



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 07:44 PM UTC

PDB ID : 2OZ0 / pdb_00002oz0
Title : Mechanistic and Structural Studies of H373Q Flavocytochrome b2: Effects of Mutating the Active Site Base
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Deposited on : 2007-02-23
Resolution : 2.80 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) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

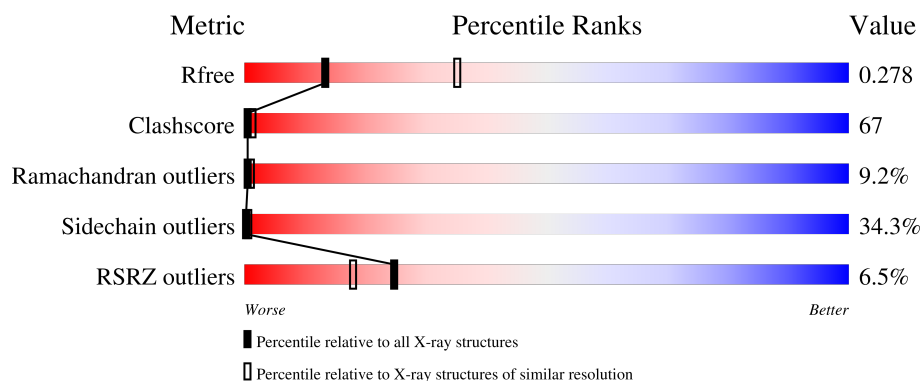
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	511	7% 8% 29% 39% 20% .
1	B	511	5% 6% 22% 28% 22% 23%

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	569	X	-	X	-
3	FMN	B	570	-	-	X	-
4	PYR	B	571	-	X	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7042 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.

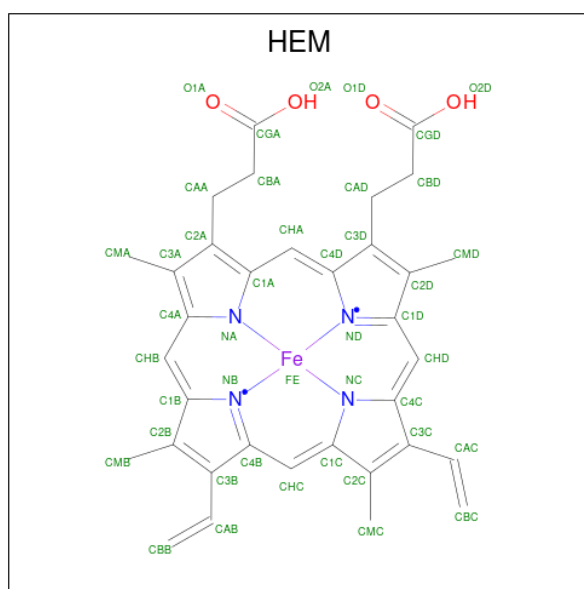
- Molecule 1 is a protein called Cytochrome b2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	492	Total	C	N	O	S	0	0	0
			3833	2441	649	728	15			
1	B	396	Total	C	N	O	S	0	0	0
			3081	1953	524	593	11			

There are 2 discrepancies between the modelled and reference sequences:

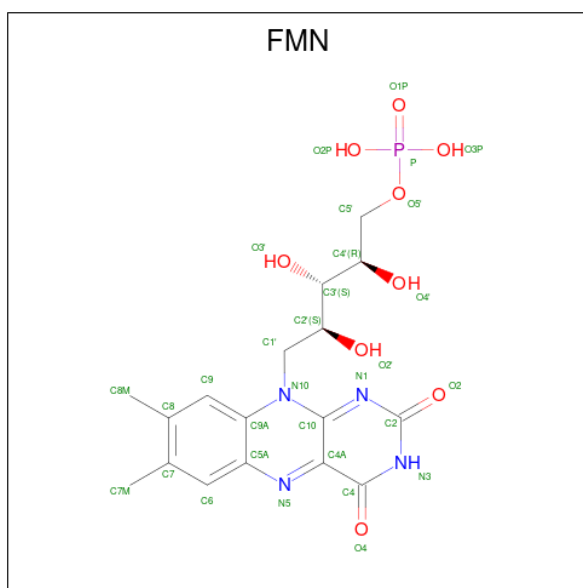
Chain	Residue	Modelled	Actual	Comment	Reference
A	373	GLN	HIS	engineered mutation	UNP P00175
B	373	GLN	HIS	engineered mutation	UNP P00175

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



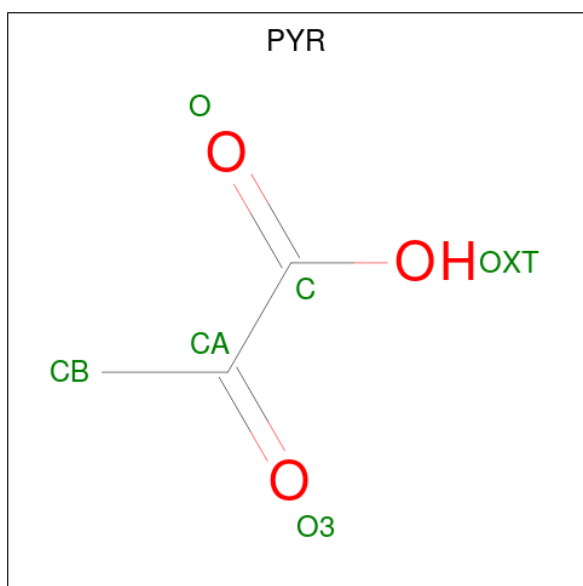
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- 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		

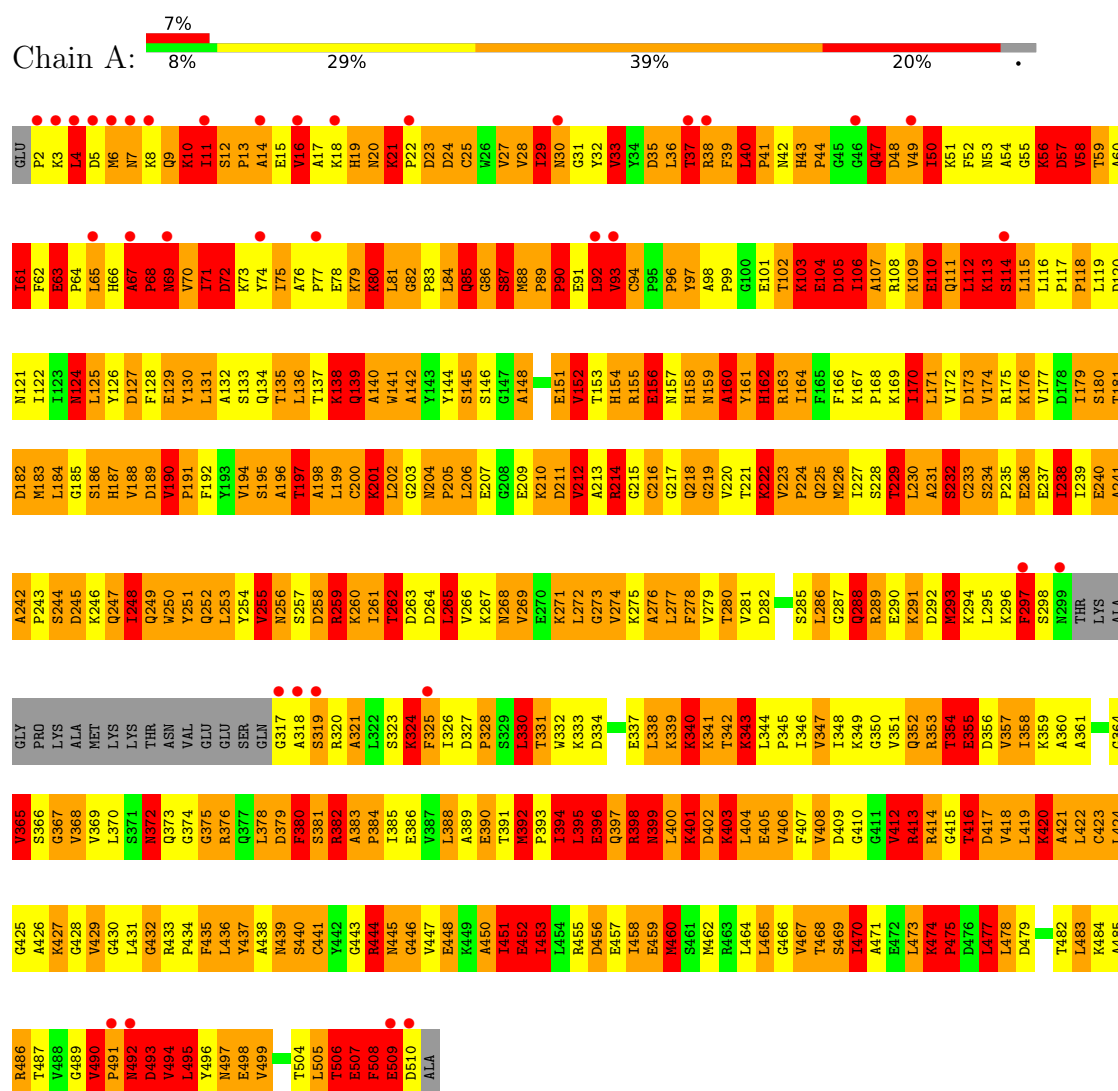
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	7	Total 7	O 7	0	0
5	B	10	Total 10	O 10	0	0

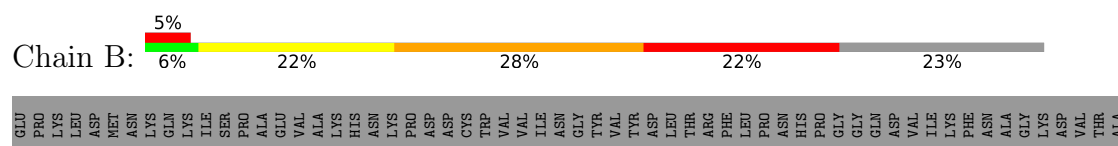
3 Residue-property plots

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Cytochrome b2



• Molecule 1: Cytochrome b2



L483	K484	A485	R486	T487	Y488	G489	Y490	P491	N492	D493	Y494	L495	Y496	N497	E498	Y499	Y500	E501	T504	L505	T506	E507	F508	E509	D510	ALA																																		
L422	C423	L424	G425	A426	K427	G428	V429	G430	L431	G432	R433	L436	Y437	A438	M439	S440	C441	Y442	G443	R444	N445	G446	Y447	E448	K449	A450	I451	E452	I453	L454	R455	D456	E457	I458	E459	M460	S461	M462	R463	L464	L465	G466	V467	T468	S469	I470	A471	E472	L473	K474	P475	D476	L477	L478	D479	L480	S481	T482		
E362	I363	G364	V365	S366	G367	V368	V369	L370	S371	N372	Q373	G374	G375	R376	Q377	L378	D379	F380	R381	R382	G443	A383	P384	I385	E386	V387	L388	A389	E390	T391	M392	P393	I394	L395	E396	Q397	R398	N399	L400	K401	D402	K403	L404	E405	V406	F407	V408	D409	G410	G411	V412	R413	R414	G415	T416	D417	V418	L419	K420	A421
ALA	GLY	PRO	LYS	ALA	MET	LYS	LYS	THR	ASN	VAL	GLU	GLU	SER	GLN	G317	A318	S319	R320	A321	L322	S323	K324	F325	I326	D327	P328	S329	L330	T331	W332	K333	D334	I335	E336	E337	L338	K339	K340	K341	T342	K343	L344	P345	I346	V347	I348	K349	G350	V351	Q352	R353	T354	E355	D356	V357	I358	K359	A360	A361	
A241	A242	P243	S244	D245	K246	MET	LYS	T248	Q249	W250	Y251	Q252	L253	Y254	V255	N256	S257	R258	K260	L261	T262	D263	D264	L265	V266	K267	N268	E269	E270	K271	L272	G273	V274	A275	A276	L277	F278	V279	T280	V281	D282	A283	P284	S285	L286	I287	R289	E290	K291	D292	M293	K294	L295	D296	F297	S298	N299	THR	LYS	
T181	D182	M183	L184	G185	S186	H187	V188	D189	Y190	P191	F192	Y193	V194	S195	A196	T197	A198	L199	C200	K201	L202	G203	N204	P205	L206	E207	G208	E209	K210	D211	V212	A213	R214	G215	C216	G217	Q218	G219	V220	T221	K222	V223	P224	Q225	M226	I227	S228	T229	L230	K231	S232	C233	S234	P235	E236	E237	I238	I239	E240	
N121	I122	I123	N124	L125	Y126	D127	F128	E129	Y130	L131	A132	S133	Q134	T135	L136	T137	K138	Q139	A140	W141	A142	Y143	Y144	S145	S146	G147	A148	N149	D150	F151	V152	T153	H154	R155	E156	M157	H158	N159	A160	Y161	H162	R163	I164	F165	F166	K167	P168	K169	L170	L171	V172	D173	V174	R175	K176	V177	D178	I179	S180	
ILE	PHE	GLU	PRO	LEU	HIS	ALA	PRO	ASN	VAL	ILE	ASP	LYS	TYR	ILE	ALA	PRO	GLU	LYS	LYS	LEU	GLY	PRO	LEU	GLN	GLY	SER	MET	PRO	PRO	GLU	LEU	VAL	CYS	PRO	PRO	TYR	A98	P99	G100	T101	T102	K103	E104	D105	I106	A107	R108	K109	E110	Q111	L112	K113	S114	L115	L116	P117	P118	I119	D120	

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	163.69Å 163.69Å 112.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.80 50.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	87.6 (50.00-2.80) 87.5 (50.00-2.80)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.206 , 0.278 0.227 , 0.278	Depositor DCC
R_{free} test set	2123 reflections (3.33%)	wwPDB-VP
Wilson B-factor (Å ²)	62.3	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 64.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7042	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	2.46	200/3907 (5.1%)	3.24	535/5291 (10.1%)
1	B	2.32	130/3130 (4.2%)	3.18	424/4230 (10.0%)
All	All	2.40	330/7037 (4.7%)	3.21	959/9521 (10.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	2	57
1	B	4	64
All	All	6	121

All (330) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	421	ALA	CA-CB	-14.29	1.30	1.53
1	A	248	ILE	CA-CB	-13.07	1.35	1.54
1	A	223	VAL	C-O	12.90	1.33	1.24
1	A	89	PRO	C-N	-12.78	1.19	1.33
1	A	61	ILE	C-O	-11.71	1.11	1.23
1	B	123	ILE	CA-CB	-11.60	1.38	1.54
1	A	470	ILE	CA-CB	-11.47	1.38	1.54
1	A	266	VAL	CA-CB	-11.34	1.40	1.54
1	A	509	GLU	C-O	11.24	1.40	1.23
1	B	406	VAL	CA-CB	-10.89	1.40	1.54
1	A	222	LYS	C-O	10.55	1.36	1.23
1	B	196	ALA	CA-CB	10.55	1.66	1.53
1	B	495	LEU	C-O	-10.35	1.12	1.24
1	B	163	ARG	C-O	10.32	1.39	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	351	VAL	CA-CB	-10.18	1.43	1.54
1	B	491	PRO	C-N	10.14	1.46	1.33
1	A	426	ALA	CA-CB	-10.11	1.36	1.53
1	B	407	PHE	C-N	-10.05	1.20	1.33
1	A	351	VAL	C-O	-10.01	1.12	1.24
1	B	389	ALA	CA-CB	-10.00	1.36	1.53
1	A	358	ILE	CA-CB	-9.94	1.42	1.54
1	B	137	THR	CB-CG2	9.92	1.85	1.52
1	B	289	ARG	CG-CD	9.85	1.81	1.52
1	B	447	VAL	CA-CB	-9.85	1.41	1.54
1	B	160	ALA	CA-CB	-9.78	1.35	1.53
1	A	154	HIS	CA-C	-9.63	1.40	1.52
1	A	142	ALA	CA-CB	-9.55	1.38	1.53
1	B	406	VAL	C-N	-9.30	1.20	1.33
1	A	418	VAL	CA-CB	-9.30	1.43	1.54
1	A	360	ALA	CA-CB	-9.27	1.39	1.53
1	A	40	LEU	C-N	9.25	1.43	1.34
1	B	369	VAL	CA-CB	-9.09	1.43	1.54
1	B	289	ARG	CB-CG	9.09	1.79	1.52
1	B	290	GLU	CA-C	-9.00	1.41	1.52
1	A	242	ALA	CA-CB	-8.99	1.38	1.53
1	A	93	VAL	CA-CB	8.96	1.66	1.54
1	B	441	CYS	CA-C	-8.96	1.43	1.52
1	A	390	GLU	C-N	-8.94	1.21	1.33
1	A	116	LEU	CA-C	-8.94	1.43	1.53
1	A	321	ALA	C-O	-8.94	1.12	1.24
1	A	343	LYS	CB-CG	8.86	1.79	1.52
1	A	413	ARG	CG-CD	8.82	1.78	1.52
1	A	407	PHE	C-O	-8.81	1.10	1.24
1	A	420	LYS	CA-C	8.80	1.64	1.52
1	B	433	ARG	C-N	8.62	1.45	1.34
1	A	465	LEU	N-CA	-8.57	1.34	1.46
1	B	167	LYS	C-O	-8.57	1.13	1.24
1	A	219	GLY	C-O	8.54	1.32	1.23
1	B	465	LEU	N-CA	-8.53	1.34	1.46
1	A	57	ASP	C-N	-8.50	1.22	1.33
1	A	129	GLU	N-CA	-8.47	1.36	1.46
1	B	175	ARG	CG-CD	8.40	1.77	1.52
1	A	196	ALA	CA-CB	-8.32	1.41	1.53
1	B	335	ILE	CA-CB	8.28	1.65	1.54
1	B	317	GLY	C-N	-8.26	1.22	1.33
1	A	238	ILE	CA-CB	-8.24	1.42	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	463	ARG	C-O	8.23	1.34	1.24
1	B	223	VAL	C-O	8.21	1.34	1.24
1	A	197	THR	N-CA	-8.21	1.36	1.45
1	A	446	GLY	C-O	8.19	1.34	1.23
1	A	198	ALA	CA-CB	-8.15	1.39	1.53
1	A	251	TYR	C-O	8.12	1.33	1.23
1	A	187	HIS	CA-C	-8.11	1.43	1.52
1	A	196	ALA	CA-C	-8.10	1.42	1.52
1	B	253	LEU	N-CA	-8.02	1.36	1.46
1	B	218	GLN	CA-C	7.98	1.63	1.52
1	A	278	PHE	N-CA	-7.96	1.36	1.46
1	A	392	MET	C-N	7.92	1.44	1.33
1	B	467	VAL	CA-CB	-7.90	1.44	1.55
1	A	406	VAL	CA-CB	-7.89	1.45	1.54
1	B	417	ASP	C-O	7.86	1.33	1.24
1	A	470	ILE	N-CA	-7.85	1.36	1.46
1	A	485	ALA	CA-CB	-7.81	1.41	1.53
1	A	428	GLY	C-O	-7.78	1.13	1.23
1	B	99	PRO	N-CD	7.78	1.58	1.47
1	A	212	VAL	N-CA	-7.77	1.37	1.46
1	A	440	SER	C-O	-7.75	1.14	1.24
1	A	286	LEU	CG-CD1	7.72	1.78	1.52
1	A	228	SER	C-O	7.70	1.33	1.23
1	B	474	LYS	C-N	7.68	1.43	1.33
1	B	368	VAL	CA-CB	-7.63	1.46	1.55
1	B	122	ILE	CA-CB	-7.57	1.44	1.54
1	A	424	LEU	CA-C	-7.56	1.42	1.52
1	A	163	ARG	CA-C	-7.54	1.42	1.52
1	B	429	VAL	CA-CB	7.52	1.64	1.54
1	B	492	ASN	C-O	7.46	1.34	1.23
1	A	152	VAL	CA-C	-7.46	1.42	1.52
1	B	253	LEU	CA-C	-7.38	1.43	1.52
1	A	416	THR	CA-CB	-7.35	1.41	1.53
1	B	176	LYS	CA-C	-7.29	1.43	1.52
1	A	343	LYS	CD-CE	7.26	1.74	1.52
1	A	508	PHE	C-N	7.25	1.46	1.33
1	B	173	ASP	CA-C	-7.21	1.43	1.52
1	A	190	VAL	CA-CB	-7.19	1.44	1.54
1	A	242	ALA	CA-C	-7.18	1.44	1.52
1	B	202	LEU	C-O	-7.17	1.15	1.24
1	B	446	GLY	C-O	7.15	1.33	1.23
1	A	227	ILE	C-O	7.12	1.32	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	340	LYS	CE-NZ	7.12	1.70	1.49
1	A	330	LEU	CA-C	-7.11	1.43	1.52
1	A	282	ASP	C-O	7.10	1.33	1.23
1	A	423	CYS	CA-C	-7.07	1.42	1.52
1	A	155	ARG	CA-CB	-7.07	1.42	1.53
1	B	428	GLY	N-CA	6.97	1.51	1.45
1	B	289	ARG	CA-CB	6.95	1.61	1.52
1	A	195	SER	CA-C	-6.95	1.43	1.53
1	A	275	LYS	CA-C	-6.95	1.43	1.52
1	B	462	MET	N-CA	-6.89	1.37	1.46
1	A	218	GLN	N-CA	-6.87	1.38	1.46
1	B	289	ARG	NE-CZ	6.85	1.40	1.33
1	A	490	VAL	CA-C	6.84	1.59	1.52
1	B	285	SER	CA-C	-6.84	1.44	1.52
1	B	99	PRO	C-O	6.83	1.32	1.24
1	B	290	GLU	C-O	-6.80	1.16	1.24
1	A	370	LEU	CA-CB	-6.79	1.44	1.53
1	A	129	GLU	CA-CB	-6.78	1.42	1.53
1	B	186	SER	N-CA	6.78	1.55	1.45
1	B	488	VAL	C-O	6.77	1.31	1.24
1	B	253	LEU	C-O	6.75	1.31	1.23
1	A	410	GLY	N-CA	-6.73	1.35	1.45
1	A	491	PRO	CA-C	6.70	1.58	1.52
1	A	276	ALA	C-O	6.70	1.31	1.23
1	A	417	ASP	C-O	6.69	1.31	1.24
1	B	189	ASP	C-N	-6.68	1.25	1.33
1	A	340	LYS	CD-CE	6.68	1.72	1.52
1	A	266	VAL	CB-CG2	-6.63	1.30	1.52
1	A	249	GLN	CA-C	6.61	1.60	1.52
1	A	33	VAL	N-CA	6.60	1.53	1.46
1	A	341	LYS	CG-CD	6.59	1.72	1.52
1	B	167	LYS	CE-NZ	6.59	1.69	1.49
1	A	330	LEU	CA-CB	-6.55	1.43	1.53
1	A	375	GLY	C-N	-6.53	1.24	1.33
1	A	403	LYS	C-O	-6.52	1.15	1.24
1	B	198	ALA	N-CA	6.48	1.54	1.46
1	B	197	THR	N-CA	-6.47	1.37	1.47
1	A	255	VAL	CA-CB	-6.47	1.46	1.54
1	A	277	LEU	CA-CB	-6.46	1.41	1.53
1	A	202	LEU	C-O	-6.46	1.16	1.24
1	A	347	VAL	CA-CB	-6.43	1.46	1.54
1	A	348	ILE	C-O	6.43	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	180	SER	C-N	-6.42	1.24	1.33
1	B	187	HIS	C-N	-6.41	1.25	1.33
1	B	441	CYS	CB-SG	6.39	2.02	1.81
1	A	368	VAL	C-O	-6.38	1.16	1.23
1	A	412	VAL	CA-CB	-6.38	1.46	1.54
1	A	429	VAL	C-O	-6.38	1.17	1.24
1	A	220	VAL	CA-C	-6.35	1.44	1.53
1	B	470	ILE	CA-CB	-6.33	1.45	1.54
1	A	323	SER	CA-C	-6.32	1.44	1.52
1	B	222	LYS	C-O	6.31	1.30	1.23
1	A	189	ASP	CA-C	-6.30	1.44	1.52
1	B	175	ARG	C-O	-6.30	1.16	1.24
1	A	253	LEU	C-O	6.29	1.31	1.24
1	A	478	LEU	CA-C	-6.28	1.45	1.52
1	A	191	PRO	CA-C	6.26	1.61	1.52
1	A	444	ARG	CZ-NH2	6.26	1.41	1.33
1	A	279	VAL	CA-CB	-6.25	1.46	1.54
1	A	233	CYS	CA-C	-6.23	1.44	1.53
1	A	450	ALA	CA-CB	-6.23	1.43	1.53
1	A	225	GLN	CD-NE2	6.22	1.46	1.33
1	A	154	HIS	CA-CB	-6.19	1.43	1.53
1	B	345	PRO	C-O	6.19	1.32	1.24
1	A	56	LYS	CA-C	6.18	1.60	1.52
1	B	261	ILE	N-CA	6.17	1.54	1.46
1	A	382	ARG	C-O	-6.14	1.15	1.23
1	B	368	VAL	CB-CG1	-6.13	1.32	1.52
1	A	169	LYS	CG-CD	-6.13	1.34	1.52
1	B	382	ARG	CA-CB	-6.12	1.43	1.53
1	B	286	LEU	CA-C	6.10	1.61	1.53
1	A	495	LEU	C-O	-6.08	1.17	1.24
1	A	164	ILE	CA-CB	-6.07	1.47	1.54
1	A	418	VAL	C-O	6.07	1.31	1.24
1	A	390	GLU	CG-CD	6.05	1.67	1.52
1	A	339	LYS	N-CA	-6.05	1.38	1.46
1	A	421	ALA	C-O	6.04	1.31	1.24
1	A	274	VAL	CB-CG2	6.03	1.72	1.52
1	A	155	ARG	CA-C	-6.02	1.45	1.52
1	B	440	SER	N-CA	-6.01	1.38	1.46
1	A	414	ARG	C-O	6.00	1.31	1.23
1	B	252	GLN	CA-C	-6.00	1.45	1.52
1	B	431	LEU	C-O	-5.99	1.16	1.23
1	A	190	VAL	C-O	-5.98	1.19	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	106	ILE	CG1-CD1	5.96	1.75	1.51
1	A	367	GLY	C-O	5.94	1.30	1.24
1	A	490	VAL	C-O	-5.94	1.17	1.24
1	A	297	PHE	C-N	-5.94	1.26	1.33
1	B	423	CYS	N-CA	-5.93	1.38	1.46
1	B	464	LEU	CA-CB	-5.93	1.42	1.53
1	A	126	TYR	CA-CB	-5.93	1.43	1.53
1	A	353	ARG	CA-C	-5.91	1.45	1.52
1	A	134	GLN	CA-C	-5.89	1.44	1.52
1	A	343	LYS	CA-C	5.88	1.60	1.52
1	A	331	THR	CA-C	-5.87	1.45	1.52
1	A	242	ALA	N-CA	-5.87	1.36	1.46
1	A	146	SER	CA-C	-5.87	1.45	1.52
1	B	231	ALA	N-CA	5.86	1.53	1.45
1	B	439	ASN	CA-C	-5.86	1.45	1.52
1	A	422	LEU	CA-CB	-5.85	1.44	1.53
1	B	322	LEU	CA-C	5.85	1.60	1.52
1	A	368	VAL	CB-CG1	-5.81	1.33	1.52
1	A	297	PHE	CA-C	5.77	1.58	1.53
1	A	145	SER	N-CA	-5.76	1.38	1.46
1	A	417	ASP	CB-CG	5.75	1.66	1.52
1	B	368	VAL	N-CA	5.75	1.53	1.46
1	A	298	SER	C-N	-5.74	1.25	1.33
1	B	501	GLU	CD-OE1	5.73	1.36	1.25
1	A	63	GLU	C-O	-5.73	1.19	1.24
1	B	360	ALA	C-N	5.73	1.41	1.33
1	B	262	THR	CA-CB	5.72	1.61	1.53
1	A	130	TYR	CA-CB	-5.71	1.44	1.53
1	B	168	PRO	N-CD	-5.71	1.39	1.47
1	A	224	PRO	N-CA	5.71	1.54	1.47
1	A	261	ILE	CA-CB	-5.69	1.46	1.54
1	B	488	VAL	CA-C	5.69	1.60	1.52
1	B	382	ARG	CB-CG	-5.67	1.35	1.52
1	B	104	GLU	N-CA	-5.66	1.38	1.46
1	A	453	ILE	C-O	-5.66	1.17	1.24
1	A	405	GLU	CA-C	-5.66	1.46	1.52
1	A	231	ALA	CA-CB	-5.64	1.43	1.53
1	A	110	GLU	N-CA	-5.64	1.38	1.46
1	A	10	LYS	N-CA	5.62	1.53	1.46
1	A	64	PRO	N-CD	5.62	1.55	1.47
1	A	493	ASP	N-CA	-5.62	1.39	1.46
1	A	378	LEU	C-N	-5.62	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	317	GLY	CA-C	5.60	1.62	1.52
1	A	194	VAL	C-O	5.58	1.30	1.23
1	B	251	TYR	CA-C	-5.58	1.45	1.52
1	A	407	PHE	CA-CB	-5.57	1.44	1.53
1	A	496	TYR	CA-CB	-5.57	1.44	1.53
1	B	182	ASP	N-CA	-5.56	1.39	1.46
1	A	420	LYS	CG-CD	5.55	1.69	1.52
1	A	107	ALA	N-CA	5.54	1.53	1.46
1	B	420	LYS	N-CA	-5.52	1.39	1.46
1	A	428	GLY	N-CA	5.51	1.53	1.45
1	B	406	VAL	C-O	-5.51	1.18	1.24
1	B	116	LEU	C-N	-5.51	1.26	1.33
1	A	118	PRO	CA-C	-5.50	1.46	1.52
1	A	65	LEU	N-CA	5.50	1.51	1.46
1	A	234	SER	C-O	-5.49	1.16	1.23
1	B	122	ILE	N-CA	-5.47	1.39	1.46
1	B	468	THR	N-CA	5.47	1.53	1.46
1	A	12	SER	N-CA	-5.47	1.38	1.46
1	B	159	ASN	N-CA	-5.47	1.39	1.46
1	B	450	ALA	CA-CB	-5.45	1.45	1.53
1	A	357	VAL	CA-CB	-5.44	1.47	1.54
1	A	126	TYR	N-CA	-5.43	1.39	1.46
1	A	90	PRO	C-N	-5.43	1.26	1.33
1	B	190	VAL	C-O	-5.42	1.17	1.24
1	B	344	LEU	N-CA	5.41	1.53	1.46
1	A	416	THR	C-O	5.40	1.30	1.24
1	A	419	LEU	N-CA	-5.40	1.40	1.46
1	B	500	TYR	CG-CD1	-5.40	1.28	1.39
1	B	477	LEU	C-O	-5.40	1.16	1.24
1	B	223	VAL	CA-C	-5.39	1.47	1.52
1	A	3	LYS	N-CA	5.38	1.53	1.46
1	B	123	ILE	CA-C	-5.38	1.46	1.52
1	B	423	CYS	C-O	5.38	1.30	1.24
1	B	103	LYS	C-N	-5.37	1.26	1.33
1	B	222	LYS	CA-C	-5.37	1.46	1.52
1	B	289	ARG	CZ-NH2	5.37	1.40	1.33
1	A	395	LEU	CA-C	-5.35	1.45	1.52
1	B	428	GLY	C-O	5.35	1.29	1.24
1	A	154	HIS	C-O	-5.34	1.17	1.24
1	A	163	ARG	CZ-NH1	5.34	1.40	1.32
1	B	124	ASN	CA-C	-5.33	1.46	1.52
1	B	205	PRO	C-O	5.33	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	389	ALA	C-O	-5.33	1.18	1.24
1	B	289	ARG	CZ-NH1	5.33	1.40	1.32
1	A	343	LYS	CG-CD	5.32	1.68	1.52
1	B	407	PHE	C-O	5.31	1.30	1.23
1	B	351	VAL	CA-CB	-5.31	1.48	1.54
1	B	323	SER	N-CA	5.30	1.52	1.46
1	B	431	LEU	CG-CD1	5.30	1.70	1.52
1	A	229	THR	C-O	-5.30	1.17	1.24
1	A	216	CYS	CA-C	-5.30	1.45	1.52
1	A	330	LEU	N-CA	-5.30	1.39	1.45
1	A	124	ASN	CA-CB	-5.29	1.46	1.53
1	B	219	GLY	CA-C	-5.28	1.47	1.52
1	B	324	LYS	N-CA	5.27	1.52	1.46
1	A	419	LEU	C-O	5.25	1.30	1.24
1	A	125	LEU	CA-CB	-5.25	1.45	1.53
1	A	232	SER	C-O	-5.24	1.17	1.24
1	A	345	PRO	C-O	5.24	1.29	1.23
1	A	89	PRO	CA-C	5.21	1.57	1.52
1	A	85	GLN	CA-C	5.21	1.59	1.52
1	A	77	PRO	N-CA	5.21	1.54	1.47
1	A	356	ASP	CG-OD2	5.20	1.35	1.25
1	B	260	LYS	CG-CD	5.20	1.68	1.52
1	B	322	LEU	N-CA	5.19	1.53	1.46
1	B	241	ALA	N-CA	5.18	1.53	1.45
1	A	161	TYR	CD1-CE1	5.17	1.54	1.38
1	A	140	ALA	N-CA	5.17	1.52	1.46
1	A	485	ALA	N-CA	-5.17	1.40	1.46
1	A	417	ASP	CG-OD1	5.17	1.35	1.25
1	A	245	ASP	C-O	-5.17	1.17	1.24
1	A	474	LYS	CG-CD	5.17	1.68	1.52
1	A	176	LYS	CG-CD	5.16	1.68	1.52
1	A	298	SER	N-CA	-5.16	1.39	1.46
1	A	486	ARG	CB-CG	5.16	1.68	1.52
1	B	430	GLY	CA-C	-5.16	1.48	1.52
1	B	204	ASN	N-CA	5.15	1.51	1.46
1	A	229	THR	CA-CB	-5.15	1.44	1.53
1	B	101	GLU	CA-C	-5.15	1.45	1.52
1	A	420	LYS	CB-CG	5.15	1.67	1.52
1	A	223	VAL	CB-CG1	-5.14	1.35	1.52
1	B	232	SER	CA-C	5.14	1.60	1.52
1	B	261	ILE	C-O	5.14	1.30	1.24
1	A	390	GLU	CD-OE2	5.13	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	162	HIS	CA-CB	-5.12	1.44	1.53
1	A	354	THR	CA-CB	-5.11	1.45	1.53
1	A	484	LYS	C-O	-5.10	1.17	1.24
1	A	497	ASN	CA-CB	-5.09	1.45	1.53
1	B	468	THR	CA-C	5.09	1.59	1.52
1	B	187	HIS	CA-C	5.07	1.58	1.52
1	B	493	ASP	C-N	-5.07	1.27	1.33
1	A	469	SER	C-O	5.06	1.30	1.23
1	A	168	PRO	N-CA	-5.05	1.41	1.47
1	A	207	GLU	C-O	5.04	1.29	1.24
1	A	57	ASP	CA-CB	-5.04	1.46	1.53
1	A	243	PRO	CA-CB	-5.03	1.45	1.53
1	B	475	PRO	N-CD	5.03	1.54	1.47
1	B	98	ALA	C-N	5.03	1.45	1.33
1	B	124	ASN	C-N	-5.03	1.27	1.34
1	B	135	THR	CB-OG1	-5.03	1.35	1.43
1	B	497	ASN	CA-C	-5.03	1.46	1.52
1	B	449	LYS	C-O	-5.03	1.18	1.24
1	A	144	TYR	CA-CB	-5.02	1.45	1.53
1	B	385	ILE	N-CA	-5.01	1.40	1.46
1	A	496	TYR	C-O	-5.01	1.18	1.24
1	A	76	ALA	C-N	5.01	1.39	1.34

All (959) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	382	ARG	O-C-N	-36.59	81.14	122.85
1	A	89	PRO	CA-C-N	28.72	153.30	119.98
1	A	89	PRO	C-N-CA	28.72	153.30	119.98
1	A	395	LEU	O-C-N	-28.28	92.14	122.12
1	B	317	GLY	CA-C-N	24.00	167.38	121.54
1	B	317	GLY	C-N-CA	24.00	167.38	121.54
1	A	396	GLU	O-C-N	-23.64	96.79	122.08
1	A	160	ALA	O-C-N	-20.36	100.53	122.12
1	A	297	PHE	CA-C-N	18.75	152.10	123.23
1	A	297	PHE	C-N-CA	18.75	152.10	123.23
1	B	267	LYS	CA-C-O	17.28	140.18	119.79
1	A	382	ARG	CA-C-O	16.93	141.79	121.81
1	B	202	LEU	CA-C-O	16.93	138.49	120.55
1	B	267	LYS	O-C-N	-16.64	100.04	122.33
1	B	276	ALA	N-CA-C	16.49	130.64	108.38
1	B	103	LYS	CA-C-N	16.28	146.65	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	103	LYS	C-N-CA	16.28	146.65	120.60
1	B	473	LEU	O-C-N	-16.27	100.95	122.59
1	A	90	PRO	CA-C-N	15.64	151.41	121.54
1	A	90	PRO	C-N-CA	15.64	151.41	121.54
1	A	492	ASN	CA-C-N	15.63	151.40	121.54
1	A	492	ASN	C-N-CA	15.63	151.40	121.54
1	A	160	ALA	CA-C-O	15.58	137.45	120.63
1	B	189	ASP	CA-C-N	14.39	148.75	122.13
1	B	189	ASP	C-N-CA	14.39	148.75	122.13
1	B	179	ILE	O-C-N	-14.00	105.07	122.57
1	A	102	THR	CA-C-O	13.60	134.32	121.67
1	A	451	ILE	CA-C-N	13.55	138.83	120.54
1	A	451	ILE	C-N-CA	13.55	138.83	120.54
1	A	167	LYS	O-C-N	-13.48	109.24	121.37
1	B	202	LEU	O-C-N	-13.44	107.88	122.12
1	B	105	ASP	CA-C-O	13.42	139.70	120.51
1	A	490	VAL	O-C-N	13.24	135.44	121.14
1	A	12	SER	CA-C-N	13.12	136.24	119.84
1	A	12	SER	C-N-CA	13.12	136.24	119.84
1	A	395	LEU	CA-C-O	13.03	134.70	120.63
1	A	321	ALA	O-C-N	-13.01	105.29	122.59
1	A	102	THR	O-C-N	-12.81	103.84	121.78
1	B	406	VAL	O-C-N	-12.79	109.36	123.18
1	A	298	SER	CA-C-N	12.72	144.59	121.70
1	A	298	SER	C-N-CA	12.72	144.59	121.70
1	A	509	GLU	CA-C-O	-12.70	103.19	119.06
1	B	135	THR	O-C-N	-12.54	105.91	122.59
1	B	494	VAL	O-C-N	12.42	134.81	121.90
1	B	375	GLY	CA-C-N	-12.32	102.67	122.26
1	B	375	GLY	C-N-CA	-12.32	102.67	122.26
1	A	211	ASP	CA-C-N	-12.25	105.12	120.56
1	A	211	ASP	C-N-CA	-12.25	105.12	120.56
1	B	365	VAL	CA-C-N	12.25	137.02	122.44
1	B	365	VAL	C-N-CA	12.25	137.02	122.44
1	A	392	MET	CA-C-N	-12.19	105.88	119.28
1	A	392	MET	C-N-CA	-12.19	105.88	119.28
1	A	324	LYS	CA-C-N	12.13	144.72	121.54
1	A	324	LYS	C-N-CA	12.13	144.72	121.54
1	B	199	LEU	O-C-N	-11.82	108.84	122.91
1	A	89	PRO	O-C-N	-11.81	107.53	121.46
1	A	392	MET	CA-C-O	11.78	129.17	118.33
1	A	271	LYS	O-C-N	-11.76	109.66	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	492	ASN	CA-C-O	-11.68	108.67	121.99
1	B	344	LEU	CA-C-N	-11.62	105.32	119.84
1	B	344	LEU	C-N-CA	-11.62	105.32	119.84
1	A	43	HIS	CA-C-N	11.55	134.28	119.84
1	A	43	HIS	C-N-CA	11.55	134.28	119.84
1	A	57	ASP	CA-C-N	11.53	142.73	121.97
1	A	57	ASP	C-N-CA	11.53	142.73	121.97
1	A	163	ARG	N-CA-C	-11.53	98.01	112.88
1	B	105	ASP	O-C-N	-11.50	107.29	122.59
1	A	115	LEU	O-C-N	11.45	137.42	122.42
1	B	107	ALA	N-CA-C	-11.43	96.49	111.24
1	B	256	ASN	CA-C-N	11.42	143.36	121.54
1	B	256	ASN	C-N-CA	11.42	143.36	121.54
1	A	223	VAL	N-CA-C	11.39	118.53	109.19
1	A	69	ASN	CA-C-N	11.35	135.24	120.60
1	A	69	ASN	C-N-CA	11.35	135.24	120.60
1	B	247	GLN	O-C-N	-11.26	109.54	123.06
1	B	265	LEU	CA-C-O	11.21	132.43	120.55
1	A	327	ASP	CA-C-N	-11.01	106.08	119.84
1	A	327	ASP	C-N-CA	-11.01	106.08	119.84
1	A	254	TYR	CA-C-N	-10.99	106.49	121.66
1	A	254	TYR	C-N-CA	-10.99	106.49	121.66
1	A	396	GLU	CA-C-O	10.97	133.14	121.07
1	A	57	ASP	CA-C-O	-10.97	108.15	120.54
1	A	116	LEU	CA-C-N	10.82	131.52	120.38
1	A	116	LEU	C-N-CA	10.82	131.52	120.38
1	A	394	ILE	CA-C-O	10.78	132.60	121.17
1	B	223	VAL	CB-CA-C	-10.71	91.86	111.36
1	A	40	LEU	CA-C-N	-10.70	108.24	120.12
1	A	40	LEU	C-N-CA	-10.70	108.24	120.12
1	B	185	GLY	O-C-N	-10.67	108.83	122.70
1	A	179	ILE	O-C-N	-10.64	109.27	122.57
1	B	189	ASP	CA-CB-CG	10.59	123.19	112.60
1	B	202	LEU	N-CA-C	10.43	122.65	111.28
1	B	428	GLY	CA-C-N	-10.42	108.68	123.06
1	B	428	GLY	C-N-CA	-10.42	108.68	123.06
1	B	338	LEU	O-C-N	-10.40	111.09	122.12
1	B	212	VAL	N-CA-CB	10.31	121.86	110.62
1	A	490	VAL	N-CA-C	-10.29	99.45	109.02
1	A	68	PRO	CA-C-N	10.27	141.16	121.54
1	A	68	PRO	C-N-CA	10.27	141.16	121.54
1	B	112	LEU	N-CA-C	-10.24	100.20	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	459	GLU	CA-C-N	10.20	134.31	120.54
1	A	459	GLU	C-N-CA	10.20	134.31	120.54
1	A	152	VAL	N-CA-C	10.17	122.36	111.58
1	A	420	LYS	N-CA-C	-10.15	100.22	111.28
1	A	406	VAL	N-CA-C	10.14	122.86	108.36
1	B	462	MET	N-CA-C	-10.13	100.32	111.36
1	B	172	VAL	O-C-N	-10.12	111.41	122.95
1	B	246	LYS	O-C-N	-10.08	108.82	122.33
1	B	491	PRO	CA-C-N	-10.03	102.21	121.06
1	B	491	PRO	C-N-CA	-10.03	102.21	121.06
1	B	339	LYS	CA-C-N	10.00	134.08	120.38
1	B	339	LYS	C-N-CA	10.00	134.08	120.38
1	A	21	LYS	CA-C-N	9.96	132.29	119.84
1	A	21	LYS	C-N-CA	9.96	132.29	119.84
1	A	12	SER	N-CA-C	9.94	131.78	109.81
1	A	245	ASP	N-CA-C	9.90	123.30	111.82
1	A	57	ASP	N-CA-CB	9.87	126.44	110.16
1	A	234	SER	CA-C-N	-9.80	107.59	119.84
1	A	234	SER	C-N-CA	-9.80	107.59	119.84
1	A	201	LYS	N-CA-C	-9.78	101.37	113.20
1	B	187	HIS	CA-CB-CG	9.74	123.55	113.80
1	B	493	ASP	CA-C-N	9.68	132.95	120.56
1	B	493	ASP	C-N-CA	9.68	132.95	120.56
1	A	112	LEU	CA-C-O	-9.68	109.36	120.20
1	A	321	ALA	CA-C-O	9.64	134.30	120.51
1	B	242	ALA	CA-C-N	-9.63	107.80	119.84
1	B	242	ALA	C-N-CA	-9.63	107.80	119.84
1	A	508	PHE	CA-C-N	-9.63	105.38	122.42
1	A	508	PHE	C-N-CA	-9.63	105.38	122.42
1	A	402	ASP	CA-CB-CG	9.58	122.18	112.60
1	B	218	GLN	CA-C-N	-9.49	114.03	122.47
1	B	218	GLN	C-N-CA	-9.49	114.03	122.47
1	A	173	ASP	N-CA-C	-9.46	93.75	109.46
1	A	297	PHE	N-CA-CB	9.40	124.86	110.11
1	A	188	VAL	N-CA-C	9.38	123.29	108.85
1	A	403	LYS	O-C-N	-9.32	110.20	122.59
1	A	159	ASN	CA-CB-CG	9.31	121.91	112.60
1	A	328	PRO	O-C-N	-9.29	110.10	122.64
1	A	467	VAL	N-CA-C	9.27	124.29	108.90
1	B	146	SER	CA-C-N	9.27	137.14	121.47
1	B	146	SER	C-N-CA	9.27	137.14	121.47
1	A	204	ASN	CA-C-N	9.25	130.39	120.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	204	ASN	C-N-CA	9.25	130.39	120.12
1	B	356	ASP	CA-C-N	-9.24	107.52	120.74
1	B	356	ASP	C-N-CA	-9.24	107.52	120.74
1	B	433	ARG	CA-C-N	-9.23	109.37	118.97
1	B	433	ARG	C-N-CA	-9.23	109.37	118.97
1	A	296	LYS	CA-C-N	9.23	135.16	122.79
1	A	296	LYS	C-N-CA	9.23	135.16	122.79
1	B	250	TRP	CA-C-N	-9.22	110.14	123.05
1	B	250	TRP	C-N-CA	-9.22	110.14	123.05
1	A	71	ILE	CA-C-N	9.20	139.12	121.54
1	A	71	ILE	C-N-CA	9.20	139.12	121.54
1	A	82	GLY	CA-C-N	9.19	129.27	119.90
1	A	82	GLY	C-N-CA	9.19	129.27	119.90
1	A	142	ALA	N-CA-C	-9.19	101.22	111.14
1	A	105	ASP	CA-CB-CG	9.17	121.77	112.60
1	B	382	ARG	N-CA-C	9.14	122.59	110.53
1	B	327	ASP	CA-C-N	-9.08	108.49	119.84
1	B	327	ASP	C-N-CA	-9.08	108.49	119.84
1	B	347	VAL	CA-C-N	9.07	138.30	121.97
1	B	347	VAL	C-N-CA	9.07	138.30	121.97
1	B	99	PRO	O-C-N	-9.06	110.40	122.64
1	B	318	ALA	CA-C-N	9.03	138.79	121.54
1	B	318	ALA	C-N-CA	9.03	138.79	121.54
1	A	33	VAL	N-CA-C	9.03	121.48	108.48
1	A	23	ASP	CA-C-N	9.03	136.76	123.13
1	A	23	ASP	C-N-CA	9.03	136.76	123.13
1	A	342	THR	N-CA-C	9.00	122.98	108.76
1	A	115	LEU	N-CA-C	-8.98	102.33	113.38
1	A	56	LYS	CA-C-N	8.96	134.82	122.19
1	A	56	LYS	C-N-CA	8.96	134.82	122.19
1	B	499	VAL	CB-CA-C	-8.93	97.60	112.16
1	A	138	LYS	O-C-N	-8.93	110.72	122.59
1	B	242	ALA	O-C-N	-8.90	114.53	121.47
1	A	281	VAL	CB-CA-C	-8.89	100.56	111.85
1	B	361	ALA	CA-C-N	8.87	132.51	120.44
1	B	361	ALA	C-N-CA	8.87	132.51	120.44
1	B	357	VAL	N-CA-C	-8.85	102.24	110.82
1	A	112	LEU	O-C-N	8.84	132.28	122.20
1	A	509	GLU	O-C-N	-8.84	111.64	122.25
1	B	105	ASP	CA-CB-CG	8.83	121.43	112.60
1	A	467	VAL	CA-C-N	-8.80	108.42	122.23
1	A	467	VAL	C-N-CA	-8.80	108.42	122.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	320	ARG	CD-NE-CZ	8.77	136.68	124.40
1	A	474	LYS	CA-C-N	8.77	128.93	119.28
1	A	474	LYS	C-N-CA	8.77	128.93	119.28
1	B	135	THR	CA-C-O	8.77	133.05	120.51
1	B	474	LYS	CA-C-N	-8.75	109.65	119.28
1	B	474	LYS	C-N-CA	-8.75	109.65	119.28
1	A	369	VAL	CA-C-N	-8.66	109.08	121.99
1	A	369	VAL	C-N-CA	-8.66	109.08	121.99
1	A	223	VAL	N-CA-CB	-8.64	102.40	111.64
1	A	112	LEU	CA-C-N	8.60	137.96	121.54
1	A	112	LEU	C-N-CA	8.60	137.96	121.54
1	B	279	VAL	O-C-N	-8.57	112.49	122.94
1	A	327	ASP	CA-C-O	8.55	127.96	119.49
1	B	492	ASN	O-C-N	-8.55	112.22	122.65
1	A	175	ARG	N-CA-C	-8.54	101.92	111.14
1	B	115	LEU	N-CA-CB	8.50	121.89	110.59
1	A	70	VAL	N-CA-C	8.49	119.28	110.36
1	B	235	PRO	CA-C-N	8.48	131.65	120.28
1	B	235	PRO	C-N-CA	8.48	131.65	120.28
1	B	226	MET	O-C-N	8.47	132.85	122.86
1	B	178	ASP	CA-CB-CG	8.46	121.06	112.60
1	B	476	ASP	CA-CB-CG	8.46	121.06	112.60
1	A	63	GLU	CA-C-O	8.44	127.09	119.08
1	B	201	LYS	CA-C-N	8.42	131.56	120.28
1	B	201	LYS	C-N-CA	8.42	131.56	120.28
1	B	419	LEU	CB-CG-CD2	-8.41	85.47	110.70
1	B	289	ARG	CB-CG-CD	8.38	130.58	111.30
1	A	247	GLN	CA-C-N	-8.36	110.67	122.71
1	A	247	GLN	C-N-CA	-8.36	110.67	122.71
1	B	473	LEU	CA-C-O	8.35	132.45	120.51
1	B	102	THR	O-C-N	-8.31	111.53	122.59
1	B	339	LYS	O-C-N	-8.30	113.32	122.12
1	A	297	PHE	CA-CB-CG	8.28	122.08	113.80
1	B	178	ASP	CA-C-N	8.26	136.84	121.97
1	B	178	ASP	C-N-CA	8.26	136.84	121.97
1	A	199	LEU	CA-C-N	-8.26	107.43	122.38
1	A	199	LEU	C-N-CA	-8.26	107.43	122.38
1	B	199	LEU	N-CA-C	8.26	122.43	111.28
1	A	169	LYS	CA-CB-CG	-8.20	97.69	114.10
1	B	179	ILE	CA-C-O	8.19	131.02	120.78
1	B	281	VAL	CB-CA-C	-8.18	97.88	111.29
1	A	490	VAL	CA-C-O	8.15	126.96	119.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	101	GLU	CA-C-N	8.12	137.05	121.54
1	B	101	GLU	C-N-CA	8.12	137.05	121.54
1	B	292	ASP	CA-CB-CG	8.10	120.70	112.60
1	B	198	ALA	CA-C-N	8.09	134.28	122.63
1	B	198	ALA	C-N-CA	8.09	134.28	122.63
1	A	452	GLU	CA-CB-CG	8.09	130.28	114.10
1	B	328	PRO	CA-N-CD	-8.09	100.67	112.00
1	A	58	VAL	O-C-N	-8.05	112.50	122.57
1	B	133	SER	O-C-N	-8.05	112.80	122.22
1	A	5	ASP	CA-CB-CG	8.04	120.64	112.60
1	A	375	GLY	CA-C-N	-8.04	107.70	122.09
1	A	375	GLY	C-N-CA	-8.04	107.70	122.09
1	B	483	LEU	CA-C-N	-8.04	110.46	122.83
1	B	483	LEU	C-N-CA	-8.04	110.46	122.83
1	A	169	LYS	N-CA-C	8.03	122.06	110.10
1	A	89	PRO	C-N-CD	-8.02	92.12	125.00
1	A	64	PRO	CA-N-CD	-8.02	100.78	112.00
1	B	99	PRO	CA-N-CD	-7.97	100.85	112.00
1	B	258	ASP	CA-CB-CG	7.96	120.56	112.60
1	B	388	LEU	O-C-N	7.94	131.81	122.20
1	A	489	GLY	N-CA-C	-7.92	97.46	112.51
1	B	238	ILE	CA-C-N	7.92	136.22	121.97
1	B	238	ILE	C-N-CA	7.92	136.22	121.97
1	A	445	ASN	N-CA-C	7.92	119.99	111.36
1	A	493	ASP	N-CA-C	7.91	127.65	110.80
1	B	112	LEU	CA-C-N	7.89	136.62	121.54
1	B	112	LEU	C-N-CA	7.89	136.62	121.54
1	A	110	GLU	N-CA-C	-7.89	103.22	113.17
1	B	376	ARG	N-CA-C	-7.89	103.47	113.72
1	B	214	ARG	CD-NE-CZ	7.87	135.42	124.40
1	B	188	VAL	CA-CB-CG2	7.87	123.77	110.40
1	B	327	ASP	CA-CB-CG	7.84	120.44	112.60
1	B	383	ALA	CA-C-N	7.83	128.25	119.32
1	B	383	ALA	C-N-CA	7.83	128.25	119.32
1	A	413	ARG	CB-CG-CD	7.82	129.29	111.30
1	A	382	ARG	CA-C-N	-7.82	110.25	121.20
1	A	382	ARG	C-N-CA	-7.82	110.25	121.20
1	B	397	GLN	CA-C-N	-7.81	109.97	122.24
1	B	397	GLN	C-N-CA	-7.81	109.97	122.24
1	A	473	LEU	N-CA-C	-7.79	96.88	109.96
1	B	154	HIS	O-C-N	-7.76	112.27	122.59
1	A	223	VAL	CA-C-N	7.76	128.05	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	223	VAL	C-N-CA	7.76	128.05	119.90
1	A	292	ASP	CA-CB-CG	7.75	120.35	112.60
1	B	427	LYS	CA-C-N	-7.75	111.05	121.27
1	B	427	LYS	C-N-CA	-7.75	111.05	121.27
1	A	136	LEU	CA-C-N	7.74	135.35	121.97
1	A	136	LEU	C-N-CA	7.74	135.35	121.97
1	A	458	ILE	N-CA-C	-7.74	103.31	110.82
1	B	379	ASP	CA-CB-CG	7.74	120.33	112.60
1	A	456	ASP	CA-CB-CG	7.72	120.32	112.60
1	A	172	VAL	O-C-N	-7.71	114.86	123.10
1	B	134	GLN	CA-C-O	7.71	130.41	121.78
1	B	157	ASN	CA-CB-CG	7.70	120.30	112.60
1	A	3	LYS	CA-C-O	-7.68	112.98	121.05
1	B	130	TYR	CA-C-N	7.68	130.57	120.28
1	B	130	TYR	C-N-CA	7.68	130.57	120.28
1	B	166	PHE	N-CA-C	7.68	121.97	109.76
1	B	153	THR	O-C-N	-7.67	113.87	122.08
1	B	283	ALA	CA-C-N	7.67	128.06	119.32
1	B	283	ALA	C-N-CA	7.67	128.06	119.32
1	B	187	HIS	CA-C-O	-7.66	112.45	121.11
1	B	433	ARG	CD-NE-CZ	7.66	135.12	124.40
1	B	507	GLU	CA-C-N	7.65	136.16	121.54
1	B	507	GLU	C-N-CA	7.65	136.16	121.54
1	A	135	THR	CA-C-O	7.64	128.73	119.64
1	A	248	ILE	N-CA-C	7.64	119.75	108.45
1	A	83	PRO	N-CA-C	7.61	123.17	111.15
1	A	199	LEU	N-CA-C	7.60	119.80	110.91
1	A	493	ASP	O-C-N	-7.59	112.50	122.59
1	B	389	ALA	CA-C-N	-7.58	108.31	121.66
1	B	389	ALA	C-N-CA	-7.58	108.31	121.66
1	A	492	ASN	CA-C-O	-7.57	112.69	120.71
1	A	507	GLU	CA-C-N	7.57	136.00	121.54
1	A	507	GLU	C-N-CA	7.57	136.00	121.54
1	B	356	ASP	CA-CB-CG	7.57	120.17	112.60
1	A	357	VAL	CA-C-N	-7.57	110.10	120.46
1	A	357	VAL	C-N-CA	-7.57	110.10	120.46
1	A	413	ARG	CB-CA-C	7.57	120.93	109.13
1	A	6	MET	CA-C-N	7.52	135.91	121.54
1	A	6	MET	C-N-CA	7.52	135.91	121.54
1	B	251	TYR	N-CA-CB	7.52	122.35	110.55
1	A	320	ARG	CA-C-N	7.50	135.86	121.54
1	A	320	ARG	C-N-CA	7.50	135.86	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	149	ASN	CA-CB-CG	7.47	120.07	112.60
1	A	183	MET	O-C-N	7.45	132.82	123.28
1	B	342	THR	N-CA-C	7.45	119.89	108.42
1	B	273	GLY	CA-C-N	7.43	135.35	121.97
1	B	273	GLY	C-N-CA	7.43	135.35	121.97
1	A	382	ARG	N-CA-C	7.43	120.58	110.55
1	A	63	GLU	O-C-N	7.39	126.22	120.38
1	A	41	PRO	CA-N-CD	-7.39	101.66	112.00
1	A	365	VAL	N-CA-C	-7.38	93.99	109.34
1	A	507	GLU	N-CA-C	7.38	126.51	110.80
1	B	167	LYS	CA-C-N	-7.37	113.10	120.98
1	B	167	LYS	C-N-CA	-7.37	113.10	120.98
1	A	11	ILE	N-CA-C	7.36	124.66	109.34
1	A	212	VAL	N-CA-CB	7.36	119.16	110.55
1	B	169	LYS	CA-C-N	7.33	133.68	122.68
1	B	169	LYS	C-N-CA	7.33	133.68	122.68
1	B	493	ASP	CA-CB-CG	7.33	119.93	112.60
1	A	400	LEU	CA-C-O	7.32	129.81	121.32
1	A	486	ARG	CA-C-N	-7.31	110.53	122.81
1	A	486	ARG	C-N-CA	-7.31	110.53	122.81
1	B	258	ASP	O-C-N	-7.30	112.88	122.59
1	A	317	GLY	CA-C-N	7.29	135.47	121.54
1	A	317	GLY	C-N-CA	7.29	135.47	121.54
1	B	495	LEU	CA-CB-CG	-7.28	90.81	116.30
1	A	163	ARG	CA-C-N	-7.27	113.72	123.10
1	A	163	ARG	C-N-CA	-7.27	113.72	123.10
1	A	88	MET	O-C-N	-7.27	116.34	121.65
1	A	420	LYS	CA-C-N	-7.26	109.98	120.29
1	A	420	LYS	C-N-CA	-7.26	109.98	120.29
1	B	392	MET	CA-C-N	-7.26	112.15	119.56
1	B	392	MET	C-N-CA	-7.26	112.15	119.56
1	A	87	SER	CA-C-N	7.25	134.93	122.38
1	A	87	SER	C-N-CA	7.25	134.93	122.38
1	B	281	VAL	N-CA-C	7.23	124.38	109.34
1	B	317	GLY	CA-C-O	-7.23	105.62	120.80
1	B	504	THR	CA-C-N	-7.22	111.40	122.09
1	B	504	THR	C-N-CA	-7.22	111.40	122.09
1	A	183	MET	CA-C-N	-7.22	112.06	122.68
1	A	183	MET	C-N-CA	-7.22	112.06	122.68
1	A	317	GLY	O-C-N	7.22	134.56	123.00
1	A	182	ASP	CA-CB-CG	7.22	119.82	112.60
1	A	200	CYS	N-CA-C	-7.22	104.21	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	440	SER	CA-C-N	-7.22	109.05	120.17
1	B	440	SER	C-N-CA	-7.22	109.05	120.17
1	A	357	VAL	CB-CA-C	-7.22	102.40	112.14
1	B	104	GLU	CB-CG-CD	7.20	124.84	112.60
1	A	320	ARG	N-CA-C	-7.20	104.37	113.01
1	B	261	ILE	CB-CA-C	-7.16	99.55	111.29
1	A	327	ASP	CA-CB-CG	7.14	119.74	112.60
1	A	492	ASN	CA-CB-CG	7.12	119.72	112.60
1	A	67	ALA	CA-C-N	-7.12	110.94	119.84
1	A	67	ALA	C-N-CA	-7.12	110.94	119.84
1	A	92	LEU	CA-C-O	7.12	128.04	119.43
1	B	325	PHE	CA-C-N	-7.11	111.84	121.66
1	B	325	PHE	C-N-CA	-7.11	111.84	121.66
1	A	184	LEU	CA-C-O	7.11	130.95	122.14
1	A	118	PRO	CB-CA-C	-7.09	102.63	111.64
1	A	135	THR	CA-C-N	-7.08	109.82	120.94
1	A	135	THR	C-N-CA	-7.08	109.82	120.94
1	A	215	GLY	CA-C-N	-7.07	111.34	122.65
1	A	215	GLY	C-N-CA	-7.07	111.34	122.65
1	A	36	LEU	CA-C-N	7.04	134.99	121.54
1	A	36	LEU	C-N-CA	7.04	134.99	121.54
1	A	64	PRO	O-C-N	-7.04	113.14	122.64
1	A	162	HIS	CA-C-N	-7.02	111.65	122.60
1	A	162	HIS	C-N-CA	-7.02	111.65	122.60
1	B	230	LEU	O-C-N	-7.00	113.28	122.59
1	A	160	ALA	N-CA-C	6.99	119.78	111.33
1	B	354	THR	N-CA-C	6.96	119.52	111.02
1	A	402	ASP	CA-C-O	6.96	128.06	119.78
1	A	475	PRO	CA-C-N	6.96	131.83	120.63
1	A	475	PRO	C-N-CA	6.96	131.83	120.63
1	A	190	VAL	N-CA-CB	-6.95	104.22	111.87
1	A	56	LYS	N-CA-C	6.94	118.64	108.86
1	A	244	SER	CA-C-N	-6.94	109.76	120.31
1	A	244	SER	C-N-CA	-6.94	109.76	120.31
1	A	290	GLU	O-C-N	-6.93	114.30	122.20
1	B	102	THR	CA-CB-OG1	6.93	120.00	109.60
1	A	8	LYS	CA-C-O	-6.91	112.93	121.78
1	A	163	ARG	NE-CZ-NH2	-6.91	112.98	119.20
1	B	137	THR	CB-CA-C	-6.90	97.85	109.65
1	B	134	GLN	O-C-N	-6.89	112.62	121.92
1	A	167	LYS	CA-C-O	6.89	130.13	120.83
1	B	420	LYS	N-CA-CB	-6.87	99.96	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	197	THR	N-CA-CB	-6.87	98.25	110.90
1	A	102	THR	CA-C-N	-6.86	113.08	122.82
1	A	102	THR	C-N-CA	-6.86	113.08	122.82
1	A	357	VAL	N-CA-C	6.85	117.61	110.62
1	B	447	VAL	CB-CA-C	-6.85	100.05	111.29
1	B	177	VAL	CA-C-N	6.83	132.41	122.77
1	B	177	VAL	C-N-CA	6.83	132.41	122.77
1	B	482	THR	CA-C-O	6.83	127.44	119.32
1	B	331	THR	CA-C-N	6.81	134.54	121.54
1	B	331	THR	C-N-CA	6.81	134.54	121.54
1	A	179	ILE	CA-C-N	-6.80	109.17	122.02
1	A	179	ILE	C-N-CA	-6.80	109.17	122.02
1	B	352	GLN	CA-C-O	6.80	126.47	118.79
1	A	151	GLU	CA-C-O	6.79	129.23	120.81
1	A	341	LYS	N-CA-C	-6.79	105.33	112.93
1	A	486	ARG	NE-CZ-NH1	-6.79	114.71	121.50
1	A	319	SER	CA-CB-OG	6.79	124.67	111.10
1	B	190	VAL	CA-CB-CG1	6.77	121.91	110.40
1	B	480	LEU	CB-CA-C	-6.76	100.07	111.02
1	A	180	SER	N-CA-C	-6.75	99.89	110.36
1	B	406	VAL	CA-C-N	6.75	133.43	122.29
1	B	406	VAL	C-N-CA	6.75	133.43	122.29
1	A	125	LEU	N-CA-CB	-6.75	99.94	110.06
1	B	296	LYS	CA-C-N	6.75	133.18	122.59
1	B	296	LYS	C-N-CA	6.75	133.18	122.59
1	A	267	LYS	N-CA-C	-6.74	103.94	111.28
1	A	490	VAL	CA-CB-CG2	6.74	121.85	110.40
1	B	119	LEU	O-C-N	-6.74	113.63	122.59
1	A	58	VAL	CA-CB-CG1	6.73	121.84	110.40
1	B	255	VAL	CA-CB-CG2	6.73	121.83	110.40
1	B	211	ASP	CA-CB-CG	6.72	119.32	112.60
1	A	158	HIS	CA-CB-CG	6.71	120.52	113.80
1	B	412	VAL	N-CA-CB	6.71	118.64	111.46
1	B	277	LEU	N-CA-C	6.71	119.67	108.20
1	A	172	VAL	CA-C-N	-6.70	112.75	122.19
1	A	172	VAL	C-N-CA	-6.70	112.75	122.19
1	A	169	LYS	CD-CE-NZ	-6.70	90.47	111.90
1	A	491	PRO	N-CA-C	-6.69	99.63	110.74
1	B	456	ASP	CA-CB-CG	6.69	119.29	112.60
1	A	48	ASP	CA-CB-CG	6.67	119.27	112.60
1	A	388	LEU	CB-CG-CD1	-6.67	90.70	110.70
1	A	356	ASP	CA-C-N	-6.64	111.36	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	356	ASP	C-N-CA	-6.64	111.36	120.46
1	A	397	GLN	O-C-N	-6.63	113.77	122.59
1	A	126	TYR	N-CA-C	6.63	120.23	111.75
1	A	425	GLY	CA-C-N	-6.62	111.48	120.87
1	A	425	GLY	C-N-CA	-6.62	111.48	120.87
1	A	264	ASP	CA-CB-CG	6.61	119.21	112.60
1	A	379	ASP	CA-CB-CG	6.61	119.21	112.60
1	A	39	PHE	CA-CB-CG	6.61	120.41	113.80
1	B	491	PRO	O-C-N	6.60	131.55	122.64
1	B	494	VAL	CA-C-N	6.60	129.02	120.44
1	B	494	VAL	C-N-CA	6.60	129.02	120.44
1	B	346	ILE	CA-C-N	6.58	132.19	123.11
1	B	346	ILE	C-N-CA	6.58	132.19	123.11
1	A	452	GLU	CA-C-O	-6.57	113.87	120.90
1	B	280	THR	CB-CA-C	-6.56	102.07	112.05
1	B	259	ARG	CA-C-O	6.56	129.90	120.51
1	A	117	PRO	CB-CA-C	-6.56	102.92	110.92
1	A	25	CYS	N-CA-C	6.55	119.14	107.80
1	A	509	GLU	CB-CA-C	-6.54	97.52	109.15
1	A	11	ILE	CA-C-N	6.53	137.73	121.80
1	A	11	ILE	C-N-CA	6.53	137.73	121.80
1	A	127	ASP	N-CA-C	-6.52	104.01	112.23
1	A	420	LYS	CG-CD-CE	6.51	126.28	111.30
1	A	269	VAL	N-CA-C	6.51	118.04	110.62
1	A	63	GLU	CA-C-N	-6.50	111.71	119.84
1	A	63	GLU	C-N-CA	-6.50	111.71	119.84
1	A	89	PRO	N-CA-C	6.49	118.62	110.70
1	B	285	SER	CA-C-N	-6.49	108.99	122.03
1	B	285	SER	C-N-CA	-6.49	108.99	122.03
1	A	245	ASP	CB-CG-OD1	-6.48	103.49	118.40
1	B	139	GLN	N-CA-CB	-6.47	100.62	110.33
1	A	393	PRO	CA-N-CD	-6.47	102.94	112.00
1	B	343	LYS	N-CA-C	-6.46	105.41	113.55
1	A	297	PHE	CA-C-O	-6.46	112.88	121.86
1	B	409	ASP	CA-CB-CG	6.45	119.05	112.60
1	A	246	LYS	N-CA-C	-6.45	105.71	112.93
1	A	133	SER	CA-C-N	-6.44	112.24	122.29
1	A	133	SER	C-N-CA	-6.44	112.24	122.29
1	B	170	ILE	CA-CB-CG2	6.44	121.45	110.50
1	A	155	ARG	CA-CB-CG	-6.44	101.22	114.10
1	B	445	ASN	CA-CB-CG	6.43	119.03	112.60
1	A	420	LYS	CB-CA-C	6.42	121.46	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	432	GLY	CA-C-N	-6.42	111.65	120.26
1	A	432	GLY	C-N-CA	-6.42	111.65	120.26
1	B	357	VAL	CA-CB-CG1	6.42	121.32	110.40
1	A	444	ARG	CG-CD-NE	6.42	126.12	112.00
1	B	212	VAL	N-CA-C	6.42	116.53	110.30
1	B	398	ARG	CA-C-N	6.42	133.80	121.54
1	B	398	ARG	C-N-CA	6.42	133.80	121.54
1	A	151	GLU	CA-C-N	-6.42	110.95	121.34
1	A	151	GLU	C-N-CA	-6.42	110.95	121.34
1	B	99	PRO	CA-C-N	6.41	133.97	121.41
1	B	99	PRO	C-N-CA	6.41	133.97	121.41
1	B	509	GLU	N-CA-C	6.41	119.88	110.59
1	A	114	SER	N-CA-CB	6.39	121.29	110.49
1	A	439	ASN	CA-CB-CG	6.39	118.99	112.60
1	B	405	GLU	N-CA-C	-6.37	99.25	109.96
1	A	365	VAL	CA-C-N	-6.37	112.13	122.26
1	A	365	VAL	C-N-CA	-6.37	112.13	122.26
1	A	350	GLY	N-CA-C	-6.37	105.57	116.01
1	A	135	THR	CA-CB-OG1	6.36	119.15	109.60
1	A	156	GLU	N-CA-C	6.36	118.22	111.28
1	B	151	GLU	CA-C-N	-6.36	112.96	120.72
1	B	151	GLU	C-N-CA	-6.36	112.96	120.72
1	B	129	GLU	CA-C-N	-6.36	112.26	120.65
1	B	129	GLU	C-N-CA	-6.36	112.26	120.65
1	B	475	PRO	CA-N-CD	-6.36	103.10	112.00
1	A	392	MET	C-N-CD	6.35	151.05	125.00
1	B	496	TYR	N-CA-CB	-6.35	100.05	110.40
1	A	79	LYS	N-CA-C	-6.33	105.69	113.41
1	A	191	PRO	O-C-N	-6.32	114.11	122.64
1	A	353	ARG	NE-CZ-NH2	-6.31	113.52	119.20
1	A	61	ILE	CA-CB-CG1	6.30	121.12	110.40
1	A	212	VAL	N-CA-C	6.30	116.47	110.42
1	B	327	ASP	C-N-CD	6.30	150.82	125.00
1	B	102	THR	OG1-CB-CG2	6.29	121.89	109.30
1	A	430	GLY	O-C-N	-6.29	118.01	123.80
1	B	100	GLY	CA-C-N	6.29	133.39	122.95
1	B	100	GLY	C-N-CA	6.29	133.39	122.95
1	A	113	LYS	CA-C-O	6.29	129.50	120.51
1	A	258	ASP	CA-CB-CG	6.28	118.88	112.60
1	A	404	LEU	CA-C-N	-6.28	113.82	122.30
1	A	404	LEU	C-N-CA	-6.28	113.82	122.30
1	A	23	ASP	CA-CB-CG	6.27	118.87	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	218	GLN	CB-CG-CD	-6.27	101.94	112.60
1	A	190	VAL	CA-C-N	-6.25	112.03	119.84
1	A	190	VAL	C-N-CA	-6.25	112.03	119.84
1	A	268	ASN	CA-C-N	-6.24	111.73	120.53
1	A	268	ASN	C-N-CA	-6.24	111.73	120.53
1	A	361	ALA	CA-C-N	6.23	129.25	120.28
1	A	361	ALA	C-N-CA	6.23	129.25	120.28
1	A	171	LEU	CA-C-N	-6.23	114.29	122.94
1	A	171	LEU	C-N-CA	-6.23	114.29	122.94
1	A	405	GLU	CA-C-O	-6.22	113.46	120.43
1	B	368	VAL	CB-CA-C	-6.22	102.22	111.80
1	A	327	ASP	C-N-CD	6.22	150.50	125.00
1	B	426	ALA	CA-C-N	-6.21	111.47	120.29
1	B	426	ALA	C-N-CA	-6.21	111.47	120.29
1	A	141	TRP	CE2-CD2-CG	-6.21	99.75	107.20
1	A	218	GLN	CA-C-N	-6.21	115.72	122.55
1	A	218	GLN	C-N-CA	-6.21	115.72	122.55
1	A	112	LEU	N-CA-CB	6.20	119.93	110.14
1	A	414	ARG	CA-C-N	-6.19	112.40	120.14
1	A	414	ARG	C-N-CA	-6.19	112.40	120.14
1	B	117	PRO	CA-C-N	6.19	127.57	119.84
1	B	117	PRO	C-N-CA	6.19	127.57	119.84
1	B	372	ASN	CA-C-O	6.17	129.34	120.51
1	B	272	LEU	N-CA-C	6.17	121.89	113.37
1	A	29	ILE	CB-CA-C	6.17	118.75	110.42
1	A	368	VAL	N-CA-CB	-6.17	102.08	112.44
1	B	123	ILE	CA-C-N	-6.16	111.78	121.87
1	B	123	ILE	C-N-CA	-6.16	111.78	121.87
1	A	171	LEU	O-C-N	-6.14	115.21	122.58
1	A	328	PRO	CA-N-CD	-6.14	103.40	112.00
1	A	407	PHE	CA-C-O	-6.14	113.29	121.46
1	A	383	ALA	CA-C-N	6.14	126.59	119.47
1	A	383	ALA	C-N-CA	6.14	126.59	119.47
1	B	177	VAL	O-C-N	6.14	129.56	123.00
1	A	122	ILE	N-CA-C	-6.13	100.87	109.21
1	A	418	VAL	CA-C-N	-6.13	112.47	120.44
1	A	418	VAL	C-N-CA	-6.13	112.47	120.44
1	B	412	VAL	CB-CA-C	6.13	118.04	111.35
1	B	111	GLN	O-C-N	-6.13	115.65	122.03
1	B	444	ARG	CA-C-O	6.13	126.92	119.38
1	A	372	ASN	N-CA-C	-6.12	102.97	110.61
1	A	40	LEU	C-N-CD	6.11	150.06	125.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	101	GLU	N-CA-C	6.10	120.55	112.25
1	B	464	LEU	CB-CG-CD1	6.10	128.99	110.70
1	B	490	VAL	N-CA-CB	-6.09	102.68	111.21
1	B	343	LYS	CB-CA-C	6.09	118.78	109.34
1	B	246	LYS	CA-C-N	-6.08	112.35	121.05
1	B	246	LYS	C-N-CA	-6.08	112.35	121.05
1	A	394	ILE	CA-C-N	-6.08	112.06	120.38
1	A	394	ILE	C-N-CA	-6.08	112.06	120.38
1	B	261	ILE	CA-C-N	6.07	129.99	120.89
1	B	261	ILE	C-N-CA	6.07	129.99	120.89
1	B	463	ARG	N-CA-C	-6.07	104.23	111.69
1	B	485	ALA	CA-C-N	-6.07	113.71	123.23
1	B	485	ALA	C-N-CA	-6.07	113.71	123.23
1	A	323	SER	N-CA-C	-6.06	97.89	110.80
1	A	25	CYS	CA-C-O	6.06	127.88	120.25
1	B	387	VAL	N-CA-CB	6.05	117.22	110.62
1	B	257	SER	CA-C-N	6.05	133.09	121.54
1	B	257	SER	C-N-CA	6.05	133.09	121.54
1	A	126	TYR	CA-C-N	-6.04	110.40	120.68
1	A	126	TYR	C-N-CA	-6.04	110.40	120.68
1	A	490	VAL	CA-CB-CG1	6.04	120.67	110.40
1	A	206	LEU	CA-CB-CG	-6.03	95.19	116.30
1	B	168	PRO	N-CA-C	6.03	120.11	110.40
1	B	487	THR	CB-CA-C	-6.03	99.86	109.80
1	A	368	VAL	CA-C-O	-6.02	115.34	121.67
1	A	348	ILE	CA-C-N	-6.01	114.42	122.72
1	A	348	ILE	C-N-CA	-6.01	114.42	122.72
1	A	399	ASN	CA-CB-CG	6.01	118.61	112.60
1	B	120	ASP	CA-CB-CG	6.01	118.61	112.60
1	A	57	ASP	CA-CB-CG	6.00	118.60	112.60
1	A	47	GLN	CA-C-N	6.00	133.00	121.54
1	A	47	GLN	C-N-CA	6.00	133.00	121.54
1	A	188	VAL	CB-CA-C	-6.00	101.58	110.82
1	B	391	THR	CA-CB-OG1	5.99	118.59	109.60
1	A	468	THR	CA-C-N	-5.99	112.05	121.87
1	A	468	THR	C-N-CA	-5.99	112.05	121.87
1	B	417	ASP	N-CA-C	-5.99	104.44	110.97
1	B	417	ASP	N-CA-CB	-5.97	101.20	109.91
1	A	440	SER	CA-C-O	-5.96	114.24	120.92
1	A	490	VAL	N-CA-CB	5.96	116.13	109.99
1	A	280	THR	CB-CA-C	-5.96	100.52	110.29
1	B	178	ASP	N-CA-CB	5.96	120.12	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	437	TYR	O-C-N	5.95	128.94	122.15
1	A	170	ILE	CA-CB-CG2	5.95	120.61	110.50
1	B	263	ASP	CA-CB-CG	-5.95	106.65	112.60
1	B	254	TYR	N-CA-C	5.95	117.98	108.41
1	B	407	PHE	CA-C-N	-5.94	114.26	122.69
1	B	407	PHE	C-N-CA	-5.94	114.26	122.69
1	A	353	ARG	NE-CZ-NH1	5.93	127.43	121.50
1	B	104	GLU	CA-CB-CG	5.93	125.97	114.10
1	A	214	ARG	CD-NE-CZ	-5.93	116.09	124.40
1	A	48	ASP	N-CA-CB	-5.93	100.47	110.49
1	A	444	ARG	NE-CZ-NH2	5.93	124.53	119.20
1	A	319	SER	CA-C-O	5.92	128.98	120.51
1	A	483	LEU	CA-C-N	-5.92	112.82	122.65
1	A	483	LEU	C-N-CA	-5.92	112.82	122.65
1	A	471	ALA	CA-C-N	-5.92	113.20	122.73
1	A	471	ALA	C-N-CA	-5.92	113.20	122.73
1	B	372	ASN	CB-CG-ND2	5.91	125.26	116.40
1	A	199	LEU	CB-CA-C	-5.90	101.95	112.27
1	B	172	VAL	CA-CB-CG1	5.88	120.39	110.40
1	A	394	ILE	O-C-N	-5.87	116.16	121.91
1	B	354	THR	CA-CB-CG2	5.86	120.45	110.50
1	A	406	VAL	O-C-N	-5.85	116.53	123.03
1	B	429	VAL	CA-C-N	-5.85	117.12	122.80
1	B	429	VAL	C-N-CA	-5.85	117.12	122.80
1	A	379	ASP	CA-C-N	5.85	132.72	121.54
1	A	379	ASP	C-N-CA	5.85	132.72	121.54
1	A	240	GLU	CA-CB-CG	5.84	125.78	114.10
1	B	178	ASP	N-CA-C	5.83	117.90	108.34
1	B	223	VAL	O-C-N	5.82	127.74	121.10
1	B	365	VAL	N-CA-CB	5.82	120.83	111.23
1	A	508	PHE	CA-CB-CG	5.82	119.61	113.80
1	A	155	ARG	O-C-N	-5.81	115.96	122.12
1	B	223	VAL	CA-C-N	5.81	127.11	119.84
1	B	223	VAL	C-N-CA	5.81	127.11	119.84
1	B	372	ASN	CA-CB-CG	5.81	118.41	112.60
1	A	240	GLU	CA-C-O	5.81	126.74	119.59
1	A	205	PRO	N-CA-C	-5.79	107.25	114.20
1	A	10	LYS	CA-C-O	-5.78	112.25	120.51
1	A	35	ASP	CA-C-N	5.77	134.27	121.80
1	A	35	ASP	C-N-CA	5.77	134.27	121.80
1	A	229	THR	N-CA-C	-5.77	105.34	112.38
1	B	391	THR	N-CA-CB	5.77	118.56	110.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	286	LEU	CA-CB-CG	-5.77	96.10	116.30
1	B	379	ASP	O-C-N	5.77	129.91	122.81
1	A	355	GLU	N-CA-C	-5.77	104.63	111.03
1	A	278	PHE	N-CA-CB	-5.76	100.90	110.47
1	A	290	GLU	CA-C-N	-5.76	111.06	121.14
1	A	290	GLU	C-N-CA	-5.76	111.06	121.14
1	A	86	GLY	CA-C-N	5.75	132.53	121.54
1	A	86	GLY	C-N-CA	5.75	132.53	121.54
1	B	340	LYS	N-CA-C	5.75	118.29	111.33
1	B	147	GLY	O-C-N	-5.75	117.35	123.45
1	B	470	ILE	O-C-N	-5.75	116.10	121.90
1	A	428	GLY	CA-C-N	-5.74	113.57	122.69
1	A	428	GLY	C-N-CA	-5.74	113.57	122.69
1	B	455	ARG	CA-C-O	5.73	126.56	119.79
1	A	250	TRP	CA-C-N	-5.73	114.11	122.65
1	A	250	TRP	C-N-CA	-5.73	114.11	122.65
1	A	117	PRO	CA-C-N	5.73	126.06	119.93
1	A	117	PRO	C-N-CA	5.73	126.06	119.93
1	A	197	THR	N-CA-CB	-5.73	101.69	110.85
1	A	58	VAL	CA-CB-CG2	5.72	120.13	110.40
1	A	279	VAL	N-CA-CB	-5.72	104.48	111.00
1	A	243	PRO	CA-C-N	-5.72	113.70	122.62
1	A	243	PRO	C-N-CA	-5.72	113.70	122.62
1	A	29	ILE	CA-CB-CG2	5.72	120.22	110.50
1	B	354	THR	N-CA-CB	5.72	118.52	109.82
1	A	23	ASP	O-C-N	5.71	130.19	122.59
1	A	505	LEU	CA-C-O	-5.71	115.21	121.89
1	B	227	ILE	CA-CB-CG1	5.71	120.10	110.40
1	A	245	ASP	CA-CB-CG	-5.70	106.90	112.60
1	A	400	LEU	N-CA-CB	5.70	119.95	111.51
1	A	276	ALA	CA-C-N	-5.70	114.96	122.99
1	A	276	ALA	C-N-CA	-5.70	114.96	122.99
1	B	355	GLU	N-CA-C	5.70	117.49	111.28
1	A	152	VAL	CA-C-O	-5.69	114.14	120.46
1	A	61	ILE	N-CA-CB	5.69	119.42	110.31
1	B	230	LEU	CA-C-N	-5.69	111.25	120.87
1	B	230	LEU	C-N-CA	-5.69	111.25	120.87
1	B	262	THR	CA-C-N	-5.69	111.47	120.63
1	B	262	THR	C-N-CA	-5.69	111.47	120.63
1	B	326	ILE	N-CA-CB	5.69	116.73	110.53
1	B	259	ARG	NE-CZ-NH1	-5.68	115.82	121.50
1	A	114	SER	O-C-N	-5.68	115.04	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	101	GLU	CB-CA-C	5.68	119.03	111.14
1	A	151	GLU	O-C-N	-5.67	112.39	122.21
1	A	291	LYS	N-CA-C	-5.66	105.88	112.89
1	B	430	GLY	N-CA-C	5.66	120.78	110.71
1	B	363	ILE	O-C-N	-5.66	115.50	122.57
1	B	419	LEU	N-CA-CB	-5.66	101.51	110.22
1	A	393	PRO	CB-CA-C	5.65	121.03	112.21
1	B	168	PRO	CB-CA-C	-5.65	101.59	110.96
1	B	351	VAL	CA-C-N	-5.64	112.47	121.44
1	B	351	VAL	C-N-CA	-5.64	112.47	121.44
1	B	507	GLU	N-CA-C	5.64	122.81	110.80
1	A	216	CYS	CB-CA-C	-5.64	101.03	110.56
1	A	341	LYS	CA-C-N	-5.64	110.81	121.63
1	A	341	LYS	C-N-CA	-5.64	110.81	121.63
1	B	168	PRO	CA-C-N	5.64	131.40	122.94
1	B	168	PRO	C-N-CA	5.64	131.40	122.94
1	B	328	PRO	O-C-N	-5.64	115.03	122.64
1	A	196	ALA	O-C-N	5.63	129.63	123.27
1	B	367	GLY	O-C-N	5.63	128.49	123.59
1	B	256	ASN	CA-CB-CG	5.62	118.22	112.60
1	A	228	SER	N-CA-C	5.62	119.08	110.20
1	A	174	VAL	CB-CA-C	-5.62	102.07	111.29
1	B	392	MET	CA-C-O	5.62	123.80	118.63
1	A	408	VAL	CB-CA-C	-5.61	102.10	111.29
1	B	335	ILE	CA-C-N	5.60	132.24	121.54
1	B	335	ILE	C-N-CA	5.60	132.24	121.54
1	B	154	HIS	CA-CB-CG	5.60	119.40	113.80
1	A	493	ASP	CA-C-O	5.59	128.51	120.51
1	B	193	TYR	O-C-N	-5.59	115.68	123.34
1	A	494	VAL	O-C-N	-5.59	115.58	122.57
1	B	420	LYS	CA-C-O	5.59	126.44	120.24
1	A	378	LEU	O-C-N	-5.59	116.09	123.13
1	B	190	VAL	CA-C-N	-5.58	112.86	119.84
1	B	190	VAL	C-N-CA	-5.58	112.86	119.84
1	B	297	PHE	N-CA-C	5.58	118.17	109.52
1	A	348	ILE	N-CA-CB	-5.58	104.69	111.21
1	B	207	GLU	N-CA-C	5.58	120.09	113.12
1	A	479	ASP	CB-CA-C	-5.57	101.84	111.30
1	B	149	ASN	N-CA-CB	5.57	119.90	110.49
1	A	458	ILE	CA-C-N	5.56	128.05	120.54
1	A	458	ILE	C-N-CA	5.56	128.05	120.54
1	B	132	ALA	O-C-N	5.56	127.80	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	248	ILE	CB-CG1-CD1	-5.56	102.13	113.80
1	A	24	ASP	CA-CB-CG	5.55	118.15	112.60
1	A	499	VAL	N-CA-C	5.55	120.17	112.35
1	B	297	PHE	CA-C-N	5.55	132.13	121.54
1	B	297	PHE	C-N-CA	5.55	132.13	121.54
1	A	94	CYS	CA-C-N	-5.54	114.67	120.38
1	A	94	CYS	C-N-CA	-5.54	114.67	120.38
1	B	379	ASP	CA-C-N	5.54	130.72	122.74
1	B	379	ASP	C-N-CA	5.54	130.72	122.74
1	B	184	LEU	CA-C-O	5.54	129.00	122.14
1	A	281	VAL	N-CA-C	5.54	117.43	112.17
1	B	433	ARG	CA-C-O	5.53	127.74	120.16
1	A	397	GLN	CA-C-N	-5.53	113.77	122.95
1	A	397	GLN	C-N-CA	-5.53	113.77	122.95
1	A	262	THR	CA-CB-CG2	5.52	119.89	110.50
1	A	376	ARG	CA-C-O	5.52	125.65	119.41
1	A	298	SER	N-CA-CB	5.52	121.03	110.82
1	A	443	GLY	O-C-N	-5.51	117.37	123.05
1	A	227	ILE	N-CA-C	5.51	116.52	108.58
1	A	288	GLN	CA-C-N	5.51	130.18	122.41
1	A	288	GLN	C-N-CA	5.51	130.18	122.41
1	B	167	LYS	CG-CD-CE	5.51	123.98	111.30
1	B	470	ILE	CB-CA-C	-5.51	104.00	112.05
1	A	241	ALA	CA-C-O	5.51	125.74	119.18
1	A	413	ARG	CA-CB-CG	-5.51	103.08	114.10
1	A	451	ILE	CA-CB-CG1	5.51	119.76	110.40
1	B	361	ALA	N-CA-C	5.51	117.72	111.11
1	A	418	VAL	CA-C-O	5.50	126.78	121.05
1	B	169	LYS	CA-CB-CG	5.50	125.10	114.10
1	B	280	THR	CA-C-O	-5.50	115.92	122.13
1	B	253	LEU	O-C-N	5.50	130.06	123.36
1	A	251	TYR	CA-C-N	-5.49	114.46	122.65
1	A	251	TYR	C-N-CA	-5.49	114.46	122.65
1	B	412	VAL	O-C-N	-5.49	116.49	122.64
1	A	398	ARG	CA-CB-CG	5.49	125.07	114.10
1	A	394	ILE	CA-CB-CG1	5.49	119.73	110.40
1	B	457	GLU	CA-C-N	-5.48	113.66	120.56
1	B	457	GLU	C-N-CA	-5.48	113.66	120.56
1	B	286	LEU	CB-CA-C	5.48	120.86	110.51
1	A	345	PRO	CA-C-N	-5.48	116.40	123.19
1	A	345	PRO	C-N-CA	-5.48	116.40	123.19
1	B	293	MET	O-C-N	5.48	129.88	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	170	ILE	CA-CB-CG1	5.48	119.71	110.40
1	B	372	ASN	OD1-CG-ND2	-5.47	117.12	122.60
1	A	190	VAL	N-CA-C	-5.47	102.83	109.01
1	B	318	ALA	CB-CA-C	5.47	121.31	110.42
1	A	453	ILE	CB-CA-C	-5.46	104.76	112.14
1	A	265	LEU	CB-CG-CD2	-5.46	94.31	110.70
1	B	253	LEU	CB-CA-C	-5.46	100.09	109.65
1	A	37	THR	CA-CB-OG1	5.46	117.79	109.60
1	A	8	LYS	CA-C-N	5.46	131.97	121.54
1	A	8	LYS	C-N-CA	5.46	131.97	121.54
1	B	218	GLN	N-CA-CB	-5.46	101.27	110.49
1	A	97	TYR	CB-CA-C	5.46	119.86	111.95
1	A	408	VAL	CG1-CB-CG2	-5.46	98.80	110.80
1	A	81	LEU	N-CA-C	5.45	117.08	111.03
1	A	139	GLN	CA-C-N	-5.45	112.92	120.38
1	A	139	GLN	C-N-CA	-5.45	112.92	120.38
1	B	112	LEU	O-C-N	5.45	128.36	122.15
1	A	499	VAL	CA-C-N	5.45	129.08	121.24
1	A	499	VAL	C-N-CA	5.45	129.08	121.24
1	A	429	VAL	N-CA-C	5.44	117.73	108.86
1	A	7	ASN	CA-C-N	5.43	132.77	123.05
1	A	7	ASN	C-N-CA	5.43	132.77	123.05
1	B	470	ILE	CA-C-N	-5.43	112.06	120.31
1	B	470	ILE	C-N-CA	-5.43	112.06	120.31
1	A	238	ILE	CA-C-N	-5.43	112.41	120.82
1	A	238	ILE	C-N-CA	-5.43	112.41	120.82
1	B	376	ARG	O-C-N	5.42	129.02	122.35
1	B	474	LYS	C-N-CD	5.42	147.23	125.00
1	B	461	SER	CA-C-N	-5.41	112.61	120.29
1	B	461	SER	C-N-CA	-5.41	112.61	120.29
1	A	365	VAL	N-CA-CB	-5.41	102.31	111.23
1	A	423	CYS	CB-CA-C	-5.40	98.92	110.32
1	A	477	LEU	O-C-N	-5.40	114.74	122.41
1	B	98	ALA	N-CA-CB	5.40	118.50	110.40
1	B	112	LEU	CA-C-O	-5.40	114.70	120.42
1	B	447	VAL	N-CA-C	5.40	120.57	109.34
1	B	212	VAL	CB-CA-C	5.39	118.55	111.81
1	A	16	VAL	N-CA-C	-5.39	105.74	113.07
1	B	346	ILE	O-C-N	5.38	129.07	123.26
1	B	186	SER	CB-CA-C	-5.38	98.46	110.19
1	B	361	ALA	CA-C-O	-5.38	115.14	120.90
1	A	11	ILE	O-C-N	-5.38	115.85	122.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	288	GLN	CB-CA-C	5.38	119.40	110.74
1	A	509	GLU	CA-C-N	5.37	131.37	121.70
1	A	509	GLU	C-N-CA	5.37	131.37	121.70
1	B	336	GLU	CA-C-N	5.37	131.79	121.54
1	B	336	GLU	C-N-CA	5.37	131.79	121.54
1	B	475	PRO	O-C-N	-5.37	115.29	122.22
1	A	435	PHE	CA-C-N	-5.37	113.29	120.54
1	A	435	PHE	C-N-CA	-5.37	113.29	120.54
1	B	351	VAL	CB-CA-C	-5.37	105.44	111.45
1	A	435	PHE	CA-C-O	5.36	126.12	119.79
1	B	366	SER	N-CA-C	5.36	119.17	111.02
1	B	99	PRO	N-CA-C	5.35	123.49	112.47
1	A	510	ASP	CA-CB-CG	5.35	117.95	112.60
1	B	152	VAL	O-C-N	-5.34	116.23	121.94
1	A	420	LYS	CA-CB-CG	5.33	124.76	114.10
1	A	405	GLU	CA-C-N	-5.33	116.22	122.93
1	A	405	GLU	C-N-CA	-5.33	116.22	122.93
1	B	207	GLU	CA-C-N	5.32	128.68	120.00
1	B	207	GLU	C-N-CA	5.32	128.68	120.00
1	B	264	ASP	CA-CB-CG	5.32	117.92	112.60
1	A	136	LEU	O-C-N	5.32	129.14	122.86
1	A	210	LYS	O-C-N	-5.31	116.60	122.07
1	A	465	LEU	N-CA-C	-5.31	106.80	113.28
1	A	368	VAL	CA-C-N	-5.31	116.19	123.14
1	A	368	VAL	C-N-CA	-5.31	116.19	123.14
1	B	367	GLY	CA-C-N	5.31	130.07	121.95
1	B	367	GLY	C-N-CA	5.31	130.07	121.95
1	B	477	LEU	N-CA-C	-5.30	106.85	113.15
1	A	417	ASP	CA-C-N	-5.28	113.08	120.53
1	A	417	ASP	C-N-CA	-5.28	113.08	120.53
1	B	139	GLN	CA-C-O	5.28	125.78	119.60
1	B	463	ARG	NE-CZ-NH1	5.28	126.78	121.50
1	A	70	VAL	N-CA-CB	5.28	116.37	110.51
1	A	184	LEU	N-CA-CB	-5.28	103.31	111.65
1	A	470	ILE	CA-C-N	-5.28	109.17	121.52
1	A	470	ILE	C-N-CA	-5.28	109.17	121.52
1	A	298	SER	N-CA-C	5.27	119.56	107.48
1	A	144	TYR	N-CA-C	-5.27	105.21	111.69
1	A	287	GLY	CA-C-N	-5.27	115.38	123.07
1	A	287	GLY	C-N-CA	-5.27	115.38	123.07
1	A	171	LEU	CA-C-O	5.26	127.80	121.65
1	B	318	ALA	O-C-N	-5.26	115.60	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	GLU	C-N-CD	5.25	146.54	125.00
1	A	93	VAL	CB-CA-C	5.25	118.00	110.33
1	A	195	SER	CA-C-N	-5.25	115.47	122.72
1	A	195	SER	C-N-CA	-5.25	115.47	122.72
1	B	143	TYR	O-C-N	5.25	127.48	122.07
1	B	193	TYR	CA-C-N	-5.25	112.53	121.97
1	B	193	TYR	C-N-CA	-5.25	112.53	121.97
1	B	482	THR	CA-CB-OG1	5.25	117.47	109.60
1	B	423	CYS	N-CA-CB	-5.25	101.68	110.39
1	A	222	LYS	N-CA-C	5.24	117.22	108.99
1	B	98	ALA	O-C-N	5.24	131.39	123.00
1	B	123	ILE	CB-CA-C	-5.24	102.70	111.29
1	B	429	VAL	N-CA-C	5.23	116.02	108.48
1	B	398	ARG	CD-NE-CZ	5.23	131.72	124.40
1	B	431	LEU	CD1-CG-CD2	5.22	122.29	110.80
1	B	504	THR	N-CA-CB	-5.22	102.46	111.55
1	A	97	TYR	N-CA-CB	5.22	120.04	111.58
1	A	146	SER	CB-CA-C	-5.21	101.08	110.36
1	A	106	ILE	CA-C-N	-5.21	113.51	120.54
1	A	106	ILE	C-N-CA	-5.21	113.51	120.54
1	B	354	THR	CB-CA-C	5.21	119.20	110.92
1	A	296	LYS	CA-CB-CG	5.20	124.51	114.10
1	B	267	LYS	CA-CB-CG	5.20	124.51	114.10
1	A	185	GLY	O-C-N	-5.20	115.94	122.70
1	B	256	ASN	CA-C-O	-5.20	115.36	121.44
1	B	353	ARG	NE-CZ-NH1	-5.20	116.31	121.50
1	A	402	ASP	N-CA-C	-5.19	106.81	112.72
1	A	210	LYS	N-CA-C	5.18	116.62	111.07
1	A	467	VAL	O-C-N	-5.18	117.17	123.02
1	B	212	VAL	CA-CB-CG1	5.18	119.21	110.40
1	A	261	ILE	N-CA-CB	-5.17	102.70	111.23
1	A	262	THR	O-C-N	5.17	127.40	122.03
1	A	248	ILE	CG1-CB-CG2	-5.16	95.23	110.70
1	B	365	VAL	CB-CA-C	5.16	119.74	111.29
1	A	444	ARG	NE-CZ-NH1	-5.15	116.35	121.50
1	A	212	VAL	CA-C-N	-5.15	113.38	120.28
1	A	212	VAL	C-N-CA	-5.15	113.38	120.28
1	B	346	ILE	CA-CB-CG2	5.14	119.25	110.50
1	B	187	HIS	N-CA-C	-5.14	101.49	109.72
1	B	157	ASN	CA-C-N	-5.14	113.45	120.44
1	B	157	ASN	C-N-CA	-5.14	113.45	120.44
1	A	396	GLU	CB-CG-CD	-5.13	103.87	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	108	ARG	CD-NE-CZ	5.13	131.59	124.40
1	B	172	VAL	CB-CA-C	5.13	117.28	110.91
1	B	357	VAL	CA-C-N	5.13	127.76	120.53
1	B	357	VAL	C-N-CA	5.13	127.76	120.53
1	A	7	ASN	CA-CB-CG	5.13	117.73	112.60
1	A	49	VAL	CA-CB-CG2	5.13	119.11	110.40
1	B	191	PRO	CA-C-O	5.12	129.93	120.60
1	B	187	HIS	CA-C-N	5.12	131.19	121.97
1	B	187	HIS	C-N-CA	5.12	131.19	121.97
1	B	169	LYS	CG-CD-CE	5.12	123.08	111.30
1	B	218	GLN	O-C-N	-5.12	115.78	122.59
1	B	492	ASN	CA-C-N	5.12	130.71	123.14
1	B	492	ASN	C-N-CA	5.12	130.71	123.14
1	B	157	ASN	O-C-N	-5.11	116.70	122.12
1	A	181	THR	CA-C-N	-5.11	113.93	122.21
1	A	181	THR	C-N-CA	-5.11	113.93	122.21
1	B	234	SER	N-CA-CB	-5.10	100.60	109.73
1	B	121	ASN	CA-CB-CG	5.10	117.70	112.60
1	B	348	ILE	CA-CB-CG1	5.09	119.06	110.40
1	B	355	GLU	N-CA-CB	5.09	117.60	110.12
1	B	275	LYS	CA-C-O	5.08	125.61	119.31
1	A	19	HIS	N-CA-C	-5.08	106.21	114.09
1	B	468	THR	N-CA-CB	-5.08	104.24	111.00
1	B	157	ASN	CB-CG-ND2	5.08	124.02	116.40
1	A	380	PHE	N-CA-CB	5.08	119.07	110.49
1	B	423	CYS	CA-C-O	5.07	125.61	119.38
1	B	171	LEU	CA-C-O	5.07	127.09	120.81
1	A	400	LEU	CB-CA-C	5.06	120.16	111.45
1	B	344	LEU	C-N-CD	5.06	145.75	125.00
1	B	180	SER	N-CA-C	-5.06	101.72	109.41
1	B	272	LEU	CB-CA-C	5.06	120.33	110.57
1	A	352	GLN	CA-C-N	-5.05	112.69	122.09
1	A	352	GLN	C-N-CA	-5.05	112.69	122.09
1	A	439	ASN	CB-CG-ND2	5.05	123.98	116.40
1	A	496	TYR	CB-CA-C	-5.05	102.89	110.92
1	B	342	THR	O-C-N	5.05	128.46	123.46
1	A	181	THR	O-C-N	-5.05	116.89	122.75
1	A	343	LYS	CA-CB-CG	5.05	124.19	114.10
1	A	403	LYS	CA-CB-CG	5.04	124.19	114.10
1	B	357	VAL	CA-C-O	5.04	126.96	120.96
1	A	127	ASP	CA-C-N	-5.04	113.52	120.28
1	A	127	ASP	C-N-CA	-5.04	113.52	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	323	SER	CA-C-N	-5.04	112.55	120.60
1	A	323	SER	C-N-CA	-5.04	112.55	120.60
1	B	405	GLU	CB-CG-CD	5.04	121.16	112.60
1	B	447	VAL	CA-C-N	-5.03	112.26	121.52
1	B	447	VAL	C-N-CA	-5.03	112.26	121.52
1	A	11	ILE	CA-CB-CG1	5.03	118.95	110.40
1	B	212	VAL	CA-CB-CG2	5.03	118.95	110.40
1	B	454	LEU	CD1-CG-CD2	-5.02	99.75	110.80
1	B	292	ASP	CA-C-N	5.02	131.13	121.54
1	B	292	ASP	C-N-CA	5.02	131.13	121.54
1	B	261	ILE	O-C-N	5.02	128.84	122.57
1	A	103	LYS	CA-C-N	5.02	131.12	121.54
1	A	103	LYS	C-N-CA	5.02	131.12	121.54
1	B	255	VAL	CA-CB-CG1	5.01	118.93	110.40
1	B	507	GLU	N-CA-CB	5.01	118.97	110.49
1	A	184	LEU	O-C-N	-5.01	116.70	122.86
1	A	298	SER	CB-CA-C	5.01	119.38	111.77
1	A	155	ARG	CA-C-N	-5.00	113.58	120.28
1	A	155	ARG	C-N-CA	-5.00	113.58	120.28

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	11	ILE	CA
1	A	298	SER	CA
1	B	102	THR	CB
1	B	149	ASN	CA
1	B	272	LEU	CA
1	B	507	GLU	CA

All (121) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	10	LYS	Mainchain
1	A	104	GLU	Peptide
1	A	106	ILE	Peptide,Mainchain
1	A	11	ILE	Peptide
1	A	114	SER	Mainchain
1	A	138	LYS	Mainchain
1	A	139	GLN	Mainchain
1	A	148	ALA	Mainchain
1	A	151	GLU	Mainchain

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Mol	Chain	Res	Type	Group
1	A	154	HIS	Sidechain
1	A	160	ALA	Mainchain
1	A	181	THR	Mainchain
1	A	222	LYS	Peptide
1	A	231	ALA	Peptide
1	A	273	GLY	Peptide
1	A	293	MET	Mainchain
1	A	297	PHE	Peptide,Mainchain
1	A	31	GLY	Peptide
1	A	321	ALA	Mainchain
1	A	324	LYS	Peptide
1	A	326	ILE	Mainchain
1	A	380	PHE	Mainchain
1	A	382	ARG	Mainchain
1	A	384	PRO	Mainchain
1	A	395	LEU	Mainchain
1	A	396	GLU	Mainchain
1	A	403	LYS	Peptide
1	A	441	CYS	Mainchain
1	A	445	ASN	Peptide
1	A	452	GLU	Mainchain
1	A	460	MET	Mainchain
1	A	47	GLN	Peptide
1	A	475	PRO	Mainchain
1	A	491	PRO	Mainchain
1	A	492	ASN	Peptide
1	A	493	ASP	Mainchain
1	A	50	ILE	Peptide
1	A	506	THR	Peptide
1	A	507	GLU	Peptide,Sidechain,Mainchain
1	A	508	PHE	Peptide
1	A	509	GLU	Peptide
1	A	56	LYS	Peptide
1	A	57	ASP	Peptide
1	A	58	VAL	Mainchain
1	A	59	THR	Mainchain
1	A	67	ALA	Mainchain
1	A	72	ASP	Sidechain,Mainchain
1	A	80	LYS	Mainchain
1	A	85	GLN	Peptide
1	A	90	PRO	Peptide
1	A	92	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	A	96	PRO	Peptide
1	B	104	GLU	Mainchain
1	B	105	ASP	Sidechain
1	B	106	ILE	Peptide
1	B	111	GLN	Mainchain
1	B	112	LEU	Mainchain
1	B	113	LYS	Peptide
1	B	114	SER	Mainchain
1	B	118	PRO	Mainchain
1	B	119	LEU	Mainchain
1	B	120	ASP	Peptide
1	B	127	ASP	Sidechain
1	B	151	GLU	Mainchain
1	B	153	THR	Mainchain
1	B	154	HIS	Mainchain
1	B	172	VAL	Mainchain
1	B	187	HIS	Peptide,Mainchain
1	B	195	SER	Peptide
1	B	199	LEU	Mainchain
1	B	200	CYS	Mainchain
1	B	208	GLY	Mainchain
1	B	210	LYS	Peptide
1	B	211	ASP	Mainchain
1	B	224	PRO	Mainchain
1	B	229	THR	Mainchain
1	B	231	ALA	Peptide
1	B	242	ALA	Mainchain
1	B	246	LYS	Mainchain
1	B	247	GLN	Mainchain
1	B	255	VAL	Mainchain
1	B	256	ASN	Peptide
1	B	257	SER	Mainchain
1	B	263	ASP	Mainchain
1	B	266	VAL	Mainchain
1	B	267	LYS	Mainchain
1	B	270	GLU	Mainchain
1	B	295	LEU	Mainchain
1	B	296	LYS	Peptide,Mainchain
1	B	317	GLY	Peptide,Mainchain
1	B	324	LYS	Peptide
1	B	327	ASP	Mainchain
1	B	331	THR	Mainchain

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Mol	Chain	Res	Type	Group
1	B	332	TRP	Mainchain
1	B	336	GLU	Mainchain
1	B	339	LYS	Mainchain
1	B	353	ARG	Mainchain
1	B	363	ILE	Mainchain
1	B	364	GLY	Mainchain
1	B	370	LEU	Mainchain
1	B	378	LEU	Mainchain
1	B	380	PHE	Mainchain
1	B	394	ILE	Peptide
1	B	396	GLU	Mainchain
1	B	475	PRO	Mainchain
1	B	492	ASN	Peptide,Mainchain
1	B	493	ASP	Peptide,Mainchain
1	B	506	THR	Mainchain
1	B	98	ALA	Mainchain
1	B	99	PRO	Peptide,Mainchain

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	3833	0	3894	441	1
1	B	3081	0	3140	519	1
2	A	43	0	30	15	0
3	A	31	0	17	14	0
3	B	31	0	18	14	0
4	B	6	0	0	1	0
5	A	7	0	0	0	0
5	B	10	0	0	1	0
All	All	7042	0	7099	948	1

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 67.

All (948) 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:B:175:ARG:CD	1:B:175:ARG:CG	1.77	1.63
1:A:413:ARG:CD	1:A:413:ARG:CG	1.78	1.61
1:A:343:LYS:CB	1:A:343:LYS:CG	1.79	1.60
1:A:286:LEU:CD1	1:A:286:LEU:CG	1.78	1.59
1:B:106:ILE:CD1	1:B:106:ILE:CG1	1.75	1.59
1:B:289:ARG:CD	1:B:289:ARG:CG	1.82	1.58
1:B:289:ARG:CG	1:B:289:ARG:CB	1.79	1.56
1:B:167:LYS:CE	1:B:167:LYS:NZ	1.69	1.55
1:B:137:THR:CB	1:B:137:THR:CG2	1.85	1.51
1:A:340:LYS:NZ	1:A:340:LYS:CE	1.70	1.49
1:B:347:VAL:HG12	1:B:367:GLY:CA	1.41	1.47
1:B:441:CYS:CB	1:B:441:CYS:SG	2.02	1.47
1:B:278:PHE:CE2	1:B:347:VAL:HG21	1.46	1.46
1:B:347:VAL:CG1	1:B:367:GLY:HA3	1.51	1.36
1:B:347:VAL:HG12	1:B:367:GLY:C	1.55	1.31
1:B:278:PHE:CD2	1:B:347:VAL:HG23	1.65	1.30
1:B:228:SER:HA	1:B:252:GLN:NE2	1.50	1.25
1:B:278:PHE:CE2	1:B:347:VAL:CG2	2.19	1.25
1:B:430:GLY:C	1:B:431:LEU:HD12	1.59	1.25
1:B:431:LEU:HD12	1:B:431:LEU:N	1.44	1.23
1:B:109:LYS:O	1:B:113:LYS:HB2	1.37	1.23
1:B:229:THR:OG1	1:B:253:LEU:HA	1.31	1.23
1:B:227:ILE:HD12	1:B:250:TRP:O	1.28	1.22
1:B:278:PHE:CD2	1:B:347:VAL:CG2	2.20	1.22
1:B:361:ALA:CB	1:B:400:LEU:HD23	1.72	1.20
1:A:252:GLN:OE1	3:A:569:FMN:N3	1.74	1.18
1:B:431:LEU:N	1:B:431:LEU:CD1	2.06	1.18
1:B:447:VAL:O	1:B:451:ILE:HD12	1.42	1.17
1:B:233:CYS:HB2	1:B:238:ILE:HD11	1.18	1.14
1:A:2:PRO:HD2	1:A:71:ILE:HD13	1.19	1.14
1:B:227:ILE:CD1	1:B:250:TRP:O	1.95	1.14
1:B:412:VAL:O	1:B:413:ARG:HD3	1.49	1.13
1:A:110:GLU:HA	1:A:113:LYS:HB2	1.21	1.12
2:A:560:HEM:HHC	2:A:560:HEM:HBB2	1.16	1.12
1:B:136:LEU:HD23	1:B:136:LEU:H	1.13	1.12
1:B:276:ALA:HB2	1:B:345:PRO:HD2	1.15	1.11
1:B:196:ALA:HB2	1:B:226:MET:CE	1.80	1.11
1:B:347:VAL:CG1	1:B:367:GLY:CA	2.18	1.10
1:A:108:ARG:O	1:A:112:LEU:HD12	1.51	1.10
1:B:234:SER:OG	1:B:237:GLU:HB2	1.51	1.09
1:B:196:ALA:HB2	1:B:226:MET:HE3	1.29	1.09
1:A:396:GLU:O	1:A:398:ARG:N	1.87	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:ASN:HD22	1:A:257:SER:N	1.50	1.08
1:A:102:THR:O	1:A:103:LYS:C	1.89	1.07
1:A:102:THR:HB	1:A:104:GLU:HG2	1.32	1.07
1:A:110:GLU:O	1:A:113:LYS:HB3	1.52	1.07
1:B:361:ALA:HB1	1:B:400:LEU:HD23	1.13	1.07
1:A:70:VAL:HG23	1:A:71:ILE:HD12	1.34	1.05
1:A:204:ASN:HD22	1:A:439:ASN:ND2	1.51	1.05
1:B:448:GLU:HA	1:B:451:ILE:CD1	1.86	1.04
1:A:218:GLN:NE2	1:A:444:ARG:HH11	1.55	1.04
1:B:265:LEU:O	1:B:266:VAL:O	1.77	1.03
1:A:33:VAL:HG13	1:A:82:GLY:O	1.58	1.03
1:B:196:ALA:CB	1:B:226:MET:CE	2.36	1.03
1:B:229:THR:H	1:B:252:GLN:NE2	1.56	1.02
1:B:246:LYS:O	1:B:247:GLN:O	1.77	1.02
1:A:29:ILE:CD1	1:A:58:VAL:HG12	1.91	1.01
2:A:560:HEM:HHC	2:A:560:HEM:CBB	1.91	1.00
1:A:29:ILE:HD11	1:A:58:VAL:HG12	1.38	1.00
1:B:448:GLU:HA	1:B:451:ILE:HD13	1.39	0.99
1:B:104:GLU:C	1:B:106:ILE:H	1.56	0.99
1:B:276:ALA:CB	1:B:345:PRO:HD2	1.92	0.99
1:A:462:MET:HE1	1:A:469:SER:C	1.89	0.98
1:B:447:VAL:O	1:B:451:ILE:CD1	2.11	0.98
1:A:2:PRO:CD	1:A:71:ILE:HD13	1.94	0.97
1:B:286:LEU:HD21	1:B:323:SER:HB3	1.43	0.97
1:B:234:SER:OG	1:B:237:GLU:CB	2.12	0.96
1:B:246:LYS:O	1:B:247:GLN:C	2.06	0.95
1:A:59:THR:HG23	1:A:63:GLU:HG2	1.49	0.95
1:A:67:ALA:C	1:A:70:VAL:HG13	1.92	0.94
1:B:347:VAL:HG12	1:B:367:GLY:HA3	1.13	0.94
1:A:218:GLN:NE2	1:A:444:ARG:NH1	2.16	0.94
1:A:110:GLU:CA	1:A:113:LYS:HB2	1.98	0.93
1:B:153:THR:O	1:B:154:HIS:C	2.06	0.93
1:B:265:LEU:O	1:B:266:VAL:C	2.09	0.93
1:A:209:GLU:HB3	1:A:238:ILE:HD13	1.51	0.93
1:A:204:ASN:HD22	1:A:439:ASN:HD21	1.13	0.93
1:B:109:LYS:O	1:B:113:LYS:CB	2.16	0.93
1:B:183:MET:HE2	1:B:428:GLY:HA3	1.50	0.93
1:B:248:ILE:HG13	1:B:249:GLN:N	1.81	0.93
1:B:233:CYS:CB	1:B:238:ILE:HD11	1.99	0.92
1:B:228:SER:HA	1:B:252:GLN:HE22	1.26	0.92
1:B:317:GLY:N	1:B:320:ARG:NH2	2.17	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:LEU:HD13	1:B:328:PRO:HG2	1.51	0.92
1:A:218:GLN:HE22	1:A:444:ARG:NH1	1.68	0.92
1:A:204:ASN:ND2	1:A:439:ASN:HD21	1.67	0.91
1:B:248:ILE:HG13	1:B:249:GLN:H	1.34	0.91
1:A:413:ARG:NH2	3:A:569:FMN:O3P	2.03	0.91
1:B:201:LYS:HB2	1:B:232:SER:CB	2.00	0.91
1:B:108:ARG:HH12	1:B:137:THR:HA	1.35	0.90
2:A:560:HEM:HHD	2:A:560:HEM:HBC2	1.52	0.90
1:B:267:LYS:O	1:B:268:ASN:C	2.00	0.90
1:B:353:ARG:NH1	1:B:356:ASP:OD1	2.05	0.90
1:B:387:VAL:O	1:B:391:THR:HG23	1.72	0.89
1:B:229:THR:OG1	1:B:253:LEU:CA	2.19	0.89
1:B:175:ARG:CG	1:B:175:ARG:HH11	1.84	0.89
1:B:236:GLU:HB3	1:B:272:LEU:HD11	1.53	0.89
1:B:104:GLU:C	1:B:106:ILE:N	2.28	0.88
1:B:361:ALA:HB1	1:B:400:LEU:CD2	2.01	0.88
1:A:160:ALA:O	1:A:161:TYR:C	2.14	0.88
1:B:392:MET:HE1	1:B:406:VAL:HG21	1.56	0.87
1:A:218:GLN:HE22	1:A:444:ARG:HH11	0.88	0.87
1:A:395:LEU:O	1:A:396:GLU:C	2.01	0.87
1:B:233:CYS:HB2	1:B:238:ILE:CD1	2.03	0.87
1:A:210:LYS:HG2	1:A:241:ALA:CB	2.04	0.87
1:A:102:THR:O	1:A:103:LYS:O	1.93	0.86
1:A:229:THR:H	1:A:252:GLN:NE2	1.72	0.86
1:B:229:THR:N	1:B:252:GLN:HE22	1.72	0.86
1:A:60:ALA:O	1:A:96:PRO:HB3	1.75	0.86
1:B:255:VAL:HG13	1:B:330:LEU:HD11	1.55	0.86
1:A:223:VAL:HG13	1:A:224:PRO:HD2	1.58	0.85
1:B:229:THR:H	1:B:252:GLN:HE22	1.19	0.85
1:B:465:LEU:O	1:B:465:LEU:HD23	1.75	0.85
1:A:102:THR:C	1:A:103:LYS:HD3	2.01	0.85
1:B:278:PHE:HE2	1:B:347:VAL:HG21	1.34	0.85
1:B:136:LEU:H	1:B:136:LEU:CD2	1.90	0.85
1:B:137:THR:HG22	1:B:139:GLN:HB3	1.57	0.85
1:B:228:SER:CA	1:B:252:GLN:HE22	1.90	0.84
1:B:442:TYR:HB2	1:B:446:GLY:HA3	1.58	0.84
1:A:29:ILE:HD11	1:A:58:VAL:CG1	2.07	0.84
1:A:196:ALA:H	1:A:226:MET:HE2	1.42	0.84
1:B:347:VAL:HG11	1:B:367:GLY:HA3	1.56	0.84
1:A:199:LEU:HD21	2:A:560:HEM:HAA1	1.60	0.84
1:A:25:CYS:SG	1:A:54:ALA:HB1	2.18	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:THR:CG2	1:B:139:GLN:HB3	2.08	0.83
1:A:256:ASN:ND2	1:A:257:SER:N	2.27	0.83
1:A:372:ASN:C	1:A:372:ASN:HD22	1.87	0.83
1:B:136:LEU:HD23	1:B:136:LEU:N	1.93	0.82
1:B:394:ILE:HA	1:B:397:GLN:OE1	1.79	0.82
1:A:269:VAL:HA	1:A:272:LEU:HD12	1.60	0.82
2:A:560:HEM:HBB2	2:A:560:HEM:CHC	2.05	0.82
1:A:229:THR:H	1:A:252:GLN:HE22	1.26	0.82
1:A:179:ILE:HA	1:A:470:ILE:CD1	2.10	0.82
1:A:173:ASP:OD2	1:B:329:SER:HB2	1.78	0.81
1:A:413:ARG:HG3	1:A:413:ARG:HH11	1.44	0.81
1:A:448:GLU:HA	1:A:451:ILE:HG13	1.63	0.81
1:B:179:ILE:HA	1:B:470:ILE:CD1	2.10	0.81
1:B:196:ALA:CB	1:B:226:MET:HE2	2.11	0.81
1:B:234:SER:OG	1:B:237:GLU:OE1	1.96	0.81
1:A:217:GLY:O	1:A:222:LYS:NZ	2.12	0.81
1:B:346:ILE:HG22	1:B:365:VAL:HG11	1.61	0.81
1:B:354:THR:OG1	1:B:391:THR:HG22	1.78	0.81
1:B:276:ALA:HB2	1:B:345:PRO:CD	2.06	0.81
1:B:196:ALA:CB	1:B:226:MET:HE3	2.03	0.81
1:A:353:ARG:HH11	1:A:355:GLU:HB2	1.45	0.80
1:A:210:LYS:HG2	1:A:241:ALA:HB2	1.62	0.80
1:B:378:LEU:HD22	1:B:379:ASP:O	1.82	0.80
1:B:132:ALA:O	1:B:136:LEU:HD23	1.82	0.79
1:A:54:ALA:O	1:A:56:LYS:NZ	2.15	0.79
1:B:179:ILE:HA	1:B:470:ILE:HD12	1.63	0.79
1:B:454:LEU:O	1:B:458:ILE:HG12	1.83	0.79
1:B:146:SER:HB3	1:B:291:LYS:HB2	1.65	0.79
1:B:229:THR:OG1	1:B:252:GLN:O	2.00	0.79
1:A:373:GLN:HG3	3:A:569:FMN:H1'1	1.63	0.79
1:A:2:PRO:HG2	1:A:71:ILE:HB	1.64	0.79
1:B:398:ARG:HB2	1:B:400:LEU:HD13	1.63	0.79
1:B:130:TYR:O	1:B:133:SER:OG	2.00	0.79
1:B:175:ARG:HH11	1:B:175:ARG:HG3	1.48	0.78
1:B:175:ARG:NH1	1:B:175:ARG:CB	2.47	0.78
1:B:201:LYS:HB2	1:B:232:SER:HB3	1.65	0.78
1:B:414:ARG:O	1:B:417:ASP:HB2	1.83	0.78
1:B:433:ARG:O	1:B:437:TYR:CD2	2.35	0.78
1:A:226:MET:HE1	1:A:349:LYS:HD2	1.65	0.78
1:A:286:LEU:CD1	1:A:286:LEU:HG	2.09	0.78
1:A:498:GLU:HG2	1:B:505:LEU:HD11	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:VAL:O	1:B:269:VAL:HG22	1.84	0.78
1:B:322:LEU:HD13	1:B:328:PRO:CG	2.14	0.78
1:A:109:LYS:HE2	1:A:109:LYS:HA	1.65	0.78
1:A:395:LEU:O	1:A:396:GLU:O	2.01	0.78
1:A:53:ASN:ND2	1:A:94:CYS:SG	2.57	0.78
1:A:252:GLN:OE1	3:A:569:FMN:C2	2.32	0.77
1:A:493:ASP:O	1:A:494:VAL:C	2.25	0.77
1:B:181:THR:O	1:B:188:VAL:HG23	1.84	0.77
1:B:213:ALA:HB2	1:B:225:GLN:HE22	1.49	0.77
1:A:38:ARG:NH2	1:A:75:ILE:HB	1.98	0.77
1:B:433:ARG:HB3	1:B:437:TYR:CE2	2.19	0.77
1:B:371:SER:HB2	1:B:409:ASP:OD1	1.85	0.77
1:B:228:SER:CA	1:B:252:GLN:NE2	2.39	0.77
1:B:196:ALA:HB3	1:B:226:MET:CE	2.14	0.77
1:B:283:ALA:N	1:B:284:PRO:CD	2.47	0.77
1:B:229:THR:N	1:B:252:GLN:NE2	2.30	0.76
1:A:32:TYR:HE1	1:A:82:GLY:HA2	1.49	0.76
1:A:179:ILE:HA	1:A:470:ILE:HD12	1.67	0.76
1:A:223:VAL:HG13	1:A:224:PRO:CD	2.15	0.76
1:A:204:ASN:ND2	1:A:439:ASN:ND2	2.26	0.76
1:A:256:ASN:HD22	1:A:257:SER:H	1.32	0.76
1:B:228:SER:HA	1:B:252:GLN:HE21	1.50	0.76
1:A:171:LEU:HD12	1:B:332:TRP:CE2	2.20	0.76
1:B:461:SER:O	1:B:465:LEU:HB2	1.85	0.76
1:B:184:LEU:HD22	1:B:250:TRP:CZ2	2.21	0.76
1:A:332:TRP:CZ2	1:A:359:LYS:HD3	2.20	0.76
1:B:275:LYS:HB2	1:B:275:LYS:NZ	2.01	0.75
1:A:347:VAL:HA	1:A:367:GLY:O	1.86	0.75
1:B:196:ALA:O	3:B:570:FMN:C4A	2.34	0.75
1:B:448:GLU:HA	1:B:451:ILE:HD12	1.68	0.75
1:A:41:PRO:HA	1:A:47:GLN:HG3	1.69	0.75
1:A:398:ARG:O	1:A:399:ASN:C	2.27	0.75
1:B:251:TYR:HB3	1:B:277:LEU:CD2	2.16	0.75
1:B:164:ILE:HB	1:B:420:LYS:HE2	1.69	0.75
1:B:410:GLY:HA2	3:B:570:FMN:P	2.27	0.74
1:B:447:VAL:HG12	1:B:451:ILE:HD11	1.70	0.74
1:A:42:ASN:OD1	1:A:324:LYS:HB2	1.85	0.74
1:B:317:GLY:N	1:B:320:ARG:HH21	1.85	0.74
1:A:110:GLU:HG2	1:A:113:LYS:HD3	1.69	0.74
1:A:392:MET:CE	1:A:395:LEU:HD12	2.17	0.74
1:B:228:SER:OG	3:B:570:FMN:O4	2.05	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:SER:OG	1:B:246:LYS:NZ	2.20	0.74
1:B:431:LEU:CD1	1:B:431:LEU:H	2.00	0.74
1:B:447:VAL:O	1:B:447:VAL:HG12	1.84	0.74
1:A:194:VAL:HG22	1:A:435:PHE:CD2	2.22	0.74
1:A:506:THR:OG1	1:B:127:ASP:OD1	2.05	0.74
1:B:325:PHE:HD1	1:B:325:PHE:H	1.35	0.74
1:A:56:LYS:C	1:A:58:VAL:HG23	2.13	0.73
1:A:60:ALA:HB2	1:A:94:CYS:O	1.87	0.73
1:A:256:ASN:ND2	1:A:257:SER:H	1.86	0.73
1:A:60:ALA:CB	1:A:94:CYS:O	2.36	0.73
1:A:84:LEU:HD11	1:A:87:SER:HA	1.71	0.73
1:A:256:ASN:ND2	1:A:258:ASP:H	1.85	0.73
1:B:361:ALA:CB	1:B:400:LEU:CD2	2.60	0.73
1:B:262:THR:O	1:B:266:VAL:HG23	1.89	0.73
1:A:110:GLU:O	1:A:113:LYS:CB	2.32	0.72
1:A:392:MET:HE3	1:A:395:LEU:HD12	1.71	0.72
1:B:183:MET:HE2	1:B:428:GLY:CA	2.19	0.72
1:B:196:ALA:HB2	1:B:226:MET:HE2	1.69	0.72
1:B:196:ALA:O	3:B:570:FMN:C10	2.37	0.72
1:A:62:PHE:HZ	1:A:70:VAL:HG21	1.55	0.72
1:A:339:LYS:HD2	1:A:340:LYS:NZ	2.04	0.72
1:A:373:GLN:HG3	3:A:569:FMN:C1'	2.20	0.72
1:B:137:THR:HG22	1:B:139:GLN:H	1.52	0.72
1:B:163:ARG:HH21	1:B:486:ARG:HA	1.53	0.72
1:B:193:TYR:O	1:B:194:VAL:C	2.29	0.72
1:B:221:THR:HG22	1:B:222:LYS:N	2.05	0.72
1:B:175:ARG:CG	1:B:175:ARG:NH1	2.52	0.71
1:B:278:PHE:HD2	1:B:347:VAL:HG23	1.51	0.71
1:B:331:THR:HG22	1:B:333:LYS:H	1.55	0.71
1:B:491:PRO:C	1:B:492:ASN:O	2.34	0.71
1:B:252:GLN:HA	1:B:278:PHE:O	1.91	0.71
1:B:347:VAL:CG1	1:B:367:GLY:C	2.50	0.71
1:B:212:VAL:HG12	1:B:439:ASN:OD1	1.90	0.71
1:B:388:LEU:HD23	1:B:392:MET:HG2	1.73	0.71
1:B:199:LEU:HB3	1:B:202:LEU:HD12	1.72	0.71
1:A:506:THR:HG1	1:B:127:ASP:CG	1.99	0.70
1:A:413:ARG:CG	1:A:413:ARG:HH11	2.03	0.70
1:B:201:LYS:HB2	1:B:232:SER:OG	1.90	0.70
1:A:182:ASP:HB2	1:A:187:HIS:HA	1.74	0.70
1:B:442:TYR:HB2	1:B:446:GLY:CA	2.22	0.70
1:A:61:ILE:HD11	1:A:94:CYS:HB3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:GLU:O	1:A:241:ALA:HB2	1.91	0.69
1:B:236:GLU:HA	1:B:239:ILE:HG22	1.74	0.69
1:B:283:ALA:HA	1:B:377:GLN:NE2	2.06	0.69
1:A:498:GLU:HG2	1:B:505:LEU:CD1	2.22	0.69
1:A:247:GLN:C	1:A:248:ILE:HG22	2.18	0.69
1:A:413:ARG:HG3	1:A:413:ARG:NH1	2.07	0.69
1:A:462:MET:CE	1:A:469:SER:C	2.66	0.69
1:B:362:GLU:C	1:B:364:GLY:H	2.01	0.69
1:A:62:PHE:CZ	1:A:70:VAL:HG21	2.28	0.69
1:B:211:ASP:HB3	1:B:439:ASN:HD21	1.56	0.69
1:A:62:PHE:HZ	1:A:70:VAL:CG2	2.06	0.69
1:B:180:SER:HA	1:B:189:ASP:O	1.93	0.69
1:B:227:ILE:HD11	1:B:250:TRP:H	1.58	0.68
1:B:255:VAL:CG1	1:B:330:LEU:HD11	2.23	0.68
1:B:259:ARG:HG3	1:B:259:ARG:HH11	1.57	0.68
1:A:75:ILE:HD11	1:A:80:LYS:HG2	1.75	0.68
1:B:209:GLU:CD	1:B:231:ALA:HB1	2.18	0.68
1:B:184:LEU:O	1:B:186:SER:N	2.25	0.68
1:B:161:TYR:CE1	1:B:385:ILE:HD13	2.27	0.68
1:B:180:SER:CB	1:B:189:ASP:O	2.41	0.68
1:B:184:LEU:HD22	1:B:250:TRP:HZ2	1.58	0.68
1:B:286:LEU:N	1:B:286:LEU:HD22	2.08	0.68
1:B:98:ALA:HB1	1:B:101:GLU:HG3	1.74	0.68
1:B:236:GLU:HB3	1:B:272:LEU:CD1	2.23	0.68
1:A:171:LEU:HD12	1:B:332:TRP:CD2	2.29	0.68
1:A:148:ALA:O	1:A:379:ASP:OD2	2.11	0.68
1:A:257:SER:HB2	1:A:324:LYS:O	1.94	0.68
1:B:262:THR:O	1:B:264:ASP:N	2.27	0.67
1:A:32:TYR:HE1	1:A:82:GLY:CA	2.07	0.67
1:A:9:GLN:O	1:A:10:LYS:HB3	1.94	0.67
1:B:214:ARG:HG2	1:B:214:ARG:HH11	1.59	0.67
1:A:269:VAL:HA	1:A:272:LEU:CD1	2.25	0.67
1:B:108:ARG:NH1	1:B:136:LEU:O	2.27	0.67
1:A:353:ARG:HD3	1:A:355:GLU:OE1	1.94	0.67
1:B:283:ALA:N	1:B:284:PRO:HD2	2.10	0.67
1:B:124:ASN:HD22	1:B:126:TYR:N	1.92	0.67
1:B:152:VAL:O	1:B:153:THR:C	2.36	0.67
1:A:108:ARG:O	1:A:112:LEU:CD1	2.39	0.67
1:A:196:ALA:O	3:A:569:FMN:O2'	2.08	0.67
1:B:259:ARG:HH11	1:B:259:ARG:CG	2.06	0.67
1:B:98:ALA:HB1	1:B:101:GLU:CB	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ALA:HB1	1:A:96:PRO:CD	2.25	0.66
1:B:214:ARG:HB3	1:B:444:ARG:HD2	1.77	0.66
1:A:14:ALA:O	1:A:17:ALA:HB3	1.96	0.66
1:A:61:ILE:HG23	1:A:97:TYR:HB2	1.78	0.66
1:B:136:LEU:CD2	1:B:136:LEU:N	2.55	0.66
1:B:267:LYS:O	1:B:269:VAL:N	2.28	0.66
1:A:27:VAL:HG22	1:A:56:LYS:O	1.95	0.66
1:A:339:LYS:HD2	1:A:340:LYS:HZ1	1.59	0.66
1:B:262:THR:C	1:B:264:ASP:N	2.47	0.66
1:A:4:LEU:HB3	1:A:32:TYR:HE2	1.61	0.66
1:B:102:THR:HB	1:B:104:GLU:HG3	1.77	0.66
1:A:382:ARG:O	1:A:383:ALA:C	2.13	0.66
1:A:50:ILE:O	1:A:54:ALA:HB2	1.96	0.65
1:A:196:ALA:N	1:A:226:MET:HE2	2.11	0.65
1:A:213:ALA:HB2	1:A:225:GLN:HE22	1.61	0.65
1:A:394:ILE:O	1:A:395:LEU:C	2.34	0.65
1:A:110:GLU:C	1:A:113:LYS:CB	2.69	0.65
1:A:506:THR:OG1	1:B:127:ASP:CG	2.40	0.65
1:B:346:ILE:HB	1:B:365:VAL:HG21	1.77	0.65
1:A:209:GLU:CB	1:A:238:ILE:HD13	2.26	0.65
1:B:248:ILE:CG1	1:B:249:GLN:N	2.57	0.65
1:B:396:GLU:HG3	1:B:401:LYS:NZ	2.12	0.65
1:B:167:LYS:NZ	1:B:167:LYS:CD	2.60	0.64
1:B:219:GLY:O	1:B:222:LYS:NZ	2.26	0.64
1:B:98:ALA:HB1	1:B:101:GLU:CG	2.27	0.64
1:A:179:ILE:HD11	1:A:455:ARG:HG3	1.80	0.64
1:B:153:THR:HG21	1:B:381:SER:HB3	1.79	0.64
1:B:184:LEU:CD2	1:B:250:TRP:CZ2	2.81	0.64
1:B:392:MET:N	1:B:393:PRO:HD2	2.12	0.64
1:B:197:THR:OG1	1:B:436:LEU:HG	1.98	0.63
1:B:236:GLU:HA	1:B:239:ILE:CG2	2.28	0.63
1:A:148:ALA:HB2	1:A:376:ARG:O	1.98	0.63
1:B:105:ASP:O	1:B:109:LYS:HB2	1.98	0.63
1:A:19:HIS:O	1:A:21:LYS:N	2.31	0.63
1:A:212:VAL:HG12	1:A:439:ASN:OD1	1.99	0.63
1:B:174:VAL:HG21	1:B:463:ARG:HB3	1.80	0.63
1:A:105:ASP:HA	1:A:108:ARG:HB2	1.80	0.63
1:B:102:THR:O	1:B:104:GLU:N	2.31	0.63
1:B:174:VAL:HG23	1:B:174:VAL:O	1.98	0.63
1:B:234:SER:OG	1:B:237:GLU:HB3	1.98	0.63
1:B:239:ILE:CD1	1:B:274:VAL:HG13	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ASP:OD2	1:B:329:SER:CB	2.45	0.62
1:A:179:ILE:HA	1:A:470:ILE:HD11	1.81	0.62
1:A:179:ILE:CA	1:A:470:ILE:HD12	2.29	0.62
1:B:439:ASN:HD22	1:B:443:GLY:HA2	1.64	0.62
1:A:124:ASN:HD22	1:A:124:ASN:C	2.06	0.62
1:A:201:LYS:HB2	1:A:232:SER:CB	2.30	0.62
1:A:396:GLU:O	1:A:397:GLN:C	2.27	0.62
1:B:382:ARG:NH2	1:B:390:GLU:OE2	2.33	0.62
1:A:179:ILE:C	1:A:470:ILE:HD12	2.25	0.62
1:B:111:GLN:HB3	1:B:135:THR:HG22	1.82	0.62
1:B:195:SER:O	1:B:197:THR:HG22	1.98	0.62
1:B:239:ILE:HD11	1:B:274:VAL:HG13	1.82	0.62
1:B:286:LEU:CD2	1:B:323:SER:HB3	2.25	0.62
1:B:198:ALA:HB2	3:B:570:FMN:O4	2.00	0.62
1:B:430:GLY:CA	1:B:431:LEU:HD12	2.28	0.62
1:B:491:PRO:O	1:B:492:ASN:O	2.16	0.62
1:B:262:THR:O	1:B:263:ASP:C	2.38	0.62
1:A:257:SER:CB	1:A:324:LYS:O	2.48	0.61
1:B:337:GLU:C	1:B:341:LYS:HE2	2.25	0.61
1:B:371:SER:CB	1:B:409:ASP:OD1	2.48	0.61
1:B:175:ARG:NH1	1:B:175:ARG:HB3	2.15	0.61
1:B:268:ASN:O	1:B:268:ASN:ND2	2.33	0.61
1:A:265:LEU:HD22	1:A:265:LEU:O	2.00	0.61
1:A:265:LEU:HD22	1:A:265:LEU:C	2.25	0.61
1:B:153:THR:HG23	1:B:381:SER:O	2.00	0.61
1:B:282:ASP:OD2	1:B:373:GLN:HG3	2.01	0.61
1:A:211:ASP:O	1:A:212:VAL:C	2.36	0.61
1:A:177:VAL:HG12	1:A:468:THR:HA	1.83	0.61
1:A:242:ALA:HB1	1:A:247:GLN:OE1	2.00	0.61
1:B:354:THR:HG21	1:B:394:ILE:CD1	2.31	0.61
1:A:4:LEU:HD22	1:A:80:LYS:HD2	1.83	0.61
1:A:60:ALA:HB1	1:A:96:PRO:HD3	1.82	0.61
1:A:164:ILE:O	1:A:420:LYS:CE	2.49	0.61
1:B:175:ARG:HH11	1:B:175:ARG:CB	2.10	0.61
1:B:494:VAL:O	1:B:498:GLU:HB2	2.01	0.61
1:A:110:GLU:C	1:A:113:LYS:HB2	2.26	0.61
1:A:171:LEU:HD12	1:B:332:TRP:CZ2	2.36	0.61
1:A:223:VAL:CG1	1:A:224:PRO:CD	2.78	0.61
1:B:182:ASP:HA	1:B:188:VAL:HG23	1.81	0.61
1:B:451:ILE:HD12	1:B:451:ILE:H	1.66	0.61
1:B:123:ILE:CG2	1:B:123:ILE:O	2.43	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:LYS:HD3	1:B:232:SER:HB3	1.81	0.60
1:B:412:VAL:O	1:B:413:ARG:CD	2.39	0.60
1:B:261:ILE:HG22	1:B:261:ILE:O	2.00	0.60
1:A:19:HIS:O	1:A:24:ASP:O	2.19	0.60
1:A:462:MET:HE1	1:A:470:ILE:N	2.16	0.60
1:A:163:ARG:NH2	1:A:486:ARG:HA	2.16	0.60
1:A:29:ILE:CD1	1:A:58:VAL:CG1	2.72	0.60
1:A:70:VAL:HG23	1:A:71:ILE:CD1	2.23	0.60
1:A:38:ARG:NH1	1:A:39:PHE:HB3	2.17	0.60
1:A:59:THR:HG23	1:A:63:GLU:CG	2.29	0.60
1:A:67:ALA:O	1:A:70:VAL:HG13	2.01	0.60
1:B:175:ARG:O	1:B:463:ARG:NH2	2.34	0.60
1:A:84:LEU:HG	1:A:86:GLY:O	2.01	0.59
1:A:27:VAL:HG13	1:A:28:VAL:N	2.17	0.59
1:A:160:ALA:O	1:A:162:HIS:N	2.34	0.59
1:A:268:ASN:O	1:A:269:VAL:C	2.42	0.59
1:A:394:ILE:O	1:A:395:LEU:O	2.20	0.59
1:B:163:ARG:NH2	1:B:486:ARG:HG3	2.17	0.59
1:B:318:ALA:C	1:B:320:ARG:H	2.05	0.59
1:B:388:LEU:CD2	1:B:392:MET:HG2	2.32	0.59
1:A:349:LYS:NZ	3:A:569:FMN:O2'	2.34	0.59
1:B:362:GLU:C	1:B:364:GLY:N	2.60	0.59
1:A:106:ILE:O	1:A:107:ALA:C	2.45	0.59
1:B:137:THR:C	1:B:139:GLN:N	2.59	0.59
1:B:254:TYR:O	1:B:255:VAL:C	2.43	0.59
1:A:204:ASN:C	1:A:206:LEU:H	2.09	0.59
1:A:234:SER:O	1:A:238:ILE:HG13	2.03	0.59
1:A:10:LYS:HG2	1:A:11:ILE:N	2.17	0.59
1:A:109:LYS:HA	1:A:112:LEU:HD13	1.84	0.59
1:B:447:VAL:O	1:B:447:VAL:CG1	2.50	0.59
1:A:179:ILE:CA	1:A:470:ILE:CD1	2.81	0.59
1:B:213:ALA:CB	1:B:225:GLN:HE22	2.15	0.59
1:A:263:ASP:OD2	1:A:341:LYS:HD2	2.02	0.58
1:B:111:GLN:O	1:B:112:LEU:C	2.46	0.58
1:A:179:ILE:C	1:A:470:ILE:CD1	2.76	0.58
1:B:207:GLU:HG3	1:B:214:ARG:HH22	1.68	0.58
1:A:413:ARG:HH22	3:A:569:FMN:P	2.26	0.58
1:A:433:ARG:HG3	3:A:569:FMN:O1P	2.03	0.58
1:A:252:GLN:OE1	3:A:569:FMN:O2	2.21	0.58
1:B:132:ALA:O	1:B:136:LEU:CD2	2.51	0.58
1:B:286:LEU:HD22	1:B:286:LEU:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ILE:HD13	1:A:59:THR:OG1	2.03	0.58
1:A:42:ASN:OD1	1:A:324:LYS:N	2.29	0.58
1:A:98:ALA:O	1:A:99:PRO:C	2.46	0.58
1:B:123:ILE:O	1:B:123:ILE:HG22	1.92	0.58
1:B:330:LEU:HD23	1:B:331:THR:H	1.69	0.58
1:A:58:VAL:O	1:A:59:THR:C	2.43	0.57
1:B:399:ASN:ND2	5:B:587:HOH:O	2.36	0.57
1:A:222:LYS:C	1:A:223:VAL:HG23	2.29	0.57
1:B:440:SER:O	1:B:441:CYS:HB3	2.04	0.57
1:A:57:ASP:C	1:A:58:VAL:HG23	2.28	0.57
1:B:365:VAL:HG13	1:B:366:SER:H	1.69	0.57
1:B:227:ILE:CD1	1:B:250:TRP:C	2.76	0.57
1:B:275:LYS:O	1:B:276:ALA:HB2	2.04	0.57
1:A:332:TRP:CD1	1:A:332:TRP:H	2.22	0.57
1:B:387:VAL:O	1:B:388:LEU:C	2.46	0.57
1:B:258:ASP:HB3	1:B:261:ILE:HG13	1.86	0.57
1:A:136:LEU:HD21	1:A:440:SER:HB3	1.85	0.57
1:A:182:ASP:CB	1:A:187:HIS:HA	2.35	0.57
1:A:29:ILE:CG1	1:A:58:VAL:HG12	2.35	0.56
1:A:69:ASN:O	1:A:73:LYS:HB2	2.05	0.56
1:A:223:VAL:CG1	1:A:224:PRO:HD2	2.34	0.56
1:B:163:ARG:NH2	1:B:486:ARG:CB	2.68	0.56
1:B:176:LYS:HB2	1:B:176:LYS:NZ	2.21	0.56
1:B:221:THR:CG2	1:B:222:LYS:N	2.68	0.56
1:A:450:ALA:O	1:A:451:ILE:C	2.47	0.56
1:B:325:PHE:CD1	1:B:325:PHE:N	2.74	0.56
1:A:183:MET:O	1:A:184:LEU:C	2.49	0.56
1:B:137:THR:C	1:B:139:GLN:H	2.11	0.56
1:B:392:MET:N	1:B:393:PRO:CD	2.67	0.56
1:A:29:ILE:HG12	1:A:58:VAL:CG1	2.35	0.56
1:A:338:LEU:HD23	1:A:341:LYS:HE3	1.86	0.56
1:A:456:ASP:O	1:A:460:MET:HB2	2.06	0.56
2:A:560:HEM:HBA2	2:A:560:HEM:HHA	1.87	0.56
1:B:225:GLN:O	1:B:250:TRP:HB2	2.06	0.56
1:A:177:VAL:HG12	1:A:468:THR:HG22	1.88	0.56
1:A:36:LEU:HA	1:A:38:ARG:HH11	1.70	0.56
1:A:57:ASP:O	1:A:93:VAL:HA	2.06	0.56
1:A:272:LEU:HD12	1:A:272:LEU:H	1.71	0.56
1:B:318:ALA:O	1:B:320:ARG:N	2.33	0.56
1:A:473:LEU:O	1:A:474:LYS:HG2	2.06	0.55
1:A:157:ASN:HD22	1:A:384:PRO:HD2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:THR:CG2	1:B:137:THR:CA	2.77	0.55
1:B:353:ARG:NH1	1:B:356:ASP:CG	2.64	0.55
1:B:282:ASP:C	1:B:284:PRO:HD2	2.31	0.55
1:B:362:GLU:O	1:B:364:GLY:N	2.39	0.55
1:A:402:ASP:C	1:A:404:LEU:H	2.14	0.55
1:A:431:LEU:HB2	1:A:435:PHE:HE2	1.72	0.55
1:B:433:ARG:CB	1:B:437:TYR:CE2	2.88	0.55
1:B:201:LYS:CD	1:B:232:SER:HB3	2.37	0.55
1:B:207:GLU:HG3	1:B:214:ARG:NH2	2.22	0.55
1:A:372:ASN:C	1:A:372:ASN:ND2	2.54	0.55
1:B:210:LYS:HD3	1:B:237:GLU:HG2	1.87	0.55
1:B:431:LEU:H	1:B:431:LEU:HD13	1.71	0.55
1:A:158:HIS:O	1:A:159:ASN:C	2.50	0.55
1:A:392:MET:HE1	1:A:395:LEU:HD12	1.88	0.55
1:B:109:LYS:HZ2	1:B:112:LEU:HD13	1.72	0.55
1:B:137:THR:O	1:B:139:GLN:N	2.39	0.55
1:B:333:LYS:C	1:B:335:ILE:H	2.12	0.55
1:A:25:CYS:SG	1:A:54:ALA:CB	2.92	0.55
1:A:203:GLY:HA3	1:A:440:SER:OG	2.07	0.55
1:A:256:ASN:HD22	1:A:258:ASP:H	1.55	0.55
1:A:29:ILE:CG1	1:A:58:VAL:CG1	2.84	0.54
1:A:229:THR:HG22	1:A:230:LEU:HD13	1.88	0.54
1:B:196:ALA:HB2	1:B:226:MET:HB3	1.89	0.54
1:A:32:TYR:CE1	1:A:82:GLY:CA	2.88	0.54
1:A:447:VAL:O	1:A:450:ALA:HB3	2.07	0.54
1:B:152:VAL:O	1:B:153:THR:O	2.26	0.54
1:B:124:ASN:HD22	1:B:126:TYR:H	1.53	0.54
1:A:38:ARG:HD3	1:A:39:PHE:H	1.73	0.54
1:A:157:ASN:HD22	1:A:384:PRO:CD	2.21	0.54
1:A:197:THR:HG22	1:A:197:THR:O	2.05	0.54
1:B:223:VAL:O	1:B:224:PRO:O	2.26	0.54
1:A:402:ASP:O	1:A:404:LEU:N	2.40	0.54
1:B:184:LEU:N	1:B:405:GLU:OE1	2.26	0.54
1:B:258:ASP:O	1:B:260:LYS:N	2.41	0.54
1:B:482:THR:O	1:B:483:LEU:C	2.49	0.54
1:B:177:VAL:HG13	1:B:462:MET:HE2	1.88	0.54
1:B:409:ASP:OD2	3:B:570:FMN:O3'	2.10	0.54
1:B:275:LYS:HB2	1:B:275:LYS:HZ3	1.72	0.54
1:B:351:VAL:HG12	1:B:352:GLN:N	2.22	0.54
1:B:400:LEU:O	1:B:403:LYS:HB2	2.07	0.54
1:B:252:GLN:NE2	1:B:252:GLN:O	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:477:LEU:O	1:B:478:LEU:HD23	2.08	0.54
1:A:113:LYS:C	1:A:115:LEU:N	2.63	0.54
1:A:192:PHE:CD1	1:A:192:PHE:C	2.85	0.54
1:A:402:ASP:C	1:A:404:LEU:N	2.66	0.54
1:B:333:LYS:HA	1:B:336:GLU:HG2	1.90	0.54
1:B:388:LEU:CD2	1:B:392:MET:CG	2.86	0.54
1:B:354:THR:HG21	1:B:394:ILE:HD13	1.89	0.54
1:A:124:ASN:C	1:A:124:ASN:ND2	2.64	0.53
1:B:282:ASP:CG	1:B:373:GLN:HG3	2.34	0.53
1:A:494:VAL:O	1:A:495:LEU:C	2.49	0.53
1:A:4:LEU:HB3	1:A:32:TYR:CE2	2.42	0.53
1:A:155:ARG:CZ	1:B:491:PRO:HB2	2.39	0.53
1:A:354:THR:OG1	1:A:391:THR:HG23	2.08	0.53
1:B:449:LYS:O	1:B:452:GLU:HB2	2.09	0.53
1:B:361:ALA:HB2	1:B:404:LEU:HD23	1.89	0.53
1:B:361:ALA:HB3	1:B:400:LEU:HD23	1.80	0.53
1:A:163:ARG:NH2	1:B:488:VAL:O	2.38	0.53
1:A:372:ASN:ND2	1:A:375:GLY:H	2.07	0.53
1:B:137:THR:O	1:B:140:ALA:N	2.42	0.53
1:B:422:LEU:C	1:B:424:LEU:N	2.65	0.53
1:A:406:VAL:O	1:A:406:VAL:HG12	2.06	0.53
1:B:180:SER:CA	1:B:189:ASP:O	2.57	0.53
1:B:259:ARG:O	1:B:263:ASP:HB2	2.09	0.53
1:B:108:ARG:HG2	1:B:108:ARG:HH11	1.73	0.53
1:A:260:LYS:O	1:A:261:ILE:C	2.49	0.53
1:A:487:THR:O	1:B:490:VAL:HG13	2.09	0.53
1:B:132:ALA:HA	1:B:136:LEU:HD21	1.90	0.53
1:A:256:ASN:HA	1:A:325:PHE:O	2.07	0.53
1:B:222:LYS:HE2	1:B:244:SER:HB2	1.90	0.52
1:B:260:LYS:O	1:B:263:ASP:N	2.42	0.52
1:B:286:LEU:HD21	1:B:323:SER:CB	2.29	0.52
1:B:347:VAL:HG12	1:B:368:VAL:N	2.19	0.52
1:A:164:ILE:O	1:A:420:LYS:HE3	2.09	0.52
1:A:372:ASN:ND2	1:A:372:ASN:O	2.43	0.52
1:B:262:THR:C	1:B:264:ASP:H	2.16	0.52
1:B:349:LYS:NZ	3:B:570:FMN:O2	2.39	0.52
1:A:110:GLU:HA	1:A:113:LYS:CB	2.15	0.52
1:A:166:PHE:CE2	1:A:416:THR:HG22	2.43	0.52
1:A:352:GLN:OE1	1:A:381:SER:OG	2.17	0.52
1:A:402:ASP:O	1:A:403:LYS:C	2.49	0.52
1:A:474:LYS:O	1:A:477:LEU:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:VAL:HG13	1:B:192:PHE:H	1.74	0.52
1:B:254:TYR:CE1	1:B:280:THR:HB	2.45	0.52
1:B:369:VAL:HG22	1:B:407:PHE:HB2	1.91	0.52
1:B:337:GLU:HG3	1:B:341:LYS:NZ	2.24	0.52
1:B:433:ARG:HG2	3:B:570:FMN:C8M	2.39	0.52
2:A:560:HEM:HHA	2:A:560:HEM:CBA	2.40	0.52
1:B:101:GLU:OE2	1:B:137:THR:HG23	2.09	0.52
1:B:148:ALA:O	1:B:149:ASN:C	2.51	0.52
1:B:159:ASN:O	1:B:160:ALA:C	2.49	0.52
1:B:259:ARG:CG	1:B:259:ARG:NH1	2.73	0.52
1:A:188:VAL:HG12	1:A:189:ASP:N	2.23	0.52
1:A:353:ARG:O	1:A:354:THR:C	2.51	0.52
1:A:431:LEU:HB2	1:A:435:PHE:CE2	2.44	0.52
1:B:175:ARG:HB3	1:B:175:ARG:CZ	2.39	0.52
1:B:332:TRP:CZ2	1:B:359:LYS:HD3	2.44	0.52
1:B:124:ASN:ND2	1:B:127:ASP:H	2.08	0.52
1:B:396:GLU:CG	1:B:401:LYS:NZ	2.73	0.52
1:B:446:GLY:O	1:B:447:VAL:C	2.51	0.52
1:B:475:PRO:C	1:B:477:LEU:N	2.68	0.52
1:B:127:ASP:O	1:B:128:PHE:C	2.50	0.52
1:B:137:THR:HG21	1:B:139:GLN:HB3	1.89	0.52
1:A:38:ARG:CZ	1:A:39:PHE:HB3	2.40	0.52
1:A:251:TYR:CE1	1:A:265:LEU:HD13	2.45	0.52
1:B:212:VAL:HG22	1:B:225:GLN:OE1	2.10	0.52
1:B:243:PRO:O	1:B:244:SER:C	2.50	0.52
1:A:35:ASP:OD1	1:A:37:THR:HG22	2.11	0.51
1:B:109:LYS:NZ	1:B:112:LEU:HD13	2.25	0.51
1:B:366:SER:O	1:B:404:LEU:HD13	2.11	0.51
1:A:473:LEU:C	1:A:474:LYS:CG	2.84	0.51
1:B:163:ARG:CZ	1:B:486:ARG:HB2	2.40	0.51
1:B:337:GLU:O	1:B:340:LYS:HB2	2.10	0.51
1:A:110:GLU:HG2	1:A:113:LYS:CD	2.39	0.51
1:A:171:LEU:CD1	1:B:332:TRP:CD2	2.94	0.51
1:B:104:GLU:C	1:B:107:ALA:H	2.18	0.51
1:B:505:LEU:O	1:B:506:THR:O	2.28	0.51
1:B:333:LYS:O	1:B:335:ILE:N	2.44	0.51
1:B:103:LYS:HA	1:B:105:ASP:OD1	2.11	0.51
1:B:227:ILE:HD11	1:B:250:TRP:N	2.24	0.51
1:A:110:GLU:C	1:A:113:LYS:HB3	2.27	0.51
1:B:179:ILE:C	1:B:470:ILE:CD1	2.84	0.51
1:B:281:VAL:HG11	1:B:348:ILE:HG23	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ALA:C	1:A:96:PRO:HB3	2.35	0.51
1:B:228:SER:C	1:B:252:GLN:HE22	2.18	0.51
1:B:333:LYS:C	1:B:335:ILE:N	2.67	0.51
1:B:396:GLU:HG3	1:B:401:LYS:HZ2	1.76	0.51
1:B:405:GLU:HB3	1:B:407:PHE:CE2	2.46	0.51
1:B:190:VAL:HG13	1:B:192:PHE:CD2	2.46	0.51
1:B:184:LEU:O	1:B:185:GLY:C	2.54	0.50
1:B:433:ARG:O	1:B:437:TYR:HD2	1.91	0.50
1:B:236:GLU:O	1:B:240:GLU:HB2	2.10	0.50
1:B:281:VAL:HG11	1:B:348:ILE:CG2	2.40	0.50
1:A:132:ALA:HA	1:A:441:CYS:SG	2.52	0.50
1:A:414:ARG:HH21	1:B:150:ASP:CG	2.18	0.50
1:B:229:THR:HG21	1:B:254:TYR:H	1.76	0.50
1:B:409:ASP:O	1:B:410:GLY:O	2.29	0.50
1:A:22:PRO:HB2	1:A:51:LYS:HG2	1.93	0.50
1:B:422:LEU:C	1:B:424:LEU:H	2.15	0.50
1:A:198:ALA:O	1:A:199:LEU:HB2	2.12	0.50
1:A:331:THR:O	1:A:332:TRP:C	2.53	0.50
1:A:405:GLU:OE1	1:A:427:LYS:HG2	2.12	0.50
1:B:108:ARG:HH22	1:B:138:LYS:HG3	1.77	0.50
1:A:57:ASP:CA	1:A:58:VAL:HG23	2.42	0.50
1:B:470:ILE:O	1:B:470:ILE:HG22	2.08	0.50
1:A:233:CYS:HB3	1:A:237:GLU:OE1	2.12	0.50
1:A:347:VAL:HG22	1:A:367:GLY:C	2.37	0.50
1:A:278:PHE:HA	1:A:347:VAL:O	2.11	0.50
1:A:412:VAL:HG12	1:A:431:LEU:HD21	1.93	0.50
1:B:98:ALA:HB1	1:B:101:GLU:HB2	1.94	0.50
1:B:412:VAL:HG13	1:B:417:ASP:HB3	1.94	0.50
1:A:210:LYS:HG2	1:A:241:ALA:HB1	1.93	0.49
1:B:108:ARG:HH12	1:B:137:THR:CA	2.17	0.49
1:A:255:VAL:HG11	1:A:330:LEU:HD21	1.94	0.49
1:B:219:GLY:C	1:B:221:THR:N	2.69	0.49
1:B:332:TRP:CE2	1:B:359:LYS:HD3	2.47	0.49
1:B:163:ARG:NH2	1:B:486:ARG:HB2	2.26	0.49
1:B:233:CYS:CB	1:B:238:ILE:CD1	2.77	0.49
1:B:463:ARG:C	1:B:465:LEU:N	2.70	0.49
1:A:174:VAL:O	1:A:174:VAL:HG23	2.11	0.49
1:A:239:ILE:HG23	1:A:249:GLN:HE22	1.76	0.49
1:A:286:LEU:CD1	1:A:286:LEU:CD2	2.80	0.49
1:A:432:GLY:O	1:A:433:ARG:C	2.54	0.49
1:B:108:ARG:NH2	1:B:138:LYS:HG3	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:LYS:O	1:B:114:SER:C	2.54	0.49
1:B:116:LEU:HD12	1:B:442:TYR:CZ	2.48	0.49
1:B:180:SER:O	1:B:181:THR:HB	2.12	0.49
1:B:144:TYR:OH	1:B:200:CYS:HA	2.13	0.49
1:B:281:VAL:CG1	1:B:348:ILE:HG23	2.42	0.49
1:B:447:VAL:HG12	1:B:451:ILE:CD1	2.41	0.49
1:A:28:VAL:O	1:A:57:ASP:OD1	2.30	0.49
1:A:271:LYS:C	1:A:273:GLY:H	2.21	0.49
1:A:417:ASP:O	1:A:418:VAL:C	2.52	0.49
1:B:463:ARG:C	1:B:465:LEU:H	2.19	0.49
1:A:29:ILE:HG12	1:A:58:VAL:HG11	1.93	0.49
1:A:67:ALA:C	1:A:70:VAL:CG1	2.77	0.49
1:A:509:GLU:HG2	1:B:115:LEU:O	2.13	0.49
1:B:353:ARG:HH11	1:B:356:ASP:CG	2.21	0.49
1:A:13:PRO:HA	1:A:88:MET:HG2	1.95	0.49
1:A:110:GLU:CA	1:A:113:LYS:CB	2.82	0.49
1:B:256:ASN:HD22	1:B:258:ASP:H	1.60	0.49
1:B:475:PRO:C	1:B:477:LEU:H	2.20	0.49
1:A:66:HIS:HE1	2:A:560:HEM:C1D	2.31	0.49
1:A:118:PRO:O	1:A:121:ASN:HB2	2.13	0.49
1:B:322:LEU:CD1	1:B:328:PRO:HG2	2.35	0.49
1:B:230:LEU:O	1:B:231:ALA:C	2.53	0.48
1:B:253:LEU:O	1:B:279:VAL:HA	2.12	0.48
1:B:352:GLN:HG3	1:B:371:SER:O	2.11	0.48
1:B:505:LEU:C	1:B:506:THR:O	2.55	0.48
1:B:207:GLU:O	1:B:210:LYS:HB2	2.14	0.48
1:B:351:VAL:HG12	1:B:352:GLN:H	1.78	0.48
1:A:385:ILE:HG23	1:A:386:GLU:H	1.78	0.48
1:B:194:VAL:HG12	1:B:195:SER:N	2.28	0.48
1:B:236:GLU:CA	1:B:239:ILE:HG22	2.42	0.48
1:B:275:LYS:HB2	1:B:275:LYS:HZ2	1.76	0.48
1:A:439:ASN:O	1:A:440:SER:C	2.53	0.48
1:B:394:ILE:HG23	1:B:397:GLN:HE22	1.77	0.48
1:A:223:VAL:HA	1:A:224:PRO:HD3	1.51	0.48
1:B:161:TYR:O	1:B:420:LYS:HE2	2.13	0.48
1:A:198:ALA:H	3:A:569:FMN:C6	2.26	0.48
1:B:137:THR:O	1:B:138:LYS:C	2.57	0.48
1:A:111:GLN:O	1:A:115:LEU:HB3	2.14	0.48
1:A:198:ALA:H	3:A:569:FMN:H6	1.79	0.48
1:A:383:ALA:HB1	1:A:385:ILE:HG22	1.96	0.48
1:B:164:ILE:HB	1:B:420:LYS:CE	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:VAL:C	1:A:18:LYS:N	2.72	0.48
1:A:212:VAL:O	1:A:213:ALA:C	2.55	0.48
1:A:222:LYS:HE3	1:A:244:SER:OG	2.14	0.48
1:A:55:GLY:C	1:A:56:LYS:HG3	2.39	0.47
1:A:256:ASN:HD22	1:A:257:SER:CA	2.24	0.47
1:B:500:TYR:CG	1:B:501:GLU:N	2.81	0.47
1:A:194:VAL:HG22	1:A:435:PHE:CG	2.49	0.47
1:A:252:GLN:HG2	1:A:253:LEU:N	2.28	0.47
1:B:295:LEU:HA	1:B:297:PHE:O	2.13	0.47
1:B:396:GLU:HG3	1:B:401:LYS:HZ3	1.78	0.47
1:B:405:GLU:HB3	1:B:407:PHE:HE2	1.78	0.47
1:B:454:LEU:O	1:B:454:LEU:HG	2.13	0.47
1:A:89:PRO:HA	1:A:90:PRO:HD2	1.24	0.47
1:A:200:CYS:C	1:A:202:LEU:N	2.71	0.47
1:B:179:ILE:CA	1:B:470:ILE:CD1	2.86	0.47
1:B:188:VAL:O	1:B:189:ASP:C	2.56	0.47
1:B:216:CYS:HB3	1:B:223:VAL:O	2.14	0.47
1:A:29:ILE:O	1:A:30:ASN:C	2.58	0.47
1:A:196:ALA:HB2	1:A:226:MET:HG2	1.97	0.47
1:A:344:LEU:HA	1:A:344:LEU:HD23	1.53	0.47
1:B:184:LEU:HD13	1:B:405:GLU:OE1	2.13	0.47
1:A:16:VAL:C	1:A:18:LYS:H	2.21	0.47
1:A:107:ALA:O	1:A:111:GLN:HB2	2.14	0.47
1:B:177:VAL:HG11	1:B:462:MET:HG2	1.96	0.47
1:A:67:ALA:HA	1:A:68:PRO:HD3	1.74	0.47
1:A:339:LYS:NZ	1:A:364:GLY:O	2.34	0.47
1:B:106:ILE:HA	1:B:109:LYS:HB2	1.96	0.47
1:B:149:ASN:HB3	1:B:290:GLU:OE2	2.15	0.47
1:B:369:VAL:HG12	1:B:371:SER:HB2	1.97	0.47
1:B:116:LEU:HA	1:B:117:PRO:HD3	1.79	0.47
1:B:317:GLY:N	1:B:320:ARG:HH22	2.07	0.47
1:B:410:GLY:HA2	3:B:570:FMN:O5'	2.15	0.47
1:B:439:ASN:ND2	1:B:443:GLY:HA2	2.28	0.47
1:A:68:PRO:O	1:A:70:VAL:HG22	2.14	0.47
1:B:107:ALA:O	1:B:109:LYS:N	2.47	0.47
1:B:166:PHE:CE2	1:B:416:THR:HG22	2.50	0.47
1:A:47:GLN:HE21	1:A:47:GLN:HB3	1.59	0.47
1:A:414:ARG:O	1:A:415:GLY:C	2.55	0.47
1:B:216:CYS:CB	1:B:223:VAL:O	2.63	0.47
1:A:36:LEU:O	1:A:38:ARG:N	2.48	0.46
1:A:67:ALA:O	1:A:70:VAL:CG1	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:LEU:HA	1:A:232:SER:OG	2.15	0.46
1:A:466:GLY:O	1:A:467:VAL:HG13	2.15	0.46
1:B:410:GLY:CA	3:B:570:FMN:O5'	2.63	0.46
1:A:27:VAL:CG2	1:A:56:LYS:H	2.29	0.46
1:B:137:THR:CG2	1:B:139:GLN:H	2.26	0.46
1:B:496:TYR:O	1:B:496:TYR:CD1	2.69	0.46
1:A:118:PRO:O	1:A:119:LEU:C	2.57	0.46
1:A:415:GLY:O	1:A:416:THR:C	2.57	0.46
1:A:453:ILE:O	1:A:457:GLU:HG3	2.15	0.46
1:B:207:GLU:CG	1:B:214:ARG:HH22	2.28	0.46
1:B:337:GLU:HB3	1:B:341:LYS:HE3	1.96	0.46
1:A:62:PHE:CE1	1:A:66:HIS:CD2	3.04	0.46
1:A:164:ILE:O	1:A:420:LYS:HE2	2.15	0.46
1:A:473:LEU:O	1:A:474:LYS:CG	2.64	0.46
1:B:457:GLU:O	1:B:458:ILE:C	2.56	0.46
1:A:137:THR:O	1:A:138:LYS:C	2.58	0.46
1:A:462:MET:HE1	1:A:469:SER:CA	2.42	0.46
2:A:560:HEM:HHD	2:A:560:HEM:CBC	2.34	0.46
1:B:282:ASP:OD1	1:B:373:GLN:HG3	2.16	0.46
1:A:382:ARG:O	1:A:384:PRO:CD	2.64	0.46
1:B:254:TYR:OH	4:B:571:PYR:O3	2.29	0.46
1:B:344:LEU:HD23	1:B:344:LEU:HA	1.18	0.46
1:A:115:LEU:HD12	1:A:115:LEU:HA	1.83	0.46
1:A:229:THR:O	1:A:229:THR:CG2	2.61	0.46
1:B:251:TYR:O	1:B:278:PHE:N	2.31	0.46
1:B:440:SER:O	1:B:441:CYS:CB	2.59	0.46
1:A:280:THR:HA	1:A:349:LYS:HB3	1.98	0.45
1:A:398:ARG:O	1:A:400:LEU:HG	2.16	0.45
1:B:416:THR:O	1:B:420:LYS:HB2	2.15	0.45
1:A:6:MET:HB2	1:A:32:TYR:OH	2.16	0.45
1:A:43:HIS:HA	1:A:44:PRO:HD2	1.44	0.45
1:B:163:ARG:NH2	1:B:486:ARG:HA	2.28	0.45
1:B:229:THR:OG1	1:B:252:GLN:C	2.58	0.45
1:B:252:GLN:HG2	1:B:253:LEU:N	2.31	0.45
1:B:354:THR:HG1	1:B:391:THR:HG22	1.81	0.45
1:A:104:GLU:C	1:A:106:ILE:N	2.73	0.45
1:A:182:ASP:HB2	1:A:186:SER:O	2.17	0.45
1:A:206:LEU:HA	1:A:206:LEU:HD12	1.31	0.45
1:B:283:ALA:HA	1:B:377:GLN:HE21	1.80	0.45
1:A:4:LEU:HD22	1:A:80:LYS:CD	2.46	0.45
1:A:204:ASN:HA	1:A:205:PRO:HD3	1.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ASP:N	1:A:58:VAL:HG23	2.30	0.45
1:A:66:HIS:CE1	2:A:560:HEM:C1D	3.04	0.45
1:B:356:ASP:O	1:B:357:VAL:C	2.54	0.45
1:B:422:LEU:HA	1:B:422:LEU:HD23	1.58	0.45
1:B:439:ASN:O	1:B:441:CYS:N	2.49	0.45
1:B:163:ARG:NH2	1:B:486:ARG:CG	2.79	0.45
1:B:433:ARG:CB	1:B:437:TYR:HE2	2.29	0.45
1:A:36:LEU:HD12	1:A:38:ARG:HH12	1.82	0.45
1:A:422:LEU:C	1:A:424:LEU:N	2.72	0.45
1:B:174:VAL:CG2	1:B:463:ARG:HB3	2.46	0.45
1:B:327:ASP:C	1:B:329:SER:H	2.25	0.45
1:A:166:PHE:HE2	1:A:416:THR:HG22	1.80	0.45
1:B:110:GLU:O	1:B:113:LYS:O	2.34	0.45
1:B:188:VAL:O	1:B:189:ASP:O	2.35	0.45
1:B:222:LYS:HE2	1:B:244:SER:CB	2.47	0.45
1:B:406:VAL:C	1:B:407:PHE:CD2	2.95	0.45
1:A:131:LEU:O	1:A:132:ALA:C	2.60	0.45
1:B:214:ARG:HH11	1:B:444:ARG:HD3	1.82	0.45
1:B:214:ARG:HD3	1:B:241:ALA:HB1	1.99	0.45
1:B:175:ARG:CG	1:B:175:ARG:NE	2.69	0.44
1:B:175:ARG:CG	1:B:175:ARG:CZ	2.95	0.44
1:A:508:PHE:HA	1:B:115:LEU:O	2.17	0.44
1:B:218:GLN:HE21	1:B:218:GLN:HB2	1.22	0.44
1:B:251:TYR:HB3	1:B:277:LEU:HD21	1.98	0.44
1:B:353:ARG:NH2	1:B:355:GLU:HG2	2.32	0.44
1:B:413:ARG:NH2	3:B:570:FMN:O1P	2.50	0.44
1:A:288:GLN:NE2	1:A:293:MET:HE1	2.31	0.44
1:B:296:LYS:HE2	1:B:296:LYS:HB3	1.50	0.44
1:A:57:ASP:HB3	1:A:93:VAL:HG23	1.99	0.44
1:A:196:ALA:O	3:A:569:FMN:C10	2.66	0.44
1:A:435:PHE:O	1:A:436:LEU:C	2.61	0.44
1:B:108:ARG:NH1	1:B:108:ARG:HG2	2.32	0.44
1:B:413:ARG:NH1	3:B:570:FMN:O1P	2.50	0.44
1:A:38:ARG:HH21	1:A:75:ILE:HB	1.77	0.44
1:A:55:GLY:O	1:A:56:LYS:HG3	2.17	0.44
1:A:127:ASP:O	1:A:128:PHE:C	2.60	0.44
1:A:490:VAL:O	1:A:492:ASN:HB2	2.18	0.44
1:B:137:THR:HG22	1:B:139:GLN:N	2.25	0.44
1:A:155:ARG:NH2	1:B:491:PRO:HB2	2.32	0.44
1:A:226:MET:HA	1:A:250:TRP:HB2	1.99	0.44
1:A:235:PRO:O	1:A:236:GLU:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:LYS:HZ1	3:A:569:FMN:C2'	2.30	0.44
1:A:416:THR:O	1:A:419:LEU:HB2	2.18	0.44
1:A:452:GLU:O	1:A:453:ILE:C	2.60	0.44
1:B:159:ASN:O	1:B:161:TYR:N	2.51	0.44
1:A:469:SER:O	1:A:470:ILE:C	2.60	0.44
1:B:227:ILE:HD13	1:B:250:TRP:O	2.04	0.44
1:A:59:THR:O	1:A:60:ALA:C	2.61	0.43
1:A:61:ILE:HG23	1:A:97:TYR:CB	2.47	0.43
1:A:268:ASN:ND2	1:A:272:LEU:HD11	2.33	0.43
1:A:400:LEU:O	1:A:401:LYS:C	2.57	0.43
1:B:151:GLU:C	1:B:155:ARG:HH11	2.26	0.43
1:B:285:SER:HA	1:B:322:LEU:HA	2.00	0.43
1:B:383:ALA:HA	1:B:384:PRO:HD3	1.75	0.43
1:A:347:VAL:HG22	1:A:367:GLY:O	2.18	0.43
1:A:453:ILE:HG23	1:A:453:ILE:HD13	1.62	0.43
1:B:98:ALA:O	1:B:101:GLU:HG2	2.19	0.43
3:B:570:FMN:HM83	3:B:570:FMN:HM71	1.83	0.43
1:A:156:GLU:O	1:A:157:ASN:C	2.61	0.43
1:A:260:LYS:C	1:A:262:THR:N	2.76	0.43
1:B:222:LYS:HE3	1:B:222:LYS:HB3	1.60	0.43
1:B:351:VAL:CG1	1:B:352:GLN:N	2.81	0.43
1:A:43:HIS:CD2	2:A:560:HEM:NB	2.87	0.43
1:A:60:ALA:O	1:A:96:PRO:CB	2.59	0.43
1:A:473:LEU:HD23	1:A:473:LEU:HA	1.55	0.43
1:A:487:THR:H	1:B:489:GLY:HA2	1.84	0.43
1:B:462:MET:HE2	1:B:468:THR:C	2.42	0.43
1:A:40:LEU:O	1:A:47:GLN:HG3	2.17	0.43
1:A:401:LYS:HD2	1:A:402:ASP:OD1	2.19	0.43
1:A:495:LEU:HD12	1:A:495:LEU:HA	1.84	0.43
1:B:151:GLU:N	1:B:379:ASP:OD2	2.52	0.43
1:B:249:GLN:O	1:B:250:TRP:CD1	2.71	0.43
1:B:439:ASN:O	1:B:443:GLY:HA2	2.18	0.43
1:A:135:THR:O	1:A:136:LEU:C	2.57	0.43
1:A:339:LYS:O	1:A:339:LYS:HG2	2.18	0.43
1:B:101:GLU:O	1:B:103:LYS:N	2.51	0.43
1:A:141:TRP:O	1:A:142:ALA:C	2.57	0.43
1:A:163:ARG:HH21	1:A:486:ARG:HA	1.83	0.43
1:A:212:VAL:HG22	1:A:225:GLN:OE1	2.19	0.43
1:A:226:MET:CE	1:A:349:LYS:HD2	2.43	0.43
1:A:238:ILE:O	1:A:238:ILE:HG22	2.19	0.43
1:A:250:TRP:CD1	1:A:276:ALA:HB3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:VAL:HG12	1:B:195:SER:H	1.82	0.43
1:A:119:LEU:C	1:A:121:ASN:H	2.26	0.43
1:A:162:HIS:N	1:A:162:HIS:ND1	2.66	0.43
1:A:286:LEU:HD21	1:A:289:ARG:HH22	1.84	0.43
1:A:474:LYS:HA	1:A:475:PRO:HD3	1.72	0.43
1:B:162:HIS:C	1:B:164:ILE:H	2.27	0.43
1:B:220:VAL:O	1:B:220:VAL:HG12	2.19	0.43
1:A:218:GLN:HE21	1:A:218:GLN:HB3	1.52	0.43
1:A:355:GLU:O	1:A:358:ILE:N	2.51	0.43
1:A:497:ASN:O	1:A:498:GLU:C	2.62	0.43
1:B:152:VAL:N	1:B:379:ASP:OD1	2.51	0.43
1:A:14:ALA:HA	1:A:17:ALA:HB2	2.01	0.42
1:A:38:ARG:HD3	1:A:39:PHE:N	2.34	0.42
1:A:40:LEU:C	1:A:42:ASN:H	2.27	0.42
1:A:103:LYS:HD3	1:A:103:LYS:N	2.33	0.42
1:A:196:ALA:H	1:A:226:MET:CE	2.23	0.42
1:A:478:LEU:HD23	1:A:478:LEU:HA	1.31	0.42
1:B:249:GLN:HB3	1:B:274:VAL:HG12	2.01	0.42
1:B:283:ALA:N	1:B:284:PRO:HD3	2.32	0.42
1:A:372:ASN:HD22	1:A:374:GLY:H	1.67	0.42
1:B:109:LYS:HA	1:B:109:LYS:HD3	1.68	0.42
1:B:204:ASN:HB3	1:B:208:GLY:H	1.85	0.42
1:A:43:HIS:CD2	2:A:560:HEM:C4B	3.07	0.42
1:A:119:LEU:C	1:A:121:ASN:N	2.77	0.42
1:A:129:GLU:O	1:A:130:TYR:C	2.59	0.42
1:A:253:LEU:HA	1:A:253:LEU:HD12	1.72	0.42
1:A:438:ALA:O	1:A:439:ASN:C	2.62	0.42
1:B:147:GLY:O	1:B:148:ALA:C	2.60	0.42
1:B:154:HIS:O	1:B:154:HIS:ND1	2.52	0.42
1:B:165:PHE:O	1:B:479:ASP:N	2.48	0.42
1:B:239:ILE:CD1	1:B:274:VAL:CG1	2.97	0.42
1:A:268:ASN:O	1:A:272:LEU:HD12	2.18	0.42
1:B:195:SER:OG	1:B:196:ALA:N	2.53	0.42
1:B:433:ARG:HG2	3:B:570:FMN:HM81	2.01	0.42
1:B:137:THR:CG2	1:B:137:THR:HB	2.23	0.42
1:A:230:LEU:HG	2:A:560:HEM:HMA3	2.01	0.42
1:A:365:VAL:HG13	1:A:366:SER:N	2.33	0.42
1:B:268:ASN:C	1:B:268:ASN:ND2	2.76	0.42
1:B:419:LEU:HA	1:B:419:LEU:HD23	1.83	0.42
1:A:179:ILE:HD13	1:A:459:GLU:HG3	2.01	0.42
1:A:210:LYS:HB2	1:A:210:LYS:HE3	1.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:LEU:O	1:A:423:CYS:C	2.56	0.42
1:B:195:SER:O	1:B:197:THR:CG2	2.67	0.42
1:A:27:VAL:HG22	1:A:56:LYS:H	1.85	0.42
1:A:28:VAL:HG23	1:A:33:VAL:HG12	2.01	0.42
1:A:239:ILE:HD12	1:A:272:LEU:HB2	2.01	0.42
1:B:235:PRO:O	1:B:239:ILE:HG22	2.19	0.42
1:A:68:PRO:C	1:A:70:VAL:H	2.28	0.42
1:B:163:ARG:HH22	1:B:486:ARG:HG3	1.82	0.42
1:B:286:LEU:CD2	1:B:323:SER:CB	2.96	0.42
1:B:286:LEU:HD11	1:B:326:ILE:HD11	2.02	0.42
1:A:41:PRO:HA	1:A:47:GLN:CG	2.44	0.42
1:A:179:ILE:O	1:A:470:ILE:CD1	2.67	0.42
1:A:219:GLY:HA3	1:A:448:GLU:OE2	2.20	0.42
1:A:278:PHE:CE2	1:A:347:VAL:HG11	2.55	0.42
1:B:213:ALA:HB2	1:B:225:GLN:NE2	2.27	0.42
1:A:188:VAL:HG12	1:A:190:VAL:H	1.85	0.41
1:B:104:GLU:O	1:B:106:ILE:N	2.52	0.41
1:B:179:ILE:C	1:B:470:ILE:HD13	2.44	0.41
1:A:56:LYS:C	1:A:58:VAL:CG2	2.89	0.41
1:A:74:TYR:CD1	2:A:560:HEM:CMB	3.04	0.41
1:A:112:LEU:HD12	1:A:112:LEU:H	1.84	0.41
1:A:293:MET:O	1:A:295:LEU:N	2.53	0.41
1:B:98:ALA:CB	1:B:101:GLU:HG3	2.47	0.41
1:B:276:ALA:HB1	1:B:345:PRO:O	2.20	0.41
1:A:170:ILE:HB	1:B:356:ASP:OD2	2.20	0.41
1:A:180:SER:HB2	1:A:188:VAL:O	2.21	0.41
1:A:229:THR:HG22	1:A:229:THR:O	2.13	0.41
1:A:272:LEU:CD1	1:A:272:LEU:H	2.32	0.41
1:B:265:LEU:HA	1:B:268:ASN:HB3	2.03	0.41
1:A:43:HIS:O	1:A:43:HIS:ND1	2.54	0.41
1:A:119:LEU:HD12	1:A:119:LEU:HA	1.70	0.41
1:A:409:ASP:OD1	1:A:409:ASP:C	2.63	0.41
1:A:420:LYS:O	1:A:421:ALA:C	2.59	0.41
1:A:132:ALA:HB2	1:A:437:TYR:HB3	2.02	0.41
1:A:191:PRO:HD2	1:A:192:PHE:CD2	2.56	0.41
1:A:197:THR:HG21	1:A:436:LEU:HD21	2.03	0.41
1:B:110:GLU:HA	1:B:113:LYS:HB3	2.03	0.41
1:B:244:SER:O	1:B:247:GLN:HB3	2.20	0.41
1:B:495:LEU:HA	1:B:495:LEU:HD12	1.04	0.41
1:A:259:ARG:HH12	1:A:334:ASP:CG	2.27	0.41
1:A:412:VAL:HG12	1:A:412:VAL:O	2.17	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:VAL:CG1	1:B:462:MET:HG2	2.51	0.41
1:B:217:GLY:HA3	1:B:247:GLN:OE1	2.21	0.41
1:B:227:ILE:HD13	1:B:251:TYR:HD2	1.85	0.41
1:B:346:ILE:CG2	1:B:365:VAL:HG11	2.42	0.41
1:B:394:ILE:C	1:B:396:GLU:N	2.79	0.41
1:A:66:HIS:HE1	2:A:560:HEM:CHD	2.33	0.41
1:A:152:VAL:N	1:A:379:ASP:OD1	2.53	0.41
1:A:239:ILE:HD13	1:A:239:ILE:HG21	1.81	0.41
1:A:257:SER:OG	1:A:324:LYS:O	2.37	0.41
1:A:357:VAL:O	1:A:357:VAL:HG12	2.18	0.41
1:B:490:VAL:HA	1:B:491:PRO:HD3	1.83	0.41
1:A:259:ARG:CG	1:A:259:ARG:HH11	2.32	0.41
1:A:433:ARG:O	1:A:434:PRO:C	2.59	0.41
1:B:295:LEU:HD23	1:B:296:LYS:H	1.84	0.41
1:B:418:VAL:O	1:B:421:ALA:HB3	2.20	0.41
1:B:437:TYR:O	1:B:438:ALA:C	2.64	0.41
1:A:201:LYS:O	1:A:205:PRO:HA	2.21	0.41
1:A:214:ARG:HB3	1:A:444:ARG:HB3	2.03	0.41
1:A:258:ASP:O	1:A:260:LYS:N	2.53	0.41
1:B:262:THR:C	1:B:266:VAL:HG23	2.46	0.41
1:B:347:VAL:CG1	1:B:367:GLY:N	2.79	0.41
1:B:414:ARG:HA	1:B:457:GLU:OE1	2.20	0.41
1:B:443:GLY:O	1:B:447:VAL:HG23	2.21	0.41
1:A:210:LYS:HD3	1:A:237:GLU:HB3	2.03	0.41
1:A:382:ARG:O	1:A:384:PRO:HD3	2.21	0.41
1:A:453:ILE:HG21	1:A:453:ILE:HD12	1.58	0.41
1:B:190:VAL:CG1	1:B:192:PHE:H	2.34	0.41
1:B:278:PHE:HA	1:B:347:VAL:O	2.21	0.41
1:B:332:TRP:CH2	1:B:359:LYS:HB3	2.56	0.41
1:A:256:ASN:HD22	1:A:258:ASP:N	2.16	0.40
1:B:199:LEU:O	1:B:202:LEU:HB2	2.21	0.40
1:A:132:ALA:CA	1:A:441:CYS:SG	3.09	0.40
1:A:139:GLN:HG3	1:A:140:ALA:N	2.37	0.40
1:A:259:ARG:HH11	1:A:259:ARG:HG3	1.86	0.40
1:A:179:ILE:CA	1:A:470:ILE:HD11	2.48	0.40
1:A:204:ASN:C	1:A:206:LEU:N	2.76	0.40
1:B:151:GLU:O	1:B:152:VAL:C	2.63	0.40
1:B:347:VAL:HA	1:B:367:GLY:O	2.22	0.40
1:B:469:SER:C	1:B:471:ALA:N	2.80	0.40
1:B:108:ARG:NH1	1:B:137:THR:HA	2.18	0.40
1:B:133:SER:HB3	1:B:141:TRP:CH2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:THR:OG1	1:B:391:THR:CG2	2.61	0.40
1:B:449:LYS:HD2	1:B:453:ILE:HG13	2.01	0.40
1:B:500:TYR:CD1	1:B:500:TYR:C	2.98	0.40
1:A:106:ILE:HA	1:A:109:LYS:HB2	2.03	0.40

All (1) 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:353:ARG:NH2	1:B:169:LYS:CG[6_555]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	488/511 (96%)	381 (78%)	67 (14%)	40 (8%)	0	1
1	B	392/511 (77%)	273 (70%)	78 (20%)	41 (10%)	0	1
All	All	880/1022 (86%)	654 (74%)	145 (16%)	81 (9%)	0	1

All (81) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	11	ILE
1	A	20	ASN
1	A	37	THR
1	A	48	ASP
1	A	58	VAL
1	A	69	ASN
1	A	72	ASP
1	A	106	ILE

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Mol	Chain	Res	Type
1	A	113	LYS
1	A	114	SER
1	A	259	ARG
1	A	319	SER
1	A	380	PHE
1	B	99	PRO
1	B	102	THR
1	B	103	LYS
1	B	105	ASP
1	B	119	LEU
1	B	167	LYS
1	B	185	GLY
1	B	243	PRO
1	B	298	SER
1	B	318	ALA
1	B	319	SER
1	B	395	LEU
1	B	508	PHE
1	A	7	ASN
1	A	13	PRO
1	A	14	ALA
1	A	44	PRO
1	A	80	LYS
1	A	105	ASP
1	A	318	ALA
1	A	325	PHE
1	A	399	ASN
1	A	401	LYS
1	B	120	ASP
1	B	149	ASN
1	B	189	ASP
1	B	218	GLN
1	B	224	PRO
1	B	255	VAL
1	B	258	ASP
1	B	364	GLY
1	B	372	ASN
1	B	410	GLY
1	B	440	SER
1	B	473	LEU
1	A	4	LEU
1	A	52	PHE

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Mol	Chain	Res	Type
1	A	68	PRO
1	A	138	LYS
1	B	108	ARG
1	B	114	SER
1	B	154	HIS
1	B	191	PRO
1	B	363	ILE
1	A	23	ASP
1	A	104	GLU
1	A	493	ASP
1	A	498	GLU
1	B	113	LYS
1	B	211	ASP
1	B	263	ASP
1	B	377	GLN
1	A	71	ILE
1	A	294	LYS
1	A	446	GLY
1	B	397	GLN
1	B	506	THR
1	A	274	VAL
1	A	403	LYS
1	A	508	PHE
1	A	40	LEU
1	B	266	VAL
1	B	194	VAL
1	A	494	VAL
1	B	365	VAL
1	B	348	ILE
1	B	447	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	424/440 (96%)	282 (66%)	142 (34%)	0 1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	340/440 (77%)	220 (65%)	120 (35%)	0	0
All	All	764/880 (87%)	502 (66%)	262 (34%)	0	0

All (262) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	10	LYS
1	A	11	ILE
1	A	12	SER
1	A	15	GLU
1	A	16	VAL
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	38	ARG
1	A	40	LEU
1	A	47	GLN
1	A	49	VAL
1	A	50	ILE
1	A	57	ASP
1	A	58	VAL
1	A	61	ILE
1	A	63	GLU
1	A	65	LEU
1	A	69	ASN
1	A	72	ASP
1	A	75	ILE
1	A	78	GLU
1	A	79	LYS
1	A	81	LEU
1	A	84	LEU
1	A	85	GLN
1	A	87	SER
1	A	91	GLU
1	A	92	LEU
1	A	93	VAL
1	A	101	GLU

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Mol	Chain	Res	Type
1	A	103	LYS
1	A	105	ASP
1	A	106	ILE
1	A	109	LYS
1	A	110	GLU
1	A	111	GLN
1	A	112	LEU
1	A	120	ASP
1	A	124	ASN
1	A	125	LEU
1	A	131	LEU
1	A	139	GLN
1	A	145	SER
1	A	152	VAL
1	A	153	THR
1	A	156	GLU
1	A	162	HIS
1	A	170	ILE
1	A	176	LYS
1	A	186	SER
1	A	190	VAL
1	A	195	SER
1	A	197	THR
1	A	201	LYS
1	A	212	VAL
1	A	214	ARG
1	A	216	CYS
1	A	221	THR
1	A	222	LYS
1	A	226	MET
1	A	229	THR
1	A	230	LEU
1	A	232	SER
1	A	236	GLU
1	A	238	ILE
1	A	240	GLU
1	A	245	ASP
1	A	248	ILE
1	A	252	GLN
1	A	255	VAL
1	A	256	ASN
1	A	259	ARG

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Mol	Chain	Res	Type
1	A	260	LYS
1	A	262	THR
1	A	265	LEU
1	A	272	LEU
1	A	277	LEU
1	A	285	SER
1	A	288	GLN
1	A	289	ARG
1	A	291	LYS
1	A	293	MET
1	A	297	PHE
1	A	328	PRO
1	A	330	LEU
1	A	333	LYS
1	A	337	GLU
1	A	338	LEU
1	A	340	LYS
1	A	342	THR
1	A	343	LYS
1	A	346	ILE
1	A	354	THR
1	A	355	GLU
1	A	365	VAL
1	A	368	VAL
1	A	372	ASN
1	A	378	LEU
1	A	381	SER
1	A	388	LEU
1	A	390	GLU
1	A	392	MET
1	A	394	ILE
1	A	396	GLU
1	A	398	ARG
1	A	401	LYS
1	A	408	VAL
1	A	412	VAL
1	A	413	ARG
1	A	416	THR
1	A	420	LYS
1	A	427	LYS
1	A	429	VAL
1	A	436	LEU

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Mol	Chain	Res	Type
1	A	444	ARG
1	A	448	GLU
1	A	451	ILE
1	A	452	GLU
1	A	453	ILE
1	A	458	ILE
1	A	460	MET
1	A	464	LEU
1	A	465	LEU
1	A	470	ILE
1	A	474	LYS
1	A	477	LEU
1	A	482	THR
1	A	483	LEU
1	A	490	VAL
1	A	493	ASP
1	A	495	LEU
1	A	499	VAL
1	A	504	THR
1	A	505	LEU
1	A	506	THR
1	A	507	GLU
1	B	99	PRO
1	B	101	GLU
1	B	102	THR
1	B	103	LYS
1	B	104	GLU
1	B	105	ASP
1	B	106	ILE
1	B	108	ARG
1	B	109	LYS
1	B	110	GLU
1	B	112	LEU
1	B	116	LEU
1	B	122	ILE
1	B	124	ASN
1	B	131	LEU
1	B	134	GLN
1	B	136	LEU
1	B	139	GLN
1	B	149	ASN
1	B	155	ARG

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Mol	Chain	Res	Type
1	B	164	ILE
1	B	169	LYS
1	B	170	ILE
1	B	172	VAL
1	B	175	ARG
1	B	176	LYS
1	B	178	ASP
1	B	179	ILE
1	B	184	LEU
1	B	187	HIS
1	B	188	VAL
1	B	190	VAL
1	B	197	THR
1	B	201	LYS
1	B	206	LEU
1	B	207	GLU
1	B	209	GLU
1	B	212	VAL
1	B	214	ARG
1	B	216	CYS
1	B	222	LYS
1	B	223	VAL
1	B	227	ILE
1	B	230	LEU
1	B	234	SER
1	B	236	GLU
1	B	239	ILE
1	B	246	LYS
1	B	247	GLN
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	259	ARG
1	B	261	ILE
1	B	263	ASP
1	B	271	LYS
1	B	275	LYS
1	B	277	LEU
1	B	280	THR

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Mol	Chain	Res	Type
1	B	281	VAL
1	B	286	LEU
1	B	289	ARG
1	B	291	LYS
1	B	296	LYS
1	B	320	ARG
1	B	322	LEU
1	B	325	PHE
1	B	330	LEU
1	B	337	GLU
1	B	339	LYS
1	B	342	THR
1	B	348	ILE
1	B	352	GLN
1	B	353	ARG
1	B	355	GLU
1	B	357	VAL
1	B	365	VAL
1	B	366	SER
1	B	372	ASN
1	B	373	GLN
1	B	378	LEU
1	B	382	ARG
1	B	385	ILE
1	B	388	LEU
1	B	391	THR
1	B	395	LEU
1	B	397	GLN
1	B	398	ARG
1	B	403	LYS
1	B	404	LEU
1	B	408	VAL
1	B	416	THR
1	B	420	LYS
1	B	423	CYS
1	B	427	LYS
1	B	429	VAL
1	B	431	LEU
1	B	436	LEU
1	B	440	SER
1	B	449	LYS
1	B	458	ILE

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Mol	Chain	Res	Type
1	B	459	GLU
1	B	460	MET
1	B	464	LEU
1	B	468	THR
1	B	470	ILE
1	B	477	LEU
1	B	482	THR
1	B	483	LEU
1	B	484	LYS
1	B	490	VAL
1	B	494	VAL
1	B	495	LEU
1	B	498	GLU
1	B	501	GLU
1	B	504	THR
1	B	510	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	30	ASN
1	A	47	GLN
1	A	53	ASN
1	A	124	ASN
1	A	139	GLN
1	A	157	ASN
1	A	218	GLN
1	A	225	GLN
1	A	249	GLN
1	A	252	GLN
1	A	256	ASN
1	A	268	ASN
1	A	288	GLN
1	A	372	ASN
1	A	377	GLN
1	A	439	ASN
1	A	497	ASN
1	B	124	ASN
1	B	218	GLN
1	B	225	GLN
1	B	249	GLN

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Mol	Chain	Res	Type
1	B	252	GLN
1	B	256	ASN
1	B	268	ASN
1	B	439	ASN
1	B	445	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	$\# Z > 2$
4	PYR	B	571	-	5,5,5	3.49	3 (60%)	3,6,6	0.71	0
3	FMN	A	569	-	33,33,33	0.98	1 (3%)	48,50,50	2.17	15 (31%)
3	FMN	B	570	-	33,33,33	1.09	2 (6%)	48,50,50	2.24	15 (31%)
2	HEM	A	560	1	50,50,50	2.48	19 (38%)	67,82,82	2.50	23 (34%)

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
4	PYR	B	571	-	-	4/4/4/4	-
3	FMN	A	569	-	1/1/4/4	3/18/18/18	0/3/3/3
3	FMN	B	570	-	-	5/18/18/18	0/3/3/3
2	HEM	A	560	1	-	9/14/54/54	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	560	HEM	C3D-C2D	7.30	1.52	1.36
2	A	560	HEM	FE-ND	7.27	2.17	1.94
4	B	571	PYR	CA-C	-5.51	1.36	1.54
4	B	571	PYR	O-C	4.78	1.34	1.22
2	A	560	HEM	FE-NA	4.34	2.09	1.95
2	A	560	HEM	CBA-CGA	3.94	1.59	1.50
2	A	560	HEM	CAB-C3B	3.91	1.57	1.47
2	A	560	HEM	CHC-C1C	-3.30	1.31	1.38
2	A	560	HEM	CAA-C2A	3.17	1.59	1.51
2	A	560	HEM	CBB-CAB	3.13	1.45	1.30
2	A	560	HEM	FE-NC	-3.12	1.84	1.95
2	A	560	HEM	CBD-CGD	3.10	1.57	1.50
2	A	560	HEM	CHA-C4D	-3.08	1.32	1.38
2	A	560	HEM	CAD-C3D	2.90	1.58	1.51
2	A	560	HEM	CBA-CAA	2.78	1.61	1.51
2	A	560	HEM	O1D-CGD	2.68	1.30	1.22
2	A	560	HEM	FE-NB	-2.54	1.87	1.94
2	A	560	HEM	C3C-C2C	-2.46	1.32	1.37
4	B	571	PYR	O3-CA	2.43	1.28	1.23
2	A	560	HEM	C1C-NC	-2.37	1.35	1.39
3	A	569	FMN	C9A-N10	-2.32	1.37	1.41
3	B	570	FMN	P-O5'	-2.09	1.53	1.60
3	B	570	FMN	P-O1P	2.08	1.56	1.50
2	A	560	HEM	C3B-C4B	-2.04	1.41	1.44
2	A	560	HEM	CHC-C4B	-2.01	1.34	1.39

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	570	FMN	C4'-C3'-C2'	6.53	124.44	113.57
2	A	560	HEM	CHC-C4B-NB	6.52	131.44	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	560	HEM	CAA-CBA-CGA	6.36	130.53	113.67
3	B	570	FMN	O5'-P-O1P	6.29	123.43	106.44
3	A	569	FMN	C4'-C3'-C2'	6.12	123.75	113.57
2	A	560	HEM	C3D-C4D-ND	5.37	116.06	110.17
2	A	560	HEM	C4D-C3D-C2D	-5.19	99.34	106.89
2	A	560	HEM	CHA-C4D-ND	-4.49	118.82	124.37
2	A	560	HEM	CAD-CBD-CGD	4.43	125.41	113.67
3	A	569	FMN	O3'-C3'-C2'	-4.39	98.95	108.93
2	A	560	HEM	CHA-C1A-NA	4.38	131.81	123.86
2	A	560	HEM	C3B-C2B-C1B	4.37	109.69	106.41
2	A	560	HEM	CHB-C1B-NB	4.34	129.74	124.37
3	A	569	FMN	O3'-C3'-C4'	4.27	118.63	108.93
2	A	560	HEM	O2A-CGA-O1A	-4.22	112.48	123.33
2	A	560	HEM	CAD-C3D-C4D	3.94	131.56	124.70
3	B	570	FMN	O3P-P-O5'	3.82	116.64	106.67
3	A	569	FMN	O4'-C4'-C5'	3.79	118.35	109.99
2	A	560	HEM	C4A-C3A-C2A	3.79	111.15	106.82
3	B	570	FMN	O4'-C4'-C3'	3.74	118.00	109.25
2	A	560	HEM	CHA-C1A-C2A	-3.74	117.12	125.30
2	A	560	HEM	O2A-CGA-CBA	3.73	125.79	114.00
3	A	569	FMN	O2-C2-N1	3.66	127.88	121.80
3	A	569	FMN	C1'-C2'-C3'	3.66	119.57	109.66
3	A	569	FMN	C5'-C4'-C3'	-3.65	105.34	112.22
2	A	560	HEM	C4A-CHB-C1B	-3.55	117.91	126.25
3	A	569	FMN	O2'-C2'-C3'	3.46	117.34	109.25
3	B	570	FMN	O4'-C4'-C5'	3.43	117.56	109.99
3	B	570	FMN	C9A-C5A-N5	-3.40	118.85	122.45
3	B	570	FMN	O3'-C3'-C2'	-3.37	101.27	108.93
2	A	560	HEM	C2B-C1B-NB	-3.37	105.97	109.84
3	B	570	FMN	O2P-P-O1P	-3.27	98.09	110.83
3	A	569	FMN	C9A-C5A-N5	-3.24	119.01	122.45
2	A	560	HEM	CHC-C4B-C3B	-3.20	118.68	125.07
3	A	569	FMN	C6-C5A-N5	3.07	123.54	118.44
2	A	560	HEM	CMB-C2B-C1B	-2.90	120.50	125.03
3	A	569	FMN	O2'-C2'-C1'	2.78	121.64	110.20
3	B	570	FMN	O2'-C2'-C3'	2.63	115.40	109.25
3	A	569	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	569	FMN	C7M-C7-C6	2.51	123.99	119.57
3	B	570	FMN	C7M-C7-C6	2.44	123.88	119.57
2	A	560	HEM	C4C-CHD-C1D	2.40	131.12	126.02
2	A	560	HEM	C1B-NB-C4B	2.36	108.00	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	570	FMN	O3P-P-O2P	-2.33	99.08	107.80
2	A	560	HEM	C3A-C4A-NA	-2.30	106.46	110.14
2	A	560	HEM	CMA-C3A-C2A	-2.29	120.76	125.62
3	B	570	FMN	C6-C7-C8	-2.23	116.41	119.69
3	A	569	FMN	N3-C2-N1	-2.21	114.81	119.50
3	A	569	FMN	C4-C4A-N5	2.14	121.16	118.21
2	A	560	HEM	CBC-CAC-C3C	-2.08	117.15	127.53
3	B	570	FMN	O2'-C2'-C1'	2.02	118.52	110.20
3	B	570	FMN	O2P-P-O5'	2.02	111.93	106.67

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	569	FMN	C2'

All (21) torsion outliers are listed below:

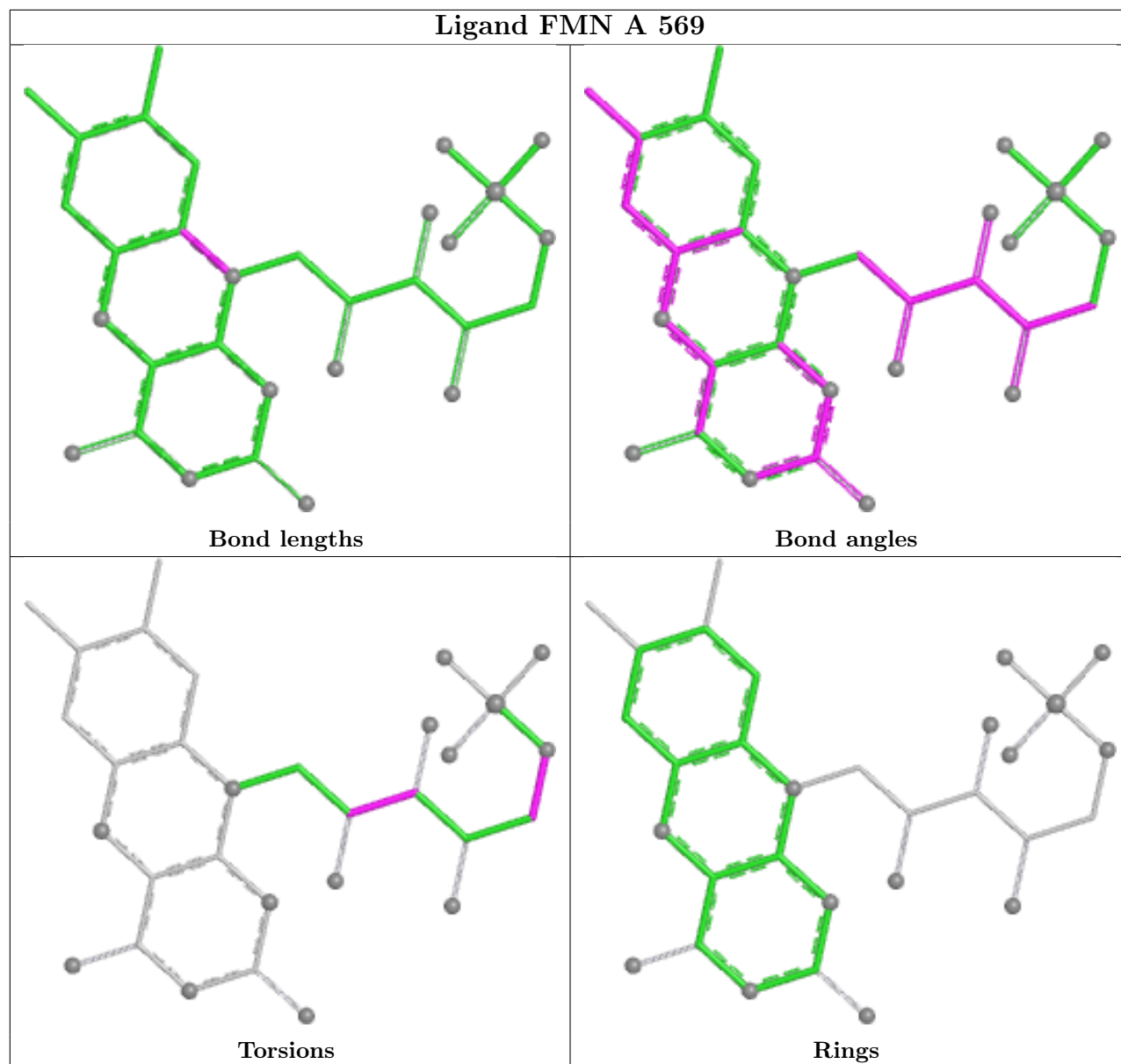
Mol	Chain	Res	Type	Atoms
2	A	560	HEM	C3D-CAD-CBD-CGD
4	B	571	PYR	O-C-CA-O3
4	B	571	PYR	OXT-C-CA-O3
3	A	569	FMN	O2'-C2'-C3'-C4'
3	A	569	FMN	O2'-C2'-C3'-O3'
2	A	560	HEM	C1A-C2A-CAA-CBA
3	B	570	FMN	C2'-C3'-C4'-O4'
3	A	569	FMN	C4'-C5'-O5'-P
3	B	570	FMN	C4'-C5'-O5'-P
3	B	570	FMN	O2'-C2'-C3'-C4'
4	B	571	PYR	O-C-CA-CB
2	A	560	HEM	C4B-C3B-CAB-CBB
4	B	571	PYR	OXT-C-CA-CB
2	A	560	HEM	C2A-CAA-CBA-CGA
3	B	570	FMN	O4'-C4'-C5'-O5'
2	A	560	HEM	CAA-CBA-CGA-O1A
2	A	560	HEM	CAA-CBA-CGA-O2A
2	A	560	HEM	CAD-CBD-CGD-O1D
2	A	560	HEM	CAD-CBD-CGD-O2D
2	A	560	HEM	C4C-C3C-CAC-CBC
3	B	570	FMN	O3'-C3'-C4'-O4'

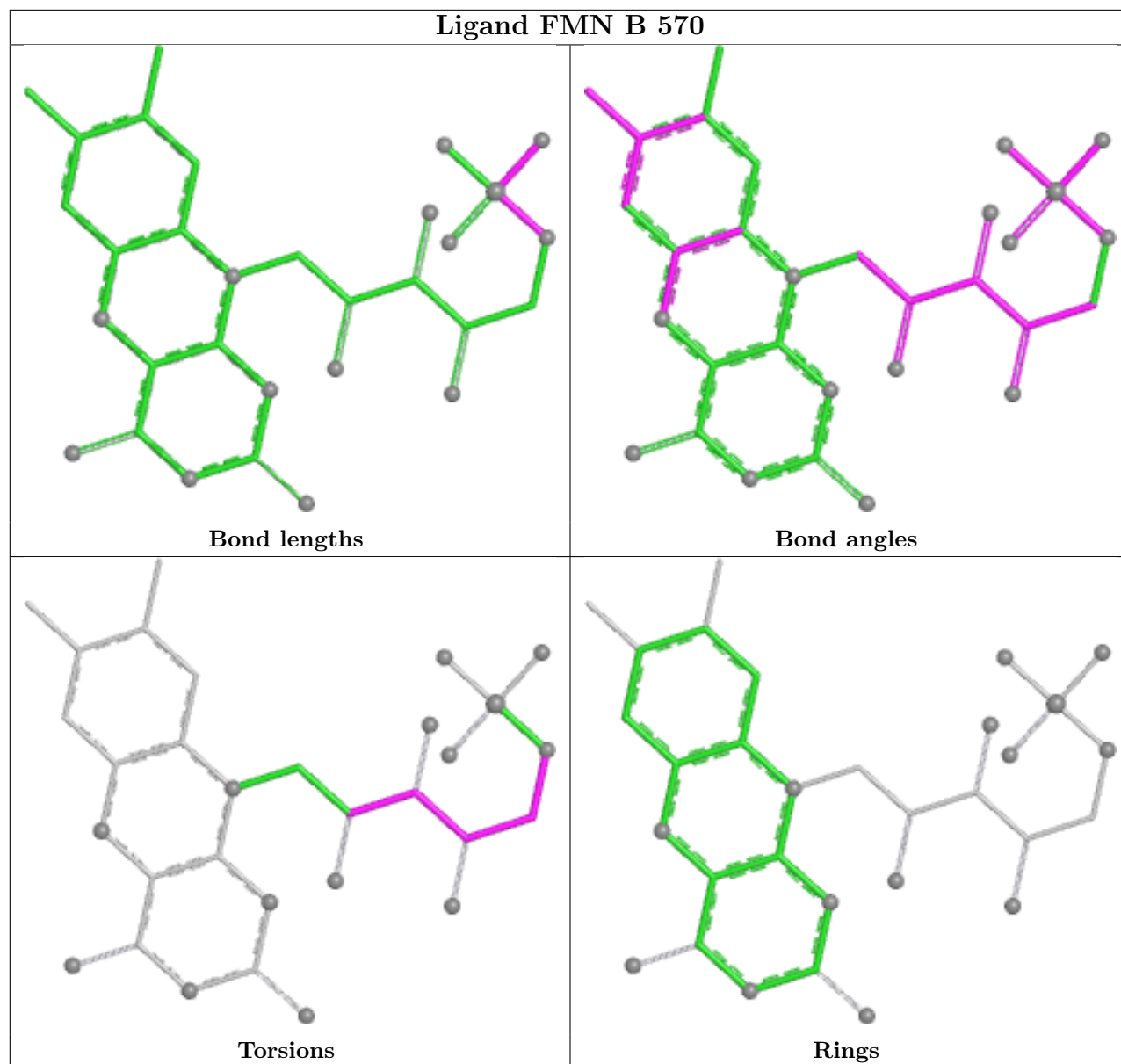
There are no ring outliers.

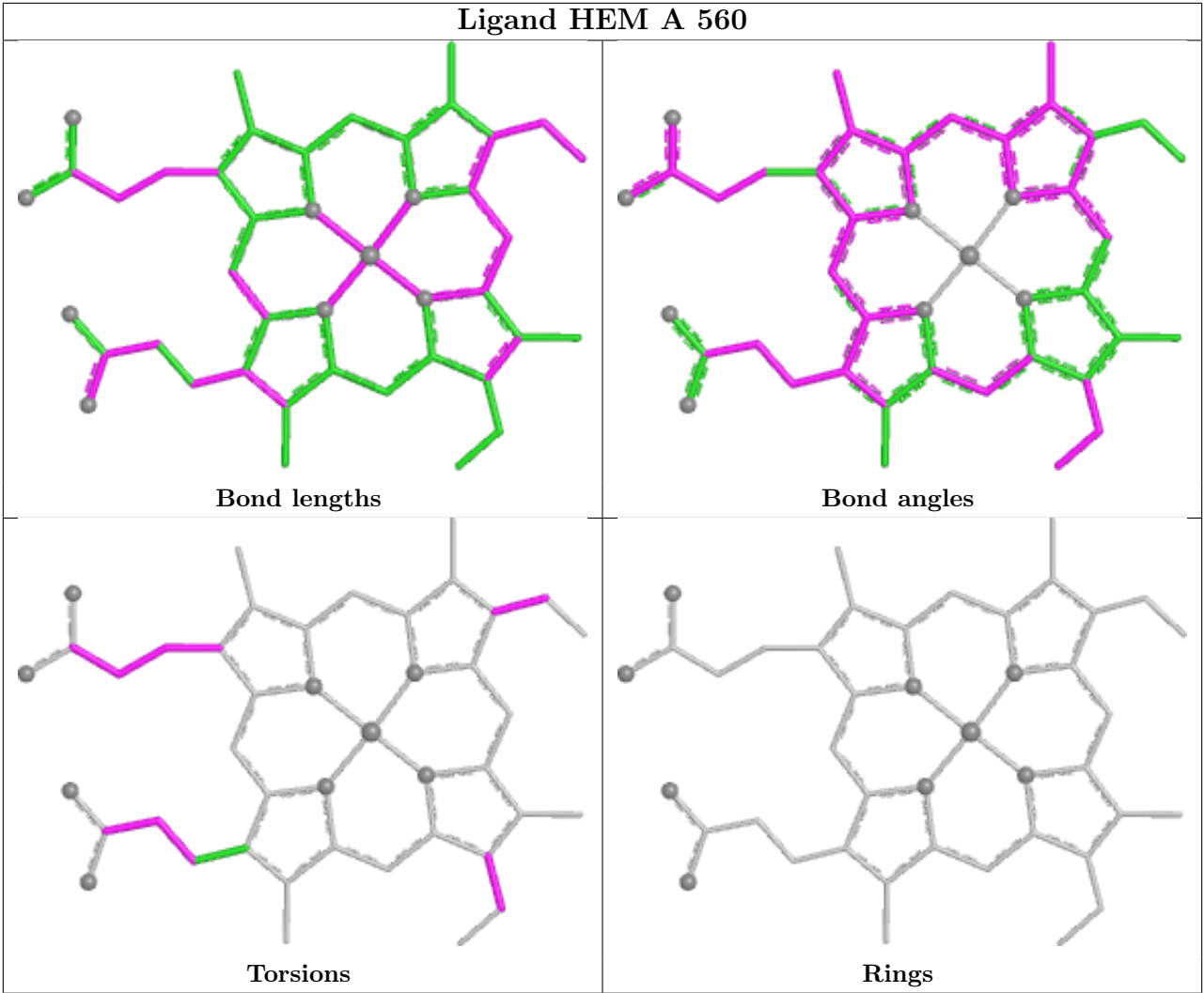
4 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	571	PYR	1	0
3	A	569	FMN	14	0
3	B	570	FMN	14	0
2	A	560	HEM	15	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	89:PRO	C	90:PRO	N	1.19

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	492/511 (96%)	0.15	35 (7%)	22 16	19, 52, 147, 183	0
1	B	396/511 (77%)	0.34	23 (5%)	29 22	18, 65, 107, 171	0
All	All	888/1022 (86%)	0.23	58 (6%)	25 18	18, 58, 138, 183	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	491	PRO	5.6
1	B	98	ALA	5.6
1	B	321	ALA	5.4
1	B	317	GLY	5.1
1	B	323	SER	5.1
1	A	509	GLU	5.0
1	A	3	LYS	4.9
1	A	4	LEU	4.7
1	B	322	LEU	4.5
1	A	299	ASN	4.5
1	A	2	PRO	4.4
1	B	492	ASN	4.1
1	A	65	LEU	4.1
1	A	318	ALA	4.0
1	B	318	ALA	3.7
1	A	317	GLY	3.6
1	A	18	LYS	3.4
1	A	7	ASN	3.2
1	A	325	PHE	3.1
1	A	92	LEU	3.1
1	A	77	PRO	3.0
1	A	492	ASN	2.9
1	B	297	PHE	2.9
1	A	297	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	46	GLY	2.8
1	A	5	ASP	2.8
1	A	69	ASN	2.8
1	B	380	PHE	2.7
1	A	11	ILE	2.7
1	A	114	SER	2.7
1	B	112	LEU	2.7
1	A	93	VAL	2.7
1	A	6	MET	2.6
1	A	74	TYR	2.5
1	B	238	ILE	2.5
1	B	282	ASP	2.4
1	B	324	LYS	2.4
1	B	319	SER	2.4
1	A	14	ALA	2.4
1	A	319	SER	2.3
1	A	510	ASP	2.3
1	B	296	LYS	2.3
1	A	30	ASN	2.3
1	B	320	ARG	2.3
1	A	16	VAL	2.3
1	B	325	PHE	2.2
1	B	506	THR	2.2
1	A	67	ALA	2.2
1	B	241	ALA	2.2
1	A	22	PRO	2.1
1	A	49	VAL	2.1
1	B	246	LYS	2.1
1	A	8	LYS	2.1
1	B	286	LEU	2.1
1	A	38	ARG	2.1
1	B	114	SER	2.1
1	A	37	THR	2.1
1	B	99	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

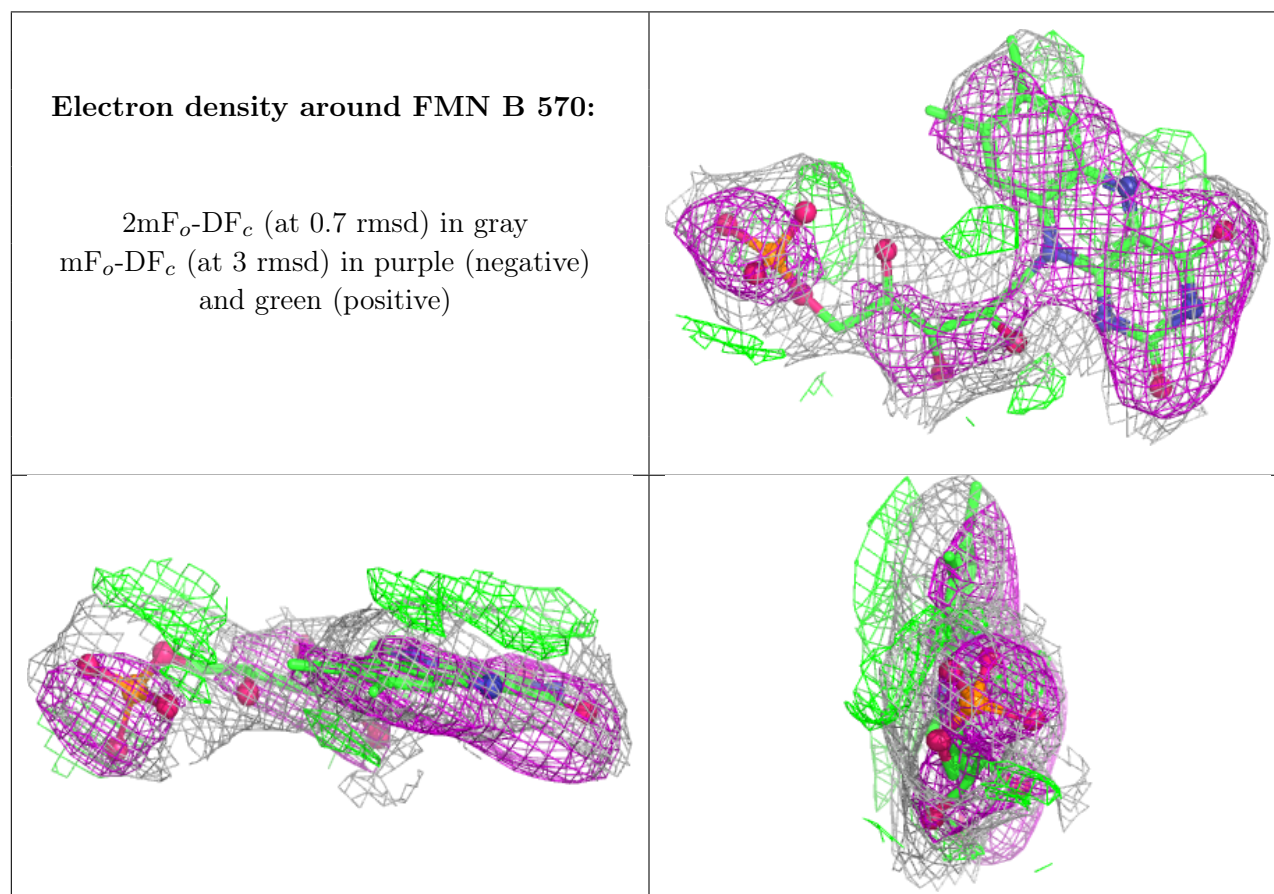
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

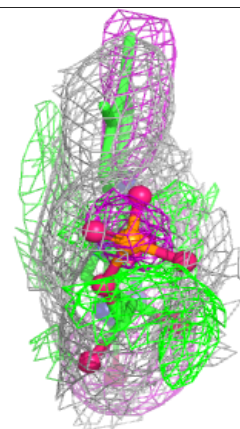
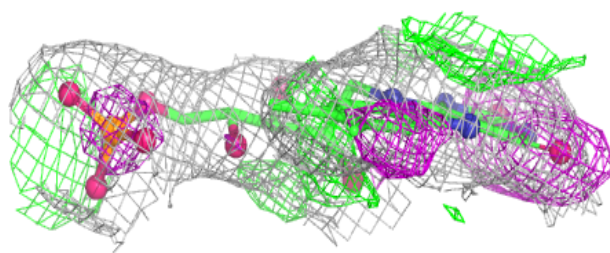
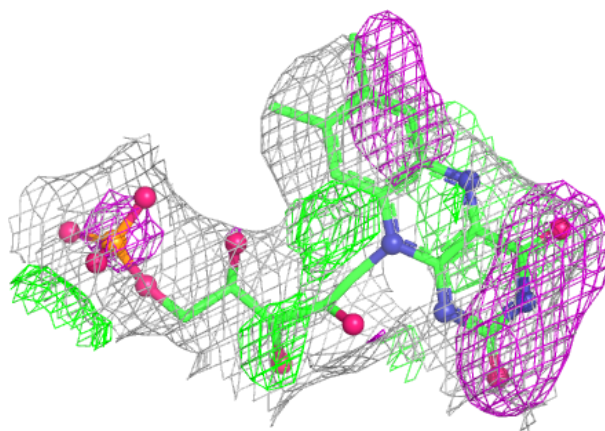
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	PYR	B	571	6/6	0.81	0.37	120,125,128,133	0
3	FMN	B	570	31/31	0.86	0.13	16,21,24,26	0
3	FMN	A	569	31/31	0.91	0.10	10,14,17,18	0
2	HEM	A	560	43/43	0.95	0.13	90,98,116,122	0

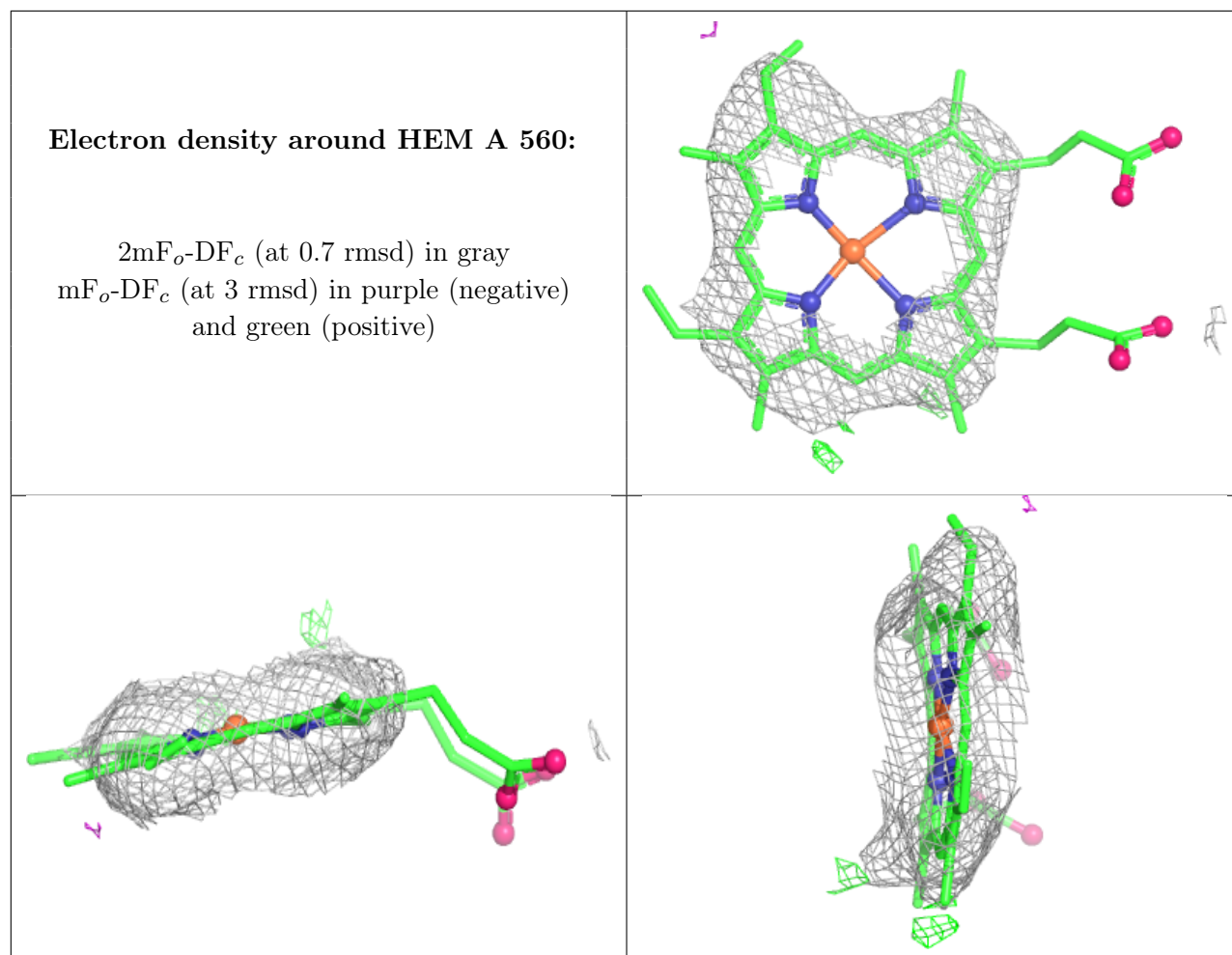
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around FMN A 569:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.