



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:52 PM UTC

PDB ID : 1FCB / pdb_00001fcb
Title : MOLECULAR STRUCTURE OF FLAVOCYTOCHROME B2 AT 2.4
ANGSTROMS RESOLUTION
Authors : Mathews, F.S.; Xia, Z.-X.
Deposited on : 1990-01-16
Resolution : 2.40 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

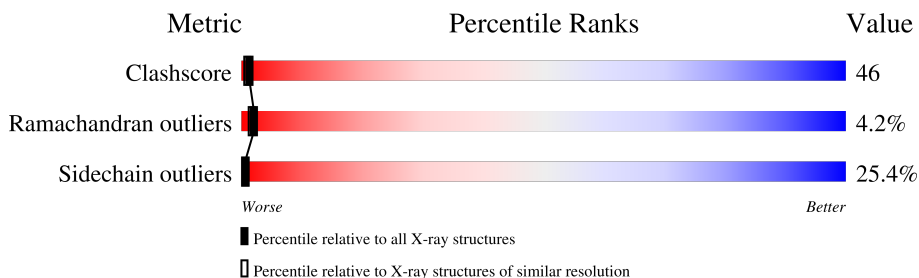
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

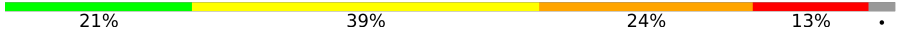
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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
3	FMN	A	570	X	-	-	-
4	PYR	B	580	-	X	-	-

2 Entry composition [i](#)

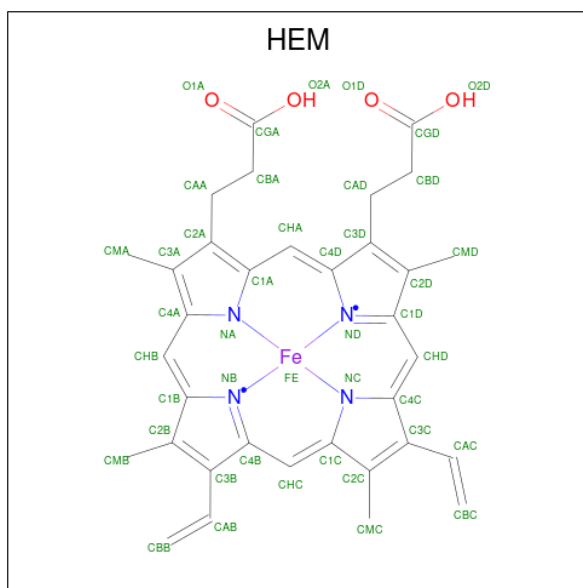
There are 5 unique types of molecules in this entry. The entry contains 7342 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

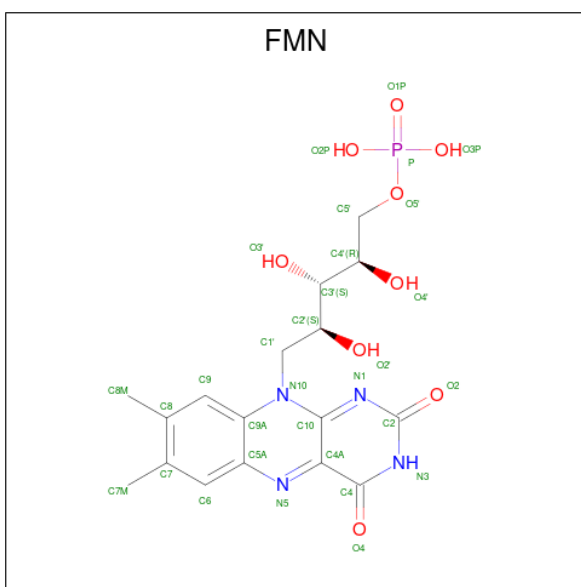
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	0	0
			3841	2446	652	728	15			
1	B	400	Total	C	N	O	S	0	0	0
			3107	1968	529	599	11			

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



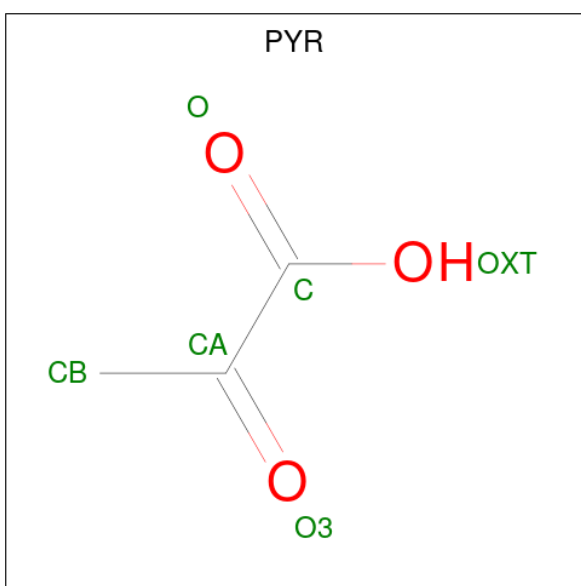
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



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

- Molecule 4 is PYRUVIC ACID (CCD ID: PYR) (formula: $C_3H_4O_3$).



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

- Molecule 5 is water.

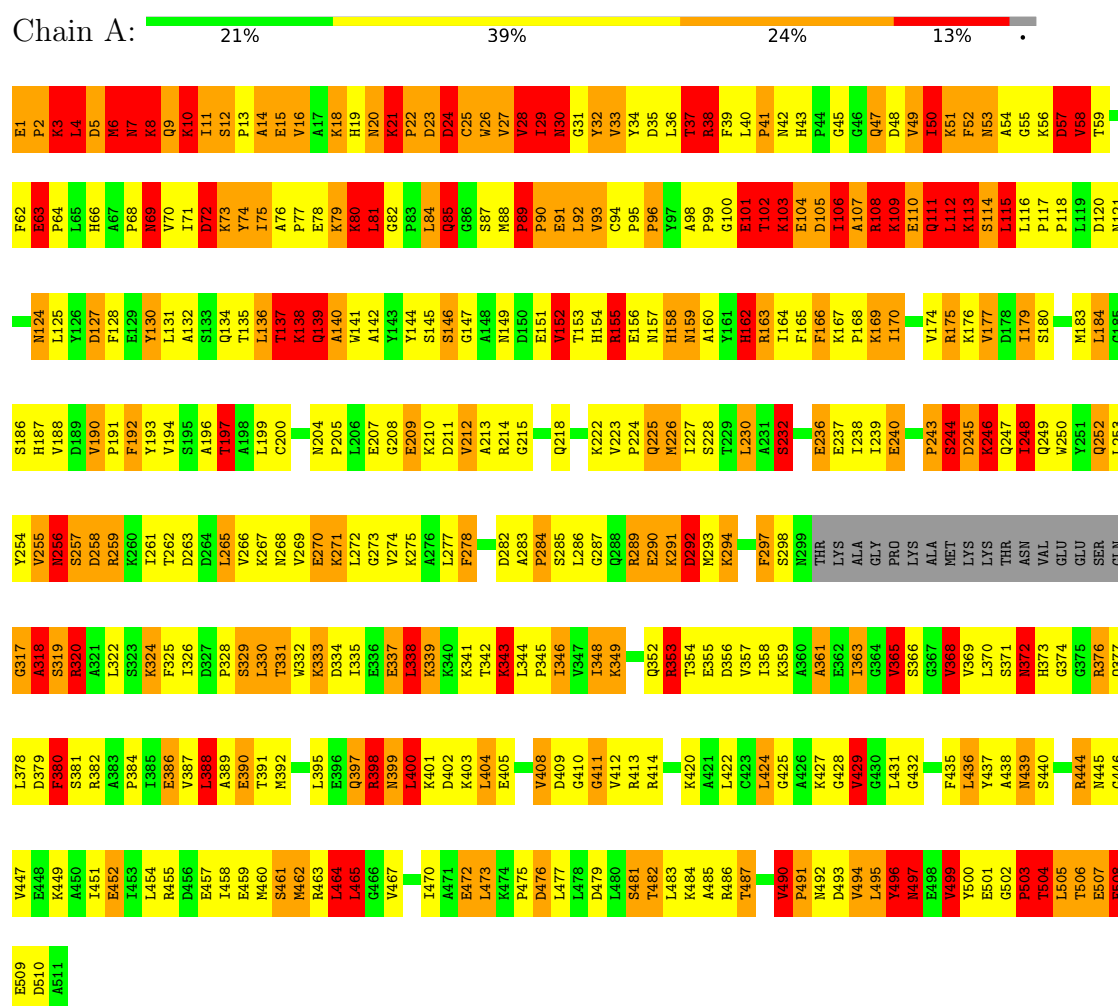
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	182	Total 182	O 182	0	0
5	B	101	Total 101	O 101	0	0

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



T506	R444	G375	MET	G185	I122	ILE
E507	N445	R376	LYS	S186	I123	PHE
F508	G446	Q377	LYS	I248	N124	GLU
E509	V447	L378	THR	Q249	L125	PRO
D510	E448	D379	ASN	W250	D126	LEU
A511	K449	F380	V312	Y251	D127	HIS
	A450	S381	E313	Q252	F128	ALA
	I451	R382	E314	F192	E129	PRO
	E452	A383	S315	Y193	Y130	ASN
	T453	P384	Q316	V194	L131	VAL
	L454	I385	Q317	S195	A132	ILE
	R455	E386	A318	A196	S133	ASP
		V387	S319	T197	Q134	LYS
		L388	R320	D258	Q134	LYS
	I458	A389		A198	T135	TYR
	E459	E390		L199	L136	ILE
	M460	T391	S323	I261	T137	ALA
	S461	M392	K324	K201	K138	PRO
	M462	P393	F325	L202	Q139	GLU
	R463	I394	I326	G203	A140	LYS
	L464	L395	D327	N204		
	L465	L396	P328	P205	Y143	
	G466	E396	S329	L206	Y144	GLY
	V467	Q397	L330	E207	S145	PRO
	T468	R398	T331	G208	S146	LEU
	S469	M399	K332	E208	G147	GLN
	I470	L400	K333	K210	A148	GLY
	A471	K401	D394	D211	N149	SER
	E472	D402	I335	V212	D150	MET
	L473	K403	E336	A213	E151	PRO
	K474	L404	E337	K275	V152	PRO
	P475	E405	I338	A276	T153	GLU
	D476	V406	K339	L277	H154	LEU
	L477	F407		Q217	R155	VAL
	L478	V408	K343	Q218	E156	VAL
	D479	D409		G219	N157	CYS
	L480	G410	I346	V220	PRO	PRO
	S481	G411	V347	T221	PRO	TYR
	T482	V412	I348	K222	M159	ALA
	L483	R413	K349	V223	A160	ALA
	K484	R414	G350	P224	Y161	PRO
	A485		V351	Q225	H162	
	R486	D417	Q352	M226	R163	E101
	T487	V418	R353	I227	I164	T102
	V488	L419	E354	S228	F165	K103
	G489	K420	E355	T229	F166	E104
	V490	A421	D292	L230	K167	D105
	N492	L422	M293	A231	I106	I106
	D493		K294	S232	R108	A107
	V494	Y429	L295	C233	I170	R108
	L495	R433	K296	P235	L171	K109
	Y496	L436	S297	E236	V172	E110
	N497	L437	S298	E237	D173	Q111
	E498	Y437	N299	I238	V174	L112
	Y499	A438	THR	I239	R175	K113
	Y500	L439	LYS	E240	K176	S114
		S440	ALA	A241	V177	L115
		C441	L370	A242	D178	L116
	P503	Y442	S371	A242		P117
	T504	G443	N372	P243		
	L505		R373	S244	D182	D120
			G374	ALA	M183	N121

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	165.51Å 165.51Å 113.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	5.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (5.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROFFT	Depositor
R, R_{free}	0.188 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7342	wwPDB-VP
Average B, all atoms (Å ²)	35.0	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, FMN, HEM

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	2/3916 (0.1%)	3.19	535/5303 (10.1%)
1	B	1.24	5/3156 (0.2%)	3.25	500/4263 (11.7%)
All	All	1.25	7/7072 (0.1%)	3.22	1035/9566 (10.8%)

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	4
1	B	0	2
All	All	0	6

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	282	ASP	N-CA	5.80	1.53	1.46
1	B	482	THR	CA-CB	5.61	1.61	1.53
1	A	102	THR	CA-CB	5.53	1.60	1.52
1	B	420	LYS	N-CA	5.48	1.52	1.46
1	B	463	ARG	NE-CZ	5.39	1.39	1.33
1	A	438	ALA	N-CA	5.09	1.52	1.46
1	B	451	ILE	CA-CB	5.07	1.60	1.54

All (1035) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	382	ARG	CD-NE-CZ	25.17	159.64	124.40
1	A	108	ARG	CD-NE-CZ	21.15	154.01	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	289	ARG	CD-NE-CZ	20.16	152.63	124.40
1	A	353	ARG	NE-CZ-NH1	19.59	141.09	121.50
1	B	259	ARG	NE-CZ-NH2	19.52	136.77	119.20
1	A	155	ARG	NE-CZ-NH2	19.29	136.56	119.20
1	B	155	ARG	CD-NE-CZ	18.81	150.73	124.40
1	A	297	PHE	CA-CB-CG	16.78	130.58	113.80
1	B	488	VAL	CA-C-O	-16.20	104.21	120.25
1	A	497	ASN	CA-CB-CG	16.15	128.75	112.60
1	A	240	GLU	CA-CB-CG	15.61	145.32	114.10
1	B	188	VAL	O-C-N	15.11	138.70	122.98
1	B	353	ARG	CD-NE-CZ	14.84	145.17	124.40
1	A	268	ASN	OD1-CG-ND2	-14.69	107.91	122.60
1	B	139	GLN	OE1-CD-NE2	14.39	136.99	122.60
1	A	353	ARG	CB-CG-CD	14.39	144.40	111.30
1	B	190	VAL	O-C-N	14.31	131.73	121.72
1	B	353	ARG	CB-CG-CD	14.29	144.18	111.30
1	A	376	ARG	NE-CZ-NH1	14.27	135.76	121.50
1	B	413	ARG	CD-NE-CZ	14.22	144.31	124.40
1	B	124	ASN	OD1-CG-ND2	-13.86	108.74	122.60
1	A	507	GLU	N-CA-C	13.65	126.24	111.36
1	A	163	ARG	CD-NE-CZ	13.43	143.20	124.40
1	A	452	GLU	CA-CB-CG	13.33	140.75	114.10
1	A	353	ARG	NE-CZ-NH2	-13.24	107.28	119.20
1	A	70	VAL	N-CA-C	13.20	122.93	110.53
1	A	379	ASP	CA-CB-CG	-13.09	99.51	112.60
1	A	115	LEU	N-CA-C	-13.01	96.04	114.12
1	A	108	ARG	CA-CB-CG	13.00	140.11	114.10
1	A	329	SER	CA-C-O	-12.67	104.53	119.35
1	A	89	PRO	N-CA-C	-12.63	95.29	110.70
1	A	414	ARG	NE-CZ-NH1	-12.55	108.95	121.50
1	B	353	ARG	CA-CB-CG	12.50	139.10	114.10
1	A	476	ASP	CA-CB-CG	-12.45	100.15	112.60
1	B	253	LEU	N-CA-C	12.31	128.79	108.73
1	B	463	ARG	CD-NE-CZ	-11.69	108.04	124.40
1	B	391	THR	CA-CB-CG2	11.63	130.28	110.50
1	A	24	ASP	CA-CB-CG	-11.55	101.05	112.60
1	B	318	ALA	N-CA-C	-11.46	97.79	112.23
1	B	334	ASP	CA-CB-CG	11.46	124.06	112.60
1	A	149	ASN	CA-CB-CG	11.40	124.00	112.60
1	A	445	ASN	OD1-CG-ND2	-11.22	111.38	122.60
1	B	163	ARG	NE-CZ-NH2	-11.17	109.15	119.20
1	A	157	ASN	CA-C-N	11.03	135.63	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	157	ASN	C-N-CA	11.03	135.63	120.63
1	B	115	LEU	N-CA-C	-10.93	97.14	111.24
1	B	121	ASN	O-C-N	10.85	134.86	122.27
1	B	455	ARG	NE-CZ-NH2	10.85	128.96	119.20
1	B	124	ASN	CB-CA-C	-10.84	89.33	111.22
1	A	490	VAL	N-CA-CB	10.82	121.14	109.99
1	A	382	ARG	CD-NE-CZ	10.82	139.55	124.40
1	B	390	GLU	CA-CB-CG	10.73	135.56	114.10
1	B	386	GLU	O-C-N	-10.73	109.92	122.15
1	B	166	PHE	CA-C-O	-10.69	108.63	121.56
1	B	233	CYS	CA-C-O	-10.69	108.32	121.89
1	B	134	GLN	OE1-CD-NE2	-10.66	111.94	122.60
1	A	297	PHE	N-CA-CB	10.64	122.58	110.35
1	A	179	ILE	O-C-N	-10.62	110.89	122.05
1	A	158	HIS	CA-CB-CG	-10.59	103.21	113.80
1	B	379	ASP	CA-CB-CG	-10.52	102.08	112.60
1	A	212	VAL	CB-CA-C	10.49	126.69	112.22
1	B	115	LEU	CB-CA-C	10.47	128.13	110.86
1	A	411	GLY	CA-C-N	10.44	140.76	121.97
1	A	411	GLY	C-N-CA	10.44	140.76	121.97
1	A	137	THR	N-CA-CB	-10.44	94.70	110.04
1	B	452	GLU	CA-CB-CG	10.39	134.89	114.10
1	B	162	HIS	CA-CB-CG	-10.32	103.48	113.80
1	B	259	ARG	CD-NE-CZ	-10.23	110.08	124.40
1	B	175	ARG	NE-CZ-NH2	10.22	128.40	119.20
1	A	104	GLU	CB-CG-CD	-10.18	95.30	112.60
1	B	188	VAL	CA-C-O	-10.17	108.48	121.40
1	A	38	ARG	CD-NE-CZ	-10.16	110.17	124.40
1	B	391	THR	N-CA-C	10.15	122.11	111.14
1	A	269	VAL	CA-C-O	-10.11	110.44	120.95
1	B	175	ARG	NE-CZ-NH1	-10.04	111.46	121.50
1	A	58	VAL	N-CA-CB	-9.97	95.33	112.08
1	A	465	LEU	CA-C-N	9.92	140.85	121.41
1	A	465	LEU	C-N-CA	9.92	140.85	121.41
1	B	191	PRO	CA-C-N	9.90	138.25	122.21
1	B	191	PRO	C-N-CA	9.90	138.25	122.21
1	A	444	ARG	NE-CZ-NH1	-9.88	111.62	121.50
1	B	197	THR	N-CA-CB	-9.88	95.49	110.90
1	B	184	LEU	N-CA-CB	-9.87	94.12	111.40
1	A	237	GLU	CB-CA-C	-9.84	92.42	110.63
1	B	328	PRO	N-CA-C	-9.82	102.41	114.20
1	B	156	GLU	CA-C-N	9.78	133.74	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	156	GLU	C-N-CA	9.78	133.74	120.54
1	B	259	ARG	NE-CZ-NH1	-9.78	111.72	121.50
1	A	163	ARG	NE-CZ-NH2	-9.77	110.41	119.20
1	A	408	VAL	CA-CB-CG2	9.76	126.99	110.40
1	B	123	ILE	N-CA-C	9.73	120.91	111.67
1	A	386	GLU	N-CA-CB	9.69	125.22	110.30
1	A	245	ASP	N-CA-C	-9.62	101.05	113.17
1	B	166	PHE	O-C-N	9.61	135.50	123.10
1	A	113	LYS	CA-C-N	-9.60	109.19	122.82
1	A	113	LYS	C-N-CA	-9.60	109.19	122.82
1	A	368	VAL	CA-CB-CG2	9.56	126.65	110.40
1	B	463	ARG	N-CA-CB	-9.56	96.07	110.12
1	A	492	ASN	CB-CA-C	9.50	126.88	110.45
1	B	182	ASP	CA-CB-CG	-9.47	103.13	112.60
1	B	200	CYS	CA-C-O	-9.46	107.18	119.10
1	B	121	ASN	N-CA-C	-9.45	100.99	114.12
1	A	464	LEU	O-C-N	-9.43	110.14	122.39
1	B	155	ARG	NE-CZ-NH2	-9.42	110.72	119.20
1	A	353	ARG	CA-CB-CG	9.41	132.93	114.10
1	A	190	VAL	N-CA-CB	-9.38	98.08	111.21
1	B	256	ASN	CA-C-O	-9.36	111.36	121.56
1	B	126	TYR	CA-C-N	9.31	133.11	120.54
1	B	126	TYR	C-N-CA	9.31	133.11	120.54
1	A	175	ARG	CD-NE-CZ	9.31	137.43	124.40
1	A	104	GLU	N-CA-C	9.28	124.19	113.15
1	A	255	VAL	CA-C-O	9.26	131.59	121.04
1	B	226	MET	O-C-N	9.26	133.77	123.22
1	A	236	GLU	CB-CG-CD	9.24	128.31	112.60
1	A	155	ARG	NH1-CZ-NH2	-9.24	107.29	119.30
1	A	106	ILE	CB-CA-C	9.23	124.13	112.04
1	B	196	ALA	CA-C-O	9.23	131.57	121.05
1	B	139	GLN	CB-CG-CD	-9.23	96.91	112.60
1	B	186	SER	CA-CB-OG	9.20	129.51	111.10
1	A	109	LYS	CB-CA-C	9.20	128.34	110.67
1	B	233	CYS	O-C-N	9.17	133.48	122.84
1	B	326	ILE	CB-CA-C	9.16	123.43	111.53
1	A	361	ALA	O-C-N	-9.14	112.44	122.12
1	A	359	LYS	CA-C-O	-9.13	110.87	120.55
1	A	179	ILE	CA-C-N	9.10	135.23	120.94
1	A	179	ILE	C-N-CA	9.10	135.23	120.94
1	B	256	ASN	O-C-N	9.09	133.59	122.86
1	B	414	ARG	NE-CZ-NH2	9.07	127.37	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	465	LEU	CA-CB-CG	9.06	148.02	116.30
1	B	320	ARG	CD-NE-CZ	-9.06	111.71	124.40
1	B	272	LEU	O-C-N	9.06	134.28	122.42
1	A	384	PRO	O-C-N	-9.05	111.22	122.17
1	A	159	ASN	CA-C-O	-9.05	110.86	120.63
1	A	376	ARG	NH1-CZ-NH2	-9.04	107.54	119.30
1	B	397	GLN	CB-CG-CD	-9.04	97.23	112.60
1	B	267	LYS	CA-C-O	-9.04	111.33	120.82
1	B	414	ARG	CD-NE-CZ	-9.03	111.76	124.40
1	B	325	PHE	CA-CB-CG	9.01	122.81	113.80
1	B	391	THR	CA-C-O	-9.01	111.42	120.70
1	B	291	LYS	CA-C-O	-9.01	111.42	120.70
1	A	197	THR	OG1-CB-CG2	9.00	127.30	109.30
1	A	101	GLU	CA-C-N	8.96	136.59	122.26
1	A	101	GLU	C-N-CA	8.96	136.59	122.26
1	A	496	TYR	N-CA-CB	-8.96	96.31	110.19
1	B	149	ASN	OD1-CG-ND2	-8.96	113.64	122.60
1	A	472	GLU	CG-CD-OE2	-8.95	97.81	118.40
1	A	262	THR	O-C-N	8.95	131.75	122.09
1	A	487	THR	N-CA-CB	-8.94	97.21	111.43
1	A	73	LYS	N-CA-C	8.91	123.46	112.23
1	A	145	SER	N-CA-C	8.91	123.46	112.23
1	A	222	LYS	N-CA-CB	8.90	125.09	110.85
1	B	476	ASP	O-C-N	8.89	134.64	122.37
1	B	281	VAL	N-CA-CB	-8.88	100.80	112.26
1	A	152	VAL	CA-CB-CG1	8.87	125.47	110.40
1	A	244	SER	N-CA-CB	8.86	124.19	110.46
1	B	331	THR	N-CA-CB	-8.83	97.32	111.62
1	B	159	ASN	CA-C-O	-8.80	110.15	120.10
1	A	190	VAL	CA-CB-CG1	8.74	125.25	110.40
1	A	377	GLN	OE1-CD-NE2	-8.72	113.88	122.60
1	A	8	LYS	N-CA-C	8.68	129.29	110.80
1	A	297	PHE	CB-CA-C	-8.68	99.85	111.74
1	B	385	ILE	N-CA-CB	8.68	122.34	110.54
1	A	115	LEU	CB-CA-C	8.66	123.94	109.38
1	A	261	ILE	CA-C-N	8.65	132.20	120.44
1	A	261	ILE	C-N-CA	8.65	132.20	120.44
1	B	476	ASP	CA-CB-CG	-8.64	103.96	112.60
1	A	139	GLN	OE1-CD-NE2	8.63	131.23	122.60
1	B	477	LEU	N-CA-C	-8.63	102.75	113.28
1	A	429	VAL	CA-C-O	-8.62	110.58	120.67
1	A	58	VAL	CA-C-O	8.62	129.88	119.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	164	ILE	O-C-N	8.56	131.87	123.14
1	B	486	ARG	NE-CZ-NH1	8.56	130.06	121.50
1	A	486	ARG	CD-NE-CZ	8.55	136.37	124.40
1	B	429	VAL	CA-CB-CG1	8.54	124.92	110.40
1	A	102	THR	CA-C-O	-8.52	112.10	122.41
1	B	410	GLY	CA-C-N	8.52	137.29	120.77
1	B	410	GLY	C-N-CA	8.52	137.29	120.77
1	B	401	LYS	N-CA-C	8.51	120.56	111.28
1	B	135	THR	CA-CB-OG1	-8.47	96.89	109.60
1	A	409	ASP	CA-C-N	8.47	138.00	121.41
1	A	409	ASP	C-N-CA	8.47	138.00	121.41
1	A	277	LEU	O-C-N	8.46	133.08	123.27
1	A	467	VAL	CA-C-N	-8.45	109.10	122.29
1	A	467	VAL	C-N-CA	-8.45	109.10	122.29
1	B	399	ASN	O-C-N	8.44	133.82	122.59
1	B	274	VAL	N-CA-C	-8.43	97.92	109.55
1	B	500	TYR	CA-C-O	-8.38	111.36	120.92
1	A	243	PRO	CA-C-O	-8.38	105.35	120.60
1	B	405	GLU	CG-CD-OE1	8.36	137.62	118.40
1	A	92	LEU	N-CA-C	-8.35	101.09	113.61
1	B	326	ILE	CA-C-O	8.35	131.96	120.86
1	B	164	ILE	O-C-N	8.34	131.65	123.14
1	A	494	VAL	CA-C-O	8.33	129.70	120.46
1	B	291	LYS	O-C-N	8.32	131.07	122.09
1	A	399	ASN	CA-C-O	-8.31	111.90	121.54
1	B	226	MET	N-CA-CB	8.27	123.80	110.16
1	B	229	THR	CA-C-O	-8.27	109.86	119.61
1	A	164	ILE	CA-C-O	-8.26	111.31	120.72
1	A	259	ARG	NH1-CZ-NH2	-8.24	108.59	119.30
1	A	214	ARG	CA-C-O	-8.23	112.22	120.70
1	B	139	GLN	CG-CD-NE2	-8.23	104.06	116.40
1	A	359	LYS	O-C-N	8.22	130.83	122.12
1	B	151	GLU	CG-CD-OE1	8.21	137.28	118.40
1	B	348	ILE	CA-CB-CG2	8.20	124.44	110.50
1	A	365	VAL	CA-C-O	-8.19	110.54	120.78
1	A	388	LEU	CA-C-O	-8.19	112.23	120.82
1	A	444	ARG	CG-CD-NE	-8.18	94.00	112.00
1	B	373	HIS	CA-C-O	-8.18	110.75	120.57
1	B	353	ARG	NE-CZ-NH2	-8.18	111.84	119.20
1	A	381	SER	CA-C-N	8.18	135.85	120.97
1	A	381	SER	C-N-CA	8.18	135.85	120.97
1	A	491	PRO	CA-C-N	-8.16	108.56	122.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	491	PRO	C-N-CA	-8.16	108.56	122.67
1	B	225	GLN	CA-C-O	-8.15	111.58	120.30
1	B	408	VAL	CA-C-O	-8.14	112.19	120.90
1	A	130	TYR	O-C-N	-8.13	113.69	122.07
1	B	490	VAL	N-CA-CB	8.13	118.37	109.99
1	A	472	GLU	CB-CG-CD	-8.13	98.78	112.60
1	A	139	GLN	CB-CG-CD	-8.12	98.79	112.60
1	A	184	LEU	N-CA-CB	-8.11	99.70	111.70
1	B	260	LYS	N-CA-C	-8.08	102.05	112.23
1	B	190	VAL	CB-CA-C	8.06	118.60	109.89
1	A	335	ILE	N-CA-CB	8.04	119.96	110.55
1	B	276	ALA	O-C-N	8.03	131.32	123.29
1	A	282	ASP	CA-C-O	-8.02	110.23	119.78
1	B	197	THR	OG1-CB-CG2	8.01	125.32	109.30
1	B	441	CYS	CA-C-O	-8.01	110.23	119.60
1	B	108	ARG	CD-NE-CZ	8.00	135.60	124.40
1	B	355	GLU	CA-C-O	-8.00	111.06	120.10
1	A	479	ASP	CA-CB-CG	-7.98	104.62	112.60
1	A	37	THR	N-CA-C	7.98	119.61	111.07
1	A	290	GLU	N-CA-C	7.97	120.88	111.71
1	A	105	ASP	CA-CB-CG	-7.95	104.65	112.60
1	B	173	ASP	CA-CB-CG	-7.95	104.65	112.60
1	A	214	ARG	NE-CZ-NH2	-7.93	112.06	119.20
1	B	113	LYS	N-CA-C	7.91	122.79	108.17
1	A	117	PRO	O-C-N	7.90	130.78	121.46
1	A	256	ASN	OD1-CG-ND2	-7.90	114.70	122.60
1	A	363	ILE	CA-CB-CG2	7.89	123.91	110.50
1	B	354	THR	CA-CB-OG1	-7.89	97.77	109.60
1	A	355	GLU	CA-C-O	-7.88	112.12	120.63
1	B	266	VAL	CB-CA-C	7.88	122.06	111.97
1	B	486	ARG	N-CA-C	-7.88	95.89	108.73
1	A	484	LYS	N-CA-CB	7.85	121.40	110.56
1	A	349	LYS	CA-C-O	-7.85	111.96	120.36
1	A	170	ILE	CA-C-N	7.84	133.50	122.36
1	A	170	ILE	C-N-CA	7.84	133.50	122.36
1	B	404	LEU	CA-C-N	-7.84	111.91	122.72
1	B	404	LEU	C-N-CA	-7.84	111.91	122.72
1	B	164	ILE	CA-C-O	-7.82	111.81	120.72
1	A	128	PHE	CA-CB-CG	7.80	121.60	113.80
1	B	459	GLU	N-CA-CB	7.79	121.31	110.01
1	B	104	GLU	CB-CA-C	-7.78	94.46	109.95
1	B	252	GLN	CB-CG-CD	7.78	125.83	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	GLN	OE1-CD-NE2	7.78	130.38	122.60
1	A	277	LEU	CA-C-O	-7.76	111.99	120.30
1	B	454	LEU	CA-C-N	7.76	131.02	120.54
1	B	454	LEU	C-N-CA	7.76	131.02	120.54
1	B	199	LEU	N-CA-C	7.76	122.38	111.52
1	A	420	LYS	O-C-N	7.75	130.05	122.07
1	A	232	SER	N-CA-CB	-7.74	97.89	110.42
1	B	175	ARG	CD-NE-CZ	-7.74	113.57	124.40
1	A	405	GLU	CG-CD-OE1	7.73	136.18	118.40
1	B	159	ASN	O-C-N	7.72	131.25	122.22
1	A	357	VAL	CA-C-N	7.71	130.28	120.56
1	A	357	VAL	C-N-CA	7.71	130.28	120.56
1	B	397	GLN	CB-CA-C	-7.69	93.37	110.21
1	B	124	ASN	CB-CG-ND2	7.69	127.93	116.40
1	A	232	SER	CB-CA-C	-7.68	95.53	110.11
1	B	167	LYS	CG-CD-CE	7.67	128.94	111.30
1	A	170	ILE	CA-CB-CG2	7.66	123.53	110.50
1	B	439	ASN	CB-CG-ND2	7.66	127.89	116.40
1	A	115	LEU	N-CA-CB	7.66	121.45	110.88
1	A	110	GLU	CA-C-O	7.65	128.73	120.24
1	A	236	GLU	N-CA-CB	7.65	121.48	110.16
1	A	248	ILE	CA-CB-CG2	7.64	123.48	110.50
1	A	414	ARG	NH1-CZ-NH2	7.63	129.22	119.30
1	A	320	ARG	N-CA-C	-7.63	103.95	113.18
1	A	404	LEU	CA-C-O	-7.62	109.92	120.21
1	A	196	ALA	CA-C-O	7.62	129.61	120.92
1	A	29	ILE	CB-CA-C	-7.62	102.10	111.32
1	B	100	GLY	CA-C-N	7.62	136.09	121.54
1	B	100	GLY	C-N-CA	7.62	136.09	121.54
1	A	459	GLU	CA-C-N	7.60	131.36	120.79
1	A	459	GLU	C-N-CA	7.60	131.36	120.79
1	B	253	LEU	N-CA-CB	-7.60	98.04	110.42
1	B	286	LEU	CA-C-O	-7.60	112.03	120.69
1	B	412	VAL	CB-CA-C	7.58	119.42	111.23
1	A	365	VAL	CG1-CB-CG2	7.58	127.48	110.80
1	A	297	PHE	N-CA-C	-7.58	101.10	110.65
1	B	390	GLU	CA-C-N	7.58	130.74	120.44
1	B	390	GLU	C-N-CA	7.58	130.74	120.44
1	B	386	GLU	CA-C-O	7.57	128.45	120.42
1	A	127	ASP	CA-CB-CG	7.57	120.17	112.60
1	B	348	ILE	CA-C-N	7.56	132.51	122.30
1	B	348	ILE	C-N-CA	7.56	132.51	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	251	TYR	CB-CG-CD1	7.52	132.08	120.80
1	B	145	SER	N-CA-C	7.52	122.21	112.89
1	A	398	ARG	NE-CZ-NH1	7.50	129.00	121.50
1	A	353	ARG	NH1-CZ-NH2	-7.50	109.56	119.30
1	A	265	LEU	CD1-CG-CD2	7.49	127.28	110.80
1	B	103	LYS	N-CA-CB	-7.49	100.68	111.84
1	A	473	LEU	CA-C-O	-7.48	109.81	120.51
1	B	283	ALA	O-C-N	7.47	127.63	121.05
1	A	268	ASN	CB-CG-OD1	7.47	135.74	120.80
1	A	432	GLY	CA-C-N	7.46	132.01	120.97
1	A	432	GLY	C-N-CA	7.46	132.01	120.97
1	B	397	GLN	OE1-CD-NE2	7.46	130.06	122.60
1	B	152	VAL	CA-CB-CG1	7.45	123.07	110.40
1	A	8	LYS	N-CA-CB	-7.43	97.93	110.49
1	B	260	LYS	N-CA-CB	7.40	121.69	110.30
1	B	506	THR	CA-C-N	7.39	132.95	121.19
1	B	506	THR	C-N-CA	7.39	132.95	121.19
1	B	287	GLY	CA-C-N	7.39	133.13	122.85
1	B	287	GLY	C-N-CA	7.39	133.13	122.85
1	B	155	ARG	NE-CZ-NH1	7.39	128.89	121.50
1	A	389	ALA	O-C-N	7.38	129.94	122.12
1	A	495	LEU	CB-CA-C	7.37	124.27	110.63
1	A	15	GLU	N-CA-C	-7.34	103.28	111.28
1	B	159	ASN	CB-CG-ND2	7.34	127.41	116.40
1	B	348	ILE	O-C-N	-7.33	114.62	122.83
1	A	214	ARG	O-C-N	7.33	130.00	122.09
1	A	380	PHE	CA-CB-CG	-7.33	106.47	113.80
1	B	250	TRP	CA-CB-CG	7.31	127.50	113.60
1	A	29	ILE	N-CA-CB	7.29	120.97	112.15
1	B	125	LEU	N-CA-C	-7.29	103.04	112.23
1	B	402	ASP	N-CA-C	-7.28	104.37	113.18
1	A	420	LYS	CA-C-O	-7.28	113.17	120.82
1	A	444	ARG	CD-NE-CZ	-7.27	114.22	124.40
1	B	192	PHE	CA-CB-CG	7.25	121.05	113.80
1	A	112	LEU	O-C-N	7.24	131.38	122.34
1	A	368	VAL	N-CA-CB	-7.23	97.18	112.00
1	A	286	LEU	CA-C-N	7.21	126.95	120.10
1	A	286	LEU	C-N-CA	7.21	126.95	120.10
1	B	420	LYS	N-CA-CB	7.21	120.52	110.07
1	A	176	LYS	CA-CB-CG	7.20	128.51	114.10
1	B	290	GLU	N-CA-C	7.18	121.15	112.38
1	A	444	ARG	O-C-N	7.18	129.73	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	189	ASP	CA-CB-CG	7.18	119.78	112.60
1	B	269	VAL	CA-C-O	-7.17	113.03	120.71
1	A	160	ALA	CA-C-O	-7.17	110.81	119.49
1	B	228	SER	O-C-N	7.17	131.99	122.96
1	A	205	PRO	O-C-N	-7.16	112.60	122.27
1	A	278	PHE	CA-C-O	-7.15	113.10	120.54
1	A	135	THR	CA-CB-OG1	-7.15	98.88	109.60
1	A	328	PRO	CA-C-O	7.13	128.71	118.86
1	B	268	ASN	CA-C-O	-7.13	110.86	119.49
1	A	210	LYS	CB-CG-CD	-7.13	94.90	111.30
1	B	487	THR	N-CA-CB	-7.13	100.09	111.43
1	A	499	VAL	CA-CB-CG2	7.12	122.51	110.40
1	B	163	ARG	NH1-CZ-NH2	7.12	128.56	119.30
1	B	190	VAL	CA-C-O	-7.12	112.37	121.13
1	B	231	ALA	N-CA-CB	-7.12	99.08	109.83
1	B	479	ASP	CA-C-N	7.12	134.58	122.26
1	B	479	ASP	C-N-CA	7.12	134.58	122.26
1	B	285	SER	CA-C-O	-7.12	112.80	121.06
1	A	504	THR	CA-CB-CG2	7.10	122.57	110.50
1	A	204	ASN	OD1-CG-ND2	-7.10	115.50	122.60
1	A	381	SER	N-CA-C	-7.09	99.98	110.48
1	B	244	SER	CA-C-O	-7.07	113.33	121.68
1	B	251	TYR	CA-C-N	-7.07	113.37	122.77
1	B	251	TYR	C-N-CA	-7.07	113.37	122.77
1	B	414	ARG	NE-CZ-NH1	-7.06	114.44	121.50
1	B	478	LEU	CA-C-O	7.06	129.14	121.16
1	A	339	LYS	CA-CB-CG	7.05	128.20	114.10
1	A	444	ARG	CA-C-O	-7.05	113.02	120.63
1	A	175	ARG	N-CA-C	-7.05	102.66	112.45
1	A	380	PHE	CB-CA-C	7.05	124.44	110.42
1	B	292	ASP	CA-CB-CG	-7.04	105.56	112.60
1	B	379	ASP	CA-C-O	7.03	128.89	120.81
1	B	446	GLY	O-C-N	7.02	129.00	122.19
1	A	265	LEU	CA-C-O	-7.01	112.99	120.42
1	A	384	PRO	CA-C-N	7.01	130.06	120.46
1	A	384	PRO	C-N-CA	7.01	130.06	120.46
1	A	28	VAL	CA-C-O	-7.00	113.04	120.53
1	A	454	LEU	CB-CA-C	6.95	121.88	110.90
1	A	492	ASN	OD1-CG-ND2	6.93	129.53	122.60
1	A	429	VAL	CB-CA-C	6.93	120.94	110.62
1	A	144	TYR	O-C-N	6.92	129.57	122.09
1	A	461	SER	CA-CB-OG	-6.92	97.26	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	155	ARG	O-C-N	6.90	130.02	122.15
1	A	431	LEU	O-C-N	6.89	131.67	123.33
1	A	377	GLN	CG-CD-NE2	6.89	126.74	116.40
1	A	464	LEU	CA-C-O	6.89	127.82	119.49
1	A	297	PHE	O-C-N	6.88	133.13	122.67
1	A	218	GLN	CA-C-O	-6.88	111.67	119.79
1	A	490	VAL	O-C-N	6.88	128.57	121.14
1	A	329	SER	CB-CA-C	6.87	121.56	110.09
1	B	282	ASP	CA-C-N	-6.87	115.28	122.28
1	B	282	ASP	C-N-CA	-6.87	115.28	122.28
1	A	69	ASN	CA-C-O	-6.85	111.87	119.95
1	A	359	LYS	CB-CA-C	-6.84	99.43	110.79
1	A	490	VAL	N-CA-C	-6.84	102.66	109.02
1	A	292	ASP	CA-CB-CG	6.83	119.44	112.60
1	B	448	GLU	CB-CG-CD	6.83	124.22	112.60
1	B	229	THR	N-CA-C	-6.83	103.46	112.34
1	B	404	LEU	N-CA-CB	-6.82	98.93	111.13
1	A	14	ALA	N-CA-C	-6.81	105.60	114.04
1	B	390	GLU	CB-CA-C	-6.81	99.28	110.85
1	A	429	VAL	CA-CB-CG1	6.80	121.96	110.40
1	B	386	GLU	CG-CD-OE1	6.80	134.04	118.40
1	A	132	ALA	CA-C-N	6.80	130.07	120.28
1	A	132	ALA	C-N-CA	6.80	130.07	120.28
1	B	260	LYS	O-C-N	6.79	131.43	122.33
1	A	170	ILE	N-CA-CB	-6.79	99.07	112.24
1	A	58	VAL	CA-CB-CG2	6.78	121.93	110.40
1	A	162	HIS	CA-CB-CG	-6.75	107.05	113.80
1	A	292	ASP	N-CA-CB	-6.75	100.14	110.13
1	B	388	LEU	CD1-CG-CD2	6.75	125.64	110.80
1	B	172	VAL	CB-CA-C	6.74	120.66	110.62
1	B	368	VAL	CA-CB-CG1	6.73	121.85	110.40
1	A	26	TRP	N-CA-CB	6.73	122.59	111.08
1	A	342	THR	CA-C-O	-6.73	113.48	120.89
1	B	368	VAL	N-CA-CB	-6.73	100.32	111.36
1	B	237	GLU	N-CA-CB	6.73	120.58	110.22
1	B	422	LEU	O-C-N	-6.73	114.99	122.12
1	B	378	LEU	CA-C-N	6.72	130.37	120.95
1	B	378	LEU	C-N-CA	6.72	130.37	120.95
1	B	449	LYS	CA-C-O	-6.72	113.29	120.42
1	A	458	ILE	CB-CG1-CD1	6.72	127.92	113.80
1	A	170	ILE	O-C-N	-6.72	114.30	122.36
1	B	155	ARG	CA-CB-CG	-6.72	100.67	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	ILE	O-C-N	6.71	129.38	121.80
1	B	476	ASP	CA-C-O	-6.70	111.17	119.28
1	B	355	GLU	CA-CB-CG	6.70	127.50	114.10
1	B	507	GLU	N-CA-C	6.70	122.36	111.37
1	A	12	SER	CA-C-O	6.69	127.25	120.03
1	B	412	VAL	CA-C-O	-6.69	112.53	120.76
1	B	436	LEU	CA-C-O	-6.69	113.75	120.90
1	B	462	MET	CA-CB-CG	-6.68	100.73	114.10
1	A	68	PRO	CB-CA-C	-6.68	101.86	111.62
1	B	399	ASN	OD1-CG-ND2	6.67	129.27	122.60
1	B	438	ALA	N-CA-C	-6.67	103.94	111.14
1	A	372	ASN	CB-CA-C	6.66	121.63	110.44
1	B	387	VAL	N-CA-C	-6.66	104.00	110.72
1	B	508	PHE	N-CA-CB	6.65	121.72	110.49
1	A	293	MET	CA-C-N	6.64	129.84	120.28
1	A	293	MET	C-N-CA	6.64	129.84	120.28
1	A	358	ILE	O-C-N	6.63	128.41	121.91
1	A	163	ARG	CA-C-N	-6.63	114.55	123.10
1	A	163	ARG	C-N-CA	-6.63	114.55	123.10
1	B	168	PRO	CB-CA-C	-6.62	102.31	110.98
1	B	294	LYS	CB-CA-C	6.61	123.58	110.42
1	B	486	ARG	CA-CB-CG	6.60	127.30	114.10
1	B	362	GLU	O-C-N	-6.58	115.15	122.12
1	B	263	ASP	N-CA-C	-6.57	102.76	111.24
1	B	103	LYS	O-C-N	6.57	131.00	122.40
1	B	390	GLU	CG-CD-OE1	6.56	133.50	118.40
1	A	263	ASP	CA-CB-CG	-6.55	106.05	112.60
1	B	481	SER	CA-CB-OG	-6.55	98.00	111.10
1	A	227	ILE	CA-C-O	6.55	127.58	120.57
1	B	121	ASN	CA-CB-CG	-6.54	106.06	112.60
1	B	182	ASP	CB-CG-OD1	6.53	133.42	118.40
1	A	337	GLU	CA-CB-CG	-6.52	101.05	114.10
1	B	102	THR	CA-CB-OG1	-6.52	99.82	109.60
1	B	225	GLN	OE1-CD-NE2	-6.51	116.09	122.60
1	A	389	ALA	CA-C-O	-6.50	113.66	120.55
1	B	335	ILE	O-C-N	6.50	128.53	121.83
1	B	163	ARG	CG-CD-NE	-6.50	97.69	112.00
1	B	207	GLU	O-C-N	6.50	129.49	122.34
1	A	326	ILE	O-C-N	6.50	128.80	122.30
1	B	237	GLU	CA-CB-CG	6.50	127.09	114.10
1	A	255	VAL	N-CA-CB	6.49	118.30	110.31
1	A	491	PRO	N-CA-C	-6.49	99.11	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	GLU	CG-CD-OE1	6.48	133.31	118.40
1	A	439	ASN	OD1-CG-ND2	-6.48	116.12	122.60
1	B	277	LEU	CA-C-N	-6.48	114.41	122.84
1	B	277	LEU	C-N-CA	-6.48	114.41	122.84
1	B	500	TYR	CB-CA-C	-6.48	99.80	109.90
1	A	53	ASN	OD1-CG-ND2	-6.47	116.13	122.60
1	B	250	TRP	CA-C-N	-6.47	113.79	122.72
1	B	250	TRP	C-N-CA	-6.47	113.79	122.72
1	A	6	MET	N-CA-C	-6.47	97.02	110.80
1	A	197	THR	CA-CB-CG2	6.47	121.50	110.50
1	A	408	VAL	N-CA-CB	-6.47	99.33	111.62
1	A	320	ARG	CD-NE-CZ	-6.46	115.35	124.40
1	B	226	MET	CA-C-O	-6.46	113.24	120.54
1	A	192	PHE	N-CA-C	-6.45	99.60	109.41
1	B	137	THR	N-CA-C	-6.45	101.84	110.55
1	A	159	ASN	O-C-N	6.44	128.95	122.12
1	B	266	VAL	CA-CB-CG2	-6.44	99.45	110.40
1	B	446	GLY	CA-C-O	-6.43	113.85	120.66
1	A	282	ASP	O-C-N	6.42	130.25	122.35
1	A	236	GLU	CA-CB-CG	6.42	126.94	114.10
1	A	330	LEU	CA-C-N	6.42	133.61	122.82
1	A	330	LEU	C-N-CA	6.42	133.61	122.82
1	B	109	LYS	CA-C-O	-6.42	113.73	120.92
1	B	147	GLY	CA-C-N	6.42	130.68	121.50
1	B	147	GLY	C-N-CA	6.42	130.68	121.50
1	A	45	GLY	CA-C-O	-6.41	109.41	120.57
1	A	402	ASP	CB-CA-C	6.41	121.78	110.37
1	B	355	GLU	CG-CD-OE1	6.41	133.14	118.40
1	A	4	LEU	CB-CA-C	6.41	123.17	110.42
1	A	196	ALA	O-C-N	-6.41	115.01	122.95
1	A	199	LEU	N-CA-C	6.40	120.23	111.39
1	A	146	SER	CA-C-N	6.40	130.22	122.03
1	A	146	SER	C-N-CA	6.40	130.22	122.03
1	B	290	GLU	O-C-N	6.39	130.70	122.39
1	B	209	GLU	CG-CD-OE1	6.39	133.09	118.40
1	B	404	LEU	CA-C-O	-6.39	112.93	120.60
1	B	390	GLU	N-CA-C	-6.39	104.40	111.36
1	B	401	LYS	CA-C-O	-6.38	113.78	120.55
1	B	475	PRO	CA-C-N	-6.38	110.82	122.38
1	B	475	PRO	C-N-CA	-6.38	110.82	122.38
1	A	255	VAL	CB-CA-C	6.38	120.84	111.33
1	A	397	GLN	O-C-N	6.37	128.88	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	440	SER	O-C-N	-6.37	113.79	122.33
1	A	91	GLU	CA-C-N	6.37	132.22	122.29
1	A	91	GLU	C-N-CA	6.37	132.22	122.29
1	B	297	PHE	N-CA-C	-6.37	105.50	113.20
1	A	506	THR	N-CA-CB	6.37	120.54	110.23
1	A	462	MET	CA-CB-CG	-6.36	101.39	114.10
1	A	410	GLY	CA-C-N	6.34	131.81	120.77
1	A	410	GLY	C-N-CA	6.34	131.81	120.77
1	B	105	ASP	CA-CB-CG	-6.34	106.26	112.60
1	B	370	LEU	N-CA-C	-6.34	100.02	109.15
1	A	50	ILE	CB-CA-C	6.33	120.22	111.92
1	A	452	GLU	CB-CG-CD	6.33	123.36	112.60
1	A	449	LYS	CA-C-N	6.33	128.66	120.44
1	A	449	LYS	C-N-CA	6.33	128.66	120.44
1	B	398	ARG	CB-CA-C	6.32	119.63	109.27
1	A	68	PRO	CA-C-N	-6.31	112.63	122.67
1	A	68	PRO	C-N-CA	-6.31	112.63	122.67
1	B	460	MET	CA-C-O	-6.31	114.20	120.82
1	B	192	PHE	CA-C-O	6.30	128.52	121.40
1	B	290	GLU	CA-C-N	6.30	129.01	120.44
1	B	290	GLU	C-N-CA	6.30	129.01	120.44
1	A	193	TYR	O-C-N	6.30	130.43	123.25
1	B	459	GLU	CA-CB-CG	6.29	126.69	114.10
1	B	468	THR	O-C-N	6.28	129.08	122.23
1	B	460	MET	N-CA-C	-6.27	104.36	111.07
1	B	381	SER	N-CA-C	-6.27	101.20	110.48
1	A	370	LEU	N-CA-C	-6.27	98.95	108.67
1	A	365	VAL	CB-CA-C	6.26	121.56	111.29
1	B	446	GLY	N-CA-C	-6.26	104.76	112.77
1	B	391	THR	O-C-N	6.25	128.84	122.09
1	A	138	LYS	N-CA-CB	6.25	119.44	110.06
1	A	153	THR	O-C-N	6.25	128.50	122.07
1	A	154	HIS	O-C-N	-6.25	115.50	122.12
1	B	249	GLN	N-CA-CB	6.24	122.29	111.00
1	B	408	VAL	CA-CB-CG1	6.24	121.00	110.40
1	B	242	ALA	O-C-N	6.24	126.49	121.38
1	A	147	GLY	CA-C-O	-6.23	114.52	121.31
1	B	191	PRO	O-C-N	-6.23	114.23	122.64
1	A	270	GLU	CA-C-O	-6.22	113.95	120.55
1	B	402	ASP	N-CA-CB	6.22	120.86	110.41
1	A	155	ARG	CD-NE-CZ	-6.22	115.70	124.40
1	B	479	ASP	CA-CB-CG	-6.22	106.38	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	467	VAL	CB-CA-C	6.21	120.80	110.30
1	A	348	ILE	CB-CA-C	6.21	118.47	110.96
1	B	227	ILE	O-C-N	6.19	130.35	123.10
1	A	162	HIS	CB-CG-CD2	6.19	139.25	131.20
1	B	289	ARG	O-C-N	6.18	130.18	122.63
1	A	425	GLY	O-C-N	-6.18	115.37	122.42
1	B	354	THR	N-CA-C	6.18	118.02	111.28
1	A	94	CYS	N-CA-C	6.18	117.68	109.83
1	A	215	GLY	N-CA-C	-6.17	106.70	114.16
1	B	377	GLN	OE1-CD-NE2	6.17	128.77	122.60
1	A	156	GLU	CA-C-N	6.16	128.86	120.54
1	A	156	GLU	C-N-CA	6.16	128.86	120.54
1	B	160	ALA	N-CA-C	-6.16	105.02	112.54
1	A	273	GLY	CA-C-O	-6.15	111.69	119.19
1	B	230	LEU	CA-C-O	6.15	127.21	119.95
1	A	371	SER	CA-C-O	6.14	127.80	121.23
1	A	120	ASP	CB-CG-OD2	-6.14	104.27	118.40
1	B	352	GLN	O-C-N	6.13	130.32	122.04
1	B	225	GLN	CA-C-N	6.13	130.83	122.19
1	B	225	GLN	C-N-CA	6.13	130.83	122.19
1	B	320	ARG	O-C-N	6.13	130.58	122.43
1	A	186	SER	CA-C-N	6.12	130.26	121.50
1	A	186	SER	C-N-CA	6.12	130.26	121.50
1	A	38	ARG	NE-CZ-NH1	-6.12	115.38	121.50
1	A	28	VAL	O-C-N	6.12	130.26	123.10
1	B	162	HIS	N-CA-CB	6.12	121.09	110.39
1	A	293	MET	CA-C-O	6.12	127.44	120.90
1	A	199	LEU	N-CA-CB	-6.11	102.66	111.70
1	B	262	THR	N-CA-C	-6.11	105.79	113.18
1	B	271	LYS	N-CA-C	-6.11	105.68	113.01
1	A	374	GLY	N-CA-C	-6.11	105.50	114.90
1	B	138	LYS	CA-CB-CG	-6.10	101.90	114.10
1	A	47	GLN	CB-CG-CD	-6.09	102.24	112.60
1	A	436	LEU	N-CA-CB	6.09	118.85	110.01
1	A	197	THR	N-CA-CB	-6.09	100.10	111.13
1	A	413	ARG	CB-CG-CD	6.09	125.31	111.30
1	A	365	VAL	N-CA-CB	-6.09	101.18	111.23
1	A	73	LYS	N-CA-CB	-6.08	100.94	110.30
1	A	343	LYS	CA-CB-CG	-6.08	101.94	114.10
1	A	399	ASN	CA-CB-CG	6.08	118.68	112.60
1	B	152	VAL	N-CA-CB	6.05	119.23	110.52
1	A	372	ASN	OD1-CG-ND2	6.04	128.64	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	173	ASP	CB-CG-OD1	6.04	132.30	118.40
1	A	410	GLY	O-C-N	6.04	130.56	122.70
1	B	388	LEU	CB-CA-C	-6.04	100.41	110.68
1	A	371	SER	O-C-N	-6.04	116.96	123.42
1	A	212	VAL	CA-CB-CG2	6.03	120.65	110.40
1	B	408	VAL	N-CA-CB	-6.03	101.48	111.36
1	A	405	GLU	CG-CD-OE2	-6.02	104.55	118.40
1	A	75	ILE	CB-CA-C	6.02	119.54	110.63
1	B	447	VAL	CA-C-O	-6.02	114.47	120.85
1	B	124	ASN	CA-CB-CG	6.02	118.62	112.60
1	B	326	ILE	O-C-N	-6.02	114.20	122.62
1	B	169	LYS	CB-CA-C	-6.01	99.38	109.48
1	B	224	PRO	CB-CA-C	6.01	118.92	111.23
1	A	53	ASN	CA-C-N	6.00	133.00	121.54
1	A	53	ASN	C-N-CA	6.00	133.00	121.54
1	B	259	ARG	NH1-CZ-NH2	-6.00	111.50	119.30
1	A	465	LEU	CB-CA-C	6.00	120.09	109.65
1	A	339	LYS	N-CA-CB	-6.00	100.13	110.32
1	A	507	GLU	CA-C-O	-5.99	114.07	120.42
1	B	115	LEU	N-CA-CB	-5.98	101.27	110.07
1	B	159	ASN	CA-CB-CG	-5.98	106.62	112.60
1	B	266	VAL	N-CA-CB	-5.97	103.57	110.55
1	B	117	PRO	N-CA-C	-5.97	103.42	110.70
1	A	291	LYS	CB-CA-C	-5.97	99.22	110.67
1	B	357	VAL	N-CA-C	-5.96	104.70	110.72
1	B	449	LYS	O-C-N	5.96	128.94	122.15
1	B	283	ALA	CA-C-O	-5.95	115.36	121.07
1	A	507	GLU	CB-CA-C	-5.95	100.74	110.85
1	B	206	LEU	CA-C-O	-5.95	112.78	119.79
1	A	372	ASN	N-CA-C	-5.94	104.16	113.02
1	B	122	ILE	O-C-N	5.94	129.48	122.83
1	B	353	ARG	NE-CZ-NH1	5.93	127.43	121.50
1	A	188	VAL	CA-C-O	-5.93	114.40	121.28
1	B	102	THR	CA-C-N	-5.93	113.59	122.07
1	B	102	THR	C-N-CA	-5.93	113.59	122.07
1	B	174	VAL	O-C-N	5.93	129.98	122.57
1	B	153	THR	CA-CB-OG1	-5.92	100.71	109.60
1	B	369	VAL	N-CA-CB	5.92	118.92	111.46
1	B	509	GLU	N-CA-C	5.91	123.39	110.80
1	B	111	GLN	N-CA-C	-5.91	104.02	111.11
1	B	421	ALA	CA-C-O	-5.90	114.30	120.55
1	A	215	GLY	O-C-N	-5.89	116.02	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	337	GLU	N-CA-CB	5.89	119.30	110.22
1	B	437	TYR	N-CA-C	5.89	117.70	111.28
1	B	470	ILE	O-C-N	-5.89	116.12	121.89
1	B	219	GLY	CA-C-N	5.89	129.96	120.30
1	B	219	GLY	C-N-CA	5.89	129.96	120.30
1	A	271	LYS	CA-C-O	-5.88	114.18	120.42
1	B	253	LEU	CB-CA-C	-5.88	100.66	110.19
1	B	394	ILE	CA-C-N	5.88	128.08	120.44
1	B	394	ILE	C-N-CA	5.88	128.08	120.44
1	B	288	GLN	CA-C-N	5.87	131.46	122.77
1	B	288	GLN	C-N-CA	5.87	131.46	122.77
1	A	377	GLN	CA-C-N	5.87	130.23	121.72
1	A	377	GLN	C-N-CA	5.87	130.23	121.72
1	A	141	TRP	O-C-N	5.87	128.84	122.15
1	A	169	LYS	N-CA-CB	5.87	119.99	110.43
1	A	380	PHE	N-CA-CB	5.86	120.40	110.49
1	A	508	PHE	N-CA-CB	5.86	120.40	110.49
1	B	191	PRO	N-CA-CB	-5.86	97.09	103.25
1	A	149	ASN	OD1-CG-ND2	-5.86	116.74	122.60
1	A	159	ASN	OD1-CG-ND2	-5.86	116.74	122.60
1	B	124	ASN	CA-C-N	5.86	130.64	120.68
1	B	124	ASN	C-N-CA	5.86	130.64	120.68
1	B	291	LYS	N-CA-C	-5.84	104.83	111.14
1	A	240	GLU	CB-CG-CD	5.84	122.53	112.60
1	B	282	ASP	OD1-CG-OD2	-5.84	108.88	122.90
1	B	354	THR	CA-C-N	5.84	128.69	120.28
1	B	354	THR	C-N-CA	5.84	128.69	120.28
1	A	80	LYS	CB-CG-CD	5.83	124.72	111.30
1	A	75	ILE	CA-C-N	-5.83	111.82	120.68
1	A	75	ILE	C-N-CA	-5.83	111.82	120.68
1	A	236	GLU	CB-CA-C	-5.83	100.94	110.85
1	B	270	GLU	CB-CA-C	-5.83	99.48	110.67
1	B	383	ALA	CA-C-N	5.83	126.23	119.47
1	B	383	ALA	C-N-CA	5.83	126.23	119.47
1	A	445	ASN	CA-C-N	5.81	126.40	120.00
1	A	445	ASN	C-N-CA	5.81	126.40	120.00
1	B	325	PHE	CA-C-N	-5.81	114.96	123.10
1	B	325	PHE	C-N-CA	-5.81	114.96	123.10
1	A	424	LEU	CA-C-N	-5.81	113.45	122.69
1	A	424	LEU	C-N-CA	-5.81	113.45	122.69
1	A	317	GLY	O-C-N	-5.81	113.71	123.00
1	A	166	PHE	N-CA-CB	-5.80	101.91	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	223	VAL	O-C-N	5.80	127.72	121.10
1	A	38	ARG	NE-CZ-NH2	5.80	124.42	119.20
1	B	131	LEU	CA-C-O	-5.79	114.73	120.70
1	A	257	SER	CB-CA-C	-5.79	99.56	110.67
1	A	297	PHE	CA-C-O	-5.79	113.11	122.20
1	B	123	ILE	CA-C-O	-5.79	114.61	120.69
1	B	237	GLU	CG-CD-OE1	5.79	131.72	118.40
1	A	155	ARG	NE-CZ-NH1	-5.79	115.71	121.50
1	A	142	ALA	CB-CA-C	-5.78	101.02	110.85
1	A	151	GLU	CG-CD-OE2	5.78	131.69	118.40
1	B	226	MET	CG-SD-CE	-5.78	88.18	100.90
1	A	398	ARG	CB-CG-CD	5.78	124.59	111.30
1	B	282	ASP	N-CA-CB	-5.78	102.13	110.56
1	A	331	THR	CA-C-N	5.77	128.02	120.28
1	A	331	THR	C-N-CA	5.77	128.02	120.28
1	A	459	GLU	N-CA-CB	5.77	118.37	110.01
1	B	318	ALA	CA-C-O	5.76	126.59	119.79
1	A	506	THR	CA-C-N	5.76	128.47	120.29
1	A	506	THR	C-N-CA	5.76	128.47	120.29
1	A	266	VAL	CA-CB-CG1	5.76	120.19	110.40
1	A	379	ASP	O-C-N	-5.76	116.22	123.01
1	A	75	ILE	O-C-N	5.76	129.48	123.26
1	A	271	LYS	CB-CA-C	-5.76	101.06	110.85
1	B	448	GLU	N-CA-C	-5.76	105.75	112.89
1	B	174	VAL	CA-C-O	-5.75	113.59	120.78
1	B	200	CYS	O-C-N	5.75	130.08	122.43
1	A	319	SER	CA-CB-OG	-5.75	99.60	111.10
1	B	233	CYS	N-CA-C	-5.75	101.95	110.46
1	A	270	GLU	O-C-N	5.74	128.21	122.12
1	A	397	GLN	CB-CG-CD	-5.74	102.84	112.60
1	B	190	VAL	N-CA-CB	-5.74	105.56	111.87
1	B	390	GLU	CB-CG-CD	5.74	122.36	112.60
1	A	66	HIS	CB-CG-CD2	-5.74	123.74	131.20
1	A	397	GLN	CA-C-O	-5.74	114.47	120.55
1	B	176	LYS	CA-C-N	-5.74	113.57	122.69
1	B	176	LYS	C-N-CA	-5.74	113.57	122.69
1	B	490	VAL	N-CA-C	-5.73	103.69	109.02
1	A	446	GLY	N-CA-C	-5.73	105.44	112.77
1	A	352	GLN	N-CA-C	5.73	120.09	112.30
1	A	365	VAL	CA-CB-CG1	5.73	120.14	110.40
1	A	427	LYS	N-CA-CB	-5.73	101.48	110.30
1	B	443	GLY	CA-C-N	5.73	128.74	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	443	GLY	C-N-CA	5.73	128.74	120.38
1	B	493	ASP	N-CA-C	5.73	117.40	109.15
1	B	157	ASN	OD1-CG-ND2	-5.73	116.87	122.60
1	A	465	LEU	N-CA-CB	-5.71	102.03	110.53
1	B	245	ASP	CA-CB-CG	5.71	118.31	112.60
1	B	136	LEU	CA-C-O	5.70	128.49	121.99
1	B	385	ILE	N-CA-C	-5.70	104.80	110.62
1	A	249	GLN	N-CA-CB	5.70	120.66	110.80
1	A	137	THR	CA-C-O	-5.70	115.51	121.55
1	A	285	SER	CA-C-O	-5.70	114.11	120.66
1	B	318	ALA	CA-C-N	5.70	128.70	120.38
1	B	318	ALA	C-N-CA	5.70	128.70	120.38
1	A	51	LYS	CA-CB-CG	5.70	125.50	114.10
1	A	274	VAL	N-CA-C	-5.70	103.77	110.21
1	A	237	GLU	CG-CD-OE1	5.69	131.50	118.40
1	A	174	VAL	O-C-N	-5.69	115.46	122.57
1	A	259	ARG	NE-CZ-NH1	5.69	127.19	121.50
1	A	494	VAL	N-CA-C	-5.69	105.55	111.58
1	A	505	LEU	CA-C-O	-5.69	114.50	121.67
1	A	104	GLU	CA-CB-CG	5.68	125.47	114.10
1	A	451	ILE	CA-C-N	5.68	128.36	120.29
1	A	451	ILE	C-N-CA	5.68	128.36	120.29
1	B	396	GLU	CB-CG-CD	5.68	122.26	112.60
1	B	147	GLY	N-CA-C	-5.67	99.73	113.18
1	B	500	TYR	N-CA-C	5.67	118.55	110.10
1	A	63	GLU	O-C-N	5.67	127.84	121.32
1	B	155	ARG	CA-C-O	-5.67	114.41	120.42
1	B	422	LEU	CA-C-N	5.67	128.44	120.28
1	B	422	LEU	C-N-CA	5.67	128.44	120.28
1	B	450	ALA	N-CA-C	-5.66	105.11	111.28
1	B	412	VAL	O-C-N	5.66	128.85	122.68
1	B	349	LYS	CB-CG-CD	5.65	124.30	111.30
1	B	439	ASN	OD1-CG-ND2	-5.65	116.95	122.60
1	B	476	ASP	CB-CG-OD1	-5.65	105.41	118.40
1	B	494	VAL	CB-CA-C	5.64	120.54	111.29
1	A	475	PRO	N-CA-CB	5.63	109.61	103.30
1	B	408	VAL	O-C-N	5.63	129.62	123.09
1	A	379	ASP	CA-C-N	5.63	132.30	121.54
1	A	379	ASP	C-N-CA	5.63	132.30	121.54
1	B	112	LEU	CA-CB-CG	5.63	136.01	116.30
1	B	478	LEU	O-C-N	-5.63	116.06	123.16
1	B	220	VAL	N-CA-CB	-5.63	100.58	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	346	ILE	N-CA-C	5.62	116.40	108.36
1	B	353	ARG	O-C-N	5.62	129.44	123.42
1	A	369	VAL	CB-CA-C	5.62	119.00	111.19
1	B	167	LYS	CA-CB-CG	-5.62	102.86	114.10
1	B	486	ARG	CB-CG-CD	-5.62	98.37	111.30
1	B	137	THR	CA-C-N	5.62	128.12	120.54
1	B	137	THR	C-N-CA	5.62	128.12	120.54
1	A	291	LYS	O-C-N	5.62	129.18	122.27
1	B	240	GLU	CB-CA-C	5.61	120.10	110.79
1	B	272	LEU	CA-C-O	-5.61	112.75	119.15
1	B	396	GLU	CG-CD-OE1	5.61	131.30	118.40
1	A	445	ASN	CA-C-O	-5.61	113.17	119.79
1	A	227	ILE	O-C-N	-5.60	116.81	123.03
1	B	444	ARG	NE-CZ-NH1	-5.60	115.90	121.50
1	A	21	LYS	N-CA-CB	-5.59	103.37	111.25
1	A	166	PHE	CB-CA-C	-5.58	99.66	109.71
1	B	140	ALA	N-CA-CB	5.58	118.07	109.98
1	A	118	PRO	N-CA-C	-5.58	102.34	111.21
1	A	139	GLN	CB-CA-C	5.57	121.64	109.99
1	A	479	ASP	CB-CG-OD2	-5.57	105.59	118.40
1	A	294	LYS	N-CA-CB	-5.57	101.64	110.22
1	A	187	HIS	CA-C-O	-5.56	114.35	120.69
1	B	405	GLU	CG-CD-OE2	-5.56	105.61	118.40
1	A	207	GLU	O-C-N	5.56	127.82	121.93
1	A	322	LEU	CA-C-N	5.56	131.72	121.94
1	A	322	LEU	C-N-CA	5.56	131.72	121.94
1	A	74	TYR	CA-C-N	-5.55	115.87	123.14
1	A	74	TYR	C-N-CA	-5.55	115.87	123.14
1	B	337	GLU	N-CA-C	-5.55	105.33	111.71
1	B	364	GLY	N-CA-C	5.55	123.75	113.76
1	A	48	ASP	CA-C-O	-5.55	114.98	120.70
1	B	386	GLU	CG-CD-OE2	-5.55	105.64	118.40
1	B	433	ARG	N-CA-C	5.55	120.46	113.25
1	A	205	PRO	CB-CA-C	5.54	120.20	112.11
1	A	400	LEU	CB-CA-C	5.54	119.54	110.17
1	B	270	GLU	N-CA-CB	5.54	118.87	110.28
1	A	24	ASP	O-C-N	-5.54	115.22	122.59
1	A	507	GLU	CA-CB-CG	5.53	125.15	114.10
1	A	331	THR	N-CA-CB	-5.52	102.65	111.43
1	A	137	THR	OG1-CB-CG2	5.52	120.34	109.30
1	A	270	GLU	N-CA-CB	5.52	118.24	110.12
1	B	219	GLY	N-CA-C	-5.52	105.19	112.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	325	PHE	CA-C-N	-5.52	117.72	122.96
1	A	325	PHE	C-N-CA	-5.52	117.72	122.96
1	B	101	GLU	N-CA-CB	-5.51	101.17	110.49
1	B	123	ILE	CA-C-N	5.51	133.68	123.32
1	B	123	ILE	C-N-CA	5.51	133.68	123.32
1	B	120	ASP	CA-CB-CG	-5.51	107.09	112.60
1	A	169	LYS	CA-C-N	5.51	130.00	122.34
1	A	169	LYS	C-N-CA	5.51	130.00	122.34
1	B	292	ASP	CB-CG-OD1	-5.51	105.73	118.40
1	A	492	ASN	CA-C-N	5.50	132.06	121.54
1	A	492	ASN	C-N-CA	5.50	132.06	121.54
1	B	447	VAL	N-CA-C	5.50	116.28	110.72
1	A	381	SER	O-C-N	-5.50	116.75	122.96
1	B	135	THR	N-CA-C	5.50	120.14	113.38
1	A	91	GLU	CA-C-O	5.50	128.37	120.51
1	A	255	VAL	CA-CB-CG1	5.50	119.74	110.40
1	B	104	GLU	CA-C-N	5.49	127.64	120.28
1	B	104	GLU	C-N-CA	5.49	127.64	120.28
1	B	372	ASN	OD1-CG-ND2	5.49	128.09	122.60
1	A	114	SER	CB-CA-C	-5.49	103.44	112.06
1	A	318	ALA	N-CA-C	-5.49	99.11	110.80
1	A	169	LYS	CA-CB-CG	-5.48	103.14	114.10
1	A	66	HIS	CA-C-N	5.48	128.27	120.49
1	A	66	HIS	C-N-CA	5.48	128.27	120.49
1	B	372	ASN	N-CA-C	-5.47	104.27	112.54
1	A	57	ASP	CA-CB-CG	-5.47	107.13	112.60
1	A	163	ARG	CG-CD-NE	-5.47	99.97	112.00
1	B	455	ARG	CA-C-O	-5.47	115.05	120.90
1	A	32	TYR	N-CA-C	5.45	118.59	110.52
1	B	263	ASP	CB-CA-C	5.45	119.85	110.86
1	B	390	GLU	OE1-CD-OE2	-5.45	109.83	122.90
1	A	500	TYR	N-CA-C	5.45	118.98	110.32
1	B	131	LEU	CA-C-N	5.45	127.84	120.38
1	B	131	LEU	C-N-CA	5.45	127.84	120.38
1	B	228	SER	CB-CA-C	-5.44	102.09	110.26
1	A	104	GLU	CG-CD-OE2	-5.44	105.88	118.40
1	A	140	ALA	N-CA-C	-5.44	105.37	112.23
1	A	226	MET	N-CA-CB	5.44	119.29	110.42
1	B	218	GLN	N-CA-C	5.44	119.92	113.28
1	A	451	ILE	CB-CA-C	-5.44	104.80	112.14
1	A	176	LYS	CA-C-O	-5.43	114.46	120.38
1	B	255	VAL	CB-CA-C	5.43	119.42	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	205	PRO	CA-CB-CG	-5.43	94.19	104.50
1	B	165	PHE	CA-CB-CG	-5.43	108.37	113.80
1	B	380	PHE	CA-CB-CG	-5.43	108.37	113.80
1	B	373	HIS	CA-CB-CG	5.42	119.22	113.80
1	A	180	SER	CA-C-O	-5.42	115.65	121.56
1	A	503	PRO	CB-CA-C	5.41	120.49	111.56
1	B	121	ASN	CA-C-N	-5.41	114.22	121.80
1	B	121	ASN	C-N-CA	-5.41	114.22	121.80
1	B	491	PRO	N-CA-C	-5.41	101.33	112.47
1	A	457	GLU	N-CA-CB	5.41	118.07	110.12
1	B	253	LEU	CA-C-O	-5.41	114.57	120.36
1	A	405	GLU	CA-C-N	5.41	130.46	123.11
1	A	405	GLU	C-N-CA	5.41	130.46	123.11
1	B	265	LEU	CB-CA-C	5.41	119.28	110.96
1	A	428	GLY	CA-C-N	-5.40	115.60	123.06
1	A	428	GLY	C-N-CA	-5.40	115.60	123.06
1	B	449	LYS	CA-C-N	5.40	127.52	120.28
1	B	449	LYS	C-N-CA	5.40	127.52	120.28
1	B	458	ILE	O-C-N	5.40	127.52	121.90
1	A	69	ASN	CA-CB-CG	-5.40	107.20	112.60
1	A	476	ASP	CA-C-O	-5.39	112.96	119.49
1	A	163	ARG	NH1-CZ-NH2	5.39	126.30	119.30
1	A	258	ASP	CA-CB-CG	5.39	117.99	112.60
1	B	194	VAL	CB-CA-C	5.39	117.48	110.96
1	B	149	ASN	N-CA-CB	-5.38	101.39	110.49
1	A	387	VAL	CB-CA-C	5.38	119.41	112.14
1	A	333	LYS	O-C-N	-5.38	116.42	122.12
1	A	113	LYS	O-C-N	5.38	129.75	122.59
1	A	412	VAL	CA-C-N	-5.38	113.75	121.98
1	A	412	VAL	C-N-CA	-5.38	113.75	121.98
1	A	42	ASN	CA-CB-CG	-5.38	107.22	112.60
1	A	169	LYS	O-C-N	5.38	129.34	123.27
1	B	397	GLN	CG-CD-OE1	-5.38	110.05	120.80
1	B	400	LEU	CA-C-O	-5.37	112.78	119.18
1	A	96	PRO	CB-CA-C	5.37	118.01	110.60
1	A	112	LEU	N-CA-C	-5.37	106.40	113.17
1	B	172	VAL	N-CA-C	-5.37	100.75	108.48
1	B	250	TRP	CA-C-O	-5.37	114.83	121.11
1	B	331	THR	CA-CB-CG2	5.37	119.62	110.50
1	B	248	ILE	CA-CB-CG2	5.36	119.62	110.50
1	A	387	VAL	N-CA-C	-5.34	105.17	110.62
1	A	277	LEU	CB-CA-C	-5.34	101.29	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	112	LEU	O-C-N	5.34	130.30	122.39
1	B	237	GLU	CG-CD-OE2	-5.34	106.11	118.40
1	A	248	ILE	CB-CA-C	5.34	118.51	110.98
1	A	447	VAL	CA-C-N	5.34	127.38	120.44
1	A	447	VAL	C-N-CA	5.34	127.38	120.44
1	B	251	TYR	N-CA-CB	5.34	119.13	110.43
1	B	437	TYR	CA-C-N	5.33	127.69	120.44
1	B	437	TYR	C-N-CA	5.33	127.69	120.44
1	B	398	ARG	N-CA-C	-5.33	106.66	114.39
1	A	253	LEU	CA-C-O	5.33	126.24	120.43
1	B	292	ASP	CB-CG-OD2	5.33	130.66	118.40
1	B	433	ARG	NE-CZ-NH2	5.33	123.99	119.20
1	A	487	THR	N-CA-C	5.32	117.50	109.41
1	B	250	TRP	CB-CA-C	5.32	120.50	109.38
1	A	444	ARG	N-CA-C	5.32	117.77	111.33
1	B	403	LYS	N-CA-C	5.32	119.48	112.89
1	B	355	GLU	O-C-N	5.31	128.44	122.22
1	B	124	ASN	CA-C-O	-5.31	115.17	121.60
1	A	384	PRO	N-CA-CB	-5.30	97.36	103.30
1	A	459	GLU	O-C-N	5.30	127.53	122.07
1	B	386	GLU	N-CA-CB	-5.30	102.31	110.16
1	B	439	ASN	CA-C-O	-5.30	114.26	120.20
1	B	472	GLU	N-CA-CB	-5.30	102.14	110.46
1	B	221	THR	CA-C-O	5.29	126.20	120.43
1	A	176	LYS	O-C-N	5.29	129.53	123.29
1	A	267	LYS	CA-C-N	5.29	127.63	120.65
1	A	267	LYS	C-N-CA	5.29	127.63	120.65
1	A	72	ASP	CA-CB-CG	-5.28	107.32	112.60
1	A	390	GLU	CA-CB-CG	5.28	124.67	114.10
1	B	154	HIS	CA-C-O	5.28	126.37	120.82
1	B	369	VAL	CA-C-N	5.27	129.89	121.66
1	B	369	VAL	C-N-CA	5.27	129.89	121.66
1	A	7	ASN	O-C-N	5.27	129.60	122.59
1	B	500	TYR	CA-CB-CG	-5.27	104.41	113.90
1	A	146	SER	O-C-N	-5.26	115.23	122.23
1	B	146	SER	CA-CB-OG	-5.26	100.58	111.10
1	A	262	THR	CA-CB-CG2	5.26	119.44	110.50
1	A	380	PHE	CA-C-N	-5.25	112.67	121.39
1	A	380	PHE	C-N-CA	-5.25	112.67	121.39
1	A	284	PRO	N-CA-C	-5.25	106.56	113.65
1	B	126	TYR	O-C-N	-5.25	115.81	122.27
1	B	264	ASP	CA-C-N	5.25	127.58	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	264	ASP	C-N-CA	5.25	127.58	120.65
1	A	139	GLN	N-CA-CB	-5.24	101.86	110.40
1	A	334	ASP	N-CA-C	-5.23	105.66	111.36
1	B	129	GLU	CB-CG-CD	-5.23	103.72	112.60
1	B	173	ASP	CA-C-O	-5.22	114.40	120.62
1	A	294	LYS	O-C-N	5.22	128.33	122.22
1	B	482	THR	CA-C-N	5.22	127.28	120.28
1	B	482	THR	C-N-CA	5.22	127.28	120.28
1	A	24	ASP	OD1-CG-OD2	5.22	135.42	122.90
1	B	374	GLY	CA-C-O	5.22	126.36	119.58
1	A	481	SER	CB-CA-C	5.21	121.31	110.32
1	B	103	LYS	N-CA-C	-5.21	104.45	111.54
1	A	342	THR	CA-CB-CG2	5.21	119.36	110.50
1	B	163	ARG	CB-CG-CD	-5.21	99.32	111.30
1	A	107	ALA	CA-C-O	-5.21	115.33	120.90
1	A	490	VAL	CA-CB-CG1	5.20	119.24	110.40
1	B	167	LYS	N-CA-CB	-5.20	103.57	111.21
1	A	401	LYS	N-CA-C	5.20	117.34	111.11
1	B	151	GLU	CG-CD-OE2	-5.20	106.45	118.40
1	B	253	LEU	CA-C-N	-5.20	115.86	122.77
1	B	253	LEU	C-N-CA	-5.20	115.86	122.77
1	B	391	THR	N-CA-CB	5.20	117.60	110.07
1	A	259	ARG	NE-CZ-NH2	5.19	123.87	119.20
1	B	143	TYR	O-C-N	5.19	127.41	122.07
1	B	362	GLU	CA-C-N	5.19	129.65	122.28
1	B	362	GLU	C-N-CA	5.19	129.65	122.28
1	B	256	ASN	CB-CA-C	-5.18	100.00	109.54
1	A	420	LYS	N-CA-CB	5.18	117.52	110.01
1	A	153	THR	CA-CB-OG1	-5.18	101.83	109.60
1	B	102	THR	CB-CA-C	5.18	119.78	111.91
1	B	157	ASN	CA-C-O	5.18	126.44	120.90
1	B	473	LEU	CB-CA-C	5.17	120.72	110.42
1	A	437	TYR	CA-C-O	-5.17	114.50	120.24
1	B	348	ILE	CB-CG1-CD1	-5.17	102.95	113.80
1	A	424	LEU	CA-C-O	-5.17	112.35	119.12
1	B	436	LEU	N-CA-C	-5.17	104.91	111.11
1	A	136	LEU	O-C-N	5.16	128.68	122.79
1	A	338	LEU	CA-C-O	5.16	126.02	120.55
1	B	459	GLU	CB-CA-C	-5.16	102.78	110.88
1	B	139	GLN	CB-CA-C	5.16	120.17	110.63
1	B	346	ILE	CB-CG1-CD1	-5.16	102.97	113.80
1	A	165	PHE	CB-CG-CD2	5.15	129.46	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	287	GLY	O-C-N	5.15	129.25	122.91
1	A	163	ARG	N-CA-C	-5.15	106.68	113.17
1	A	225	GLN	CA-C-O	-5.15	114.80	120.36
1	A	246	LYS	CB-CG-CD	5.15	123.15	111.30
1	A	208	GLY	O-C-N	5.15	129.39	122.70
1	A	372	ASN	CA-CB-CG	5.15	117.75	112.60
1	A	93	VAL	CA-CB-CG1	5.14	119.13	110.40
1	B	232	SER	CB-CA-C	-5.13	100.81	110.67
1	B	187	HIS	CG-CD2-NE2	-5.13	102.07	107.20
1	A	324	LYS	CA-CB-CG	-5.13	103.84	114.10
1	A	391	THR	N-CA-C	5.13	116.68	111.14
1	B	166	PHE	CA-CB-CG	5.13	118.93	113.80
1	B	261	ILE	CB-CA-C	-5.12	105.23	112.14
1	A	15	GLU	CG-CD-OE1	5.12	130.17	118.40
1	B	417	ASP	N-CA-C	-5.12	105.78	111.36
1	A	38	ARG	N-CA-CB	-5.12	101.90	110.39
1	B	325	PHE	N-CA-CB	5.11	118.20	110.28
1	A	356	ASP	O-C-N	-5.11	115.41	122.46
1	B	314	GLU	CB-CG-CD	5.11	121.28	112.60
1	A	358	ILE	CA-C-O	-5.10	115.77	121.17
1	A	354	THR	N-CA-C	5.09	116.83	111.28
1	A	163	ARG	CB-CG-CD	-5.09	99.59	111.30
1	A	331	THR	OG1-CB-CG2	-5.09	99.12	109.30
1	B	330	LEU	CA-CB-CG	5.08	134.10	116.30
1	B	465	LEU	O-C-N	5.08	129.42	122.46
1	A	39	PHE	N-CA-C	5.08	117.94	111.69
1	A	332	TRP	O-C-N	5.08	127.51	122.12
1	A	137	THR	CA-C-N	5.08	127.34	120.38
1	A	137	THR	C-N-CA	5.08	127.34	120.38
1	B	458	ILE	CA-CB-CG2	5.08	119.13	110.50
1	A	444	ARG	N-CA-CB	5.07	117.67	110.06
1	A	259	ARG	CB-CA-C	5.07	120.01	110.63
1	A	486	ARG	N-CA-C	-5.07	100.25	108.41
1	B	244	SER	CA-CB-OG	-5.07	100.97	111.10
1	A	225	GLN	CB-CG-CD	5.07	121.21	112.60
1	B	452	GLU	N-CA-CB	5.07	117.66	110.16
1	B	238	ILE	CA-C-O	-5.06	114.45	120.78
1	A	209	GLU	CB-CG-CD	5.06	121.20	112.60
1	A	66	HIS	N-CA-CB	-5.06	103.01	111.20
1	A	158	HIS	N-CA-CB	5.06	117.31	109.98
1	A	177	VAL	CA-C-O	-5.06	115.00	120.36
1	B	232	SER	CA-C-N	5.06	131.42	122.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	232	SER	C-N-CA	5.06	131.42	122.67
1	A	51	LYS	CB-CG-CD	-5.05	99.67	111.30
1	B	257	SER	N-CA-C	-5.05	105.77	111.28
1	B	380	PHE	N-CA-CB	5.05	119.02	110.49
1	A	24	ASP	CB-CG-OD1	-5.05	106.79	118.40
1	B	379	ASP	N-CA-CB	5.04	117.37	109.85
1	A	167	LYS	O-C-N	5.04	125.91	121.37
1	A	41	PRO	N-CA-C	-5.04	107.29	113.84
1	A	209	GLU	CA-CB-CG	5.04	124.18	114.10
1	B	145	SER	CA-C-O	-5.04	113.06	119.31
1	A	429	VAL	CA-CB-CG2	5.04	118.96	110.40
1	A	346	ILE	CA-C-N	-5.03	116.55	123.14
1	A	346	ILE	C-N-CA	-5.03	116.55	123.14
1	B	225	GLN	O-C-N	5.03	129.11	123.27
1	B	277	LEU	CB-CA-C	-5.03	101.81	110.16
1	B	490	VAL	O-C-N	5.03	126.57	121.14
1	A	271	LYS	CA-CB-CG	5.03	124.15	114.10
1	A	366	SER	CB-CA-C	-5.02	99.36	109.55
1	A	212	VAL	N-CA-C	-5.02	105.65	110.72
1	B	444	ARG	NE-CZ-NH2	5.02	123.72	119.20
1	B	397	GLN	N-CA-C	5.02	118.89	112.87
1	B	239	ILE	N-CA-CB	5.01	116.07	110.51
1	B	152	VAL	CA-C-N	5.01	126.99	120.28
1	B	152	VAL	C-N-CA	5.01	126.99	120.28
1	B	449	LYS	CA-CB-CG	-5.00	104.09	114.10

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	320	ARG	Sidechain
1	A	353	ARG	Sidechain
1	A	376	ARG	Sidechain
1	A	38	ARG	Sidechain
1	B	163	ARG	Sidechain
1	B	463	ARG	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	3841	0	3900	416	2
1	B	3107	0	3156	270	0
2	A	43	0	30	9	0
3	A	31	0	17	0	0
3	B	31	0	18	2	0
4	B	6	0	0	0	0
5	A	182	0	0	10	0
5	B	101	0	0	11	0
All	All	7342	0	7121	651	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 46.

All (651) 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:10:LYS:O	1:A:10:LYS:HD3	1.18	1.33
1:A:24:ASP:HA	1:A:37:THR:CG2	1.60	1.27
1:A:1:GLU:N	1:A:71:ILE:HD12	1.49	1.27
1:A:1:GLU:H3	1:A:2:PRO:CD	1.50	1.25
1:A:24:ASP:CA	1:A:37:THR:HG21	1.66	1.25
1:A:24:ASP:O	1:A:37:THR:HG22	1.36	1.24
1:A:10:LYS:HZ2	1:A:85:GLN:NE2	1.37	1.22
1:A:26:TRP:CE3	1:A:81:LEU:HD23	1.75	1.21
1:A:33:VAL:HG23	1:A:82:GLY:O	1.37	1.20
1:A:1:GLU:N	1:A:71:ILE:CD1	2.05	1.18
1:A:1:GLU:N	1:A:2:PRO:HD2	1.51	1.17
1:A:496:TYR:HD1	1:A:496:TYR:C	1.53	1.15
1:B:398:ARG:O	1:B:399:ASN:HB2	1.45	1.14
1:B:396:GLU:HG3	1:B:401:LYS:HD3	1.28	1.11
1:A:113:LYS:CE	1:A:115:LEU:HD13	1.80	1.11
1:A:9:GLN:HG2	1:A:11:ILE:HD11	1.32	1.10
1:A:495:LEU:HD12	1:B:503:PRO:HB2	1.23	1.10
1:B:313:GLU:O	1:B:314:GLU:HB2	1.41	1.08
1:A:113:LYS:HE2	1:A:115:LEU:HD13	1.12	1.07
1:A:317:GLY:HA3	1:A:320:ARG:HH11	0.97	1.07
1:A:79:LYS:N	1:A:79:LYS:HD2	1.70	1.06
1:A:494:VAL:HG21	1:B:503:PRO:HD2	1.18	1.06
1:A:317:GLY:HA3	1:A:320:ARG:NH1	1.71	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:GLU:H1	1:A:71:ILE:CD1	1.63	1.06
1:A:1:GLU:CA	1:A:71:ILE:HD12	1.85	1.05
1:B:197:THR:CG2	1:B:436:LEU:HD21	1.86	1.05
1:A:503:PRO:O	1:A:504:THR:HB	1.58	1.04
1:A:1:GLU:H3	1:A:2:PRO:HD2	0.97	1.04
1:A:10:LYS:O	1:A:10:LYS:CD	2.05	1.04
1:A:248:ILE:HD11	1:A:250:TRP:NE1	1.71	1.04
1:A:494:VAL:CG2	1:B:503:PRO:HD2	1.87	1.03
1:A:6:MET:HG2	1:A:7:ASN:H	1.24	1.03
1:A:491:PRO:HD3	5:A:732:HOH:O	1.57	1.02
1:B:108:ARG:C	1:B:112:LEU:HD23	1.85	1.02
1:A:146:SER:HB3	1:A:291:LYS:HD2	1.40	1.01
1:A:496:TYR:C	1:A:496:TYR:CD1	2.31	1.01
1:B:509:GLU:HG3	1:B:510:ASP:H	1.25	1.00
1:A:6:MET:HG2	1:A:7:ASN:N	1.71	1.00
1:A:35:ASP:OD1	1:A:37:THR:HG22	1.60	1.00
1:A:226:MET:HE2	1:A:252:GLN:HB2	1.40	1.00
1:A:1:GLU:H1	1:A:71:ILE:HD12	1.02	0.99
1:B:509:GLU:CG	1:B:510:ASP:H	1.71	0.99
1:B:396:GLU:HG3	1:B:401:LYS:CD	1.91	0.99
1:B:197:THR:HG21	1:B:436:LEU:HD21	1.44	0.99
1:A:137:THR:HG22	1:A:140:ALA:H	1.24	0.98
1:A:102:THR:O	1:A:102:THR:HG22	1.62	0.98
1:A:24:ASP:C	1:A:37:THR:CG2	2.37	0.98
1:A:10:LYS:NZ	1:A:85:GLN:NE2	2.12	0.97
1:A:257:SER:HB2	1:A:324:LYS:HG3	1.45	0.97
1:A:24:ASP:O	1:A:37:THR:CG2	2.12	0.96
1:A:35:ASP:OD1	1:A:37:THR:CG2	2.12	0.96
1:A:2:PRO:O	1:A:3:LYS:CE	2.14	0.96
1:A:16:VAL:CG1	1:A:88:MET:HE1	1.95	0.96
1:B:313:GLU:O	1:B:314:GLU:CB	2.12	0.95
1:A:9:GLN:HG2	1:A:11:ILE:CD1	1.97	0.94
1:A:10:LYS:HZ2	1:A:85:GLN:HE22	1.08	0.94
1:A:29:ILE:HD12	1:A:58:VAL:HG12	1.47	0.94
1:A:26:TRP:CE3	1:A:81:LEU:CD2	2.51	0.93
1:A:495:LEU:HD12	1:B:503:PRO:CB	1.97	0.93
1:A:69:ASN:H	1:A:69:ASN:HD22	1.15	0.92
1:A:110:GLU:O	1:A:113:LYS:CG	2.19	0.91
1:A:257:SER:CB	1:A:324:LYS:HG3	2.00	0.91
1:B:108:ARG:O	1:B:112:LEU:HD23	1.71	0.91
1:B:115:LEU:O	1:B:116:LEU:C	2.13	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:LYS:HE2	1:A:115:LEU:CD1	1.99	0.91
1:A:2:PRO:O	1:A:3:LYS:NZ	2.04	0.91
1:A:10:LYS:NZ	1:A:85:GLN:HE22	1.67	0.91
1:A:2:PRO:O	1:A:3:LYS:HE3	1.69	0.90
1:B:113:LYS:O	1:B:115:LEU:HD23	1.72	0.89
1:A:2:PRO:C	1:A:3:LYS:HG2	1.96	0.89
1:A:113:LYS:O	1:A:114:SER:C	2.13	0.89
1:A:317:GLY:CA	1:A:320:ARG:HH11	1.85	0.89
1:A:113:LYS:O	1:A:113:LYS:HG3	1.72	0.89
1:B:102:THR:C	1:B:103:LYS:HD2	1.96	0.89
1:A:9:GLN:O	1:A:10:LYS:HB3	1.73	0.88
5:A:593:HOH:O	1:B:491:PRO:HD3	1.70	0.88
1:B:113:LYS:C	1:B:115:LEU:H	1.76	0.87
1:A:29:ILE:HD12	1:A:58:VAL:CG1	2.03	0.87
1:B:197:THR:HG21	1:B:436:LEU:CD2	2.03	0.87
1:A:90:PRO:O	1:A:92:LEU:N	2.06	0.86
1:B:396:GLU:HG3	1:B:401:LYS:CE	2.06	0.86
1:A:226:MET:CE	1:A:252:GLN:HB2	2.06	0.86
1:A:112:LEU:C	1:A:112:LEU:HD12	1.98	0.86
1:A:11:ILE:O	1:A:85:GLN:HB2	1.76	0.85
1:A:33:VAL:CG2	1:A:82:GLY:O	2.22	0.85
1:B:509:GLU:HG3	1:B:510:ASP:N	1.91	0.85
1:A:155:ARG:HE	1:B:491:PRO:HB3	1.42	0.84
1:A:270:GLU:OE1	1:A:343:LYS:HE3	1.77	0.84
1:A:112:LEU:HD12	1:A:113:LYS:N	1.92	0.83
1:B:113:LYS:C	1:B:115:LEU:N	2.29	0.83
1:B:396:GLU:CG	1:B:401:LYS:HD3	2.07	0.83
1:A:146:SER:HB3	1:A:291:LYS:CD	2.09	0.82
1:A:496:TYR:HD1	1:A:496:TYR:O	1.61	0.82
1:A:510:ASP:H	1:B:115:LEU:HD13	1.41	0.82
1:A:9:GLN:O	1:A:10:LYS:CB	2.27	0.82
1:A:32:TYR:HE2	1:A:80:LYS:HB3	1.45	0.82
1:B:120:ASP:C	1:B:121:ASN:HD22	1.88	0.82
1:A:2:PRO:HG3	1:A:72:ASP:OD1	1.78	0.82
1:A:24:ASP:HA	1:A:37:THR:HG21	0.82	0.82
1:A:510:ASP:CA	1:B:115:LEU:CD1	2.58	0.81
1:A:22:PRO:O	1:A:24:ASP:N	2.13	0.81
1:A:510:ASP:N	1:B:115:LEU:HD13	1.93	0.81
1:A:1:GLU:CA	1:A:71:ILE:CD1	2.57	0.81
1:A:6:MET:SD	1:A:8:LYS:HD2	2.20	0.81
1:B:496:TYR:CD1	1:B:496:TYR:C	2.57	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:THR:HG22	1:A:140:ALA:N	1.96	0.80
1:A:78:GLU:C	1:A:79:LYS:HD2	2.05	0.80
1:A:1:GLU:N	1:A:2:PRO:CD	2.20	0.80
1:A:88:MET:C	1:A:89:PRO:O	2.19	0.80
1:B:251:TYR:OH	5:B:594:HOH:O	1.99	0.80
1:A:26:TRP:CZ3	1:A:81:LEU:HD23	2.16	0.80
1:A:88:MET:O	1:A:89:PRO:C	2.24	0.80
1:A:24:ASP:CA	1:A:37:THR:CG2	2.41	0.79
1:A:510:ASP:CA	1:B:115:LEU:HD13	2.11	0.79
1:A:16:VAL:HG11	1:A:88:MET:HE1	1.63	0.79
1:A:244:SER:HB2	1:A:246:LYS:H	1.46	0.79
1:A:50:ILE:HG23	2:A:560:HEM:CBC	2.12	0.79
1:A:110:GLU:O	1:A:113:LYS:HG3	1.82	0.79
1:A:6:MET:CG	1:A:7:ASN:N	2.44	0.79
1:A:110:GLU:O	1:A:113:LYS:HG2	1.83	0.78
1:A:26:TRP:CZ3	1:A:81:LEU:CD2	2.66	0.78
1:A:24:ASP:C	1:A:37:THR:HG22	2.03	0.78
1:A:130:TYR:CE2	1:A:134:GLN:NE2	2.50	0.78
1:B:248:ILE:HB	1:B:275:LYS:HD2	1.66	0.78
1:A:20:ASN:H	1:A:20:ASN:HD22	1.32	0.77
1:A:29:ILE:CD1	1:A:58:VAL:CG1	2.63	0.77
1:A:29:ILE:CD1	1:A:58:VAL:HG12	2.13	0.77
1:A:102:THR:O	1:A:104:GLU:N	2.18	0.77
1:A:257:SER:HB2	1:A:324:LYS:CG	2.15	0.77
1:A:146:SER:CB	1:A:291:LYS:HD2	2.15	0.77
1:B:286:LEU:CD1	5:B:645:HOH:O	2.32	0.77
1:B:320:ARG:HG3	1:B:320:ARG:O	1.71	0.76
1:A:1:GLU:H2	1:A:71:ILE:CD1	1.98	0.76
1:A:248:ILE:CD1	1:A:250:TRP:NE1	2.49	0.76
1:B:312:VAL:O	1:B:314:GLU:N	2.18	0.76
1:A:101:GLU:OE2	1:A:138:LYS:HG3	1.87	0.75
1:A:24:ASP:HA	1:A:37:THR:CB	2.16	0.75
1:A:256:ASN:HD22	1:A:258:ASP:H	1.32	0.74
1:A:211:ASP:HB3	1:A:439:ASN:HD21	1.51	0.74
1:A:27:VAL:HG13	1:A:29:ILE:HD13	1.69	0.74
1:A:248:ILE:HD11	1:A:250:TRP:CE2	2.21	0.74
1:A:22:PRO:C	1:A:24:ASP:H	1.94	0.74
1:A:9:GLN:CG	1:A:11:ILE:CD1	2.65	0.74
1:A:40:LEU:HD12	1:A:47:GLN:HG2	1.69	0.73
1:A:84:LEU:HD11	1:A:88:MET:HG2	1.67	0.73
1:A:113:LYS:CG	1:A:113:LYS:O	2.34	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:GLU:N	1:A:71:ILE:HB	2.04	0.73
1:A:113:LYS:CE	1:A:115:LEU:CD1	2.60	0.73
1:A:26:TRP:CZ3	1:A:81:LEU:HG	2.23	0.73
1:A:503:PRO:O	1:A:504:THR:CB	2.35	0.73
1:B:315:SER:O	1:B:316:GLN:HB3	1.89	0.72
1:A:1:GLU:N	1:A:71:ILE:HD13	2.05	0.72
1:A:507:GLU:O	1:A:508:PHE:HB2	1.90	0.72
1:A:1:GLU:H2	1:A:2:PRO:HD2	1.51	0.72
1:A:6:MET:HG2	1:A:8:LYS:H	1.53	0.71
1:A:228:SER:HA	1:A:252:GLN:HE21	1.54	0.71
1:B:163:ARG:O	5:B:607:HOH:O	2.07	0.71
1:B:196:ALA:H	1:B:226:MET:HE2	1.53	0.71
1:A:226:MET:HE1	1:A:349:LYS:CD	2.20	0.71
1:A:35:ASP:OD1	1:A:37:THR:HG23	1.91	0.71
1:B:217:GLY:HA3	1:B:247:GLN:NE2	2.05	0.71
1:B:229:THR:OG1	1:B:253:LEU:HA	1.90	0.70
1:A:2:PRO:C	1:A:3:LYS:CG	2.63	0.70
1:A:101:GLU:OE1	1:A:108:ARG:NH1	2.24	0.70
1:B:339:LYS:HG3	1:B:346:ILE:CD1	2.21	0.70
1:A:79:LYS:N	1:A:79:LYS:CD	2.46	0.70
1:A:270:GLU:OE1	1:A:343:LYS:CE	2.39	0.70
1:B:496:TYR:C	1:B:496:TYR:HD1	1.99	0.70
1:A:112:LEU:O	1:A:114:SER:N	2.25	0.69
1:B:113:LYS:O	1:B:113:LYS:HG2	1.90	0.69
1:A:24:ASP:N	1:A:24:ASP:OD1	2.23	0.69
1:A:75:ILE:CD1	2:A:560:HEM:HBB1	2.22	0.69
1:A:226:MET:HE2	1:A:252:GLN:CB	2.18	0.69
1:B:226:MET:HE3	1:B:252:GLN:CB	2.23	0.68
1:A:16:VAL:HG12	1:A:88:MET:HE1	1.75	0.68
1:B:109:LYS:HA	1:B:112:LEU:HG	1.75	0.68
1:B:108:ARG:C	1:B:112:LEU:CD2	2.65	0.68
1:A:256:ASN:HD22	1:A:257:SER:N	1.92	0.67
1:A:197:THR:CG2	1:A:436:LEU:HD21	2.24	0.67
1:A:155:ARG:HH21	1:B:491:PRO:HB2	1.60	0.67
1:A:3:LYS:O	1:A:4:LEU:HB2	1.93	0.66
1:A:158:HIS:ND1	1:A:411:GLY:O	2.27	0.66
1:A:1:GLU:H2	1:A:71:ILE:HD13	1.60	0.66
1:A:8:LYS:O	1:A:9:GLN:C	2.37	0.66
1:A:1:GLU:H1	1:A:71:ILE:CG1	2.09	0.66
1:A:102:THR:O	1:A:102:THR:CG2	2.29	0.66
1:B:248:ILE:HD11	1:B:250:TRP:NE1	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:SER:OG	1:B:324:LYS:HG2	1.95	0.66
1:A:1:GLU:HA	1:A:71:ILE:CD1	2.26	0.66
1:A:69:ASN:HD22	1:A:69:ASN:N	1.88	0.66
1:A:9:GLN:CG	1:A:11:ILE:HD13	2.26	0.66
1:B:249:GLN:H	1:B:275:LYS:HE3	1.59	0.66
1:A:15:GLU:CD	1:A:18:LYS:HZ1	2.04	0.66
1:A:16:VAL:HG11	1:A:88:MET:CE	2.26	0.66
1:A:32:TYR:CE2	1:A:80:LYS:HB3	2.28	0.66
1:A:15:GLU:CD	1:A:18:LYS:NZ	2.54	0.65
1:B:228:SER:HA	1:B:252:GLN:HG3	1.77	0.65
1:A:386:GLU:OE1	5:A:583:HOH:O	2.14	0.65
1:A:490:VAL:HG23	1:A:491:PRO:O	1.96	0.65
1:B:227:ILE:HG13	1:B:250:TRP:O	1.97	0.65
1:B:316:GLN:HB2	1:B:320:ARG:HA	1.78	0.65
1:B:396:GLU:OE2	1:B:401:LYS:NZ	2.26	0.65
1:A:26:TRP:CZ3	1:A:81:LEU:CG	2.79	0.65
1:A:110:GLU:C	1:A:113:LYS:HG2	2.22	0.65
1:A:5:ASP:O	1:A:6:MET:HB3	1.95	0.65
1:A:24:ASP:C	1:A:37:THR:HG21	2.13	0.65
1:A:338:LEU:HD13	1:A:346:ILE:HD13	1.79	0.64
1:B:398:ARG:O	1:B:399:ASN:CB	2.31	0.64
1:A:1:GLU:N	1:A:71:ILE:CB	2.61	0.64
1:A:93:VAL:O	1:A:93:VAL:HG23	1.98	0.64
1:A:73:LYS:HE3	1:A:74:TYR:CZ	2.32	0.64
1:A:112:LEU:C	1:A:112:LEU:CD1	2.69	0.64
1:A:108:ARG:HH12	1:A:138:LYS:N	1.95	0.64
1:A:163:ARG:O	5:A:709:HOH:O	2.15	0.64
1:A:21:LYS:HG3	1:A:22:PRO:HD2	1.78	0.64
1:A:90:PRO:C	1:A:92:LEU:H	2.00	0.64
1:B:197:THR:HG21	1:B:436:LEU:CG	2.27	0.64
1:A:197:THR:HG21	1:A:436:LEU:HD21	1.78	0.64
1:B:104:GLU:OE2	1:B:138:LYS:HD3	1.97	0.64
1:B:102:THR:HA	1:B:103:LYS:HD2	1.80	0.63
1:B:196:ALA:CB	1:B:226:MET:HE2	2.28	0.63
1:A:9:GLN:HG3	1:A:11:ILE:HD13	1.81	0.63
1:B:102:THR:CA	1:B:103:LYS:HD2	2.27	0.63
1:A:331:THR:HG22	1:A:333:LYS:H	1.63	0.63
1:B:217:GLY:HA3	1:B:247:GLN:HE22	1.62	0.63
1:B:190:VAL:HG11	1:B:221:THR:HG21	1.80	0.63
1:B:387:VAL:O	1:B:391:THR:HG23	1.98	0.63
1:B:239:ILE:N	1:B:239:ILE:HD12	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:LYS:O	1:B:343:LYS:HG2	1.99	0.63
1:A:40:LEU:CD1	1:A:47:GLN:OE1	2.46	0.63
1:A:346:ILE:HB	1:A:365:VAL:HG22	1.80	0.63
1:B:354:THR:OG1	1:B:391:THR:HG22	1.99	0.63
1:A:108:ARG:HH22	1:A:138:LYS:HG2	1.64	0.63
1:A:31:GLY:O	1:A:84:LEU:HB3	1.98	0.62
1:B:102:THR:O	1:B:103:LYS:C	2.43	0.62
1:A:22:PRO:O	1:A:24:ASP:OD1	2.17	0.62
1:B:320:ARG:O	1:B:320:ARG:CG	2.43	0.62
1:B:226:MET:HG2	1:B:252:GLN:HB3	1.81	0.62
1:B:239:ILE:HD12	1:B:239:ILE:H	1.64	0.62
1:A:388:LEU:HD13	1:A:424:LEU:CB	2.28	0.62
1:A:9:GLN:O	1:A:10:LYS:CG	2.48	0.62
1:A:29:ILE:O	1:A:30:ASN:HB2	1.97	0.62
1:A:248:ILE:HD11	1:A:250:TRP:CD1	2.33	0.62
1:A:491:PRO:CD	5:A:732:HOH:O	2.28	0.62
1:B:496:TYR:CD1	1:B:496:TYR:O	2.53	0.62
1:B:286:LEU:HD12	5:B:645:HOH:O	1.95	0.62
1:B:207:GLU:O	1:B:210:LYS:HB2	2.00	0.62
1:B:105:ASP:OD1	1:B:105:ASP:N	2.28	0.61
1:A:102:THR:C	1:A:104:GLU:N	2.57	0.61
1:B:204:ASN:ND2	1:B:211:ASP:HB2	2.16	0.61
1:B:382:ARG:HH12	1:B:390:GLU:CD	2.07	0.61
1:A:15:GLU:OE2	1:A:18:LYS:NZ	2.33	0.61
1:A:16:VAL:CG2	1:A:33:VAL:CG1	2.78	0.61
1:B:133:SER:OG	1:B:134:GLN:NE2	2.33	0.61
1:B:388:LEU:HD22	1:B:392:MET:HG2	1.81	0.61
1:B:331:THR:CG2	1:B:333:LYS:HB2	2.30	0.61
1:A:9:GLN:O	1:A:10:LYS:HG3	2.00	0.61
1:A:88:MET:O	1:A:89:PRO:O	2.17	0.61
1:B:226:MET:HE3	1:B:252:GLN:HB2	1.83	0.61
1:A:3:LYS:C	1:A:5:ASP:H	2.08	0.61
1:A:243:PRO:HD2	1:A:247:GLN:OE1	2.00	0.61
1:A:257:SER:OG	1:A:324:LYS:HG3	2.00	0.61
1:A:4:LEU:O	1:A:6:MET:N	2.32	0.60
1:A:28:VAL:HG11	1:A:84:LEU:HD22	1.81	0.60
1:A:89:PRO:HG2	1:A:92:LEU:HD12	1.83	0.60
1:A:482:THR:HB	1:B:486:ARG:O	1.99	0.60
1:A:388:LEU:HD13	1:A:424:LEU:HB2	1.82	0.60
1:A:40:LEU:HD11	1:A:47:GLN:OE1	2.01	0.60
1:A:110:GLU:CA	1:A:113:LYS:HG2	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:LYS:O	1:A:22:PRO:O	2.19	0.60
1:A:239:ILE:HD13	1:A:272:LEU:HB3	1.83	0.60
1:B:108:ARG:HH22	1:B:138:LYS:HG3	1.67	0.60
1:B:105:ASP:O	1:B:106:ILE:C	2.44	0.60
1:B:113:LYS:O	1:B:115:LEU:N	2.34	0.60
1:B:248:ILE:HD11	1:B:250:TRP:HE1	1.66	0.60
1:A:1:GLU:H1	1:A:71:ILE:HB	1.67	0.60
1:B:136:LEU:HB3	1:B:140:ALA:HB3	1.83	0.59
1:B:177:VAL:HG22	1:B:468:THR:HA	1.84	0.59
1:A:1:GLU:HB3	1:A:62:PHE:HE2	1.67	0.59
1:A:162:HIS:ND1	1:A:162:HIS:N	2.49	0.59
1:A:508:PHE:CE2	1:B:116:LEU:HD23	2.38	0.59
1:A:155:ARG:NE	1:B:491:PRO:HB3	2.16	0.59
1:A:166:PHE:CD1	1:A:465:LEU:HD21	2.38	0.59
1:B:243:PRO:HD2	1:B:247:GLN:HE22	1.67	0.59
1:B:327:ASP:C	1:B:329:SER:H	2.10	0.59
1:A:495:LEU:CD1	1:B:503:PRO:HB2	2.16	0.59
1:A:155:ARG:HE	1:B:491:PRO:CB	2.15	0.58
1:B:281:VAL:HG22	1:B:349:LYS:O	2.03	0.58
1:B:339:LYS:HA	1:B:346:ILE:HD11	1.85	0.58
1:A:30:ASN:H	1:A:59:THR:HG1	1.50	0.58
1:A:168:PRO:O	1:B:353:ARG:HD2	2.03	0.58
1:A:16:VAL:CG2	1:A:33:VAL:HG11	2.32	0.58
1:A:508:PHE:HZ	1:B:135:THR:CG2	2.15	0.58
1:B:419:LEU:HD21	1:B:458:ILE:HG23	1.84	0.58
1:A:226:MET:CE	1:A:252:GLN:CB	2.80	0.58
1:A:84:LEU:HD11	1:A:88:MET:CG	2.33	0.58
1:B:108:ARG:O	1:B:111:GLN:HB2	2.04	0.58
1:A:113:LYS:HE3	1:A:115:LEU:HD13	1.79	0.58
1:B:260:LYS:O	1:B:260:LYS:CG	2.50	0.58
1:B:349:LYS:NZ	3:B:570:FMN:O2'	2.36	0.58
1:B:286:LEU:HD13	5:B:645:HOH:O	2.00	0.57
1:A:78:GLU:H	1:A:78:GLU:CD	2.10	0.57
1:A:108:ARG:O	1:A:112:LEU:HG	2.04	0.57
1:A:124:ASN:HD22	1:A:124:ASN:C	2.12	0.57
1:A:499:VAL:HG22	1:B:505:LEU:HD11	1.87	0.57
1:B:115:LEU:HD23	1:B:115:LEU:N	2.18	0.57
1:B:256:ASN:HD22	1:B:258:ASP:H	1.53	0.57
1:B:113:LYS:O	1:B:113:LYS:CG	2.52	0.57
1:B:196:ALA:HB3	1:B:226:MET:HE2	1.87	0.57
1:A:15:GLU:OE1	1:A:18:LYS:NZ	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:TRP:CH2	1:A:81:LEU:HG	2.39	0.56
1:A:502:GLY:O	1:A:503:PRO:O	2.23	0.56
1:A:110:GLU:HA	1:A:113:LYS:HB3	1.86	0.56
1:A:13:PRO:CG	1:A:87:SER:O	2.52	0.56
1:A:50:ILE:HG23	2:A:560:HEM:CAC	2.34	0.56
1:A:496:TYR:CD1	1:A:497:ASN:N	2.73	0.56
1:A:2:PRO:HG2	1:A:3:LYS:H	1.70	0.56
1:B:186:SER:OG	1:B:248:ILE:HG21	2.04	0.56
1:B:497:ASN:N	1:B:497:ASN:HD22	2.03	0.56
1:A:98:ALA:O	1:A:99:PRO:C	2.47	0.56
1:A:256:ASN:ND2	1:A:258:ASP:H	2.02	0.56
1:A:81:LEU:HD13	1:A:81:LEU:N	2.19	0.56
1:A:89:PRO:O	1:A:90:PRO:O	2.24	0.56
1:A:230:LEU:HD22	1:A:254:TYR:CE2	2.40	0.56
1:A:23:ASP:O	1:A:24:ASP:HB3	2.05	0.56
1:B:227:ILE:O	1:B:252:GLN:N	2.31	0.56
1:B:213:ALA:HA	1:B:225:GLN:NE2	2.20	0.56
1:B:288:GLN:HG3	1:B:293:MET:SD	2.47	0.56
1:A:12:SER:OG	1:A:85:GLN:NE2	2.39	0.55
1:B:197:THR:HG23	1:B:436:LEU:HD11	1.88	0.55
1:B:509:GLU:CG	1:B:510:ASP:N	2.47	0.55
1:A:494:VAL:CG2	1:A:495:LEU:N	2.70	0.55
1:A:1:GLU:H2	1:A:71:ILE:HG21	1.71	0.55
5:A:593:HOH:O	1:B:491:PRO:CD	2.43	0.55
1:B:136:LEU:HD13	1:B:140:ALA:HB1	1.88	0.55
1:B:234:SER:O	1:B:235:PRO:C	2.49	0.55
1:B:196:ALA:HB3	1:B:226:MET:CE	2.36	0.55
1:A:337:GLU:O	1:A:341:LYS:HD2	2.06	0.54
1:A:481:SER:OG	1:B:484:LYS:NZ	2.40	0.54
1:B:213:ALA:CA	1:B:225:GLN:HE22	2.19	0.54
1:A:248:ILE:CD1	1:A:250:TRP:CD1	2.91	0.54
1:A:289:ARG:NH1	1:A:292:ASP:OD1	2.41	0.54
1:B:327:ASP:C	1:B:329:SER:N	2.65	0.54
1:A:159:ASN:HB3	1:B:488:VAL:HG11	1.90	0.54
1:B:313:GLU:N	1:B:313:GLU:OE1	2.40	0.54
1:B:442:TYR:HB2	1:B:446:GLY:HA3	1.89	0.54
1:A:1:GLU:H1	1:A:71:ILE:CB	2.20	0.54
1:A:20:ASN:HD22	1:A:20:ASN:N	1.96	0.54
1:A:361:ALA:HB2	1:A:404:LEU:HD22	1.89	0.54
1:B:339:LYS:HG3	1:B:346:ILE:HD12	1.90	0.54
1:A:476:ASP:OD1	1:A:476:ASP:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:VAL:HG23	1:A:495:LEU:N	2.23	0.54
1:B:313:GLU:OE1	1:B:313:GLU:CA	2.56	0.54
1:A:105:ASP:OD1	1:A:105:ASP:N	2.41	0.54
1:A:179:ILE:HD11	1:A:455:ARG:HG3	1.90	0.53
1:A:114:SER:O	1:A:115:LEU:HD12	2.09	0.53
1:A:289:ARG:NH1	1:A:292:ASP:CG	2.66	0.53
1:A:75:ILE:HD12	2:A:560:HEM:HBB1	1.89	0.53
1:A:348:ILE:HD12	1:A:365:VAL:HG11	1.89	0.53
1:A:18:LYS:HE2	1:A:19:HIS:CE1	2.43	0.53
1:B:197:THR:HG22	1:B:197:THR:O	2.08	0.53
1:A:13:PRO:HG2	1:A:87:SER:O	2.08	0.53
1:A:16:VAL:HG21	1:A:33:VAL:CG1	2.39	0.53
1:A:226:MET:HE1	1:A:349:LYS:HD2	1.89	0.53
1:A:460:MET:HE2	1:B:318:ALA:HA	1.91	0.53
1:A:485:ALA:HB1	1:B:487:THR:HG22	1.90	0.53
1:A:49:VAL:HG21	2:A:560:HEM:CMD	2.39	0.53
1:B:257:SER:OG	1:B:324:LYS:O	2.26	0.53
1:B:104:GLU:OE2	1:B:138:LYS:CD	2.56	0.52
1:A:49:VAL:O	1:A:53:ASN:OD1	2.27	0.52
1:A:63:GLU:HB3	1:A:64:PRO:HD3	1.91	0.52
1:A:73:LYS:HE3	1:A:74:TYR:OH	2.09	0.52
1:A:16:VAL:HG21	1:A:33:VAL:HG13	1.90	0.52
1:A:11:ILE:O	1:A:85:GLN:CB	2.55	0.52
1:A:102:THR:O	1:A:103:LYS:C	2.53	0.52
1:A:155:ARG:NH2	1:B:491:PRO:HB2	2.23	0.52
1:B:449:LYS:HA	1:B:452:GLU:HG2	1.91	0.52
1:A:22:PRO:C	1:A:24:ASP:N	2.56	0.52
1:B:474:LYS:H	1:B:477:LEU:HD23	1.74	0.52
1:A:508:PHE:HE2	1:B:116:LEU:HD23	1.72	0.52
1:B:107:ALA:O	1:B:108:ARG:C	2.51	0.52
1:A:108:ARG:NH1	1:A:137:THR:HA	2.23	0.52
1:A:213:ALA:HB2	1:A:225:GLN:HE22	1.75	0.52
1:A:283:ALA:N	1:A:284:PRO:CD	2.73	0.52
1:B:326:ILE:O	1:B:327:ASP:C	2.45	0.52
1:A:49:VAL:HG21	2:A:560:HEM:HMD2	1.91	0.52
1:A:11:ILE:HG22	1:A:12:SER:H	1.74	0.51
1:B:369:VAL:HG22	1:B:407:PHE:HB2	1.91	0.51
1:A:84:LEU:CD1	1:A:88:MET:CE	2.89	0.51
1:A:275:LYS:NZ	5:A:577:HOH:O	2.42	0.51
1:B:102:THR:O	1:B:103:LYS:HB2	2.09	0.51
1:B:167:LYS:HE3	5:B:680:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:ILE:O	1:B:328:PRO:HD3	2.11	0.51
1:A:113:LYS:O	1:A:114:SER:O	2.27	0.51
1:A:422:LEU:HD13	1:A:470:ILE:HD12	1.92	0.51
1:A:102:THR:C	1:A:104:GLU:H	2.18	0.51
1:A:32:TYR:HE2	1:A:80:LYS:CB	2.20	0.51
1:A:152:VAL:HG21	1:A:380:PHE:CE1	2.46	0.51
1:A:22:PRO:O	1:A:23:ASP:C	2.51	0.51
1:B:102:THR:C	1:B:104:GLU:N	2.64	0.51
1:B:214:ARG:O	1:B:218:GLN:HG2	2.11	0.51
1:B:325:PHE:HD1	1:B:325:PHE:H	1.58	0.51
1:A:510:ASP:CA	1:B:115:LEU:HD11	2.38	0.50
1:B:190:VAL:CG1	1:B:221:THR:HG21	2.41	0.50
1:A:29:ILE:O	1:A:30:ASN:CB	2.60	0.50
1:A:40:LEU:HD12	1:A:47:GLN:CG	2.41	0.50
1:B:228:SER:O	1:B:231:ALA:HB2	2.11	0.50
1:B:473:LEU:O	1:B:474:LYS:HG2	2.12	0.50
1:A:110:GLU:HA	1:A:113:LYS:HG2	1.92	0.50
1:B:113:LYS:O	1:B:115:LEU:CD2	2.54	0.50
1:B:339:LYS:CG	1:B:346:ILE:HD12	2.42	0.50
1:B:108:ARG:O	1:B:111:GLN:CB	2.59	0.50
1:B:197:THR:CG2	1:B:436:LEU:HD11	2.42	0.50
1:A:108:ARG:NH1	1:A:136:LEU:O	2.45	0.49
1:A:495:LEU:C	1:A:495:LEU:HD23	2.36	0.49
1:A:499:VAL:HG22	1:B:505:LEU:CD1	2.41	0.49
1:B:459:GLU:CD	5:B:625:HOH:O	2.55	0.49
1:B:273:GLY:O	1:B:275:LYS:HE2	2.12	0.49
1:A:40:LEU:HG	1:A:41:PRO:HD3	1.95	0.49
1:A:107:ALA:HA	1:A:110:GLU:OE1	2.13	0.49
1:B:507:GLU:O	1:B:508:PHE:HB2	2.13	0.49
1:B:192:PHE:HA	1:B:429:VAL:O	2.12	0.49
1:B:384:PRO:HG2	1:B:409:ASP:O	2.13	0.49
1:A:24:ASP:C	1:A:37:THR:HB	2.37	0.49
1:A:34:TYR:CE1	1:A:80:LYS:HG3	2.47	0.49
1:A:75:ILE:HG22	1:A:80:LYS:HD2	1.94	0.49
1:A:388:LEU:HD13	1:A:424:LEU:HB3	1.93	0.49
1:B:190:VAL:HG21	1:B:223:VAL:HG22	1.94	0.49
1:B:197:THR:HG21	1:B:436:LEU:HG	1.95	0.49
1:B:316:GLN:HB2	1:B:320:ARG:CA	2.43	0.48
1:A:398:ARG:HB2	1:A:400:LEU:HG	1.93	0.48
1:B:162:HIS:HE1	5:B:635:HOH:O	1.95	0.48
1:B:339:LYS:CG	1:B:346:ILE:CD1	2.91	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:GLU:O	1:A:294:LYS:HB2	2.14	0.48
1:B:289:ARG:HH12	1:B:292:ASP:CG	2.21	0.48
1:A:487:THR:H	1:B:489:GLY:HA2	1.78	0.48
1:B:248:ILE:CD1	1:B:250:TRP:NE1	2.75	0.48
1:A:13:PRO:HG3	1:A:87:SER:O	2.13	0.48
1:B:204:ASN:ND2	1:B:211:ASP:CB	2.77	0.48
1:B:382:ARG:NH1	1:B:390:GLU:OE1	2.46	0.48
1:A:43:HIS:CE1	2:A:560:HEM:ND	2.81	0.48
1:A:69:ASN:H	1:A:69:ASN:ND2	1.94	0.48
1:A:228:SER:HA	1:A:252:GLN:NE2	2.26	0.48
1:A:113:LYS:HE3	1:A:115:LEU:CD1	2.41	0.48
1:B:197:THR:HG23	1:B:436:LEU:HD21	1.89	0.48
1:B:326:ILE:O	1:B:328:PRO:N	2.47	0.48
1:B:490:VAL:O	1:B:491:PRO:C	2.56	0.48
1:B:402:ASP:OD1	1:B:402:ASP:O	2.31	0.48
1:A:226:MET:HE1	1:A:349:LYS:HD3	1.92	0.48
1:B:129:GLU:HB2	1:B:437:TYR:CD2	2.49	0.48
1:A:20:ASN:HA	1:A:54:ALA:HB1	1.96	0.47
1:A:111:GLN:NE2	5:A:640:HOH:O	2.47	0.47
1:B:227:ILE:HD11	1:B:249:GLN:HG2	1.95	0.47
1:B:286:LEU:HB2	5:B:645:HOH:O	2.13	0.47
1:A:34:TYR:HA	1:A:79:LYS:O	2.14	0.47
1:A:40:LEU:N	1:A:41:PRO:HD2	2.29	0.47
1:B:337:GLU:HA	1:B:337:GLU:OE1	2.12	0.47
1:B:419:LEU:HD12	1:B:461:SER:HB3	1.96	0.47
1:A:93:VAL:O	1:A:93:VAL:CG2	2.62	0.47
1:A:223:VAL:HA	1:A:224:PRO:HD3	1.74	0.47
1:B:229:THR:OG1	1:B:254:TYR:N	2.47	0.47
1:A:1:GLU:H3	1:A:2:PRO:HD3	1.63	0.47
1:A:3:LYS:HE3	1:A:3:LYS:HB3	1.69	0.47
1:A:84:LEU:HD13	1:A:88:MET:HE3	1.97	0.47
1:A:137:THR:CG2	1:A:139:GLN:HG3	2.44	0.47
1:A:1:GLU:HA	1:A:71:ILE:HD12	1.77	0.47
1:A:84:LEU:CD1	1:A:88:MET:HE3	2.44	0.47
1:A:192:PHE:HA	1:A:429:VAL:O	2.14	0.47
1:A:209:GLU:OE2	1:A:232:SER:HB2	2.14	0.47
1:B:115:LEU:O	1:B:116:LEU:O	2.32	0.47
1:B:234:SER:HB2	1:B:235:PRO:HD2	1.96	0.47
1:B:282:ASP:OD1	1:B:373:HIS:ND1	2.33	0.47
1:B:316:GLN:HG3	1:B:320:ARG:HB2	1.95	0.47
1:B:388:LEU:HD22	1:B:392:MET:CG	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:VAL:CG1	1:B:221:THR:CG2	2.93	0.47
1:B:249:GLN:H	1:B:275:LYS:CE	2.27	0.47
1:A:1:GLU:N	1:A:71:ILE:CG1	2.73	0.47
1:A:38:ARG:HH11	1:A:38:ARG:HD3	1.25	0.47
1:A:69:ASN:N	1:A:69:ASN:ND2	2.56	0.47
1:B:496:TYR:HD1	1:B:497:ASN:HD22	1.62	0.47
1:A:490:VAL:O	1:A:491:PRO:C	2.57	0.46
1:A:10:LYS:HD3	1:A:10:LYS:C	2.23	0.46
1:A:13:PRO:HA	1:A:88:MET:HE2	1.96	0.46
1:B:102:THR:C	1:B:103:LYS:CD	2.79	0.46
1:B:351:VAL:HG21	1:B:368:VAL:HG22	1.96	0.46
1:A:112:LEU:C	1:A:114:SER:N	2.74	0.46
1:B:114:SER:C	1:B:115:LEU:HD23	2.41	0.46
1:B:326:ILE:O	1:B:328:PRO:CD	2.63	0.46
1:A:13:PRO:HA	1:A:88:MET:CE	2.45	0.46
1:A:106:ILE:O	1:A:107:ALA:C	2.57	0.46
1:A:461:SER:O	1:A:465:LEU:HB2	2.16	0.46
1:A:482:THR:CB	1:B:486:ARG:O	2.64	0.46
1:A:24:ASP:O	1:A:25:CYS:C	2.58	0.46
1:A:155:ARG:HH11	1:A:155:ARG:HD3	1.39	0.46
1:A:27:VAL:CG1	1:A:29:ILE:HD13	2.43	0.46
1:A:40:LEU:O	1:A:47:GLN:HG2	2.16	0.46
1:A:162:HIS:CE1	5:A:701:HOH:O	2.69	0.46
1:A:257:SER:CB	1:A:324:LYS:CG	2.81	0.46
1:A:496:TYR:CD1	1:A:496:TYR:O	2.53	0.46
1:A:13:PRO:HB3	1:A:89:PRO:HD3	1.97	0.46
1:A:24:ASP:C	1:A:37:THR:CB	2.88	0.46
1:A:197:THR:HG23	1:A:436:LEU:HD21	1.95	0.46
1:A:363:ILE:HD13	1:A:363:ILE:HG21	1.74	0.46
1:B:248:ILE:CD1	1:B:250:TRP:HE1	2.26	0.46
1:A:256:ASN:ND2	1:A:257:SER:N	2.62	0.46
1:A:18:LYS:HE2	1:A:18:LYS:HB3	1.67	0.46
1:B:143:TYR:O	1:B:376:ARG:NH2	2.39	0.46
1:B:392:MET:N	1:B:393:PRO:CD	2.79	0.46
1:A:109:LYS:O	1:A:112:LEU:CD1	2.65	0.45
1:B:197:THR:HA	3:B:570:FMN:C5A	2.46	0.45
1:B:259:ARG:HH11	1:B:259:ARG:HD2	1.14	0.45
1:A:5:ASP:O	1:A:6:MET:CB	2.62	0.45
1:A:177:VAL:HG21	1:A:463:ARG:HG2	1.99	0.45
1:A:317:GLY:O	1:A:318:ALA:HB3	2.17	0.45
1:A:348:ILE:O	1:A:368:VAL:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:LEU:HD22	1:B:115:LEU:HA	1.53	0.45
1:B:204:ASN:HD21	1:B:211:ASP:CB	2.29	0.45
1:B:204:ASN:HD22	1:B:211:ASP:HB2	1.80	0.45
1:B:317:GLY:O	1:B:320:ARG:HB3	2.16	0.45
1:A:81:LEU:N	1:A:81:LEU:CD1	2.79	0.45
1:B:234:SER:H	1:B:237:GLU:HG3	1.80	0.45
1:B:156:GLU:CD	1:B:163:ARG:HH22	2.25	0.45
1:A:1:GLU:HB3	1:A:62:PHE:CE2	2.51	0.45
1:A:211:ASP:HB3	1:A:439:ASN:ND2	2.26	0.45
1:A:14:ALA:O	1:A:18:LYS:HB2	2.16	0.45
1:A:183:MET:CE	1:A:191:PRO:HA	2.47	0.45
1:B:260:LYS:O	1:B:260:LYS:HG2	2.11	0.45
1:A:20:ASN:C	1:A:54:ALA:HB1	2.42	0.44
1:A:20:ASN:CA	1:A:54:ALA:HB1	2.47	0.44
1:A:98:ALA:HB1	1:A:101:GLU:HB2	1.99	0.44
2:A:560:HEM:HBB2	2:A:560:HEM:CMB	2.48	0.44
1:B:182:ASP:HA	1:B:186:SER:O	2.17	0.44
1:A:28:VAL:HG23	1:A:56:LYS:O	2.15	0.44
1:A:108:ARG:HH12	1:A:137:THR:C	2.25	0.44
1:B:113:LYS:O	1:B:114:SER:C	2.58	0.44
1:B:462:MET:HE1	1:B:470:ILE:HD13	1.98	0.44
1:B:500:TYR:CD1	1:B:500:TYR:C	2.89	0.44
1:A:24:ASP:CA	1:A:37:THR:CB	2.87	0.44
1:A:95:PRO:HB2	1:A:96:PRO:CD	2.46	0.44
1:B:108:ARG:HB3	1:B:112:LEU:HD21	1.99	0.44
1:A:78:GLU:OE2	1:A:78:GLU:N	2.37	0.44
1:A:102:THR:HB	1:A:104:GLU:CG	2.47	0.44
1:A:499:VAL:HG12	1:A:499:VAL:O	2.17	0.44
1:A:506:THR:O	1:B:130:TYR:CD1	2.71	0.44
1:B:379:ASP:O	1:B:380:PHE:HB2	2.18	0.44
1:B:469:SER:O	1:B:472:GLU:HB2	2.16	0.44
1:A:15:GLU:OE1	1:A:19:HIS:HE1	2.01	0.44
1:B:228:SER:C	1:B:230:LEU:N	2.75	0.44
1:B:466:GLY:C	1:B:467:VAL:HG13	2.43	0.44
1:A:460:MET:HB3	5:B:656:HOH:O	2.17	0.44
1:A:256:ASN:O	1:A:259:ARG:HD3	2.17	0.44
1:A:13:PRO:HB3	1:A:89:PRO:CD	2.48	0.43
1:A:28:VAL:HB	1:A:57:ASP:OD2	2.18	0.43
1:B:146:SER:OG	1:B:291:LYS:HB2	2.18	0.43
1:A:197:THR:CG2	1:A:200:CYS:SG	3.06	0.43
1:B:259:ARG:HH22	1:B:334:ASP:CG	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:PRO:HA	1:A:47:GLN:CG	2.48	0.43
1:A:344:LEU:HA	1:A:345:PRO:HD3	1.92	0.43
1:B:111:GLN:O	1:B:115:LEU:HB3	2.18	0.43
1:A:40:LEU:HD12	1:A:40:LEU:C	2.43	0.43
1:A:124:ASN:O	1:A:127:ASP:HB2	2.18	0.43
1:A:494:VAL:HG21	1:B:503:PRO:CD	2.13	0.43
1:B:320:ARG:HH21	1:B:320:ARG:HD3	1.50	0.43
1:A:26:TRP:O	1:A:55:GLY:HA2	2.18	0.43
1:A:485:ALA:C	1:A:487:THR:HG23	2.44	0.43
1:B:197:THR:CG2	1:B:197:THR:O	2.67	0.43
1:A:4:LEU:HD22	1:A:4:LEU:HA	1.40	0.43
1:B:248:ILE:HG21	1:B:248:ILE:HD13	1.76	0.43
1:B:278:PHE:CE2	1:B:347:VAL:HG11	2.54	0.43
1:A:21:LYS:C	1:A:22:PRO:O	2.61	0.43
1:A:424:LEU:HA	1:A:424:LEU:HD23	1.77	0.43
1:A:508:PHE:HZ	1:B:135:THR:HG22	1.83	0.43
1:A:226:MET:HE3	1:A:278:PHE:HB2	2.01	0.42
1:B:187:HIS:ND1	1:B:187:HIS:C	2.77	0.42
1:B:447:VAL:O	1:B:451:ILE:HG13	2.19	0.42
1:A:460:MET:CE	1:B:318:ALA:HA	2.48	0.42
1:B:394:ILE:O	1:B:397:GLN:HB2	2.20	0.42
1:B:396:GLU:OE2	1:B:401:LYS:CD	2.67	0.42
1:A:226:MET:CE	1:A:252:GLN:HG3	2.49	0.42
1:B:146:SER:OG	1:B:291:LYS:HD2	2.20	0.42
1:B:190:VAL:CG2	1:B:223:VAL:HG22	2.49	0.42
1:A:47:GLN:O	1:A:51:LYS:HB2	2.19	0.42
1:B:171:LEU:HD23	1:B:171:LEU:HA	1.85	0.42
1:B:218:GLN:OE1	1:B:448:GLU:OE1	2.38	0.42
1:B:454:LEU:O	1:B:458:ILE:HG13	2.19	0.42
1:A:6:MET:HE2	1:A:6:MET:HB2	1.91	0.42
1:A:289:ARG:HH12	1:A:292:ASP:CG	2.27	0.42
1:B:259:ARG:NH1	1:B:334:ASP:OD2	2.42	0.42
1:A:76:ALA:HA	1:A:77:PRO:HD3	1.94	0.42
1:A:155:ARG:NE	1:B:491:PRO:CB	2.79	0.42
1:B:223:VAL:HG12	1:B:224:PRO:O	2.19	0.42
1:A:482:THR:HG21	1:B:486:ARG:HB3	2.02	0.42
1:B:107:ALA:O	1:B:111:GLN:HB2	2.19	0.42
1:B:209:GLU:H	1:B:209:GLU:HG2	1.38	0.42
1:B:127:ASP:O	1:B:131:LEU:HD22	2.20	0.42
1:B:259:ARG:NH2	1:B:334:ASP:OD2	2.51	0.42
1:B:108:ARG:NH1	1:B:137:THR:HA	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:MET:CG	1:A:8:LYS:HD2	2.50	0.41
1:B:190:VAL:HG13	1:B:221:THR:CG2	2.51	0.41
1:A:226:MET:CE	1:A:252:GLN:CG	2.98	0.41
1:A:464:LEU:HD13	1:B:285:SER:HB3	2.01	0.41
1:B:108:ARG:CZ	1:B:136:LEU:O	2.68	0.41
1:A:100:GLY:O	1:A:102:THR:N	2.53	0.41
1:A:110:GLU:C	1:A:113:LYS:H	2.29	0.41
1:A:162:HIS:HE1	5:A:701:HOH:O	2.02	0.41
1:A:444:ARG:HH11	1:A:444:ARG:HD2	1.35	0.41
1:B:267:LYS:HZ3	1:B:267:LYS:HG3	1.54	0.41
1:B:382:ARG:NH1	1:B:390:GLU:CD	2.77	0.41
1:A:29:ILE:CD1	1:A:58:VAL:HG11	2.45	0.41
1:A:34:TYR:CD1	1:A:80:LYS:HG3	2.55	0.41
1:B:120:ASP:O	1:B:121:ASN:ND2	2.48	0.41
1:B:190:VAL:HG11	1:B:221:THR:CG2	2.49	0.41
1:B:236:GLU:OE2	1:B:268:ASN:ND2	2.50	0.41
1:B:260:LYS:O	1:B:260:LYS:HG3	2.19	0.41
1:A:15:GLU:OE2	1:A:15:GLU:HA	2.21	0.41
1:B:213:ALA:HA	1:B:225:GLN:HE22	1.80	0.41
1:B:241:ALA:O	1:B:242:ALA:C	2.63	0.41
1:B:497:ASN:N	1:B:497:ASN:ND2	2.67	0.41
1:A:121:ASN:HA	1:B:297:PHE:CE2	2.56	0.41
1:A:194:VAL:HG22	1:A:435:PHE:CD1	2.56	0.41
1:A:473:LEU:HD23	1:A:473:LEU:HA	1.80	0.41
1:B:419:LEU:HD11	1:B:461:SER:HB2	2.03	0.41
1:A:51:LYS:HD3	1:A:52:PHE:CE1	2.56	0.41
1:A:392:MET:HG3	1:A:424:LEU:O	2.20	0.41
1:A:493:ASP:CG	1:A:496:TYR:HB3	2.46	0.41
1:B:197:THR:CG2	1:B:436:LEU:CD2	2.70	0.41
1:B:255:VAL:HB	1:B:262:THR:HG21	2.02	0.41
1:A:436:LEU:HD23	1:A:436:LEU:HA	1.92	0.41
1:A:494:VAL:CG2	1:A:495:LEU:H	2.34	0.41
2:A:560:HEM:HBB2	2:A:560:HEM:HMB2	2.03	0.41
1:B:289:ARG:NH1	1:B:292:ASP:CG	2.79	0.41
1:B:470:ILE:HD12	1:B:473:LEU:HD12	2.03	0.41
1:A:11:ILE:O	1:A:85:GLN:N	2.43	0.41
1:A:25:CYS:C	1:A:26:TRP:HD1	2.29	0.41
1:A:121:ASN:HA	1:B:297:PHE:CD2	2.56	0.41
1:A:317:GLY:O	1:A:318:ALA:CB	2.69	0.41
1:A:333:LYS:O	1:A:337:GLU:HG2	2.21	0.41
1:A:348:ILE:CD1	1:A:365:VAL:HG11	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:ASN:O	1:A:373:HIS:CB	2.69	0.41
1:B:178:ASP:O	1:B:469:SER:HA	2.21	0.41
1:B:317:GLY:H	1:B:319:SER:HB2	1.85	0.41
1:A:317:GLY:C	1:A:319:SER:H	2.29	0.40
1:B:109:LYS:CA	1:B:109:LYS:HE3	2.51	0.40
1:B:202:LEU:HD23	1:B:202:LEU:HA	1.90	0.40
1:B:394:ILE:O	1:B:397:GLN:CB	2.70	0.40
1:A:112:LEU:HA	1:A:116:LEU:HG	2.04	0.40
1:A:337:GLU:O	1:A:341:LYS:CD	2.69	0.40
1:B:377:GLN:HB3	5:B:662:HOH:O	2.20	0.40
1:B:108:ARG:HB3	1:B:112:LEU:CD2	2.51	0.40
1:A:26:TRP:CD2	1:A:81:LEU:CD2	3.00	0.40
1:B:190:VAL:HA	1:B:191:PRO:HD3	1.84	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ARG:NH2	1:A:245:ASP:OD1[3_665]	2.09	0.11
1:A:38:ARG:CZ	1:A:245:ASP:OD1[3_665]	2.12	0.08

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	490/511 (96%)	438 (89%)	27 (6%)	25 (5%)		
1	B	396/511 (78%)	353 (89%)	31 (8%)	12 (3%)		
All	All	886/1022 (87%)	791 (89%)	58 (6%)	37 (4%)		

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	5	ASP
1	A	7	ASN
1	A	10	LYS
1	A	22	PRO
1	A	23	ASP
1	A	24	ASP
1	A	25	CYS
1	A	81	LEU
1	A	90	PRO
1	A	91	GLU
1	A	103	LYS
1	A	298	SER
1	A	503	PRO
1	A	504	THR
1	A	508	PHE
1	B	101	GLU
1	B	313	GLU
1	B	314	GLU
1	B	316	GLN
1	B	508	PHE
1	B	510	ASP
1	A	2	PRO
1	A	30	ASN
1	A	85	GLN
1	A	113	LYS
1	B	503	PRO
1	A	6	MET
1	A	318	ALA
1	A	380	PHE
1	B	315	SER
1	B	481	SER
1	B	399	ASN
1	B	120	ASP
1	A	9	GLN
1	B	191	PRO
1	A	89	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	423/440 (96%)	315 (74%)	108 (26%)	0	0
1	B	342/440 (78%)	256 (75%)	86 (25%)	0	1
All	All	765/880 (87%)	571 (75%)	194 (25%)	0	1

All (194) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLU
1	A	3	LYS
1	A	4	LEU
1	A	6	MET
1	A	8	LYS
1	A	10	LYS
1	A	11	ILE
1	A	16	VAL
1	A	18	LYS
1	A	20	ASN
1	A	21	LYS
1	A	27	VAL
1	A	28	VAL
1	A	29	ILE
1	A	30	ASN
1	A	33	VAL
1	A	36	LEU
1	A	37	THR
1	A	38	ARG
1	A	49	VAL
1	A	50	ILE
1	A	52	PHE
1	A	57	ASP
1	A	58	VAL
1	A	63	GLU
1	A	69	ASN
1	A	72	ASP
1	A	79	LYS
1	A	80	LYS
1	A	81	LEU
1	A	84	LEU
1	A	85	GLN
1	A	101	GLU

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Mol	Chain	Res	Type
1	A	102	THR
1	A	103	LYS
1	A	106	ILE
1	A	108	ARG
1	A	109	LYS
1	A	111	GLN
1	A	112	LEU
1	A	113	LYS
1	A	115	LEU
1	A	124	ASN
1	A	125	LEU
1	A	131	LEU
1	A	137	THR
1	A	138	LYS
1	A	139	GLN
1	A	152	VAL
1	A	155	ARG
1	A	162	HIS
1	A	169	LYS
1	A	170	ILE
1	A	175	ARG
1	A	184	LEU
1	A	190	VAL
1	A	197	THR
1	A	212	VAL
1	A	230	LEU
1	A	232	SER
1	A	236	GLU
1	A	240	GLU
1	A	244	SER
1	A	246	LYS
1	A	248	ILE
1	A	252	GLN
1	A	255	VAL
1	A	256	ASN
1	A	265	LEU
1	A	271	LYS
1	A	292	ASP
1	A	297	PHE
1	A	329	SER
1	A	330	LEU
1	A	338	LEU

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Mol	Chain	Res	Type
1	A	339	LYS
1	A	343	LYS
1	A	353	ARG
1	A	365	VAL
1	A	368	VAL
1	A	372	ASN
1	A	378	LEU
1	A	388	LEU
1	A	390	GLU
1	A	395	LEU
1	A	397	GLN
1	A	398	ARG
1	A	399	ASN
1	A	400	LEU
1	A	403	LYS
1	A	408	VAL
1	A	429	VAL
1	A	452	GLU
1	A	462	MET
1	A	464	LEU
1	A	465	LEU
1	A	472	GLU
1	A	477	LEU
1	A	482	THR
1	A	483	LEU
1	A	490	VAL
1	A	496	TYR
1	A	497	ASN
1	A	499	VAL
1	A	501	GLU
1	A	504	THR
1	A	505	LEU
1	A	509	GLU
1	B	102	THR
1	B	103	LYS
1	B	105	ASP
1	B	109	LYS
1	B	111	GLN
1	B	112	LEU
1	B	115	LEU
1	B	120	ASP
1	B	125	LEU

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Mol	Chain	Res	Type
1	B	131	LEU
1	B	133	SER
1	B	134	GLN
1	B	139	GLN
1	B	152	VAL
1	B	170	ILE
1	B	176	LYS
1	B	177	VAL
1	B	184	LEU
1	B	186	SER
1	B	188	VAL
1	B	195	SER
1	B	197	THR
1	B	209	GLU
1	B	220	VAL
1	B	222	LYS
1	B	225	GLN
1	B	230	LEU
1	B	236	GLU
1	B	237	GLU
1	B	244	SER
1	B	245	ASP
1	B	248	ILE
1	B	249	GLN
1	B	252	GLN
1	B	255	VAL
1	B	256	ASN
1	B	257	SER
1	B	260	LYS
1	B	263	ASP
1	B	267	LYS
1	B	268	ASN
1	B	275	LYS
1	B	294	LYS
1	B	295	LEU
1	B	312	VAL
1	B	313	GLU
1	B	320	ARG
1	B	323	SER
1	B	324	LYS
1	B	325	PHE
1	B	330	LEU

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Mol	Chain	Res	Type
1	B	331	THR
1	B	337	GLU
1	B	343	LYS
1	B	353	ARG
1	B	355	GLU
1	B	365	VAL
1	B	368	VAL
1	B	370	LEU
1	B	373	HIS
1	B	378	LEU
1	B	388	LEU
1	B	391	THR
1	B	396	GLU
1	B	397	GLN
1	B	398	ARG
1	B	404	LEU
1	B	408	VAL
1	B	429	VAL
1	B	448	GLU
1	B	462	MET
1	B	464	LEU
1	B	477	LEU
1	B	481	SER
1	B	483	LEU
1	B	484	LYS
1	B	488	VAL
1	B	490	VAL
1	B	492	ASN
1	B	496	TYR
1	B	497	ASN
1	B	498	GLU
1	B	504	THR
1	B	506	THR
1	B	508	PHE
1	B	509	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	HIS
1	A	20	ASN
1	A	53	ASN

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Mol	Chain	Res	Type
1	A	69	ASN
1	A	85	GLN
1	A	124	ASN
1	A	139	GLN
1	A	157	ASN
1	A	159	ASN
1	A	218	GLN
1	A	225	GLN
1	A	249	GLN
1	A	252	GLN
1	A	256	ASN
1	A	372	ASN
1	A	377	GLN
1	A	439	ASN
1	B	121	ASN
1	B	124	ASN
1	B	134	GLN
1	B	139	GLN
1	B	204	ASN
1	B	218	GLN
1	B	225	GLN
1	B	247	GLN
1	B	249	GLN
1	B	252	GLN
1	B	256	ASN
1	B	377	GLN
1	B	492	ASN
1	B	497	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	A	560	1	50,50,50	1.42	11 (22%)	67,82,82	1.59	12 (17%)
3	FMN	B	570	-	33,33,33	1.07	1 (3%)	48,50,50	2.25	15 (31%)
4	PYR	B	580	-	5,5,5	5.53	4 (80%)	3,6,6	4.69	2 (66%)
3	FMN	A	570	-	33,33,33	0.99	1 (3%)	48,50,50	2.17	15 (31%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	560	1	-	3/14/54/54	-
3	FMN	B	570	-	-	5/18/18/18	0/3/3/3
4	PYR	B	580	-	-	0/4/4/4	-
3	FMN	A	570	-	1/1/4/4	3/18/18/18	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	580	PYR	CB-CA	8.85	1.67	1.50
4	B	580	PYR	O3-CA	7.15	1.39	1.23
4	B	580	PYR	CA-C	-4.33	1.40	1.54
2	A	560	HEM	CAC-C3C	3.21	1.55	1.47
2	A	560	HEM	FE-NA	2.77	2.04	1.95
2	A	560	HEM	CMD-C2D	2.72	1.56	1.50
2	A	560	HEM	FE-ND	2.56	2.02	1.94
2	A	560	HEM	FE-NC	2.53	2.03	1.95
2	A	560	HEM	CAB-C3B	2.34	1.53	1.47
3	A	570	FMN	C9A-N10	-2.31	1.37	1.41
2	A	560	HEM	CAD-C3D	2.27	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	560	HEM	CMA-C3A	2.23	1.55	1.50
2	A	560	HEM	CMC-C2C	2.21	1.55	1.50
2	A	560	HEM	O2A-CGA	-2.21	1.23	1.30
4	B	580	PYR	O-C	2.19	1.28	1.22
3	B	570	FMN	P-O5'	-2.12	1.53	1.60
2	A	560	HEM	C3B-C2B	-2.00	1.33	1.37

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	580	PYR	O3-CA-CB	-7.71	102.50	119.77
3	B	570	FMN	C4'-C3'-C2'	6.53	124.43	113.57
3	B	570	FMN	O2P-P-O5'	6.43	123.44	106.67
3	A	570	FMN	C4'-C3'-C2'	6.11	123.74	113.57
2	A	560	HEM	CAA-CBA-CGA	4.81	126.42	113.67
2	A	560	HEM	O1A-CGA-CBA	-4.39	109.18	123.09
3	A	570	FMN	O3'-C3'-C2'	-4.38	98.97	108.93
3	A	570	FMN	O3'-C3'-C4'	4.27	118.64	108.93
2	A	560	HEM	CHD-C1D-ND	4.17	128.91	124.42
3	A	570	FMN	O4'-C4'-C5'	3.80	118.36	109.99
2	A	560	HEM	O2A-CGA-CBA	3.79	125.97	114.00
3	B	570	FMN	O5'-P-O1P	3.77	116.62	106.44
3	B	570	FMN	O4'-C4'-C3'	3.75	118.03	109.25
3	A	570	FMN	C1'-C2'-C3'	3.66	119.59	109.66
3	A	570	FMN	C5'-C4'-C3'	-3.66	105.32	112.22
3	A	570	FMN	O2-C2-N1	3.64	127.85	121.80
3	A	570	FMN	O2'-C2'-C3'	3.46	117.34	109.25
3	B	570	FMN	C9A-C5A-N5	-3.44	118.81	122.45
3	B	570	FMN	O4'-C4'-C5'	3.41	117.51	109.99
3	B	570	FMN	O3'-C3'-C2'	-3.37	101.27	108.93
2	A	560	HEM	CMB-C2B-C1B	-3.30	119.88	125.03
3	A	570	FMN	C9A-C5A-N5	-3.22	119.04	122.45
3	A	570	FMN	C6-C5A-N5	3.06	123.53	118.44
3	B	570	FMN	O3P-P-O1P	-3.02	99.07	110.83
3	A	570	FMN	O2'-C2'-C1'	2.78	121.62	110.20
3	B	570	FMN	O2'-C2'-C3'	2.62	115.38	109.25
3	B	570	FMN	O3P-P-O2P	-2.59	98.08	107.80
2	A	560	HEM	O1D-CGD-CBD	-2.57	114.93	123.09
3	A	570	FMN	C10-N1-C2	2.53	122.33	116.85
3	B	570	FMN	O3'-C3'-C4'	2.52	114.66	108.93
3	A	570	FMN	C7M-C7-C6	2.51	123.99	119.57
3	B	570	FMN	C7M-C7-C6	2.46	123.91	119.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	560	HEM	C4C-CHD-C1D	-2.39	120.94	126.02
2	A	560	HEM	CBD-CAD-C3D	-2.37	105.97	112.53
2	A	560	HEM	CBB-CAB-C3B	-2.31	115.98	127.53
2	A	560	HEM	CHC-C4B-NB	-2.23	122.02	124.42
3	B	570	FMN	C6-C7-C8	-2.23	116.41	119.69
2	A	560	HEM	O2D-CGD-CBD	2.22	121.03	114.00
3	A	570	FMN	N3-C2-N1	-2.21	114.81	119.50
2	A	560	HEM	CBC-CAC-C3C	-2.18	116.64	127.53
3	A	570	FMN	C4-C4A-N5	2.15	121.18	118.21
4	B	580	PYR	OXT-C-CA	2.10	119.41	113.59
3	B	570	FMN	O3P-P-O5'	2.03	111.96	106.67
3	B	570	FMN	O2'-C2'-C1'	2.03	118.53	110.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	570	FMN	C2'

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	570	FMN	O2'-C2'-C3'-C4'
3	A	570	FMN	O2'-C2'-C3'-O3'
3	B	570	FMN	C2'-C3'-C4'-O4'
3	A	570	FMN	C4'-C5'-O5'-P
3	B	570	FMN	C4'-C5'-O5'-P
3	B	570	FMN	O2'-C2'-C3'-C4'
3	B	570	FMN	O4'-C4'-C5'-O5'
2	A	560	HEM	CAD-CBD-CGD-O2D
2	A	560	HEM	CAD-CBD-CGD-O1D
3	B	570	FMN	O3'-C3'-C4'-O4'
2	A	560	HEM	CAA-CBA-CGA-O2A

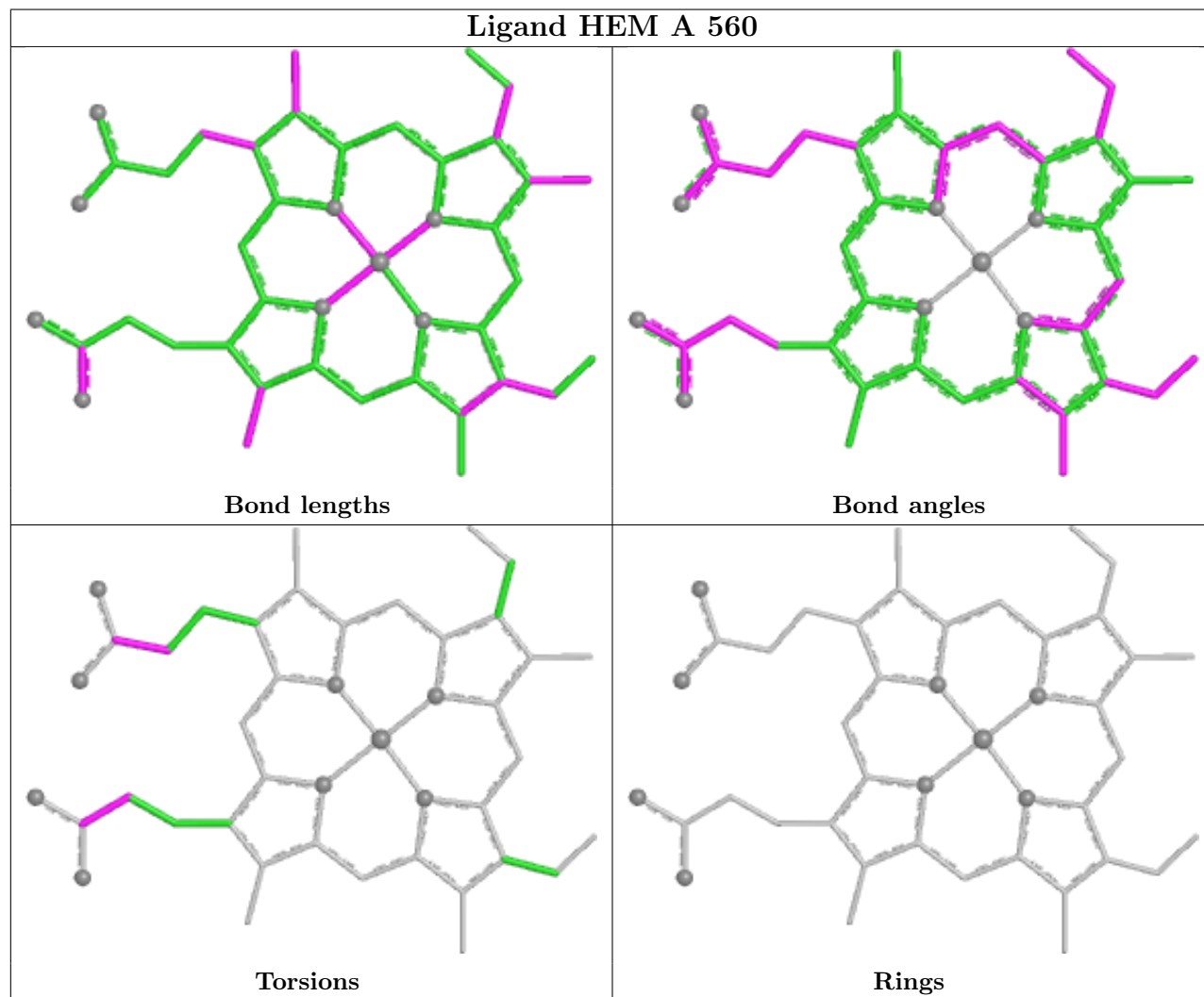
There are no ring outliers.

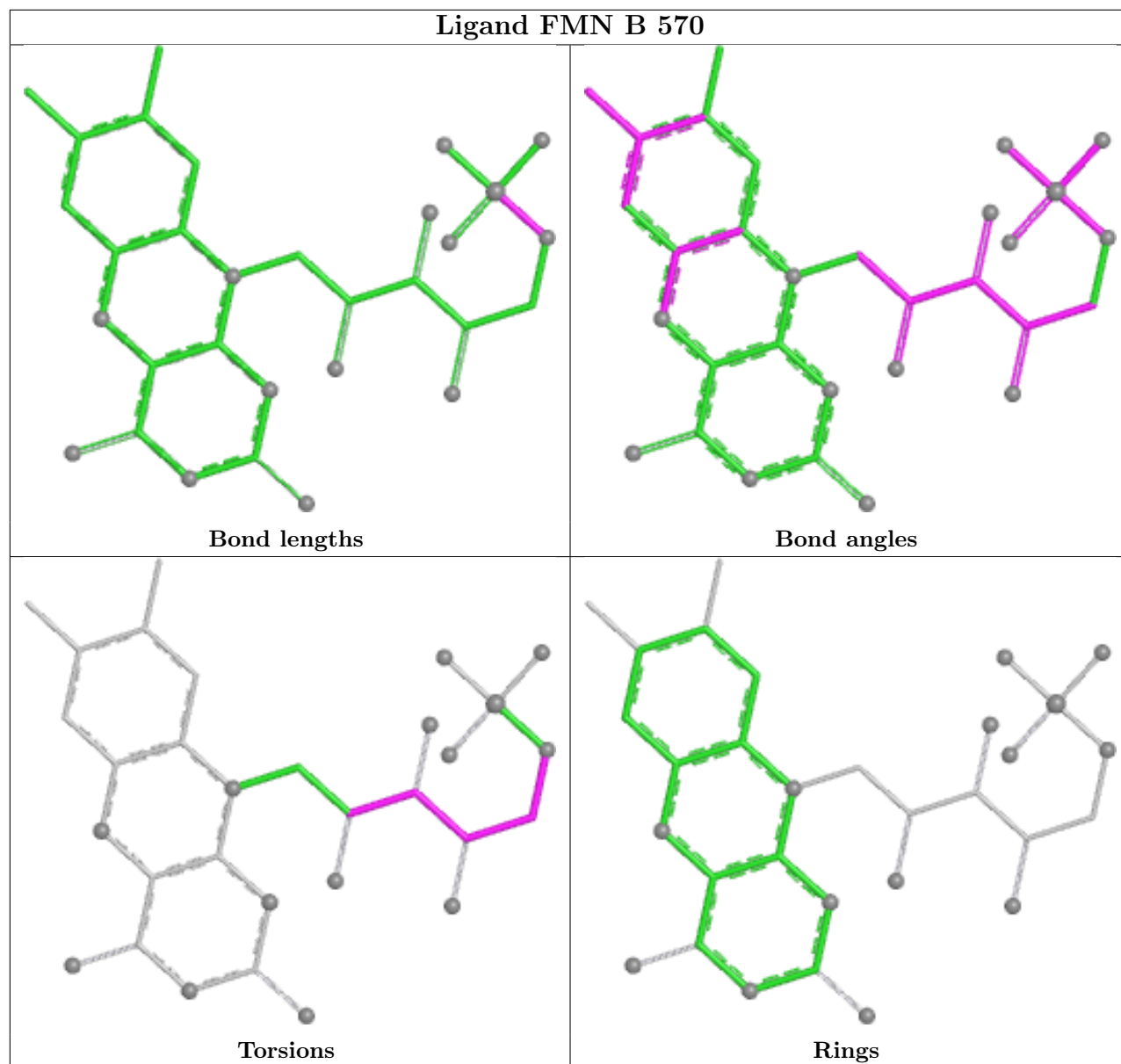
2 monomers are involved in 11 short contacts:

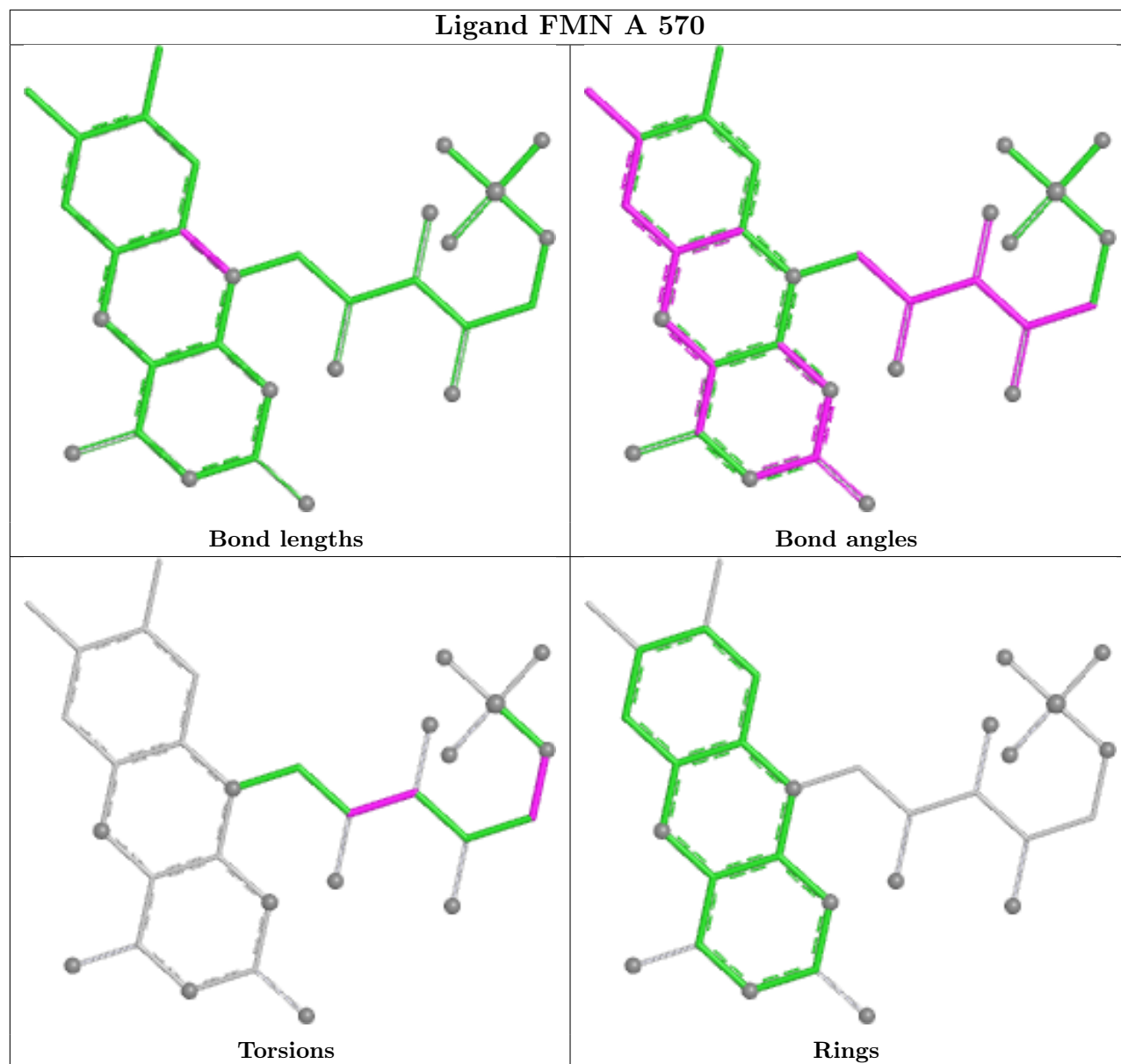
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	560	HEM	9	0
3	B	570	FMN	2	0

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.