



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:29 AM UTC

PDB ID : 7CAT / pdb_00007cat
Title : The NADPH binding site on beef liver catalase
Authors : Murthy, M.R.N.; Reid III, T.J.; Sicignano, A.; Tanaka, N.; Fita, I.; Rossmann, M.G.
Deposited on : 1984-11-15
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

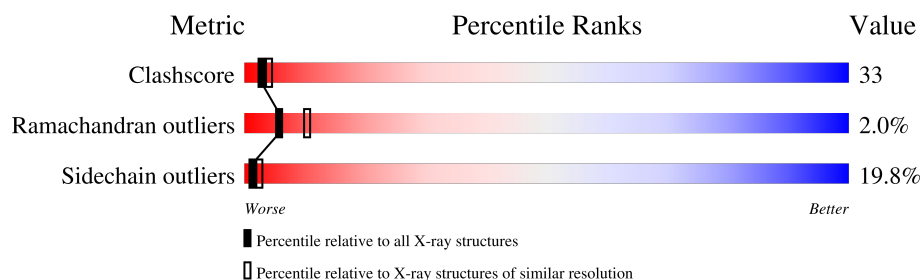
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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

Note EDS was not executed.

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

2 Entry composition [i](#)

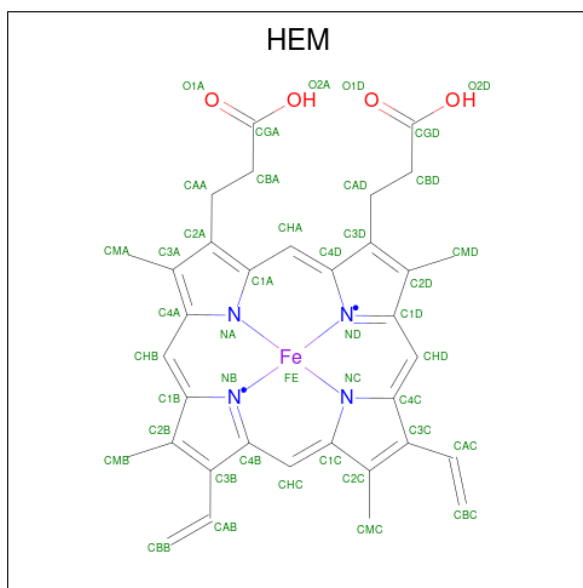
There are 4 unique types of molecules in this entry. The entry contains 8298 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CATALASE.

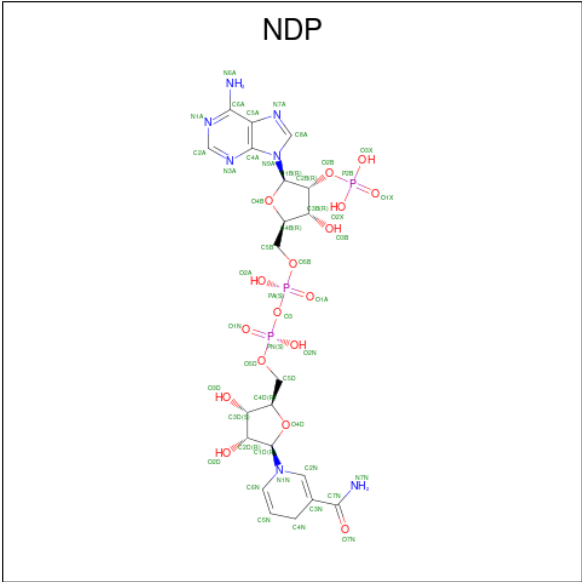
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	0	0	0
			4008	2543	714	737	14			
1	B	498	Total	C	N	O	S	0	0	0
			4008	2543	714	737	14			

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

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is water.

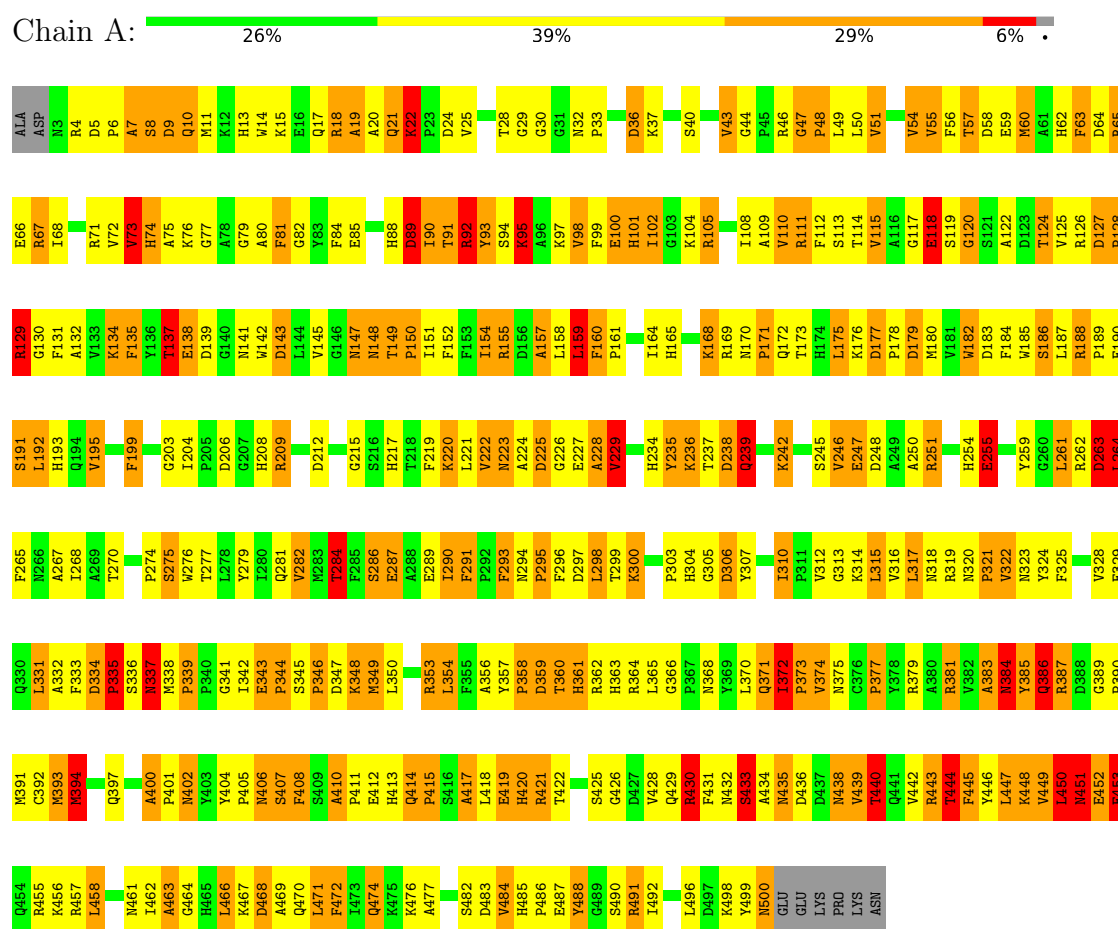
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	50	Total	O	0	0
			50	50		
4	B	50	Total	O	0	0
			50	50		

3 Residue-property plots

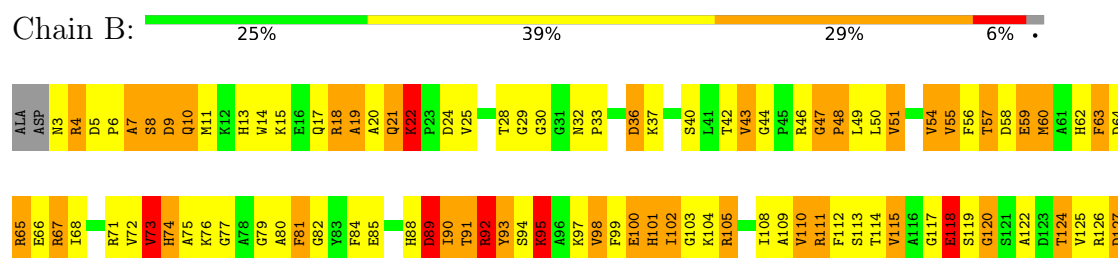
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

• Molecule 1: CATALASE



• Molecule 1: CATALASE



P390	P391	V328	D263	E190	P128
M391	C392	E329	L264	S191	R129
N393	Q330	R331	F265	L192	G130
N394	L331	A332	N266	H193	F131
Q397	F333	K332	A267	Q194	A132
A400	D334	A335	T270	V195	V133
P401	P336	P337	A269	F199	K134
M402	N337	S338	T271	G203	L136
Y403	K338	P339	S275	L204	E138
Y404	P339	F340	K276	P205	D139
P405	Q340	G341	T277	D206	G140
M406	G341	L342	L278	G207	G141
A469	S407	I342	Y279	H208	W142
F408	P408	E343	Y279	R209	D143
S409	P344	P344	T280		L144
A410	S345	S345	Q281	D212	V145
P411	P346	P346	V282		G146
E412	D347	F348	M283	G215	N147
H413	D347	F348	T284	S216	N148
H413	K348	F348	F285	H217	T149
Q414	N349	E287	S286	T218	P150
P415	L350	E287	E287	F219	P151
S416		A288	A288	K220	F152
A417	R353	E289	E289	L221	F153
L418	L354	I290	I290	V222	F154
E419	F355	F291	F291	N223	R155
H420	A356	F292	F292	A224	D156
R421	Y357	F293	F293	D225	A157
T422	P358	N294	N294	G226	L158
S425	D359	P295	P295	E227	L159
G426	T360	D296	D296	A228	F160
D427	H361	D297	D297	V229	P161
V428	R362	L298	L298		
Q429	R364	T299	T299	H234	T164
R430	L365	K300	K300	Y235	H165
F431	G366			K236	K168
M432	P367	P303	P303	T237	R169
N433	S368	H304	H304	D238	N170
A434	V369	G305	G305	Q239	R171
GLU	M435	D306	D306	K242	
GLU	D436	Y307	Y307		T172
LVS	L437			S245	T173
PRO	M438	I310	I310	V246	H174
LVS	V439	F311	F311	D245	L175
ASN	T440	G312	G312	E247	K176
	Q441	G313	G313	D248	D177
	V442	K314	K314	A249	P178
	R443	L315	L315	A250	D179
	T444	V316	V316	R251	M180
	F445	L317	L317		V181
	Y446	N318	N318	H254	W182
	L447	R319	R319	E255	D183
	K448	P320	P320		F184
	V449	P321	P321	D258	W185
	L450	N322	N322	Y259	S186
	N451	V323	V323	G260	L187
	E452	N324	N324	L261	R188
		Y324	Y324	L261	R188
		F205	F205	P262	R189

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	142.00Å 142.00Å 103.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.50 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (8.50-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	0.212 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8298	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.87	65/4128 (1.6%)	2.67	372/5607 (6.6%)
1	B	1.87	64/4128 (1.6%)	2.67	373/5607 (6.7%)
All	All	1.87	129/8256 (1.6%)	2.67	745/11214 (6.6%)

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

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

All (129) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	426	GLY	N-CA	9.43	1.54	1.45
1	B	426	GLY	N-CA	9.36	1.54	1.45
1	B	151	ILE	N-CA	8.24	1.56	1.46
1	A	151	ILE	N-CA	8.21	1.56	1.46
1	A	364	ARG	NE-CZ	7.90	1.41	1.33
1	B	364	ARG	NE-CZ	7.89	1.41	1.33
1	A	124	THR	CA-CB	7.74	1.62	1.52
1	B	124	THR	CA-CB	7.70	1.62	1.52
1	A	185	TRP	C-O	7.63	1.33	1.24
1	B	185	TRP	C-O	7.54	1.32	1.24
1	B	164	ILE	CA-CB	7.45	1.63	1.54
1	A	164	ILE	CA-CB	7.42	1.63	1.54
1	A	360	THR	C-O	7.41	1.33	1.24
1	B	160	PHE	C-O	7.38	1.32	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	360	THR	C-O	7.37	1.33	1.24
1	A	160	PHE	C-O	7.26	1.32	1.24
1	B	120	GLY	N-CA	7.10	1.53	1.45
1	A	120	GLY	N-CA	7.08	1.53	1.45
1	A	310	ILE	C-O	7.05	1.31	1.23
1	B	310	ILE	C-O	6.98	1.31	1.23
1	B	343	GLU	N-CA	6.68	1.55	1.46
1	A	469	ALA	N-CA	6.67	1.54	1.45
1	B	420	HIS	CE1-NE2	-6.67	1.25	1.32
1	A	343	GLU	N-CA	6.66	1.55	1.46
1	A	420	HIS	CE1-NE2	-6.61	1.25	1.32
1	B	469	ALA	N-CA	6.61	1.54	1.45
1	A	28	THR	C-O	6.57	1.32	1.23
1	A	323	ASN	C-N	-6.53	1.25	1.33
1	B	28	THR	C-O	6.51	1.32	1.23
1	B	323	ASN	C-N	-6.51	1.25	1.33
1	A	171	PRO	N-CD	6.50	1.56	1.47
1	B	139	ASP	N-CA	6.49	1.53	1.46
1	B	171	PRO	N-CD	6.48	1.56	1.47
1	A	139	ASP	N-CA	6.43	1.53	1.46
1	B	238	ASP	N-CA	6.43	1.54	1.46
1	B	275	SER	C-N	-6.42	1.24	1.33
1	B	363	HIS	C-N	-6.42	1.25	1.33
1	A	363	HIS	C-N	-6.41	1.25	1.33
1	A	275	SER	C-N	-6.41	1.24	1.33
1	A	321	PRO	C-O	-6.39	1.16	1.23
1	B	321	PRO	C-O	-6.39	1.16	1.23
1	B	261	LEU	CA-CB	-6.34	1.43	1.53
1	A	238	ASP	N-CA	6.32	1.54	1.46
1	A	385	TYR	N-CA	6.32	1.53	1.46
1	A	109	ALA	C-N	-6.30	1.25	1.33
1	A	261	LEU	CA-CB	-6.30	1.43	1.53
1	B	109	ALA	C-N	-6.24	1.25	1.33
1	B	385	TYR	N-CA	6.17	1.53	1.46
1	B	310	ILE	CA-CB	6.10	1.59	1.54
1	B	410	ALA	CA-CB	-6.10	1.43	1.53
1	A	305	GLY	N-CA	6.08	1.53	1.45
1	A	410	ALA	CA-CB	-6.08	1.43	1.53
1	B	228	ALA	C-N	-6.07	1.28	1.33
1	B	410	ALA	N-CA	6.02	1.55	1.45
1	B	300	LYS	C-O	6.02	1.31	1.23
1	B	305	GLY	N-CA	6.01	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	300	LYS	C-O	6.01	1.31	1.23
1	A	410	ALA	N-CA	6.00	1.55	1.45
1	A	310	ILE	CA-CB	5.97	1.59	1.54
1	B	67	ARG	CD-NE	-5.94	1.38	1.46
1	A	228	ALA	C-N	-5.90	1.28	1.33
1	B	62	HIS	CE1-NE2	5.89	1.38	1.32
1	B	246	VAL	C-N	-5.87	1.25	1.33
1	A	246	VAL	C-N	-5.86	1.25	1.33
1	A	67	ARG	CD-NE	-5.86	1.38	1.46
1	A	62	HIS	CE1-NE2	5.85	1.38	1.32
1	B	165	HIS	C-N	-5.81	1.26	1.33
1	A	130	GLY	C-O	5.80	1.29	1.23
1	B	130	GLY	C-O	5.80	1.29	1.23
1	A	165	HIS	C-N	-5.77	1.26	1.33
1	A	329	GLU	N-CA	5.76	1.53	1.46
1	A	384	ASN	N-CA	5.72	1.55	1.46
1	B	329	GLU	N-CA	5.71	1.53	1.46
1	B	10	GLN	C-O	5.69	1.30	1.24
1	A	336	SER	N-CA	-5.68	1.38	1.46
1	A	10	GLN	C-O	5.67	1.30	1.24
1	B	384	ASN	N-CA	5.65	1.54	1.46
1	B	336	SER	N-CA	-5.64	1.38	1.46
1	A	74	HIS	C-N	-5.61	1.26	1.33
1	B	74	HIS	C-N	-5.59	1.26	1.33
1	B	203	GLY	N-CA	5.49	1.52	1.45
1	A	203	GLY	N-CA	5.47	1.52	1.45
1	B	222	VAL	C-O	5.47	1.30	1.24
1	A	472	PHE	CA-CB	-5.44	1.44	1.53
1	B	472	PHE	CA-CB	-5.43	1.44	1.53
1	A	348	LYS	C-O	5.42	1.30	1.24
1	A	222	VAL	C-O	5.41	1.30	1.24
1	B	348	LYS	C-O	5.39	1.30	1.24
1	A	204	ILE	CA-CB	5.39	1.61	1.54
1	B	204	ILE	CA-CB	5.36	1.61	1.54
1	B	362	ARG	CD-NE	-5.33	1.38	1.46
1	A	463	ALA	C-O	5.33	1.30	1.24
1	B	29	GLY	N-CA	5.32	1.53	1.45
1	B	435	ASN	N-CA	5.31	1.53	1.46
1	A	29	GLY	N-CA	5.29	1.53	1.45
1	B	75	ALA	C-N	-5.28	1.26	1.33
1	A	435	ASN	N-CA	5.28	1.52	1.46
1	B	291	PHE	N-CA	5.27	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	291	PHE	N-CA	5.27	1.53	1.46
1	B	463	ALA	C-O	5.27	1.30	1.24
1	A	362	ARG	CD-NE	-5.26	1.38	1.46
1	A	343	GLU	CA-C	-5.25	1.46	1.52
1	B	343	GLU	CA-C	-5.25	1.46	1.52
1	A	75	ALA	C-N	-5.23	1.26	1.33
1	B	325	PHE	C-N	-5.20	1.26	1.34
1	A	325	PHE	C-N	-5.19	1.26	1.34
1	B	261	LEU	N-CA	5.17	1.52	1.46
1	A	323	ASN	N-CA	-5.13	1.40	1.46
1	A	362	ARG	C-O	5.11	1.30	1.24
1	A	261	LEU	N-CA	5.10	1.52	1.46
1	B	242	LYS	CA-CB	-5.10	1.44	1.53
1	B	208	HIS	CA-CB	5.09	1.62	1.53
1	A	208	HIS	CA-CB	5.09	1.61	1.53
1	B	362	ARG	C-O	5.08	1.30	1.24
1	A	186	SER	C-N	-5.08	1.26	1.33
1	A	242	LYS	CA-CB	-5.08	1.44	1.53
1	A	329	GLU	CA-CB	-5.07	1.45	1.53
1	B	323	ASN	N-CA	-5.07	1.40	1.46
1	A	381	ARG	NE-CZ	5.06	1.38	1.33
1	B	329	GLU	CA-CB	-5.06	1.45	1.53
1	B	134	LYS	CE-NZ	5.05	1.64	1.49
1	B	377	PRO	CA-CB	-5.05	1.48	1.53
1	A	425	SER	C-O	5.04	1.29	1.24
1	A	377	PRO	CA-CB	-5.03	1.48	1.53
1	B	42	THR	N-CA	5.03	1.52	1.45
1	A	119	SER	C-O	5.03	1.30	1.24
1	B	119	SER	C-O	5.01	1.30	1.24
1	A	134	LYS	CE-NZ	5.01	1.64	1.49
1	B	186	SER	C-N	-5.00	1.26	1.33

All (745) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	67	ARG	CD-NE-CZ	21.05	153.88	124.40
1	A	67	ARG	CD-NE-CZ	21.02	153.82	124.40
1	A	472	PHE	CA-CB-CG	17.55	131.35	113.80
1	B	472	PHE	CA-CB-CG	17.51	131.31	113.80
1	A	139	ASP	CA-CB-CG	15.76	128.36	112.60
1	B	139	ASP	CA-CB-CG	15.73	128.33	112.60
1	A	74	HIS	CA-C-N	14.00	139.04	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	HIS	C-N-CA	14.00	139.04	120.28
1	B	74	HIS	CA-C-N	14.00	139.04	120.28
1	B	74	HIS	C-N-CA	14.00	139.04	120.28
1	B	343	GLU	CA-CB-CG	13.47	141.04	114.10
1	A	343	GLU	CA-CB-CG	13.46	141.02	114.10
1	B	28	THR	CA-C-O	-12.82	107.39	121.88
1	A	28	THR	CA-C-O	-12.81	107.41	121.88
1	A	111	ARG	CD-NE-CZ	11.51	140.51	124.40
1	B	111	ARG	CD-NE-CZ	11.49	140.48	124.40
1	A	263	ASP	CA-CB-CG	11.35	123.95	112.60
1	B	368	ASN	CA-C-O	-11.34	107.96	121.34
1	A	368	ASN	CA-C-O	-11.32	107.98	121.34
1	B	263	ASP	CA-CB-CG	11.30	123.90	112.60
1	B	461	ASN	CA-CB-CG	11.09	123.69	112.60
1	A	461	ASN	CA-CB-CG	11.07	123.67	112.60
1	A	364	ARG	CD-NE-CZ	-10.95	109.07	124.40
1	B	364	ARG	CD-NE-CZ	-10.92	109.12	124.40
1	B	261	LEU	CA-CB-CG	10.80	154.11	116.30
1	A	261	LEU	CA-CB-CG	10.78	154.04	116.30
1	B	92	ARG	CA-C-N	10.71	135.01	120.44
1	B	92	ARG	C-N-CA	10.71	135.01	120.44
1	A	92	ARG	CA-C-N	10.66	134.94	120.44
1	A	92	ARG	C-N-CA	10.66	134.94	120.44
1	B	407	SER	CA-C-O	-10.45	105.80	119.80
1	A	407	SER	CA-C-O	-10.43	105.82	119.80
1	B	179	ASP	CA-CB-CG	10.19	122.79	112.60
1	A	179	ASP	CA-CB-CG	10.14	122.74	112.60
1	A	254	HIS	CA-CB-CG	10.14	123.94	113.80
1	B	254	HIS	CA-CB-CG	10.10	123.90	113.80
1	A	239	GLN	OE1-CD-NE2	-10.05	112.55	122.60
1	A	71	ARG	CD-NE-CZ	10.04	138.46	124.40
1	B	239	GLN	OE1-CD-NE2	-10.05	112.55	122.60
1	B	71	ARG	CD-NE-CZ	10.03	138.44	124.40
1	B	453	GLU	CA-C-N	9.95	133.97	120.54
1	B	453	GLU	C-N-CA	9.95	133.97	120.54
1	A	453	GLU	CA-C-N	9.93	133.95	120.54
1	A	453	GLU	C-N-CA	9.93	133.95	120.54
1	B	386	GLN	CB-CG-CD	9.92	129.46	112.60
1	A	386	GLN	CB-CG-CD	9.91	129.45	112.60
1	A	221	LEU	CA-C-O	-9.56	110.57	120.71
1	B	221	LEU	CA-C-O	-9.54	110.59	120.71
1	B	191	SER	CA-C-N	9.46	134.69	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	191	SER	C-N-CA	9.46	134.69	120.31
1	A	191	SER	CA-C-N	9.45	134.67	120.31
1	A	191	SER	C-N-CA	9.45	134.67	120.31
1	A	335	PRO	CA-C-N	9.35	143.39	121.52
1	A	335	PRO	C-N-CA	9.35	143.39	121.52
1	B	335	PRO	CA-C-N	9.34	143.38	121.52
1	B	335	PRO	C-N-CA	9.34	143.38	121.52
1	B	102	ILE	O-C-N	8.95	132.33	122.75
1	B	225	ASP	CA-C-O	-8.93	108.55	119.18
1	A	102	ILE	O-C-N	8.92	132.30	122.75
1	A	225	ASP	CA-C-O	-8.89	108.60	119.18
1	A	443	ARG	CD-NE-CZ	8.79	136.70	124.40
1	B	443	ARG	CD-NE-CZ	8.78	136.69	124.40
1	B	59	GLU	CB-CG-CD	8.73	127.44	112.60
1	A	59	GLU	CB-CG-CD	8.71	127.42	112.60
1	B	57	THR	CB-CA-C	8.68	126.58	110.70
1	B	247	GLU	CA-CB-CG	8.66	131.42	114.10
1	A	247	GLU	CA-CB-CG	8.66	131.42	114.10
1	A	57	THR	CB-CA-C	8.65	126.53	110.70
1	A	54	VAL	CA-C-O	-8.55	110.09	120.78
1	B	54	VAL	CA-C-O	-8.53	110.12	120.78
1	A	336	SER	CA-CB-OG	8.48	128.07	111.10
1	B	336	SER	CA-CB-OG	8.48	128.06	111.10
1	B	99	PHE	CA-CB-CG	8.48	122.28	113.80
1	B	451	ASN	CA-CB-CG	8.45	121.05	112.60
1	A	99	PHE	CA-CB-CG	8.43	122.23	113.80
1	A	451	ASN	CA-CB-CG	8.41	121.01	112.60
1	A	468	ASP	CA-CB-CG	8.39	120.99	112.60
1	B	54	VAL	CA-C-N	8.37	130.78	122.66
1	B	54	VAL	C-N-CA	8.37	130.78	122.66
1	B	19	ALA	N-CA-C	-8.35	103.23	113.50
1	B	468	ASP	CA-CB-CG	8.35	120.95	112.60
1	A	54	VAL	CA-C-N	8.34	130.75	122.66
1	A	54	VAL	C-N-CA	8.34	130.75	122.66
1	A	19	ALA	N-CA-C	-8.34	103.25	113.50
1	A	425	SER	CA-C-N	-8.30	109.45	120.91
1	A	425	SER	C-N-CA	-8.30	109.45	120.91
1	A	410	ALA	CB-CA-C	8.28	124.83	109.51
1	A	93	TYR	CA-C-O	-8.27	112.18	120.70
1	B	147	ASN	CA-C-O	-8.27	111.59	121.60
1	B	425	SER	CA-C-N	-8.27	109.49	120.91
1	B	425	SER	C-N-CA	-8.27	109.49	120.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	147	ASN	CA-C-O	-8.27	111.59	121.60
1	B	410	ALA	CB-CA-C	8.27	124.81	109.51
1	B	93	TYR	CA-C-O	-8.26	112.19	120.70
1	A	375	ASN	OD1-CG-ND2	-8.24	114.36	122.60
1	B	375	ASN	OD1-CG-ND2	-8.22	114.38	122.60
1	B	328	VAL	CB-CA-C	8.21	118.96	110.91
1	A	328	VAL	CB-CA-C	8.21	118.95	110.91
1	B	24	ASP	CA-CB-CG	8.20	120.80	112.60
1	B	420	HIS	CA-C-N	8.15	132.31	120.82
1	B	420	HIS	C-N-CA	8.15	132.31	120.82
1	B	281	GLN	CA-C-O	-8.14	111.67	121.28
1	A	24	ASP	CA-CB-CG	8.14	120.74	112.60
1	B	408	PHE	CA-C-N	8.13	135.91	123.47
1	B	408	PHE	C-N-CA	8.13	135.91	123.47
1	B	275	SER	CA-C-N	8.12	136.33	122.37
1	B	275	SER	C-N-CA	8.12	136.33	122.37
1	A	135	PHE	CA-CB-CG	8.12	121.92	113.80
1	A	408	PHE	CA-C-N	8.11	135.88	123.47
1	A	408	PHE	C-N-CA	8.11	135.88	123.47
1	A	275	SER	CA-C-N	8.09	136.28	122.37
1	A	275	SER	C-N-CA	8.09	136.28	122.37
1	A	281	GLN	CA-C-O	-8.09	111.74	121.28
1	A	420	HIS	CA-C-N	8.08	132.22	120.82
1	A	420	HIS	C-N-CA	8.08	132.22	120.82
1	B	135	PHE	CA-CB-CG	8.08	121.88	113.80
1	B	234	HIS	CA-C-O	-8.04	111.39	120.32
1	B	450	LEU	CB-CA-C	8.03	125.25	109.35
1	A	450	LEU	CB-CA-C	8.01	125.22	109.35
1	A	234	HIS	CA-C-O	-8.01	111.43	120.32
1	A	438	ASN	CA-C-O	-8.01	109.98	119.35
1	A	92	ARG	NE-CZ-NH1	7.99	129.49	121.50
1	B	438	ASN	CA-C-O	-7.99	110.01	119.35
1	B	92	ARG	NE-CZ-NH1	7.98	129.48	121.50
1	B	89	ASP	CA-CB-CG	-7.94	104.66	112.60
1	A	435	ASN	CB-CA-C	7.93	123.34	110.09
1	A	291	PHE	CA-CB-CG	7.93	121.73	113.80
1	A	89	ASP	CA-CB-CG	-7.93	104.67	112.60
1	B	291	PHE	CA-CB-CG	7.90	121.70	113.80
1	B	435	ASN	CB-CA-C	7.90	123.28	110.09
1	A	129	ARG	CD-NE-CZ	-7.83	113.44	124.40
1	B	129	ARG	CD-NE-CZ	-7.82	113.45	124.40
1	B	62	HIS	CA-CB-CG	-7.78	106.02	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	363	HIS	CA-C-N	7.75	130.88	120.65
1	A	363	HIS	C-N-CA	7.75	130.88	120.65
1	A	62	HIS	CA-CB-CG	-7.74	106.06	113.80
1	A	168	LYS	CA-CB-CG	7.74	129.58	114.10
1	B	363	HIS	CA-C-N	7.73	130.85	120.65
1	B	363	HIS	C-N-CA	7.73	130.85	120.65
1	A	430	ARG	NE-CZ-NH1	-7.73	113.77	121.50
1	B	430	ARG	NE-CZ-NH1	-7.73	113.77	121.50
1	B	168	LYS	CA-CB-CG	7.72	129.54	114.10
1	A	368	ASN	OD1-CG-ND2	-7.71	114.89	122.60
1	A	305	GLY	N-CA-C	-7.70	102.92	112.77
1	A	386	GLN	CA-CB-CG	7.69	129.47	114.10
1	B	368	ASN	OD1-CG-ND2	-7.68	114.92	122.60
1	B	157	ALA	CA-C-N	7.67	131.58	120.38
1	B	157	ALA	C-N-CA	7.67	131.58	120.38
1	B	386	GLN	CA-CB-CG	7.67	129.45	114.10
1	B	305	GLY	N-CA-C	-7.67	102.95	112.77
1	A	157	ALA	CA-C-N	7.67	131.57	120.38
1	A	157	ALA	C-N-CA	7.67	131.57	120.38
1	B	229	VAL	N-CA-CB	-7.67	99.78	111.05
1	A	229	VAL	N-CA-CB	-7.65	99.80	111.05
1	A	322	VAL	CB-CA-C	7.63	121.56	111.94
1	A	371	GLN	OE1-CD-NE2	-7.62	114.98	122.60
1	A	8	SER	N-CA-C	7.62	120.47	111.71
1	B	127	ASP	CA-CB-CG	7.62	120.22	112.60
1	A	127	ASP	CA-CB-CG	7.61	120.21	112.60
1	B	322	VAL	CB-CA-C	7.61	121.53	111.94
1	B	8	SER	N-CA-C	7.60	120.45	111.71
1	B	371	GLN	OE1-CD-NE2	-7.58	115.02	122.60
1	A	58	ASP	CA-C-O	7.57	129.00	120.90
1	A	226	GLY	N-CA-C	-7.56	104.36	115.63
1	B	226	GLY	N-CA-C	-7.56	104.37	115.63
1	A	228	ALA	CA-C-N	7.56	132.09	121.96
1	A	228	ALA	C-N-CA	7.56	132.09	121.96
1	B	228	ALA	CA-C-N	7.56	132.09	121.96
1	B	228	ALA	C-N-CA	7.56	132.09	121.96
1	B	58	ASP	CA-C-O	7.52	128.95	120.90
1	B	238	ASP	CA-CB-CG	7.48	120.08	112.60
1	A	238	ASP	CA-CB-CG	7.46	120.06	112.60
1	B	126	ARG	CA-CB-CG	7.45	128.99	114.10
1	A	126	ARG	CA-CB-CG	7.43	128.96	114.10
1	A	261	LEU	N-CA-CB	7.40	120.80	110.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	261	LEU	N-CA-CB	7.39	120.79	110.07
1	A	206	ASP	CA-C-O	-7.35	113.51	122.41
1	B	143	ASP	CA-C-O	-7.34	112.65	120.80
1	B	184	PHE	CA-C-N	7.34	130.43	120.38
1	B	184	PHE	C-N-CA	7.34	130.43	120.38
1	B	206	ASP	CA-C-O	-7.33	113.54	122.41
1	A	143	ASP	CA-C-O	-7.33	112.67	120.80
1	A	184	PHE	CA-C-N	7.32	130.40	120.38
1	A	184	PHE	C-N-CA	7.32	130.40	120.38
1	A	19	ALA	CA-C-O	7.31	127.18	119.14
1	A	490	SER	CA-C-O	-7.29	110.50	119.18
1	B	19	ALA	CA-C-O	7.28	127.14	119.14
1	A	137	THR	CA-C-O	-7.27	113.02	121.82
1	B	490	SER	CA-C-O	-7.26	110.53	119.18
1	B	137	THR	CA-C-O	-7.26	113.04	121.82
1	A	385	TYR	CB-CA-C	7.22	123.05	110.64
1	B	102	ILE	CA-C-O	-7.17	112.89	121.28
1	B	293	PHE	CA-CB-CG	7.17	120.97	113.80
1	B	385	TYR	CB-CA-C	7.17	122.97	110.64
1	A	293	PHE	CA-CB-CG	7.16	120.96	113.80
1	A	102	ILE	CA-C-O	-7.15	112.92	121.28
1	A	10	GLN	OE1-CD-NE2	-7.12	115.48	122.60
1	B	9	ASP	CA-CB-CG	7.10	119.70	112.60
1	A	9	ASP	CA-CB-CG	7.08	119.68	112.60
1	B	290	ILE	CB-CA-C	7.07	118.26	110.62
1	B	10	GLN	OE1-CD-NE2	-7.07	115.53	122.60
1	A	290	ILE	CB-CA-C	7.04	118.22	110.62
1	A	134	LYS	CA-C-O	-7.02	112.73	120.38
1	B	134	LYS	CA-C-O	-7.00	112.75	120.38
1	A	66	GLU	CA-C-N	6.99	132.04	122.19
1	A	66	GLU	C-N-CA	6.99	132.04	122.19
1	A	81	PHE	N-CA-CB	-6.98	99.89	111.20
1	B	66	GLU	CA-C-N	6.98	132.03	122.19
1	B	66	GLU	C-N-CA	6.98	132.03	122.19
1	A	94	SER	N-CA-C	6.97	120.54	108.76
1	A	418	LEU	CA-C-O	-6.97	114.16	121.55
1	B	94	SER	N-CA-C	6.96	120.53	108.76
1	B	482	SER	O-C-N	6.96	129.24	122.07
1	A	482	SER	O-C-N	6.95	129.23	122.07
1	B	81	PHE	N-CA-CB	-6.94	99.96	111.20
1	B	353	ARG	O-C-N	-6.93	114.77	122.12
1	B	418	LEU	CA-C-O	-6.92	114.22	121.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	445	PHE	O-C-N	6.90	130.54	122.20
1	A	353	ARG	O-C-N	-6.89	114.81	122.12
1	B	445	PHE	O-C-N	6.88	130.53	122.20
1	B	264	LEU	CA-C-O	-6.87	113.23	120.92
1	A	264	LEU	CA-C-O	-6.87	113.23	120.92
1	B	429	GLN	CA-CB-CG	6.83	127.77	114.10
1	A	429	GLN	CA-CB-CG	6.82	127.74	114.10
1	A	413	HIS	N-CA-CB	6.81	120.80	110.45
1	B	413	HIS	N-CA-CB	6.80	120.79	110.45
1	A	179	ASP	N-CA-C	-6.79	103.33	111.69
1	A	412	GLU	CA-CB-CG	6.79	127.69	114.10
1	B	179	ASP	N-CA-C	-6.79	103.33	111.69
1	B	412	GLU	CA-CB-CG	6.79	127.69	114.10
1	B	46	ARG	O-C-N	6.79	131.29	122.19
1	B	7	ALA	CA-C-N	6.78	130.04	120.28
1	B	7	ALA	C-N-CA	6.78	130.04	120.28
1	A	281	GLN	N-CA-C	-6.75	99.30	110.17
1	A	46	ARG	O-C-N	6.75	131.23	122.19
1	A	111	ARG	NE-CZ-NH1	6.75	128.25	121.50
1	B	318	ASN	CA-CB-CG	6.75	119.35	112.60
1	B	111	ARG	NE-CZ-NH1	6.75	128.25	121.50
1	A	7	ALA	CA-C-N	6.74	129.99	120.28
1	A	7	ALA	C-N-CA	6.74	129.99	120.28
1	B	414	GLN	CA-C-O	6.74	126.43	119.49
1	A	414	GLN	CA-C-O	6.73	126.43	119.49
1	A	219	PHE	CA-CB-CG	-6.73	107.07	113.80
1	A	370	LEU	CA-C-N	6.72	133.63	122.54
1	A	370	LEU	C-N-CA	6.72	133.63	122.54
1	B	219	PHE	CA-CB-CG	-6.72	107.08	113.80
1	B	281	GLN	N-CA-C	-6.72	99.34	110.17
1	B	55	VAL	N-CA-C	-6.72	106.46	111.90
1	A	55	VAL	N-CA-C	-6.71	106.46	111.90
1	A	318	ASN	CA-CB-CG	6.70	119.30	112.60
1	A	429	GLN	CA-C-N	6.70	133.06	123.14
1	A	429	GLN	C-N-CA	6.70	133.06	123.14
1	A	32	ASN	CB-CG-ND2	6.70	126.45	116.40
1	B	370	LEU	CA-C-N	6.69	133.58	122.54
1	B	370	LEU	C-N-CA	6.69	133.58	122.54
1	A	159	LEU	CA-CB-CG	6.68	139.67	116.30
1	B	429	GLN	CA-C-N	6.67	133.01	123.14
1	B	429	GLN	C-N-CA	6.67	133.01	123.14
1	B	32	ASN	CB-CG-ND2	6.66	126.40	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	159	LEU	CA-CB-CG	6.66	139.62	116.30
1	A	129	ARG	CA-C-N	6.64	127.08	120.31
1	A	129	ARG	C-N-CA	6.64	127.08	120.31
1	A	215	GLY	CA-C-N	6.63	134.21	121.54
1	A	215	GLY	C-N-CA	6.63	134.21	121.54
1	B	215	GLY	CA-C-N	6.62	134.18	121.54
1	B	215	GLY	C-N-CA	6.62	134.18	121.54
1	A	261	LEU	N-CA-C	-6.61	104.00	111.14
1	B	261	LEU	N-CA-C	-6.61	104.00	111.14
1	B	304	HIS	CA-CB-CG	6.60	120.40	113.80
1	B	129	ARG	CA-C-N	6.60	127.04	120.31
1	B	129	ARG	C-N-CA	6.60	127.04	120.31
1	B	33	PRO	CA-C-N	6.59	132.34	122.91
1	B	33	PRO	C-N-CA	6.59	132.34	122.91
1	A	143	ASP	CA-CB-CG	6.59	119.19	112.60
1	A	304	HIS	CA-CB-CG	6.59	120.39	113.80
1	A	193	HIS	CA-C-N	6.59	131.88	120.68
1	A	193	HIS	C-N-CA	6.59	131.88	120.68
1	B	193	HIS	CA-C-N	6.58	131.86	120.68
1	B	193	HIS	C-N-CA	6.58	131.86	120.68
1	A	386	GLN	OE1-CD-NE2	-6.57	116.03	122.60
1	A	419	GLU	CB-CG-CD	6.57	123.77	112.60
1	B	55	VAL	CA-C-N	6.57	128.98	120.44
1	B	55	VAL	C-N-CA	6.57	128.98	120.44
1	B	419	GLU	CB-CG-CD	6.57	123.77	112.60
1	A	89	ASP	CB-CA-C	6.57	121.20	109.38
1	B	113	SER	O-C-N	6.57	129.86	123.29
1	B	89	ASP	CB-CA-C	6.55	121.18	109.38
1	A	390	PRO	CA-C-O	-6.55	114.10	121.43
1	B	386	GLN	OE1-CD-NE2	-6.55	116.05	122.60
1	A	55	VAL	CA-C-N	6.55	128.95	120.44
1	A	55	VAL	C-N-CA	6.55	128.95	120.44
1	B	143	ASP	CA-CB-CG	6.54	119.14	112.60
1	A	33	PRO	CA-C-N	6.54	132.26	122.91
1	A	33	PRO	C-N-CA	6.54	132.26	122.91
1	B	390	PRO	CA-C-O	-6.54	114.11	121.43
1	B	281	GLN	OE1-CD-NE2	-6.53	116.07	122.60
1	A	113	SER	O-C-N	6.53	129.82	123.29
1	A	343	GLU	CB-CA-C	6.53	123.03	110.17
1	B	190	GLU	N-CA-C	-6.52	105.04	112.87
1	A	190	GLU	N-CA-C	-6.52	105.05	112.87
1	B	343	GLU	CB-CA-C	6.51	122.99	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	281	GLN	OE1-CD-NE2	-6.51	116.09	122.60
1	A	404	TYR	CA-C-O	6.48	124.65	119.59
1	A	126	ARG	O-C-N	6.46	131.10	122.96
1	A	468	ASP	CA-C-O	-6.46	111.47	119.28
1	A	242	LYS	O-C-N	6.45	131.17	122.59
1	B	349	MET	CA-C-N	6.45	129.45	120.29
1	B	349	MET	C-N-CA	6.45	129.45	120.29
1	A	92	ARG	NH1-CZ-NH2	-6.45	110.92	119.30
1	A	126	ARG	N-CA-C	-6.44	100.12	109.59
1	B	499	TYR	CA-C-N	6.44	133.30	121.70
1	B	499	TYR	C-N-CA	6.44	133.30	121.70
1	A	349	MET	CA-C-N	6.44	129.43	120.29
1	A	349	MET	C-N-CA	6.44	129.43	120.29
1	B	404	TYR	CA-C-O	6.43	124.61	119.59
1	A	499	TYR	CA-C-N	6.42	133.26	121.70
1	A	499	TYR	C-N-CA	6.42	133.26	121.70
1	A	29	GLY	O-C-N	-6.42	113.63	122.68
1	B	468	ASP	CA-C-O	-6.42	111.51	119.28
1	B	118	GLU	CA-C-O	-6.42	114.63	121.88
1	B	242	LYS	O-C-N	6.42	131.13	122.59
1	A	389	GLY	CA-C-N	6.41	126.43	119.89
1	A	389	GLY	C-N-CA	6.41	126.43	119.89
1	B	92	ARG	NH1-CZ-NH2	-6.41	110.97	119.30
1	B	188	ARG	NE-CZ-NH1	-6.41	115.09	121.50
1	B	126	ARG	N-CA-C	-6.40	100.18	109.59
1	B	29	GLY	O-C-N	-6.40	113.66	122.68
1	B	187	LEU	N-CA-CB	-6.39	101.14	110.53
1	B	389	GLY	CA-C-N	6.39	126.40	119.89
1	B	389	GLY	C-N-CA	6.39	126.40	119.89
1	B	126	ARG	O-C-N	6.38	131.00	122.96
1	A	118	GLU	CA-C-O	-6.37	114.68	121.88
1	A	188	ARG	NE-CZ-NH1	-6.37	115.13	121.50
1	B	56	PHE	CA-CB-CG	-6.35	107.45	113.80
1	A	187	LEU	N-CA-CB	-6.34	101.20	110.53
1	A	56	PHE	CA-CB-CG	-6.33	107.47	113.80
1	A	334	ASP	CA-CB-CG	6.33	118.93	112.60
1	A	138	GLU	CB-CG-CD	6.32	123.34	112.60
1	B	334	ASP	CA-CB-CG	6.31	118.91	112.60
1	B	284	THR	CA-C-O	-6.31	114.93	121.87
1	B	492	ILE	CA-C-O	-6.30	114.05	121.05
1	A	284	THR	CA-C-O	-6.30	114.94	121.87
1	A	36	ASP	CA-C-O	-6.30	112.52	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	138	GLU	CB-CG-CD	6.30	123.30	112.60
1	A	492	ILE	CA-C-O	-6.29	114.07	121.05
1	B	36	ASP	CA-C-O	-6.28	112.54	120.20
1	A	182	TRP	CB-CA-C	6.27	122.71	110.67
1	B	169	ARG	CD-NE-CZ	6.27	133.18	124.40
1	B	182	TRP	CB-CA-C	6.27	122.71	110.67
1	B	261	LEU	O-C-N	6.27	128.86	122.09
1	A	261	LEU	O-C-N	6.25	128.84	122.09
1	A	169	ARG	CD-NE-CZ	6.24	133.14	124.40
1	B	209	ARG	CD-NE-CZ	-6.24	115.66	124.40
1	B	384	ASN	CA-CB-CG	-6.23	106.37	112.60
1	A	209	ARG	CD-NE-CZ	-6.22	115.69	124.40
1	B	488	TYR	N-CA-C	-6.22	104.41	111.07
1	B	466	LEU	O-C-N	6.22	129.91	122.27
1	B	115	VAL	CA-C-O	-6.21	114.69	120.34
1	A	384	ASN	CA-CB-CG	-6.21	106.39	112.60
1	B	361	HIS	CA-CB-CG	-6.21	107.59	113.80
1	A	115	VAL	CA-C-O	-6.20	114.69	120.34
1	A	442	VAL	N-CA-CB	6.20	117.38	110.62
1	B	63	PHE	CA-CB-CG	6.20	120.00	113.80
1	B	149	THR	CA-CB-OG1	-6.19	100.31	109.60
1	A	393	MET	N-CA-C	6.19	119.30	111.69
1	B	25	VAL	CA-C-N	6.19	130.16	121.24
1	B	25	VAL	C-N-CA	6.19	130.16	121.24
1	A	63	PHE	CA-CB-CG	6.19	119.99	113.80
1	A	488	TYR	N-CA-C	-6.18	104.45	111.07
1	A	25	VAL	CA-C-N	6.17	130.13	121.24
1	A	25	VAL	C-N-CA	6.17	130.13	121.24
1	B	442	VAL	N-CA-CB	6.17	117.34	110.62
1	A	361	HIS	CA-CB-CG	-6.17	107.64	113.80
1	A	149	THR	CA-CB-OG1	-6.16	100.36	109.60
1	B	434	ALA	CA-C-N	-6.16	112.37	122.54
1	B	434	ALA	C-N-CA	-6.16	112.37	122.54
1	B	368	ASN	O-C-N	6.16	130.27	121.95
1	B	290	ILE	N-CA-CB	-6.16	105.00	112.33
1	A	368	ASN	O-C-N	6.16	130.26	121.95
1	A	290	ILE	N-CA-CB	-6.16	105.01	112.33
1	A	466	LEU	O-C-N	6.15	129.84	122.27
1	A	250	ALA	CA-C-N	6.15	128.44	120.44
1	A	250	ALA	C-N-CA	6.15	128.44	120.44
1	A	319	ARG	CD-NE-CZ	-6.14	115.80	124.40
1	B	353	ARG	NE-CZ-NH2	-6.14	113.67	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	353	ARG	NE-CZ-NH2	-6.14	113.68	119.20
1	B	319	ARG	CD-NE-CZ	-6.14	115.81	124.40
1	B	393	MET	N-CA-C	6.14	119.24	111.69
1	A	20	ALA	N-CA-C	-6.13	102.98	111.81
1	B	188	ARG	NE-CZ-NH2	6.13	124.72	119.20
1	B	250	ALA	CA-C-N	6.13	128.41	120.44
1	B	250	ALA	C-N-CA	6.13	128.41	120.44
1	A	303	PRO	CA-C-O	-6.13	114.67	121.23
1	A	434	ALA	CA-C-N	-6.13	112.43	122.54
1	A	434	ALA	C-N-CA	-6.13	112.43	122.54
1	B	66	GLU	N-CA-C	6.13	118.93	111.82
1	B	303	PRO	CA-C-O	-6.11	114.69	121.23
1	B	20	ALA	N-CA-C	-6.11	103.02	111.81
1	A	457	ARG	CD-NE-CZ	6.10	132.94	124.40
1	A	66	GLU	N-CA-C	6.10	118.89	111.82
1	A	175	LEU	CA-C-N	6.07	130.19	121.50
1	A	175	LEU	C-N-CA	6.07	130.19	121.50
1	B	175	LEU	CA-C-N	6.07	130.19	121.50
1	B	175	LEU	C-N-CA	6.07	130.19	121.50
1	A	188	ARG	NE-CZ-NH2	6.07	124.66	119.20
1	B	168	LYS	N-CA-CB	6.07	120.74	110.49
1	B	379	ARG	CA-CB-CG	6.06	126.22	114.10
1	A	59	GLU	CA-C-O	6.06	126.84	120.42
1	A	379	ARG	CA-CB-CG	6.05	126.21	114.10
1	B	491	ARG	N-CA-C	-6.04	104.78	111.36
1	B	134	LYS	CD-CE-NZ	-6.03	92.59	111.90
1	A	30	GLY	N-CA-C	-6.03	106.25	115.66
1	B	281	GLN	CG-CD-OE1	6.03	132.86	120.80
1	A	168	LYS	N-CA-CB	6.03	120.67	110.49
1	B	457	ARG	CD-NE-CZ	6.03	132.84	124.40
1	B	449	VAL	N-CA-C	-6.02	106.38	113.42
1	A	414	GLN	OE1-CD-NE2	6.02	128.62	122.60
1	B	262	ARG	O-C-N	6.02	128.35	122.09
1	A	491	ARG	N-CA-C	-6.01	104.81	111.36
1	B	238	ASP	N-CA-C	-6.01	105.95	113.28
1	B	414	GLN	OE1-CD-NE2	6.01	128.61	122.60
1	A	134	LYS	CD-CE-NZ	-6.01	92.68	111.90
1	A	281	GLN	CG-CD-OE1	6.01	132.81	120.80
1	A	67	ARG	CA-CB-CG	6.00	126.11	114.10
1	A	290	ILE	CA-CB-CG2	6.00	120.70	110.50
1	B	30	GLY	N-CA-C	-6.00	106.30	115.66
1	B	59	GLU	CA-C-O	6.00	126.78	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	55	VAL	CA-C-O	6.00	125.94	120.30
1	B	290	ILE	CA-CB-CG2	5.99	120.68	110.50
1	B	67	ARG	CA-CB-CG	5.99	126.07	114.10
1	B	242	LYS	N-CA-C	-5.98	98.06	110.80
1	A	323	ASN	CA-C-N	5.98	128.54	120.65
1	A	323	ASN	C-N-CA	5.98	128.54	120.65
1	B	55	VAL	CA-C-O	5.98	125.92	120.30
1	A	242	LYS	N-CA-C	-5.97	98.08	110.80
1	B	323	ASN	CA-C-N	5.97	128.53	120.65
1	B	323	ASN	C-N-CA	5.97	128.53	120.65
1	B	349	MET	O-C-N	-5.97	115.80	122.12
1	A	449	VAL	N-CA-C	-5.96	106.45	113.42
1	A	75	ALA	CA-C-N	5.96	131.22	123.00
1	A	75	ALA	C-N-CA	5.96	131.22	123.00
1	B	119	SER	N-CA-C	5.96	119.65	112.38
1	A	238	ASP	N-CA-C	-5.96	106.02	113.28
1	A	318	ASN	N-CA-CB	-5.95	99.75	111.60
1	B	75	ALA	CA-C-N	5.95	131.22	123.00
1	B	75	ALA	C-N-CA	5.95	131.22	123.00
1	A	47	GLY	O-C-N	5.95	127.72	121.77
1	B	318	ASN	N-CA-CB	-5.94	99.78	111.60
1	A	65	ARG	CA-C-N	5.94	129.34	120.31
1	A	65	ARG	C-N-CA	5.94	129.34	120.31
1	A	262	ARG	O-C-N	5.94	128.27	122.09
1	A	349	MET	O-C-N	-5.93	115.83	122.12
1	B	47	GLY	O-C-N	5.93	127.70	121.77
1	B	366	GLY	CA-C-N	5.93	127.25	119.84
1	B	366	GLY	C-N-CA	5.93	127.25	119.84
1	A	270	THR	CA-CB-OG1	-5.93	100.71	109.60
1	B	65	ARG	CA-C-N	5.92	129.31	120.31
1	B	65	ARG	C-N-CA	5.92	129.31	120.31
1	B	270	THR	CA-CB-OG1	-5.92	100.72	109.60
1	A	119	SER	N-CA-C	5.91	119.59	112.38
1	A	366	GLY	CA-C-N	5.91	127.23	119.84
1	A	366	GLY	C-N-CA	5.91	127.23	119.84
1	A	32	ASN	OD1-CG-ND2	-5.91	116.69	122.60
1	B	449	VAL	O-C-N	5.89	128.65	122.17
1	A	449	VAL	O-C-N	5.88	128.64	122.17
1	A	306	ASP	CA-C-O	-5.88	114.64	120.70
1	A	322	VAL	CA-C-N	5.88	131.20	122.86
1	A	322	VAL	C-N-CA	5.88	131.20	122.86
1	B	32	ASN	OD1-CG-ND2	-5.87	116.73	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	383	ALA	CA-C-N	-5.86	110.46	121.95
1	A	383	ALA	C-N-CA	-5.86	110.46	121.95
1	B	322	VAL	CA-C-N	5.86	131.18	122.86
1	B	322	VAL	C-N-CA	5.86	131.18	122.86
1	B	383	ALA	CA-C-N	-5.85	110.48	121.95
1	B	383	ALA	C-N-CA	-5.85	110.48	121.95
1	A	358	PRO	CB-CA-C	5.84	120.21	111.68
1	A	126	ARG	CA-C-O	-5.84	113.81	120.58
1	A	255	GLU	CA-CB-CG	5.83	125.77	114.10
1	B	433	SER	N-CA-C	-5.83	105.53	114.16
1	A	445	PHE	CA-C-O	-5.83	114.20	121.02
1	B	358	PRO	CB-CA-C	5.83	120.19	111.68
1	B	126	ARG	CA-C-O	-5.83	113.82	120.58
1	B	255	GLU	CA-CB-CG	5.83	125.75	114.10
1	B	400	ALA	N-CA-C	5.82	118.06	109.50
1	B	420	HIS	CA-CB-CG	5.82	119.62	113.80
1	B	306	ASP	CA-C-O	-5.82	114.71	120.70
1	B	88	HIS	CA-C-N	-5.82	114.50	122.93
1	B	88	HIS	C-N-CA	-5.82	114.50	122.93
1	A	400	ALA	N-CA-C	5.81	118.05	109.50
1	B	139	ASP	N-CA-C	-5.81	106.00	112.57
1	A	88	HIS	CA-C-N	-5.81	114.51	122.93
1	A	88	HIS	C-N-CA	-5.81	114.51	122.93
1	A	433	SER	N-CA-C	-5.81	105.56	114.16
1	B	358	PRO	N-CA-C	-5.80	106.61	113.86
1	A	295	PRO	N-CD-CG	-5.80	94.50	103.20
1	B	295	PRO	N-CD-CG	-5.80	94.50	103.20
1	A	358	PRO	N-CA-C	-5.79	106.62	113.86
1	A	190	GLU	CB-CG-CD	5.79	122.45	112.60
1	A	192	LEU	N-CA-CB	-5.79	101.31	110.28
1	A	374	VAL	CA-C-O	-5.79	112.68	119.85
1	B	444	THR	CA-CB-OG1	-5.77	100.94	109.60
1	A	118	GLU	N-CA-C	-5.77	102.39	110.35
1	B	445	PHE	CA-C-O	-5.77	114.27	121.02
1	A	139	ASP	N-CA-C	-5.77	106.05	112.57
1	A	383	ALA	CA-C-O	-5.76	112.99	120.25
1	B	190	GLU	CB-CG-CD	5.76	122.39	112.60
1	A	332	ALA	CA-C-N	5.76	130.08	122.30
1	A	332	ALA	C-N-CA	5.76	130.08	122.30
1	B	192	LEU	N-CA-CB	-5.76	101.35	110.28
1	A	420	HIS	CA-CB-CG	5.76	119.56	113.80
1	B	332	ALA	CA-C-N	5.76	130.07	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	332	ALA	C-N-CA	5.76	130.07	122.30
1	A	444	THR	CA-CB-OG1	-5.75	100.97	109.60
1	B	118	GLU	N-CA-C	-5.75	102.41	110.35
1	B	265	PHE	O-C-N	5.75	127.99	122.07
1	B	129	ARG	NE-CZ-NH2	5.75	124.37	119.20
1	A	129	ARG	NE-CZ-NH2	5.74	124.37	119.20
1	A	265	PHE	O-C-N	5.74	127.98	122.07
1	B	177	ASP	N-CA-CB	-5.74	98.79	110.50
1	B	374	VAL	CA-C-O	-5.74	112.73	119.85
1	B	60	MET	CA-C-N	5.73	127.96	120.28
1	B	60	MET	C-N-CA	5.73	127.96	120.28
1	A	177	ASP	N-CA-CB	-5.72	98.82	110.50
1	A	341	GLY	CA-C-N	5.72	131.79	122.69
1	A	341	GLY	C-N-CA	5.72	131.79	122.69
1	B	383	ALA	CA-C-O	-5.72	113.04	120.25
1	B	284	THR	N-CA-CB	-5.71	102.10	110.26
1	B	199	PHE	CA-CB-CG	-5.71	108.09	113.80
1	B	341	GLY	CA-C-N	5.69	131.73	122.69
1	B	341	GLY	C-N-CA	5.69	131.73	122.69
1	A	135	PHE	CA-C-O	-5.68	114.19	120.38
1	B	135	PHE	CA-C-O	-5.67	114.20	120.38
1	B	265	PHE	CA-C-N	5.67	127.81	120.44
1	B	265	PHE	C-N-CA	5.67	127.81	120.44
1	A	60	MET	CA-C-N	5.66	127.87	120.28
1	A	60	MET	C-N-CA	5.66	127.87	120.28
1	A	199	PHE	CA-CB-CG	-5.66	108.14	113.80
1	A	112	PHE	CA-C-O	-5.66	114.76	121.66
1	B	112	PHE	CA-C-O	-5.65	114.77	121.66
1	A	284	THR	N-CA-CB	-5.64	102.19	110.26
1	A	265	PHE	CA-C-N	5.62	127.75	120.44
1	A	265	PHE	C-N-CA	5.62	127.75	120.44
1	B	291	PHE	N-CA-C	-5.62	101.39	109.48
1	B	251	ARG	CA-CB-CG	5.62	125.33	114.10
1	B	263	ASP	CB-CA-C	5.61	121.58	110.42
1	A	263	ASP	CB-CA-C	5.60	121.57	110.42
1	A	414	GLN	CB-CA-C	5.60	119.85	110.55
1	A	291	PHE	N-CA-C	-5.60	101.41	109.48
1	A	251	ARG	CA-CB-CG	5.59	125.29	114.10
1	A	73	VAL	CA-C-O	-5.59	115.43	121.19
1	B	221	LEU	N-CA-C	-5.59	100.59	109.59
1	B	414	GLN	CB-CA-C	5.58	119.82	110.55
1	B	73	VAL	CA-C-O	-5.58	115.45	121.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	ARG	CB-CG-CD	5.58	124.12	111.30
1	B	359	ASP	CB-CG-OD2	-5.58	105.58	118.40
1	B	111	ARG	CB-CG-CD	5.57	124.11	111.30
1	B	100	GLU	CA-C-O	-5.57	112.09	119.10
1	A	221	LEU	N-CA-C	-5.56	100.64	109.59
1	A	100	GLU	CA-C-O	-5.56	112.10	119.10
1	A	359	ASP	CB-CG-OD2	-5.56	105.62	118.40
1	A	68	ILE	CA-C-O	-5.55	112.52	119.95
1	B	199	PHE	CA-C-O	-5.55	112.77	119.59
1	B	440	THR	CA-CB-OG1	-5.54	101.28	109.60
1	B	360	THR	N-CA-CB	-5.53	101.78	110.46
1	A	199	PHE	CA-C-O	-5.53	112.79	119.59
1	B	68	ILE	CA-C-O	-5.52	112.55	119.95
1	A	22	LYS	N-CA-C	-5.52	97.61	109.81
1	A	360	THR	N-CA-CB	-5.52	101.80	110.46
1	A	440	THR	CA-CB-OG1	-5.52	101.33	109.60
1	B	22	LYS	N-CA-C	-5.51	97.63	109.81
1	B	483	ASP	CA-C-O	-5.51	114.03	120.20
1	A	217	HIS	N-CA-CB	5.50	117.91	110.38
1	A	109	ALA	CA-C-O	-5.49	114.91	121.56
1	A	221	LEU	O-C-N	5.49	130.18	123.21
1	B	217	HIS	N-CA-CB	5.48	117.89	110.38
1	B	221	LEU	O-C-N	5.47	130.16	123.21
1	B	109	ALA	CA-C-O	-5.46	114.95	121.56
1	B	110	VAL	CA-C-O	-5.46	114.80	120.64
1	A	72	VAL	CB-CA-C	5.46	120.62	112.16
1	A	483	ASP	CA-C-O	-5.46	114.09	120.20
1	A	110	VAL	CA-C-O	-5.45	114.80	120.64
1	B	397	GLN	OE1-CD-NE2	-5.45	117.15	122.60
1	B	372	ILE	CA-CB-CG1	5.44	119.64	110.40
1	B	72	VAL	CB-CA-C	5.43	120.58	112.16
1	B	122	ALA	CB-CA-C	5.42	118.59	109.48
1	A	397	GLN	OE1-CD-NE2	-5.42	117.18	122.60
1	A	344	PRO	CB-CA-C	-5.42	103.88	110.98
1	A	262	ARG	CD-NE-CZ	-5.42	116.81	124.40
1	A	372	ILE	CA-CB-CG1	5.42	119.61	110.40
1	A	36	ASP	O-C-N	5.41	130.21	123.28
1	A	425	SER	CA-C-O	-5.41	114.51	120.24
1	B	320	ASN	CA-C-O	-5.41	115.73	120.60
1	B	362	ARG	NE-CZ-NH1	5.41	126.91	121.50
1	A	429	GLN	CA-C-O	-5.40	115.63	121.36
1	B	187	LEU	CB-CA-C	5.40	119.12	109.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	366	GLY	O-C-N	5.40	127.17	121.77
1	A	187	LEU	CB-CA-C	5.40	119.12	109.29
1	B	344	PRO	CB-CA-C	-5.40	103.91	110.98
1	B	470	GLN	CA-C-O	-5.40	115.68	121.56
1	B	36	ASP	O-C-N	5.39	130.19	123.28
1	B	461	ASN	N-CA-C	-5.39	105.10	110.97
1	A	366	GLY	O-C-N	5.39	127.16	121.77
1	B	262	ARG	CD-NE-CZ	-5.39	116.86	124.40
1	A	49	LEU	CA-C-O	5.38	126.46	120.43
1	A	320	ASN	CA-C-O	-5.38	115.75	120.60
1	A	362	ARG	NE-CZ-NH1	5.38	126.88	121.50
1	A	470	GLN	CA-C-O	-5.38	115.69	121.56
1	B	49	LEU	CA-C-O	5.38	126.46	120.43
1	B	425	SER	CA-C-O	-5.38	114.53	120.24
1	A	119	SER	CA-C-N	-5.38	113.15	122.83
1	A	119	SER	C-N-CA	-5.38	113.15	122.83
1	A	122	ALA	CB-CA-C	5.38	118.52	109.48
1	B	164	ILE	CB-CG1-CD1	5.38	125.10	113.80
1	B	119	SER	CA-C-N	-5.37	113.17	122.83
1	B	119	SER	C-N-CA	-5.37	113.17	122.83
1	A	461	ASN	N-CA-C	-5.36	105.12	110.97
1	A	346	PRO	CB-CA-C	5.36	118.44	110.88
1	A	164	ILE	CB-CG1-CD1	5.36	125.05	113.80
1	A	337	ASN	N-CA-C	-5.36	102.16	109.71
1	A	91	THR	CA-CB-OG1	-5.35	101.58	109.60
1	B	429	GLN	CA-C-O	-5.35	115.69	121.36
1	B	105	ARG	CB-CA-C	-5.34	99.94	109.71
1	B	91	THR	CA-CB-OG1	-5.34	101.60	109.60
1	B	337	ASN	N-CA-C	-5.34	102.18	109.71
1	A	422	THR	O-C-N	5.33	129.13	123.42
1	A	105	ARG	CB-CA-C	-5.33	99.95	109.71
1	B	346	PRO	CB-CA-C	5.33	118.39	110.88
1	B	419	GLU	CA-CB-CG	5.32	124.74	114.10
1	A	419	GLU	CA-CB-CG	5.32	124.74	114.10
1	B	457	ARG	NE-CZ-NH1	5.32	126.82	121.50
1	B	169	ARG	N-CA-C	5.32	118.40	109.95
1	A	432	ASN	CA-C-O	-5.31	116.03	121.87
1	B	111	ARG	NE-CZ-NH2	-5.31	114.42	119.20
1	A	286	SER	CA-CB-OG	-5.30	100.49	111.10
1	B	422	THR	O-C-N	5.30	129.10	123.42
1	B	432	ASN	CA-C-O	-5.30	116.04	121.87
1	B	286	SER	CA-CB-OG	-5.29	100.51	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	ASP	N-CA-CB	5.29	118.77	110.46
1	A	417	ALA	CB-CA-C	5.29	119.67	110.72
1	B	450	LEU	N-CA-CB	-5.29	101.42	111.00
1	B	225	ASP	N-CA-CB	5.29	118.76	110.46
1	B	289	GLU	CB-CG-CD	5.28	121.58	112.60
1	B	359	ASP	CA-CB-CG	5.28	117.88	112.60
1	B	417	ALA	CB-CA-C	5.28	119.65	110.72
1	A	111	ARG	NE-CZ-NH2	-5.28	114.45	119.20
1	A	169	ARG	N-CA-C	5.28	118.35	109.95
1	A	457	ARG	NE-CZ-NH1	5.28	126.78	121.50
1	A	289	GLU	CB-CG-CD	5.28	121.57	112.60
1	A	359	ASP	CA-CB-CG	5.27	117.87	112.60
1	B	259	TYR	CA-C-N	5.27	126.73	120.14
1	B	259	TYR	C-N-CA	5.27	126.73	120.14
1	B	265	PHE	N-CA-CB	5.27	117.65	110.01
1	B	325	PHE	N-CA-CB	5.27	117.83	109.82
1	A	450	LEU	N-CA-CB	-5.26	101.47	111.00
1	B	95	LYS	CB-CA-C	-5.26	101.00	110.37
1	A	265	PHE	N-CA-CB	5.25	117.63	110.01
1	B	393	MET	CA-C-O	-5.25	114.41	120.24
1	A	318	ASN	CB-CA-C	5.25	121.79	110.41
1	B	318	ASN	CB-CA-C	5.24	121.78	110.41
1	A	203	GLY	N-CA-C	-5.24	106.45	112.73
1	A	393	MET	CA-C-O	-5.24	114.43	120.24
1	A	95	LYS	CB-CA-C	-5.23	101.05	110.37
1	A	325	PHE	N-CA-CB	5.23	117.77	109.82
1	A	431	PHE	CA-CB-CG	-5.23	108.57	113.80
1	B	203	GLY	N-CA-C	-5.23	106.46	112.73
1	A	259	TYR	CA-C-N	5.23	126.67	120.14
1	A	259	TYR	C-N-CA	5.23	126.67	120.14
1	B	117	GLY	CA-C-N	5.22	131.68	121.66
1	B	117	GLY	C-N-CA	5.22	131.68	121.66
1	B	11	MET	N-CA-CB	5.21	118.36	110.28
1	A	11	MET	N-CA-CB	5.21	118.36	110.28
1	A	362	ARG	NE-CZ-NH2	-5.21	114.51	119.20
1	B	362	ARG	NE-CZ-NH2	-5.21	114.51	119.20
1	A	464	GLY	CA-C-O	-5.20	115.14	120.45
1	B	387	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	B	431	PHE	CA-CB-CG	-5.20	108.60	113.80
1	A	117	GLY	CA-C-N	5.20	131.64	121.66
1	A	117	GLY	C-N-CA	5.20	131.64	121.66
1	A	343	GLU	CA-C-N	5.19	125.09	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	343	GLU	C-N-CA	5.19	125.09	119.85
1	A	134	LYS	CB-CA-C	-5.18	100.75	109.72
1	A	134	LYS	O-C-N	5.18	129.40	123.29
1	B	393	MET	CB-CA-C	-5.18	101.22	110.70
1	A	387	ARG	NE-CZ-NH2	5.18	123.86	119.20
1	B	134	LYS	O-C-N	5.18	129.40	123.29
1	B	464	GLY	CA-C-O	-5.18	115.17	120.45
1	B	343	GLU	CA-C-N	5.17	125.07	119.85
1	B	343	GLU	C-N-CA	5.17	125.07	119.85
1	A	393	MET	CB-CA-C	-5.17	101.24	110.70
1	A	188	ARG	O-C-N	5.16	125.40	121.27
1	A	335	PRO	O-C-N	-5.16	115.92	122.17
1	B	474	GLN	O-C-N	5.16	127.40	122.03
1	B	44	GLY	O-C-N	5.16	126.93	121.77
1	B	134	LYS	CB-CA-C	-5.16	100.80	109.72
1	B	199	PHE	O-C-N	5.16	128.97	122.37
1	A	111	ARG	N-CA-C	-5.16	100.49	108.90
1	A	444	THR	OG1-CB-CG2	5.16	119.61	109.30
1	B	247	GLU	CG-CD-OE2	-5.15	106.56	118.40
1	A	313	GLY	CA-C-O	-5.14	115.95	121.35
1	B	314	LYS	CA-CB-CG	5.14	124.39	114.10
1	B	111	ARG	N-CA-C	-5.14	100.52	108.90
1	B	444	THR	OG1-CB-CG2	5.14	119.58	109.30
1	B	335	PRO	O-C-N	-5.14	115.95	122.17
1	A	474	GLN	O-C-N	5.13	127.37	122.03
1	A	199	PHE	O-C-N	5.13	128.94	122.37
1	A	247	GLU	CG-CD-OE2	-5.13	106.60	118.40
1	B	111	ARG	N-CA-CB	5.13	119.30	110.68
1	B	143	ASP	O-C-N	5.13	129.19	123.19
1	A	314	LYS	CA-CB-CG	5.12	124.35	114.10
1	A	375	ASN	CB-CG-ND2	5.12	124.08	116.40
1	A	44	GLY	O-C-N	5.12	126.89	121.77
1	B	313	GLY	CA-C-O	-5.12	115.98	121.35
1	B	422	THR	N-CA-C	-5.12	100.96	108.79
1	A	111	ARG	N-CA-CB	5.12	119.27	110.68
1	A	137	THR	CA-CB-OG1	-5.12	101.93	109.60
1	A	143	ASP	O-C-N	5.11	129.17	123.19
1	B	73	VAL	CA-CB-CG1	5.11	119.08	110.40
1	B	188	ARG	O-C-N	5.11	125.35	121.27
1	B	137	THR	CA-CB-OG1	-5.10	101.94	109.60
1	B	375	ASN	CB-CG-ND2	5.10	124.05	116.40
1	A	422	THR	N-CA-C	-5.09	101.00	108.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	452	GLU	N-CA-C	-5.08	107.63	113.88
1	B	461	ASN	CA-C-O	-5.08	115.67	121.00
1	A	73	VAL	CA-CB-CG1	5.07	119.02	110.40
1	A	392	CYS	CA-C-N	5.06	129.24	120.58
1	A	392	CYS	C-N-CA	5.06	129.24	120.58
1	B	291	PHE	CB-CA-C	5.06	117.56	109.62
1	A	461	ASN	CA-C-O	-5.05	115.69	121.00
1	A	291	PHE	CB-CA-C	5.05	117.55	109.62
1	B	224	ALA	CA-C-O	-5.05	112.74	119.10
1	A	284	THR	OG1-CB-CG2	5.04	119.38	109.30
1	A	421	ARG	CD-NE-CZ	-5.04	117.34	124.40
1	A	452	GLU	N-CA-C	-5.04	107.68	113.88
1	A	299	THR	CA-CB-OG1	-5.04	102.04	109.60
1	B	103	GLY	N-CA-C	-5.04	108.69	114.69
1	B	392	CYS	CA-C-N	5.04	129.19	120.58
1	B	392	CYS	C-N-CA	5.04	129.19	120.58
1	A	224	ALA	CA-C-O	-5.04	112.76	119.10
1	A	300	LYS	CA-CB-CG	-5.04	104.03	114.10
1	B	300	LYS	CA-CB-CG	-5.03	104.04	114.10
1	B	284	THR	OG1-CB-CG2	5.02	119.35	109.30
1	B	299	THR	CA-CB-OG1	-5.02	102.07	109.60
1	A	343	GLU	CG-CD-OE1	5.01	129.92	118.40
1	B	421	ARG	CD-NE-CZ	-5.01	117.38	124.40
1	B	343	GLU	CG-CD-OE1	5.00	129.91	118.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	430	ARG	Sidechain
1	B	430	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4008	0	3833	275	3

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4008	0	3833	265	3
2	A	43	0	30	11	0
2	B	43	0	30	12	0
3	A	48	0	26	3	0
3	B	48	0	26	3	0
4	A	50	0	0	4	1
4	B	50	0	0	3	1
All	All	8298	0	7778	522	4

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 33.

All (522) 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:155:ARG:NH2	1:B:438:ASN:HD21	1.22	1.35
1:A:155:ARG:NH2	1:A:438:ASN:HD21	1.22	1.34
1:A:155:ARG:HH22	1:A:438:ASN:ND2	1.22	1.33
1:B:155:ARG:HH22	1:B:438:ASN:ND2	1.22	1.32
1:A:177:ASP:HB3	1:A:180:MET:HE2	1.14	1.08
1:B:177:ASP:HB3	1:B:180:MET:HE2	1.14	1.07
1:A:322:VAL:HA	1:B:172:GLN:NE2	1.79	0.98
1:A:172:GLN:NE2	1:B:322:VAL:HA	1.79	0.96
1:B:384:ASN:C	1:B:384:ASN:HD22	1.66	0.96
1:A:384:ASN:C	1:A:384:ASN:HD22	1.66	0.96
1:A:172:GLN:HE21	1:B:322:VAL:HA	1.29	0.96
1:A:444:THR:O	1:A:448:LYS:HG2	1.66	0.95
1:B:177:ASP:CB	1:B:180:MET:HE2	1.96	0.95
1:A:322:VAL:HA	1:B:172:GLN:HE21	1.30	0.95
1:B:444:THR:O	1:B:448:LYS:HG2	1.66	0.95
1:A:173:THR:HG21	1:A:175:LEU:HD12	1.49	0.94
1:A:177:ASP:CB	1:A:180:MET:HE2	1.97	0.94
1:B:173:THR:HG21	1:B:175:LEU:HD12	1.49	0.94
1:A:406:ASN:ND2	1:A:408:PHE:H	1.71	0.89
1:A:406:ASN:HD22	1:A:408:PHE:H	1.20	0.89
1:B:148:ASN:H	1:B:148:ASN:HD22	1.20	0.88
1:A:220:LYS:HE3	1:A:420:HIS:CD2	2.09	0.87
1:B:220:LYS:HE3	1:B:420:HIS:CD2	2.09	0.87
1:B:406:ASN:ND2	1:B:408:PHE:H	1.71	0.87
1:B:406:ASN:HD22	1:B:408:PHE:H	1.20	0.86
1:A:229:VAL:HG13	1:A:282:VAL:HG23	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:ASP:HB3	1:B:180:MET:CE	2.05	0.85
1:A:148:ASN:HD22	1:A:148:ASN:H	1.20	0.85
1:A:189:PRO:O	1:A:192:LEU:HD12	1.76	0.85
1:B:189:PRO:O	1:B:192:LEU:HD12	1.76	0.85
1:B:229:VAL:HG13	1:B:282:VAL:HG23	1.57	0.84
1:A:90:ILE:HD13	1:A:312:VAL:HG13	1.58	0.83
1:B:90:ILE:HD13	1:B:312:VAL:HG13	1.58	0.83
1:A:177:ASP:HB3	1:A:180:MET:CE	2.05	0.81
1:B:179:ASP:O	1:B:183:ASP:HB2	1.82	0.80
1:B:142:TRP:HB2	1:B:339:PRO:HD3	1.65	0.79
1:A:179:ASP:O	1:A:183:ASP:HB2	1.82	0.78
1:A:142:TRP:HB2	1:A:339:PRO:HD3	1.65	0.78
1:A:487:GLU:O	1:A:491:ARG:HG3	1.84	0.78
1:B:384:ASN:C	1:B:384:ASN:ND2	2.42	0.78
1:A:384:ASN:C	1:A:384:ASN:ND2	2.41	0.77
1:A:384:ASN:HD22	1:A:385:TYR:N	1.82	0.77
1:B:384:ASN:HD22	1:B:385:TYR:N	1.82	0.77
1:B:487:GLU:O	1:B:491:ARG:HG3	1.83	0.77
1:B:173:THR:CG2	1:B:175:LEU:HD12	2.15	0.76
1:A:458:LEU:CD1	1:A:462:ILE:HD11	2.16	0.76
1:A:173:THR:CG2	1:A:175:LEU:HD12	2.15	0.76
1:A:251:ARG:O	1:A:255:GLU:HB2	1.86	0.75
1:A:223:ASN:C	1:A:223:ASN:HD22	1.94	0.75
1:B:17:GLN:O	1:B:17:GLN:HG2	1.86	0.75
1:B:458:LEU:CD1	1:B:462:ILE:HD11	2.16	0.75
1:A:17:GLN:O	1:A:17:GLN:HG2	1.85	0.75
1:A:451:ASN:O	1:A:455:ARG:HG3	1.87	0.74
1:B:223:ASN:C	1:B:223:ASN:HD22	1.94	0.74
1:B:98:VAL:HG23	1:B:137:THR:CG2	2.17	0.74
1:B:79:GLY:O	1:B:80:ALA:HB2	1.88	0.74
1:A:98:VAL:HG23	1:A:137:THR:HB	1.68	0.74
1:B:251:ARG:O	1:B:255:GLU:HB2	1.86	0.74
1:B:74:HIS:O	1:B:111:ARG:NH2	2.20	0.74
1:B:98:VAL:HG23	1:B:137:THR:HB	1.68	0.73
1:A:284:THR:HG22	1:A:286:SER:H	1.53	0.73
1:B:170:ASN:ND2	1:B:172:GLN:H	1.87	0.73
1:B:284:THR:HG22	1:B:286:SER:H	1.53	0.73
1:B:451:ASN:O	1:B:455:ARG:HG3	1.87	0.73
1:A:98:VAL:HG23	1:A:137:THR:CG2	2.17	0.73
1:A:79:GLY:O	1:A:80:ALA:HB2	1.88	0.73
1:A:170:ASN:ND2	1:A:172:GLN:H	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:496:LEU:O	1:B:500:ASN:HB2	1.89	0.73
1:B:297:ASP:OD1	1:B:300:LYS:HE2	1.89	0.73
1:A:108:ILE:HD13	1:A:315:LEU:HD12	1.69	0.72
1:B:458:LEU:O	1:B:462:ILE:HG13	1.90	0.72
1:A:297:ASP:OD1	1:A:300:LYS:HE2	1.89	0.72
1:B:108:ILE:HD13	1:B:315:LEU:HD12	1.69	0.72
1:B:458:LEU:O	1:B:458:LEU:HD12	1.90	0.71
1:A:458:LEU:O	1:A:462:ILE:HG13	1.90	0.71
1:A:458:LEU:O	1:A:458:LEU:HD12	1.90	0.71
1:A:496:LEU:O	1:A:500:ASN:HB2	1.89	0.71
1:B:223:ASN:ND2	1:B:225:ASP:H	1.88	0.71
1:A:74:HIS:O	1:A:111:ARG:NH2	2.20	0.71
1:B:134:LYS:HE3	1:B:331:LEU:CD2	2.21	0.70
1:A:223:ASN:ND2	1:A:225:ASP:H	1.88	0.70
1:A:134:LYS:HE3	1:A:331:LEU:CD2	2.21	0.70
1:A:446:TYR:HA	1:A:450:LEU:HD22	1.74	0.70
1:A:170:ASN:HD22	1:A:172:GLN:H	1.40	0.70
1:B:446:TYR:HA	1:B:450:LEU:HD22	1.74	0.70
1:B:383:ALA:HB1	1:B:411:PRO:HG3	1.73	0.69
1:B:170:ASN:HD22	1:B:172:GLN:H	1.39	0.69
1:A:383:ALA:HB1	1:A:411:PRO:HG3	1.73	0.69
1:B:155:ARG:NH2	1:B:438:ASN:ND2	2.02	0.68
1:A:172:GLN:HE21	1:B:322:VAL:CA	2.05	0.68
1:A:275:SER:HA	1:A:315:LEU:O	1.94	0.68
1:B:447:LEU:HB2	1:B:448:LYS:HD3	1.76	0.68
1:A:284:THR:HB	1:A:287:GLU:HG3	1.75	0.68
1:B:275:SER:HA	1:B:315:LEU:O	1.93	0.68
1:A:131:PHE:C	1:A:131:PHE:HD1	2.03	0.67
1:B:458:LEU:HD11	1:B:462:ILE:HD11	1.76	0.67
1:A:322:VAL:CA	1:B:172:GLN:HE21	2.05	0.67
1:A:458:LEU:HD11	1:A:462:ILE:HD11	1.77	0.67
1:B:43:VAL:HG13	1:B:48:PRO:HD2	1.77	0.67
1:B:284:THR:HB	1:B:287:GLU:HG3	1.75	0.67
1:A:374:VAL:O	1:A:374:VAL:HG22	1.95	0.67
1:A:447:LEU:HB2	1:A:448:LYS:HD3	1.76	0.66
1:B:131:PHE:HD1	1:B:131:PHE:C	2.03	0.66
1:A:43:VAL:HG13	1:A:48:PRO:HD2	1.77	0.66
1:A:149:THR:OG1	1:A:150:PRO:HD2	1.96	0.66
1:B:149:THR:OG1	1:B:150:PRO:HD2	1.95	0.66
1:B:374:VAL:HG22	1:B:374:VAL:O	1.95	0.66
1:B:342:ILE:O	1:B:343:GLU:HB2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:SER:O	1:A:476:LYS:NZ	2.27	0.66
1:A:92:ARG:O	1:A:223:ASN:HB3	1.96	0.65
1:B:43:VAL:O	1:B:47:GLY:HA3	1.96	0.65
1:B:467:LYS:HE2	1:B:468:ASP:OD2	1.96	0.65
1:A:155:ARG:NH2	1:A:438:ASN:ND2	2.02	0.65
1:B:148:ASN:HD22	1:B:148:ASN:N	1.94	0.65
1:A:348:LYS:CE	4:A:551:HOH:O	2.45	0.65
1:B:98:VAL:CG2	1:B:137:THR:HG22	2.27	0.65
1:A:98:VAL:CG2	1:A:137:THR:HG22	2.27	0.65
1:A:487:GLU:CG	1:A:491:ARG:HD2	2.27	0.65
1:B:186:SER:O	1:B:476:LYS:NZ	2.27	0.65
1:A:371:GLN:NE2	1:A:393:MET:H	1.95	0.64
1:A:467:LYS:HE2	1:A:468:ASP:OD2	1.96	0.64
1:A:148:ASN:HD22	1:A:148:ASN:N	1.94	0.64
2:A:507:HEM:HBB2	2:A:507:HEM:HMB2	1.79	0.64
1:A:342:ILE:O	1:A:343:GLU:HB2	1.95	0.64
1:B:98:VAL:CG2	1:B:137:THR:CG2	2.76	0.64
1:A:371:GLN:HE22	1:A:393:MET:H	1.45	0.64
1:B:92:ARG:O	1:B:223:ASN:HB3	1.96	0.64
1:B:371:GLN:NE2	1:B:393:MET:H	1.95	0.64
1:A:43:VAL:O	1:A:47:GLY:HA3	1.96	0.64
1:A:372:ILE:O	1:A:373:PRO:C	2.41	0.64
1:B:487:GLU:CG	1:B:491:ARG:HD2	2.27	0.64
1:B:348:LYS:CE	4:B:509:HOH:O	2.45	0.64
1:B:371:GLN:HE22	1:B:393:MET:H	1.44	0.64
1:B:371:GLN:HE21	1:B:393:MET:HB2	1.64	0.63
1:A:371:GLN:HE21	1:A:393:MET:HB2	1.64	0.63
1:B:131:PHE:C	1:B:131:PHE:CD1	2.76	0.63
1:A:98:VAL:CG2	1:A:137:THR:CG2	2.76	0.63
1:A:406:ASN:HD22	1:A:406:ASN:C	2.07	0.63
1:B:458:LEU:CD1	1:B:462:ILE:CD1	2.77	0.63
1:B:466:LEU:HD12	1:B:466:LEU:O	1.99	0.63
1:A:385:TYR:OH	1:A:411:PRO:O	2.16	0.62
1:B:372:ILE:O	1:B:373:PRO:C	2.41	0.62
1:A:466:LEU:HD12	1:A:466:LEU:O	1.99	0.62
1:B:406:ASN:HD22	1:B:406:ASN:C	2.07	0.62
1:A:458:LEU:CD1	1:A:462:ILE:CD1	2.77	0.62
1:B:100:GLU:O	1:B:101:HIS:HB3	2.00	0.62
1:A:100:GLU:O	1:A:101:HIS:HB3	2.00	0.61
1:A:471:LEU:HD21	1:A:500:ASN:OD1	2.00	0.61
1:A:18:ARG:O	1:A:21:GLN:NE2	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:ASN:ND2	1:A:406:ASN:C	2.57	0.61
1:A:229:VAL:CG1	1:A:282:VAL:HG23	2.30	0.61
1:B:18:ARG:O	1:B:21:GLN:NE2	2.32	0.61
1:B:410:ALA:HB1	1:B:411:PRO:HD2	1.82	0.61
1:B:471:LEU:HD21	1:B:500:ASN:OD1	2.00	0.61
1:A:410:ALA:HB1	1:A:411:PRO:HD2	1.82	0.61
1:A:131:PHE:C	1:A:131:PHE:CD1	2.76	0.61
1:A:90:ILE:CD1	1:A:312:VAL:HG13	2.30	0.61
1:B:406:ASN:HD22	1:B:408:PHE:N	1.96	0.60
1:B:471:LEU:HD22	1:B:474:GLN:NE2	2.16	0.60
1:A:173:THR:HG22	1:A:175:LEU:HG	1.83	0.60
1:A:152:PHE:HB3	1:A:298:LEU:HD13	1.84	0.60
1:B:385:TYR:OH	1:B:411:PRO:O	2.16	0.60
1:A:73:VAL:O	1:A:74:HIS:HB2	2.01	0.60
1:B:152:PHE:HB3	1:B:298:LEU:HD13	1.84	0.60
1:B:384:ASN:ND2	1:B:386:GLN:H	2.00	0.60
1:A:110:VAL:HG21	1:A:317:LEU:HD11	1.84	0.60
1:B:245:SER:OG	1:B:248:ASP:HB2	2.01	0.60
1:B:406:ASN:ND2	1:B:406:ASN:C	2.58	0.60
1:B:453:GLU:HA	1:B:453:GLU:OE2	2.01	0.60
1:B:73:VAL:O	1:B:74:HIS:HB2	2.01	0.60
1:B:90:ILE:CD1	1:B:312:VAL:HG13	2.30	0.60
1:A:471:LEU:HD22	1:A:474:GLN:NE2	2.16	0.60
1:B:229:VAL:CG1	1:B:282:VAL:HG23	2.30	0.60
1:B:458:LEU:HD11	1:B:462:ILE:CD1	2.32	0.60
1:A:147:ASN:CG	2:A:507:HEM:HAC	2.27	0.60
1:A:245:SER:OG	1:A:248:ASP:HB2	2.01	0.59
1:A:360:THR:HG21	2:A:507:HEM:HMA3	1.83	0.59
1:A:209:ARG:HG2	1:A:274:PRO:HB3	1.83	0.59
1:A:458:LEU:HD11	1:A:462:ILE:CD1	2.32	0.59
1:A:453:GLU:OE2	1:A:453:GLU:HA	2.01	0.59
1:A:189:PRO:C	1:A:191:SER:H	2.10	0.59
1:B:189:PRO:C	1:B:191:SER:H	2.10	0.59
1:B:110:VAL:HG21	1:B:317:LEU:HD11	1.84	0.58
1:B:147:ASN:CG	2:B:507:HEM:HAC	2.27	0.58
1:A:110:VAL:HA	1:A:132:ALA:O	2.03	0.58
1:A:476:LYS:O	1:A:477:ALA:C	2.46	0.58
1:B:173:THR:HG22	1:B:175:LEU:HG	1.83	0.58
1:B:209:ARG:HG2	1:B:274:PRO:HB3	1.83	0.58
1:A:60:MET:HE1	1:A:63:PHE:HD2	1.69	0.58
1:A:384:ASN:ND2	1:A:386:GLN:H	2.00	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:MET:HE1	1:B:63:PHE:HD2	1.69	0.58
1:A:406:ASN:HD22	1:A:408:PHE:N	1.96	0.58
1:B:360:THR:HG21	2:B:507:HEM:HMA3	1.83	0.58
1:B:110:VAL:HA	1:B:132:ALA:O	2.03	0.57
1:B:356:ALA:O	1:B:360:THR:HG22	2.04	0.57
1:B:476:LYS:O	1:B:477:ALA:C	2.46	0.57
1:B:134:LYS:HE3	1:B:331:LEU:HD22	1.86	0.57
1:A:487:GLU:HG2	1:A:491:ARG:HD2	1.87	0.57
1:B:487:GLU:HG2	1:B:491:ARG:HD2	1.87	0.57
1:A:356:ALA:O	1:A:360:THR:HG22	2.04	0.57
1:A:173:THR:CG2	1:A:175:LEU:CD1	2.82	0.57
1:A:142:TRP:HB2	1:A:339:PRO:CD	2.35	0.56
1:A:64:ASP:HB3	1:B:360:THR:HB	1.88	0.56
1:B:173:THR:CG2	1:B:175:LEU:CD1	2.82	0.56
1:A:134:LYS:HE3	1:A:331:LEU:HD22	1.86	0.56
1:A:236:LYS:HG3	1:A:279:TYR:CE2	2.40	0.56
1:A:294:ASN:ND2	1:A:296:PHE:H	2.03	0.56
1:B:236:LYS:HG3	1:B:279:TYR:CE2	2.41	0.55
1:B:394:MET:HE3	1:B:394:MET:HA	1.88	0.55
1:B:100:GLU:O	1:B:100:GLU:CG	2.55	0.55
1:B:294:ASN:ND2	1:B:296:PHE:H	2.03	0.55
1:A:192:LEU:HD22	1:A:484:VAL:HG11	1.89	0.55
1:B:142:TRP:HB2	1:B:339:PRO:CD	2.35	0.55
1:A:446:TYR:HA	1:A:450:LEU:CD2	2.36	0.55
1:B:446:TYR:HA	1:B:450:LEU:CD2	2.36	0.55
1:A:360:THR:HB	1:B:64:ASP:HB3	1.87	0.55
1:A:394:MET:HE3	1:A:394:MET:HA	1.88	0.55
1:B:160:PHE:HB3	1:B:161:PRO:HD3	1.89	0.55
2:B:507:HEM:HMB1	2:B:507:HEM:HBB2	1.88	0.55
1:B:446:TYR:CE2	1:B:455:ARG:HD3	2.43	0.55
1:A:147:ASN:ND2	2:A:507:HEM:HAC	2.22	0.54
1:A:361:HIS:NE2	2:A:507:HEM:O2A	2.40	0.54
1:B:189:PRO:C	1:B:191:SER:N	2.63	0.54
1:A:189:PRO:C	1:A:191:SER:N	2.63	0.54
1:B:306:ASP:HB3	1:B:307:TYR:CE2	2.43	0.54
1:A:463:ALA:O	1:A:467:LYS:HB3	2.07	0.54
1:A:485:HIS:CD2	1:A:486:PRO:HD2	2.43	0.54
1:B:463:ALA:O	1:B:467:LYS:HB3	2.07	0.54
1:A:306:ASP:HB3	1:A:307:TYR:CE2	2.43	0.54
1:B:51:VAL:O	1:B:51:VAL:CG1	2.55	0.54
1:B:179:ASP:O	1:B:183:ASP:CB	2.52	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:LEU:HD22	1:B:484:VAL:HG11	1.89	0.54
1:B:361:HIS:NE2	2:B:507:HEM:O2A	2.40	0.54
1:B:127:ASP:C	1:B:128:PRO:O	2.48	0.54
1:B:77:GLY:O	1:B:324:TYR:OH	2.19	0.54
1:B:173:THR:HG22	1:B:175:LEU:CG	2.38	0.54
1:A:100:GLU:O	1:A:100:GLU:CG	2.55	0.54
1:A:170:ASN:HD22	1:A:173:THR:H	1.56	0.54
1:B:147:ASN:ND2	2:B:507:HEM:HAC	2.22	0.54
1:A:446:TYR:CE2	1:A:455:ARG:HD3	2.42	0.53
1:A:453:GLU:OE2	1:A:453:GLU:CA	2.55	0.53
1:A:173:THR:HG22	1:A:175:LEU:CG	2.38	0.53
1:B:212:ASP:OD1	1:B:237:THR:HG22	2.09	0.53
1:A:160:PHE:HB3	1:A:161:PRO:HD3	1.89	0.53
1:B:485:HIS:CD2	1:B:486:PRO:HD2	2.43	0.53
1:A:51:VAL:O	1:A:51:VAL:CG1	2.55	0.53
1:A:179:ASP:O	1:A:183:ASP:CB	2.52	0.53
1:A:95:LYS:HG2	1:A:222:VAL:O	2.09	0.53
1:A:155:ARG:NE	1:A:433:SER:O	2.35	0.53
1:A:282:VAL:HG12	1:A:310:ILE:CD1	2.39	0.53
1:B:95:LYS:HG2	1:B:222:VAL:O	2.09	0.52
1:B:282:VAL:HG12	1:B:310:ILE:CD1	2.39	0.52
1:A:212:ASP:OD1	1:A:237:THR:HG22	2.09	0.52
1:A:127:ASP:C	1:A:128:PRO:O	2.48	0.52
1:B:453:GLU:OE2	1:B:453:GLU:CA	2.55	0.52
1:A:400:ALA:O	1:A:401:PRO:C	2.52	0.52
1:B:148:ASN:H	1:B:148:ASN:ND2	1.98	0.52
1:A:157:ALA:HB2	2:A:507:HEM:HBB1	1.91	0.52
1:B:170:ASN:HD22	1:B:173:THR:H	1.56	0.52
1:A:172:GLN:NE2	1:B:321:PRO:O	2.43	0.52
1:A:36:ASP:HB3	1:B:430:ARG:HD3	1.92	0.52
1:A:50:LEU:HD12	1:B:428:VAL:HG13	1.92	0.52
1:A:170:ASN:HD22	1:A:172:GLN:N	2.07	0.52
1:A:321:PRO:O	1:B:172:GLN:NE2	2.43	0.52
1:A:428:VAL:HG13	1:B:50:LEU:HD12	1.92	0.52
1:B:400:ALA:O	1:B:401:PRO:C	2.52	0.52
1:B:85:GLU:HA	1:B:104:LYS:O	2.10	0.52
1:A:85:GLU:HA	1:A:104:LYS:O	2.10	0.51
1:B:386:GLN:O	1:B:387:ARG:NH1	2.43	0.51
1:A:155:ARG:HD2	1:A:433:SER:HB2	1.92	0.51
1:B:157:ALA:HB2	2:B:507:HEM:HBB1	1.91	0.51
1:A:430:ARG:HD3	1:B:36:ASP:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:ARG:HD2	1:B:433:SER:HB2	1.92	0.51
1:A:178:PRO:O	1:A:182:TRP:HB2	2.10	0.50
1:A:220:LYS:CE	1:A:420:HIS:CD2	2.90	0.50
1:B:178:PRO:O	1:B:182:TRP:HB2	2.10	0.50
1:A:82:GLY:HA3	1:A:316:VAL:O	2.12	0.50
1:A:386:GLN:O	1:A:387:ARG:NH1	2.43	0.50
1:A:179:ASP:O	1:A:183:ASP:N	2.42	0.50
1:B:82:GLY:HA3	1:B:316:VAL:O	2.12	0.50
1:B:435:ASN:C	1:B:436:ASP:O	2.55	0.50
1:B:179:ASP:O	1:B:183:ASP:N	2.42	0.50
1:B:155:ARG:NE	1:B:433:SER:O	2.35	0.50
1:B:439:VAL:O	1:B:440:THR:C	2.55	0.50
1:B:98:VAL:HG23	1:B:137:THR:CB	2.41	0.50
1:A:236:LYS:O	1:A:276:TRP:HA	2.12	0.49
1:B:170:ASN:HD22	1:B:172:GLN:N	2.07	0.49
1:B:345:SER:HB2	1:B:346:PRO:CD	2.43	0.49
1:B:276:TRP:HZ3	1:B:317:LEU:HD22	1.77	0.49
1:B:236:LYS:O	1:B:276:TRP:HA	2.12	0.49
1:B:334:ASP:O	1:B:337:ASN:HB2	2.13	0.49
1:A:236:LYS:HG3	1:A:279:TYR:HE2	1.78	0.49
1:B:129:ARG:H	1:B:148:ASN:ND2	2.10	0.49
1:B:238:ASP:OD1	1:B:275:SER:OG	2.26	0.49
1:B:223:ASN:ND2	1:B:225:ASP:N	2.59	0.49
1:A:51:VAL:O	1:A:51:VAL:HG13	2.13	0.49
1:A:439:VAL:O	1:A:440:THR:C	2.55	0.49
1:A:141:ASN:OD1	1:A:377:PRO:HA	2.13	0.49
1:A:173:THR:CG2	1:A:175:LEU:CG	2.91	0.49
1:A:334:ASP:O	1:A:337:ASN:HB2	2.13	0.49
1:B:141:ASN:OD1	1:B:377:PRO:HA	2.13	0.49
1:A:331:LEU:HD13	1:A:333:PHE:CZ	2.48	0.48
1:A:345:SER:HB2	1:A:346:PRO:CD	2.42	0.48
1:A:9:ASP:HB3	1:A:13:HIS:CE1	2.49	0.48
1:B:51:VAL:O	1:B:51:VAL:HG13	2.13	0.48
1:B:458:LEU:HD12	1:B:462:ILE:CD1	2.43	0.48
1:A:129:ARG:H	1:A:148:ASN:ND2	2.10	0.48
1:A:239:GLN:OE1	1:A:275:SER:N	2.38	0.48
1:A:276:TRP:HZ3	1:A:317:LEU:HD22	1.77	0.48
1:B:173:THR:CG2	1:B:175:LEU:CG	2.91	0.48
1:A:192:LEU:HD22	1:A:484:VAL:CG1	2.43	0.48
1:A:19:ALA:C	1:A:21:GLN:H	2.22	0.48
1:B:192:LEU:HD22	1:B:484:VAL:CG1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ILE:HG13	1:A:349:MET:HE2	1.96	0.48
1:B:239:GLN:OE1	1:B:275:SER:N	2.38	0.48
1:A:435:ASN:C	1:A:436:ASP:O	2.55	0.48
1:A:458:LEU:HD12	1:A:462:ILE:CD1	2.43	0.48
1:B:9:ASP:HB3	1:B:13:HIS:CE1	2.49	0.48
1:B:134:LYS:HE2	1:B:134:LYS:HB2	1.57	0.48
1:B:157:ALA:CB	2:B:507:HEM:HBB1	2.44	0.48
1:A:223:ASN:C	1:A:223:ASN:ND2	2.64	0.48
1:B:74:HIS:CE1	1:B:115:VAL:HG22	2.49	0.47
1:B:154:ILE:HG13	1:B:349:MET:HE2	1.96	0.47
1:A:77:GLY:O	1:A:324:TYR:OH	2.19	0.47
1:A:449:VAL:HG21	3:A:508:NDP:O4D	2.14	0.47
1:A:74:HIS:CE1	1:A:115:VAL:HG22	2.49	0.47
1:B:331:LEU:HD13	1:B:333:PHE:CZ	2.48	0.47
1:B:19:ALA:C	1:B:21:GLN:H	2.22	0.47
1:B:449:VAL:HG21	3:B:508:NDP:O4D	2.14	0.47
1:B:236:LYS:HG3	1:B:279:TYR:HE2	1.78	0.47
1:A:147:ASN:HB2	2:A:507:HEM:HAC	1.97	0.47
1:A:157:ALA:CB	2:A:507:HEM:HBB1	2.44	0.47
1:B:173:THR:CG2	1:B:175:LEU:HG	2.44	0.47
1:A:98:VAL:HG23	1:A:137:THR:CB	2.41	0.47
1:A:391:MET:HE3	1:A:393:MET:CE	2.45	0.47
1:A:223:ASN:ND2	1:A:225:ASP:N	2.59	0.47
1:A:238:ASP:OD1	1:A:275:SER:OG	2.26	0.47
1:B:484:VAL:HG22	1:B:488:TYR:HD1	1.80	0.47
1:A:100:GLU:O	1:A:100:GLU:HG3	2.15	0.46
1:B:220:LYS:CE	1:B:420:HIS:CD2	2.90	0.46
1:B:415:PRO:C	1:B:417:ALA:H	2.23	0.46
1:A:239:GLN:OE1	1:A:274:PRO:HA	2.15	0.46
1:A:291:PHE:CE1	1:A:293:PHE:HB2	2.51	0.46
1:B:6:PRO:O	1:B:7:ALA:C	2.58	0.46
1:A:134:LYS:HB2	1:A:134:LYS:HE2	1.57	0.46
1:A:159:LEU:HD11	1:A:188:ARG:CZ	2.46	0.46
1:B:357:TYR:N	1:B:358:PRO:HD2	2.29	0.46
1:B:374:VAL:O	1:B:374:VAL:CG2	2.63	0.46
1:A:90:ILE:CD1	1:A:312:VAL:CG1	2.94	0.46
1:B:22:LYS:HD3	1:B:22:LYS:HA	1.77	0.46
1:B:90:ILE:CD1	1:B:312:VAL:CG1	2.94	0.46
1:B:100:GLU:O	1:B:100:GLU:HG3	2.15	0.46
1:B:170:ASN:HA	1:B:171:PRO:HD3	1.87	0.46
1:B:391:MET:HE3	1:B:393:MET:CE	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:LYS:HE2	4:B:522:HOH:O	2.15	0.46
1:B:135:PHE:CD1	1:B:142:TRP:CE3	3.04	0.46
1:B:239:GLN:OE1	1:B:274:PRO:HA	2.15	0.46
1:A:89:ASP:OD1	1:A:89:ASP:C	2.56	0.46
1:A:15:LYS:HE2	4:A:514:HOH:O	2.15	0.46
1:A:65:ARG:HH12	1:B:359:ASP:CG	2.24	0.46
1:A:90:ILE:HD13	1:A:312:VAL:CG1	2.38	0.46
1:A:348:LYS:HE2	4:A:551:HOH:O	2.13	0.46
1:A:359:ASP:CG	1:B:65:ARG:HH12	2.24	0.46
1:B:149:THR:OG1	1:B:150:PRO:CD	2.64	0.46
1:A:357:TYR:N	1:A:358:PRO:HD2	2.29	0.46
1:B:5:ASP:O	1:B:8:SER:HB2	2.16	0.46
1:B:90:ILE:HD13	1:B:312:VAL:CG1	2.38	0.46
1:B:276:TRP:CZ3	1:B:317:LEU:HD22	2.51	0.46
1:A:5:ASP:O	1:A:8:SER:HB2	2.16	0.46
1:A:276:TRP:CZ3	1:A:317:LEU:HD22	2.51	0.46
1:A:371:GLN:HE22	1:A:393:MET:N	2.13	0.46
1:B:81:PHE:CD1	1:B:81:PHE:N	2.84	0.46
1:B:147:ASN:HB2	2:B:507:HEM:HAC	1.97	0.46
1:B:159:LEU:HD11	1:B:188:ARG:CZ	2.46	0.46
1:B:177:ASP:HA	1:B:178:PRO:HD3	1.85	0.46
1:A:50:LEU:HA	1:A:50:LEU:HD23	1.63	0.45
1:A:173:THR:CG2	1:A:175:LEU:HG	2.44	0.45
1:A:357:TYR:H	1:A:358:PRO:HD2	1.81	0.45
1:B:263:ASP:O	1:B:264:LEU:C	2.59	0.45
1:A:135:PHE:CD1	1:A:142:TRP:CE3	3.04	0.45
1:A:188:ARG:O	1:A:191:SER:HB3	2.16	0.45
1:A:484:VAL:HG22	1:A:488:TYR:HD1	1.80	0.45
1:B:357:TYR:H	1:B:358:PRO:HD2	1.82	0.45
1:A:142:TRP:HA	1:A:337:ASN:O	2.16	0.45
1:B:188:ARG:O	1:B:191:SER:HB3	2.16	0.45
1:B:487:GLU:HG2	1:B:491:ARG:CD	2.46	0.45
1:A:81:PHE:CD1	1:A:81:PHE:N	2.84	0.45
1:A:335:PRO:O	1:A:338:MET:HE3	2.17	0.45
1:A:415:PRO:C	1:A:417:ALA:H	2.23	0.45
1:B:142:TRP:HA	1:B:337:ASN:O	2.16	0.45
1:A:6:PRO:O	1:A:7:ALA:C	2.58	0.45
1:A:487:GLU:HG2	1:A:491:ARG:CD	2.46	0.45
1:B:335:PRO:O	1:B:338:MET:HE3	2.16	0.45
1:B:429:GLN:HE21	1:B:429:GLN:HB2	1.60	0.45
1:A:453:GLU:O	1:A:456:LYS:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:VAL:HG21	1:B:137:THR:HG22	1.99	0.45
1:B:294:ASN:C	1:B:294:ASN:HD22	2.25	0.45
1:B:331:LEU:HD13	1:B:333:PHE:CE2	2.52	0.45
1:A:98:VAL:HG21	1:A:137:THR:HG22	1.99	0.45
1:A:228:ALA:HB2	1:A:420:HIS:CE1	2.52	0.45
1:A:294:ASN:C	1:A:294:ASN:HD22	2.25	0.45
1:A:97:LYS:O	1:A:100:GLU:HB3	2.17	0.45
1:B:282:VAL:HG12	1:B:310:ILE:HD12	1.99	0.45
1:B:371:GLN:HE22	1:B:393:MET:N	2.13	0.44
1:B:453:GLU:O	1:B:456:LYS:HG2	2.17	0.44
1:A:353:ARG:O	1:A:354:LEU:C	2.59	0.44
1:A:444:THR:O	1:A:445:PHE:C	2.60	0.44
1:B:291:PHE:CE1	1:B:293:PHE:HB2	2.51	0.44
1:A:484:VAL:O	1:A:484:VAL:HG23	2.18	0.44
1:B:97:LYS:O	1:B:100:GLU:HB3	2.17	0.44
1:B:430:ARG:HH11	1:B:430:ARG:HD2	1.58	0.44
1:A:209:ARG:HH11	1:A:209:ARG:HD3	1.63	0.44
1:A:471:LEU:O	1:A:472:PHE:C	2.61	0.44
1:B:402:ASN:C	1:B:402:ASN:HD22	2.25	0.44
1:A:79:GLY:O	1:A:80:ALA:CB	2.58	0.44
1:A:236:LYS:HB3	1:A:236:LYS:HE2	1.46	0.44
1:A:331:LEU:HD13	1:A:333:PHE:CE2	2.52	0.44
1:A:381:ARG:HH11	1:A:381:ARG:HD3	1.59	0.44
1:B:147:ASN:CB	2:B:507:HEM:HAC	2.48	0.44
1:B:449:VAL:HG21	3:B:508:NDP:C4D	2.48	0.44
1:B:444:THR:O	1:B:445:PHE:C	2.60	0.44
1:A:282:VAL:HG12	1:A:310:ILE:HD12	1.99	0.43
1:A:354:LEU:HD12	1:A:354:LEU:HA	1.63	0.43
1:B:63:PHE:C	1:B:65:ARG:H	2.26	0.43
1:B:145:VAL:HG22	1:B:333:PHE:HB3	2.00	0.43
1:A:145:VAL:HG22	1:A:333:PHE:HB3	2.00	0.43
1:B:228:ALA:HB2	1:B:420:HIS:CE1	2.52	0.43
1:B:484:VAL:O	1:B:484:VAL:HG23	2.18	0.43
1:A:449:VAL:HG21	3:A:508:NDP:C4D	2.47	0.43
1:A:108:ILE:O	1:A:108:ILE:HG13	2.15	0.43
1:A:84:PHE:O	1:A:105:ARG:HA	2.19	0.43
1:B:435:ASN:O	1:B:436:ASP:C	2.61	0.43
1:A:147:ASN:CB	2:A:507:HEM:HAC	2.48	0.43
1:A:402:ASN:C	1:A:402:ASN:HD22	2.25	0.43
1:B:50:LEU:HA	1:B:50:LEU:HD23	1.63	0.43
1:B:236:LYS:HE2	1:B:236:LYS:HB3	1.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:THR:HG21	2:B:507:HEM:CMA	2.47	0.43
1:A:92:ARG:H	1:A:92:ARG:HG3	1.62	0.43
1:A:134:LYS:HG3	1:A:143:ASP:OD2	2.19	0.43
1:A:157:ALA:CB	2:A:507:HEM:CBB	2.97	0.43
1:A:293:PHE:O	1:A:295:PRO:CD	2.67	0.43
1:B:134:LYS:HG3	1:B:143:ASP:OD2	2.18	0.43
1:B:293:PHE:O	1:B:295:PRO:CD	2.67	0.43
1:B:353:ARG:O	1:B:354:LEU:C	2.59	0.43
1:A:360:THR:HG21	2:A:507:HEM:CMA	2.47	0.43
1:B:84:PHE:O	1:B:105:ARG:HA	2.19	0.43
1:B:445:PHE:O	1:B:449:VAL:HB	2.19	0.43
1:A:22:LYS:HD3	1:A:22:LYS:HA	1.77	0.42
1:B:108:ILE:O	1:B:108:ILE:HG13	2.15	0.42
1:A:263:ASP:O	1:A:264:LEU:C	2.59	0.42
1:B:110:VAL:CG2	1:B:317:LEU:HD11	2.48	0.42
1:A:63:PHE:C	1:A:65:ARG:H	2.26	0.42
1:A:149:THR:OG1	1:A:150:PRO:CD	2.64	0.42
1:A:343:GLU:HA	1:A:344:PRO:HD3	1.96	0.42
1:A:374:VAL:O	1:A:374:VAL:CG2	2.63	0.42
1:B:157:ALA:CB	2:B:507:HEM:CBB	2.97	0.42
1:A:152:PHE:CB	1:A:298:LEU:HD13	2.49	0.42
1:B:471:LEU:O	1:B:472:PHE:C	2.61	0.42
2:B:507:HEM:HBB2	2:B:507:HEM:CMB	2.50	0.42
1:A:189:PRO:O	1:A:192:LEU:HB2	2.20	0.42
1:A:298:LEU:HD12	1:A:349:MET:HG3	2.02	0.42
1:A:337:ASN:HD22	1:A:337:ASN:HA	1.67	0.42
1:B:90:ILE:O	1:B:93:TYR:HB2	2.20	0.42
3:B:508:NDP:C6N	3:B:508:NDP:H4B	2.50	0.42
1:A:347:ASP:HB3	1:A:350:LEU:HB3	2.02	0.42
1:B:349:MET:O	1:B:353:ARG:HG3	2.20	0.42
1:A:177:ASP:HA	1:A:178:PRO:HD3	1.85	0.42
1:A:435:ASN:O	1:A:436:ASP:C	2.61	0.42
1:A:120:GLY:H	1:B:120:GLY:H	1.68	0.42
1:A:410:ALA:HB1	1:A:411:PRO:CD	2.50	0.42
1:B:3:ASN:HB3	1:B:4:ARG:H	1.67	0.42
1:A:118:GLU:H	1:A:118:GLU:HG2	1.04	0.42
1:A:445:PHE:O	1:A:449:VAL:HB	2.19	0.42
3:A:508:NDP:C6N	3:A:508:NDP:H4B	2.50	0.41
1:B:189:PRO:O	1:B:192:LEU:HB2	2.20	0.41
1:A:90:ILE:O	1:A:93:TYR:HB2	2.20	0.41
1:A:284:THR:CG2	1:A:286:SER:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:HIS:HA	1:A:486:PRO:HD2	1.83	0.41
1:B:89:ASP:C	1:B:89:ASP:OD1	2.56	0.41
1:A:135:PHE:CE1	1:A:142:TRP:CZ3	3.09	0.41
1:B:298:LEU:HD12	1:B:349:MET:HG3	2.02	0.41
1:B:421:ARG:HE	1:B:421:ARG:HB3	1.60	0.41
1:A:98:VAL:HG23	1:A:137:THR:HG21	2.01	0.41
1:A:110:VAL:CG2	1:A:317:LEU:HD11	2.48	0.41
1:A:349:MET:O	1:A:353:ARG:HG3	2.20	0.41
1:B:14:TRP:CZ3	1:B:18:ARG:HD2	2.56	0.41
1:B:293:PHE:O	1:B:295:PRO:HD3	2.20	0.41
1:B:307:TYR:N	1:B:307:TYR:CD2	2.88	0.41
1:A:14:TRP:CZ3	1:A:18:ARG:HD2	2.56	0.41
1:A:67:ARG:NH2	1:B:168:LYS:HE3	2.35	0.41
1:B:404:TYR:HA	1:B:405:PRO:HA	1.93	0.41
1:A:371:GLN:NE2	1:A:393:MET:HB2	2.33	0.41
1:B:118:GLU:H	1:B:118:GLU:HG2	1.04	0.41
1:B:235:TYR:HA	1:B:277:THR:O	2.21	0.41
1:A:209:ARG:HB2	4:A:533:HOH:O	2.21	0.41
1:A:293:PHE:O	1:A:295:PRO:HD3	2.20	0.41
1:B:135:PHE:CE1	1:B:142:TRP:CZ3	3.09	0.41
1:A:118:GLU:HG3	1:B:120:GLY:CA	2.51	0.41
1:A:168:LYS:HE3	1:B:67:ARG:NH2	2.35	0.41
1:A:195:VAL:O	1:A:199:PHE:HD1	2.04	0.41
1:A:307:TYR:N	1:A:307:TYR:CD2	2.88	0.41
1:B:273:TYR:HA	1:B:274:PRO:HD2	1.95	0.41
1:A:5:ASP:HA	1:A:6:PRO:HD3	1.88	0.41
1:A:415:PRO:C	1:A:417:ALA:N	2.79	0.41
1:B:258:ASP:O	1:B:261:LEU:N	2.53	0.41
1:B:223:ASN:C	1:B:223:ASN:ND2	2.64	0.40
1:B:347:ASP:HB3	1:B:350:LEU:HB3	2.02	0.40
1:B:358:PRO:O	1:B:362:ARG:HD2	2.22	0.40
1:A:64:ASP:OD1	1:B:359:ASP:OD2	2.39	0.40
1:A:92:ARG:O	1:A:223:ASN:CB	2.68	0.40
1:A:235:TYR:HA	1:A:277:THR:O	2.21	0.40
1:A:294:ASN:ND2	1:A:294:ASN:C	2.78	0.40
1:B:114:THR:HG22	1:B:129:ARG:HD2	2.04	0.40
1:A:120:GLY:CA	1:B:118:GLU:HG3	2.51	0.40
1:A:154:ILE:HG13	1:A:349:MET:CE	2.51	0.40
1:A:170:ASN:HA	1:A:171:PRO:HD3	1.87	0.40
1:B:294:ASN:ND2	1:B:294:ASN:C	2.78	0.40
1:B:410:ALA:HB1	1:B:411:PRO:CD	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:THR:HG22	1:A:129:ARG:HD2	2.03	0.40
1:B:59:GLU:HB2	4:B:524:HOH:O	2.21	0.40
1:A:294:ASN:HA	1:A:295:PRO:HD2	1.77	0.40
1:A:359:ASP:OD2	1:B:64:ASP:OD1	2.39	0.40

All (4) 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:419:GLU:OE2	1:B:430:ARG:NH1[6_556]	1.98	0.22
1:A:430:ARG:NH1	1:B:419:GLU:OE2[6_556]	1.98	0.22
1:B:10:GLN:NE2	4:B:551:HOH:O[6_556]	2.13	0.07
1:A:10:GLN:NE2	4:A:543:HOH:O[6_556]	2.14	0.06

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	496/506 (98%)	434 (88%)	52 (10%)	10 (2%)	6	10
1	B	496/506 (98%)	434 (88%)	52 (10%)	10 (2%)	6	10
All	All	992/1012 (98%)	868 (88%)	104 (10%)	20 (2%)	6	10

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	267	ALA
1	B	267	ALA
1	A	54	VAL
1	A	440	THR
1	B	54	VAL
1	B	440	THR

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Mol	Chain	Res	Type
1	A	451	ASN
1	B	451	ASN
1	A	101	HIS
1	A	268	ILE
1	A	373	PRO
1	B	101	HIS
1	B	268	ILE
1	B	373	PRO
1	A	22	LYS
1	A	394	MET
1	B	22	LYS
1	B	394	MET
1	A	128	PRO
1	B	128	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	430/437 (98%)	345 (80%)	85 (20%)	1	2
1	B	430/437 (98%)	345 (80%)	85 (20%)	1	2
All	All	860/874 (98%)	690 (80%)	170 (20%)	1	2

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	18	ARG
1	A	21	GLN
1	A	37	LYS
1	A	40	SER
1	A	43	VAL
1	A	48	PRO
1	A	51	VAL
1	A	55	VAL

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Mol	Chain	Res	Type
1	A	57	THR
1	A	73	VAL
1	A	76	LYS
1	A	89	ASP
1	A	90	ILE
1	A	91	THR
1	A	92	ARG
1	A	95	LYS
1	A	98	VAL
1	A	102	ILE
1	A	118	GLU
1	A	124	THR
1	A	125	VAL
1	A	129	ARG
1	A	137	THR
1	A	138	GLU
1	A	148	ASN
1	A	150	PRO
1	A	154	ILE
1	A	155	ARG
1	A	158	LEU
1	A	159	LEU
1	A	176	LYS
1	A	195	VAL
1	A	220	LYS
1	A	223	ASN
1	A	227	GLU
1	A	229	VAL
1	A	235	TYR
1	A	236	LYS
1	A	239	GLN
1	A	242	LYS
1	A	246	VAL
1	A	247	GLU
1	A	255	GLU
1	A	261	LEU
1	A	263	ASP
1	A	264	LEU
1	A	282	VAL
1	A	284	THR
1	A	287	GLU
1	A	290	ILE

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Mol	Chain	Res	Type
1	A	298	LEU
1	A	315	LEU
1	A	317	LEU
1	A	331	LEU
1	A	335	PRO
1	A	337	ASN
1	A	339	PRO
1	A	354	LEU
1	A	365	LEU
1	A	372	ILE
1	A	384	ASN
1	A	386	GLN
1	A	394	MET
1	A	402	ASN
1	A	405	PRO
1	A	406	ASN
1	A	407	SER
1	A	414	GLN
1	A	415	PRO
1	A	421	ARG
1	A	433	SER
1	A	439	VAL
1	A	443	ARG
1	A	444	THR
1	A	447	LEU
1	A	448	LYS
1	A	450	LEU
1	A	452	GLU
1	A	453	GLU
1	A	458	LEU
1	A	471	LEU
1	A	484	VAL
1	A	498	LYS
1	A	500	ASN
1	B	4	ARG
1	B	18	ARG
1	B	21	GLN
1	B	37	LYS
1	B	40	SER
1	B	43	VAL
1	B	48	PRO
1	B	51	VAL

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Mol	Chain	Res	Type
1	B	55	VAL
1	B	57	THR
1	B	73	VAL
1	B	76	LYS
1	B	89	ASP
1	B	90	ILE
1	B	91	THR
1	B	92	ARG
1	B	95	LYS
1	B	98	VAL
1	B	102	ILE
1	B	118	GLU
1	B	124	THR
1	B	125	VAL
1	B	129	ARG
1	B	137	THR
1	B	138	GLU
1	B	148	ASN
1	B	150	PRO
1	B	154	ILE
1	B	155	ARG
1	B	158	LEU
1	B	159	LEU
1	B	176	LYS
1	B	195	VAL
1	B	220	LYS
1	B	223	ASN
1	B	227	GLU
1	B	229	VAL
1	B	235	TYR
1	B	236	LYS
1	B	239	GLN
1	B	242	LYS
1	B	246	VAL
1	B	247	GLU
1	B	255	GLU
1	B	261	LEU
1	B	263	ASP
1	B	264	LEU
1	B	282	VAL
1	B	284	THR
1	B	287	GLU

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Mol	Chain	Res	Type
1	B	290	ILE
1	B	298	LEU
1	B	315	LEU
1	B	317	LEU
1	B	331	LEU
1	B	335	PRO
1	B	337	ASN
1	B	339	PRO
1	B	354	LEU
1	B	365	LEU
1	B	372	ILE
1	B	384	ASN
1	B	386	GLN
1	B	394	MET
1	B	402	ASN
1	B	405	PRO
1	B	406	ASN
1	B	407	SER
1	B	414	GLN
1	B	415	PRO
1	B	421	ARG
1	B	433	SER
1	B	439	VAL
1	B	443	ARG
1	B	444	THR
1	B	447	LEU
1	B	448	LYS
1	B	450	LEU
1	B	452	GLU
1	B	453	GLU
1	B	458	LEU
1	B	471	LEU
1	B	484	VAL
1	B	498	LYS
1	B	500	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	10	GLN
1	A	13	HIS

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Mol	Chain	Res	Type
1	A	17	GLN
1	A	21	GLN
1	A	39	ASN
1	A	101	HIS
1	A	148	ASN
1	A	167	GLN
1	A	170	ASN
1	A	172	GLN
1	A	223	ASN
1	A	234	HIS
1	A	243	ASN
1	A	272	ASN
1	A	281	GLN
1	A	294	ASN
1	A	330	GLN
1	A	337	ASN
1	A	371	GLN
1	A	384	ASN
1	A	396	ASN
1	A	397	GLN
1	A	402	ASN
1	A	406	ASN
1	A	414	GLN
1	A	420	HIS
1	A	429	GLN
1	A	438	ASN
1	A	474	GLN
1	A	485	HIS
1	B	3	ASN
1	B	10	GLN
1	B	13	HIS
1	B	17	GLN
1	B	21	GLN
1	B	39	ASN
1	B	101	HIS
1	B	148	ASN
1	B	167	GLN
1	B	170	ASN
1	B	172	GLN
1	B	223	ASN
1	B	234	HIS
1	B	243	ASN

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Mol	Chain	Res	Type
1	B	272	ASN
1	B	281	GLN
1	B	294	ASN
1	B	330	GLN
1	B	337	ASN
1	B	371	GLN
1	B	384	ASN
1	B	396	ASN
1	B	397	GLN
1	B	402	ASN
1	B	406	ASN
1	B	414	GLN
1	B	420	HIS
1	B	429	GLN
1	B	438	ASN
1	B	474	GLN
1	B	485	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
3	NDP	B	508	-	51,52,52	1.76	10 (19%)	71,80,80	1.80	10 (14%)
2	HEM	A	507	1	50,50,50	1.21	6 (12%)	67,82,82	1.27	8 (11%)
2	HEM	B	507	1	50,50,50	1.22	6 (12%)	67,82,82	1.26	8 (11%)
3	NDP	A	508	-	51,52,52	1.76	10 (19%)	71,80,80	1.81	10 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NDP	B	508	-	-	6/34/77/77	0/5/5/5
2	HEM	A	507	1	-	4/14/54/54	-
2	HEM	B	507	1	-	4/14/54/54	-
3	NDP	A	508	-	-	6/34/77/77	0/5/5/5

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	508	NDP	PN-O3	-5.97	1.53	1.59
3	A	508	NDP	PN-O3	-5.94	1.53	1.59
3	A	508	NDP	C4N-C3N	-4.65	1.41	1.50
3	B	508	NDP	C4N-C3N	-4.63	1.41	1.50
3	A	508	NDP	P2B-O2B	4.41	1.67	1.59
3	B	508	NDP	P2B-O2B	4.35	1.67	1.59
3	B	508	NDP	C4N-C5N	-4.02	1.38	1.49
3	A	508	NDP	C4N-C5N	-4.01	1.38	1.49
3	A	508	NDP	C7N-C3N	3.52	1.56	1.48
3	B	508	NDP	C7N-C3N	3.50	1.56	1.48
3	A	508	NDP	O4B-C1B	3.08	1.49	1.42
3	B	508	NDP	O4B-C1B	3.05	1.49	1.42
2	B	507	HEM	FE-NB	2.79	2.03	1.94
2	A	507	HEM	FE-NB	2.78	2.03	1.94
2	B	507	HEM	CAC-C3C	2.49	1.54	1.47
2	B	507	HEM	C2A-C3A	-2.48	1.32	1.38
2	A	507	HEM	C2A-C3A	-2.47	1.32	1.38
2	A	507	HEM	CAC-C3C	2.45	1.53	1.47
2	B	507	HEM	CMA-C3A	2.39	1.55	1.50
2	A	507	HEM	CAB-C3B	2.39	1.53	1.47
2	B	507	HEM	CAB-C3B	2.39	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	507	HEM	CMA-C3A	2.37	1.55	1.50
3	B	508	NDP	C2A-N1A	2.19	1.37	1.33
3	A	508	NDP	C2A-N1A	2.18	1.37	1.33
3	B	508	NDP	PA-O2A	-2.14	1.45	1.55
3	A	508	NDP	PA-O2A	-2.13	1.45	1.55
3	A	508	NDP	PN-O2N	-2.07	1.45	1.55
3	B	508	NDP	PN-O2N	-2.06	1.45	1.55
3	B	508	NDP	PN-O5D	2.04	1.67	1.59
3	A	508	NDP	PN-O5D	2.02	1.67	1.59
2	B	507	HEM	O2D-CGD	-2.01	1.24	1.30
2	A	507	HEM	C3B-C2B	-2.00	1.33	1.37

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	508	NDP	C2B-C1B-N9A	7.92	126.79	113.75
3	B	508	NDP	C2B-C1B-N9A	7.91	126.77	113.75
3	A	508	NDP	O2X-P2B-O2B	5.72	128.15	105.85
3	B	508	NDP	O2X-P2B-O2B	5.72	128.15	105.85
3	B	508	NDP	O2N-PN-O3	4.59	119.67	107.27
3	A	508	NDP	O2N-PN-O3	4.57	119.62	107.27
3	A	508	NDP	O3X-P2B-O2B	-4.24	89.31	105.85
3	B	508	NDP	O3X-P2B-O2B	-4.24	89.33	105.85
2	B	507	HEM	O2D-CGD-O1D	3.76	133.01	123.33
2	A	507	HEM	O2D-CGD-O1D	3.76	133.00	123.33
3	A	508	NDP	O4B-C1B-C2B	-3.19	101.10	106.59
3	B	508	NDP	O4B-C1B-C2B	-3.19	101.10	106.59
3	A	508	NDP	C6N-N1N-C2N	3.00	122.53	119.32
3	B	508	NDP	C6N-N1N-C2N	2.92	122.45	119.32
2	B	507	HEM	O1D-CGD-CBD	-2.86	114.01	123.09
2	A	507	HEM	O1D-CGD-CBD	-2.86	114.02	123.09
3	A	508	NDP	O4B-C1B-N9A	-2.81	102.69	108.09
3	B	508	NDP	O4B-C1B-N9A	-2.78	102.75	108.09
2	A	507	HEM	CHC-C1C-NC	-2.69	121.52	124.45
2	B	507	HEM	CHC-C1C-NC	-2.66	121.56	124.45
2	B	507	HEM	O1A-CGA-CBA	-2.65	114.70	123.09
2	A	507	HEM	O1A-CGA-CBA	-2.62	114.77	123.09
2	B	507	HEM	CAA-C2A-C1A	-2.60	119.87	124.94
2	A	507	HEM	CAA-C2A-C1A	-2.58	119.90	124.94
3	B	508	NDP	O2A-PA-O3	2.55	114.17	107.27
3	A	508	NDP	O2A-PA-O3	2.55	114.16	107.27
3	A	508	NDP	C3N-C2N-N1N	-2.55	119.47	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	508	NDP	C3N-C2N-N1N	-2.48	119.56	123.20
2	A	507	HEM	CHA-C1A-NA	2.35	128.13	123.86
2	B	507	HEM	CHA-C1A-NA	2.32	128.07	123.86
2	B	507	HEM	CAA-C2A-C3A	2.18	131.96	127.07
2	A	507	HEM	CAA-C2A-C3A	2.17	131.94	127.07
3	A	508	NDP	C1D-N1N-C2N	-2.11	117.66	121.14
3	B	508	NDP	C1D-N1N-C2N	-2.08	117.71	121.14
2	A	507	HEM	C1A-CHA-C4D	-2.07	121.38	126.25
2	B	507	HEM	C1A-CHA-C4D	-2.04	121.45	126.25

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	507	HEM	C2C-C3C-CAC-CBC
2	B	507	HEM	C2C-C3C-CAC-CBC
2	A	507	HEM	C4C-C3C-CAC-CBC
2	B	507	HEM	C4C-C3C-CAC-CBC
3	A	508	NDP	O4B-C4B-C5B-O5B
3	B	508	NDP	O4B-C4B-C5B-O5B
3	A	508	NDP	PN-O3-PA-O2A
3	B	508	NDP	PN-O3-PA-O2A
3	A	508	NDP	O4D-C1D-N1N-C6N
3	B	508	NDP	O4D-C1D-N1N-C6N
3	A	508	NDP	PN-O3-PA-O1A
3	B	508	NDP	PN-O3-PA-O1A
2	B	507	HEM	CAD-CBD-CGD-O2D
2	A	507	HEM	CAD-CBD-CGD-O2D
2	B	507	HEM	CAD-CBD-CGD-O1D
2	A	507	HEM	CAD-CBD-CGD-O1D
3	A	508	NDP	C2B-C1B-N9A-C4A
3	B	508	NDP	C2B-C1B-N9A-C4A
3	A	508	NDP	C2B-C1B-N9A-C8A
3	B	508	NDP	C2B-C1B-N9A-C8A

There are no ring outliers.

4 monomers are involved in 29 short contacts:

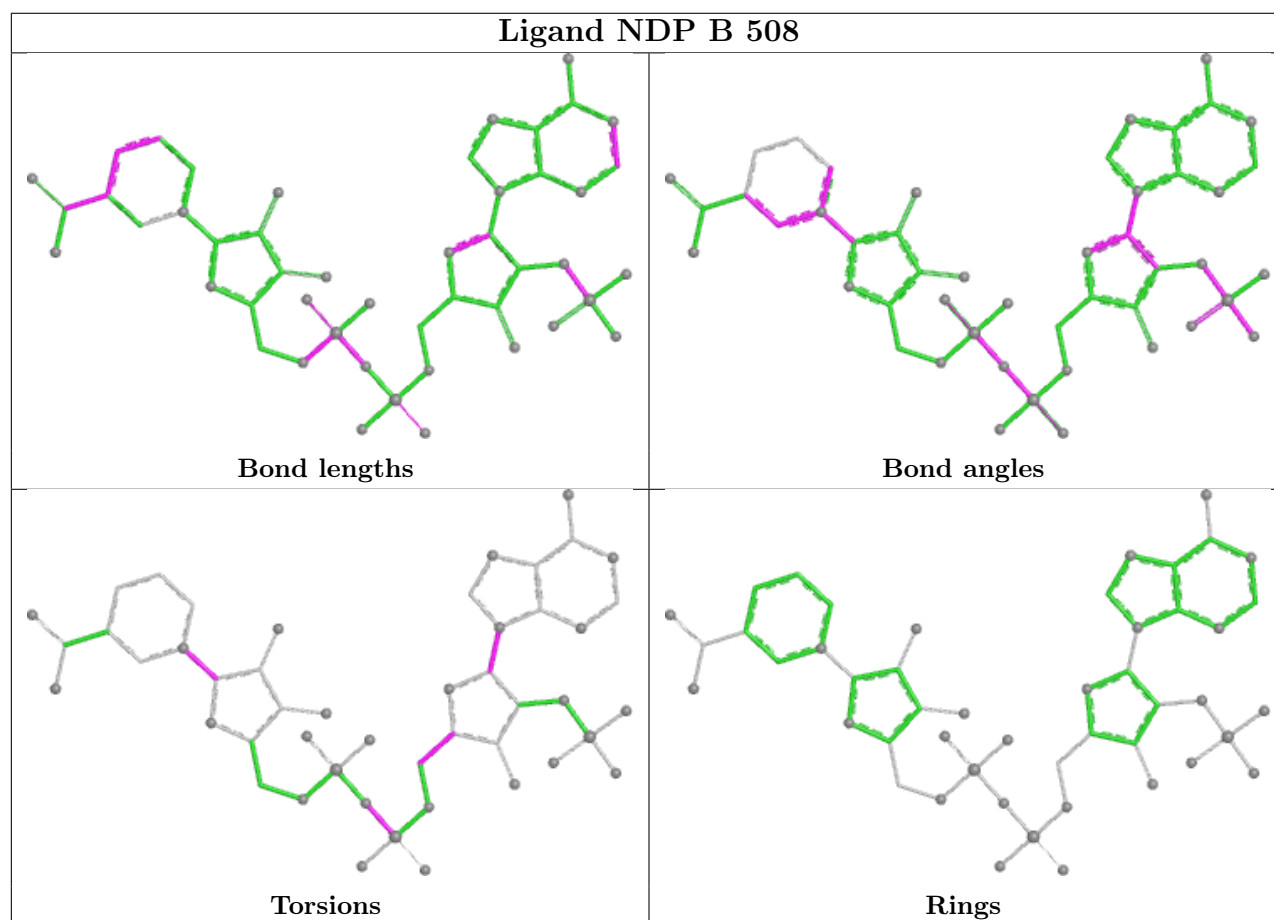
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	508	NDP	3	0
2	A	507	HEM	11	0

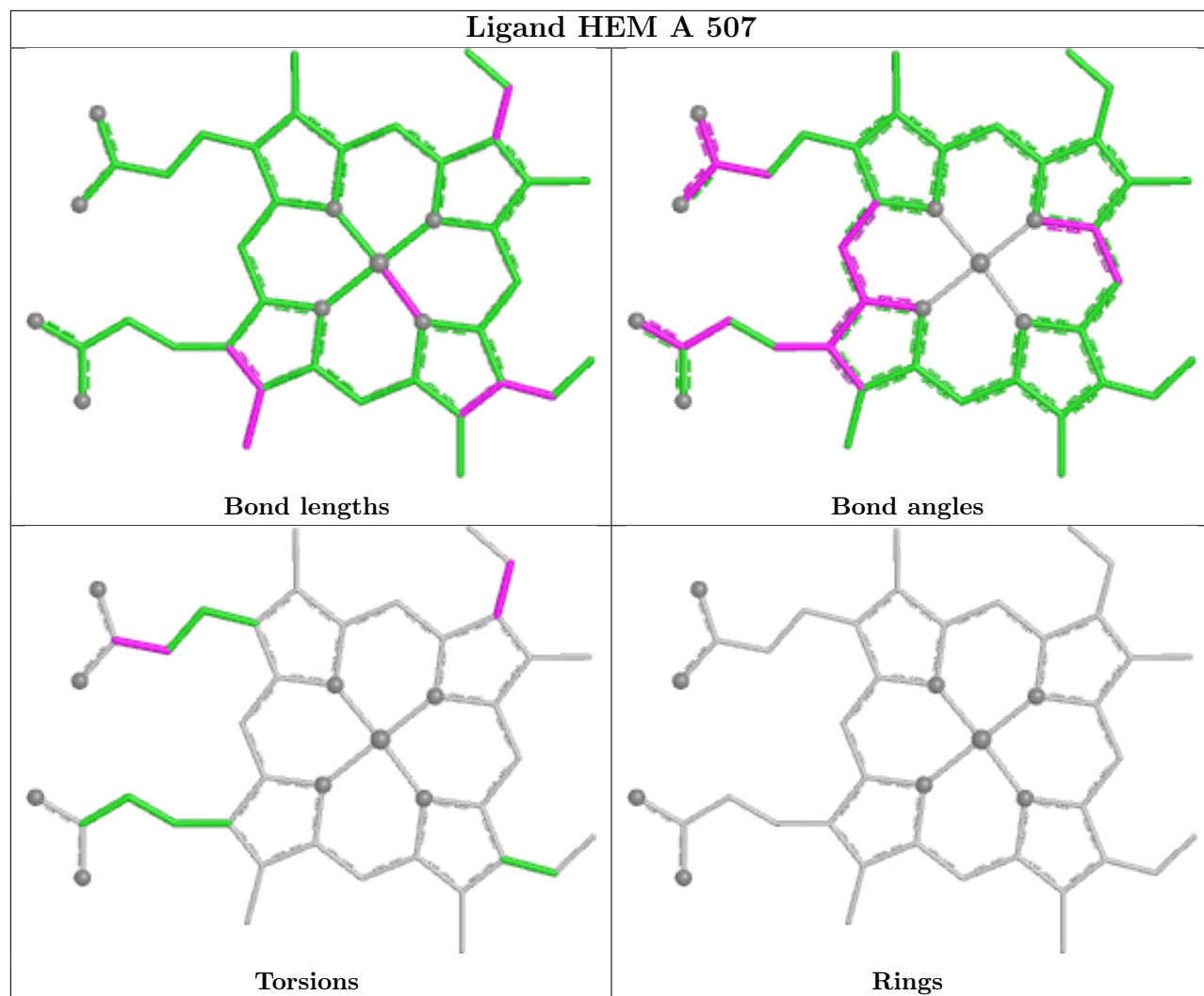
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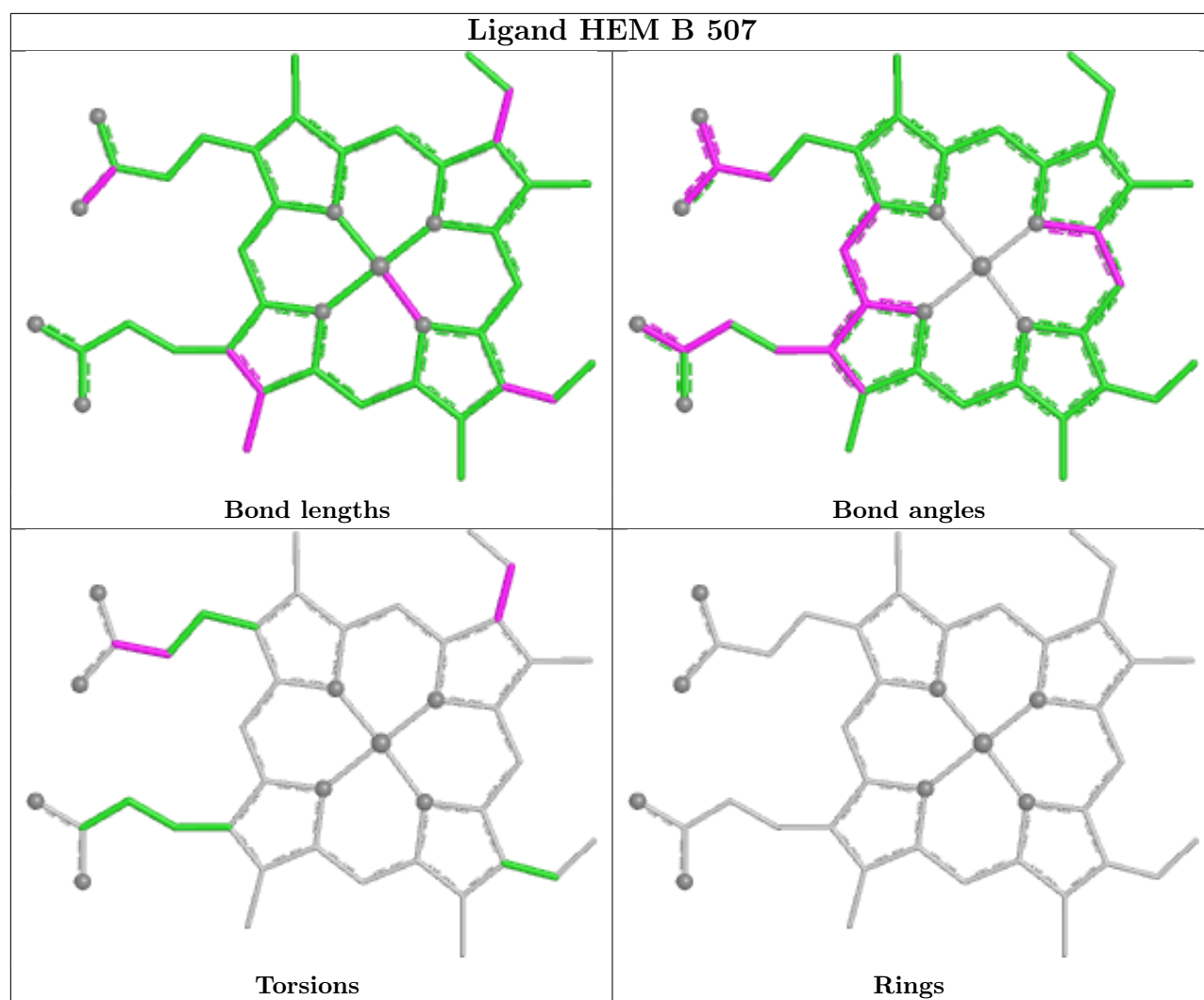
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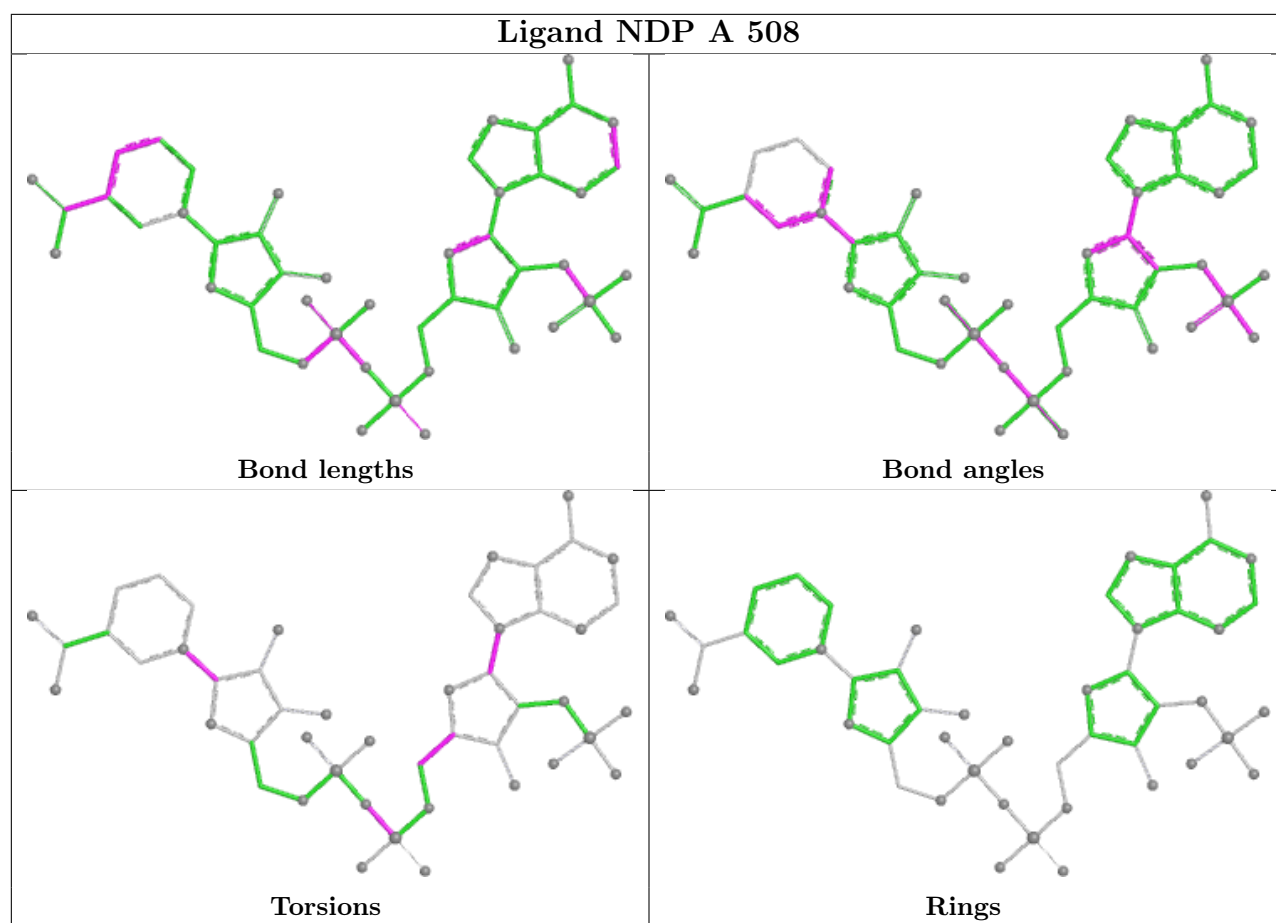
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	507	HEM	12	0
3	A	508	NDP	3	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.