



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:26 PM UTC

PDB ID : 1LTD / pdb_00001ltd
Title : THE 2.6 ANGSTROMS REFINED STRUCTURE OF THE ESCHERICHIA COLI RECOMBINANT SACCHAROMYCES CEREVISIAE FLAVOCYTOCHROME B2-SULPHITE COMPLEX
Authors : Tegoni, M.; Cambillau, C.
Deposited on : 1994-01-14
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

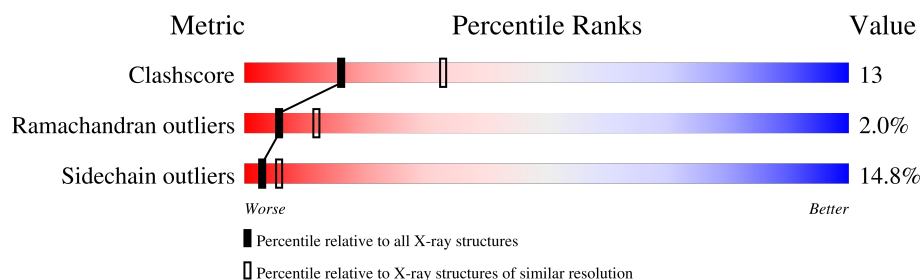
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	506	
1	B	506	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FMN	A	570	X	-	-	-
3	FMN	B	570	X	-	-	-

2 Entry composition [i](#)

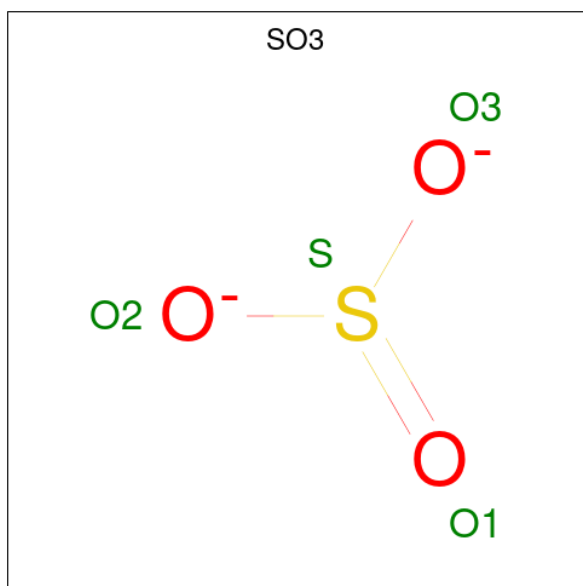
There are 5 unique types of molecules in this entry. The entry contains 7075 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 B2.

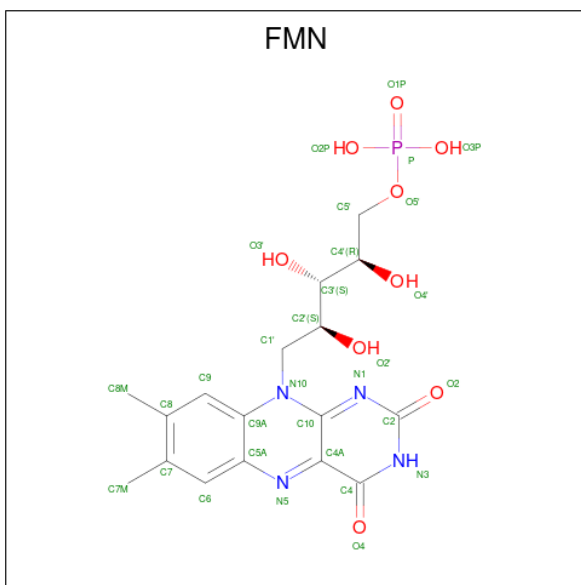
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	0	1
			3742	2386	633	709	14			
1	B	387	Total	C	N	O	S	0	0	1
			3014	1913	513	577	11			

- Molecule 2 is SULFITE ION (CCD ID: SO3) (formula: O₃S).



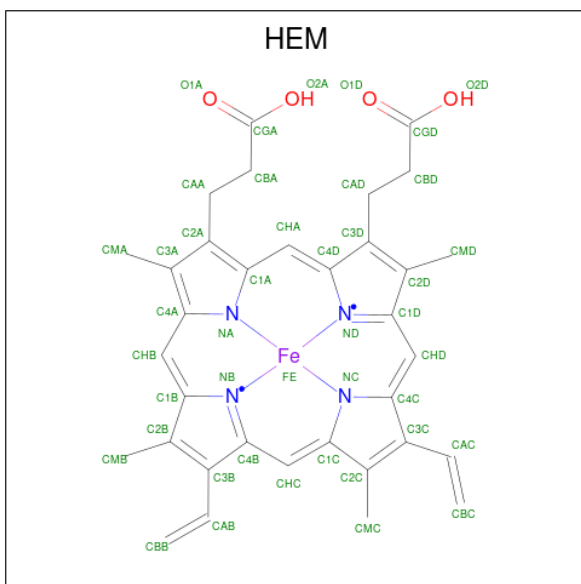
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			4	3	1		
2	B	1	Total	O	S	0	0
			4	3	1		

- Molecule 3 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 31	C 17	N 4	O 9	P 1	0	0
3	B	1	Total 31	C 17	N 4	O 9	P 1	0	0

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 5 is water.

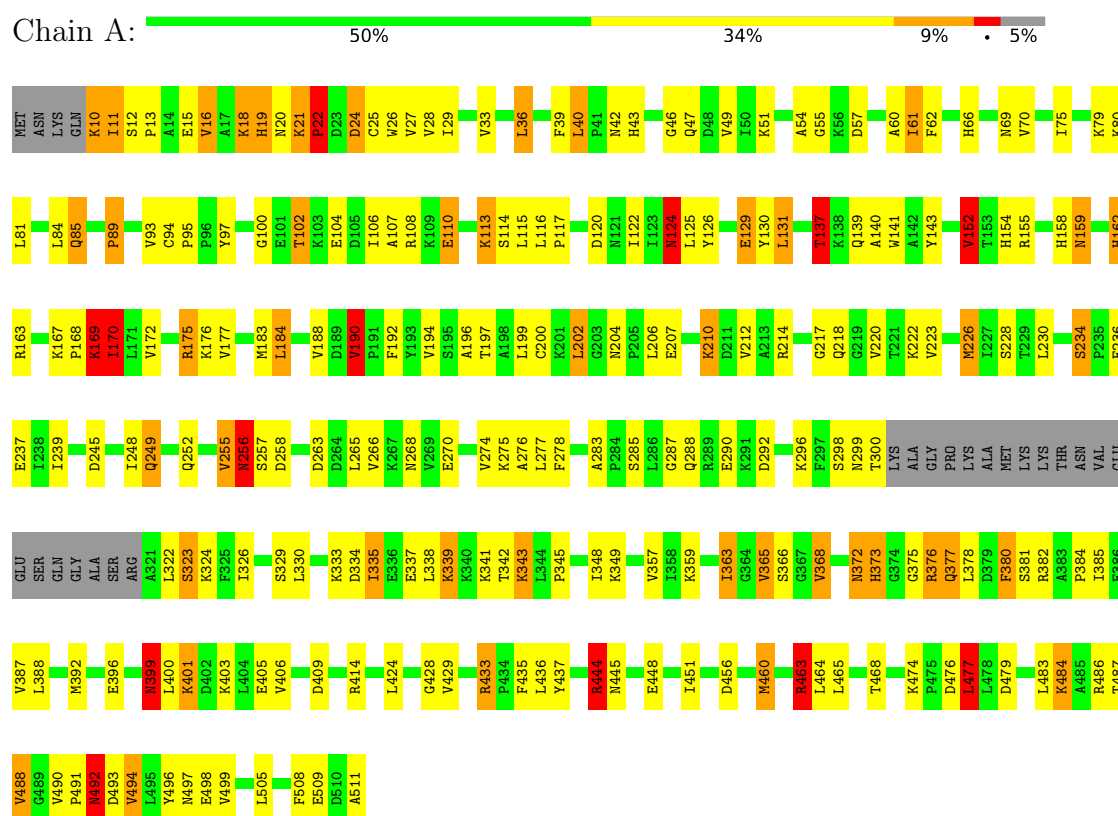
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	145	Total 145	O 145	0	0
5	B	61	Total 61	O 61	0	0

3 Residue-property plots

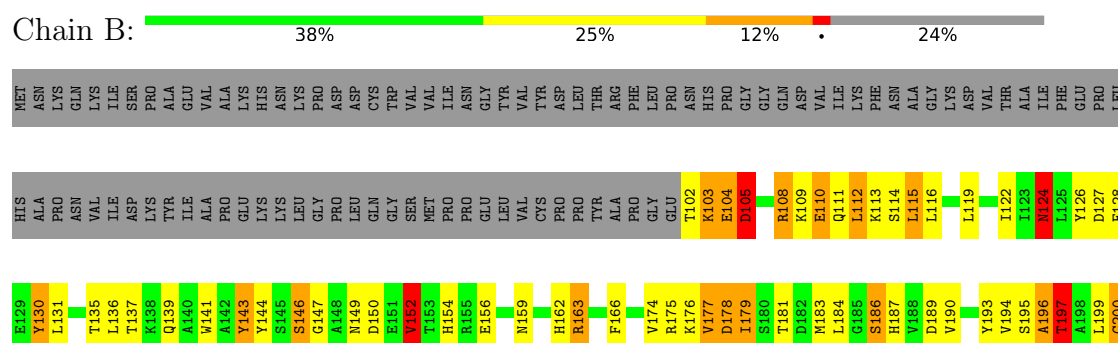
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

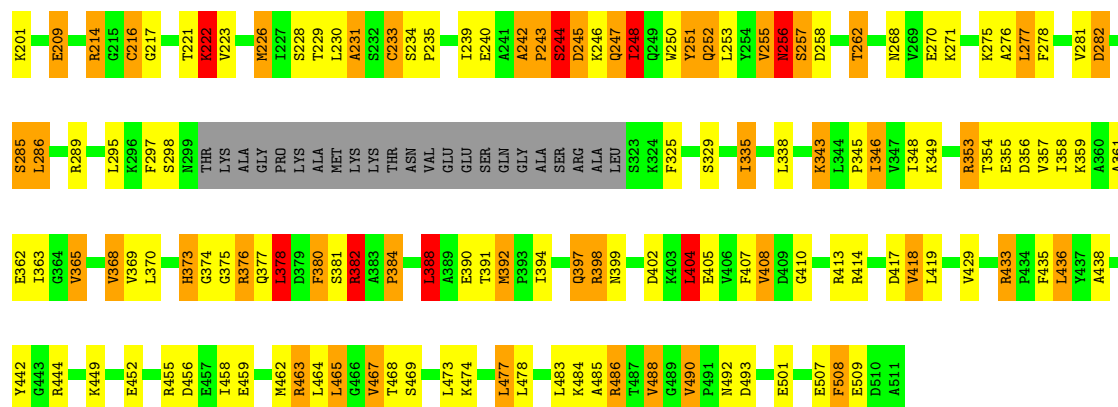
Note EDS was not executed.

• Molecule 1: FLAVOCYTOCHROME B2



• Molecule 1: FLAVOCYTOCHROME B2





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	164.50Å 164.50Å 114.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.173 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7075	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, SO3, FMN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.26	14/3816 (0.4%)	2.12	142/5170 (2.7%)
1	B	1.27	15/3063 (0.5%)	2.11	111/4138 (2.7%)
All	All	1.26	29/6879 (0.4%)	2.11	253/9308 (2.7%)

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	1
All	All	0	4

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	154	HIS	CD2-NE2	-8.36	1.28	1.37
1	B	392	MET	CA-CB	-7.53	1.47	1.54
1	B	373	HIS	CD2-NE2	-7.32	1.29	1.37
1	A	152	VAL	CA-CB	7.28	1.65	1.54
1	B	298	SER	C-N	-7.01	1.23	1.33
1	B	194	VAL	CA-CB	-7.01	1.45	1.54
1	A	405	GLU	CA-CB	-6.84	1.43	1.53
1	A	299	ASN	C-N	-6.70	1.24	1.33
1	B	459	GLU	CA-CB	-6.68	1.43	1.53
1	B	162	HIS	CD2-NE2	-6.23	1.30	1.37
1	A	19	HIS	CD2-NE2	-6.21	1.31	1.37
1	B	384	PRO	CA-CB	-6.17	1.45	1.53
1	B	187	HIS	CD2-NE2	-6.00	1.31	1.37
1	B	179	ILE	CA-CB	5.90	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	373	HIS	CD2-NE2	-5.80	1.31	1.37
1	A	384	PRO	CA-CB	-5.68	1.45	1.53
1	B	418	VAL	CA-CB	5.65	1.61	1.54
1	A	158	HIS	CD2-NE2	-5.64	1.31	1.37
1	B	456	ASP	CA-CB	-5.48	1.44	1.53
1	A	382	ARG	CA-CB	-5.43	1.44	1.53
1	B	388	LEU	CA-CB	-5.39	1.45	1.53
1	A	162	HIS	CD2-NE2	-5.31	1.32	1.37
1	A	493	ASP	N-CA	-5.27	1.39	1.46
1	B	255	VAL	CA-CB	5.23	1.59	1.54
1	B	154	HIS	CD2-NE2	-5.18	1.32	1.37
1	A	141	TRP	NE1-CE2	-5.18	1.31	1.37
1	A	499	VAL	CA-CB	5.16	1.61	1.54
1	A	479	ASP	CA-CB	-5.06	1.46	1.53
1	B	467	VAL	CA-CB	-5.05	1.46	1.54

All (253) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	190	VAL	N-CA-CB	-16.96	97.25	111.67
1	B	507	GLU	N-CA-C	10.79	127.15	113.55
1	A	70	VAL	N-CA-C	10.12	120.94	110.72
1	A	124	ASN	OD1-CG-ND2	-9.82	112.78	122.60
1	B	377	GLN	CA-C-O	-9.81	113.57	119.55
1	A	170	ILE	N-CA-CB	-9.60	100.22	112.60
1	B	181	THR	N-CA-C	-9.10	96.18	108.74
1	A	382	ARG	NE-CZ-NH2	-9.00	111.10	119.20
1	B	189	ASP	N-CA-C	8.94	121.02	111.28
1	A	256	ASN	OD1-CG-ND2	-8.71	113.89	122.60
1	A	376	ARG	NE-CZ-NH1	8.65	130.16	121.50
1	B	127	ASP	CA-CB-CG	8.54	121.14	112.60
1	A	19	HIS	CB-CG-CD2	-8.38	120.31	131.20
1	A	190	VAL	O-C-N	-8.28	114.20	121.57
1	A	381	SER	N-CA-C	-8.26	98.26	110.48
1	B	435	PHE	CA-CB-CG	-8.24	105.56	113.80
1	A	373	HIS	CA-CB-CG	8.23	122.03	113.80
1	A	476	ASP	CA-CB-CG	8.14	120.74	112.60
1	A	326	ILE	N-CA-C	-8.09	96.06	107.80
1	A	115	LEU	N-CA-C	-8.09	103.40	113.18
1	B	199	LEU	N-CA-C	8.04	122.47	111.54
1	B	335	ILE	N-CA-C	-7.99	102.91	110.42
1	B	149	ASN	CB-CG-ND2	7.99	128.38	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	256	ASN	OD1-CG-ND2	-7.94	114.66	122.60
1	B	152	VAL	CA-C-O	-7.89	111.95	120.47
1	A	409	ASP	CA-CB-CG	7.76	120.36	112.60
1	A	497	ASN	OD1-CG-ND2	-7.74	114.86	122.60
1	B	244	SER	N-CA-C	7.58	126.94	110.80
1	A	170	ILE	CB-CA-C	7.45	121.40	111.19
1	A	226	MET	CG-SD-CE	-7.41	84.60	100.90
1	B	398	ARG	N-CA-C	-7.40	104.34	113.15
1	B	463	ARG	NE-CZ-NH2	-7.40	112.54	119.20
1	A	40	LEU	N-CA-C	7.37	123.74	113.57
1	A	292	ASP	CA-CB-CG	7.36	119.95	112.60
1	B	368	VAL	CA-CB-CG2	-7.33	97.95	110.40
1	A	256	ASN	CA-CB-CG	7.32	119.92	112.60
1	A	493	ASP	N-CA-CB	-7.25	98.25	110.49
1	A	334	ASP	CA-CB-CG	-7.23	105.37	112.60
1	B	408	VAL	O-C-N	-7.22	113.55	122.57
1	B	149	ASN	OD1-CG-ND2	-7.21	115.39	122.60
1	A	342	THR	CA-CB-OG1	-7.17	98.84	109.60
1	A	69	ASN	OD1-CG-ND2	-7.08	115.52	122.60
1	A	283	ALA	CA-C-N	7.05	126.75	119.56
1	A	283	ALA	C-N-CA	7.05	126.75	119.56
1	A	380	PHE	CA-CB-CG	-6.98	106.82	113.80
1	A	256	ASN	CB-CG-ND2	6.97	126.86	116.40
1	A	43	HIS	CB-CG-CD2	-6.88	122.25	131.20
1	A	190	VAL	CB-CA-C	6.87	120.72	110.97
1	B	268	ASN	OD1-CG-ND2	-6.79	115.81	122.60
1	A	435	PHE	CA-CB-CG	-6.76	107.04	113.80
1	B	410	GLY	O-C-N	6.75	131.48	122.70
1	A	268	ASN	OD1-CG-ND2	-6.74	115.86	122.60
1	B	256	ASN	CB-CG-ND2	6.73	126.49	116.40
1	A	486	ARG	NE-CZ-NH2	-6.71	113.16	119.20
1	B	508	PHE	N-CA-CB	6.69	121.79	110.49
1	A	496	TYR	N-CA-C	-6.68	103.93	111.14
1	A	365	VAL	O-C-N	-6.65	115.69	122.54
1	A	445	ASN	OD1-CG-ND2	-6.63	115.97	122.60
1	B	474	LYS	CA-C-N	6.62	126.25	119.56
1	B	474	LYS	C-N-CA	6.62	126.25	119.56
1	A	42	ASN	OD1-CG-ND2	-6.61	115.99	122.60
1	A	372	ASN	OD1-CG-ND2	-6.59	116.01	122.60
1	A	387	VAL	N-CA-C	-6.59	104.06	110.72
1	A	401	LYS	N-CA-C	6.57	119.27	111.33
1	A	492	ASN	OD1-CG-ND2	-6.56	116.04	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	ASN	CB-CG-ND2	6.55	126.23	116.40
1	A	69	ASN	CB-CG-ND2	6.53	126.20	116.40
1	B	103	LYS	CA-C-N	6.51	129.00	120.28
1	B	103	LYS	C-N-CA	6.51	129.00	120.28
1	B	262	THR	CA-CB-OG1	-6.50	99.85	109.60
1	A	357	VAL	N-CA-C	-6.49	104.43	110.53
1	A	376	ARG	NE-CZ-NH2	-6.49	113.36	119.20
1	B	124	ASN	OD1-CG-ND2	-6.48	116.12	122.60
1	A	493	ASP	CA-CB-CG	6.48	119.08	112.60
1	A	154	HIS	CB-CG-CD2	-6.43	122.83	131.20
1	A	167	LYS	CA-C-N	6.40	126.77	119.92
1	A	167	LYS	C-N-CA	6.40	126.77	119.92
1	A	433	ARG	N-CA-C	6.38	122.22	113.16
1	A	19	HIS	CB-CG-ND1	6.37	132.26	122.70
1	A	80	LYS	N-CA-C	-6.37	97.27	108.23
1	B	110	GLU	N-CA-C	-6.36	104.44	111.82
1	B	226	MET	CG-SD-CE	-6.34	86.94	100.90
1	A	444	ARG	CG-CD-NE	-6.34	98.05	112.00
1	A	323	SER	O-C-N	-6.33	117.31	123.26
1	B	362	GLU	CA-CB-CG	-6.33	101.45	114.10
1	B	197	THR	N-CA-CB	-6.25	100.10	110.47
1	A	399	ASN	CA-CB-CG	-6.24	106.36	112.60
1	B	141	TRP	CG-CD2-CE3	6.21	140.11	133.90
1	B	376	ARG	N-CA-C	-6.20	105.66	113.72
1	B	103	LYS	N-CA-C	6.19	123.99	110.80
1	B	114	SER	CA-C-N	-6.17	111.24	121.92
1	B	114	SER	C-N-CA	-6.17	111.24	121.92
1	A	492	ASN	O-C-N	6.15	131.73	122.94
1	A	365	VAL	CB-CA-C	6.14	118.33	111.45
1	A	167	LYS	CB-CG-CD	-6.14	97.18	111.30
1	A	499	VAL	O-C-N	-6.13	115.33	122.07
1	A	433	ARG	O-C-N	-6.10	114.97	120.71
1	A	474	LYS	O-C-N	-6.10	116.79	121.55
1	B	474	LYS	O-C-N	-6.08	114.33	121.32
1	A	204	ASN	OD1-CG-ND2	-6.04	116.56	122.60
1	B	382	ARG	NE-CZ-NH2	-6.03	113.77	119.20
1	B	147	GLY	O-C-N	-6.03	118.11	123.65
1	B	196	ALA	N-CA-C	6.01	119.43	109.46
1	A	335	ILE	N-CA-C	-6.00	104.66	110.72
1	B	193	TYR	O-C-N	-5.99	117.01	123.42
1	B	348	ILE	O-C-N	-5.99	116.12	122.83
1	B	214	ARG	CA-CB-CG	-5.97	102.15	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	353	ARG	O-C-N	-5.97	116.58	123.33
1	A	365	VAL	N-CA-CB	-5.95	99.72	111.15
1	A	376	ARG	O-C-N	-5.95	115.20	122.34
1	B	242	ALA	CA-C-N	5.94	127.27	119.84
1	B	242	ALA	C-N-CA	5.94	127.27	119.84
1	B	378	LEU	CB-CA-C	-5.94	100.30	110.22
1	A	377	GLN	CG-CD-NE2	5.93	125.30	116.40
1	A	249	GLN	CA-CB-CG	-5.90	102.30	114.10
1	B	115	LEU	CA-C-O	-5.90	112.65	119.14
1	A	342	THR	CA-CB-CG2	5.89	120.52	110.50
1	B	297	PHE	N-CA-C	-5.89	99.58	109.07
1	B	231	ALA	CA-C-O	-5.88	114.58	121.16
1	A	43	HIS	ND1-CG-CD2	5.88	111.97	106.10
1	A	322	LEU	N-CA-C	-5.86	102.09	110.59
1	A	491	PRO	CA-C-N	-5.86	112.54	123.03
1	A	491	PRO	C-N-CA	-5.86	112.54	123.03
1	A	363	ILE	CB-CG1-CD1	-5.85	101.51	113.80
1	A	108	ARG	CB-CG-CD	-5.85	97.85	111.30
1	A	248	ILE	CB-CG1-CD1	-5.83	101.55	113.80
1	B	362	GLU	CA-C-O	-5.81	114.35	120.63
1	B	110	GLU	CB-CG-CD	5.80	122.47	112.60
1	A	29	ILE	CA-CB-CG2	-5.80	100.64	110.50
1	A	484	LYS	N-CA-CB	-5.80	102.42	110.65
1	A	159	ASN	OD1-CG-ND2	-5.77	116.83	122.60
1	B	438	ALA	N-CA-C	-5.75	104.70	110.97
1	B	490	VAL	CA-C-N	5.75	126.08	119.93
1	B	490	VAL	C-N-CA	5.75	126.08	119.93
1	A	168	PRO	N-CA-C	5.74	120.24	111.34
1	B	197	THR	CA-CB-OG1	-5.74	100.98	109.60
1	B	478	LEU	CA-C-O	5.74	127.60	121.11
1	A	491	PRO	CA-C-O	-5.72	114.93	121.56
1	A	368	VAL	N-CA-CB	-5.72	101.98	111.36
1	A	220	VAL	N-CA-C	-5.71	104.57	112.50
1	B	402	ASP	CA-C-O	5.70	126.39	119.38
1	A	486	ARG	NE-CZ-NH1	5.70	127.19	121.50
1	A	329	SER	CA-C-O	-5.69	113.24	119.95
1	B	282	ASP	CA-CB-CG	5.69	118.29	112.60
1	B	162	HIS	CA-CB-CG	-5.69	108.11	113.80
1	B	257	SER	N-CA-C	-5.68	105.17	111.36
1	A	61	ILE	CB-CA-C	-5.66	104.60	112.02
1	B	380	PHE	CA-CB-CG	-5.66	108.14	113.80
1	B	374	GLY	N-CA-C	-5.63	106.41	115.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	357	VAL	N-CA-C	-5.62	105.14	110.42
1	B	251	TYR	N-CA-C	-5.61	100.55	109.59
1	B	143	TYR	CA-C-O	-5.61	113.52	119.97
1	B	248	ILE	CB-CG1-CD1	-5.60	102.04	113.80
1	A	275	LYS	N-CA-C	5.59	120.79	113.30
1	A	484	LYS	O-C-N	-5.56	114.61	122.06
1	B	404	LEU	O-C-N	-5.55	116.78	123.27
1	A	339	LYS	N-CA-C	-5.54	105.25	111.28
1	A	234	SER	CA-C-O	-5.53	114.67	120.70
1	B	195	SER	N-CA-C	-5.53	102.27	110.46
1	A	334	ASP	N-CA-C	5.51	117.28	111.28
1	B	349	LYS	CG-CD-CE	-5.50	98.65	111.30
1	B	221	THR	CA-C-O	5.50	126.75	120.54
1	A	43	HIS	CG-CD2-NE2	-5.49	101.71	107.20
1	A	292	ASP	CB-CA-C	-5.49	102.51	110.96
1	B	186	SER	N-CA-C	5.49	117.77	110.53
1	B	285	SER	N-CA-C	-5.47	100.98	109.24
1	B	233	CYS	N-CA-C	-5.47	99.69	108.55
1	A	39	PHE	CA-C-O	-5.46	114.70	120.55
1	A	85	GLN	OE1-CD-NE2	-5.46	117.14	122.60
1	A	387	VAL	CB-CA-C	-5.46	104.69	112.22
1	A	372	ASN	CA-C-O	5.45	126.10	119.78
1	B	234	SER	CA-C-N	5.45	125.10	119.05
1	B	234	SER	C-N-CA	5.45	125.10	119.05
1	A	365	VAL	N-CA-C	-5.44	104.06	110.21
1	B	166	PHE	CA-C-O	-5.43	115.31	121.72
1	B	368	VAL	CA-CB-CG1	5.43	119.63	110.40
1	B	162	HIS	CB-CG-CD2	-5.41	124.17	131.20
1	A	172	VAL	N-CA-C	-5.40	100.70	108.48
1	A	368	VAL	N-CA-C	-5.40	101.22	108.35
1	A	162	HIS	CB-CG-CD2	-5.37	124.22	131.20
1	B	130	TYR	CA-C-O	-5.37	115.17	120.70
1	B	130	TYR	N-CA-C	-5.37	105.34	111.14
1	A	274	VAL	O-C-N	-5.34	117.03	122.54
1	A	11	ILE	N-CA-C	-5.34	100.95	108.27
1	A	122	ILE	O-C-N	-5.33	116.86	122.83
1	A	129	GLU	CB-CA-C	-5.33	102.28	110.81
1	A	117	PRO	CB-CA-C	5.33	117.42	110.92
1	A	66	HIS	CB-CG-CD2	-5.32	124.29	131.20
1	A	343	LYS	CA-CB-CG	5.31	124.72	114.10
1	B	243	PRO	N-CA-C	5.31	123.41	112.47
1	A	285	SER	N-CA-C	-5.30	101.01	109.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	184	LEU	N-CA-CB	-5.30	103.86	111.70
1	B	433	ARG	N-CA-C	5.29	120.81	113.45
1	B	124	ASN	CB-CG-ND2	5.29	124.34	116.40
1	B	200	CYS	CB-CA-C	-5.29	99.89	110.42
1	A	484	LYS	N-CA-C	-5.29	107.36	112.97
1	B	159	ASN	CA-C-O	-5.28	114.13	120.10
1	B	373	HIS	CA-CB-CG	5.28	119.08	113.80
1	A	406	VAL	O-C-N	-5.28	116.00	122.97
1	B	286	LEU	N-CA-CB	-5.28	102.49	110.35
1	A	463	ARG	CB-CA-C	-5.27	102.84	110.96
1	A	10	LYS	CB-CG-CD	5.27	123.42	111.30
1	B	353	ARG	CA-C-O	-5.26	115.09	120.99
1	B	141	TRP	CB-CG-CD1	-5.26	119.01	126.90
1	A	477	LEU	N-CA-C	-5.26	105.72	113.61
1	B	408	VAL	N-CA-CB	-5.26	102.55	111.23
1	A	155	ARG	CA-CB-CG	-5.26	103.58	114.10
1	A	377	GLN	OE1-CD-NE2	-5.25	117.35	122.60
1	A	392	MET	O-C-N	-5.25	115.78	120.71
1	A	382	ARG	N-CA-C	5.25	117.46	110.53
1	A	268	ASN	CB-CG-ND2	5.23	124.25	116.40
1	A	275	LYS	CA-CB-CG	-5.23	103.64	114.10
1	A	89	PRO	CA-C-N	5.22	125.03	119.28
1	A	89	PRO	C-N-CA	5.22	125.03	119.28
1	A	324	LYS	N-CA-C	-5.21	106.92	113.28
1	A	194	VAL	N-CA-CB	-5.21	105.12	111.21
1	A	200	CYS	O-C-N	-5.20	115.63	122.39
1	B	240	GLU	CA-CB-CG	-5.19	103.72	114.10
1	A	202	LEU	N-CA-C	-5.19	105.62	111.28
1	B	222	LYS	N-CA-C	-5.19	99.95	108.41
1	A	488	VAL	N-CA-C	-5.17	98.56	107.24
1	B	297	PHE	N-CA-CB	5.16	118.67	110.57
1	A	372	ASN	CB-CG-ND2	5.15	124.12	116.40
1	B	216	CYS	CA-CB-SG	-5.14	102.58	114.40
1	B	417	ASP	N-CA-C	-5.13	105.77	111.36
1	B	486	ARG	NE-CZ-NH1	5.13	126.63	121.50
1	A	348	ILE	N-CA-CB	-5.13	105.21	110.95
1	B	178	ASP	CA-CB-CG	5.12	117.72	112.60
1	B	361	ALA	CA-C-O	-5.12	115.42	120.80
1	A	296	LYS	CA-CB-CG	-5.10	103.90	114.10
1	B	488	VAL	O-C-N	-5.08	117.55	122.99
1	B	493	ASP	CA-C-N	5.07	127.41	120.77
1	B	493	ASP	C-N-CA	5.07	127.41	120.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	PHE	CA-CB-CG	-5.07	108.73	113.80
1	B	271	LYS	N-CA-C	-5.07	105.65	111.07
1	B	381	SER	N-CA-C	-5.06	102.98	110.48
1	B	362	GLU	O-C-N	-5.06	116.75	122.12
1	A	169	LYS	CB-CA-C	-5.06	100.11	109.37
1	A	170	ILE	CA-CB-CG1	-5.06	101.80	110.40
1	A	12	SER	CA-C-N	5.06	126.16	119.84
1	A	12	SER	C-N-CA	5.06	126.16	119.84
1	A	210	LYS	N-CA-C	-5.05	105.90	111.71
1	A	29	ILE	CA-CB-CG1	5.05	118.98	110.40
1	A	113	LYS	CA-C-O	5.05	127.73	120.51
1	B	245	ASP	N-CA-C	5.05	121.55	110.80
1	A	263	ASP	O-C-N	-5.04	116.40	122.15
1	A	377	GLN	CA-C-O	-5.04	113.31	120.51
1	A	137	THR	CA-CB-CG2	5.03	119.06	110.50
1	B	154	HIS	CB-CG-CD2	-5.02	124.67	131.20
1	B	486	ARG	O-C-N	-5.02	116.69	122.87
1	B	485	ALA	N-CA-C	-5.01	104.33	110.65
1	B	104	GLU	N-CA-C	-5.01	105.82	111.28
1	B	247	GLN	OE1-CD-NE2	-5.00	117.60	122.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	130	TYR	Sidechain
1	A	463	ARG	Sidechain
1	A	492	ASN	Mainchain
1	B	251	TYR	Sidechain

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	3742	0	3794	103	0
1	B	3014	0	3072	94	0
2	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	4	0	0	0	0
3	A	31	0	18	1	0
3	B	31	0	17	1	0
4	A	43	0	30	5	0
5	A	145	0	0	2	0
5	B	61	0	0	2	0
All	All	7075	0	6931	182	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (182) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:VAL:HG22	1:B:490:VAL:HG21	1.49	0.95
1:A:196:ALA:H	1:A:226:MET:HE2	1.54	0.72
1:A:199:LEU:HD21	4:A:560:HEM:HAA1	1.71	0.72
1:A:372:ASN:HD22	1:A:375:GLY:H	1.36	0.72
1:A:488:VAL:HG22	1:B:490:VAL:CG2	2.19	0.71
1:B:243:PRO:HD2	1:B:247:GLN:HE22	1.55	0.71
1:B:183:MET:HE2	1:B:250:TRP:HH2	1.54	0.71
1:A:256:ASN:HD22	1:A:257:SER:N	1.88	0.71
1:A:396:GLU:HG3	1:A:401:LYS:HG3	1.75	0.69
1:B:197:THR:HG21	1:B:436:LEU:HG	1.73	0.69
1:A:61:ILE:HD12	1:A:97:TYR:HB2	1.75	0.68
1:A:137:THR:HG22	1:A:140:ALA:H	1.59	0.67
1:B:217:GLY:HA3	1:B:247:GLN:NE2	2.09	0.66
1:A:177:VAL:HG23	1:A:468:THR:HA	1.79	0.65
1:A:190:VAL:HG11	1:A:223:VAL:HG22	1.77	0.65
1:A:162:HIS:HE1	5:A:674:HOH:O	1.80	0.64
1:A:116:LEU:HD22	1:A:131:LEU:HG	1.80	0.64
1:B:109:LYS:HD2	1:B:112:LEU:HD21	1.79	0.63
1:A:511:ALA:H	1:B:115:LEU:HD13	1.63	0.63
1:A:25:CYS:SG	1:A:54:ALA:HB2	2.39	0.63
1:A:385:ILE:HD11	1:A:424:LEU:HD12	1.80	0.63
1:B:256:ASN:HD22	1:B:257:SER:N	1.97	0.62
1:A:27:VAL:HG11	1:A:36:LEU:HD22	1.81	0.62
1:A:28:VAL:HG22	1:A:33:VAL:HG22	1.81	0.62
1:B:216:CYS:O	1:B:222:LYS:HA	2.00	0.61
1:B:105:ASP:O	1:B:109:LYS:HG2	2.00	0.61
1:B:353:ARG:HD2	1:B:355:GLU:HB2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:ARG:NH2	1:B:486:ARG:HG3	2.16	0.60
1:A:143:TYR:O	1:A:376:ARG:NH2	2.33	0.60
1:A:337:GLU:O	1:A:341:LYS:HD3	2.02	0.60
1:B:354:THR:HA	1:B:391:THR:HG22	1.85	0.59
1:A:270:GLU:OE2	1:A:343:LYS:HG3	2.02	0.59
1:A:414:ARG:HD2	1:B:150:ASP:OD2	2.02	0.59
1:A:266:VAL:HG13	1:A:277:LEU:HD11	1.85	0.59
1:A:463:ARG:HD2	1:B:285:SER:OG	2.02	0.59
1:A:396:GLU:HA	1:A:401:LYS:HB2	1.86	0.57
1:A:226:MET:HE3	1:A:252:GLN:HB2	1.86	0.57
1:B:109:LYS:HA	1:B:112:LEU:HD23	1.87	0.57
1:A:169:LYS:HG2	1:A:465:LEU:O	2.05	0.56
1:A:170:ILE:HD11	1:B:282:ASP:HA	1.88	0.56
1:A:196:ALA:HB1	1:A:228:SER:HB2	1.88	0.56
1:A:465:LEU:HD23	1:B:378:LEU:HD11	1.88	0.56
1:B:256:ASN:ND2	1:B:258:ASP:H	2.05	0.55
1:A:176:LYS:HA	5:A:661:HOH:O	2.07	0.55
1:B:177:VAL:HG22	1:B:468:THR:HA	1.88	0.55
1:B:152:VAL:HG21	1:B:380:PHE:CE1	2.41	0.55
1:B:256:ASN:HD22	1:B:257:SER:H	1.56	0.54
1:A:16:VAL:HA	1:A:26:TRP:HE3	1.73	0.54
1:A:287:GLY:H	1:A:377:GLN:NE2	2.05	0.54
1:A:163:ARG:NH1	1:B:488:VAL:O	2.41	0.54
1:A:57:ASP:HB3	1:A:93:VAL:HG12	1.88	0.54
1:A:217:GLY:O	1:A:222:LYS:NZ	2.41	0.54
1:A:372:ASN:ND2	1:A:375:GLY:H	2.06	0.53
1:B:369:VAL:HG22	1:B:407:PHE:HB2	1.91	0.53
1:A:218:GLN:HE22	1:A:444:ARG:HD3	1.73	0.53
1:B:404:LEU:HD12	1:B:405:GLU:O	2.07	0.53
1:A:152:VAL:HG21	1:A:380:PHE:CE1	2.44	0.53
1:B:354:THR:OG1	1:B:391:THR:HG22	2.09	0.53
1:A:511:ALA:N	1:B:115:LEU:HD13	2.23	0.53
1:A:223:VAL:HG21	1:A:451:ILE:HG12	1.91	0.52
1:A:197:THR:HB	1:A:436:LEU:HD11	1.90	0.52
1:A:169:LYS:HA	1:B:353:ARG:HH21	1.74	0.52
1:B:375:GLY:HA2	5:B:767:HOH:O	2.10	0.52
1:B:452:GLU:HB3	1:B:455:ARG:NH2	2.24	0.52
1:B:394:ILE:HD13	1:B:397:GLN:HE22	1.75	0.52
1:B:465:LEU:HD22	1:B:477:LEU:HG	1.92	0.52
1:A:60:ALA:HB3	1:A:94:CYS:O	2.10	0.52
1:A:226:MET:HE3	1:A:252:GLN:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:VAL:HB	4:A:560:HEM:HBC2	1.92	0.51
1:A:456:ASP:O	1:A:460:MET:HB2	2.10	0.51
1:A:16:VAL:HA	1:A:26:TRP:CE3	2.45	0.51
1:B:289:ARG:HD2	5:B:764:HOH:O	2.10	0.51
1:B:373:HIS:O	1:B:376:ARG:HG3	2.11	0.51
1:A:508:PHE:HE2	1:B:116:LEU:HD23	1.75	0.51
1:B:243:PRO:HD2	1:B:247:GLN:NE2	2.24	0.51
1:B:270:GLU:OE2	1:B:343:LYS:HB3	2.11	0.51
1:B:143:TYR:O	1:B:376:ARG:NH2	2.42	0.51
1:B:209:GLU:HG3	1:B:231:ALA:HB1	1.93	0.51
1:A:210:LYS:O	1:A:214:ARG:HG3	2.10	0.50
1:A:226:MET:HE1	1:A:349:LYS:HE3	1.92	0.50
1:B:252:GLN:HA	1:B:278:PHE:O	2.11	0.50
1:A:140:ALA:HB2	1:A:202:LEU:HB3	1.92	0.50
1:A:15:GLU:O	1:A:18:LYS:HB2	2.12	0.50
1:A:373:HIS:O	1:A:376:ARG:HG3	2.12	0.50
1:B:108:ARG:O	1:B:111:GLN:HB2	2.12	0.50
1:A:124:ASN:ND2	1:A:126:TYR:HB2	2.27	0.49
1:A:256:ASN:ND2	1:A:258:ASP:H	2.10	0.49
1:B:144:TYR:O	1:B:433:ARG:HD3	2.12	0.49
1:B:235:PRO:O	1:B:239:ILE:HG13	2.13	0.49
1:B:216:CYS:HB3	1:B:223:VAL:O	2.12	0.49
1:A:252:GLN:HA	1:A:278:PHE:O	2.13	0.49
1:A:234:SER:HG	1:A:237:GLU:HG3	1.79	0.48
1:B:179:ILE:HG22	1:B:462:MET:SD	2.53	0.48
1:B:226:MET:HE3	1:B:252:GLN:HB3	1.96	0.48
1:A:61:ILE:CD1	1:A:97:TYR:HB2	2.43	0.48
1:A:487:THR:O	1:B:490:VAL:HG22	2.14	0.48
1:A:234:SER:OG	1:A:237:GLU:HG3	2.14	0.48
1:A:400:LEU:O	1:A:403:LYS:HG2	2.14	0.48
1:A:183:MET:HE2	1:A:428:GLY:HA3	1.95	0.48
1:A:494:VAL:O	1:A:498:GLU:HB2	2.13	0.48
1:A:288:GLN:HE21	1:A:290:GLU:HG2	1.78	0.48
1:A:169:LYS:HB3	1:B:353:ARG:NH2	2.29	0.47
1:A:100:GLY:H	1:A:300:THR:N	2.11	0.47
1:A:505:LEU:HD13	1:B:130:TYR:HB2	1.96	0.47
1:B:419:LEU:HD13	1:B:465:LEU:HD12	1.95	0.47
1:B:108:ARG:HH21	1:B:137:THR:HA	1.80	0.47
1:B:109:LYS:O	1:B:113:LYS:HB3	2.15	0.47
1:B:174:VAL:O	1:B:463:ARG:HD2	2.14	0.47
1:A:170:ILE:HG12	1:B:281:VAL:HG23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:ILE:HD13	1:A:363:ILE:HG21	1.67	0.46
1:A:169:LYS:HD3	1:A:477:LEU:HD11	1.98	0.46
1:B:358:ILE:HD11	1:B:394:ILE:HG21	1.98	0.46
1:A:21:LYS:HB3	1:A:24:ASP:OD1	2.15	0.46
1:B:394:ILE:HD13	1:B:397:GLN:NE2	2.30	0.46
1:B:109:LYS:HA	1:B:112:LEU:CD2	2.46	0.46
1:A:239:ILE:HD13	1:A:249:GLN:NE2	2.31	0.45
1:A:372:ASN:HD22	1:A:375:GLY:N	2.09	0.45
1:A:255:VAL:HG11	1:A:330:LEU:HD21	1.99	0.45
1:B:282:ASP:OD1	1:B:373:HIS:ND1	2.48	0.45
1:B:143:TYR:HA	1:B:289:ARG:HH22	1.81	0.45
1:B:111:GLN:HB3	1:B:135:THR:HG22	1.99	0.45
1:B:346:ILE:O	1:B:365:VAL:HB	2.17	0.45
1:A:75:ILE:HD11	4:A:560:HEM:HAB	1.98	0.44
1:B:122:ILE:HG21	1:B:128:PHE:CZ	2.52	0.44
1:A:207:GLU:CD	1:A:214:ARG:HH22	2.24	0.44
1:B:388:LEU:HD22	1:B:392:MET:HG2	1.98	0.44
1:B:244:SER:O	1:B:246:LYS:N	2.50	0.44
1:A:400:LEU:HA	1:A:403:LYS:HD3	2.00	0.44
1:B:467:VAL:HG11	1:B:477:LEU:HD21	1.98	0.44
1:B:201:LYS:HE3	1:B:233:CYS:SG	2.57	0.44
3:B:570:FMN:H9	3:B:570:FMN:H1'2	1.55	0.44
1:A:20:ASN:HB3	1:A:55:GLY:HA3	2.00	0.44
1:B:175:ARG:NH1	1:B:176:LYS:HE2	2.33	0.44
1:A:27:VAL:CG1	1:A:36:LEU:HD22	2.46	0.43
1:B:226:MET:HB3	1:B:226:MET:HE2	1.89	0.43
1:A:129:GLU:HG2	1:A:437:TYR:CD2	2.53	0.43
1:A:22:PRO:HG3	1:A:51:LYS:HG3	1.99	0.43
1:A:28:VAL:HG21	1:A:84:LEU:HD22	2.01	0.43
1:A:107:ALA:O	1:A:110:GLU:HG3	2.18	0.43
1:A:159:ASN:HB3	1:B:488:VAL:HG11	1.99	0.43
1:B:116:LEU:HB3	1:B:442:TYR:OH	2.19	0.43
1:B:358:ILE:HD11	1:B:394:ILE:CG2	2.49	0.43
1:A:49:VAL:HG11	4:A:560:HEM:HMD2	2.01	0.43
1:B:175:ARG:HH12	1:B:176:LYS:HE2	1.84	0.43
1:B:178:ASP:O	1:B:469:SER:HA	2.19	0.43
1:A:256:ASN:HD22	1:A:257:SER:H	1.67	0.42
1:A:508:PHE:CE2	1:B:116:LEU:HD23	2.54	0.42
1:B:175:ARG:HH11	1:B:175:ARG:HD2	1.70	0.42
1:A:192:PHE:HA	1:A:429:VAL:O	2.18	0.42
1:A:276:ALA:HA	1:A:345:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:GLU:HG3	1:A:401:LYS:CG	2.48	0.42
1:B:356:ASP:HA	1:B:359:LYS:HD2	2.02	0.42
1:B:119:LEU:HD22	1:B:449:LYS:HG2	2.02	0.42
1:A:230:LEU:HG	4:A:560:HEM:HAA2	2.02	0.42
1:B:124:ASN:HD22	1:B:126:TYR:N	2.17	0.42
1:B:248:ILE:HD13	1:B:248:ILE:HG21	1.73	0.42
1:B:358:ILE:HD13	1:B:398:ARG:NH1	2.35	0.42
1:B:382:ARG:NH2	1:B:390:GLU:OE1	2.53	0.42
1:A:79:LYS:HE3	1:A:79:LYS:HB3	1.89	0.41
1:A:218:GLN:HE22	1:A:444:ARG:HH11	1.68	0.41
1:B:146:SER:HB3	1:B:289:ARG:HB3	2.01	0.41
1:A:11:ILE:H	1:A:85:GLN:HG3	1.85	0.41
1:A:106:ILE:HD13	1:A:106:ILE:HA	1.89	0.41
1:A:175:ARG:HH11	1:A:175:ARG:HB2	1.86	0.41
1:A:40:LEU:O	1:A:47:GLN:HB3	2.20	0.41
1:B:276:ALA:HA	1:B:345:PRO:HD2	2.01	0.41
1:B:253:LEU:HD22	1:B:277:LEU:HD13	2.02	0.41
1:A:25:CYS:SG	1:A:54:ALA:CB	3.07	0.41
1:A:196:ALA:HB2	1:A:226:MET:HG2	2.02	0.41
1:B:229:THR:OG1	1:B:253:LEU:HA	2.21	0.41
1:B:102:THR:O	1:B:104:GLU:N	2.54	0.41
1:B:335:ILE:CG2	1:B:363:ILE:HD11	2.51	0.41
1:A:113:LYS:HE2	1:A:113:LYS:HB3	1.89	0.40
1:A:188:VAL:HG12	1:A:190:VAL:H	1.87	0.40
3:A:570:FMN:H9	3:A:570:FMN:H1'2	1.62	0.40
1:B:156:GLU:OE2	1:B:163:ARG:NH2	2.54	0.40
1:B:179:ILE:CD1	1:B:190:VAL:HG12	2.52	0.40
1:B:196:ALA:HB1	1:B:228:SER:HB2	2.01	0.40
1:B:256:ASN:HD22	1:B:258:ASP:H	1.67	0.40
1:A:139:GLN:HG3	1:A:202:LEU:HD22	2.03	0.40
1:B:214:ARG:HA	1:B:243:PRO:CD	2.51	0.40
1:B:418:VAL:HG11	1:B:458:ILE:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	478/506 (94%)	440 (92%)	29 (6%)	9 (2%)	6	13
1	B	383/506 (76%)	341 (89%)	34 (9%)	8 (2%)	5	11
All	All	861/1012 (85%)	781 (91%)	63 (7%)	17 (2%)	6	12

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	245	ASP
1	A	46	GLY
1	A	114	SER
1	B	103	LYS
1	B	473	LEU
1	A	24	ASP
1	A	104	GLU
1	A	298	SER
1	B	146	SER
1	B	508	PHE
1	A	16	VAL
1	B	200	CYS
1	A	102	THR
1	B	242	ALA
1	A	399	ASN
1	B	105	ASP
1	A	22	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	412/435 (95%)	358 (87%)	54 (13%)	4	8
1	B	333/435 (77%)	277 (83%)	56 (17%)	2	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	745/870 (86%)	635 (85%)	110 (15%)	3 6

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LYS
1	A	13	PRO
1	A	18	LYS
1	A	19	HIS
1	A	21	LYS
1	A	22	PRO
1	A	36	LEU
1	A	81	LEU
1	A	89	PRO
1	A	95	PRO
1	A	102	THR
1	A	110	GLU
1	A	120	ASP
1	A	124	ASN
1	A	125	LEU
1	A	131	LEU
1	A	137	THR
1	A	152	VAL
1	A	169	LYS
1	A	170	ILE
1	A	175	ARG
1	A	184	LEU
1	A	190	VAL
1	A	206	LEU
1	A	212	VAL
1	A	236	GLU
1	A	245	ASP
1	A	255	VAL
1	A	256	ASN
1	A	265	LEU
1	A	323	SER
1	A	333	LYS
1	A	335	ILE
1	A	338	LEU
1	A	339	LYS
1	A	359	LYS
1	A	365	VAL

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Mol	Chain	Res	Type
1	A	366	SER
1	A	368	VAL
1	A	378	LEU
1	A	388	LEU
1	A	399	ASN
1	A	433	ARG
1	A	444	ARG
1	A	448	GLU
1	A	460	MET
1	A	464	LEU
1	A	477	LEU
1	A	483	LEU
1	A	484	LYS
1	A	490	VAL
1	A	492	ASN
1	A	494	VAL
1	A	509	GLU
1	B	105	ASP
1	B	108	ARG
1	B	110	GLU
1	B	112	LEU
1	B	124	ASN
1	B	131	LEU
1	B	136	LEU
1	B	139	GLN
1	B	152	VAL
1	B	163	ARG
1	B	177	VAL
1	B	184	LEU
1	B	186	SER
1	B	197	THR
1	B	209	GLU
1	B	222	LYS
1	B	230	LEU
1	B	244	SER
1	B	248	ILE
1	B	252	GLN
1	B	255	VAL
1	B	256	ASN
1	B	262	THR
1	B	275	LYS
1	B	277	LEU

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Mol	Chain	Res	Type
1	B	286	LEU
1	B	295	LEU
1	B	325	PHE
1	B	329	SER
1	B	338	LEU
1	B	343	LYS
1	B	346	ILE
1	B	365	VAL
1	B	368	VAL
1	B	370	LEU
1	B	378	LEU
1	B	382	ARG
1	B	384	PRO
1	B	388	LEU
1	B	397	GLN
1	B	399	ASN
1	B	404	LEU
1	B	408	VAL
1	B	413	ARG
1	B	414	ARG
1	B	429	VAL
1	B	436	LEU
1	B	444	ARG
1	B	464	LEU
1	B	465	LEU
1	B	477	LEU
1	B	483	LEU
1	B	484	LYS
1	B	492	ASN
1	B	501	GLU
1	B	509	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	HIS
1	A	53	ASN
1	A	85	GLN
1	A	124	ASN
1	A	139	GLN
1	A	157	ASN
1	A	162	HIS

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Mol	Chain	Res	Type
1	A	204	ASN
1	A	218	GLN
1	A	249	GLN
1	A	252	GLN
1	A	256	ASN
1	A	288	GLN
1	A	372	ASN
1	A	377	GLN
1	A	439	ASN
1	A	497	ASN
1	B	111	GLN
1	B	124	ASN
1	B	162	HIS
1	B	225	GLN
1	B	247	GLN
1	B	252	GLN
1	B	256	ASN
1	B	377	GLN
1	B	397	GLN
1	B	439	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	FMN	A	570	2	33,33,33	1.96	9 (27%)	48,50,50	2.36	14 (29%)
3	FMN	B	570	2	33,33,33	1.75	8 (24%)	48,50,50	2.42	21 (43%)
2	SO3	B	580	3	1,3,3	0.61	0	0,3,3	-	-
2	SO3	A	580	3	1,3,3	0.71	0	0,3,3	-	-
4	HEM	A	560	1	50,50,50	1.31	7 (14%)	67,82,82	1.16	5 (7%)

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	FMN	A	570	2	2/2/4/4	10/18/18/18	0/3/3/3
3	FMN	B	570	2	2/2/4/4	10/18/18/18	0/3/3/3
4	HEM	A	560	1	-	11/14/54/54	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	570	FMN	C1'-N10	-5.08	1.35	1.47
3	B	570	FMN	C9-C8	-4.77	1.33	1.39
3	B	570	FMN	C1'-N10	-4.32	1.37	1.47
3	A	570	FMN	C6-C7	-3.93	1.34	1.39
3	A	570	FMN	C7M-C7	-3.42	1.44	1.51
4	A	560	HEM	CBB-CAB	3.40	1.46	1.30
4	A	560	HEM	CAC-C3C	-3.20	1.38	1.47
3	B	570	FMN	C2'-C3'	-2.96	1.48	1.53
4	A	560	HEM	CAB-C3B	-2.93	1.39	1.47
3	A	570	FMN	C4A-C10	-2.76	1.36	1.44
4	A	560	HEM	CBC-CAC	2.70	1.43	1.30
3	A	570	FMN	C9-C8	-2.68	1.36	1.39
3	B	570	FMN	C1'-C2'	-2.66	1.48	1.52
3	A	570	FMN	O4'-C4'	-2.48	1.38	1.43
3	A	570	FMN	C4A-N5	2.28	1.35	1.30
3	A	570	FMN	C9A-N10	-2.22	1.37	1.41
4	A	560	HEM	O2D-CGD	-2.19	1.23	1.30
3	A	570	FMN	C10-N1	2.16	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	570	FMN	C9A-N10	-2.15	1.37	1.41
3	B	570	FMN	C4A-N5	2.12	1.35	1.30
4	A	560	HEM	O2A-CGA	-2.12	1.23	1.30
3	B	570	FMN	C9A-C5A	-2.09	1.37	1.41
4	A	560	HEM	CBA-CGA	2.06	1.55	1.50
3	B	570	FMN	C9-C9A	-2.00	1.36	1.39

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	570	FMN	C4'-C3'-C2'	8.65	127.97	113.57
3	B	570	FMN	C4'-C3'-C2'	6.06	123.65	113.57
3	B	570	FMN	C4A-C10-N1	-5.47	111.18	124.59
3	B	570	FMN	C4-C4A-C10	5.28	125.98	116.93
3	A	570	FMN	C4A-C10-N1	-5.25	111.72	124.59
3	A	570	FMN	C10-N1-C2	5.13	127.97	116.85
3	A	570	FMN	C4-C4A-C10	4.60	124.82	116.93
3	B	570	FMN	O4'-C4'-C3'	4.38	119.49	109.25
3	B	570	FMN	C10-N1-C2	4.26	126.08	116.85
3	B	570	FMN	O3'-C3'-C4'	4.04	118.12	108.93
3	B	570	FMN	O4'-C4'-C5'	3.55	117.81	109.99
4	A	560	HEM	C3B-C4B-NB	3.27	111.82	109.47
3	A	570	FMN	N10-C10-N1	3.23	128.01	118.51
3	A	570	FMN	C10-C4A-N5	-3.19	118.30	124.81
3	B	570	FMN	C4-C4A-N5	-3.19	113.81	118.21
3	B	570	FMN	C4A-C10-N10	3.16	121.01	116.48
3	B	570	FMN	O5'-C5'-C4'	3.11	117.66	109.36
3	A	570	FMN	O4'-C4'-C3'	3.09	116.48	109.25
3	A	570	FMN	O5'-P-O1P	-3.06	98.18	106.44
3	B	570	FMN	N10-C10-N1	3.06	127.51	118.51
3	B	570	FMN	C1'-C2'-C3'	3.02	117.84	109.66
3	B	570	FMN	O2P-P-O5'	-2.99	98.87	106.67
4	A	560	HEM	CAA-CBA-CGA	2.81	121.11	113.67
3	B	570	FMN	O2-C2-N3	2.73	123.82	118.58
3	B	570	FMN	O2'-C2'-C1'	2.72	121.38	110.20
3	B	570	FMN	C5A-C9A-N10	2.68	120.39	117.97
3	A	570	FMN	C1'-C2'-C3'	2.62	116.75	109.66
3	B	570	FMN	C9A-N10-C10	-2.52	116.92	120.75
3	A	570	FMN	C9A-C5A-N5	-2.51	119.80	122.45
3	A	570	FMN	O2'-C2'-C1'	2.50	120.46	110.20
3	A	570	FMN	C4A-C10-N10	2.48	120.03	116.48
3	B	570	FMN	O2-C2-N1	-2.35	117.90	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	570	FMN	C10-C4A-N5	-2.34	120.03	124.81
4	A	560	HEM	CMB-C2B-C1B	2.28	128.60	125.03
3	A	570	FMN	O3'-C3'-C4'	2.20	113.93	108.93
4	A	560	HEM	O2A-CGA-CBA	2.17	120.86	114.00
4	A	560	HEM	C2A-C1A-NA	2.15	112.53	110.15
3	B	570	FMN	C9-C9A-N10	-2.11	119.02	121.85
3	B	570	FMN	C4-N3-C2	-2.07	121.96	125.64
3	A	570	FMN	C4-N3-C2	-2.01	122.08	125.64

All (4) chirality outliers are listed below:

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

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	570	FMN	N10-C1'-C2'-O2'
3	A	570	FMN	O2'-C2'-C3'-O3'
3	A	570	FMN	C2'-C3'-C4'-O4'
3	A	570	FMN	O3'-C3'-C4'-O4'
3	A	570	FMN	O3'-C3'-C4'-C5'
3	A	570	FMN	O4'-C4'-C5'-O5'
3	A	570	FMN	C4'-C5'-O5'-P
3	B	570	FMN	N10-C1'-C2'-O2'
3	B	570	FMN	C1'-C2'-C3'-O3'
3	B	570	FMN	O2'-C2'-C3'-O3'
3	B	570	FMN	C2'-C3'-C4'-O4'
3	B	570	FMN	O3'-C3'-C4'-O4'
3	B	570	FMN	O3'-C3'-C4'-C5'
3	B	570	FMN	O4'-C4'-C5'-O5'
3	B	570	FMN	C4'-C5'-O5'-P
4	A	560	HEM	C2C-C3C-CAC-CBC
4	A	560	HEM	C3D-CAD-CBD-CGD
3	A	570	FMN	O2'-C2'-C3'-C4'
3	A	570	FMN	C2'-C3'-C4'-C5'
3	B	570	FMN	O2'-C2'-C3'-C4'
4	A	560	HEM	C4C-C3C-CAC-CBC
3	B	570	FMN	C3'-C4'-C5'-O5'

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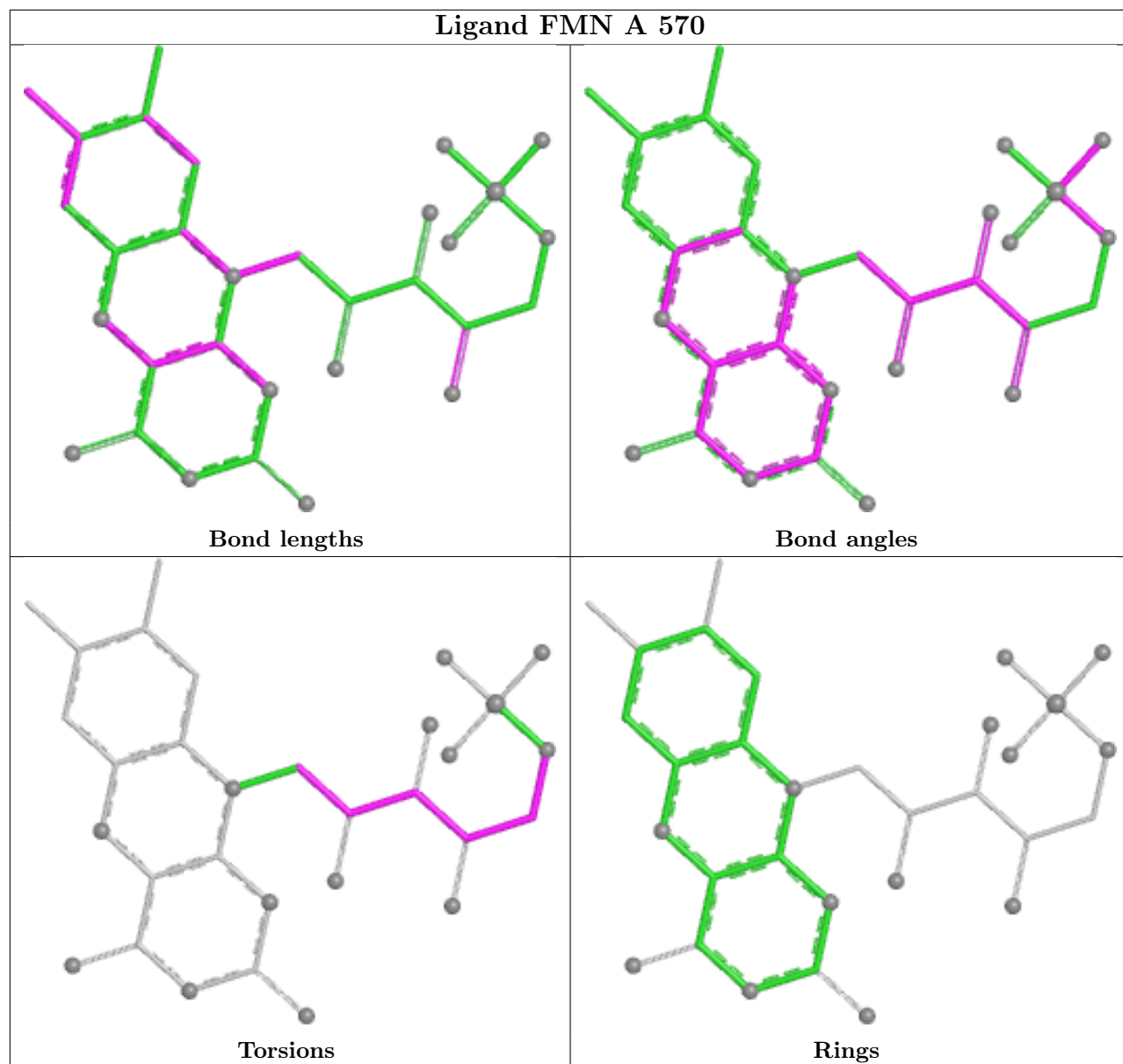
Mol	Chain	Res	Type	Atoms
3	A	570	FMN	C1'-C2'-C3'-O3'
4	A	560	HEM	C4B-C3B-CAB-CBB
4	A	560	HEM	C2B-C3B-CAB-CBB
4	A	560	HEM	CAA-CBA-CGA-O2A
4	A	560	HEM	CAA-CBA-CGA-O1A
4	A	560	HEM	CAD-CBD-CGD-O1D
4	A	560	HEM	CAD-CBD-CGD-O2D
4	A	560	HEM	C1A-C2A-CAA-CBA
4	A	560	HEM	C2A-CAA-CBA-CGA

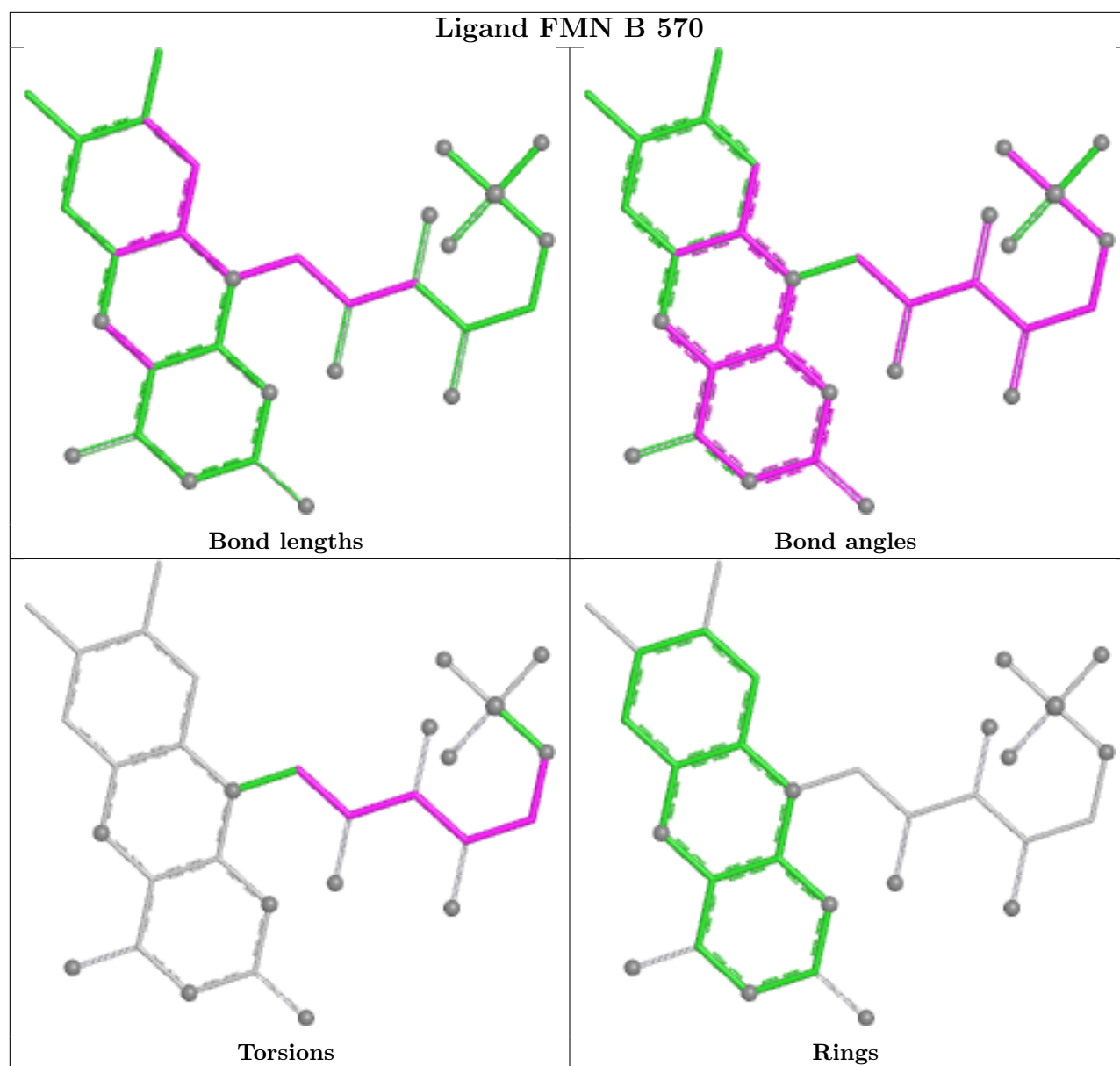
There are no ring outliers.

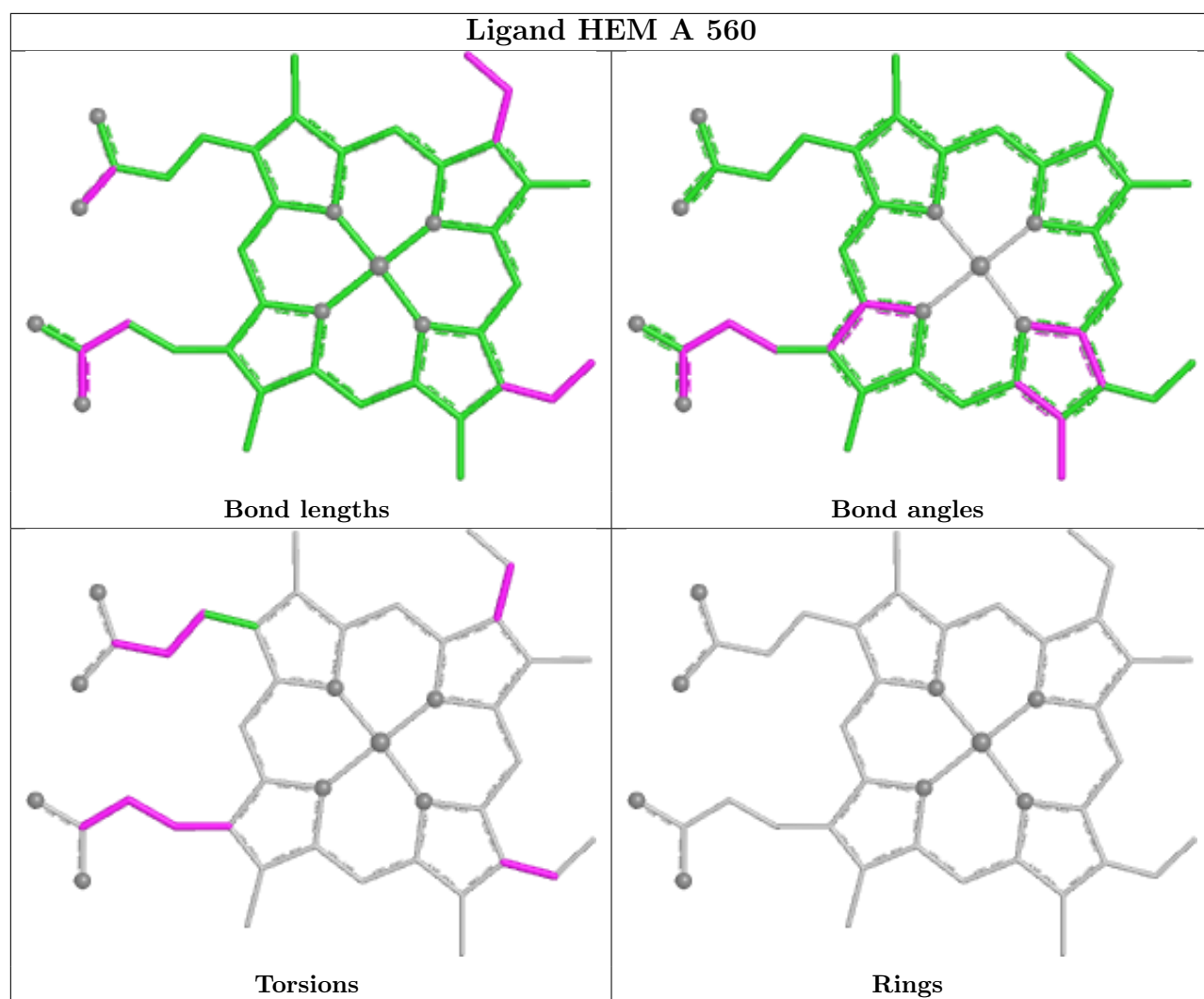
3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	570	FMN	1	0
3	B	570	FMN	1	0
4	A	560	HEM	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.