



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:55 AM UTC

PDB ID : 1LDC / pdb_00001ldc
Title : X-RAY STRUCTURE OF TWO COMPLEXES OF THE Y143F FLAVO-CYTOCHROME B2 MUTANT CRYSTALLIZED IN THE PRESENCE OF LACTATE OR PHENYL-LACTATE
Authors : Tegoni, M.; Cambillau, C.
Deposited on : 1995-04-13
Resolution : 2.90 Å(reported)

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

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

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

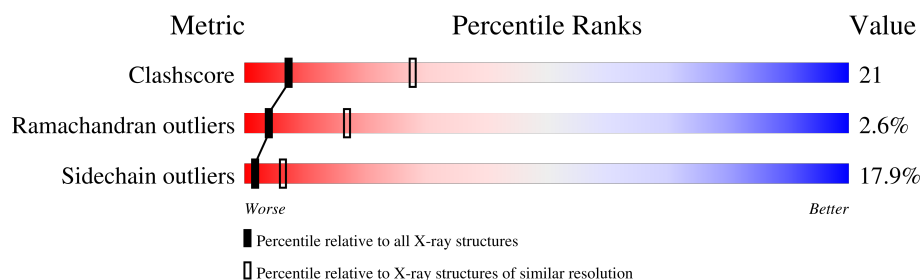
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (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 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	511	
1	B	511	

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

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

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8726 atoms, of which 1765 are hydrogens and 0 are deuteriums.

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).



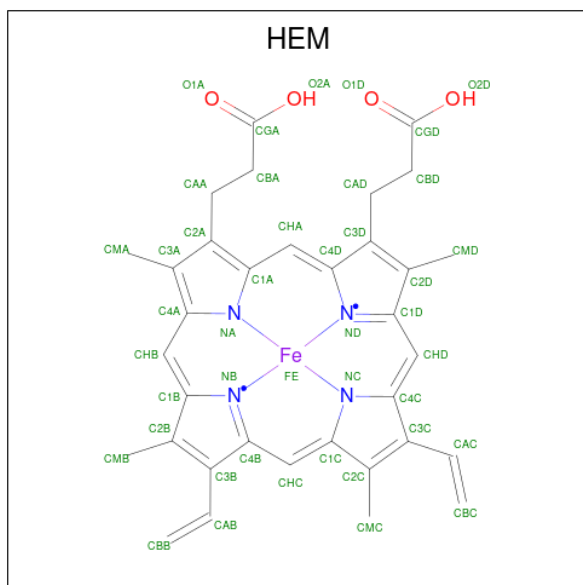
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			35	17	4	4	9	1		

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

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



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

- Molecule 5 is water.

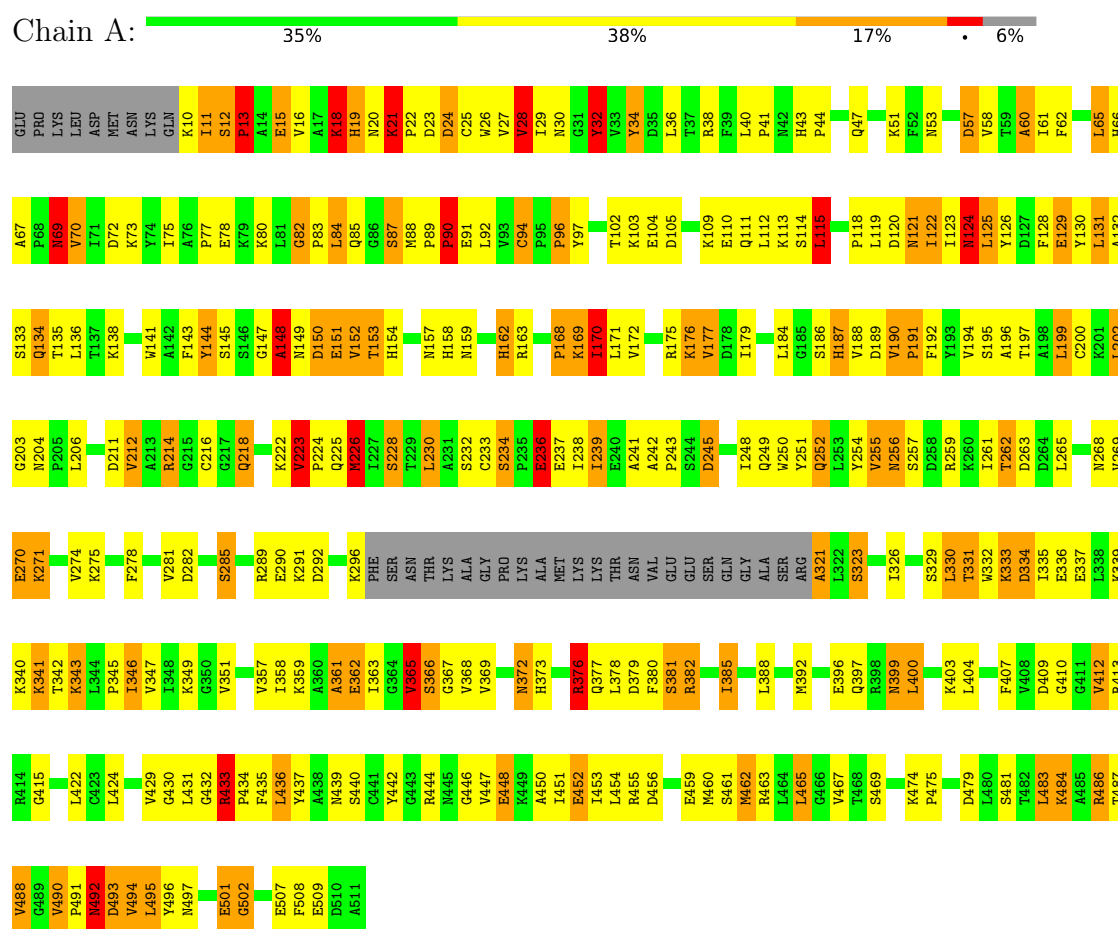
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	130	Total	H	O	0	0
			386	256	130		
5	B	11	Total	H	O	0	0
			33	22	11		

3 Residue-property plots

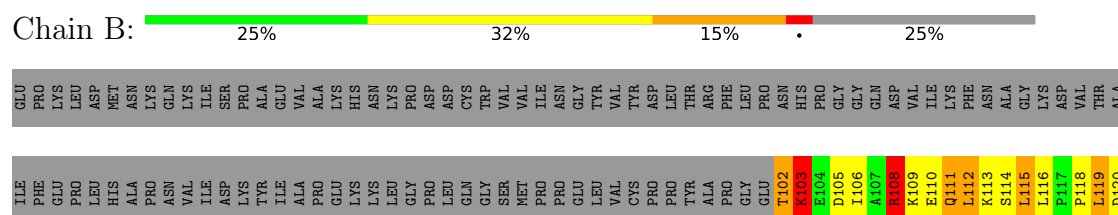
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 1: L-LACTATE DEHYDROGENASE



R463	L464	L465	G466	V467	T468	S469	E472	L473	K474	L477	L478	D479	L480	S481	T482	L483	R486	T487	V488	G489	V490	F491	M492	D493	V494	L495	Y496	N497	E498	V499	Y500	P503	T504	L505	T506	E507	F508	E509	D510	A511																	
L388	L391	T392	P393	I394	L400	K403	L404	E405	V406	F407	V408	D409	V412	R413	R414	G415	T416	D417	V418	L419	K420	A421	V429	Q430	L431	F435	L436	N438	M439	S440	C441	Y442	G443	R444	N445	G446	V447	E448	K449	A450	I451	E452	I453	L454	D455	E457	I458	E459	M460	S461	M462						
SER	LYS	F325	I326	D327	P328	S329	L330	T331	I335	E336	E337	L338	K339	K340	K341	T342	K343	L344	P345	I346	V347	I348	K349	G350	V351	T354	V357	I358	A361	E362	I363	G364	V365	S366	V368	V369	L370	S371	R372	H373	G374	G375	R376	Q377	L378	D379	F380	S381	R382	A383	P384	I385	E386	V387			
K260	T261	T262	D263	D264	K267	M268	V269	E270	K271	K275	A276	L277	F278	V279	T280	V281	D282	A283	P284	S285	L286	G287	Q288	R289	E290	K291	D292	M293	K294	L295	K296	PHE	SER	ASN	THR	LYS	ALA	GLY	PRO	LYS	ALA	MET	LYS	LYS	THR	ASN	VAL	GLU	GLU	SER	GLN	GLY	ALA	SER	ARG	ALA	LEU
D189	V190	I122	I123	N124	L125	Y126	D127	L131	A132	T135	L136	T137	K138	Q139	A140	W141	A142	S145	S146	G147	A148	N149	D150	E151	V152	T153	H154	R155	E156	H157	H158	N159	A160	Y161	H162	R163	I164	F165	F166	K167	P168	V172	D173	V174	R175	K176	V177	D178	I179	S180	T181	D182	M183	H187	V188		
D189	V190	Y193	V194	S195	A196	T197	A198	L199	C200	K201	N204	P205	L206	E209	K210	D211	V212	A213	R214	G215	C216	Q217	Q218	K222	V223	P224	Q225	M226	T229	L230	C233	S234	P235	E236	E237	P243	S244	D245	K246	Q247	I248	Q249	W250	Y251	Q252	L253	Y254	V255	N256	S257	D258	R259					

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 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.90)	Depositor
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.195 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8726	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PYR, HEM, 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	1.38	23/3794 (0.6%)	2.33	207/5140 (4.0%)
1	B	1.31	11/3030 (0.4%)	2.32	162/4094 (4.0%)
All	All	1.35	34/6824 (0.5%)	2.33	369/9234 (4.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	2
All	All	0	8

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	179	ILE	CA-CB	8.63	1.66	1.54
1	B	373	HIS	CD2-NE2	-8.17	1.28	1.37
1	A	475	PRO	CA-CB	-8.12	1.42	1.53
1	A	152	VAL	CA-CB	7.72	1.65	1.54
1	A	373	HIS	CD2-NE2	-7.72	1.29	1.37
1	A	212	VAL	CA-CB	6.93	1.63	1.54
1	A	158	HIS	CD2-NE2	-6.88	1.30	1.37
1	A	162	HIS	CD2-NE2	-6.86	1.30	1.37
1	A	501	GLU	CA-CB	-6.83	1.42	1.53
1	B	158	HIS	CD2-NE2	-6.83	1.30	1.37
1	A	32	TYR	CA-CB	-6.83	1.42	1.53
1	B	482	THR	CA-CB	6.82	1.62	1.53
1	B	154	HIS	CD2-NE2	-6.67	1.30	1.37
1	A	103	LYS	CD-CE	6.28	1.71	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	158	HIS	CG-ND1	-6.26	1.31	1.38
1	A	150	ASP	CA-CB	6.25	1.64	1.53
1	A	128	PHE	CA-CB	-6.18	1.43	1.53
1	A	346	ILE	CA-CB	6.06	1.61	1.54
1	A	19	HIS	CD2-NE2	-6.04	1.31	1.37
1	B	154	HIS	CG-ND1	-5.88	1.31	1.38
1	A	187	HIS	CD2-NE2	-5.83	1.31	1.37
1	A	382	ARG	CZ-NH1	5.75	1.40	1.32
1	A	486	ARG	CA-CB	-5.55	1.45	1.52
1	B	162	HIS	CD2-NE2	-5.46	1.31	1.37
1	A	132	ALA	CA-CB	-5.46	1.44	1.53
1	A	148	ALA	CA-C	-5.46	1.46	1.52
1	B	187	HIS	CD2-NE2	-5.40	1.31	1.37
1	A	154	HIS	CD2-NE2	-5.30	1.32	1.37
1	B	391	THR	CA-CB	5.22	1.61	1.53
1	A	154	HIS	CG-ND1	-5.21	1.32	1.38
1	A	494	VAL	CA-CB	5.20	1.62	1.54
1	A	194	VAL	CA-CB	-5.18	1.48	1.54
1	B	158	HIS	CG-ND1	-5.18	1.32	1.38
1	B	194	VAL	CA-CB	-5.16	1.47	1.54

All (369) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	372	ASN	OD1-CG-ND2	-13.45	109.15	122.60
1	B	256	ASN	OD1-CG-ND2	-13.44	109.16	122.60
1	A	492	ASN	CA-CB-CG	13.09	125.69	112.60
1	B	379	ASP	CA-C-O	-11.69	106.52	119.97
1	A	492	ASN	O-C-N	11.55	137.31	123.33
1	A	223	VAL	N-CA-CB	-10.43	96.60	111.21
1	B	435	PHE	CA-CB-CG	-10.06	103.74	113.80
1	A	150	ASP	CA-CB-CG	9.99	122.59	112.60
1	A	115	LEU	N-CA-C	-9.95	100.55	112.89
1	A	335	ILE	N-CA-C	-9.89	101.22	110.82
1	B	268	ASN	OD1-CG-ND2	-9.89	112.71	122.60
1	B	417	ASP	CA-CB-CG	9.72	122.32	112.60
1	A	157	ASN	OD1-CG-ND2	-9.59	113.01	122.60
1	B	372	ASN	OD1-CG-ND2	-9.53	113.07	122.60
1	A	497	ASN	OD1-CG-ND2	-9.50	113.10	122.60
1	B	474	LYS	O-C-N	-9.47	110.42	121.32
1	B	256	ASN	CB-CG-ND2	9.39	130.48	116.40
1	A	379	ASP	CA-C-O	-9.39	108.62	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	463	ARG	NE-CZ-NH2	-9.30	110.83	119.20
1	A	409	ASP	CA-CB-CG	9.25	121.85	112.60
1	B	212	VAL	N-CA-C	-9.16	101.81	110.42
1	A	190	VAL	N-CA-CB	-9.10	98.46	111.21
1	A	184	LEU	N-CA-CB	-9.03	98.50	112.13
1	B	380	PHE	CA-CB-CG	-8.84	104.96	113.80
1	B	327	ASP	CA-C-N	8.83	129.05	119.87
1	B	327	ASP	C-N-CA	8.83	129.05	119.87
1	B	497	ASN	OD1-CG-ND2	-8.70	113.90	122.60
1	B	124	ASN	CB-CG-ND2	8.70	129.44	116.40
1	A	94	CYS	N-CA-C	8.53	120.66	109.83
1	A	152	VAL	CA-C-O	-8.51	111.61	120.71
1	B	372	ASN	CB-CG-ND2	8.46	129.10	116.40
1	A	176	LYS	N-CA-C	-8.45	95.90	109.76
1	B	115	LEU	N-CA-C	-8.38	103.19	113.41
1	A	157	ASN	CB-CG-ND2	8.38	128.96	116.40
1	B	149	ASN	CA-CB-CG	8.31	120.91	112.60
1	A	270	GLU	N-CA-C	-8.31	102.02	112.90
1	B	124	ASN	OD1-CG-ND2	-8.26	114.34	122.60
1	B	120	ASP	CA-CB-CG	8.18	120.78	112.60
1	A	497	ASN	CB-CG-ND2	8.16	128.64	116.40
1	A	493	ASP	CA-CB-CG	8.12	120.72	112.60
1	B	289	ARG	NE-CZ-NH1	8.05	129.55	121.50
1	A	357	VAL	N-CA-C	-8.04	103.02	110.82
1	A	488	VAL	N-CA-C	-8.04	95.88	107.77
1	A	483	LEU	CB-CA-C	-8.03	98.27	110.88
1	B	357	VAL	N-CA-C	-8.02	103.00	110.53
1	A	435	PHE	CA-CB-CG	-8.01	105.79	113.80
1	A	70	VAL	N-CA-C	8.01	118.79	110.62
1	A	361	ALA	N-CA-C	-7.98	102.52	111.14
1	A	159	ASN	CB-CG-ND2	7.98	128.37	116.40
1	A	334	ASP	N-CA-C	7.97	120.88	111.71
1	A	262	THR	CA-CB-OG1	-7.95	97.68	109.60
1	A	271	LYS	N-CA-C	-7.95	102.70	111.36
1	B	159	ASN	CB-CG-ND2	7.86	128.18	116.40
1	B	282	ASP	CA-CB-CG	7.79	120.39	112.60
1	A	326	ILE	N-CA-C	-7.77	94.36	106.72
1	A	249	GLN	CA-CB-CG	-7.77	98.57	114.10
1	A	212	VAL	N-CA-C	-7.72	101.77	112.50
1	B	473	LEU	O-C-N	-7.72	112.32	122.59
1	B	341	LYS	N-CA-CB	-7.71	99.30	110.56
1	A	151	GLU	N-CA-C	7.70	122.09	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	372	ASN	CB-CG-ND2	7.70	127.94	116.40
1	A	373	HIS	CB-CG-CD2	-7.68	121.21	131.20
1	B	417	ASP	N-CA-C	-7.68	102.24	111.69
1	A	154	HIS	CB-CG-CD2	-7.67	121.23	131.20
1	A	484	LYS	N-CA-CB	-7.67	99.98	110.56
1	A	159	ASN	OD1-CG-ND2	-7.63	114.97	122.60
1	B	379	ASP	O-C-N	-7.63	112.88	122.27
1	B	167	LYS	CA-C-N	7.61	127.62	119.78
1	B	167	LYS	C-N-CA	7.61	127.62	119.78
1	B	369	VAL	CB-CA-C	-7.60	100.57	110.98
1	B	181	THR	N-CA-C	-7.58	97.67	108.96
1	B	377	GLN	OE1-CD-NE2	-7.57	115.03	122.60
1	A	21	LYS	O-C-N	-7.56	116.51	121.88
1	A	53	ASN	OD1-CG-ND2	-7.56	115.04	122.60
1	A	43	HIS	CB-CG-CD2	-7.54	121.40	131.20
1	B	189	ASP	N-CA-C	7.53	119.27	111.14
1	A	19	HIS	CA-CB-CG	-7.51	106.29	113.80
1	B	368	VAL	CA-CB-CG2	-7.49	97.67	110.40
1	B	206	LEU	N-CA-C	7.46	119.05	111.07
1	A	19	HIS	CB-CG-CD2	-7.43	121.54	131.20
1	A	372	ASN	CA-CB-CG	7.36	119.96	112.60
1	A	28	VAL	CB-CA-C	-7.36	100.83	110.84
1	B	341	LYS	CA-CB-CG	7.35	128.80	114.10
1	A	172	VAL	N-CA-C	-7.34	97.91	108.48
1	A	250	TRP	CA-C-O	-7.32	112.80	120.70
1	A	382	ARG	NE-CZ-NH2	-7.32	112.61	119.20
1	A	413	ARG	NE-CZ-NH2	-7.31	112.62	119.20
1	A	204	ASN	CA-CB-CG	7.29	119.89	112.60
1	B	172	VAL	N-CA-C	-7.26	97.67	108.12
1	B	178	ASP	CA-CB-CG	7.25	119.84	112.60
1	A	145	SER	N-CA-C	7.15	122.00	113.28
1	B	369	VAL	N-CA-CB	7.13	119.56	111.21
1	A	256	ASN	OD1-CG-ND2	-7.10	115.50	122.60
1	B	268	ASN	CB-CG-ND2	7.10	127.05	116.40
1	B	145	SER	N-CA-C	7.09	122.03	113.23
1	B	246	LYS	N-CA-C	7.07	120.02	111.82
1	A	111	GLN	CB-CG-CD	-7.04	100.63	112.60
1	A	83	PRO	N-CA-C	7.04	121.87	111.03
1	B	463	ARG	CG-CD-NE	-7.04	96.52	112.00
1	A	144	TYR	CA-C-O	-7.03	113.10	120.55
1	B	504	THR	N-CA-C	-7.03	98.62	109.24
1	B	196	ALA	N-CA-C	7.02	125.75	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	225	GLN	OE1-CD-NE2	-6.98	115.62	122.60
1	A	483	LEU	N-CA-CB	6.97	120.11	110.01
1	A	281	VAL	O-C-N	-6.94	115.41	122.14
1	A	154	HIS	CA-CB-CG	6.93	120.73	113.80
1	A	129	GLU	CB-CA-C	-6.92	100.30	110.96
1	B	158	HIS	CB-CG-CD2	-6.91	122.21	131.20
1	A	496	TYR	N-CA-C	-6.89	103.69	111.07
1	B	490	VAL	N-CA-CB	-6.89	101.56	111.21
1	A	290	GLU	O-C-N	-6.88	114.36	122.20
1	A	211	ASP	CA-C-O	-6.88	111.17	119.49
1	B	163	ARG	CA-CB-CG	6.86	127.81	114.10
1	B	194	VAL	N-CA-C	-6.85	99.89	109.21
1	B	112	LEU	N-CA-CB	-6.81	100.14	110.01
1	B	436	LEU	CA-C-O	-6.78	113.31	120.63
1	A	94	CYS	CA-C-N	6.72	124.50	119.66
1	A	94	CYS	C-N-CA	6.72	124.50	119.66
1	B	328	PRO	CA-N-CD	-6.72	102.60	112.00
1	B	327	ASP	CA-C-O	-6.70	113.39	120.23
1	A	170	ILE	O-C-N	6.65	129.67	122.76
1	A	12	SER	N-CA-C	6.64	119.89	110.40
1	A	362	GLU	CA-C-O	-6.60	113.50	120.63
1	A	184	LEU	CB-CA-C	6.60	121.10	111.73
1	A	433	ARG	N-CA-C	6.58	122.60	113.45
1	B	254	TYR	CA-C-O	-6.57	113.33	120.36
1	A	379	ASP	O-C-N	-6.57	113.03	122.36
1	B	111	GLN	CA-C-O	6.56	127.66	120.90
1	B	351	VAL	CA-C-O	-6.54	114.85	121.59
1	A	177	VAL	O-C-N	-6.52	116.21	123.26
1	A	479	ASP	CA-CB-CG	-6.52	106.08	112.60
1	A	252	GLN	OE1-CD-NE2	-6.51	116.09	122.60
1	B	102	THR	N-CA-CB	-6.46	100.51	111.50
1	B	218	GLN	N-CA-C	6.44	120.97	113.18
1	A	69	ASN	CB-CG-ND2	6.41	126.01	116.40
1	A	450	ALA	N-CA-C	-6.39	104.24	111.14
1	A	413	ARG	NH1-CZ-NH2	6.37	127.58	119.30
1	B	245	ASP	CA-CB-CG	6.36	118.96	112.60
1	B	270	GLU	CA-C-N	6.35	128.70	120.44
1	B	270	GLU	C-N-CA	6.35	128.70	120.44
1	A	28	VAL	N-CA-CB	6.34	118.60	110.99
1	B	364	GLY	O-C-N	-6.32	114.93	122.33
1	B	195	SER	N-CA-C	-6.30	100.88	110.14
1	A	169	LYS	CB-CG-CD	-6.29	96.82	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	57	ASP	N-CA-C	-6.28	97.47	108.20
1	B	151	GLU	CA-C-N	-6.27	111.77	120.74
1	B	151	GLU	C-N-CA	-6.27	111.77	120.74
1	A	225	GLN	CA-C-O	-6.26	113.43	120.32
1	A	381	SER	O-C-N	-6.24	115.91	122.96
1	A	153	THR	CA-CB-OG1	-6.22	100.27	109.60
1	A	154	HIS	CB-CG-ND1	6.22	132.03	122.70
1	A	120	ASP	CA-CB-CG	6.22	118.82	112.60
1	A	494	VAL	CA-C-O	-6.21	113.92	120.57
1	B	212	VAL	CA-C-O	-6.21	113.98	121.18
1	B	140	ALA	CA-C-O	-6.20	114.29	120.80
1	A	365	VAL	CB-CA-C	6.19	120.91	111.68
1	B	464	LEU	O-C-N	-6.18	114.99	122.22
1	A	78	GLU	CA-CB-CG	6.17	126.44	114.10
1	B	279	VAL	CA-C-O	-6.17	113.46	120.74
1	A	321	ALA	N-CA-C	-6.16	93.74	111.00
1	B	408	VAL	CA-C-O	-6.16	115.17	120.96
1	A	238	ILE	N-CA-CB	-6.15	103.36	110.55
1	A	439	ASN	OD1-CG-ND2	-6.15	116.45	122.60
1	A	226	MET	CG-SD-CE	-6.12	87.44	100.90
1	A	365	VAL	N-CA-CB	-6.11	99.59	110.95
1	A	141	TRP	CG-CD2-CE3	6.11	140.01	133.90
1	B	511	ALA	N-CA-C	-6.08	93.97	111.00
1	B	506	THR	N-CA-CB	-6.07	101.11	110.04
1	A	433	ARG	CA-C-O	-6.07	112.75	118.33
1	B	254	TYR	N-CA-C	-6.06	98.84	108.73
1	A	245	ASP	CA-CB-CG	6.04	118.64	112.60
1	B	349	LYS	CG-CD-CE	-6.03	97.43	111.30
1	A	187	HIS	CB-CG-CD2	-6.03	123.36	131.20
1	A	211	ASP	CA-C-N	-6.02	110.77	120.64
1	A	211	ASP	C-N-CA	-6.02	110.77	120.64
1	A	263	ASP	N-CA-C	-6.01	104.72	111.28
1	A	474	LYS	CA-C-N	6.01	125.56	119.19
1	A	474	LYS	C-N-CA	6.01	125.56	119.19
1	B	245	ASP	N-CA-C	-5.99	104.87	111.82
1	B	510	ASP	CA-C-O	5.99	126.73	119.31
1	B	474	LYS	CA-C-N	5.97	125.67	119.64
1	B	474	LYS	C-N-CA	5.97	125.67	119.64
1	A	179	ILE	O-C-N	-5.96	115.12	122.57
1	B	141	TRP	CG-CD2-CE3	5.95	139.85	133.90
1	B	210	LYS	N-CA-C	-5.94	104.38	111.69
1	B	199	LEU	N-CA-C	5.94	123.45	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	484	LYS	O-C-N	-5.93	114.78	122.37
1	A	254	TYR	N-CA-C	-5.93	100.04	109.59
1	B	233	CYS	O-C-N	-5.93	117.00	123.52
1	A	24	ASP	O-C-N	5.92	130.20	122.68
1	B	368	VAL	CA-CB-CG1	5.92	120.46	110.40
1	A	188	VAL	N-CA-CB	-5.91	99.67	111.91
1	A	492	ASN	OD1-CG-ND2	-5.89	116.71	122.60
1	A	188	VAL	CB-CA-C	5.89	119.89	110.82
1	A	493	ASP	N-CA-C	5.88	123.32	110.80
1	B	504	THR	CA-CB-OG1	-5.87	100.80	109.60
1	B	293	MET	CA-C-O	-5.86	114.16	121.02
1	A	296	LYS	CA-CB-CG	-5.85	102.41	114.10
1	B	142	ALA	CA-C-O	-5.84	114.19	121.02
1	B	190	VAL	CA-C-N	5.83	126.60	120.12
1	B	190	VAL	C-N-CA	5.83	126.60	120.12
1	B	495	LEU	O-C-N	-5.82	115.51	122.15
1	B	453	ILE	N-CA-C	5.81	116.28	110.23
1	A	237	GLU	CB-CA-C	-5.81	100.97	110.85
1	B	176	LYS	CA-C-O	-5.81	114.08	120.30
1	B	504	THR	CA-CB-CG2	5.81	120.38	110.50
1	A	66	HIS	ND1-CG-CD2	5.80	111.90	106.10
1	A	376	ARG	N-CA-C	-5.80	103.56	111.56
1	B	249	GLN	OE1-CD-NE2	-5.79	116.81	122.60
1	B	408	VAL	O-C-N	-5.79	117.63	123.19
1	A	189	ASP	CA-CB-CG	5.79	118.39	112.60
1	A	124	ASN	OD1-CG-ND2	-5.78	116.82	122.60
1	B	154	HIS	CB-CG-CD2	-5.78	123.68	131.20
1	B	262	THR	CA-CB-OG1	-5.77	100.95	109.60
1	A	53	ASN	CB-CG-ND2	5.77	125.05	116.40
1	A	396	GLU	CA-CB-CG	-5.76	102.57	114.10
1	A	509	GLU	N-CA-C	5.75	119.78	112.87
1	B	490	VAL	CB-CA-C	5.75	121.82	111.36
1	B	377	GLN	CG-CD-NE2	5.74	125.02	116.40
1	B	387	VAL	CA-C-N	5.72	128.26	120.54
1	B	387	VAL	C-N-CA	5.72	128.26	120.54
1	B	414	ARG	NH1-CZ-NH2	-5.72	111.87	119.30
1	A	191	PRO	O-C-N	-5.71	114.93	122.64
1	B	407	PHE	N-CA-C	-5.71	101.55	110.17
1	A	366	SER	N-CA-C	5.70	119.04	111.75
1	A	132	ALA	CA-C-O	-5.69	113.42	119.97
1	B	156	GLU	CA-CB-CG	5.69	125.48	114.10
1	A	214	ARG	CA-C-O	-5.68	114.85	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	463	ARG	NH1-CZ-NH2	5.68	126.69	119.30
1	B	154	HIS	CA-C-O	-5.65	115.07	121.00
1	A	236	GLU	CA-CB-CG	5.65	125.39	114.10
1	A	488	VAL	O-C-N	-5.64	117.31	123.18
1	A	129	GLU	N-CA-CB	5.62	118.11	109.91
1	B	348	ILE	N-CA-CB	-5.60	104.90	111.39
1	A	87	SER	N-CA-C	5.59	118.34	109.50
1	B	292	ASP	CA-CB-CG	5.59	118.19	112.60
1	A	323	SER	O-C-N	-5.56	117.96	123.46
1	A	188	VAL	CA-CB-CG1	5.55	119.84	110.40
1	B	392	MET	CA-C-O	-5.54	112.96	118.34
1	A	199	LEU	N-CA-C	5.54	122.61	110.80
1	B	383	ALA	CA-C-N	5.54	125.00	119.24
1	B	383	ALA	C-N-CA	5.54	125.00	119.24
1	B	296	LYS	CA-CB-CG	5.53	125.17	114.10
1	A	341	LYS	CA-CB-CG	5.52	125.15	114.10
1	B	413	ARG	N-CA-C	-5.52	105.98	114.16
1	A	285	SER	O-C-N	-5.52	116.20	123.21
1	B	275	LYS	N-CA-CB	-5.52	102.33	110.49
1	B	444	ARG	CB-CG-CD	5.52	123.99	111.30
1	A	159	ASN	CA-CB-CG	-5.51	107.09	112.60
1	A	136	LEU	N-CA-C	5.51	118.26	110.50
1	A	363	ILE	CB-CG1-CD1	-5.51	102.23	113.80
1	A	234	SER	CA-CB-OG	5.50	122.11	111.10
1	B	337	GLU	CA-C-O	-5.49	115.06	120.82
1	A	66	HIS	CG-CD2-NE2	-5.47	101.73	107.20
1	B	226	MET	N-CA-C	-5.46	99.99	108.90
1	A	223	VAL	CA-CB-CG2	-5.46	101.11	110.40
1	B	247	GLN	OE1-CD-NE2	-5.46	117.14	122.60
1	A	43	HIS	ND1-CG-CD2	5.46	111.56	106.10
1	A	169	LYS	CA-CB-CG	5.46	125.02	114.10
1	B	488	VAL	O-C-N	-5.45	117.45	123.18
1	B	362	GLU	O-C-N	-5.45	116.34	122.12
1	A	268	ASN	OD1-CG-ND2	-5.44	117.16	122.60
1	A	153	THR	CA-CB-CG2	5.44	119.75	110.50
1	A	436	LEU	N-CA-C	-5.43	105.39	112.23
1	B	438	ALA	N-CA-C	-5.43	105.01	111.69
1	A	459	GLU	N-CA-CB	-5.42	102.13	110.16
1	B	198	ALA	O-C-N	-5.42	116.67	122.85
1	B	279	VAL	O-C-N	-5.41	116.77	122.83
1	A	53	ASN	CA-CB-CG	5.41	118.00	112.60
1	B	500	TYR	O-C-N	-5.40	116.49	122.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	VAL	CB-CA-C	-5.39	104.86	112.14
1	B	335	ILE	N-CA-C	-5.38	105.14	111.00
1	A	365	VAL	CA-C-N	5.38	128.23	120.38
1	A	365	VAL	C-N-CA	5.38	128.23	120.38
1	A	456	ASP	CA-C-O	-5.36	115.19	120.82
1	A	379	ASP	N-CA-C	5.35	119.91	112.90
1	B	141	TRP	CA-C-O	-5.35	115.19	121.07
1	A	199	LEU	O-C-N	-5.35	115.48	122.59
1	B	146	SER	N-CA-C	5.34	122.18	110.80
1	A	342	THR	CA-CB-OG1	-5.34	101.59	109.60
1	A	228	SER	CA-CB-OG	5.34	121.77	111.10
1	A	454	LEU	N-CA-C	5.33	117.17	111.36
1	B	455	ARG	N-CA-C	-5.33	105.63	111.82
1	A	102	THR	N-CA-C	-5.31	99.48	110.80
1	B	281	VAL	N-CA-C	5.31	117.29	111.77
1	A	60	ALA	N-CA-C	5.30	117.75	111.33
1	B	189	ASP	CB-CA-C	-5.30	102.52	110.90
1	A	11	ILE	N-CA-C	-5.30	98.32	109.34
1	A	502	GLY	CA-C-N	5.30	125.59	119.92
1	A	502	GLY	C-N-CA	5.30	125.59	119.92
1	A	202	LEU	N-CA-C	-5.29	105.42	111.14
1	A	66	HIS	N-CA-C	5.29	118.06	108.69
1	B	413	ARG	CB-CG-CD	5.29	123.46	111.30
1	B	149	ASN	N-CA-C	5.28	122.05	110.80
1	A	147	GLY	CA-C-N	-5.28	115.17	122.30
1	A	147	GLY	C-N-CA	-5.28	115.17	122.30
1	B	226	MET	CG-SD-CE	-5.28	89.29	100.90
1	B	328	PRO	N-CA-C	5.27	120.52	114.03
1	B	162	HIS	CB-CG-CD2	-5.26	124.37	131.20
1	B	108	ARG	CA-C-O	-5.25	115.31	120.82
1	A	412	VAL	N-CA-CB	-5.25	105.07	110.95
1	A	168	PRO	CA-C-N	-5.24	113.73	122.64
1	A	168	PRO	C-N-CA	-5.24	113.73	122.64
1	B	498	GLU	CA-C-O	-5.22	115.32	120.70
1	B	163	ARG	N-CA-C	-5.21	106.89	113.20
1	B	166	PHE	O-C-N	-5.21	117.14	123.03
1	A	448	GLU	CB-CG-CD	-5.20	103.75	112.60
1	A	186	SER	N-CA-C	-5.20	99.72	110.80
1	A	18	LYS	CA-CB-CG	5.20	124.50	114.10
1	A	121	ASN	CA-CB-CG	5.20	117.80	112.60
1	B	271	LYS	CA-CB-CG	5.20	124.49	114.10
1	B	252	GLN	CA-C-O	5.19	126.04	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	328	PRO	N-CA-CB	5.19	108.29	103.41
1	A	373	HIS	CB-CG-ND1	5.19	130.48	122.70
1	A	368	VAL	N-CA-CB	-5.18	102.96	111.45
1	A	121	ASN	O-C-N	-5.17	115.23	122.37
1	B	404	LEU	N-CA-C	5.17	117.03	108.13
1	B	387	VAL	CG1-CB-CG2	-5.17	99.43	110.80
1	A	415	GLY	CA-C-O	-5.17	115.18	120.45
1	A	162	HIS	N-CA-C	-5.15	106.96	113.20
1	A	333	LYS	N-CA-C	-5.15	105.74	111.36
1	B	450	ALA	CB-CA-C	-5.15	101.92	110.68
1	A	271	LYS	CB-CG-CD	5.14	123.13	111.30
1	A	60	ALA	O-C-N	5.14	127.56	122.12
1	A	493	ASP	O-C-N	5.14	129.42	122.59
1	B	132	ALA	CA-C-O	-5.13	115.43	120.82
1	A	19	HIS	CB-CG-ND1	5.12	130.39	122.70
1	A	190	VAL	CB-CA-C	5.12	120.68	111.36
1	B	212	VAL	N-CA-CB	5.11	116.43	110.65
1	B	264	ASP	N-CA-C	-5.11	105.62	111.14
1	B	285	SER	N-CA-C	-5.11	101.31	109.23
1	A	188	VAL	CA-CB-CG2	-5.11	101.72	110.40
1	A	491	PRO	O-C-N	-5.11	117.14	123.01
1	A	134	GLN	CG-CD-NE2	-5.10	108.74	116.40
1	A	422	LEU	O-C-N	-5.10	115.60	122.23
1	B	235	PRO	O-C-N	5.10	128.35	122.23
1	A	148	ALA	CB-CA-C	-5.10	101.71	110.22
1	B	393	PRO	N-CA-C	-5.10	106.18	113.47
1	A	70	VAL	CA-C-O	-5.09	115.65	120.95
1	B	373	HIS	CB-CG-CD2	-5.09	124.58	131.20
1	B	465	LEU	N-CA-C	-5.09	105.92	111.82
1	A	89	PRO	CA-C-N	5.08	126.20	119.84
1	A	89	PRO	C-N-CA	5.08	126.20	119.84
1	B	326	ILE	N-CA-CB	-5.08	104.99	110.53
1	A	223	VAL	CA-C-N	5.08	124.84	119.76
1	A	223	VAL	C-N-CA	5.08	124.84	119.76
1	A	242	ALA	CA-C-N	5.08	125.52	120.04
1	A	242	ALA	C-N-CA	5.08	125.52	120.04
1	A	62	PHE	CA-C-O	-5.07	115.68	120.90
1	B	392	MET	CA-C-N	5.07	124.24	118.97
1	B	392	MET	C-N-CA	5.07	124.24	118.97
1	A	233	CYS	CA-C-O	-5.05	115.55	121.46
1	B	141	TRP	CB-CG-CD1	-5.05	119.32	126.90
1	A	382	ARG	CB-CG-CD	-5.05	99.69	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	509	GLU	CA-CB-CG	-5.05	104.00	114.10
1	A	148	ALA	N-CA-CB	5.03	118.62	110.17
1	A	382	ARG	NH1-CZ-NH2	5.03	125.84	119.30
1	A	66	HIS	CB-CG-CD2	-5.03	124.67	131.20
1	A	82	GLY	CA-C-N	5.02	125.25	119.83
1	A	82	GLY	C-N-CA	5.02	125.25	119.83
1	A	475	PRO	N-CA-CB	5.02	108.84	103.52
1	A	218	GLN	CG-CD-NE2	-5.01	108.88	116.40
1	B	168	PRO	CA-C-O	-5.01	115.74	121.56
1	A	90	PRO	N-CA-C	5.01	122.79	112.47
1	B	161	TYR	O-C-N	-5.01	115.55	122.46
1	B	486	ARG	O-C-N	-5.01	116.52	122.63
1	A	131	LEU	CA-C-O	-5.00	115.55	120.90
1	A	351	VAL	N-CA-C	5.00	116.03	109.58
1	B	457	GLU	CB-CG-CD	5.00	121.10	112.60

There are no chirality outliers.

All (8) planarity outliers are listed below:

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

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3721	809	3783	147	0
1	B	2982	666	3044	140	0
2	A	31	4	16	3	0
2	B	31	4	19	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	43	4	30	8	0
4	A	6	0	0	2	0
4	B	6	0	0	0	0
5	A	130	256	0	13	0
5	B	11	22	0	0	0
All	All	6961	1765	6892	283	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 21.

All (283) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:ARG:HH21	1:A:376:ARG:NH2	1.38	1.22
1:A:289:ARG:NH2	1:A:376:ARG:NH2	2.06	1.04
1:A:488:VAL:HG22	1:B:490:VAL:HG11	1.51	0.93
1:B:148:ALA:C	1:B:149:ASN:HD22	1.76	0.92
1:A:289:ARG:NH2	1:A:376:ARG:HH22	1.69	0.88
1:A:143:PHE:O	1:A:376:ARG:NH2	2.10	0.84
1:A:58:VAL:HA	1:A:94:CYS:SG	2.18	0.83
1:B:163:ARG:NH2	1:B:486:ARG:HG3	1.95	0.82
1:A:197:THR:HG21	1:A:436:LEU:HD21	1.61	0.81
1:A:77:PRO:HA	1:A:80:LYS:HD2	1.63	0.80
1:A:109:LYS:HA	1:A:112:LEU:HD12	1.63	0.80
3:A:560:HEM:HBA2	3:A:560:HEM:HHA	1.63	0.79
1:B:217:GLY:HA3	1:B:247:GLN:NE2	2.00	0.76
1:A:433:ARG:HD2	5:A:627:HOH:O	1.85	0.76
1:A:289:ARG:HH21	1:A:376:ARG:HH22	1.27	0.75
1:A:490:VAL:HG22	1:A:492:ASN:ND2	2.03	0.74
1:B:373:HIS:O	1:B:376:ARG:HG3	1.88	0.73
1:A:228:SER:HA	1:A:252:GLN:HE21	1.52	0.73
1:A:488:VAL:HG22	1:B:490:VAL:CG1	2.20	0.71
1:A:256:ASN:HD22	1:A:257:SER:N	1.86	0.71
1:B:276:ALA:HB2	1:B:345:PRO:HG2	1.74	0.69
1:A:70:VAL:HB	3:A:560:HEM:HMB1	1.75	0.69
1:A:465:LEU:HD23	1:B:378:LEU:HD11	1.75	0.69
1:B:201:LYS:HE3	1:B:233:CYS:SG	2.33	0.68
1:A:256:ASN:HD22	1:A:257:SER:H	1.41	0.68
1:B:400:LEU:HA	1:B:403:LYS:HD3	1.75	0.67
1:B:349:LYS:NZ	2:B:570:FMN:H2'	2.11	0.65
1:A:148:ALA:N	1:A:376:ARG:HA	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:THR:CG2	1:A:436:LEU:HD21	2.27	0.65
1:A:400:LEU:O	1:A:403:LYS:HG2	1.97	0.65
3:A:560:HEM:HHB	3:A:560:HEM:CBA	2.22	0.65
1:A:196:ALA:HB2	1:A:226:MET:HG2	1.79	0.64
1:A:133:SER:O	5:A:609:HOH:O	2.15	0.64
1:B:182:ASP:HA	1:B:187:HIS:HA	1.80	0.64
1:A:144:TYR:O	1:A:433:ARG:HD3	1.98	0.63
1:A:508:PHE:CZ	1:B:131:LEU:HD12	2.33	0.63
1:B:229:THR:OG1	1:B:253:LEU:HA	2.00	0.62
1:B:132:ALA:HB2	1:B:437:TYR:HB3	1.81	0.62
1:A:385:ILE:HD11	1:A:424:LEU:HD12	1.82	0.61
1:A:461:SER:O	1:A:465:LEU:HB2	1.99	0.61
1:B:276:ALA:CB	1:B:345:PRO:HG2	2.30	0.61
1:B:183:MET:HE3	1:B:407:PHE:HE2	1.66	0.61
3:A:560:HEM:HBA2	3:A:560:HEM:CHA	2.30	0.61
1:B:252:GLN:HA	1:B:278:PHE:O	2.01	0.61
1:B:478:LEU:HD13	1:B:480:LEU:HD21	1.83	0.61
1:B:152:VAL:HG21	1:B:380:PHE:CE2	2.36	0.60
1:A:21:LYS:HB3	1:A:24:ASP:O	2.01	0.60
1:A:124:ASN:ND2	1:A:126:TYR:HB2	2.16	0.59
1:A:40:LEU:HG	1:A:47:GLN:HB2	1.83	0.59
1:A:251:TYR:HB2	1:A:274:VAL:HG21	1.84	0.59
1:B:286:LEU:HG	1:B:289:ARG:NH2	2.17	0.59
1:A:196:ALA:HB1	1:A:228:SER:HB2	1.84	0.59
1:B:196:ALA:HB2	1:B:226:MET:HG2	1.86	0.58
1:A:22:PRO:HB3	1:A:51:LYS:HD2	1.85	0.58
1:B:431:LEU:HB2	1:B:435:PHE:CE2	2.38	0.58
1:B:270:GLU:OE2	1:B:343:LYS:HB3	2.04	0.58
1:A:218:GLN:HE22	1:A:444:ARG:HD2	1.67	0.58
1:A:349:LYS:HA	1:A:369:VAL:HB	1.85	0.58
1:A:32:TYR:CE1	1:A:82:GLY:HA2	2.38	0.58
1:A:214:ARG:HD2	1:A:444:ARG:HD3	1.85	0.58
1:B:103:LYS:O	1:B:106:ILE:HG12	2.03	0.58
1:A:392:MET:HG3	1:A:424:LEU:O	2.04	0.58
1:B:183:MET:CE	1:B:250:TRP:HH2	2.16	0.58
1:B:349:LYS:HZ1	2:B:570:FMN:H2'	1.68	0.58
1:A:412:VAL:HG21	1:A:429:VAL:CG1	2.34	0.57
1:B:212:VAL:HG12	1:B:216:CYS:SG	2.44	0.57
1:A:218:GLN:HE22	1:A:444:ARG:HH11	1.52	0.57
1:A:113:LYS:C	1:A:115:LEU:H	2.12	0.56
1:B:122:ILE:HG23	1:B:127:ASP:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:TYR:OH	1:A:202:LEU:HB2	2.04	0.56
1:A:148:ALA:H	1:A:376:ARG:HA	1.70	0.56
1:B:124:ASN:HD22	1:B:126:TYR:HB2	1.70	0.56
1:A:430:GLY:O	5:A:612:HOH:O	2.17	0.56
1:B:256:ASN:HD22	1:B:257:SER:N	2.04	0.56
1:B:174:VAL:O	1:B:463:ARG:HD2	2.06	0.56
1:B:289:ARG:HH11	1:B:376:ARG:HB2	1.70	0.56
1:A:462:MET:HG2	1:A:467:VAL:HG23	1.88	0.56
1:A:65:LEU:HD21	1:A:202:LEU:HD21	1.87	0.55
1:A:75:ILE:O	1:A:80:LYS:HE3	2.06	0.55
1:A:199:LEU:HD21	3:A:560:HEM:HAA1	1.89	0.55
1:B:109:LYS:O	1:B:113:LYS:HB3	2.07	0.55
1:B:161:TYR:CE1	1:B:385:ILE:HD13	2.41	0.55
1:B:212:VAL:HG13	1:B:447:VAL:HG11	1.89	0.55
1:A:113:LYS:O	1:A:115:LEU:N	2.40	0.55
1:A:110:GLU:HB2	1:A:113:LYS:HE3	1.88	0.55
1:B:492:ASN:HD21	1:B:494:VAL:HG22	1.72	0.55
1:A:358:ILE:O	1:A:362:GLU:HG3	2.07	0.54
1:A:442:TYR:HB2	1:A:446:GLY:HA3	1.90	0.54
1:B:194:VAL:HG11	1:B:212:VAL:HG11	1.89	0.54
1:A:110:GLU:HA	1:A:113:LYS:HG2	1.90	0.54
1:A:105:ASP:O	1:A:109:LYS:HG3	2.07	0.54
1:A:163:ARG:NH1	1:A:486:ARG:HA	2.23	0.54
1:A:125:LEU:HG	1:A:434:PRO:HB3	1.90	0.54
1:B:442:TYR:HB2	1:B:446:GLY:HA3	1.90	0.54
1:B:469:SER:O	1:B:472:GLU:HB2	2.07	0.53
1:A:431:LEU:HD23	1:A:434:PRO:HG2	1.89	0.53
1:A:75:ILE:HD11	3:A:560:HEM:HAB	1.88	0.53
1:A:162:HIS:HE1	5:A:652:HOH:O	1.90	0.53
1:A:270:GLU:HB3	1:A:343:LYS:NZ	2.23	0.53
1:B:244:SER:HB2	1:B:247:GLN:H	1.74	0.53
1:A:84:LEU:HD11	1:A:88:MET:HE2	1.91	0.53
2:A:570:FMN:O4'	2:A:570:FMN:H1'2	2.09	0.53
1:A:248:ILE:HG23	1:A:275:LYS:HD3	1.91	0.53
1:B:388:LEU:HD12	1:B:408:VAL:HG21	1.91	0.53
1:B:108:ARG:HG3	1:B:135:THR:HA	1.90	0.52
1:A:214:ARG:HA	1:A:243:PRO:HD3	1.90	0.52
1:B:387:VAL:O	1:B:391:THR:HG23	2.09	0.51
1:A:347:VAL:HA	1:A:367:GLY:O	2.10	0.51
1:B:452:GLU:HG2	1:B:455:ARG:NH2	2.25	0.51
1:B:109:LYS:HD2	1:B:112:LEU:HD23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:MET:O	1:B:295:LEU:N	2.44	0.51
1:A:28:VAL:HB	1:A:57:ASP:HA	1.93	0.51
1:B:449:LYS:HE2	1:B:453:ILE:HD11	1.92	0.51
1:B:289:ARG:HD2	1:B:376:ARG:HB3	1.93	0.50
1:B:337:GLU:HA	1:B:340:LYS:HD2	1.92	0.50
1:B:372:ASN:ND2	1:B:375:GLY:H	2.09	0.50
1:A:447:VAL:O	1:A:451:ILE:HG13	2.11	0.50
1:A:88:MET:SD	1:A:92:LEU:HD13	2.52	0.50
1:B:108:ARG:O	1:B:112:LEU:HB3	2.11	0.50
1:B:431:LEU:HB2	1:B:435:PHE:HE2	1.76	0.50
1:B:465:LEU:HD22	1:B:477:LEU:HD23	1.92	0.50
1:B:163:ARG:HH22	1:B:486:ARG:HG3	1.72	0.49
1:A:270:GLU:OE2	1:A:343:LYS:HG3	2.12	0.49
1:B:347:VAL:HG13	1:B:367:GLY:C	2.37	0.49
1:B:462:MET:HG2	1:B:467:VAL:HG23	1.94	0.49
1:A:122:ILE:HG22	1:A:453:ILE:HD11	1.93	0.49
1:B:255:VAL:HG21	1:B:330:LEU:HD21	1.94	0.49
1:B:339:LYS:HG2	1:B:346:ILE:HD12	1.95	0.49
1:B:467:VAL:HG11	1:B:477:LEU:HD21	1.95	0.49
1:A:171:LEU:O	1:B:331:THR:HA	2.12	0.49
1:A:187:HIS:HE1	5:A:602:HOH:O	1.95	0.49
1:B:256:ASN:ND2	1:B:258:ASP:H	2.09	0.49
1:B:361:ALA:CB	1:B:400:LEU:HD13	2.43	0.49
1:A:199:LEU:HA	1:A:232:SER:OG	2.14	0.48
1:A:452:GLU:HG3	1:A:455:ARG:NH2	2.29	0.48
1:A:331:THR:O	1:A:334:ASP:HB2	2.12	0.48
1:A:197:THR:CG2	1:A:200:CYS:SG	3.02	0.47
1:B:102:THR:HG21	1:B:138:LYS:NZ	2.29	0.47
1:B:179:ILE:HD11	1:B:455:ARG:HG2	1.96	0.47
1:A:153:THR:HG21	1:A:381:SER:HB3	1.97	0.47
1:A:321:ALA:N	5:A:718:HOH:O	2.47	0.47
1:A:345:PRO:HB3	1:A:366:SER:OG	2.14	0.47
1:B:283:ALA:O	1:B:326:ILE:HG21	2.14	0.47
1:B:124:ASN:ND2	1:B:126:TYR:HB2	2.29	0.47
1:B:213:ALA:HB2	1:B:225:GLN:HE22	1.79	0.47
1:A:112:LEU:HG	1:A:135:THR:HB	1.97	0.47
1:A:256:ASN:O	1:A:259:ARG:HD3	2.14	0.47
1:B:194:VAL:HG21	1:B:216:CYS:SG	2.54	0.47
1:B:183:MET:SD	1:B:188:VAL:HG21	2.55	0.47
1:A:69:ASN:HD22	1:A:73:LYS:HD3	1.79	0.47
1:A:337:GLU:HB3	1:A:341:LYS:NZ	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:GLU:O	1:A:18:LYS:HB3	2.15	0.46
1:A:214:ARG:NH1	5:A:651:HOH:O	2.48	0.46
1:A:234:SER:HB2	1:A:236:GLU:HG2	1.98	0.46
1:A:508:PHE:CE1	1:B:116:LEU:HD23	2.51	0.46
1:A:163:ARG:NH1	1:B:488:VAL:O	2.49	0.46
1:B:163:ARG:HB3	1:B:483:LEU:HA	1.97	0.46
1:B:441:CYS:HB3	1:B:442:TYR:CD1	2.50	0.46
1:B:164:ILE:HB	1:B:420:LYS:HD3	1.97	0.46
1:B:456:ASP:O	1:B:460:MET:HG3	2.16	0.46
1:B:108:ARG:HG2	1:B:135:THR:O	2.16	0.46
1:A:60:ALA:HB1	1:A:96:PRO:HG3	1.97	0.46
1:A:169:LYS:HE3	5:A:850:HOH:O	2.16	0.45
1:A:488:VAL:CG2	1:B:490:VAL:HG11	2.36	0.45
1:B:222:LYS:HD2	1:B:222:LYS:N	2.31	0.45
1:B:370:LEU:HD22	1:B:406:VAL:CG1	2.45	0.45
1:B:157:ASN:OD1	1:B:384:PRO:HD2	2.17	0.45
1:B:193:TYR:HE2	1:B:407:PHE:HD2	1.63	0.45
1:B:439:ASN:O	1:B:443:GLY:N	2.50	0.45
1:A:197:THR:HG21	1:A:436:LEU:CD2	2.40	0.45
1:B:256:ASN:HD22	1:B:257:SER:H	1.63	0.45
1:B:256:ASN:HD22	1:B:258:ASP:H	1.64	0.45
1:A:58:VAL:HG23	1:A:94:CYS:SG	2.56	0.45
1:B:148:ALA:C	1:B:149:ASN:ND2	2.59	0.45
1:B:339:LYS:HA	1:B:346:ILE:HD11	1.99	0.45
1:B:478:LEU:CD1	1:B:480:LEU:HD21	2.46	0.45
1:A:216:CYS:O	1:A:222:LYS:HA	2.17	0.45
1:A:214:ARG:NH1	1:A:241:ALA:HB1	2.32	0.45
1:B:385:ILE:HD11	1:B:421:ALA:HA	1.99	0.45
1:B:419:LEU:HD13	1:B:465:LEU:HD12	1.99	0.45
1:A:29:ILE:HB	1:A:34:TYR:HE2	1.81	0.45
1:A:192:PHE:HA	1:A:429:VAL:O	2.17	0.45
1:B:351:VAL:HG11	1:B:357:VAL:CG2	2.47	0.45
1:B:149:ASN:O	1:B:150:ASP:HB2	2.17	0.44
1:B:288:GLN:HG3	1:B:293:MET:SD	2.56	0.44
1:A:15:GLU:O	1:A:19:HIS:CE1	2.70	0.44
1:A:130:TYR:O	1:A:134:GLN:HG2	2.18	0.44
1:A:255:VAL:HG21	1:A:330:LEU:HD23	1.99	0.44
1:B:199:LEU:O	1:B:201:LYS:N	2.50	0.44
1:A:77:PRO:HA	1:A:80:LYS:CD	2.41	0.44
1:A:143:PHE:CD1	1:A:289:ARG:NH2	2.71	0.44
1:B:418:VAL:HG21	1:B:458:ILE:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:LYS:HD2	1:B:112:LEU:CD2	2.48	0.44
1:B:210:LYS:O	1:B:214:ARG:HG3	2.17	0.44
1:B:348:ILE:HD12	1:B:365:VAL:HG21	1.99	0.44
1:A:123:ILE:HG21	1:B:290:GLU:HG2	1.99	0.44
1:A:252:GLN:HA	1:A:278:PHE:O	2.17	0.44
1:A:361:ALA:HB1	1:A:400:LEU:HD22	2.00	0.44
1:B:412:VAL:HG13	1:B:417:ASP:HB2	1.99	0.44
1:A:32:TYR:HB3	1:A:34:TYR:OH	2.18	0.43
1:B:197:THR:HG21	1:B:436:LEU:HG	1.99	0.43
1:B:292:ASP:O	1:B:293:MET:C	2.60	0.43
1:A:170:ILE:HD11	1:B:282:ASP:HA	1.99	0.43
1:B:111:GLN:O	1:B:115:LEU:HB2	2.18	0.43
1:B:149:ASN:HB3	1:B:290:GLU:OE2	2.17	0.43
1:B:243:PRO:HD2	1:B:247:GLN:HE22	1.83	0.43
2:B:570:FMN:HI'2	2:B:570:FMN:H9	1.63	0.43
1:A:176:LYS:HA	5:A:640:HOH:O	2.18	0.43
1:A:110:GLU:O	1:A:113:LYS:HG2	2.19	0.43
1:A:333:LYS:HD2	1:A:333:LYS:HA	1.74	0.43
3:A:560:HEM:O1A	4:A:580:PYR:OXT	2.37	0.43
1:A:21:LYS:O	1:A:25:CYS:HB2	2.18	0.43
1:B:174:VAL:HB	1:B:463:ARG:HG3	2.01	0.43
1:B:196:ALA:CB	1:B:226:MET:HE2	2.49	0.43
2:B:570:FMN:H9	2:B:570:FMN:O4'	2.19	0.43
1:A:380:PHE:HE1	5:A:721:HOH:O	2.01	0.43
1:B:354:THR:OG1	1:B:391:THR:HG22	2.19	0.43
1:A:278:PHE:HA	1:A:347:VAL:O	2.19	0.43
1:B:230:LEU:N	1:B:230:LEU:HD12	2.34	0.43
1:B:282:ASP:C	1:B:284:PRO:HD2	2.44	0.43
1:A:187:HIS:CE1	5:A:602:HOH:O	2.69	0.42
1:A:330:LEU:HD22	1:A:334:ASP:HB3	2.00	0.42
1:A:361:ALA:HB2	1:A:404:LEU:HD22	2.01	0.42
1:B:492:ASN:ND2	1:B:494:VAL:HG22	2.33	0.42
1:A:129:GLU:HG2	1:A:437:TYR:CD2	2.54	0.42
1:B:230:LEU:HD13	1:B:254:TYR:CD2	2.54	0.42
1:B:289:ARG:NH1	1:B:377:GLN:HE21	2.17	0.42
1:B:462:MET:HG2	1:B:467:VAL:CG2	2.50	0.42
1:A:175:ARG:HH11	1:A:175:ARG:HB2	1.84	0.42
1:B:174:VAL:CG2	1:B:463:ARG:HG3	2.49	0.42
1:A:285:SER:O	1:A:377:GLN:NE2	2.53	0.42
1:B:230:LEU:CD1	1:B:254:TYR:HD2	2.33	0.42
1:B:439:ASN:OD1	1:B:443:GLY:HA2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:SER:HA	1:A:13:PRO:HD3	1.91	0.42
1:A:138:LYS:HD2	5:A:701:HOH:O	2.20	0.42
1:A:269:VAL:O	1:A:274:VAL:HG22	2.18	0.42
1:A:346:ILE:HB	1:A:365:VAL:HG22	2.02	0.42
1:A:376:ARG:NH1	4:A:580:PYR:O3	2.53	0.42
1:A:432:GLY:HA3	2:A:570:FMN:H4'	2.01	0.42
1:B:106:ILE:O	1:B:110:GLU:HG2	2.20	0.42
1:A:223:VAL:HA	1:A:224:PRO:HD3	1.95	0.42
1:A:177:VAL:HG23	1:A:463:ARG:NH1	2.35	0.41
1:A:282:ASP:O	1:A:377:GLN:HG2	2.20	0.41
1:A:330:LEU:HD22	1:A:334:ASP:CB	2.49	0.41
1:B:201:LYS:HA	1:B:204:ASN:O	2.21	0.41
1:A:337:GLU:OE1	1:A:340:LYS:HE2	2.20	0.41
2:A:570:FMN:O4'	2:A:570:FMN:H9	2.19	0.41
1:B:153:THR:HG21	1:B:381:SER:HB3	2.02	0.41
1:A:113:LYS:C	1:A:115:LEU:N	2.77	0.41
1:B:357:VAL:HG13	1:B:368:VAL:HG11	2.02	0.41
1:B:358:ILE:HD11	1:B:394:ILE:HG21	2.01	0.41
1:A:487:THR:O	1:B:490:VAL:HG12	2.20	0.41
1:B:164:ILE:HG23	1:B:480:LEU:HD23	2.02	0.41
1:B:224:PRO:HA	1:B:248:ILE:O	2.20	0.41
1:A:16:VAL:HA	1:A:26:TRP:CE3	2.55	0.41
1:B:183:MET:HE2	1:B:250:TRP:HH2	1.86	0.41
1:B:400:LEU:O	1:B:403:LYS:HB2	2.21	0.41
1:A:61:ILE:HG23	1:A:97:TYR:HB2	2.03	0.41
1:A:151:GLU:OE1	1:A:291:LYS:NZ	2.54	0.41
1:A:239:ILE:HD11	1:A:274:VAL:HG12	2.03	0.41
1:A:332:TRP:O	1:A:336:GLU:HG3	2.20	0.41
1:B:214:ARG:HA	1:B:243:PRO:CD	2.50	0.41
1:B:336:GLU:O	1:B:339:LYS:HB2	2.20	0.41
1:A:118:PRO:HA	5:A:680:HOH:O	2.20	0.41
1:A:255:VAL:HG21	1:A:330:LEU:CD2	2.50	0.41
1:B:172:VAL:HG11	1:B:466:GLY:O	2.20	0.41
1:B:217:GLY:HA3	1:B:247:GLN:HE21	1.82	0.41
1:A:67:ALA:HA	1:A:232:SER:O	2.21	0.41
1:A:230:LEU:HD12	3:A:560:HEM:HMA2	2.03	0.41
1:A:369:VAL:HG22	1:A:407:PHE:HB2	2.03	0.41
1:B:210:LYS:HD3	1:B:237:GLU:HB3	2.03	0.41
1:B:430:GLY:C	1:B:431:LEU:HD12	2.45	0.41
1:A:168:PRO:HB3	1:A:465:LEU:HA	2.04	0.41
1:A:382:ARG:HH21	1:A:484:LYS:NZ	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:TYR:CD1	1:A:436:LEU:HD13	2.56	0.40
1:B:226:MET:HE1	1:B:349:LYS:CD	2.52	0.40
1:A:447:VAL:HG12	1:A:451:ILE:HD11	2.03	0.40
1:B:371:SER:HB2	1:B:409:ASP:OD1	2.21	0.40
1:B:486:ARG:HH11	1:B:486:ARG:HD2	1.74	0.40
1:A:203:GLY:HA3	1:A:440:SER:OG	2.21	0.40
1:A:495:LEU:HD21	1:B:503:PRO:HB2	2.03	0.40
1:B:153:THR:OG1	1:B:381:SER:N	2.55	0.40
1:B:159:ASN:O	1:B:162:HIS:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

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	474/511 (93%)	425 (90%)	36 (8%)	13 (3%)	4	16
1	B	378/511 (74%)	331 (88%)	38 (10%)	9 (2%)	4	18
All	All	852/1022 (83%)	756 (89%)	74 (9%)	22 (3%)	4	17

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	PRO
1	A	104	GLU
1	A	114	SER
1	B	146	SER
1	B	149	ASN
1	A	69	ASN
1	A	399	ASN
1	A	493	ASP
1	B	103	LYS

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Mol	Chain	Res	Type
1	B	200	CYS
1	B	287	GLY
1	B	290	GLU
1	B	294	LYS
1	A	85	GLN
1	B	119	LEU
1	A	18	LYS
1	B	114	SER
1	A	13	PRO
1	A	23	ASP
1	A	149	ASN
1	A	150	ASP
1	A	410	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	411/440 (93%)	336 (82%)	75 (18%)	2	6
1	B	330/440 (75%)	272 (82%)	58 (18%)	2	6
All	All	741/880 (84%)	608 (82%)	133 (18%)	2	6

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LYS
1	A	11	ILE
1	A	13	PRO
1	A	15	GLU
1	A	20	ASN
1	A	21	LYS
1	A	27	VAL
1	A	28	VAL
1	A	30	ASN
1	A	36	LEU

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Mol	Chain	Res	Type
1	A	38	ARG
1	A	41	PRO
1	A	44	PRO
1	A	65	LEU
1	A	72	ASP
1	A	84	LEU
1	A	87	SER
1	A	90	PRO
1	A	91	GLU
1	A	96	PRO
1	A	115	LEU
1	A	119	LEU
1	A	121	ASN
1	A	122	ILE
1	A	124	ASN
1	A	125	LEU
1	A	131	LEU
1	A	152	VAL
1	A	170	ILE
1	A	190	VAL
1	A	191	PRO
1	A	195	SER
1	A	206	LEU
1	A	212	VAL
1	A	223	VAL
1	A	226	MET
1	A	230	LEU
1	A	236	GLU
1	A	239	ILE
1	A	245	ASP
1	A	255	VAL
1	A	261	ILE
1	A	262	THR
1	A	265	LEU
1	A	271	LYS
1	A	292	ASP
1	A	323	SER
1	A	329	SER
1	A	330	LEU
1	A	331	THR
1	A	339	LYS
1	A	343	LYS

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Mol	Chain	Res	Type
1	A	359	LYS
1	A	365	VAL
1	A	372	ASN
1	A	376	ARG
1	A	378	LEU
1	A	385	ILE
1	A	388	LEU
1	A	397	GLN
1	A	399	ASN
1	A	400	LEU
1	A	448	GLU
1	A	452	GLU
1	A	460	MET
1	A	462	MET
1	A	465	LEU
1	A	469	SER
1	A	481	SER
1	A	483	LEU
1	A	490	VAL
1	A	494	VAL
1	A	495	LEU
1	A	501	GLU
1	A	507	GLU
1	B	103	LYS
1	B	105	ASP
1	B	108	ARG
1	B	118	PRO
1	B	119	LEU
1	B	131	LEU
1	B	136	LEU
1	B	149	ASN
1	B	152	VAL
1	B	163	ARG
1	B	182	ASP
1	B	197	THR
1	B	206	LEU
1	B	209	GLU
1	B	236	GLU
1	B	243	PRO
1	B	244	SER
1	B	248	ILE
1	B	249	GLN

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Mol	Chain	Res	Type
1	B	252	GLN
1	B	255	VAL
1	B	256	ASN
1	B	257	SER
1	B	260	LYS
1	B	262	THR
1	B	263	ASP
1	B	267	LYS
1	B	289	ARG
1	B	295	LEU
1	B	296	LYS
1	B	328	PRO
1	B	331	THR
1	B	338	LEU
1	B	342	THR
1	B	343	LYS
1	B	368	VAL
1	B	370	LEU
1	B	372	ASN
1	B	378	LEU
1	B	384	PRO
1	B	387	VAL
1	B	388	LEU
1	B	391	THR
1	B	408	VAL
1	B	413	ARG
1	B	414	ARG
1	B	416	THR
1	B	429	VAL
1	B	436	LEU
1	B	444	ARG
1	B	461	SER
1	B	463	ARG
1	B	464	LEU
1	B	468	THR
1	B	483	LEU
1	B	492	ASN
1	B	507	GLU
1	B	509	GLU

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

Mol	Chain	Res	Type
1	A	69	ASN
1	A	85	GLN
1	A	124	ASN
1	A	134	GLN
1	A	149	ASN
1	A	157	ASN
1	A	162	HIS
1	A	218	GLN
1	A	249	GLN
1	A	252	GLN
1	A	256	ASN
1	A	268	ASN
1	A	372	ASN
1	B	124	ASN
1	B	149	ASN
1	B	225	GLN
1	B	247	GLN
1	B	256	ASN
1	B	372	ASN
1	B	492	ASN
1	B	497	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	HEM	A	560	1	50,50,50	1.63	7 (14%)	67,82,82	2.22	6 (8%)
2	FMN	B	570	-	33,33,33	1.92	10 (30%)	48,50,50	2.18	17 (35%)
4	PYR	B	580	-	5,5,5	2.13	2 (40%)	3,6,6	1.80	0
4	PYR	A	580	-	5,5,5	2.31	2 (40%)	3,6,6	1.89	1 (33%)
2	FMN	A	570	-	33,33,33	2.34	10 (30%)	48,50,50	2.77	23 (47%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	A	560	1	-	9/14/54/54	-
2	FMN	B	570	-	2/2/4/4	6/18/18/18	0/3/3/3
4	PYR	B	580	-	-	0/4/4/4	-
4	PYR	A	580	-	-	0/4/4/4	-
2	FMN	A	570	-	2/2/4/4	17/18/18/18	0/3/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	560	HEM	CAA-C2A	6.45	1.67	1.51
2	A	570	FMN	C2'-C3'	-5.90	1.43	1.53
2	A	570	FMN	C9-C8	-5.85	1.31	1.39
2	B	570	FMN	C1'-N10	-5.26	1.35	1.47
2	A	570	FMN	C1'-N10	-4.69	1.36	1.47
2	B	570	FMN	C9-C8	-4.40	1.33	1.39
2	A	570	FMN	O2'-C2'	-3.72	1.35	1.43
4	A	580	PYR	CA-C	-3.66	1.42	1.54
4	B	580	PYR	CA-C	-3.49	1.42	1.54
2	B	570	FMN	C4A-N5	3.44	1.38	1.30
3	A	560	HEM	CAC-C3C	-3.34	1.38	1.47
3	A	560	HEM	CBB-CAB	3.19	1.45	1.30
3	A	560	HEM	CAB-C3B	-3.16	1.39	1.47
3	A	560	HEM	CBC-CAC	3.00	1.44	1.30
2	A	570	FMN	O4'-C4'	-2.99	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	570	FMN	C4A-N5	2.99	1.37	1.30
4	A	580	PYR	CB-CA	2.82	1.55	1.50
2	A	570	FMN	C4A-C10	-2.81	1.35	1.44
2	B	570	FMN	C9A-C5A	-2.61	1.37	1.41
2	A	570	FMN	C6-C5A	-2.50	1.36	1.40
2	B	570	FMN	C2'-C3'	-2.40	1.49	1.53
4	B	580	PYR	OXT-C	-2.35	1.24	1.30
2	B	570	FMN	C6-C7	-2.34	1.36	1.39
2	B	570	FMN	C6-C5A	-2.32	1.36	1.40
2	A	570	FMN	C4'-C3'	-2.32	1.49	1.53
3	A	560	HEM	O2A-CGA	-2.32	1.23	1.30
2	B	570	FMN	C8M-C8	2.28	1.55	1.51
2	A	570	FMN	C9-C9A	-2.20	1.36	1.39
2	B	570	FMN	C9A-N10	-2.13	1.37	1.41
3	A	560	HEM	CHC-C1C	-2.12	1.34	1.38
2	B	570	FMN	C1'-C2'	2.05	1.55	1.52

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	560	HEM	CAA-C2A-C1A	-11.75	101.98	124.94
3	A	560	HEM	CAA-C2A-C3A	10.08	149.67	127.07
2	A	570	FMN	C4'-C3'-C2'	6.92	125.08	113.57
2	A	570	FMN	C10-N1-C2	6.59	131.12	116.85
2	A	570	FMN	C4A-C10-N1	-6.57	108.47	124.59
2	B	570	FMN	C10-N1-C2	5.46	128.68	116.85
2	B	570	FMN	C4'-C3'-C2'	4.85	121.65	113.57
2	A	570	FMN	C8M-C8-C9	-4.32	111.95	119.57
2	B	570	FMN	C4A-C10-N1	-4.21	114.27	124.59
2	A	570	FMN	C4-C4A-C10	4.16	124.07	116.93
2	B	570	FMN	O2-C2-N3	4.00	126.25	118.58
2	B	570	FMN	O4'-C4'-C3'	3.85	118.26	109.25
2	A	570	FMN	N10-C10-N1	3.78	129.63	118.51
2	A	570	FMN	C1'-C2'-C3'	3.77	119.89	109.66
2	A	570	FMN	C4A-C10-N10	3.76	121.86	116.48
2	B	570	FMN	C4A-C10-N10	3.70	121.78	116.48
2	B	570	FMN	C5A-C9A-N10	3.60	121.22	117.97
2	A	570	FMN	O2'-C2'-C3'	-3.53	100.99	109.25
2	A	570	FMN	N3-C2-N1	-3.32	112.45	119.50
3	A	560	HEM	C3B-C4B-NB	3.27	111.82	109.47
2	A	570	FMN	C5A-C9A-N10	3.18	120.84	117.97
2	A	570	FMN	C9A-N10-C10	-3.04	116.12	120.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	570	FMN	C8M-C8-C7	3.03	126.95	120.76
2	A	570	FMN	O4'-C4'-C3'	2.98	116.22	109.25
2	A	570	FMN	C9-C9A-N10	-2.94	117.90	121.85
2	A	570	FMN	O3'-C3'-C4'	2.91	115.55	108.93
2	A	570	FMN	C4-C4A-N5	-2.83	114.30	118.21
2	B	570	FMN	O5'-C5'-C4'	2.79	116.80	109.36
2	B	570	FMN	O3P-P-O2P	2.76	118.16	107.80
2	B	570	FMN	C8M-C8-C7	2.76	126.39	120.76
2	A	570	FMN	O2'-C2'-C1'	2.73	121.43	110.20
2	B	570	FMN	C4-C4A-C10	2.61	121.41	116.93
3	A	560	HEM	CAA-CBA-CGA	2.55	120.43	113.67
2	B	570	FMN	C9-C9A-N10	-2.54	118.44	121.85
2	B	570	FMN	C8M-C8-C9	-2.53	115.12	119.57
2	B	570	FMN	O5'-P-O1P	-2.51	99.66	106.44
2	B	570	FMN	C9A-N10-C10	-2.43	117.05	120.75
4	A	580	PYR	OXT-C-CA	2.43	120.32	113.59
3	A	560	HEM	CBA-CAA-C2A	2.41	119.21	112.53
2	A	570	FMN	O2-C2-N3	2.40	123.19	118.58
2	B	570	FMN	N3-C2-N1	-2.38	114.44	119.50
2	A	570	FMN	O4'-C4'-C5'	2.37	115.22	109.99
2	A	570	FMN	C7M-C7-C6	-2.25	115.60	119.57
2	A	570	FMN	C5A-C6-C7	-2.22	116.72	120.83
3	A	560	HEM	O2D-CGD-CBD	2.18	120.89	114.00
2	A	570	FMN	O5'-P-O1P	-2.14	100.66	106.44
2	B	570	FMN	O4'-C4'-C5'	2.07	114.54	109.99

All (4) chirality outliers are listed below:

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

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	570	FMN	N10-C1'-C2'-O2'
2	A	570	FMN	C1'-C2'-C3'-O3'
2	A	570	FMN	C1'-C2'-C3'-C4'
2	A	570	FMN	O2'-C2'-C3'-O3'
2	A	570	FMN	O2'-C2'-C3'-C4'

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Mol	Chain	Res	Type	Atoms
2	A	570	FMN	C2'-C3'-C4'-O4'
2	A	570	FMN	O3'-C3'-C4'-O4'
2	A	570	FMN	O3'-C3'-C4'-C5'
2	A	570	FMN	O4'-C4'-C5'-O5'
2	A	570	FMN	C5'-O5'-P-O1P
2	A	570	FMN	C5'-O5'-P-O3P
2	B	570	FMN	N10-C1'-C2'-O2'
2	B	570	FMN	C3'-C4'-C5'-O5'
2	B	570	FMN	O4'-C4'-C5'-O5'
3	A	560	HEM	C2B-C3B-CAB-CBB
3	A	560	HEM	C2C-C3C-CAC-CBC
3	A	560	HEM	C4C-C3C-CAC-CBC
2	A	570	FMN	C2'-C3'-C4'-C5'
2	B	570	FMN	O3'-C3'-C4'-O4'
2	A	570	FMN	C3'-C4'-C5'-O5'
2	A	570	FMN	C4'-C5'-O5'-P
2	B	570	FMN	C4'-C5'-O5'-P
2	B	570	FMN	C2'-C3'-C4'-O4'
3	A	560	HEM	C3D-CAD-CBD-CGD
3	A	560	HEM	C4B-C3B-CAB-CBB
2	A	570	FMN	C2'-C1'-N10-C10
3	A	560	HEM	CAA-CBA-CGA-O1A
2	A	570	FMN	C5'-O5'-P-O2P
3	A	560	HEM	CAD-CBD-CGD-O1D
3	A	560	HEM	CAD-CBD-CGD-O2D
3	A	560	HEM	CAA-CBA-CGA-O2A
2	A	570	FMN	N10-C1'-C2'-C3'

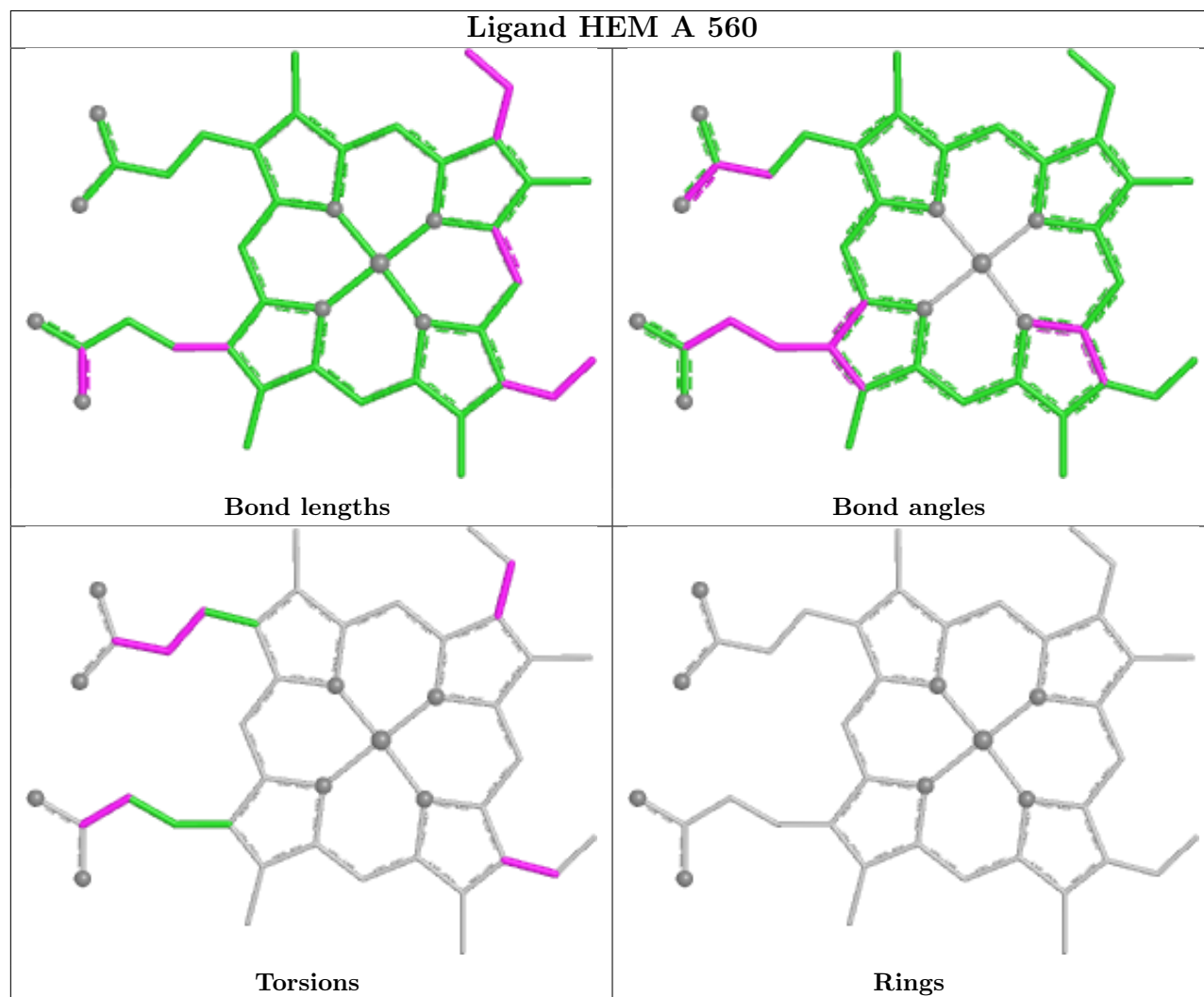
There are no ring outliers.

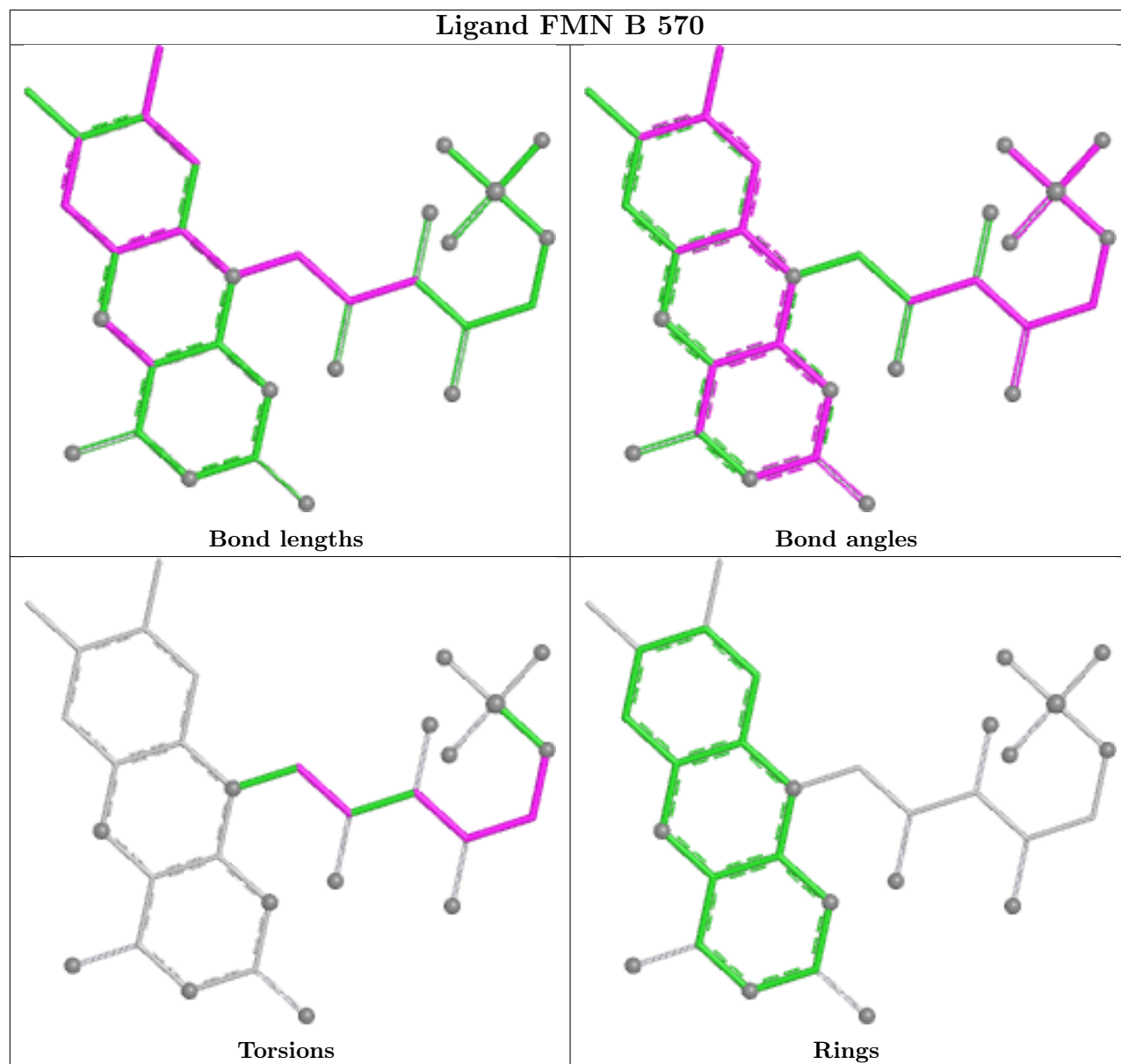
4 monomers are involved in 16 short contacts:

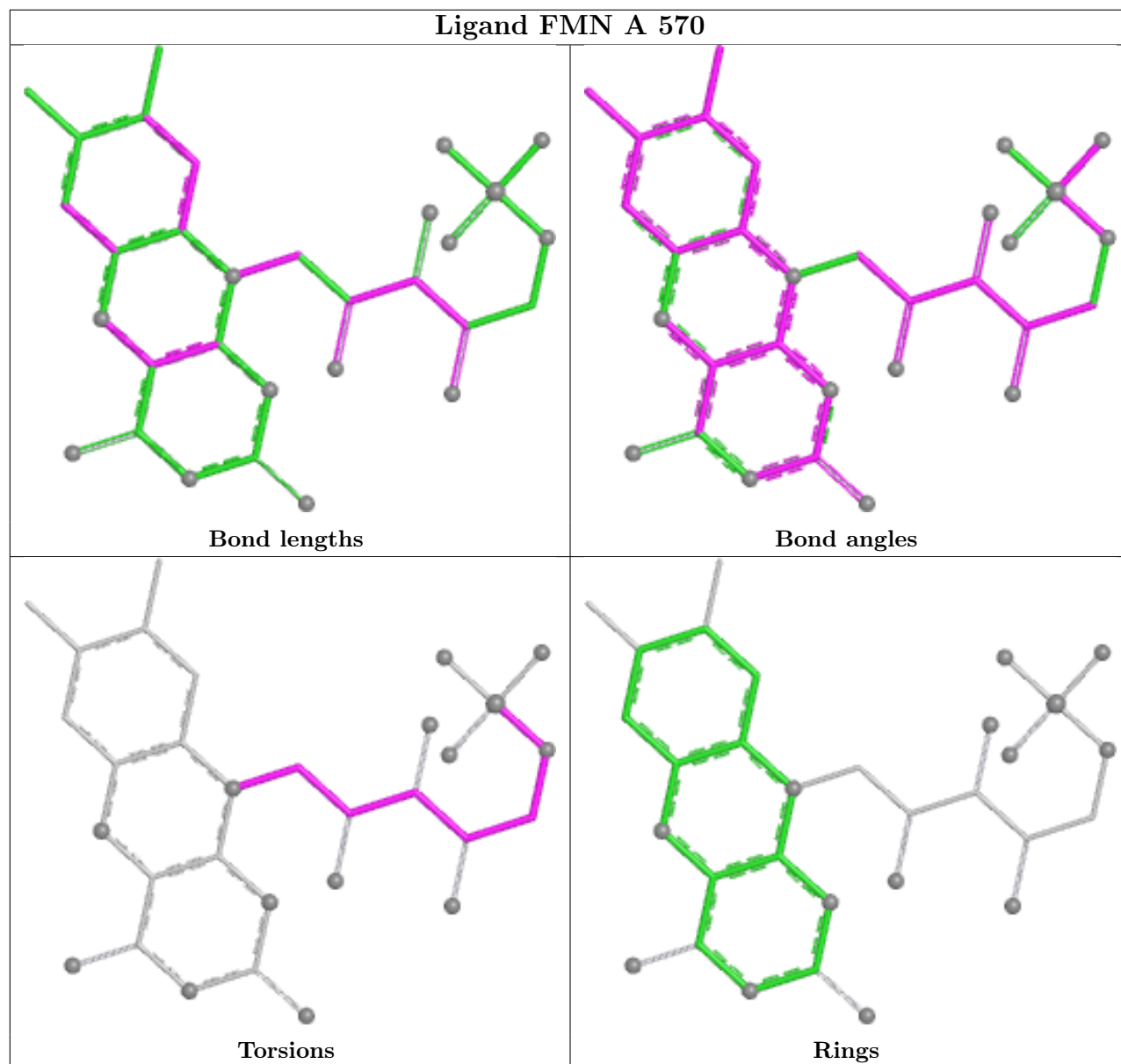
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	560	HEM	8	0
2	B	570	FMN	4	0
4	A	580	PYR	2	0
2	A	570	FMN	3	0

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.