD-OE2	-8.33	113.31	123.30
1	B	4	VAL	N-CA-CB	8.26	129.68	111.50
1	C	558	ARG	NE-CZ-NH1	-8.22	116.19	120.30
1	A	276	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	C	492	PRO	N-CA-CB	8.19	113.13	103.30
1	B	556	TYR	CB-CG-CD2	-8.11	116.13	121.00
1	D	356	ARG	NE-CZ-NH1	-8.07	116.27	120.30
1	D	279	ARG	NE-CZ-NH1	-8.05	116.27	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	218	SER	CB-CA-C	8.05	125.40	110.10
1	B	544	ARG	NE-CZ-NH1	8.03	124.32	120.30
1	C	231	ASP	CB-CG-OD2	8.03	125.53	118.30
1	B	11	GLU	CB-CG-CD	7.99	135.78	114.20
1	A	242	ARG	NE-CZ-NH1	-7.98	116.31	120.30
1	A	345	LEU	CA-CB-CG	7.97	133.63	115.30
1	C	393	ARG	NE-CZ-NH1	-7.93	116.33	120.30
1	B	328	LYS	CA-CB-CG	7.92	130.81	113.40
1	A	442	GLU	CA-CB-CG	7.89	130.75	113.40
1	A	3	GLU	C-N-CA	7.86	141.34	121.70
1	C	356	ARG	NH1-CZ-NH2	7.84	128.02	119.40
1	A	56	LYS	C-N-CA	7.83	141.29	121.70
1	B	343	ASP	CB-CG-OD1	7.83	125.35	118.30
1	A	127	ASP	CB-CG-OD2	-7.81	111.27	118.30
1	C	321	ARG	NE-CZ-NH1	-7.79	116.40	120.30
1	C	492	PRO	CA-N-CD	-7.77	100.62	111.50
1	D	194	ASP	CB-CG-OD1	7.76	125.28	118.30
1	A	512	ASP	CB-CG-OD2	7.73	125.26	118.30
1	C	326	ASP	CB-CG-OD2	7.71	125.24	118.30
1	A	275	SER	N-CA-CB	-7.70	98.95	110.50
1	B	425	ARG	NE-CZ-NH2	7.69	124.15	120.30
1	A	7	ASP	CA-CB-CG	7.69	130.31	113.40
1	B	262	ASP	CB-CG-OD2	7.60	125.14	118.30
1	B	155	GLU	OE1-CD-OE2	7.59	132.41	123.30
1	C	220	ASP	CB-CG-OD2	-7.58	111.48	118.30
1	A	234	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	C	220	ASP	CB-CG-OD1	7.55	125.09	118.30
1	B	476	ASP	CB-CG-OD2	7.54	125.08	118.30
1	C	276	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	C	377	GLU	OE1-CD-OE2	-7.47	114.33	123.30
1	B	150	LYS	CB-CA-C	7.43	125.27	110.40
1	A	44	ASP	CB-CG-OD1	-7.37	111.67	118.30
1	C	392	ASN	CA-CB-CG	7.37	129.61	113.40
1	C	326	ASP	CB-CG-OD1	-7.32	111.71	118.30
1	B	234	ARG	NE-CZ-NH2	-7.31	116.64	120.30
1	D	93	ASP	CB-CG-OD2	-7.29	111.74	118.30
1	A	47	GLU	OE1-CD-OE2	7.27	132.03	123.30
1	A	356	ARG	NE-CZ-NH1	-7.25	116.68	120.30
1	C	194	ASP	CB-CG-OD2	7.24	124.82	118.30
1	A	544	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	A	245	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	C	71	THR	CA-C-N	7.19	133.01	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	468	ASN	OD1-CG-ND2	7.18	138.42	121.90
1	C	401	ARG	CA-CB-CG	7.17	129.17	113.40
1	D	486	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	C	492	PRO	N-CD-CG	7.14	113.91	103.20
1	B	145	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	B	425	ARG	CB-CG-CD	7.08	130.02	111.60
1	B	474	GLY	O-C-N	7.07	134.00	122.70
1	B	279	ARG	NE-CZ-NH2	7.05	123.82	120.30
1	A	38	CYS	CB-CA-C	-7.01	96.38	110.40
1	A	328	LYS	CB-CA-C	-7.01	96.39	110.40
1	C	503	HIS	N-CA-CB	-7.01	97.99	110.60
1	D	552	ASP	CB-CG-OD2	-6.99	112.01	118.30
1	C	259	VAL	CG1-CB-CG2	6.99	122.08	110.90
1	A	259	VAL	CG1-CB-CG2	6.98	122.07	110.90
1	B	401	ARG	CD-NE-CZ	6.98	133.37	123.60
1	C	380	ARG	NE-CZ-NH2	6.98	123.79	120.30
1	B	11	GLU	CA-CB-CG	6.97	128.73	113.40
1	D	267	ARG	CA-C-N	6.96	130.13	116.20
1	A	496	LEU	CA-CB-CG	6.91	131.20	115.30
1	D	47	GLU	OE1-CD-OE2	6.90	131.58	123.30
1	B	294	LYS	CA-CB-CG	6.90	128.58	113.40
1	B	93	ASP	CB-CG-OD1	6.90	124.51	118.30
1	B	492	PRO	CA-N-CD	-6.88	101.86	111.50
1	B	475	LYS	O-C-N	6.84	133.65	122.70
1	B	357	ASP	CB-CG-OD2	6.84	124.45	118.30
1	A	514	LYS	CD-CE-NZ	6.82	127.38	111.70
1	A	194	ASP	CB-CG-OD2	6.79	124.41	118.30
1	D	481	ARG	NE-CZ-NH2	6.78	123.69	120.30
1	A	467	TYR	CB-CG-CD1	-6.78	116.93	121.00
1	B	267	ARG	C-N-CA	-6.76	108.10	122.30
1	A	283	ASP	CB-CG-OD2	6.75	124.38	118.30
1	D	12	MET	CA-CB-CG	6.75	124.78	113.30
1	D	558	ARG	CG-CD-NE	6.75	125.97	111.80
1	D	410	GLN	CA-CB-CG	6.73	128.21	113.40
1	C	93	ASP	CB-CG-OD1	-6.73	112.25	118.30
1	C	12	MET	CA-CB-CG	6.71	124.71	113.30
1	D	200	ARG	NE-CZ-NH2	-6.71	116.94	120.30
1	B	146	ASP	CB-CG-OD2	-6.70	112.27	118.30
1	B	175	GLU	OE1-CD-OE2	6.70	131.34	123.30
1	D	389	ARG	NE-CZ-NH2	6.70	123.65	120.30
1	D	520	GLU	OE1-CD-OE2	-6.69	115.28	123.30
1	B	350	GLN	CB-CG-CD	6.68	128.97	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	373	VAL	CA-C-O	6.68	134.13	120.10
1	D	81	VAL	CB-CA-C	-6.67	98.74	111.40
1	B	283	ASP	C-N-CA	6.64	138.30	121.70
1	D	245	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	B	246	PRO	CA-C-O	6.64	136.13	120.20
1	A	7	ASP	CB-CG-OD2	6.62	124.26	118.30
1	A	321	ARG	O-C-N	-6.58	112.17	122.70
1	A	494	TYR	CB-CG-CD2	6.58	124.95	121.00
1	C	478	GLN	CB-CG-CD	-6.58	94.51	111.60
1	C	3	GLU	C-N-CA	6.56	138.11	121.70
1	D	185	GLU	OE1-CD-OE2	-6.55	115.44	123.30
1	C	530	TYR	O-C-N	-6.54	112.24	122.70
1	C	414	GLU	OE1-CD-OE2	6.53	131.13	123.30
1	C	569	LYS	C-N-CA	6.53	138.02	121.70
1	B	492	PRO	N-CD-CG	6.52	112.98	103.20
1	D	396	ASN	CB-CA-C	6.50	123.39	110.40
1	C	238	ALA	N-CA-CB	6.48	119.18	110.10
1	A	359	GLU	CA-CB-CG	6.47	127.63	113.40
1	A	93	ASP	CA-CB-CG	-6.44	99.22	113.40
1	C	426	LYS	CA-CB-CG	6.44	127.56	113.40
1	B	357	ASP	CB-CG-OD1	-6.42	112.52	118.30
1	A	487	GLU	CA-C-N	6.40	131.29	117.20
1	C	111	LYS	CA-CB-CG	6.40	127.47	113.40
1	B	359	GLU	OE1-CD-OE2	-6.39	115.63	123.30
1	B	282	GLU	OE1-CD-OE2	6.37	130.95	123.30
1	A	341	THR	CA-C-N	6.36	128.93	116.20
1	B	468	ASN	CB-CG-OD1	-6.36	108.88	121.60
1	B	252	VAL	N-CA-CB	6.36	125.49	111.50
1	C	3	GLU	O-C-N	-6.33	112.57	122.70
1	B	31	LEU	CA-CB-CG	6.33	129.87	115.30
1	B	276	ARG	NH1-CZ-NH2	6.31	126.34	119.40
1	C	217	ASP	CB-CG-OD1	6.30	123.97	118.30
1	D	426	LYS	CA-CB-CG	6.30	127.25	113.40
1	A	283	ASP	CA-CB-CG	6.29	127.25	113.40
1	B	296	GLU	OE1-CD-OE2	6.28	130.84	123.30
1	C	161	GLY	O-C-N	-6.28	112.53	123.20
1	D	4	VAL	N-CA-CB	6.28	125.31	111.50
1	A	570	ASP	CB-CG-OD1	6.27	123.94	118.30
1	A	143	SER	CA-C-N	6.26	130.98	117.20
1	C	380	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	C	194	ASP	OD1-CG-OD2	-6.25	111.44	123.30
1	A	366	THR	CA-C-O	6.24	133.21	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	448	GLU	CA-CB-CG	6.24	127.13	113.40
1	B	249	GLY	N-CA-C	-6.24	97.51	113.10
1	D	185	GLU	N-CA-CB	-6.22	99.40	110.60
1	A	162	GLY	O-C-N	-6.22	112.75	122.70
1	D	270	ASP	CB-CG-OD1	6.20	123.88	118.30
1	D	516	GLU	N-CA-CB	-6.19	99.45	110.60
1	A	467	TYR	CB-CG-CD2	6.18	124.71	121.00
1	B	459	GLU	OE1-CD-OE2	6.18	130.72	123.30
1	C	250	ALA	N-CA-C	6.18	127.68	111.00
1	B	534	GLU	O-C-N	-6.17	112.82	122.70
1	D	204	ASP	CB-CG-OD1	6.17	123.85	118.30
1	A	79	LYS	CD-CE-NZ	6.17	125.88	111.70
1	C	425	ARG	NE-CZ-NH1	6.15	123.38	120.30
1	A	19	HIS	O-C-N	-6.15	112.86	122.70
1	C	231	ASP	CB-CG-OD1	-6.13	112.78	118.30
1	A	357	ASP	CB-CG-OD2	6.11	123.80	118.30
1	B	570	ASP	N-CA-CB	6.11	121.59	110.60
1	C	16	ASP	CA-CB-CG	6.11	126.84	113.40
1	C	146	ASP	CB-CG-OD2	-6.11	112.80	118.30
1	D	283	ASP	CA-CB-CG	6.11	126.84	113.40
1	C	145	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	C	341	THR	CA-C-N	6.09	128.37	116.20
1	A	281	LEU	O-C-N	-6.08	112.97	122.70
1	C	360	TYR	CB-CG-CD2	6.08	124.65	121.00
1	C	285	SER	C-N-CA	6.07	135.06	122.30
1	A	145	ARG	NE-CZ-NH1	-6.07	117.27	120.30
1	B	252	VAL	CB-CA-C	-6.05	99.91	111.40
1	C	44	ASP	CB-CG-OD2	6.04	123.73	118.30
1	C	194	ASP	CB-CG-OD1	6.04	123.73	118.30
1	C	380	ARG	NH1-CZ-NH2	-6.01	112.79	119.40
1	C	129	VAL	CA-CB-CG1	6.00	119.90	110.90
1	B	235	MET	CA-CB-CG	5.99	123.48	113.30
1	A	281	LEU	CA-C-O	5.98	132.65	120.10
1	D	155	GLU	OE1-CD-OE2	5.97	130.46	123.30
1	B	425	ARG	NE-CZ-NH1	-5.97	117.32	120.30
1	C	276	ARG	CD-NE-CZ	-5.96	115.25	123.60
1	C	17	SER	N-CA-CB	-5.96	101.56	110.50
1	A	155	GLU	OE1-CD-OE2	5.95	130.44	123.30
1	C	332	PHE	CA-CB-CG	5.93	128.12	113.90
1	D	223	THR	O-C-N	-5.92	113.22	122.70
1	B	401	ARG	CA-CB-CG	5.90	126.38	113.40
1	C	293	VAL	CB-CA-C	-5.90	100.19	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	338	PRO	CA-C-N	5.90	127.99	116.20
1	C	115	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	C	18	CYS	CA-CB-SG	-5.87	103.43	114.00
1	D	16	ASP	CB-CG-OD1	-5.84	113.04	118.30
1	A	264	ALA	N-CA-CB	5.83	118.26	110.10
1	A	306	ASP	CB-CG-OD2	5.83	123.54	118.30
1	A	267	ARG	O-C-N	-5.82	113.31	123.20
1	D	251	GLY	N-CA-C	5.80	127.61	113.10
1	A	367	TYR	CB-CG-CD1	5.80	124.48	121.00
1	A	345	LEU	CB-CA-C	5.80	121.21	110.20
1	B	477	ALA	N-CA-CB	-5.79	101.99	110.10
1	C	17	SER	CA-C-O	5.79	132.26	120.10
1	C	298	THR	CA-C-N	5.77	127.74	116.20
1	A	426	LYS	CA-C-N	5.76	129.88	117.20
1	B	242	ARG	CD-NE-CZ	5.76	131.67	123.60
1	B	520	GLU	CA-CB-CG	5.76	126.06	113.40
1	C	245	ARG	NE-CZ-NH1	-5.75	117.43	120.30
1	C	127	ASP	CB-CG-OD1	5.70	123.43	118.30
1	B	469	GLY	CA-C-O	5.69	130.85	120.60
1	A	218	SER	CB-CA-C	5.69	120.91	110.10
1	A	319	ASN	CA-CB-CG	5.68	125.91	113.40
1	C	211	LEU	CA-C-O	5.67	132.00	120.10
1	B	259	VAL	N-CA-CB	5.65	123.92	111.50
1	C	68	ILE	CA-CB-CG2	5.64	122.17	110.90
1	A	520	GLU	OE1-CD-OE2	-5.63	116.54	123.30
1	A	393	ARG	NE-CZ-NH2	5.63	123.12	120.30
1	C	543	ASN	OD1-CG-ND2	5.63	134.85	121.90
1	D	316	ALA	CB-CA-C	-5.63	101.66	110.10
1	B	200	ARG	NH1-CZ-NH2	5.63	125.59	119.40
1	D	231	ASP	CB-CG-OD1	5.63	123.37	118.30
1	B	477	ALA	CB-CA-C	5.63	118.54	110.10
1	B	403	LYS	CA-CB-CG	5.62	125.76	113.40
1	A	534	GLU	O-C-N	-5.62	113.72	122.70
1	A	276	ARG	CA-CB-CG	5.61	125.75	113.40
1	A	252	VAL	CA-CB-CG1	5.61	119.31	110.90
1	D	200	ARG	O-C-N	-5.61	113.73	122.70
1	C	242	ARG	NE-CZ-NH2	5.59	123.09	120.30
1	A	536	THR	CA-CB-CG2	5.59	120.22	112.40
1	D	61	LYS	N-CA-CB	5.59	120.66	110.60
1	A	242	ARG	CA-CB-CG	5.59	125.69	113.40
1	B	94	MET	CA-CB-CG	5.58	122.79	113.30
1	B	161	GLY	N-CA-C	5.58	127.05	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	200	ARG	CG-CD-NE	5.58	123.51	111.80
1	D	411	GLN	CA-CB-CG	5.55	125.62	113.40
1	D	262	ASP	CB-CG-OD1	5.55	123.29	118.30
1	C	417	TYR	CB-CG-CD2	5.54	124.33	121.00
1	C	506	MET	CA-C-N	5.54	127.27	116.20
1	A	185	GLU	CB-CA-C	5.53	121.47	110.40
1	D	68	ILE	CB-CA-C	5.53	122.67	111.60
1	A	234	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	A	329	LEU	CA-C-O	-5.53	108.50	120.10
1	C	110	ASP	CA-CB-CG	5.52	125.54	113.40
1	A	83	TYR	CB-CG-CD2	5.52	124.31	121.00
1	B	488	LEU	CA-CB-CG	5.51	127.98	115.30
1	B	380	ARG	CD-NE-CZ	5.51	131.32	123.60
1	C	506	MET	CA-C-O	-5.50	108.54	120.10
1	A	273	LEU	O-C-N	-5.50	113.90	122.70
1	B	204	ASP	CB-CG-OD2	5.50	123.25	118.30
1	D	282	GLU	N-CA-CB	-5.50	100.71	110.60
1	A	520	GLU	CA-CB-CG	5.49	125.48	113.40
1	C	272	ARG	NH1-CZ-NH2	5.49	125.44	119.40
1	C	4	VAL	N-CA-C	5.49	125.82	111.00
1	C	31	LEU	N-CA-CB	-5.48	99.43	110.40
1	C	321	ARG	NH1-CZ-NH2	5.47	125.42	119.40
1	D	546	GLY	O-C-N	-5.47	113.90	123.20
1	C	4	VAL	N-CA-CB	-5.47	99.47	111.50
1	C	367	TYR	CB-CG-CD2	5.47	124.28	121.00
1	D	400	THR	C-N-CA	5.47	135.36	121.70
1	C	425	ARG	CD-NE-CZ	5.46	131.25	123.60
1	D	396	ASN	CA-CB-CG	5.46	125.41	113.40
1	C	204	ASP	CB-CG-OD2	5.46	123.21	118.30
1	A	534	GLU	CA-C-N	5.45	129.20	117.20
1	A	367	TYR	CB-CG-CD2	-5.45	117.73	121.00
1	C	357	ASP	OD1-CG-OD2	-5.45	112.95	123.30
1	C	534	GLU	CA-CB-CG	5.45	125.38	113.40
1	A	328	LYS	CA-CB-CG	5.44	125.37	113.40
1	B	234	ARG	CD-NE-CZ	5.44	131.22	123.60
1	C	344	GLY	CA-C-O	-5.44	110.81	120.60
1	C	218	SER	N-CA-CB	-5.43	102.35	110.50
1	D	350	GLN	CB-CG-CD	5.43	125.72	111.60
1	B	262	ASP	OD1-CG-OD2	-5.41	113.03	123.30
1	B	378	ALA	N-CA-CB	5.40	117.66	110.10
1	A	219	ILE	O-C-N	-5.40	114.06	122.70
1	C	567	PHE	O-C-N	-5.39	114.08	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	563	SER	CB-CA-C	5.39	120.33	110.10
1	D	492	PRO	N-CD-CG	5.38	111.27	103.20
1	D	204	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	A	558	ARG	NH1-CZ-NH2	-5.37	113.49	119.40
1	B	421	ASP	CB-CG-OD1	-5.37	113.47	118.30
1	D	93	ASP	CB-CG-OD1	5.37	123.13	118.30
1	D	316	ALA	N-CA-CB	5.36	117.60	110.10
1	A	563	SER	N-CA-CB	-5.35	102.47	110.50
1	C	133	SER	O-C-N	-5.35	114.10	123.20
1	B	426	LYS	CD-CE-NZ	5.35	124.00	111.70
1	B	421	ASP	N-CA-CB	-5.34	100.98	110.60
1	B	145	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	B	12	MET	CB-CA-C	-5.34	99.73	110.40
1	C	18	CYS	N-CA-CB	-5.34	101.00	110.60
1	A	186	ASP	CB-CG-OD2	5.33	123.09	118.30
1	A	28	ASN	O-C-N	-5.32	114.18	122.70
1	A	252	VAL	CB-CA-C	-5.32	101.29	111.40
1	B	74	HIS	O-C-N	5.32	131.22	122.70
1	B	16	ASP	N-CA-CB	5.32	120.18	110.60
1	D	73	CYS	CB-CA-C	-5.32	99.76	110.40
1	A	156	LYS	CA-CB-CG	5.32	125.10	113.40
1	C	196	MET	CG-SD-CE	5.32	108.71	100.20
1	C	543	ASN	CB-CG-ND2	-5.32	103.94	116.70
1	C	505	THR	O-C-N	-5.31	114.20	122.70
1	A	123	LYS	CA-C-N	5.31	128.89	117.20
1	A	426	LYS	O-C-N	-5.31	114.20	122.70
1	C	200	ARG	O-C-N	-5.31	114.21	122.70
1	A	148	GLY	C-N-CA	-5.30	108.46	121.70
1	A	499	ALA	CB-CA-C	5.29	118.04	110.10
1	A	534	GLU	CG-CD-OE2	5.29	128.89	118.30
1	B	245	ARG	CA-CB-CG	5.29	125.05	113.40
1	B	196	MET	CG-SD-CE	5.28	108.65	100.20
1	D	235	MET	N-CA-C	-5.28	96.75	111.00
1	A	426	LYS	CA-CB-CG	5.28	125.00	113.40
1	A	19	HIS	CA-C-O	5.27	131.18	120.10
1	D	231	ASP	CB-CA-C	5.26	120.92	110.40
1	A	487	GLU	O-C-N	-5.26	114.29	122.70
1	D	260	LEU	O-C-N	-5.26	114.29	122.70
1	B	395	MET	CA-CB-CG	5.25	122.22	113.30
1	D	321	ARG	CD-NE-CZ	-5.24	116.26	123.60
1	B	478	GLN	N-CA-CB	-5.23	101.19	110.60
1	A	339	GLY	CA-C-O	-5.22	111.19	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	359	GLU	CA-C-N	5.22	128.69	117.20
1	D	267	ARG	NH1-CZ-NH2	5.22	125.14	119.40
1	D	10	GLY	C-N-CA	5.22	134.75	121.70
1	C	7	ASP	CB-CG-OD2	5.22	123.00	118.30
1	D	78	GLU	CB-CA-C	5.21	120.82	110.40
1	B	93	ASP	CB-CA-C	5.21	120.81	110.40
1	B	453	ILE	C-N-CA	5.19	134.67	121.70
1	C	273	LEU	O-C-N	-5.18	114.41	122.70
1	D	161	GLY	N-CA-C	5.18	126.06	113.10
1	B	81	VAL	CA-CB-CG2	5.18	118.67	110.90
1	A	367	TYR	CZ-CE2-CD2	-5.18	115.14	119.80
1	C	349	LEU	CB-CA-C	-5.18	100.36	110.20
1	C	459	GLU	CG-CD-OE1	5.17	128.65	118.30
1	D	36	GLY	O-C-N	-5.17	114.42	122.70
1	B	215	SER	O-C-N	-5.17	114.42	122.70
1	B	429	LYS	CA-CB-CG	5.17	124.78	113.40
1	D	486	ARG	CD-NE-CZ	5.17	130.84	123.60
1	D	67	GLU	CG-CD-OE2	-5.17	107.96	118.30
1	B	312	ALA	CA-C-N	5.16	126.52	116.20
1	B	533	GLY	O-C-N	-5.16	114.44	122.70
1	D	382	ASN	CA-CB-CG	5.16	124.74	113.40
1	A	89	SER	N-CA-CB	5.15	118.23	110.50
1	A	366	THR	O-C-N	-5.15	114.47	122.70
1	C	240	VAL	CA-CB-CG2	5.15	118.62	110.90
1	A	186	ASP	CA-CB-CG	5.14	124.71	113.40
1	A	16	ASP	CB-CG-OD1	-5.14	113.68	118.30
1	A	440	VAL	CB-CA-C	-5.13	101.65	111.40
1	A	271	ILE	O-C-N	-5.13	114.49	122.70
1	D	196	MET	CG-SD-CE	5.13	108.41	100.20
1	D	176	THR	C-N-CA	5.13	134.52	121.70
1	A	395	MET	CB-CA-C	-5.12	100.15	110.40
1	C	58	SER	CB-CA-C	-5.12	100.36	110.10
1	B	16	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	143	SER	O-C-N	-5.11	114.52	122.70
1	A	147	ALA	N-CA-CB	5.11	117.26	110.10
1	D	267	ARG	C-N-CA	-5.11	111.58	122.30
1	D	175	GLU	CG-CD-OE2	-5.11	108.09	118.30
1	D	85	ASP	CB-CG-OD1	-5.10	113.71	118.30
1	D	382	ASN	N-CA-CB	-5.10	101.42	110.60
1	A	167	ALA	CA-C-N	5.09	128.39	117.20
1	B	19	HIS	CA-CB-CG	-5.08	104.96	113.60
1	D	546	GLY	CA-C-O	5.08	129.75	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	395	MET	CA-CB-CG	5.08	121.94	113.30
1	A	330	LYS	CD-CE-NZ	5.08	123.38	111.70
1	B	11	GLU	OE1-CD-OE2	-5.07	117.22	123.30
1	C	9	HIS	CB-CA-C	-5.07	100.27	110.40
1	A	417	TYR	CB-CG-CD1	-5.07	117.96	121.00
1	B	301	TYR	CA-CB-CG	5.06	123.01	113.40
1	D	240	VAL	CB-CA-C	-5.05	101.80	111.40
1	B	298	THR	CA-C-N	5.05	126.30	116.20
1	D	350	GLN	CA-CB-CG	5.04	124.49	113.40
1	A	51	ALA	N-CA-CB	-5.04	103.04	110.10
1	C	247	THR	N-CA-CB	5.04	119.88	110.30
1	D	200	ARG	C-N-CA	5.03	134.28	121.70
1	C	150	LYS	CB-CA-C	5.03	120.45	110.40
1	A	72	SER	O-C-N	-5.02	114.67	122.70
1	D	235	MET	N-CA-CB	5.02	119.64	110.60
1	A	282	GLU	N-CA-CB	-5.01	101.58	110.60
1	A	556	TYR	CA-CB-CG	-5.01	103.87	113.40
1	C	225	MET	CB-CG-SD	5.01	127.44	112.40
1	D	83	TYR	CB-CG-CD2	5.01	124.01	121.00
1	A	162	GLY	CA-C-N	5.01	128.21	117.20
1	D	563	SER	CA-CB-OG	5.01	124.72	111.20
1	D	468	ASN	CB-CG-OD1	5.00	131.60	121.60
1	D	563	SER	CB-CA-C	5.00	119.61	110.10

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	146	ASP	Mainchain
1	A	491	ALA	Mainchain,Peptide
1	B	491	ALA	Mainchain,Peptide
1	C	477	ALA	Mainchain
1	C	491	ALA	Mainchain,Peptide
1	D	491	ALA	Mainchain,Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4124	0	4013	181	1
1	B	4093	0	3976	179	0
1	C	4099	0	3977	192	2
1	D	4113	0	3987	210	1
2	A	172	0	120	15	0
2	B	172	0	120	17	0
2	C	172	0	120	13	0
2	D	172	0	120	19	0
3	A	53	0	31	9	0
3	B	53	0	31	8	0
3	C	53	0	31	12	0
3	D	53	0	30	9	0
4	B	5	0	0	1	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
5	A	48	0	0	2	0
5	B	29	0	0	3	0
5	C	30	0	0	2	0
5	D	19	0	0	2	0
All	All	17470	0	16556	789	2

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 23.

All (789) 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:D:70:CYS:SG	2:D:602:HEM:HAB	1.27	1.72
1:D:18:CYS:SG	2:D:603:HEM:HAC	1.21	1.71
1:D:41:CYS:SG	2:D:604:HEM:HAC	1.13	1.70
1:B:87:CYS:SG	2:B:601:HEM:HAC	1.33	1.68
3:B:700:FAD:C2'	3:B:700:FAD:C1'	1.77	1.62
3:D:900:FAD:C1'	3:D:900:FAD:C2'	1.78	1.59
3:A:600:FAD:C2'	3:A:600:FAD:C1'	1.78	1.57
3:C:800:FAD:C2'	3:C:800:FAD:C1'	1.78	1.56
1:A:41:CYS:SG	2:A:604:HEM:HAC	1.46	1.55
1:C:87:CYS:SG	2:C:601:HEM:HAC	1.46	1.53
1:B:73:CYS:SG	2:B:602:HEM:HAC	1.48	1.51
1:D:73:CYS:SG	2:D:602:HEM:HAC	1.50	1.51
1:D:18:CYS:SG	2:D:603:HEM:CAC	2.12	1.34
1:B:73:CYS:SG	2:B:602:HEM:CAC	2.15	1.33
1:C:379:VAL:HG11	1:C:418:LEU:HD13	1.45	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:CYS:HG	2:D:603:HEM:HAC	1.22	0.95
1:A:288:VAL:HG23	1:A:526:ILE:HD11	1.46	0.95
1:D:64:LEU:HD13	1:D:159:ILE:HD12	1.53	0.91
1:C:35:ASN:HD21	1:C:71:THR:H	1.16	0.91
1:A:66:GLY:H	1:A:258:GLN:HE22	1.07	0.91
1:A:319:ASN:HD21	1:A:331:GLY:H	1.09	0.91
1:A:452:GLN:HE21	1:A:452:GLN:HA	1.35	0.91
1:A:393:ARG:HH11	1:A:478:GLN:NE2	1.67	0.91
1:A:35:ASN:HD21	1:A:71:THR:H	1.18	0.89
1:B:66:GLY:H	1:B:258:GLN:HE22	1.19	0.89
1:C:319:ASN:HD21	1:C:331:GLY:H	0.94	0.88
1:D:316:ALA:HB1	1:D:502:VAL:HG12	1.55	0.88
1:B:455:VAL:HG21	1:B:460:LEU:HD12	1.53	0.87
1:D:447:GLU:HB3	1:D:457:ALA:HB1	1.57	0.87
1:D:225:MET:HE1	1:D:260:LEU:HD23	1.57	0.84
1:A:41:CYS:HG	2:A:604:HEM:HAC	0.83	0.82
1:C:319:ASN:ND2	1:C:331:GLY:H	1.75	0.82
1:D:31:LEU:HD21	2:D:603:HEM:HAD1	1.62	0.82
1:C:421:ASP:HB2	1:C:488:LEU:HD12	1.61	0.81
1:B:73:CYS:HG	2:B:602:HEM:CAC	1.77	0.81
1:B:125:THR:HG22	1:B:304:LYS:HB3	1.63	0.81
1:D:526:ILE:HG12	1:D:529:LEU:HB2	1.63	0.81
1:D:424:ILE:HD13	1:D:486:ARG:HD2	1.62	0.80
1:A:66:GLY:H	1:A:258:GLN:NE2	1.79	0.80
1:C:392:ASN:HA	1:C:463:THR:HG21	1.64	0.80
1:C:186:ASP:HB2	1:C:240:VAL:HG11	1.64	0.79
1:D:506:MET:CE	1:D:543:ASN:HA	2.13	0.78
1:B:73:CYS:HG	2:B:602:HEM:HAC	0.96	0.78
1:B:409:LEU:HD23	1:B:414:GLU:HB3	1.64	0.78
1:C:280:ILE:HD12	1:C:347:VAL:HG13	1.64	0.77
1:C:181:LYS:H	1:C:181:LYS:HD3	1.48	0.77
1:D:471:VAL:HG22	1:D:484:LEU:HB3	1.63	0.77
1:C:175:GLU:OE2	1:C:188:LYS:HG3	1.84	0.76
1:D:52:ALA:CA	1:D:53:PRO:N	2.48	0.76
1:B:533:GLY:HA2	1:B:553:ILE:HG22	1.65	0.76
1:D:506:MET:HE2	1:D:543:ASN:HA	1.64	0.76
1:C:233:GLY:HA3	1:C:245:ARG:NH2	2.01	0.76
1:C:416:ALA:HB3	1:C:498:ILE:HD11	1.69	0.75
1:B:366:THR:HG22	1:B:498:ILE:HD12	1.68	0.75
1:C:319:ASN:HD21	1:C:331:GLY:N	1.79	0.74
1:C:421:ASP:HB3	1:C:424:ILE:HG12	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:VAL:HG13	1:A:361:ILE:HD13	1.69	0.74
1:A:62:SER:CB	2:A:601:HEM:HBB2	2.18	0.73
1:C:446:ILE:HD13	1:C:464:VAL:HG11	1.71	0.73
1:A:145:ARG:HH11	1:A:268:GLY:H	1.36	0.72
1:B:68:ILE:HD11	2:B:602:HEM:CMC	2.19	0.72
1:B:175:GLU:OE2	1:B:188:LYS:HG3	1.90	0.72
1:A:135:GLY:HA3	1:A:553:ILE:HD12	1.72	0.72
1:A:142:VAL:HG21	1:A:225:MET:HE1	1.71	0.72
1:A:177:LYS:HB2	1:A:178:PRO:HD3	1.71	0.72
1:D:453:ILE:O	1:D:454:ASP:HB2	1.89	0.72
1:D:66:GLY:H	1:D:258:GLN:HE22	1.36	0.71
1:B:319:ASN:HD21	1:B:331:GLY:H	1.36	0.71
1:C:452:GLN:HA	1:C:452:GLN:HE21	1.55	0.71
1:C:409:LEU:HD22	1:C:414:GLU:HB3	1.73	0.71
3:D:900:FAD:N10	3:D:900:FAD:C2'	2.52	0.71
1:A:366:THR:HG22	1:A:498:ILE:HD13	1.72	0.70
1:D:366:THR:HG21	1:D:380:ARG:HE	1.56	0.70
1:D:453:ILE:HG22	1:D:455:VAL:HG13	1.73	0.70
1:C:194:ASP:OD2	1:C:242:ARG:NH2	2.24	0.70
1:D:68:ILE:HD11	2:D:602:HEM:HMC2	1.73	0.70
1:A:41:CYS:SG	2:A:604:HEM:C3C	2.84	0.70
1:A:393:ARG:NH1	1:A:478:GLN:NE2	2.39	0.70
1:D:35:ASN:HD21	1:D:71:THR:H	1.38	0.70
1:C:181:LYS:H	1:C:181:LYS:CD	2.00	0.69
1:D:393:ARG:HD3	1:D:478:GLN:HE22	1.56	0.69
1:B:455:VAL:CG2	1:B:460:LEU:HD12	2.23	0.68
1:B:392:ASN:HA	1:B:463:THR:HG21	1.75	0.68
1:B:550:ILE:HG12	3:B:700:FAD:C2	2.23	0.68
1:A:319:ASN:ND2	1:A:331:GLY:H	1.89	0.68
1:D:455:VAL:HB	1:D:456:PRO:HD2	1.75	0.68
1:A:68:ILE:HD11	2:A:602:HEM:HMC2	1.76	0.68
1:A:117:ALA:HA	1:A:120:ALA:HB3	1.76	0.68
1:B:68:ILE:HD11	2:B:602:HEM:HMC1	1.74	0.68
1:A:186:ASP:HB2	1:A:240:VAL:HG11	1.74	0.68
1:D:52:ALA:O	1:D:53:PRO:N	2.27	0.68
1:B:460:LEU:O	1:B:464:VAL:HG23	1.94	0.67
1:B:549:ALA:HB3	3:B:700:FAD:N1	2.10	0.67
1:C:35:ASN:ND2	1:C:71:THR:H	1.92	0.67
1:A:6:ALA:HA	2:A:603:HEM:HBC2	1.76	0.67
1:B:58:SER:H	1:B:61:LYS:CE	2.06	0.67
1:C:326:ASP:OD2	1:C:328:LYS:HB2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:310:ILE:HD11	1:D:529:LEU:HD21	1.76	0.67
1:C:516:GLU:HG2	5:C:843:HOH:O	1.94	0.67
1:C:129:VAL:HB	1:C:308:VAL:HG22	1.77	0.67
1:C:87:CYS:SG	2:C:601:HEM:C3C	2.87	0.67
3:A:600:FAD:C3'	3:A:600:FAD:C1'	2.71	0.66
1:B:526:ILE:HG12	1:B:529:LEU:HB2	1.78	0.66
1:D:64:LEU:HD13	1:D:159:ILE:CD1	2.23	0.66
1:C:549:ALA:HB3	3:C:800:FAD:N1	2.11	0.66
1:B:58:SER:H	1:B:61:LYS:HE2	1.60	0.66
1:A:393:ARG:HH11	1:A:478:GLN:HE21	1.42	0.66
1:C:163:ASN:HD21	1:C:336:ASN:ND2	1.93	0.66
1:D:72:SER:HB2	1:D:158:PRO:HB2	1.78	0.66
1:A:26:VAL:HG21	1:A:297:TYR:HB3	1.78	0.66
1:D:68:ILE:HD11	2:D:602:HEM:CMC	2.26	0.65
1:A:393:ARG:NH1	1:A:478:GLN:HE21	1.95	0.65
1:B:280:ILE:HG13	1:B:347:VAL:HG13	1.79	0.65
1:A:319:ASN:HD21	1:A:331:GLY:N	1.91	0.65
1:B:446:ILE:HG23	1:B:460:LEU:HD22	1.78	0.65
1:A:62:SER:HB3	2:A:601:HEM:HBB2	1.78	0.65
1:B:321:ARG:NH2	1:B:346:ASP:OD1	2.20	0.65
1:A:468:ASN:ND2	1:A:487:GLU:O	2.30	0.65
1:D:514:LYS:O	1:D:515:ALA:HB3	1.97	0.65
1:B:319:ASN:ND2	1:B:331:GLY:H	1.94	0.64
1:B:28:ASN:C	1:B:28:ASN:HD22	2.00	0.64
1:D:460:LEU:O	1:D:464:VAL:HG23	1.96	0.64
1:D:288:VAL:HG22	1:D:526:ILE:HD11	1.79	0.64
1:D:73:CYS:SG	2:D:602:HEM:C3C	2.89	0.64
1:A:75:LYS:H	1:A:80:SER:HB3	1.62	0.64
1:B:389:ARG:NH2	1:B:413:GLY:HA3	2.13	0.64
1:A:68:ILE:HD11	2:A:602:HEM:CMC	2.27	0.64
1:D:393:ARG:NH1	1:D:467:TYR:HD2	1.94	0.64
1:D:135:GLY:HA3	1:D:553:ILE:HD12	1.80	0.64
1:D:117:ALA:HA	1:D:120:ALA:HB3	1.80	0.64
1:B:471:VAL:HG11	1:B:487:GLU:HA	1.80	0.64
1:C:530:TYR:CE2	1:C:563:SER:HB3	2.32	0.64
1:A:83:TYR:CE1	1:A:159:ILE:HD11	2.34	0.63
1:A:445:THR:OG1	1:A:448:GLU:HB2	1.98	0.63
1:A:26:VAL:HG21	1:A:297:TYR:CB	2.28	0.63
3:C:800:FAD:C3'	3:C:800:FAD:C1'	2.74	0.63
1:C:231:ASP:HB3	1:C:245:ARG:HG3	1.78	0.63
1:C:62:SER:CB	2:C:601:HEM:HBB2	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145:ARG:HH11	1:D:268:GLY:H	1.44	0.63
1:D:154:LEU:HD13	1:D:277:VAL:CG2	2.28	0.63
1:B:362:GLN:NE2	1:B:544:ARG:HH21	1.97	0.63
1:A:127:ASP:HB2	1:A:150:LYS:O	1.96	0.63
1:B:173:ALA:HA	1:B:215:SER:HB2	1.81	0.63
1:B:228:ASP:HB3	1:B:247:THR:OG1	1.98	0.63
1:B:449:LEU:HD22	1:B:495:ALA:HB2	1.81	0.63
1:A:514:LYS:HE3	1:A:516:GLU:OE1	1.99	0.63
3:A:600:FAD:N10	3:A:600:FAD:C2'	2.58	0.63
1:A:387:VAL:O	1:A:416:ALA:HB1	1.98	0.62
1:B:509:LEU:H	1:B:536:THR:HA	1.64	0.62
1:B:35:ASN:HD21	1:B:71:THR:H	1.46	0.62
1:A:106:PRO:HG2	1:A:109:ALA:HB2	1.81	0.62
3:B:700:FAD:C2'	3:B:700:FAD:N10	2.58	0.62
1:C:431:ILE:O	1:C:435:VAL:HG23	1.99	0.62
1:A:392:ASN:HA	1:A:463:THR:HG21	1.79	0.62
1:B:71:THR:HA	1:B:74:HIS:O	1.99	0.62
1:D:20:VAL:HG22	1:D:33:HIS:CG	2.34	0.62
1:B:337:HIS:HB2	1:B:338:PRO:HD2	1.82	0.62
1:A:246:PRO:HD2	1:A:250:ALA:O	2.00	0.62
1:D:52:ALA:O	1:D:52:ALA:CA	2.47	0.62
1:B:450:ALA:HA	1:B:455:VAL:HG22	1.81	0.62
1:C:388:ASN:ND2	1:C:390:GLU:HB2	2.15	0.62
1:D:553:ILE:HG13	1:D:554:VAL:N	2.13	0.62
1:D:52:ALA:CA	1:D:53:PRO:CD	2.79	0.61
2:A:601:HEM:HHA	2:A:601:HEM:HBA1	1.81	0.61
1:C:409:LEU:HA	1:C:414:GLU:HB3	1.82	0.61
1:B:73:CYS:CB	2:B:602:HEM:HAC	2.31	0.61
1:B:154:LEU:HD22	1:B:293:VAL:HG11	1.82	0.61
1:C:445:THR:OG1	1:C:448:GLU:HB2	2.01	0.61
1:D:431:ILE:HA	1:D:434:TYR:CD2	2.36	0.61
1:A:453:ILE:O	1:A:454:ASP:HB2	2.00	0.61
1:B:435:VAL:HG22	1:B:440:VAL:HG21	1.82	0.60
1:D:405:SER:O	1:D:409:LEU:HD12	2.01	0.60
1:D:283:ASP:CG	1:D:284:ALA:H	2.03	0.60
1:B:259:VAL:O	1:B:263:ASN:ND2	2.35	0.60
3:C:800:FAD:C1'	3:C:800:FAD:O2'	2.47	0.60
1:D:41:CYS:SG	2:D:604:HEM:C3C	2.92	0.60
1:A:283:ASP:OD2	1:A:284:ALA:N	2.34	0.60
1:B:332:PHE:HZ	1:B:409:LEU:HD11	1.66	0.60
1:C:155:GLU:OE1	3:C:800:FAD:H1B	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:ASP:OD2	1:C:245:ARG:HD2	2.00	0.60
1:D:70:CYS:SG	2:D:602:HEM:C3B	2.93	0.60
1:A:142:VAL:HG21	1:A:225:MET:CE	2.30	0.60
1:A:35:ASN:ND2	1:A:70:CYS:HB2	2.15	0.60
1:C:62:SER:HB3	2:C:601:HEM:HBB2	1.82	0.60
1:A:153:LEU:HD22	1:A:271:ILE:HG23	1.84	0.60
3:D:900:FAD:C1'	3:D:900:FAD:O2'	2.47	0.60
1:C:409:LEU:HD21	1:C:500:PRO:HG3	1.84	0.59
1:C:558:ARG:HG2	1:C:558:ARG:HH11	1.66	0.59
1:B:467:TYR:HA	1:B:470:PHE:CD2	2.36	0.59
1:C:389:ARG:HD2	1:C:412:LYS:CB	2.31	0.59
1:C:467:TYR:HA	1:C:470:PHE:CD2	2.37	0.59
1:C:131:ILE:HG12	1:C:277:VAL:HG21	1.83	0.59
1:C:388:ASN:HB3	1:C:411:GLN:HE21	1.67	0.59
1:C:514:LYS:O	1:C:515:ALA:HB3	2.03	0.59
1:C:68:ILE:O	1:C:68:ILE:HG13	2.02	0.59
1:A:294:LYS:HB2	1:A:300:TYR:CE2	2.38	0.59
1:B:527:THR:HG22	1:B:567:PHE:CZ	2.37	0.59
1:D:234:ARG:HB2	1:D:241:ASN:OD1	2.02	0.59
1:C:166:LEU:HD13	2:C:601:HEM:HMD2	1.84	0.59
1:D:218:SER:HB3	1:D:554:VAL:HG12	1.85	0.59
1:D:49:ALA:HB1	1:D:61:LYS:HB3	1.84	0.59
1:B:375:ILE:HG21	1:B:418:LEU:HD11	1.84	0.58
1:B:421:ASP:HB3	1:B:424:ILE:HG12	1.85	0.58
1:B:68:ILE:HG13	1:B:68:ILE:O	2.03	0.58
1:B:375:ILE:HG12	1:B:496:LEU:HD22	1.85	0.58
1:A:145:ARG:NH1	1:A:268:GLY:H	1.99	0.58
1:A:163:ASN:HD21	1:A:336:ASN:ND2	2.01	0.58
1:A:514:LYS:HE3	1:A:516:GLU:CD	2.24	0.58
3:B:700:FAD:C3'	3:B:700:FAD:C1'	2.76	0.58
1:A:170:GLY:HA2	1:A:252:VAL:HG21	1.85	0.58
1:C:87:CYS:O	1:C:372:GLY:HA3	2.03	0.58
1:B:375:ILE:HG21	1:B:418:LEU:CD1	2.33	0.58
1:D:470:PHE:CG	1:D:476:ASP:HA	2.39	0.58
1:C:375:ILE:HG13	1:C:496:LEU:HD22	1.86	0.58
1:D:35:ASN:ND2	1:D:70:CYS:H	2.01	0.58
1:C:558:ARG:HH11	1:C:558:ARG:CG	2.15	0.58
1:D:159:ILE:HG13	5:D:930:HOH:O	2.04	0.58
1:D:453:ILE:HD11	1:D:495:ALA:CB	2.34	0.57
3:D:900:FAD:C1'	3:D:900:FAD:C3'	2.74	0.57
1:C:343:ASP:HB3	3:C:800:FAD:H61A	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:GLN:NE2	1:A:452:GLN:HA	2.11	0.57
1:B:196:MET:CE	1:B:203:ASN:HB2	2.33	0.57
1:C:294:LYS:O	1:C:294:LYS:HG3	2.04	0.57
1:B:66:GLY:H	1:B:258:GLN:NE2	1.97	0.57
1:D:326:ASP:OD2	1:D:328:LYS:HG3	2.04	0.57
1:C:118:ILE:CD1	1:C:279:ARG:NH1	2.67	0.57
3:C:800:FAD:N10	3:C:800:FAD:C2'	2.63	0.57
1:D:83:TYR:CE1	1:D:159:ILE:HD13	2.39	0.57
1:A:470:PHE:CG	1:A:476:ASP:HA	2.40	0.57
1:A:517:VAL:HG21	1:A:529:LEU:HD22	1.87	0.57
1:B:455:VAL:HB	1:B:456:PRO:HD2	1.87	0.57
1:B:42:HIS:HB2	2:B:602:HEM:HMB2	1.86	0.56
1:A:293:VAL:HG21	1:A:303:ILE:HD12	1.86	0.56
1:A:71:THR:HA	1:A:74:HIS:O	2.05	0.56
1:B:228:ASP:OD1	1:B:247:THR:HG21	2.06	0.56
1:D:470:PHE:HA	1:D:475:LYS:O	2.05	0.56
1:B:114:GLN:HE21	1:B:279:ARG:HH21	1.54	0.56
1:D:516:GLU:HG2	1:D:525:PRO:HB3	1.87	0.56
1:D:192:ILE:HG23	1:D:208:VAL:HG12	1.88	0.56
1:C:409:LEU:CD2	1:C:414:GLU:HB3	2.36	0.56
1:C:388:ASN:HD22	1:C:390:GLU:H	1.53	0.56
1:A:28:ASN:HD21	1:A:32:THR:H	1.53	0.56
1:D:506:MET:HE3	1:D:543:ASN:HA	1.88	0.56
1:A:388:ASN:HD21	1:A:392:ASN:HB2	1.71	0.56
1:B:230:THR:OG1	1:B:247:THR:HG23	2.06	0.56
1:C:453:ILE:CG2	1:C:455:VAL:HG13	2.36	0.56
1:D:319:ASN:ND2	1:D:331:GLY:H	2.04	0.56
1:C:6:ALA:HA	2:C:603:HEM:HBC2	1.88	0.55
1:A:470:PHE:HB3	1:A:476:ASP:HA	1.87	0.55
1:B:102:ARG:NH2	1:B:157:GLU:OE1	2.39	0.55
1:B:403:LYS:O	1:B:406:ALA:HB3	2.06	0.55
1:C:421:ASP:HB3	1:C:424:ILE:CG1	2.36	0.55
1:C:453:ILE:O	1:C:454:ASP:HB2	2.07	0.55
1:D:393:ARG:HD3	1:D:478:GLN:NE2	2.20	0.55
1:B:234:ARG:HB2	1:B:241:ASN:OD1	2.07	0.55
1:D:403:LYS:O	1:D:406:ALA:HB3	2.07	0.55
1:B:122:VAL:HG22	1:B:302:VAL:HG11	1.89	0.55
1:C:380:ARG:HA	1:C:384:ALA:HB3	1.88	0.55
1:C:420:PHE:CE2	1:C:431:ILE:HG21	2.42	0.55
1:D:384:ALA:HB2	1:D:420:PHE:HB3	1.89	0.55
1:B:366:THR:HA	1:B:498:ILE:HB	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:376:THR:HG23	1:C:379:VAL:H	1.71	0.55
1:C:240:VAL:HG12	1:C:241:ASN:N	2.21	0.55
1:C:281:LEU:N	1:C:290:GLY:O	2.26	0.55
1:D:52:ALA:CA	1:D:53:PRO:HD3	2.37	0.55
1:C:376:THR:HG22	1:C:379:VAL:HG23	1.89	0.54
1:C:452:GLN:HA	1:C:452:GLN:NE2	2.21	0.54
1:C:471:VAL:CG1	1:C:487:GLU:HG3	2.37	0.54
1:D:19:HIS:ND1	1:D:34:GLU:OE2	2.40	0.54
1:A:461:ALA:O	1:A:465:THR:HG23	2.07	0.54
1:D:468:ASN:OD1	1:D:487:GLU:HB3	2.06	0.54
1:A:367:TYR:HB3	1:A:499:ALA:O	2.07	0.54
1:C:375:ILE:HG21	1:C:418:LEU:CD1	2.37	0.54
1:A:393:ARG:HH11	1:A:478:GLN:HE22	1.53	0.54
1:B:540:HIS:ND1	1:B:544:ARG:HG3	2.23	0.54
1:D:175:GLU:OE2	1:D:188:LYS:HG3	2.07	0.54
1:D:198:GLY:HA3	1:D:545:LEU:HD21	1.89	0.54
1:D:421:ASP:OD2	1:D:424:ILE:HG12	2.08	0.54
1:A:79:LYS:HG2	1:A:96:PHE:O	2.08	0.54
1:D:322:VAL:HG22	1:D:361:ILE:HD13	1.89	0.54
1:D:78:GLU:O	1:D:79:LYS:C	2.45	0.54
1:B:325:TYR:O	2:D:604:HEM:HMD2	2.08	0.54
1:A:343:ASP:HB2	5:A:609:HOH:O	2.08	0.54
1:A:459:GLU:O	1:A:463:THR:HG23	2.07	0.54
1:A:231:ASP:HB3	1:A:245:ARG:HG2	1.89	0.53
1:A:172:ASN:OD1	1:A:548:ASN:ND2	2.41	0.53
1:B:393:ARG:HD3	1:B:478:GLN:NE2	2.23	0.53
1:C:385:ILE:HG12	1:C:488:LEU:HD21	1.89	0.53
1:A:367:TYR:O	1:A:369:PRO:HD3	2.08	0.53
1:A:504:HIS:CD2	1:A:544:ARG:HE	2.27	0.53
3:A:600:FAD:O2'	3:A:600:FAD:C1'	2.51	0.53
1:B:319:ASN:HD21	1:B:330:LYS:HA	1.74	0.53
1:D:145:ARG:HG2	1:D:151:VAL:CG2	2.39	0.53
1:D:145:ARG:NH1	1:D:268:GLY:H	2.06	0.53
1:B:196:MET:HE3	1:B:203:ASN:HB2	1.90	0.53
1:B:527:THR:HG22	1:B:567:PHE:HZ	1.72	0.53
1:C:187:LYS:HB2	1:C:190:ILE:CD1	2.38	0.53
1:C:420:PHE:CE2	1:C:431:ILE:HD13	2.43	0.53
1:C:453:ILE:HG21	1:C:455:VAL:HG13	1.90	0.53
1:C:461:ALA:O	1:C:465:THR:HG22	2.09	0.53
1:A:245:ARG:HD3	1:A:249:GLY:HA2	1.90	0.53
1:B:446:ILE:CD1	1:B:464:VAL:HG11	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:SER:HB3	1:B:61:LYS:HE3	1.91	0.53
1:D:376:THR:OG1	1:D:377:GLU:N	2.41	0.53
1:D:62:SER:CB	2:D:601:HEM:HBB2	2.38	0.53
1:A:317:LYS:HB3	1:A:340:ALA:O	2.09	0.53
1:C:187:LYS:HB2	1:C:190:ILE:HD12	1.90	0.53
1:A:550:ILE:HA	1:A:553:ILE:HG12	1.90	0.53
1:B:455:VAL:HB	1:B:456:PRO:CD	2.39	0.53
1:B:393:ARG:HD3	1:B:478:GLN:HE22	1.73	0.53
1:C:172:ASN:O	1:C:551:SER:OG	2.26	0.53
1:D:389:ARG:HG3	1:D:389:ARG:HH11	1.73	0.53
1:A:176:THR:HB	1:A:178:PRO:HD2	1.89	0.52
1:A:167:ALA:HA	3:A:600:FAD:N5	2.24	0.52
1:D:179:GLN:NE2	1:D:242:ARG:HB3	2.23	0.52
1:A:206:GLU:HA	1:A:209:LYS:HD2	1.90	0.52
1:B:450:ALA:HA	1:B:455:VAL:CG2	2.40	0.52
1:B:544:ARG:HD2	1:B:549:ALA:HB2	1.91	0.52
1:C:173:ALA:HA	1:C:215:SER:HB2	1.91	0.52
1:C:315:PHE:CD1	1:C:321:ARG:HG2	2.45	0.52
1:C:429:LYS:O	1:C:430:ALA:C	2.47	0.52
1:A:458:ALA:O	1:A:462:LYS:HB2	2.09	0.52
1:B:376:THR:HG22	1:B:434:TYR:OH	2.10	0.52
1:B:288:VAL:CG2	1:B:526:ILE:HD11	2.39	0.52
1:A:35:ASN:HD22	1:A:70:CYS:HB2	1.75	0.52
1:D:377:GLU:OE1	1:D:401:ARG:HD3	2.10	0.52
1:D:467:TYR:O	1:D:470:PHE:HB2	2.09	0.52
1:D:446:ILE:HD13	1:D:464:VAL:HG11	1.92	0.52
1:D:233:GLY:HA3	1:D:245:ARG:NH2	2.24	0.52
1:B:283:ASP:CG	1:B:284:ALA:H	2.13	0.52
1:D:28:ASN:HD22	1:D:28:ASN:C	2.12	0.51
1:A:550:ILE:O	1:A:554:VAL:HG23	2.09	0.51
1:C:8:PHE:HE2	2:C:604:HEM:HHA	1.75	0.51
1:D:192:ILE:HD13	1:D:209:LYS:HG2	1.92	0.51
1:C:450:ALA:HA	1:C:455:VAL:CG2	2.40	0.51
1:B:6:ALA:HA	2:B:603:HEM:HBC2	1.92	0.51
3:B:700:FAD:O2'	3:B:700:FAD:C1'	2.52	0.51
1:A:68:ILE:C	1:A:68:ILE:HD12	2.30	0.51
1:B:187:LYS:HB2	1:B:190:ILE:HD12	1.91	0.51
1:C:387:VAL:HG12	1:C:388:ASN:O	2.10	0.51
1:C:394:PHE:O	1:C:395:MET:HB3	2.09	0.51
1:D:441:LYS:O	1:D:494:TYR:HA	2.11	0.51
1:D:498:ILE:O	1:D:498:ILE:HD12	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:ILE:HG12	1:A:529:LEU:HB2	1.93	0.51
1:B:175:GLU:HG2	1:B:186:ASP:O	2.10	0.51
1:B:362:GLN:NE2	1:B:544:ARG:NH2	2.58	0.51
1:B:446:ILE:HD11	1:B:464:VAL:HG11	1.92	0.51
1:C:37:GLN:O	1:C:40:SER:HB2	2.11	0.51
1:D:80:SER:O	1:D:97:GLY:HA2	2.11	0.51
1:B:362:GLN:HE22	1:B:544:ARG:NH2	2.09	0.51
1:C:374:MET:HE1	3:C:800:FAD:H6	1.92	0.51
1:C:455:VAL:HB	1:C:456:PRO:HD2	1.91	0.51
1:C:450:ALA:HA	1:C:455:VAL:HG22	1.93	0.51
1:D:368:SER:HB2	1:D:375:ILE:HD13	1.92	0.51
1:D:428:LEU:HB3	1:D:431:ILE:HG13	1.91	0.51
1:A:366:THR:HA	1:A:498:ILE:HB	1.92	0.51
1:B:62:SER:HB3	2:B:601:HEM:HBB2	1.93	0.51
1:A:322:VAL:HG13	1:A:361:ILE:HG21	1.93	0.50
1:C:270:ASP:OD1	1:C:272:ARG:NH2	2.43	0.50
1:D:453:ILE:CG2	1:D:455:VAL:HG13	2.41	0.50
1:A:35:ASN:ND2	1:A:71:THR:H	1.99	0.50
1:B:394:PHE:O	1:B:395:MET:HB3	2.11	0.50
1:B:540:HIS:CG	1:B:544:ARG:HG3	2.47	0.50
1:D:155:GLU:HB3	1:D:273:LEU:CD2	2.42	0.50
1:D:280:ILE:HG23	1:D:288:VAL:HG13	1.93	0.50
1:A:80:SER:O	1:A:97:GLY:HA2	2.11	0.50
1:B:441:LYS:HB2	1:B:495:ALA:HB3	1.93	0.50
1:A:181:LYS:HE3	1:A:181:LYS:H	1.77	0.50
1:A:236:GLY:N	1:A:377:GLU:OE2	2.27	0.50
1:B:153:LEU:HD22	1:B:271:ILE:HG23	1.93	0.50
1:A:135:GLY:O	1:A:136:ALA:C	2.49	0.50
1:A:388:ASN:ND2	1:A:392:ASN:H	2.09	0.50
1:B:388:ASN:OD1	1:B:411:GLN:NE2	2.44	0.50
1:C:277:VAL:HG13	1:C:291:VAL:CG2	2.42	0.50
1:D:453:ILE:HD11	1:D:495:ALA:HB3	1.94	0.50
1:B:335:THR:HG22	1:B:367:TYR:CD2	2.46	0.50
1:C:526:ILE:HG12	1:C:529:LEU:HB2	1.92	0.50
1:D:383:GLY:HA3	1:D:424:ILE:HD12	1.94	0.50
1:C:376:THR:CG2	1:C:378:ALA:HB3	2.41	0.50
1:D:385:ILE:HD13	1:D:488:LEU:HD13	1.94	0.50
1:C:28:ASN:C	1:C:28:ASN:HD22	2.16	0.49
1:A:446:ILE:HD11	1:A:493:PHE:CZ	2.47	0.49
1:B:394:PHE:HD1	1:B:407:ALA:HB1	1.76	0.49
1:C:399:THR:CG2	1:C:404:ALA:HB2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:31:LEU:HD21	2:D:603:HEM:CAD	2.39	0.49
1:D:380:ARG:HH11	1:D:380:ARG:HB2	1.77	0.49
1:A:187:LYS:HB2	1:A:190:ILE:HG13	1.94	0.49
1:B:194:ASP:OD2	1:B:242:ARG:NH2	2.45	0.49
1:A:246:PRO:HG3	1:A:255:HIS:CD2	2.47	0.49
1:D:468:ASN:OD1	1:D:487:GLU:OE1	2.30	0.49
1:A:234:ARG:HG3	1:A:235:MET:N	2.27	0.49
1:A:422:ASP:OD1	1:A:494:TYR:OH	2.22	0.49
1:B:228:ASP:O	1:B:246:PRO:HA	2.12	0.49
1:C:203:ASN:O	1:C:205:PRO:HD3	2.12	0.49
1:C:386:VAL:HG22	1:C:418:LEU:HD23	1.95	0.49
1:A:171:MET:HB2	1:A:550:ILE:HB	1.93	0.49
1:A:177:LYS:HE3	1:A:220:ASP:OD2	2.11	0.49
1:D:207:LEU:O	1:D:211:LEU:HB2	2.13	0.49
1:A:39:VAL:HG13	1:A:44:ASP:HB3	1.95	0.49
1:B:263:ASN:O	1:B:267:ARG:HG2	2.13	0.49
1:B:368:SER:OG	1:B:371:GLY:N	2.38	0.49
1:A:368:SER:HB2	1:A:375:ILE:HD13	1.93	0.49
1:B:5:LEU:HD22	1:B:9:HIS:CE1	2.48	0.49
3:C:800:FAD:O2'	3:C:800:FAD:C9A	2.61	0.49
1:D:349:LEU:HD21	1:D:355:THR:CG2	2.43	0.49
1:D:549:ALA:HB3	3:D:900:FAD:N1	2.27	0.49
1:A:154:LEU:HD23	1:A:272:ARG:HB2	1.95	0.48
1:C:346:ASP:O	1:C:350:GLN:HG2	2.12	0.48
1:A:127:ASP:O	1:A:305:ALA:HB1	2.13	0.48
1:B:389:ARG:HH21	1:B:413:GLY:HA3	1.79	0.48
1:B:5:LEU:HD23	1:B:96:PHE:CE1	2.49	0.48
1:B:453:ILE:HD11	1:B:495:ALA:HB2	1.94	0.48
1:A:293:VAL:CG2	1:A:303:ILE:HD12	2.43	0.48
1:C:240:VAL:CG1	1:C:241:ASN:N	2.76	0.48
1:C:367:TYR:HB3	1:C:499:ALA:O	2.14	0.48
1:D:128:VAL:HG22	1:D:307:ALA:HB3	1.94	0.48
1:D:459:GLU:HA	1:D:459:GLU:OE1	2.13	0.48
1:D:73:CYS:SG	2:D:602:HEM:CBC	2.89	0.48
1:A:175:GLU:OE2	1:A:188:LYS:HG3	2.13	0.48
1:A:360:TYR:CD2	1:A:542:ALA:HB1	2.49	0.48
1:A:52:ALA:HB1	1:A:53:PRO:HD2	1.94	0.48
1:B:505:THR:HB	5:B:732:HOH:O	2.13	0.48
1:C:291:VAL:HG12	1:C:303:ILE:HB	1.95	0.48
1:A:109:ALA:O	1:A:110:ASP:CB	2.61	0.48
1:A:326:ASP:OD2	1:A:328:LYS:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:GLU:O	1:B:324:LYS:HG3	2.13	0.48
1:B:533:GLY:CA	1:B:553:ILE:HG22	2.38	0.48
1:D:205:PRO:O	1:D:209:LYS:HG3	2.13	0.48
1:D:249:GLY:O	1:D:250:ALA:CB	2.62	0.48
1:D:267:ARG:HH21	1:D:267:ARG:HG3	1.78	0.48
1:B:337:HIS:CE1	1:B:339:GLY:H	2.32	0.48
1:C:459:GLU:OE1	1:C:459:GLU:HA	2.14	0.48
1:D:102:ARG:NH2	1:D:157:GLU:OE1	2.47	0.48
1:D:196:MET:CE	1:D:203:ASN:HB2	2.44	0.48
1:B:468:ASN:O	1:B:471:VAL:HB	2.14	0.48
1:C:533:GLY:HA2	1:C:553:ILE:HG22	1.96	0.48
1:D:114:GLN:O	1:D:118:ILE:HG13	2.13	0.48
2:A:601:HEM:CHA	2:A:601:HEM:HBA1	2.44	0.48
1:A:72:SER:HB2	1:A:158:PRO:HB2	1.95	0.48
1:C:421:ASP:HB3	1:C:424:ILE:CD1	2.44	0.48
1:D:225:MET:HE1	1:D:260:LEU:CD2	2.37	0.48
1:A:310:ILE:CD1	1:A:529:LEU:HD21	2.43	0.47
1:B:115:ASP:HA	1:B:118:ILE:HD12	1.96	0.47
1:C:376:THR:HG21	1:C:428:LEU:HD21	1.95	0.47
1:D:421:ASP:HB2	1:D:490:VAL:O	2.13	0.47
1:D:418:LEU:O	1:D:495:ALA:HA	2.14	0.47
1:A:41:CYS:HG	2:A:604:HEM:CAC	1.78	0.47
3:B:700:FAD:H1'1	3:B:700:FAD:H9	1.60	0.47
1:B:429:LYS:O	1:B:432:GLU:HB2	2.14	0.47
1:C:375:ILE:HG21	1:C:418:LEU:HD11	1.94	0.47
1:C:446:ILE:CD1	1:C:464:VAL:HG11	2.43	0.47
1:B:433:GLY:CA	2:B:601:HEM:HBA2	2.44	0.47
1:C:10:GLY:HA2	1:C:14:GLY:HA2	1.95	0.47
1:A:167:ALA:HA	3:A:600:FAD:C6	2.43	0.47
1:A:56:LYS:HB3	1:A:57:VAL:HG23	1.96	0.47
1:C:249:GLY:O	1:C:250:ALA:HB3	2.15	0.47
1:D:463:THR:O	1:D:464:VAL:C	2.52	0.47
1:B:428:LEU:O	1:B:429:LYS:C	2.53	0.47
1:C:87:CYS:SG	2:C:601:HEM:CBC	2.90	0.47
1:D:156:LYS:HD3	3:D:900:FAD:C4A	2.44	0.47
1:D:249:GLY:O	1:D:250:ALA:HB3	2.15	0.47
1:D:293:VAL:O	1:D:300:TYR:HA	2.15	0.47
1:D:506:MET:HG3	1:D:540:HIS:HB2	1.96	0.47
1:D:510:VAL:HG12	1:D:518:LYS:HG3	1.96	0.47
1:C:154:LEU:HD22	1:C:293:VAL:HG11	1.96	0.47
1:D:28:ASN:ND2	1:D:31:LEU:H	2.11	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:ILE:C	1:D:68:ILE:HD12	2.34	0.47
1:A:174:ALA:O	1:A:175:GLU:HB2	2.15	0.47
1:C:192:ILE:HD13	1:C:209:LYS:HG2	1.96	0.47
1:C:68:ILE:HA	5:C:824:HOH:O	2.15	0.47
1:D:319:ASN:HD21	1:D:331:GLY:H	1.61	0.47
1:A:133:SER:HB3	1:A:155:GLU:HB2	1.96	0.47
2:B:603:HEM:HHA	2:B:603:HEM:HBA2	1.97	0.47
1:C:358:LEU:HA	1:C:507:GLY:HA3	1.96	0.47
1:C:549:ALA:CB	3:C:800:FAD:H1'2	2.45	0.47
1:C:59:PRO:HG3	2:C:602:HEM:CMD	2.45	0.47
1:D:145:ARG:HG2	1:D:151:VAL:HG21	1.95	0.47
1:D:173:ALA:HA	1:D:215:SER:HB2	1.96	0.47
1:A:5:LEU:HD23	1:A:96:PHE:CE1	2.50	0.47
1:B:279:ARG:HB3	1:B:292:LEU:HB3	1.97	0.47
1:B:431:ILE:O	1:B:431:ILE:HG22	2.15	0.47
1:C:245:ARG:HA	1:C:252:VAL:HG13	1.97	0.47
1:C:421:ASP:OD1	1:C:490:VAL:O	2.33	0.47
1:B:20:VAL:HG22	1:B:33:HIS:CD2	2.50	0.47
1:C:395:MET:HG2	1:C:396:ASN:N	2.28	0.47
1:C:498:ILE:O	1:C:498:ILE:HD12	2.15	0.47
1:D:364:HIS:O	1:D:500:PRO:HA	2.15	0.47
1:A:170:GLY:HA2	1:A:252:VAL:CG2	2.45	0.46
1:B:356:ARG:NH1	1:B:357:ASP:OD2	2.44	0.46
1:B:361:ILE:HG22	1:B:361:ILE:O	2.15	0.46
1:B:35:ASN:ND2	1:B:70:CYS:H	2.14	0.46
1:C:146:ASP:CG	1:C:267:ARG:HH11	2.18	0.46
1:D:225:MET:CE	1:D:260:LEU:HD23	2.38	0.46
1:A:198:GLY:O	1:A:543:ASN:HB3	2.15	0.46
1:A:356:ARG:NE	1:A:357:ASP:OD2	2.43	0.46
1:B:240:VAL:HG13	1:B:241:ASN:N	2.29	0.46
1:B:231:ASP:HB3	1:B:245:ARG:HG3	1.97	0.46
1:C:422:ASP:OD1	1:C:492:PRO:HD2	2.15	0.46
1:D:26:VAL:HG21	1:D:297:TYR:HB3	1.97	0.46
1:D:235:MET:HE3	1:D:547:GLY:N	2.31	0.46
1:A:142:VAL:O	1:A:143:SER:C	2.54	0.46
1:B:28:ASN:C	1:B:28:ASN:ND2	2.69	0.46
1:C:421:ASP:OD1	1:C:422:ASP:N	2.47	0.46
1:D:424:ILE:HD11	1:D:486:ARG:HB2	1.97	0.46
1:A:206:GLU:OE2	1:A:209:LYS:NZ	2.48	0.46
1:A:235:MET:SD	1:A:377:GLU:HB3	2.56	0.46
1:A:504:HIS:CG	1:A:544:ARG:HE	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:PRO:O	1:B:273:LEU:HD13	2.16	0.46
1:B:402:ASP:OD1	1:B:403:LYS:N	2.44	0.46
1:B:44:ASP:OD2	1:B:44:ASP:C	2.53	0.46
1:C:26:VAL:HG21	1:C:297:TYR:HB3	1.96	0.46
1:D:367:TYR:O	1:D:369:PRO:HD3	2.15	0.46
1:D:52:ALA:HB3	1:D:52:ALA:O	2.16	0.46
3:D:900:FAD:H1'1	5:D:922:HOH:O	2.14	0.46
1:A:517:VAL:CG2	1:A:529:LEU:HD22	2.45	0.46
1:A:177:LYS:HG3	5:A:650:HOH:O	2.15	0.46
1:C:393:ARG:NH1	1:C:467:TYR:HD2	2.14	0.46
3:A:600:FAD:O3'	3:A:600:FAD:C1'	2.64	0.46
1:B:222:LEU:HD13	1:B:256:VAL:HG22	1.97	0.46
1:B:481:ARG:HA	1:B:482:PRO:HD3	1.79	0.46
1:C:164:THR:O	1:C:253:GLY:HA3	2.15	0.46
1:C:409:LEU:HD21	1:C:500:PRO:CG	2.46	0.46
1:C:420:PHE:HE2	1:C:431:ILE:HG21	1.80	0.46
1:A:118:ILE:HD13	1:A:281:LEU:CD2	2.46	0.46
1:A:375:ILE:HG12	1:A:496:LEU:HD22	1.98	0.46
1:D:376:THR:HG22	1:D:434:TYR:OH	2.15	0.46
1:A:282:GLU:O	1:A:283:ASP:HB3	2.15	0.46
1:C:177:LYS:O	1:C:181:LYS:HG2	2.15	0.46
1:C:184:ILE:HD13	1:C:241:ASN:CB	2.46	0.46
1:C:422:ASP:HB2	1:C:492:PRO:HD2	1.97	0.46
1:A:266:LYS:O	1:A:266:LYS:HG2	2.15	0.46
1:A:368:SER:HB2	1:A:375:ILE:CD1	2.46	0.46
1:C:163:ASN:ND2	1:C:336:ASN:ND2	2.62	0.46
1:D:291:VAL:HG12	1:D:303:ILE:HB	1.97	0.46
1:D:4:VAL:O	1:D:5:LEU:C	2.52	0.46
1:D:5:LEU:HD23	1:D:96:PHE:CD1	2.50	0.46
1:A:170:GLY:CA	1:A:252:VAL:HG21	2.45	0.45
1:A:422:ASP:O	1:A:426:LYS:HG3	2.15	0.45
1:A:48:LEU:HD13	1:A:60:HIS:CE1	2.51	0.45
1:C:556:TYR:O	1:C:557:GLY:C	2.54	0.45
1:D:251:GLY:O	1:D:252:VAL:C	2.54	0.45
1:C:393:ARG:O	1:C:394:PHE:HB3	2.16	0.45
1:C:471:VAL:HG11	1:C:487:GLU:HG3	1.96	0.45
1:A:186:ASP:CB	1:A:240:VAL:HG11	2.43	0.45
1:B:145:ARG:HH11	1:B:268:GLY:H	1.64	0.45
1:B:366:THR:HG21	1:B:380:ARG:HE	1.81	0.45
1:C:407:ALA:O	1:C:411:GLN:HG2	2.16	0.45
1:C:68:ILE:HD11	2:C:602:HEM:HMC3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:512:ASP:OD2	1:B:516:GLU:OE2	2.34	0.45
1:B:68:ILE:HD12	1:B:68:ILE:C	2.37	0.45
1:C:330:LYS:HB2	1:C:330:LYS:NZ	2.31	0.45
1:D:195:THR:HG22	1:D:203:ASN:ND2	2.31	0.45
1:D:240:VAL:O	1:D:242:ARG:HG2	2.16	0.45
1:D:471:VAL:HG11	1:D:487:GLU:HG2	1.97	0.45
1:C:109:ALA:O	1:C:110:ASP:CB	2.63	0.45
1:C:402:ASP:OD1	1:C:402:ASP:N	2.44	0.45
1:C:429:LYS:O	1:C:431:ILE:N	2.50	0.45
1:B:135:GLY:HA3	1:B:553:ILE:HD12	1.99	0.45
1:C:153:LEU:C	1:C:153:LEU:HD23	2.36	0.45
1:C:512:ASP:OD1	1:C:514:LYS:N	2.39	0.45
1:D:378:ALA:O	1:D:382:ASN:HB2	2.17	0.45
1:D:514:LYS:O	1:D:515:ALA:CB	2.64	0.45
1:A:145:ARG:HG2	1:A:151:VAL:CG2	2.46	0.45
1:A:544:ARG:HD2	1:A:549:ALA:HB2	1.97	0.45
1:B:326:ASP:OD2	1:B:328:LYS:HG3	2.16	0.45
1:C:28:ASN:HD21	1:C:32:THR:H	1.65	0.45
1:D:118:ILE:HD12	1:D:279:ARG:NH1	2.31	0.45
1:B:267:ARG:HG2	1:B:267:ARG:H	1.63	0.45
1:B:510:VAL:HA	5:B:734:HOH:O	2.16	0.45
1:D:232:VAL:HA	1:D:243:SER:O	2.17	0.45
1:B:26:VAL:HG21	1:B:297:TYR:HB2	1.98	0.45
1:B:276:ARG:NH2	1:B:343:ASP:OD1	2.38	0.45
1:B:396:ASN:OD1	1:B:481:ARG:HA	2.16	0.45
1:C:26:VAL:HG21	1:C:297:TYR:CB	2.46	0.45
1:B:410:GLN:HE21	1:B:410:GLN:HB2	1.38	0.45
1:C:418:LEU:O	1:C:495:ALA:HA	2.17	0.44
1:A:146:ASP:O	1:A:147:ALA:HB2	2.17	0.44
1:A:366:THR:HG21	1:A:380:ARG:HE	1.82	0.44
1:A:379:VAL:HG12	1:A:384:ALA:HB2	1.98	0.44
1:A:453:ILE:O	1:A:454:ASP:CB	2.66	0.44
1:C:424:ILE:N	1:C:424:ILE:HD13	2.32	0.44
1:D:371:GLY:CA	1:D:439:ILE:HG21	2.46	0.44
1:D:87:CYS:O	1:D:372:GLY:HA3	2.16	0.44
1:A:417:TYR:CZ	1:A:453:ILE:HG23	2.52	0.44
1:B:282:GLU:HA	1:B:287:LYS:O	2.17	0.44
1:D:336:ASN:HD22	1:D:340:ALA:CB	2.30	0.44
1:D:375:ILE:HG21	1:D:418:LEU:HD11	1.99	0.44
1:D:288:VAL:CG2	1:D:526:ILE:HD11	2.45	0.44
1:A:566:LYS:O	1:A:567:PHE:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:GLY:O	1:C:202:ILE:HG23	2.18	0.44
1:C:200:ARG:O	1:C:202:ILE:HG22	2.18	0.44
1:C:374:MET:CE	3:C:800:FAD:H6	2.48	0.44
1:D:326:ASP:OD1	1:D:328:LYS:HD2	2.17	0.44
1:A:506:MET:HE3	1:A:543:ASN:HA	2.00	0.44
1:B:449:LEU:HD22	1:B:495:ALA:CB	2.46	0.44
1:A:167:ALA:HA	3:A:600:FAD:C5X	2.48	0.44
1:D:431:ILE:HA	1:D:434:TYR:HD2	1.83	0.44
1:D:52:ALA:CB	1:D:52:ALA:O	2.66	0.44
1:A:280:ILE:HA	1:A:291:VAL:HG23	1.99	0.44
1:A:425:ARG:HH21	1:A:435:VAL:HG21	1.83	0.44
1:A:46:LYS:O	1:A:49:ALA:HB3	2.18	0.44
1:B:422:ASP:OD1	1:B:494:TYR:OH	2.36	0.44
1:C:321:ARG:NH2	1:C:342:GLY:HA3	2.32	0.44
1:C:511:ILE:HA	1:C:516:GLU:O	2.17	0.44
1:D:187:LYS:HB2	1:D:190:ILE:HG13	1.99	0.44
1:D:470:PHE:CD1	1:D:476:ASP:HA	2.52	0.44
1:D:66:GLY:H	1:D:258:GLN:NE2	2.10	0.44
1:A:177:LYS:O	1:A:181:LYS:HE3	2.18	0.44
1:B:394:PHE:CD1	1:B:407:ALA:HB1	2.52	0.44
1:B:8:PHE:HE2	2:B:604:HEM:HHA	1.83	0.44
1:C:35:ASN:ND2	1:C:69:ALA:HB1	2.33	0.44
1:C:428:LEU:HD23	1:C:431:ILE:HG13	1.99	0.44
1:A:294:LYS:HB2	1:A:300:TYR:CD2	2.53	0.43
1:A:410:GLN:HB2	1:A:410:GLN:HE21	1.38	0.43
1:A:82:ALA:O	1:A:85:ASP:HB2	2.18	0.43
1:B:283:ASP:OD2	1:B:284:ALA:N	2.51	0.43
1:D:280:ILE:HD12	1:D:347:VAL:HG13	2.00	0.43
1:A:141:ALA:O	1:A:142:VAL:O	2.36	0.43
1:A:478:GLN:HB3	1:A:479:PHE:CD1	2.53	0.43
1:B:467:TYR:O	1:B:471:VAL:HG23	2.18	0.43
1:B:166:LEU:HD21	2:B:601:HEM:CBC	2.48	0.43
1:B:26:VAL:HG21	1:B:297:TYR:CB	2.49	0.43
1:B:516:GLU:HG2	5:B:741:HOH:O	2.18	0.43
1:B:514:LYS:O	1:B:515:ALA:HB3	2.18	0.43
1:B:87:CYS:O	1:B:372:GLY:HA3	2.19	0.43
1:C:366:THR:HG23	1:C:380:ARG:HH21	1.83	0.43
1:C:512:ASP:OD1	1:C:512:ASP:C	2.56	0.43
1:D:471:VAL:CG1	1:D:487:GLU:HG2	2.48	0.43
1:A:130:ILE:O	1:A:153:LEU:HA	2.18	0.43
1:B:246:PRO:HD3	1:B:252:VAL:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:448:GLU:HA	1:B:451:LYS:HD2	2.00	0.43
1:C:514:LYS:O	1:C:515:ALA:CB	2.66	0.43
1:D:142:VAL:HG21	1:D:225:MET:HE3	1.99	0.43
1:A:145:ARG:HG2	1:A:151:VAL:HG21	2.00	0.43
1:D:155:GLU:HB3	1:D:273:LEU:HD22	1.99	0.43
1:D:383:GLY:HA3	1:D:424:ILE:CD1	2.49	0.43
1:A:225:MET:HG2	1:A:263:ASN:OD1	2.18	0.43
1:A:470:PHE:CB	1:A:476:ASP:HA	2.49	0.43
1:D:82:ALA:O	1:D:83:TYR:C	2.54	0.43
1:C:397:GLU:HB2	1:C:481:ARG:NH1	2.34	0.43
1:D:179:GLN:HE22	1:D:242:ARG:HB3	1.84	0.43
1:D:400:THR:O	1:D:403:LYS:N	2.47	0.43
1:D:44:ASP:H	1:D:47:GLU:HB2	1.83	0.43
1:A:283:ASP:CG	1:A:284:ALA:N	2.72	0.43
1:A:132:GLY:CA	3:A:600:FAD:H4B	2.49	0.43
1:B:195:THR:HG21	1:B:208:VAL:HG13	2.01	0.43
1:B:171:MET:O	1:B:244:HIS:HB2	2.19	0.43
1:B:317:LYS:O	1:B:317:LYS:HG3	2.19	0.43
1:B:349:LEU:HD21	1:B:355:THR:HG23	2.01	0.43
1:B:433:GLY:HA2	2:B:601:HEM:HBA2	2.01	0.43
1:C:127:ASP:HB2	1:C:150:LYS:O	2.19	0.43
1:D:422:ASP:HB3	1:D:490:VAL:HG12	2.00	0.43
1:D:198:GLY:O	1:D:543:ASN:HB3	2.18	0.43
1:B:234:ARG:HB2	1:B:234:ARG:HE	1.74	0.43
1:B:435:VAL:CG2	1:B:440:VAL:HG21	2.49	0.43
1:C:413:GLY:O	1:C:414:GLU:C	2.56	0.43
1:D:172:ASN:OD1	1:D:548:ASN:ND2	2.52	0.43
1:B:240:VAL:HG22	1:B:241:ASN:H	1.84	0.42
1:B:278:VAL:HG23	1:B:292:LEU:HD12	2.01	0.42
1:C:170:GLY:HA2	1:C:252:VAL:HG21	2.01	0.42
1:C:9:HIS:HA	1:C:12:MET:CE	2.49	0.42
1:D:177:LYS:HB2	1:D:178:PRO:HD3	2.00	0.42
1:D:65:ILE:HB	1:D:258:GLN:NE2	2.33	0.42
1:D:375:ILE:HG21	1:D:418:LEU:CD1	2.49	0.42
1:A:428:LEU:HB3	1:A:431:ILE:HD12	2.02	0.42
1:B:164:THR:O	1:B:253:GLY:HA3	2.19	0.42
1:C:225:MET:HG2	1:C:263:ASN:CG	2.39	0.42
1:D:204:ASP:O	1:D:208:VAL:HG23	2.19	0.42
1:D:488:LEU:HD23	1:D:488:LEU:O	2.19	0.42
1:B:127:ASP:HB2	1:B:150:LYS:H	1.84	0.42
1:B:456:PRO:HB2	1:B:459:GLU:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:42:HIS:CE1	2:D:604:HEM:ND	2.87	0.42
1:D:455:VAL:HB	1:D:456:PRO:CD	2.46	0.42
1:A:326:ASP:OD2	1:A:328:LYS:HB2	2.18	0.42
1:A:334:ALA:HA	1:A:502:VAL:O	2.19	0.42
1:A:453:ILE:CG2	1:A:455:VAL:HG13	2.49	0.42
1:C:145:ARG:NH1	1:C:267:ARG:O	2.52	0.42
1:C:184:ILE:HD13	1:C:241:ASN:HB3	2.02	0.42
1:C:367:TYR:O	1:C:369:PRO:HD3	2.19	0.42
1:C:394:PHE:O	1:C:395:MET:CB	2.67	0.42
1:D:376:THR:O	1:D:379:VAL:HG23	2.20	0.42
1:A:74:HIS:CE1	2:A:602:HEM:ND	2.87	0.42
1:B:394:PHE:CE1	1:B:395:MET:SD	3.13	0.42
1:C:180:ALA:O	1:C:181:LYS:C	2.58	0.42
1:D:119:ALA:O	1:D:121:GLY:N	2.38	0.42
1:D:192:ILE:HG23	1:D:208:VAL:CG1	2.49	0.42
2:D:601:HEM:CBD	2:D:601:HEM:HHA	2.49	0.42
1:A:272:ARG:O	1:A:275:SER:HB2	2.20	0.42
1:A:48:LEU:HD11	2:A:602:HEM:C1B	2.54	0.42
1:A:65:ILE:H	1:A:65:ILE:HG13	1.71	0.42
1:B:204:ASP:OD1	1:B:206:GLU:N	2.53	0.42
1:C:234:ARG:HB2	1:C:234:ARG:HE	1.43	0.42
1:D:450:ALA:HA	1:D:455:VAL:HG22	2.02	0.42
1:D:68:ILE:HG13	1:D:68:ILE:O	2.20	0.42
1:B:409:LEU:HD23	1:B:409:LEU:HA	1.89	0.42
1:B:171:MET:HG3	1:B:550:ILE:HG22	2.01	0.42
1:B:401:ARG:NH2	4:B:714:SO4:O1	2.38	0.42
1:C:471:VAL:HG21	1:C:487:GLU:HA	2.01	0.42
1:D:188:LYS:O	1:D:192:ILE:HG13	2.19	0.42
1:D:210:VAL:O	1:D:211:LEU:C	2.57	0.42
1:D:136:ALA:HB2	1:D:553:ILE:HB	2.01	0.42
1:A:26:VAL:CG2	1:A:297:TYR:HB3	2.49	0.42
1:C:154:LEU:HD13	1:C:293:VAL:HG22	2.01	0.42
1:C:279:ARG:HB3	1:C:292:LEU:HB2	2.01	0.42
1:D:460:LEU:HA	1:D:460:LEU:HD23	1.91	0.42
1:A:181:LYS:HE3	1:A:181:LYS:N	2.34	0.42
1:A:225:MET:HE2	1:A:263:ASN:HB2	2.01	0.42
1:C:146:ASP:OD2	1:C:267:ARG:NH1	2.51	0.42
1:C:364:HIS:O	1:C:500:PRO:HA	2.20	0.42
1:C:484:LEU:HA	1:C:485:PRO:HD2	1.89	0.42
3:C:800:FAD:H2B	3:C:800:FAD:H8A	1.90	0.42
1:D:326:ASP:C	1:D:326:ASP:OD2	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:VAL:HA	1:D:43:GLY:O	2.20	0.42
3:D:900:FAD:N10	3:D:900:FAD:O2'	2.52	0.42
1:A:433:GLY:HA3	2:A:601:HEM:HBA2	2.02	0.42
1:C:233:GLY:HA3	1:C:245:ARG:HH22	1.78	0.42
1:C:60:HIS:CD2	2:C:602:HEM:NC	2.87	0.42
1:C:80:SER:O	1:C:97:GLY:HA2	2.20	0.42
1:D:181:LYS:HA	1:D:181:LYS:HE2	2.02	0.42
1:D:26:VAL:HG11	1:D:31:LEU:HD11	2.02	0.41
1:D:319:ASN:HD21	1:D:331:GLY:N	2.17	0.41
1:D:485:PRO:HB2	1:D:486:ARG:H	1.58	0.41
1:B:32:THR:O	1:B:33:HIS:C	2.58	0.41
1:D:498:ILE:C	1:D:498:ILE:HD12	2.40	0.41
1:A:68:ILE:HG13	1:A:68:ILE:O	2.20	0.41
1:B:199:GLY:HA3	1:B:203:ASN:OD1	2.19	0.41
1:B:210:VAL:HG13	1:B:214:ASN:ND2	2.36	0.41
1:B:316:ALA:HB3	1:B:336:ASN:ND2	2.35	0.41
1:D:28:ASN:ND2	1:D:28:ASN:C	2.74	0.41
1:D:376:THR:HG23	1:D:379:VAL:HG23	2.03	0.41
1:D:37:GLN:O	1:D:40:SER:HB2	2.21	0.41
1:D:430:ALA:O	1:D:433:GLY:N	2.47	0.41
1:D:458:ALA:O	1:D:462:LYS:HB2	2.20	0.41
1:A:310:ILE:HD12	1:A:529:LEU:HD21	2.02	0.41
1:A:222:LEU:O	1:A:223:THR:C	2.59	0.41
1:A:246:PRO:O	1:A:247:THR:C	2.56	0.41
1:A:449:LEU:HD11	1:A:495:ALA:HB2	2.00	0.41
1:B:220:ASP:O	1:B:224:SER:HB3	2.20	0.41
1:B:424:ILE:O	1:B:425:ARG:C	2.58	0.41
1:C:505:THR:O	1:C:506:MET:C	2.57	0.41
1:D:105:VAL:HA	1:D:106:PRO:HD2	1.90	0.41
1:D:114:GLN:HG2	1:D:300:TYR:CE2	2.55	0.41
1:D:329:LEU:HD13	1:D:502:VAL:HG22	2.02	0.41
1:D:37:GLN:HA	1:D:40:SER:HB2	2.03	0.41
1:D:446:ILE:HG21	1:D:464:VAL:HG21	2.02	0.41
1:D:499:ALA:HA	1:D:500:PRO:HD3	1.96	0.41
3:D:900:FAD:H1'1	3:D:900:FAD:H9	1.82	0.41
1:A:26:VAL:HG21	1:A:297:TYR:HB2	2.01	0.41
1:A:433:GLY:O	1:A:437:LEU:HG	2.20	0.41
1:C:409:LEU:CD2	1:C:500:PRO:HG3	2.50	0.41
1:C:63:HIS:CD2	2:C:601:HEM:NA	2.89	0.41
1:A:409:LEU:HA	1:A:409:LEU:HD23	1.92	0.41
1:A:453:ILE:HG21	1:A:455:VAL:HG13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:602:HEM:HBA2	1:C:360:TYR:OH	2.21	0.41
1:C:376:THR:HG21	1:C:378:ALA:HB3	2.02	0.41
1:C:376:THR:HG23	1:C:378:ALA:HB3	2.03	0.41
1:D:477:ALA:O	1:D:478:GLN:C	2.59	0.41
1:C:471:VAL:HB	1:C:487:GLU:HG3	2.03	0.41
1:D:110:ASP:O	1:D:114:GLN:HG3	2.21	0.41
1:D:371:GLY:HA2	1:D:439:ILE:HG21	2.01	0.41
1:A:286:GLY:O	1:A:526:ILE:HD12	2.20	0.41
1:A:346:ASP:O	1:A:347:VAL:C	2.59	0.41
1:A:471:VAL:HG22	1:A:484:LEU:HB3	2.03	0.41
1:B:87:CYS:SG	2:B:601:HEM:CBC	2.94	0.41
1:C:425:ARG:HD2	1:C:432:GLU:OE1	2.21	0.41
1:A:204:ASP:HB3	1:A:207:LEU:HD12	2.02	0.41
1:B:186:ASP:OD2	1:B:242:ARG:HD3	2.21	0.41
1:B:499:ALA:HA	1:B:500:PRO:HD3	1.83	0.41
1:D:428:LEU:HD23	1:D:431:ILE:HG13	2.03	0.41
1:C:483:ASP:OD2	1:C:485:PRO:HD3	2.21	0.41
1:D:75:LYS:HB2	1:D:78:GLU:O	2.21	0.41
1:B:534:GLU:OE2	3:B:700:FAD:O3'	2.30	0.40
1:B:58:SER:N	1:B:61:LYS:HZ1	2.19	0.40
1:D:170:GLY:H	1:D:235:MET:HE1	1.84	0.40
1:D:94:MET:HB2	2:D:602:HEM:HMD3	2.01	0.40
1:C:116:LYS:O	1:C:120:ALA:HB2	2.22	0.40
1:C:15:CYS:HB3	1:C:22:ASP:HA	2.03	0.40
1:B:263:ASN:O	1:B:264:ALA:C	2.59	0.40
1:B:280:ILE:HG13	1:B:347:VAL:CG1	2.51	0.40
1:C:109:ALA:O	1:C:110:ASP:HB2	2.21	0.40
1:C:409:LEU:HD22	1:C:414:GLU:CB	2.49	0.40
1:C:455:VAL:HB	1:C:456:PRO:CD	2.51	0.40
1:C:8:PHE:HE2	2:C:604:HEM:CHA	2.34	0.40
1:C:398:ILE:CD1	1:C:482:PRO:HD2	2.51	0.40
1:C:395:MET:HE2	1:C:404:ALA:HB1	2.01	0.40
1:D:190:ILE:O	1:D:194:ASP:HB2	2.22	0.40
1:D:380:ARG:O	1:D:481:ARG:NH2	2.55	0.40
1:A:316:ALA:HB1	1:A:502:VAL:HG12	2.03	0.40
1:C:332:PHE:HE1	1:C:500:PRO:HB2	1.87	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:THR:OG1	1:C:247:THR:OG1[4_555]	2.12	0.08
1:C:125:THR:OG1	1:D:247:THR:OG1[4_456]	2.15	0.05

## 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	568/572 (99%)	504 (89%)	51 (9%)	13 (2%)	7	27
1	B	562/572 (98%)	495 (88%)	52 (9%)	15 (3%)	6	23
1	C	566/572 (99%)	482 (85%)	64 (11%)	20 (4%)	4	17
1	D	566/572 (99%)	488 (86%)	61 (11%)	17 (3%)	5	20
All	All	2262/2288 (99%)	1969 (87%)	228 (10%)	65 (3%)	5	21

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	VAL
1	A	142	VAL
1	A	147	ALA
1	A	454	ASP
1	B	250	ALA
1	B	357	ASP
1	B	388	ASN
1	B	454	ASP
1	C	250	ALA
1	C	284	ALA
1	C	394	PHE
1	C	401	ARG
1	C	454	ASP
1	D	120	ALA
1	D	250	ALA
1	D	357	ASP

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Mol	Chain	Res	Type
1	D	454	ASP
1	D	485	PRO
1	A	143	SER
1	A	283	ASP
1	A	513	THR
1	B	240	VAL
1	B	247	THR
1	B	251	GLY
1	B	412	LYS
1	B	478	GLN
1	C	120	ALA
1	C	414	GLU
1	C	415	SER
1	C	451	LYS
1	C	485	PRO
1	D	267	ARG
1	D	401	ARG
1	D	478	GLN
1	A	110	ASP
1	A	120	ALA
1	A	343	ASP
1	B	148	GLY
1	B	201	ASN
1	B	489	VAL
1	C	180	ALA
1	C	343	ASP
1	C	410	GLN
1	D	11	GLU
1	D	17	SER
1	D	148	GLY
1	B	215	SER
1	B	284	ALA
1	C	56	LYS
1	C	201	ASN
1	C	492	PRO
1	D	329	LEU
1	A	55	ASP
1	C	430	ALA
1	D	464	VAL
1	B	13	GLY
1	C	412	LYS
1	D	13	GLY

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Mol	Chain	Res	Type
1	D	283	ASP
1	A	4	VAL
1	A	162	GLY
1	D	369	PRO
1	C	286	GLY
1	C	398	ILE
1	D	482	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	409/429 (95%)	350 (86%)	59 (14%)	4	11
1	B	406/429 (95%)	344 (85%)	62 (15%)	3	10
1	C	405/429 (94%)	343 (85%)	62 (15%)	3	10
1	D	407/429 (95%)	346 (85%)	61 (15%)	3	10
All	All	1627/1716 (95%)	1383 (85%)	244 (15%)	3	10

All (244) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLU
1	A	16	ASP
1	A	17	SER
1	A	28	ASN
1	A	31	LEU
1	A	32	THR
1	A	55	ASP
1	A	61	LYS
1	A	67	GLU
1	A	68	ILE
1	A	79	LYS
1	A	80	SER
1	A	102	ARG
1	A	105	VAL

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Mol	Chain	Res	Type
1	A	150	LYS
1	A	156	LYS
1	A	181	LYS
1	A	211	LEU
1	A	239	SER
1	A	245	ARG
1	A	252	VAL
1	A	259	VAL
1	A	273	LEU
1	A	282	GLU
1	A	283	ASP
1	A	291	VAL
1	A	292	LEU
1	A	296	GLU
1	A	330	LYS
1	A	345	LEU
1	A	350	GLN
1	A	359	GLU
1	A	375	ILE
1	A	387	VAL
1	A	388	ASN
1	A	390	GLU
1	A	395	MET
1	A	401	ARG
1	A	402	ASP
1	A	421	ASP
1	A	423	SER
1	A	426	LYS
1	A	432	GLU
1	A	448	GLU
1	A	449	LEU
1	A	452	GLN
1	A	460	LEU
1	A	463	THR
1	A	465	THR
1	A	480	GLU
1	A	487	GLU
1	A	488	LEU
1	A	489	VAL
1	A	496	LEU
1	A	520	GLU
1	A	526	ILE

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Mol	Chain	Res	Type
1	A	529	LEU
1	A	534	GLU
1	A	570	ASP
1	B	5	LEU
1	B	16	ASP
1	B	26	VAL
1	B	28	ASN
1	B	31	LEU
1	B	54	LYS
1	B	61	LYS
1	B	68	ILE
1	B	78	GLU
1	B	79	LYS
1	B	89	SER
1	B	93	ASP
1	B	94	MET
1	B	102	ARG
1	B	105	VAL
1	B	145	ARG
1	B	165	LYS
1	B	201	ASN
1	B	206	GLU
1	B	211	LEU
1	B	224	SER
1	B	228	ASP
1	B	234	ARG
1	B	240	VAL
1	B	247	THR
1	B	252	VAL
1	B	267	ARG
1	B	282	GLU
1	B	291	VAL
1	B	294	LYS
1	B	322	VAL
1	B	345	LEU
1	B	350	GLN
1	B	374	MET
1	B	375	ILE
1	B	376	THR
1	B	377	GLU
1	B	392	ASN
1	B	395	MET

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Mol	Chain	Res	Type
1	B	405	SER
1	B	410	GLN
1	B	415	SER
1	B	423	SER
1	B	429	LYS
1	B	432	GLU
1	B	444	LYS
1	B	445	THR
1	B	452	GLN
1	B	460	LEU
1	B	463	THR
1	B	478	GLN
1	B	480	GLU
1	B	488	LEU
1	B	489	VAL
1	B	494	TYR
1	B	496	LEU
1	B	506	MET
1	B	518	LYS
1	B	522	THR
1	B	526	ILE
1	B	529	LEU
1	B	548	ASN
1	C	15	CYS
1	C	16	ASP
1	C	17	SER
1	C	21	SER
1	C	26	VAL
1	C	27	THR
1	C	28	ASN
1	C	31	LEU
1	C	40	SER
1	C	61	LYS
1	C	68	ILE
1	C	75	LYS
1	C	111	LYS
1	C	124	GLU
1	C	143	SER
1	C	145	ARG
1	C	201	ASN
1	C	202	ILE
1	C	203	ASN

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Mol	Chain	Res	Type
1	C	205	PRO
1	C	211	LEU
1	C	223	THR
1	C	224	SER
1	C	225	MET
1	C	234	ARG
1	C	242	ARG
1	C	243	SER
1	C	252	VAL
1	C	259	VAL
1	C	280	ILE
1	C	292	LEU
1	C	321	ARG
1	C	322	VAL
1	C	347	VAL
1	C	368	SER
1	C	374	MET
1	C	376	THR
1	C	388	ASN
1	C	390	GLU
1	C	392	ASN
1	C	395	MET
1	C	400	THR
1	C	402	ASP
1	C	405	SER
1	C	410	GLN
1	C	424	ILE
1	C	444	LYS
1	C	448	GLU
1	C	452	GLN
1	C	459	GLU
1	C	460	LEU
1	C	463	THR
1	C	465	THR
1	C	484	LEU
1	C	487	GLU
1	C	489	VAL
1	C	496	LEU
1	C	520	GLU
1	C	526	ILE
1	C	551	SER
1	C	558	ARG

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Mol	Chain	Res	Type
1	C	570	ASP
1	D	5	LEU
1	D	16	ASP
1	D	17	SER
1	D	28	ASN
1	D	32	THR
1	D	40	SER
1	D	45	LEU
1	D	68	ILE
1	D	72	SER
1	D	75	LYS
1	D	78	GLU
1	D	81	VAL
1	D	89	SER
1	D	101	GLU
1	D	102	ARG
1	D	111	LYS
1	D	126	THR
1	D	130	ILE
1	D	145	ARG
1	D	159	ILE
1	D	175	GLU
1	D	185	GLU
1	D	211	LEU
1	D	230	THR
1	D	235	MET
1	D	243	SER
1	D	247	THR
1	D	252	VAL
1	D	273	LEU
1	D	282	GLU
1	D	283	ASP
1	D	291	VAL
1	D	292	LEU
1	D	328	LYS
1	D	345	LEU
1	D	347	VAL
1	D	350	GLN
1	D	368	SER
1	D	376	THR
1	D	385	ILE
1	D	388	ASN

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Mol	Chain	Res	Type
1	D	392	ASN
1	D	395	MET
1	D	396	ASN
1	D	401	ARG
1	D	415	SER
1	D	444	LYS
1	D	447	GLU
1	D	449	LEU
1	D	452	GLN
1	D	459	GLU
1	D	460	LEU
1	D	462	LYS
1	D	463	THR
1	D	480	GLU
1	D	488	LEU
1	D	496	LEU
1	D	526	ILE
1	D	529	LEU
1	D	558	ARG
1	D	570	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	33	HIS
1	A	35	ASN
1	A	114	GLN
1	A	172	ASN
1	A	258	GLN
1	A	319	ASN
1	A	336	ASN
1	A	362	GLN
1	A	388	ASN
1	A	410	GLN
1	A	411	GLN
1	A	452	GLN
1	A	468	ASN
1	A	478	GLN
1	A	548	ASN
1	B	28	ASN
1	B	35	ASN

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Mol	Chain	Res	Type
1	B	114	GLN
1	B	172	ASN
1	B	258	GLN
1	B	319	ASN
1	B	336	ASN
1	B	362	GLN
1	B	388	ASN
1	B	392	ASN
1	B	410	GLN
1	B	411	GLN
1	B	452	GLN
1	B	478	GLN
1	B	548	ASN
1	C	28	ASN
1	C	35	ASN
1	C	37	GLN
1	C	114	GLN
1	C	172	ASN
1	C	319	ASN
1	C	336	ASN
1	C	362	GLN
1	C	388	ASN
1	C	411	GLN
1	C	452	GLN
1	C	548	ASN
1	D	28	ASN
1	D	35	ASN
1	D	37	GLN
1	D	172	ASN
1	D	258	GLN
1	D	319	ASN
1	D	336	ASN
1	D	350	GLN
1	D	362	GLN
1	D	382	ASN
1	D	388	ASN
1	D	411	GLN
1	D	452	GLN
1	D	478	GLN
1	D	548	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

23 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	FAD	A	600	-	51,58,58	1.79	12 (23%)	54,89,89	3.33	21 (38%)
2	HEM	A	601	1	28,50,50	2.28	6 (21%)	17,82,82	3.02	9 (52%)
2	HEM	A	602	1	28,50,50	2.15	4 (14%)	17,82,82	3.34	9 (52%)
2	HEM	A	603	1	28,50,50	2.32	5 (17%)	17,82,82	2.30	7 (41%)
2	HEM	A	604	1	28,50,50	2.21	7 (25%)	17,82,82	2.83	9 (52%)
2	HEM	B	601	1	28,50,50	2.25	5 (17%)	17,82,82	2.88	7 (41%)
2	HEM	B	602	1	28,50,50	1.98	7 (25%)	17,82,82	2.56	6 (35%)
2	HEM	B	603	1	28,50,50	2.15	8 (28%)	17,82,82	3.20	8 (47%)
2	HEM	B	604	1	28,50,50	2.14	6 (21%)	17,82,82	2.75	9 (52%)
3	FAD	B	700	-	51,58,58	1.77	8 (15%)	54,89,89	3.48	25 (46%)
4	SO4	B	714	-	4,4,4	0.55	0	6,6,6	0.52	0
2	HEM	C	601	1	28,50,50	2.11	5 (17%)	17,82,82	2.52	7 (41%)
2	HEM	C	602	1	28,50,50	2.32	6 (21%)	17,82,82	2.71	7 (41%)
2	HEM	C	603	1	28,50,50	2.13	5 (17%)	17,82,82	2.28	8 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	HEM	C	604	1	28,50,50	2.08	5 (17%)	17,82,82	4.64	10 (58%)
3	FAD	C	800	-	51,58,58	1.61	9 (17%)	54,89,89	4.02	18 (33%)
4	SO4	C	814	-	4,4,4	0.66	0	6,6,6	0.66	0
2	HEM	D	601	1	28,50,50	2.31	6 (21%)	17,82,82	2.42	4 (23%)
2	HEM	D	602	1	28,50,50	2.16	4 (14%)	17,82,82	2.30	7 (41%)
2	HEM	D	603	1	28,50,50	2.21	7 (25%)	17,82,82	1.41	3 (17%)
2	HEM	D	604	1	28,50,50	2.03	4 (14%)	17,82,82	2.77	8 (47%)
3	FAD	D	900	-	51,58,58	1.75	7 (13%)	54,89,89	3.55	21 (38%)
4	SO4	D	914	-	4,4,4	0.61	0	6,6,6	0.69	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	FAD	A	600	-	2/2/9/9	0/28/50/50	0/6/6/6
2	HEM	A	601	1	-	0/6/54/54	0/0/8/8
2	HEM	A	602	1	-	0/6/54/54	0/0/8/8
2	HEM	A	603	1	-	0/6/54/54	0/0/8/8
2	HEM	A	604	1	-	0/6/54/54	0/0/8/8
2	HEM	B	601	1	-	0/6/54/54	0/0/8/8
2	HEM	B	602	1	-	0/6/54/54	0/0/8/8
2	HEM	B	603	1	-	0/6/54/54	0/0/8/8
2	HEM	B	604	1	-	0/6/54/54	0/0/8/8
3	FAD	B	700	-	2/2/9/9	0/28/50/50	0/6/6/6
4	SO4	B	714	-	-	0/0/0/0	0/0/0/0
2	HEM	C	601	1	-	0/6/54/54	0/0/8/8
2	HEM	C	602	1	-	0/6/54/54	0/0/8/8
2	HEM	C	603	1	-	0/6/54/54	0/0/8/8
2	HEM	C	604	1	-	0/6/54/54	0/0/8/8
3	FAD	C	800	-	3/3/9/9	0/28/50/50	0/6/6/6
4	SO4	C	814	-	-	0/0/0/0	0/0/0/0
2	HEM	D	601	1	-	0/6/54/54	0/0/8/8
2	HEM	D	602	1	-	0/6/54/54	0/0/8/8
2	HEM	D	603	1	-	0/6/54/54	0/0/8/8
2	HEM	D	604	1	-	0/6/54/54	0/0/8/8
3	FAD	D	900	-	2/2/9/9	0/28/50/50	0/6/6/6
4	SO4	D	914	-	-	0/0/0/0	0/0/0/0



All (126) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	HEM	C3B-C2B	-7.08	1.31	1.40
2	D	602	HEM	C3B-C2B	-5.92	1.32	1.40
2	C	602	HEM	C3C-C2C	-5.86	1.32	1.40
2	C	602	HEM	C3B-C2B	-5.74	1.32	1.40
2	A	603	HEM	C3C-C2C	-5.74	1.32	1.40
2	B	604	HEM	C3B-C2B	-5.70	1.32	1.40
2	C	603	HEM	C3C-C2C	-5.57	1.33	1.40
2	A	603	HEM	C3B-C2B	-5.57	1.33	1.40
2	B	601	HEM	C3C-C2C	-5.42	1.33	1.40
2	D	601	HEM	C3B-C2B	-5.40	1.33	1.40
2	C	604	HEM	C3B-C2B	-5.35	1.33	1.40
2	A	604	HEM	C3C-C2C	-5.32	1.33	1.40
2	A	602	HEM	C3C-C2C	-5.28	1.33	1.40
2	D	603	HEM	C3C-C2C	-5.27	1.33	1.40
2	D	603	HEM	C3B-C2B	-5.08	1.33	1.40
2	C	601	HEM	C3B-C2B	-5.05	1.33	1.40
2	B	601	HEM	C3B-C2B	-5.03	1.33	1.40
2	D	604	HEM	C3C-C2C	-4.95	1.33	1.40
2	C	601	HEM	C3C-C2C	-4.89	1.33	1.40
2	D	601	HEM	C3C-C2C	-4.76	1.34	1.40
2	B	603	HEM	C3C-C2C	-4.71	1.34	1.40
2	A	601	HEM	C3C-C2C	-4.66	1.34	1.40
2	D	602	HEM	C3C-C2C	-4.63	1.34	1.40
2	B	604	HEM	C3C-C2C	-4.57	1.34	1.40
2	D	604	HEM	C3B-C2B	-4.44	1.34	1.40
2	C	603	HEM	C3B-C2B	-4.44	1.34	1.40
2	B	602	HEM	C3B-C2B	-4.39	1.34	1.40
2	A	604	HEM	C3B-C2B	-4.21	1.34	1.40
2	C	604	HEM	C3C-C2C	-4.18	1.34	1.40
2	B	603	HEM	C3B-C2B	-4.16	1.34	1.40
2	B	602	HEM	C3C-C2C	-4.14	1.34	1.40
2	A	602	HEM	C3B-C2B	-4.05	1.35	1.40
3	C	800	FAD	C2B-C1B	-3.21	1.48	1.53
3	D	900	FAD	C2B-C1B	-3.18	1.48	1.53
3	B	700	FAD	C2B-C1B	-3.12	1.48	1.53
3	A	600	FAD	C5'-C4'	-3.08	1.47	1.51
3	C	800	FAD	P-O1P	-2.61	1.41	1.50
3	C	800	FAD	C5'-C4'	-2.56	1.47	1.51
3	A	600	FAD	PA-O2A	-2.40	1.43	1.55
3	C	800	FAD	C1'-N10	-2.40	1.45	1.48
3	A	600	FAD	P-O2P	-2.36	1.43	1.55
3	D	900	FAD	P-O2P	-2.26	1.43	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	600	FAD	O4'-C4'	-2.26	1.38	1.43
3	A	600	FAD	P-O1P	-2.24	1.42	1.50
3	C	800	FAD	O4B-C4B	-2.12	1.40	1.45
3	A	600	FAD	C1'-N10	-2.08	1.46	1.48
3	B	700	FAD	PA-O2A	-2.05	1.44	1.55
2	C	602	HEM	CMB-C2B	2.01	1.55	1.51
2	A	604	HEM	C1A-NA	2.01	1.40	1.36
2	B	601	HEM	C1B-NB	2.02	1.39	1.36
2	B	603	HEM	CAD-C3D	2.02	1.56	1.52
2	B	603	HEM	C1B-NB	2.02	1.39	1.36
2	A	601	HEM	CAA-C2A	2.02	1.55	1.52
2	B	604	HEM	C1C-NC	2.03	1.39	1.36
3	A	600	FAD	C6-C7	2.05	1.43	1.37
2	B	602	HEM	C1C-NC	2.07	1.39	1.36
2	A	604	HEM	C1B-NB	2.08	1.39	1.36
2	D	603	HEM	C1C-NC	2.09	1.39	1.36
2	D	603	HEM	C1B-NB	2.10	1.39	1.36
2	B	604	HEM	C4D-ND	2.12	1.39	1.36
2	D	603	HEM	C4C-NC	2.14	1.39	1.36
2	A	601	HEM	CAD-C3D	2.18	1.56	1.52
3	D	900	FAD	C2-N3	2.24	1.42	1.38
3	B	700	FAD	C8-C7	2.27	1.46	1.41
2	C	604	HEM	CMC-C2C	2.27	1.56	1.51
3	B	700	FAD	C6-C7	2.28	1.43	1.37
2	C	603	HEM	C1B-NB	2.33	1.39	1.36
3	A	600	FAD	C4-C4X	2.35	1.45	1.41
3	A	600	FAD	O4B-C1B	2.44	1.44	1.41
2	B	602	HEM	CMB-C2B	2.47	1.56	1.51
2	A	604	HEM	CMD-C2D	2.51	1.56	1.51
2	B	603	HEM	CAA-C2A	2.54	1.56	1.52
2	D	601	HEM	CAA-C2A	2.57	1.56	1.52
2	B	602	HEM	C4D-ND	2.69	1.39	1.36
2	A	603	HEM	C1C-NC	2.75	1.40	1.36
2	C	601	HEM	C4C-NC	2.78	1.40	1.36
2	C	602	HEM	C1C-NC	2.80	1.40	1.36
2	B	603	HEM	C1C-NC	2.82	1.40	1.36
3	C	800	FAD	C8-C7	2.90	1.48	1.41
3	C	800	FAD	C4-C4X	2.94	1.47	1.41
3	D	900	FAD	C4-C4X	3.44	1.47	1.41
2	A	601	HEM	C3B-CAB	3.57	1.55	1.47
3	B	700	FAD	C4-C4X	3.67	1.48	1.41
2	D	601	HEM	C3B-CAB	3.73	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	700	FAD	C4-N3	3.88	1.40	1.33
2	D	601	HEM	C1B-NB	3.88	1.41	1.36
2	B	602	HEM	C3B-CAB	3.96	1.55	1.47
3	D	900	FAD	C4-N3	4.05	1.40	1.33
3	B	700	FAD	C1'-C2'	4.09	1.77	1.51
2	B	602	HEM	C3C-CAC	4.12	1.55	1.47
2	D	603	HEM	C3C-CAC	4.15	1.56	1.47
2	A	604	HEM	C3C-CAC	4.17	1.56	1.47
3	A	600	FAD	C1'-C2'	4.20	1.78	1.51
2	C	601	HEM	C3B-CAB	4.21	1.56	1.47
3	D	900	FAD	C1'-C2'	4.23	1.78	1.51
2	D	602	HEM	C3B-CAB	4.23	1.56	1.47
2	C	603	HEM	C3C-CAC	4.25	1.56	1.47
3	A	600	FAD	C4-N3	4.28	1.40	1.33
2	B	603	HEM	C3C-CAC	4.32	1.56	1.47
3	C	800	FAD	C1'-C2'	4.32	1.78	1.51
2	B	604	HEM	C3B-CAB	4.39	1.56	1.47
2	C	601	HEM	C3C-CAC	4.39	1.56	1.47
2	C	602	HEM	C3C-CAC	4.40	1.56	1.47
2	A	601	HEM	C3C-CAC	4.46	1.56	1.47
2	C	603	HEM	C3B-CAB	4.46	1.56	1.47
2	B	603	HEM	C3B-CAB	4.59	1.57	1.47
2	B	604	HEM	C3C-CAC	4.62	1.56	1.47
2	D	604	HEM	C3C-CAC	4.64	1.57	1.47
2	A	603	HEM	C3C-CAC	4.69	1.57	1.47
2	D	603	HEM	C3B-CAB	4.72	1.57	1.47
2	C	604	HEM	C3B-CAB	4.73	1.57	1.47
2	D	604	HEM	C3B-CAB	4.80	1.57	1.47
2	D	602	HEM	C3C-CAC	4.81	1.57	1.47
2	C	604	HEM	C3C-CAC	4.85	1.57	1.47
2	A	603	HEM	C3B-CAB	4.86	1.57	1.47
2	A	602	HEM	C3B-CAB	4.93	1.57	1.47
2	C	602	HEM	C3B-CAB	4.98	1.57	1.47
2	B	601	HEM	C3C-CAC	5.02	1.57	1.47
3	C	800	FAD	C5B-C4B	5.14	1.67	1.51
2	A	604	HEM	C3B-CAB	5.17	1.58	1.47
2	B	601	HEM	C3B-CAB	5.20	1.58	1.47
2	A	602	HEM	C3C-CAC	5.35	1.58	1.47
2	D	601	HEM	C3C-CAC	5.53	1.58	1.47
3	B	700	FAD	C5B-C4B	6.28	1.71	1.51
3	D	900	FAD	C5B-C4B	6.39	1.71	1.51
3	A	600	FAD	C5B-C4B	6.49	1.72	1.51

All (203) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	900	FAD	C5B-C4B-C3B	-10.83	74.02	115.29
3	A	600	FAD	C5B-C4B-C3B	-10.69	74.55	115.29
3	C	800	FAD	C5B-C4B-C3B	-10.65	74.68	115.29
3	B	700	FAD	C5B-C4B-C3B	-10.59	74.91	115.29
3	A	600	FAD	C4B-O4B-C1B	-8.69	100.52	109.77
2	A	601	HEM	CBD-CAD-C3D	-8.21	96.80	112.47
3	B	700	FAD	C1'-N10-C9A	-7.64	111.34	118.35
2	D	604	HEM	CAD-CBD-CGD	-7.46	99.91	112.66
3	D	900	FAD	C4X-C10-N10	-6.61	115.93	120.52
2	A	604	HEM	CMA-C3A-C4A	-6.18	118.96	128.46
2	D	601	HEM	CAA-CBA-CGA	-6.00	102.42	112.66
2	D	601	HEM	CAD-CBD-CGD	-5.91	102.57	112.66
3	A	600	FAD	C4X-C4-N3	-5.58	115.53	123.48
2	B	601	HEM	CAD-CBD-CGD	-5.26	103.67	112.66
2	A	603	HEM	CMA-C3A-C4A	-5.20	120.47	128.46
2	B	603	HEM	CMA-C3A-C4A	-5.18	120.50	128.46
3	B	700	FAD	O4'-C4'-C5'	-4.76	99.39	110.00
2	B	602	HEM	CMA-C3A-C4A	-4.66	121.31	128.46
2	C	604	HEM	CMA-C3A-C4A	-4.49	121.57	128.46
2	B	604	HEM	CAD-CBD-CGD	-4.43	105.10	112.66
2	C	602	HEM	CAD-CBD-CGD	-4.40	105.15	112.66
3	D	900	FAD	O4'-C4'-C5'	-4.31	100.39	110.00
2	C	604	HEM	CMD-C2D-C1D	-4.30	121.86	128.46
2	C	601	HEM	CAD-CBD-CGD	-4.27	105.36	112.66
3	C	800	FAD	C6-C5X-N5	-4.24	113.98	118.97
3	B	700	FAD	C4X-C10-N10	-4.04	117.72	120.52
3	C	800	FAD	C4X-C4-N3	-4.03	117.75	123.48
2	D	602	HEM	CMD-C2D-C1D	-3.95	122.39	128.46
3	B	700	FAD	C5X-C9A-N10	-3.95	114.72	117.66
2	A	604	HEM	CMD-C2D-C1D	-3.88	122.50	128.46
3	D	900	FAD	C9A-C5X-N5	-3.67	116.77	122.24
2	A	602	HEM	CAD-CBD-CGD	-3.67	106.40	112.66
2	B	601	HEM	CMD-C2D-C1D	-3.66	122.84	128.46
2	A	601	HEM	CAD-CBD-CGD	-3.64	106.44	112.66
2	A	602	HEM	CMA-C3A-C4A	-3.62	122.90	128.46
3	D	900	FAD	O2'-C2'-C1'	-3.60	101.46	109.79
3	C	800	FAD	O2'-C2'-C1'	-3.59	101.49	109.79
3	C	800	FAD	C1'-N10-C10	-3.57	114.84	118.50
2	A	603	HEM	CMD-C2D-C1D	-3.54	123.03	128.46
2	A	601	HEM	CMD-C2D-C1D	-3.53	123.04	128.46
2	C	601	HEM	CMD-C2D-C1D	-3.44	123.17	128.46
2	C	603	HEM	CMD-C2D-C1D	-3.42	123.20	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	HEM	CMA-C3A-C4A	-3.35	123.31	128.46
2	B	604	HEM	CMD-C2D-C1D	-3.33	123.34	128.46
2	C	602	HEM	CMD-C2D-C1D	-3.21	123.53	128.46
2	D	603	HEM	CMD-C2D-C1D	-3.14	123.64	128.46
2	B	603	HEM	CMD-C2D-C1D	-3.11	123.68	128.46
3	A	600	FAD	O2'-C2'-C1'	-3.05	102.72	109.79
2	C	604	HEM	CAA-CBA-CGA	-3.05	107.44	112.66
2	A	602	HEM	CMD-C2D-C1D	-3.02	123.82	128.46
3	A	600	FAD	O4'-C4'-C3'	-2.97	101.72	109.09
3	B	700	FAD	C4A-C5A-N7A	-2.96	106.55	109.41
2	D	604	HEM	CMA-C3A-C4A	-2.96	123.92	128.46
3	C	800	FAD	O2B-C2B-C3B	-2.96	102.36	111.83
2	B	604	HEM	CAA-CBA-CGA	-2.92	107.67	112.66
2	C	603	HEM	CMA-C3A-C4A	-2.90	124.00	128.46
2	B	603	HEM	CBA-CAA-C2A	-2.90	106.95	112.48
2	B	602	HEM	CMD-C2D-C1D	-2.87	124.06	128.46
3	B	700	FAD	C4X-C4-N3	-2.85	119.43	123.48
3	B	700	FAD	O4'-C4'-C3'	-2.80	102.14	109.09
3	D	900	FAD	C2A-N1A-C6A	-2.67	114.09	118.77
3	D	900	FAD	C4X-C4-N3	-2.62	119.75	123.48
3	A	600	FAD	C5A-C6A-N1A	-2.60	111.83	119.70
3	C	800	FAD	C4X-C10-N10	-2.55	118.75	120.52
2	A	601	HEM	CAA-CBA-CGA	-2.55	108.31	112.66
3	A	600	FAD	O5B-PA-O1A	-2.54	99.02	109.25
3	D	900	FAD	C1B-N9A-C4A	-2.53	122.27	126.64
2	C	601	HEM	CAA-CBA-CGA	-2.48	108.42	112.66
3	A	600	FAD	C4'-C3'-C2'	-2.44	108.15	113.41
3	C	800	FAD	C5A-C6A-N1A	-2.43	112.35	119.70
3	B	700	FAD	C1B-N9A-C4A	-2.42	122.45	126.64
2	D	601	HEM	CMD-C2D-C1D	-2.35	124.85	128.46
2	B	604	HEM	CMA-C3A-C4A	-2.34	124.86	128.46
3	B	700	FAD	C4'-C3'-C2'	-2.34	108.37	113.41
2	D	602	HEM	CMA-C3A-C4A	-2.30	124.93	128.46
3	C	800	FAD	C5X-C9A-N10	-2.29	115.95	117.66
3	B	700	FAD	C7-C6-C5X	-2.29	117.54	121.08
2	D	604	HEM	CMD-C2D-C1D	-2.26	124.99	128.46
3	A	600	FAD	C1B-N9A-C4A	-2.20	122.84	126.64
2	B	603	HEM	CBD-CAD-C3D	-2.20	108.27	112.47
3	A	600	FAD	C10-C4X-N5	-2.20	118.07	120.59
3	A	600	FAD	C7M-C7-C8	-2.19	116.12	120.72
2	B	604	HEM	C3C-C4C-NC	-2.17	106.84	110.94
3	B	700	FAD	O5B-PA-O1A	-2.15	100.56	109.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	700	FAD	O2'-C2'-C1'	-2.14	104.84	109.79
3	D	900	FAD	C7M-C7-C8	-2.10	116.30	120.72
2	D	603	HEM	CMA-C3A-C4A	-2.10	125.24	128.46
3	D	900	FAD	C4A-C5A-N7A	-2.09	107.39	109.41
3	B	700	FAD	C8M-C8-C7	-2.09	116.33	120.72
3	C	800	FAD	O3B-C3B-C2B	-2.05	105.26	111.83
2	A	602	HEM	CMD-C2D-C3D	2.00	128.72	124.94
3	B	700	FAD	C2B-C3B-C4B	2.01	106.53	102.62
2	C	603	HEM	CMB-C2B-C3B	2.02	128.64	124.89
2	B	601	HEM	CMB-C2B-C3B	2.03	128.66	124.89
3	C	800	FAD	C2A-N1A-C6A	2.05	122.36	118.77
2	C	603	HEM	CMD-C2D-C3D	2.08	128.86	124.94
3	B	700	FAD	C9-C8-C7	2.08	123.66	119.95
2	D	603	HEM	CMD-C2D-C3D	2.10	128.90	124.94
2	D	604	HEM	CMA-C3A-C2A	2.11	128.91	124.94
3	D	900	FAD	C1'-N10-C10	2.14	120.70	118.50
2	C	603	HEM	C4C-C3C-C2C	2.15	108.40	106.90
2	D	604	HEM	C4C-C3C-C2C	2.20	108.43	106.90
2	D	602	HEM	CMC-C2C-C3C	2.20	128.98	124.89
2	C	602	HEM	C4C-C3C-C2C	2.21	108.44	106.90
2	D	604	HEM	CMB-C2B-C3B	2.22	129.02	124.89
2	A	602	HEM	CMC-C2C-C3C	2.23	129.04	124.89
2	D	602	HEM	CMB-C2B-C3B	2.23	129.04	124.89
3	D	900	FAD	C5X-C9A-N10	2.24	119.32	117.66
2	B	601	HEM	CMD-C2D-C3D	2.25	129.18	124.94
2	D	602	HEM	CBD-CAD-C3D	2.25	116.76	112.47
3	D	900	FAD	C7M-C7-C6	2.26	126.00	120.34
2	B	603	HEM	CMB-C2B-C3B	2.28	129.12	124.89
3	B	700	FAD	C4-C4X-N5	2.29	121.19	118.68
3	B	700	FAD	O3B-C3B-C4B	2.30	117.81	111.09
2	A	604	HEM	CAA-CBA-CGA	2.32	116.63	112.66
2	A	602	HEM	CMA-C3A-C2A	2.41	129.49	124.94
2	B	601	HEM	C4C-C3C-C2C	2.44	108.60	106.90
3	D	900	FAD	C6-C5X-N5	2.47	121.86	118.97
2	A	603	HEM	CMC-C2C-C3C	2.47	129.48	124.89
2	D	602	HEM	CMD-C2D-C3D	2.49	129.63	124.94
2	B	603	HEM	CMD-C2D-C3D	2.49	129.64	124.94
2	C	602	HEM	CAA-CBA-CGA	2.49	116.92	112.66
3	A	600	FAD	O5'-C5'-C4'	2.51	116.06	109.36
2	C	601	HEM	C1D-C2D-C3D	2.54	108.76	107.00
2	D	601	HEM	CBD-CAD-C3D	2.58	117.39	112.47
3	B	700	FAD	C9-C9A-C5X	2.59	124.05	119.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	HEM	C4C-C3C-C2C	2.60	108.72	106.90
2	C	602	HEM	CMC-C2C-C3C	2.60	129.72	124.89
2	A	604	HEM	C4C-C3C-C2C	2.62	108.73	106.90
3	C	800	FAD	C6-C5X-C9A	2.64	122.43	119.00
2	A	603	HEM	C4C-C3C-C2C	2.67	108.77	106.90
2	A	603	HEM	CMB-C2B-C3B	2.67	129.85	124.89
2	C	603	HEM	CMC-C2C-C3C	2.70	129.91	124.89
2	A	604	HEM	CMD-C2D-C3D	2.71	130.04	124.94
2	C	604	HEM	CMD-C2D-C3D	2.72	130.08	124.94
2	A	601	HEM	CMA-C3A-C2A	2.75	130.13	124.94
2	A	604	HEM	CMB-C2B-C3B	2.75	130.00	124.89
2	A	603	HEM	CMD-C2D-C3D	2.78	130.18	124.94
2	C	604	HEM	CMB-C2B-C3B	2.78	130.05	124.89
2	C	601	HEM	CMB-C2B-C3B	2.81	130.11	124.89
2	C	604	HEM	C4C-C3C-C2C	2.88	108.91	106.90
2	C	604	HEM	CMC-C2C-C3C	2.92	130.30	124.89
2	B	604	HEM	CBA-CAA-C2A	2.94	118.11	112.48
2	A	604	HEM	CMC-C2C-C3C	2.95	130.37	124.89
2	D	604	HEM	CAA-CBA-CGA	2.99	117.77	112.66
2	A	601	HEM	CMC-C2C-C3C	3.00	130.46	124.89
3	B	700	FAD	O3'-C3'-C4'	3.00	116.26	108.82
3	A	600	FAD	O2A-PA-O1A	3.03	127.95	112.28
2	A	601	HEM	CMD-C2D-C3D	3.09	130.77	124.94
2	A	601	HEM	CMB-C2B-C3B	3.10	130.65	124.89
3	D	900	FAD	O2'-C2'-C3'	3.11	116.80	109.09
2	B	602	HEM	CMB-C2B-C3B	3.15	130.74	124.89
2	B	604	HEM	CMB-C2B-C3B	3.19	130.81	124.89
2	C	602	HEM	CMB-C2B-C3B	3.27	130.97	124.89
2	B	602	HEM	CMA-C3A-C2A	3.31	131.19	124.94
2	C	604	HEM	CMA-C3A-C2A	3.35	131.27	124.94
2	C	603	HEM	CAD-CBD-CGD	3.41	118.50	112.66
2	A	602	HEM	CBD-CAD-C3D	3.54	119.22	112.47
2	B	604	HEM	C4C-C3C-C2C	3.60	109.41	106.90
2	B	603	HEM	CMA-C3A-C2A	3.72	131.96	124.94
2	A	603	HEM	CMA-C3A-C2A	3.77	132.06	124.94
3	A	600	FAD	C4-C4X-N5	3.96	123.03	118.68
3	C	800	FAD	N3A-C2A-N1A	4.21	132.52	128.86
3	A	600	FAD	C4X-N5-C5X	4.22	121.21	116.76
3	D	900	FAD	C4'-C3'-C2'	4.22	122.50	113.41
2	B	601	HEM	CBA-CAA-C2A	4.34	120.77	112.48
2	B	602	HEM	CBA-CAA-C2A	4.34	120.79	112.48
3	A	600	FAD	C2A-N1A-C6A	4.35	126.38	118.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	604	HEM	CMA-C3A-C2A	4.46	133.36	124.94
2	A	602	HEM	CBA-CAA-C2A	4.48	121.06	112.48
2	A	604	HEM	CBA-CAA-C2A	4.52	121.13	112.48
3	A	600	FAD	C1'-N10-C9A	4.56	122.52	118.35
3	A	600	FAD	N6A-C6A-N1A	4.61	127.91	118.77
3	C	800	FAD	C4-N3-C2	4.84	119.40	115.16
2	C	603	HEM	CAA-CBA-CGA	4.94	121.09	112.66
2	D	604	HEM	CBA-CAA-C2A	5.17	122.37	112.48
3	C	800	FAD	O5'-C5'-C4'	5.18	123.19	109.36
3	B	700	FAD	C4X-N5-C5X	5.19	122.25	116.76
3	D	900	FAD	C4X-N5-C5X	5.36	122.42	116.76
3	B	700	FAD	C1'-N10-C10	5.43	124.07	118.50
2	B	602	HEM	CAA-CBA-CGA	5.60	122.23	112.66
2	D	602	HEM	CAA-CBA-CGA	5.78	122.54	112.66
3	D	900	FAD	O3'-C3'-C4'	5.79	123.17	108.82
2	B	604	HEM	CBD-CAD-C3D	5.80	123.52	112.47
3	C	800	FAD	N6A-C6A-N1A	6.00	130.66	118.77
2	C	601	HEM	CBD-CAD-C3D	6.23	124.35	112.47
3	A	600	FAD	O4B-C4B-C5B	6.51	131.40	109.40
3	A	600	FAD	C4-N3-C2	6.69	121.01	115.16
2	C	602	HEM	CBA-CAA-C2A	7.20	126.25	112.48
2	B	601	HEM	CBD-CAD-C3D	7.23	126.27	112.47
2	C	604	HEM	CBA-CAA-C2A	7.76	127.32	112.48
3	B	700	FAD	O4B-C4B-C5B	8.42	137.85	109.40
3	B	700	FAD	O5B-C5B-C4B	9.20	141.62	109.00
3	D	900	FAD	O4B-C4B-C5B	9.35	140.99	109.40
3	D	900	FAD	N3A-C2A-N1A	9.38	137.03	128.86
2	B	603	HEM	CAA-CBA-CGA	9.63	129.12	112.66
3	B	700	FAD	N3A-C2A-N1A	9.76	137.35	128.86
2	A	602	HEM	CAA-CBA-CGA	10.07	129.87	112.66
3	A	600	FAD	O5B-C5B-C4B	10.19	145.13	109.00
3	D	900	FAD	O5B-C5B-C4B	11.16	148.57	109.00
2	C	604	HEM	CBD-CAD-C3D	14.33	139.81	112.47
3	C	800	FAD	O5B-C5B-C4B	15.80	165.03	109.00
3	C	800	FAD	O4B-C4B-C5B	16.08	163.68	109.40

All (9) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	800	FAD	C4B
3	C	800	FAD	C4'
3	C	800	FAD	C3'

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Mol	Chain	Res	Type	Atom
3	B	700	FAD	C4'
3	B	700	FAD	C3'
3	A	600	FAD	C4'
3	A	600	FAD	C3'
3	D	900	FAD	C4'
3	D	900	FAD	C3'

There are no torsion outliers.

There are no ring outliers.

21 monomers are involved in 103 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	600	FAD	9	0
2	A	601	HEM	5	0
2	A	602	HEM	5	0
2	A	603	HEM	1	0
2	A	604	HEM	4	0
2	B	601	HEM	6	0
2	B	602	HEM	8	0
2	B	603	HEM	2	0
2	B	604	HEM	1	0
3	B	700	FAD	8	0
4	B	714	SO4	1	0
2	C	601	HEM	7	0
2	C	602	HEM	3	0
2	C	603	HEM	1	0
2	C	604	HEM	2	0
3	C	800	FAD	12	0
2	D	601	HEM	2	0
2	D	602	HEM	8	0
2	D	603	HEM	5	0
2	D	604	HEM	4	0
3	D	900	FAD	9	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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.