



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 08:36 am BST

PDB ID : 8CAT
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

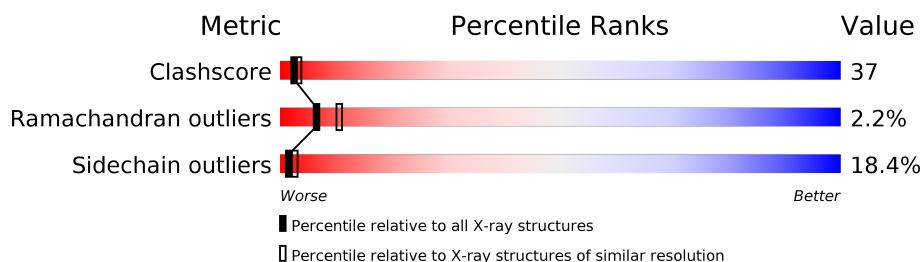
1 Overall quality at a glance

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	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NDP	A	508	X	-	-	-
3	NDP	B	508	X	-	-	-

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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 4008	C 2543	N 714	O 737	S 14	0	0	0
1	B	498	Total 4008	C 2543	N 714	O 737	S 14	0	0	0

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



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

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



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

- Molecule 4 is water.

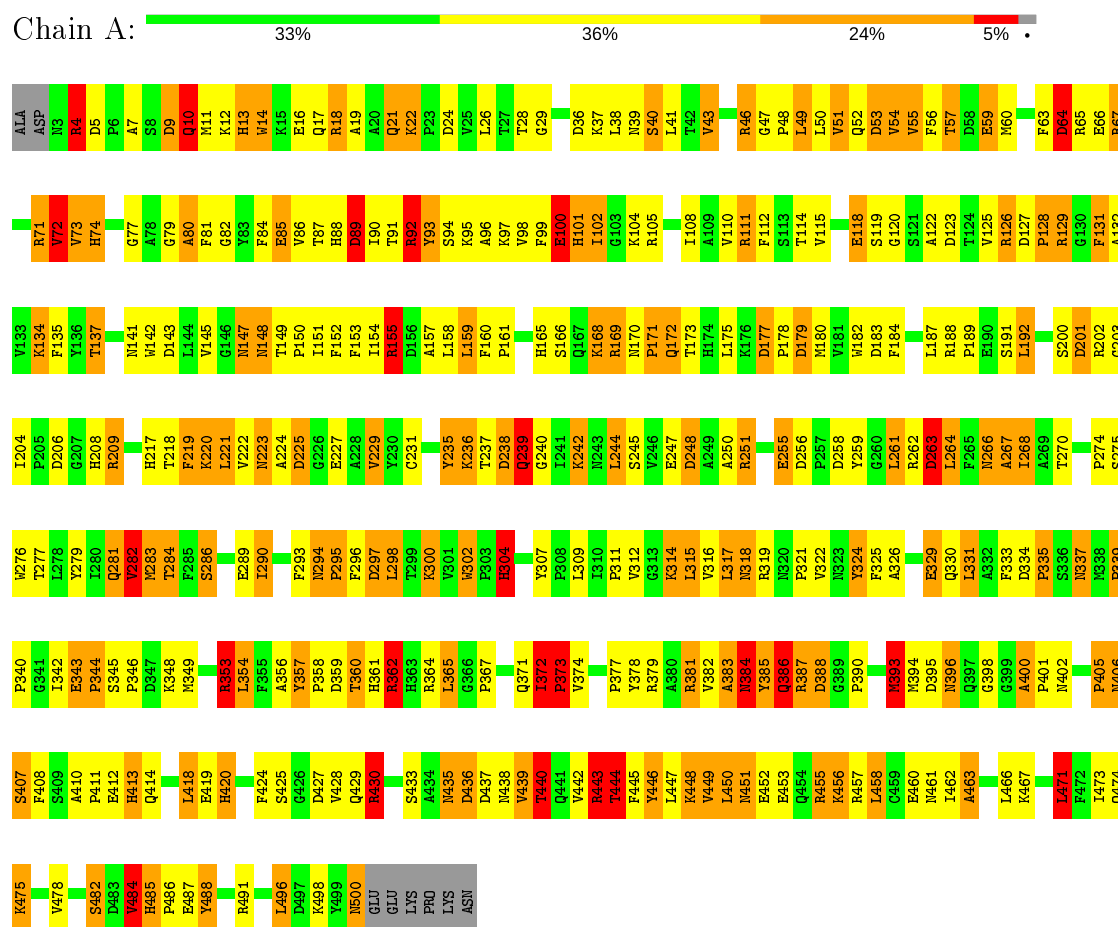
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	48	Total O 48 48	0	0
4	B	50	Total O 50 50	0	0

3 Residue-property plots

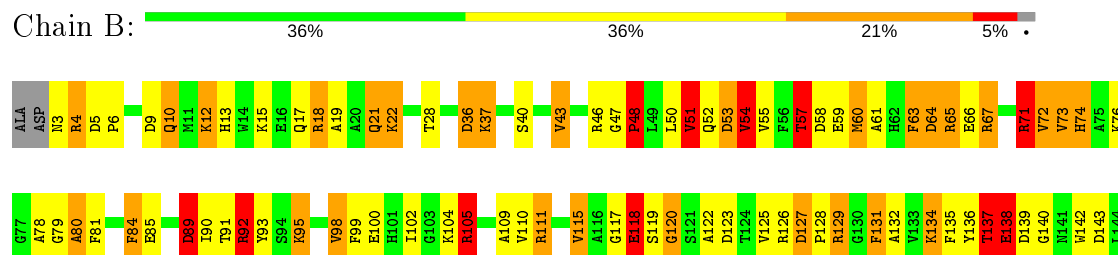
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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



LYS	D437	L365	F293	V145
PRO	M438		M294	G146
LYS	V439	L370	P295	N147
ASN	T440	Q371	F296	N148
	Q441	I372	D297	T149
	V442	P373	L298	P150
	R443	V374	T299	I151
	T444	N375	K300	F152
	P445		V301	F153
	Y446	Y378	W302	I154
	L447	Y379	W303	R155
	V449	A380	H304	D156
	K448	R381	G305	A157
	L450	V382	D306	L158
	M451	A383	Y307	L159
	E452	N384	P308	F160
	E453	Y385	L309	P161
	Q454	Q386	I310	S162
	R455	R387	P311	S163
	K456	D388	V312	F163
	R457		G313	
	L458	C392	K314	K168
	C459	M393	I315	R169
	E460	M394	V316	N170
	M461	D395	L317	P171
	L462	N396	N318	Q172
			R319	T173
			N320	H174
	L466	A400	P321	L175
	K467	P401	V322	K176
	D468	N402		D177
	A469	Y403		P178
	Q470	Y404	L331	D179
	L471	P405	A332	M180
	F472	N406	F333	V181
		S407	D334	D183
	K475	F408	P335	
	K476	S409	S336	L187
	A477	A410	N337	R188
	V478	P411	K338	P189
	K479	E412	P339	E190
		H413		S191
	D483	Q414	E343	L192
	V484	P415		H193
	H485	S416	D347	Q194
	P486	A417	K348	V195
	E487		M349	
	Y488	H420	L350	L198
		R421	Q351	
	R491		G352	D201
	Y492	S425	R353	R202
	Q493	G426	L354	
	A494	D427	F355	D206
	L495	V428	A356	
	L496	Q429		R209
	D497	R430	D359	
	K498	F431	T360	D212
	Y499	N432	H361	G213
	M500		R362	T218
	GLU	N435	H363	
	GLU	D436	R364	

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	142.00 Å 142.00 Å 103.70 Å 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}	0.191 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8296	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	1.53	22/4128 (0.5%)	2.37	195/5607 (3.5%)
1	B	1.57	20/4128 (0.5%)	2.42	229/5607 (4.1%)
All	All	1.55	42/8256 (0.5%)	2.39	424/11214 (3.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	2
All	All	0	6

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	67	ARG	CD-NE	-6.86	1.34	1.46
1	A	343	GLU	N-CA	6.53	1.59	1.46
1	A	166	SER	CB-OG	6.43	1.50	1.42
1	B	100	GLU	CD-OE2	-6.36	1.18	1.25
1	B	119	SER	CB-OG	-6.30	1.34	1.42
1	A	59	GLU	CD-OE1	6.10	1.32	1.25
1	A	364	ARG	NE-CZ	6.08	1.41	1.33
1	B	294	ASN	N-CA	6.05	1.58	1.46
1	A	171	PRO	N-CD	6.00	1.56	1.47
1	B	261	LEU	CA-CB	-5.96	1.40	1.53
1	A	29	GLY	N-CA	5.95	1.54	1.46
1	A	360	THR	C-O	5.82	1.34	1.23
1	B	305	GLY	N-CA	5.81	1.54	1.46
1	A	14	TRP	NE1-CE2	5.80	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	344	PRO	N-CD	5.74	1.55	1.47
1	A	329	GLU	CA-CB	-5.74	1.41	1.53
1	A	300	LYS	C-O	5.69	1.34	1.23
1	A	353	ARG	CZ-NH2	5.69	1.40	1.33
1	B	129	ARG	CG-CD	-5.67	1.37	1.51
1	A	155	ARG	CZ-NH2	-5.53	1.25	1.33
1	B	409	SER	CB-OG	5.51	1.49	1.42
1	B	151	ILE	N-CA	5.50	1.57	1.46
1	B	426	GLY	N-CA	5.49	1.54	1.46
1	A	65	ARG	CZ-NH2	5.45	1.40	1.33
1	B	381	ARG	CZ-NH1	5.30	1.40	1.33
1	B	48	PRO	N-CD	5.27	1.55	1.47
1	A	67	ARG	CG-CD	-5.26	1.38	1.51
1	B	120	GLY	N-CA	5.24	1.53	1.46
1	B	319	ARG	CZ-NH2	5.23	1.39	1.33
1	B	336	SER	CB-OG	-5.21	1.35	1.42
1	A	85	GLU	CD-OE1	-5.20	1.20	1.25
1	B	28	THR	C-O	5.18	1.33	1.23
1	A	56	PHE	CE2-CZ	5.15	1.47	1.37
1	A	165	HIS	CG-CD2	-5.14	1.27	1.35
1	B	118	GLU	CD-OE2	-5.14	1.20	1.25
1	B	66	GLU	CD-OE1	-5.13	1.20	1.25
1	B	162	SER	CB-OG	5.08	1.48	1.42
1	A	400	ALA	CA-CB	5.07	1.63	1.52
1	A	398	GLY	N-CA	5.05	1.53	1.46
1	B	59	GLU	CG-CD	-5.05	1.44	1.51
1	A	122	ALA	N-CA	5.05	1.56	1.46
1	B	289	GLU	CD-OE2	5.02	1.31	1.25

All (424) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	ARG	CD-NE-CZ	25.86	159.81	123.60
1	B	92	ARG	NE-CZ-NH1	23.28	131.94	120.30
1	B	126	ARG	NE-CZ-NH2	21.12	130.86	120.30
1	B	261	LEU	CA-CB-CG	20.39	162.19	115.30
1	A	362	ARG	NE-CZ-NH2	-20.36	110.12	120.30
1	A	111	ARG	NE-CZ-NH2	-20.23	110.19	120.30
1	A	362	ARG	NE-CZ-NH1	20.16	130.38	120.30
1	A	353	ARG	NE-CZ-NH1	20.11	130.36	120.30
1	A	169	ARG	NE-CZ-NH2	-19.74	110.43	120.30
1	A	353	ARG	NE-CZ-NH2	-19.55	110.52	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	430	ARG	NE-CZ-NH1	-18.83	110.89	120.30
1	A	169	ARG	NE-CZ-NH1	17.42	129.01	120.30
1	B	89	ASP	CB-CG-OD1	-17.04	102.96	118.30
1	A	111	ARG	NE-CZ-NH1	16.76	128.68	120.30
1	B	71	ARG	CD-NE-CZ	15.98	145.98	123.60
1	A	155	ARG	NE-CZ-NH1	-15.77	112.42	120.30
1	B	457	ARG	NE-CZ-NH1	15.17	127.88	120.30
1	B	188	ARG	NE-CZ-NH1	-15.13	112.73	120.30
1	B	457	ARG	NE-CZ-NH2	-14.37	113.11	120.30
1	A	364	ARG	NE-CZ-NH1	-14.33	113.14	120.30
1	B	71	ARG	NE-CZ-NH2	14.26	127.43	120.30
1	A	379	ARG	NE-CZ-NH1	14.05	127.33	120.30
1	B	364	ARG	NE-CZ-NH2	-13.20	113.70	120.30
1	B	225	ASP	CB-CG-OD1	13.16	130.14	118.30
1	B	111	ARG	NE-CZ-NH2	-13.03	113.79	120.30
1	A	261	LEU	CA-CB-CG	12.77	144.67	115.30
1	B	188	ARG	NE-CZ-NH2	12.69	126.64	120.30
1	B	111	ARG	NE-CZ-NH1	12.69	126.64	120.30
1	A	359	ASP	CB-CG-OD2	-12.63	106.93	118.30
1	B	381	ARG	NE-CZ-NH1	-12.51	114.05	120.30
1	B	155	ARG	NE-CZ-NH1	12.46	126.53	120.30
1	B	437	ASP	CB-CG-OD1	12.25	129.33	118.30
1	B	362	ARG	NE-CZ-NH1	12.21	126.41	120.30
1	A	359	ASP	CB-CG-OD1	12.03	129.12	118.30
1	B	159	LEU	CA-CB-CG	11.93	142.75	115.30
1	B	155	ARG	CD-NE-CZ	11.81	140.13	123.60
1	A	65	ARG	CD-NE-CZ	11.61	139.85	123.60
1	B	430	ARG	NE-CZ-NH2	11.53	126.07	120.30
1	B	92	ARG	NE-CZ-NH2	-11.06	114.77	120.30
1	B	129	ARG	NE-CZ-NH2	10.99	125.79	120.30
1	B	138	GLU	OE1-CD-OE2	-10.98	110.12	123.30
1	A	378	TYR	CB-CG-CD1	10.89	127.53	121.00
1	B	362	ARG	NE-CZ-NH2	-10.71	114.95	120.30
1	B	263	ASP	CB-CG-OD2	-10.62	108.74	118.30
1	A	9	ASP	CB-CG-OD1	10.40	127.66	118.30
1	B	225	ASP	CB-CG-OD2	-10.19	109.13	118.30
1	B	319	ARG	NE-CZ-NH2	-10.13	115.23	120.30
1	A	93	TYR	CB-CG-CD2	-10.10	114.94	121.00
1	A	143	ASP	CB-CG-OD2	-10.05	109.25	118.30
1	A	343	GLU	CA-CB-CG	9.99	135.38	113.40
1	A	188	ARG	NE-CZ-NH1	-9.98	115.31	120.30
1	B	36	ASP	CB-CG-OD1	9.80	127.12	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	455	ARG	NE-CZ-NH1	9.79	125.19	120.30
1	A	329	GLU	OE1-CD-OE2	9.76	135.01	123.30
1	B	65	ARG	NE-CZ-NH2	9.60	125.10	120.30
1	A	251	ARG	NE-CZ-NH1	9.46	125.03	120.30
1	B	343	GLU	OE1-CD-OE2	-9.40	112.01	123.30
1	B	381	ARG	NE-CZ-NH2	9.40	125.00	120.30
1	A	89	ASP	CB-CG-OD1	-9.39	109.85	118.30
1	B	169	ARG	NE-CZ-NH1	-9.36	115.62	120.30
1	A	155	ARG	CD-NE-CZ	-9.34	110.53	123.60
1	A	378	TYR	CB-CG-CD2	-9.32	115.41	121.00
1	B	262	ARG	NE-CZ-NH1	-9.28	115.66	120.30
1	A	126	ARG	NE-CZ-NH1	9.26	124.93	120.30
1	A	53	ASP	CB-CG-OD2	-9.09	110.12	118.30
1	B	359	ASP	CB-CG-OD2	-9.08	110.13	118.30
1	B	386	GLN	CB-CG-CD	9.07	135.18	111.60
1	A	455	ARG	NE-CZ-NH2	-8.97	115.81	120.30
1	A	364	ARG	CD-NE-CZ	-8.89	111.15	123.60
1	B	127	ASP	CB-CG-OD1	8.88	126.29	118.30
1	B	81	PHE	CB-CG-CD1	-8.86	114.60	120.80
1	B	53	ASP	CB-CG-OD1	8.84	126.26	118.30
1	B	343	GLU	CA-CB-CG	8.82	132.82	113.40
1	B	450	LEU	CB-CA-C	8.72	126.77	110.20
1	B	168	LYS	CA-CB-CG	8.71	132.55	113.40
1	A	335	PRO	C-N-CA	8.68	143.39	121.70
1	B	254	HIS	CA-CB-CG	8.66	128.33	113.60
1	B	386	GLN	CA-CB-CG	8.65	132.44	113.40
1	B	364	ARG	CD-NE-CZ	-8.63	111.52	123.60
1	A	251	ARG	CA-CB-CG	8.56	132.24	113.40
1	B	65	ARG	NE-CZ-NH1	-8.52	116.04	120.30
1	B	353	ARG	NE-CZ-NH2	-8.48	116.06	120.30
1	B	343	GLU	CG-CD-OE1	8.46	135.22	118.30
1	B	59	GLU	OE1-CD-OE2	-8.45	113.16	123.30
1	B	202	ARG	NE-CZ-NH2	-8.44	116.08	120.30
1	B	255	GLU	CA-CB-CG	8.43	131.94	113.40
1	B	429	GLN	CA-CB-CG	8.43	131.94	113.40
1	B	347	ASP	CB-CG-OD2	8.40	125.86	118.30
1	B	134	LYS	CD-CE-NZ	-8.33	92.53	111.70
1	B	472	PHE	CA-CB-CG	8.26	133.72	113.90
1	B	497	ASP	CB-CG-OD2	-8.23	110.89	118.30
1	A	457	ARG	CD-NE-CZ	8.23	135.12	123.60
1	B	334	ASP	CB-CG-OD1	8.22	125.70	118.30
1	B	497	ASP	CB-CG-OD1	8.20	125.68	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	89	ASP	OD1-CG-OD2	8.17	138.82	123.30
1	B	175	LEU	CA-CB-CG	8.17	134.09	115.30
1	B	408	PHE	C-N-CA	8.15	142.08	121.70
1	B	450	LEU	CA-CB-CG	8.15	134.04	115.30
1	A	430	ARG	CD-NE-CZ	-8.11	112.24	123.60
1	B	262	ARG	NE-CZ-NH2	-8.11	116.24	120.30
1	A	71	ARG	NE-CZ-NH1	8.09	124.34	120.30
1	B	201	ASP	CB-CG-OD2	-8.09	111.02	118.30
1	B	187	LEU	CB-CA-C	8.02	125.43	110.20
1	A	93	TYR	CB-CG-CD1	7.99	125.79	121.00
1	B	314	LYS	CA-CB-CG	7.98	130.95	113.40
1	B	123	ASP	CB-CG-OD2	-7.95	111.14	118.30
1	A	179	ASP	CB-CG-OD2	7.91	125.42	118.30
1	B	494	ALA	CB-CA-C	7.90	121.96	110.10
1	A	179	ASP	CA-CB-CG	7.89	130.76	113.40
1	A	457	ARG	NE-CZ-NH1	7.89	124.25	120.30
1	B	457	ARG	CD-NE-CZ	7.88	134.64	123.60
1	A	373	PRO	N-CA-CB	-7.87	93.85	103.30
1	A	412	GLU	CA-CB-CG	7.87	130.70	113.40
1	A	324	TYR	CB-CG-CD2	7.85	125.71	121.00
1	B	468	ASP	CB-CG-OD1	7.83	125.35	118.30
1	B	60	MET	CA-CB-CG	7.82	126.60	113.30
1	B	67	ARG	NE-CZ-NH2	7.82	124.21	120.30
1	A	159	LEU	CA-CB-CG	7.77	133.16	115.30
1	B	206	ASP	CB-CG-OD2	7.76	125.28	118.30
1	A	67	ARG	CA-CB-CG	7.73	130.40	113.40
1	B	443	ARG	CD-NE-CZ	7.72	134.41	123.60
1	B	126	ARG	NE-CZ-NH1	-7.70	116.45	120.30
1	A	388	ASP	CB-CG-OD1	-7.67	111.40	118.30
1	B	262	ARG	NH1-CZ-NH2	7.64	127.80	119.40
1	A	155	ARG	NE-CZ-NH2	7.60	124.10	120.30
1	A	201	ASP	CB-CG-OD2	-7.55	111.50	118.30
1	B	483	ASP	CB-CG-OD1	7.55	125.10	118.30
1	B	298	LEU	CA-CB-CG	7.55	132.66	115.30
1	B	436	ASP	CB-CG-OD2	7.52	125.07	118.30
1	A	365	LEU	CA-CB-CG	7.52	132.59	115.30
1	B	378	TYR	CB-CG-CD1	7.51	125.51	121.00
1	A	357	TYR	CB-CG-CD2	-7.50	116.50	121.00
1	B	169	ARG	NE-CZ-NH2	7.36	123.98	120.30
1	A	263	ASP	CB-CG-OD1	7.34	124.91	118.30
1	A	80	ALA	CB-CA-C	7.33	121.10	110.10
1	A	67	ARG	CG-CD-NE	7.31	127.15	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	123	ASP	CB-CG-OD1	7.30	124.87	118.30
1	B	247	GLU	CA-CB-CG	7.28	129.42	113.40
1	B	129	ARG	NE-CZ-NH1	-7.25	116.68	120.30
1	B	275	SER	C-N-CA	7.20	139.71	121.70
1	A	65	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	B	105	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	B	67	ARG	NE-CZ-NH1	-7.19	116.70	120.30
1	B	111	ARG	CD-NE-CZ	7.18	133.65	123.60
1	B	343	GLU	N-CA-CB	-7.14	97.76	110.60
1	B	256	ASP	CB-CG-OD1	7.11	124.70	118.30
1	A	248	ASP	CB-CG-OD2	-7.10	111.91	118.30
1	A	364	ARG	NH1-CZ-NH2	7.08	127.19	119.40
1	A	188	ARG	CD-NE-CZ	-7.04	113.74	123.60
1	A	343	GLU	CB-CA-C	7.04	124.48	110.40
1	A	10	GLN	CB-CG-CD	7.04	129.90	111.60
1	A	256	ASP	CB-CG-OD1	7.04	124.63	118.30
1	B	126	ARG	CA-CB-CG	7.01	128.82	113.40
1	A	92	ARG	NE-CZ-NH2	7.01	123.80	120.30
1	B	251	ARG	NE-CZ-NH2	6.98	123.79	120.30
1	A	353	ARG	CD-NE-CZ	6.96	133.35	123.60
1	A	221	LEU	O-C-N	6.94	133.80	122.70
1	A	435	ASN	CB-CA-C	6.94	124.27	110.40
1	B	209	ARG	CD-NE-CZ	-6.92	113.91	123.60
1	A	16	GLU	OE1-CD-OE2	6.91	131.59	123.30
1	B	261	LEU	O-C-N	6.91	133.75	122.70
1	A	263	ASP	CA-CB-CG	6.90	128.57	113.40
1	A	437	ASP	CB-CG-OD1	6.87	124.48	118.30
1	B	483	ASP	CB-CG-OD2	-6.87	112.12	118.30
1	B	74	HIS	C-N-CA	6.86	138.85	121.70
1	B	89	ASP	CA-CB-CG	-6.83	98.38	113.40
1	A	122	ALA	CB-CA-C	6.81	120.32	110.10
1	A	238	ASP	CB-CG-OD2	6.79	124.41	118.30
1	B	255	GLU	OE1-CD-OE2	-6.79	115.15	123.30
1	A	28	THR	CA-C-N	6.78	129.76	116.20
1	A	446	TYR	CB-CG-CD2	6.77	125.06	121.00
1	B	312	VAL	CA-CB-CG2	6.74	121.01	110.90
1	B	334	ASP	OD1-CG-OD2	-6.74	110.50	123.30
1	B	51	VAL	C-N-CA	6.73	138.52	121.70
1	A	302	TRP	CA-CB-CG	6.72	126.47	113.70
1	B	364	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	A	259	TYR	CB-CG-CD1	-6.72	116.97	121.00
1	A	471	LEU	CB-CA-C	6.71	122.96	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	379	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	A	335	PRO	CA-CB-CG	-6.65	91.36	104.00
1	B	381	ARG	CD-NE-CZ	-6.65	114.29	123.60
1	B	92	ARG	C-N-CA	6.65	138.32	121.70
1	B	111	ARG	O-C-N	6.61	133.28	122.70
1	B	468	ASP	OD1-CG-OD2	-6.61	110.75	123.30
1	A	111	ARG	N-CA-CB	6.60	122.48	110.60
1	B	98	VAL	CG1-CB-CG2	-6.56	100.40	110.90
1	A	49	LEU	CA-CB-CG	6.56	130.38	115.30
1	A	290	ILE	CA-CB-CG2	6.54	123.98	110.90
1	B	89	ASP	CB-CA-C	6.48	123.37	110.40
1	B	81	PHE	CB-CG-CD2	6.47	125.33	120.80
1	A	134	LYS	CD-CE-NZ	-6.47	96.83	111.70
1	B	343	GLU	CB-CG-CD	6.46	131.64	114.20
1	A	282	VAL	CA-CB-CG1	6.46	120.59	110.90
1	A	319	ARG	CD-NE-CZ	-6.45	114.56	123.60
1	A	4	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	A	247	GLU	CG-CD-OE1	6.45	131.19	118.30
1	A	440	THR	CA-CB-CG2	6.42	121.39	112.40
1	B	177	ASP	CB-CG-OD1	-6.42	112.52	118.30
1	B	385	TYR	CB-CA-C	6.42	123.24	110.40
1	B	187	LEU	CA-CB-CG	6.39	130.01	115.30
1	A	188	ARG	NE-CZ-NH2	6.39	123.50	120.30
1	B	182	TRP	CB-CA-C	6.39	123.18	110.40
1	B	54	VAL	CA-CB-CG1	6.38	120.47	110.90
1	A	284	THR	OG1-CB-CG2	6.37	124.65	110.00
1	A	209	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	A	405	PRO	CA-N-CD	-6.36	102.60	111.50
1	B	315	LEU	CA-CB-CG	6.35	129.91	115.30
1	B	84	PHE	CB-CG-CD1	-6.33	116.37	120.80
1	B	247	GLU	CG-CD-OE2	-6.31	105.68	118.30
1	B	365	LEU	N-CA-CB	-6.30	97.81	110.40
1	A	250	ALA	CB-CA-C	6.28	119.52	110.10
1	B	126	ARG	NH1-CZ-NH2	-6.25	112.52	119.40
1	B	252	LEU	CA-CB-CG	6.25	129.68	115.30
1	A	395	ASP	CB-CG-OD2	-6.24	112.68	118.30
1	B	139	ASP	CB-CG-OD2	6.24	123.91	118.30
1	B	318	ASN	CB-CA-C	6.23	122.87	110.40
1	B	468	ASP	CB-CG-OD2	6.23	123.90	118.30
1	B	359	ASP	CB-CG-OD1	6.22	123.90	118.30
1	A	172	GLN	CA-CB-CG	-6.22	99.72	113.40
1	A	143	ASP	O-C-N	6.20	132.61	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	429	GLN	CA-CB-CG	6.19	127.03	113.40
1	B	370	LEU	C-N-CA	6.18	137.15	121.70
1	A	382	VAL	CG1-CB-CG2	6.17	120.77	110.90
1	B	160	PHE	CB-CG-CD1	-6.16	116.48	120.80
1	A	4	ARG	CD-NE-CZ	6.15	132.22	123.60
1	B	85	GLU	OE1-CD-OE2	-6.13	115.94	123.30
1	B	261	LEU	N-CA-CB	6.13	122.66	110.40
1	A	251	ARG	NE-CZ-NH2	-6.13	117.24	120.30
1	A	329	GLU	CG-CD-OE2	-6.12	106.05	118.30
1	B	334	ASP	CB-CG-OD2	6.12	123.81	118.30
1	B	437	ASP	CB-CG-OD2	-6.12	112.80	118.30
1	A	379	ARG	CA-CB-CG	6.11	126.85	113.40
1	B	117	GLY	C-N-CA	6.11	136.97	121.70
1	A	387	ARG	CD-NE-CZ	-6.10	115.06	123.60
1	B	322	VAL	CA-CB-CG1	6.08	120.03	110.90
1	B	379	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	A	46	ARG	NE-CZ-NH1	-6.07	117.27	120.30
1	B	477	ALA	N-CA-CB	6.07	118.59	110.10
1	B	347	ASP	OD1-CG-OD2	-6.06	111.78	123.30
1	A	71	ARG	CD-NE-CZ	6.04	132.06	123.60
1	A	126	ARG	CA-CB-CG	6.03	126.67	113.40
1	B	421	ARG	NE-CZ-NH1	6.03	123.32	120.30
1	A	177	ASP	N-CA-CB	-6.01	99.78	110.60
1	B	28	THR	CA-C-O	-6.01	107.48	120.10
1	B	396	ASN	C-N-CA	6.00	136.69	121.70
1	A	407	SER	CA-C-O	-5.99	107.52	120.10
1	A	202	ARG	NE-CZ-NH1	-5.99	117.31	120.30
1	B	115	VAL	CA-CB-CG1	5.98	119.87	110.90
1	A	244	LEU	CA-CB-CG	5.97	129.03	115.30
1	B	163	PHE	N-CA-CB	5.93	121.28	110.60
1	B	57	THR	CB-CA-C	5.93	127.61	111.60
1	B	122	ALA	CB-CA-C	5.92	118.98	110.10
1	B	63	PHE	CB-CG-CD2	-5.90	116.67	120.80
1	A	496	LEU	CB-CA-C	5.89	121.40	110.20
1	A	427	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	B	239	GLN	CG-CD-OE1	5.89	133.39	121.60
1	A	4	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	B	388	ASP	CB-CG-OD2	5.88	123.59	118.30
1	A	100	GLU	CG-CD-OE2	-5.87	106.56	118.30
1	B	375	ASN	CB-CG-ND2	5.87	130.78	116.70
1	A	192	LEU	CA-CB-CG	5.87	128.79	115.30
1	B	58	ASP	CB-CG-OD1	5.87	123.58	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	B	338	MET	O-C-N	5.85	132.21	121.10
1	A	219	PHE	CB-CA-C	5.83	122.07	110.40
1	A	263	ASP	CB-CA-C	5.83	122.07	110.40
1	A	443	ARG	NE-CZ-NH2	5.83	123.21	120.30
1	A	52	GLN	CA-CB-CG	5.82	126.21	113.40
1	A	9	ASP	CB-CA-C	5.82	122.04	110.40
1	B	244	LEU	CA-CB-CG	5.82	128.68	115.30
1	B	450	LEU	N-CA-CB	-5.82	98.76	110.40
1	B	410	ALA	CB-CA-C	5.81	118.82	110.10
1	B	289	GLU	CA-CB-CG	5.81	126.18	113.40
1	B	445	PHE	O-C-N	5.80	131.99	122.70
1	B	137	THR	CA-CB-CG2	5.79	120.50	112.40
1	B	52	GLN	CB-CA-C	-5.79	98.83	110.40
1	A	73	VAL	CA-CB-CG1	5.78	119.56	110.90
1	A	385	TYR	CB-CG-CD2	-5.76	117.54	121.00
1	A	289	GLU	CG-CD-OE1	5.75	129.80	118.30
1	B	202	ARG	CG-CD-NE	-5.75	99.73	111.80
1	B	177	ASP	N-CA-CB	-5.74	100.27	110.60
1	B	58	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	A	360	THR	N-CA-CB	-5.73	99.41	110.30
1	A	221	LEU	CA-C-O	-5.73	108.07	120.10
1	A	385	TYR	CB-CG-CD1	5.72	124.43	121.00
1	B	412	GLU	CB-CA-C	-5.72	98.96	110.40
1	A	314	LYS	CD-CE-NZ	-5.71	98.56	111.70
1	B	71	ARG	CA-CB-CG	5.71	125.97	113.40
1	A	270	THR	CA-CB-CG2	5.71	120.39	112.40
1	B	420	HIS	C-N-CA	5.70	135.94	121.70
1	A	72	VAL	CA-CB-CG1	5.69	119.44	110.90
1	B	273	TYR	CB-CG-CD2	-5.68	117.59	121.00
1	B	413	HIS	N-CA-CB	5.68	120.83	110.60
1	B	182	TRP	N-CA-CB	-5.68	100.38	110.60
1	B	435	ASN	CB-CA-C	5.67	121.73	110.40
1	B	202	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	B	446	TYR	CA-CB-CG	5.65	124.14	113.40
1	B	92	ARG	NH1-CZ-NH2	-5.62	113.22	119.40
1	A	283	MET	CG-SD-CE	5.62	109.19	100.20
1	B	282	VAL	CA-CB-CG1	5.61	119.32	110.90
1	A	388	ASP	CB-CG-OD2	5.61	123.35	118.30
1	B	168	LYS	N-CA-CB	5.60	120.68	110.60
1	B	99	PHE	CA-CB-CG	5.59	127.33	113.90
1	B	71	ARG	NE-CZ-NH1	-5.59	117.51	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	HIS	C-N-CA	5.58	135.65	121.70
1	A	393	MET	CB-CA-C	-5.58	99.24	110.40
1	B	74	HIS	CB-CA-C	-5.58	99.24	110.40
1	A	386	GLN	CB-CG-CD	5.58	126.10	111.60
1	B	71	ARG	CB-CG-CD	5.58	126.11	111.60
1	A	184	PHE	C-N-CA	5.58	135.64	121.70
1	B	123	ASP	CB-CG-OD1	5.57	123.31	118.30
1	A	384	ASN	CB-CA-C	5.54	121.48	110.40
1	A	259	TYR	CB-CG-CD2	5.54	124.32	121.00
1	A	266	ASN	CB-CA-C	5.54	121.48	110.40
1	A	425	SER	CB-CA-C	-5.54	99.58	110.10
1	A	405	PRO	N-CD-CG	-5.52	94.92	103.20
1	A	111	ARG	CD-NE-CZ	5.51	131.32	123.60
1	B	408	PHE	O-C-N	-5.51	113.89	122.70
1	A	484	VAL	CA-CB-CG1	5.50	119.16	110.90
1	B	384	ASN	CB-CA-C	5.50	121.39	110.40
1	B	129	ARG	CG-CD-NE	5.49	123.33	111.80
1	B	263	ASP	CB-CA-C	5.48	121.36	110.40
1	B	187	LEU	CB-CG-CD1	5.48	120.31	111.00
1	A	224	ALA	CA-C-O	-5.47	108.61	120.10
1	B	143	ASP	C-N-CA	5.47	135.37	121.70
1	A	324	TYR	CG-CD2-CE2	5.47	125.67	121.30
1	B	66	GLU	OE1-CD-OE2	5.46	129.85	123.30
1	A	297	ASP	CB-CG-OD1	5.46	123.21	118.30
1	A	270	THR	N-CA-CB	5.45	120.65	110.30
1	A	247	GLU	CG-CD-OE2	-5.44	107.42	118.30
1	A	261	LEU	N-CA-CB	5.43	121.27	110.40
1	A	372	ILE	CA-CB-CG1	5.43	121.31	111.00
1	B	127	ASP	OD1-CG-OD2	-5.43	112.99	123.30
1	A	420	HIS	CA-CB-CG	5.42	122.81	113.60
1	A	64	ASP	C-N-CA	5.41	135.23	121.70
1	A	444	THR	OG1-CB-CG2	5.40	122.42	110.00
1	A	413	HIS	N-CA-CB	5.39	120.30	110.60
1	B	126	ARG	CA-C-O	-5.38	108.79	120.10
1	B	338	MET	CA-C-O	-5.38	108.80	120.10
1	A	393	MET	CA-CB-CG	-5.38	104.16	113.30
1	B	55	VAL	CA-CB-CG1	5.38	118.97	110.90
1	A	89	ASP	CB-CA-C	5.37	121.14	110.40
1	B	430	ARG	NH1-CZ-NH2	-5.37	113.49	119.40
1	B	353	ARG	NH1-CZ-NH2	5.37	125.30	119.40
1	A	29	GLY	O-C-N	-5.36	114.09	123.20
1	A	357	TYR	CB-CG-CD1	5.36	124.22	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	126	ARG	O-C-N	5.36	131.27	122.70
1	B	293	PHE	CA-CB-CG	5.35	126.75	113.90
1	A	247	GLU	CA-CB-CG	5.35	125.17	113.40
1	A	304	HIS	N-CA-CB	5.34	120.21	110.60
1	A	52	GLN	N-CA-CB	5.33	120.20	110.60
1	A	24	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	B	392	CYS	CA-CB-SG	-5.33	104.41	114.00
1	B	105	ARG	CB-CA-C	-5.33	99.75	110.40
1	A	461	ASN	CA-CB-CG	5.32	125.11	113.40
1	A	429	GLN	N-CA-CB	-5.30	101.06	110.60
1	B	209	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	A	418	LEU	CB-CA-C	5.29	120.26	110.20
1	B	72	VAL	CB-CA-C	5.29	121.45	111.40
1	A	225	ASP	CB-CG-OD2	-5.26	113.56	118.30
1	A	381	ARG	N-CA-CB	5.26	120.06	110.60
1	B	460	GLU	CG-CD-OE2	-5.26	107.79	118.30
1	B	191	SER	C-N-CA	5.25	134.84	121.70
1	B	302	TRP	N-CA-CB	5.25	120.05	110.60
1	A	153	PHE	O-C-N	5.25	131.09	122.70
1	B	219	PHE	CB-CA-C	5.25	120.89	110.40
1	B	129	ARG	CB-CG-CD	5.24	125.22	111.60
1	A	119	SER	N-CA-CB	-5.23	102.66	110.50
1	B	66	GLU	C-N-CA	5.23	134.76	121.70
1	B	251	ARG	CD-NE-CZ	-5.22	116.29	123.60
1	B	139	ASP	CB-CG-OD1	-5.22	113.60	118.30
1	B	472	PHE	CB-CG-CD2	5.22	124.45	120.80
1	A	227	GLU	OE1-CD-OE2	5.20	129.54	123.30
1	B	202	ARG	CD-NE-CZ	5.20	130.88	123.60
1	B	476	LYS	CB-CG-CD	5.20	125.12	111.60
1	B	438	ASN	CA-C-O	-5.19	109.20	120.10
1	A	258	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	475	LYS	N-CA-CB	5.19	119.94	110.60
1	A	383	ALA	CB-CA-C	-5.19	102.32	110.10
1	B	436	ASP	CB-CA-C	5.19	120.78	110.40
1	A	429	GLN	C-N-CA	5.18	134.64	121.70
1	B	140	GLY	O-C-N	5.17	130.97	122.70
1	A	414	GLN	CA-CB-CG	5.16	124.76	113.40
1	A	281	GLN	CA-CB-CG	5.16	124.75	113.40
1	B	174	HIS	CA-CB-CG	-5.16	104.83	113.60
1	B	425	SER	C-N-CA	-5.16	111.47	122.30
1	B	318	ASN	N-CA-CB	-5.15	101.33	110.60
1	B	37	LYS	CB-CG-CD	5.15	124.99	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	109	ALA	CA-C-N	5.15	128.53	117.20
1	B	242	LYS	O-C-N	5.15	130.93	122.70
1	B	228	ALA	C-N-CA	5.14	134.55	121.70
1	A	239	GLN	CB-CG-CD	5.13	124.94	111.60
1	A	318	ASN	N-CA-CB	-5.13	101.37	110.60
1	B	48	PRO	N-CA-CB	-5.13	96.96	102.60
1	B	378	TYR	CB-CG-CD2	-5.13	117.92	121.00
1	A	102	ILE	CB-CA-C	-5.12	101.36	111.60
1	B	159	LEU	CB-CG-CD2	5.12	119.70	111.00
1	B	491	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	B	28	THR	CA-C-N	5.12	126.43	116.20
1	B	158	LEU	C-N-CA	5.12	134.49	121.70
1	A	463	ALA	N-CA-CB	-5.11	102.94	110.10
1	B	105	ARG	CD-NE-CZ	-5.11	116.45	123.60
1	B	223	ASN	O-C-N	5.10	130.86	122.70
1	A	281	GLN	CG-CD-OE1	5.10	131.79	121.60
1	A	66	GLU	CG-CD-OE2	-5.10	108.11	118.30
1	A	429	GLN	CB-CA-C	5.08	120.55	110.40
1	B	187	LEU	N-CA-CB	-5.08	100.25	110.40
1	B	322	VAL	CG1-CB-CG2	-5.07	102.79	110.90
1	A	96	ALA	O-C-N	5.07	130.80	122.70
1	B	81	PHE	N-CA-CB	-5.06	101.49	110.60
1	B	403	TYR	CB-CG-CD1	-5.06	117.97	121.00
1	A	22	LYS	N-CA-C	-5.05	97.36	111.00
1	B	169	ARG	CB-CA-C	-5.05	100.30	110.40
1	B	156	ASP	CB-CG-OD1	5.05	122.84	118.30
1	A	430	ARG	NE-CZ-NH2	5.04	122.82	120.30
1	A	344	PRO	O-C-N	5.03	130.75	122.70
1	A	424	PHE	O-C-N	5.03	130.74	122.70
1	A	168	LYS	CA-CB-CG	5.02	124.45	113.40
1	A	41	LEU	CB-CG-CD2	-5.02	102.47	111.00
1	A	218	THR	CA-CB-CG2	5.01	119.42	112.40
1	A	449	VAL	O-C-N	5.01	130.72	122.70
1	A	143	ASP	CB-CG-OD1	5.01	122.81	118.30
1	A	295	PRO	N-CD-CG	-5.01	95.69	103.20
1	A	147	ASN	CA-C-O	-5.00	109.59	120.10

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	353	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	362	ARG	Sidechain
1	A	430	ARG	Sidechain
1	A	71	ARG	Sidechain
1	B	105	ARG	Sidechain
1	B	310	ILE	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	4008	0	3830	329	3
1	B	4008	0	3825	293	2
2	A	43	0	30	15	0
2	B	43	0	30	9	0
3	A	48	0	24	0	0
3	B	48	0	24	3	0
4	A	48	0	0	4	1
4	B	50	0	0	5	0
All	All	8296	0	7763	596	3

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 37.

All (596) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ARG:NH2	1:A:438:ASN:HD21	1.19	1.40
1:B:155:ARG:HH22	1:B:438:ASN:ND2	1.28	1.30
1:A:155:ARG:HH22	1:A:438:ASN:ND2	1.28	1.29
1:B:155:ARG:NH2	1:B:438:ASN:HD21	1.34	1.24
1:A:367:PRO:HG2	1:A:390:PRO:HG2	1.19	1.14
1:A:322:VAL:HA	1:B:172:GLN:NE2	1.66	1.11
1:A:487:GLU:O	1:A:491:ARG:HG3	1.52	1.08
1:A:173:THR:CG2	1:A:175:LEU:HD12	1.84	1.08
1:A:444:THR:HA	1:A:448:LYS:HD3	1.42	1.02
1:A:220:LYS:HE3	1:A:420:HIS:CD2	1.97	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:444:THR:O	1:B:448:LYS:HG2	1.62	0.99
1:A:189:PRO:O	1:A:192:LEU:HD12	1.62	0.99
1:A:148:ASN:H	1:A:148:ASN:HD22	0.99	0.99
1:B:177:ASP:HB3	1:B:180:MET:HE3	1.42	0.98
1:B:170:ASN:HD22	1:B:172:GLN:H	1.12	0.97
1:A:471:LEU:HD22	1:A:474:GLN:NE2	1.79	0.97
1:A:384:ASN:HD22	1:A:384:ASN:C	1.56	0.97
1:A:173:THR:HG21	1:A:175:LEU:HD12	1.46	0.96
1:A:371:GLN:HE21	1:A:393:MET:HB2	1.30	0.95
1:A:322:VAL:HA	1:B:172:GLN:HE22	1.30	0.94
2:A:507:HEM:HBB2	2:A:507:HEM:HMB2	1.48	0.94
1:B:173:THR:HG22	1:B:175:LEU:HG	1.49	0.93
1:A:367:PRO:HG2	1:A:390:PRO:CG	1.99	0.92
1:B:451:ASN:O	1:B:455:ARG:HG3	1.69	0.92
1:B:298:LEU:HD12	1:B:349:MET:HG3	1.53	0.91
1:A:383:ALA:HB1	1:A:411:PRO:HG3	1.50	0.91
1:B:229:VAL:HG13	1:B:282:VAL:HG23	1.52	0.91
1:B:142:TRP:HB2	1:B:339:PRO:HD3	1.52	0.90
1:B:189:PRO:O	1:B:192:LEU:HD12	1.72	0.90
1:A:220:LYS:HE3	1:A:420:HIS:HD2	1.37	0.89
1:A:384:ASN:HD22	1:A:385:TYR:N	1.72	0.88
1:B:229:VAL:CG1	1:B:282:VAL:HG23	2.03	0.87
1:B:284:THR:HG22	1:B:286:SER:H	1.40	0.87
1:B:177:ASP:HB3	1:B:180:MET:CE	2.04	0.87
1:B:406:ASN:HD22	1:B:408:PHE:H	1.18	0.87
1:B:179:ASP:O	1:B:183:ASP:HB2	1.75	0.86
1:A:92:ARG:HB2	1:A:92:ARG:HH11	1.40	0.86
1:B:450:LEU:HD23	1:B:455:ARG:HG2	1.58	0.85
1:A:384:ASN:C	1:A:384:ASN:ND2	2.30	0.84
1:A:406:ASN:ND2	1:A:408:PHE:H	1.75	0.84
1:B:406:ASN:ND2	1:B:408:PHE:H	1.74	0.84
1:A:458:LEU:O	1:A:462:ILE:HG13	1.76	0.83
1:A:223:ASN:HD22	1:A:223:ASN:C	1.82	0.83
1:B:74:HIS:O	1:B:111:ARG:NH2	2.11	0.83
1:B:251:ARG:O	1:B:255:GLU:HB2	1.77	0.83
1:B:90:ILE:HD13	1:B:312:VAL:HG13	1.60	0.82
1:A:485:HIS:CD2	1:A:486:PRO:HD2	2.14	0.82
1:A:458:LEU:HD12	1:A:458:LEU:O	1.80	0.82
1:A:148:ASN:N	1:A:148:ASN:HD22	1.78	0.82
1:A:406:ASN:C	1:A:406:ASN:HD22	1.83	0.81
1:B:496:LEU:O	1:B:500:ASN:HB2	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:GLU:O	1:A:101:HIS:HB3	1.80	0.81
1:A:148:ASN:H	1:A:148:ASN:ND2	1.79	0.81
1:A:149:THR:OG1	1:A:150:PRO:HD2	1.79	0.81
2:A:507:HEM:HBB2	2:A:507:HEM:CMB	2.11	0.80
1:A:98:VAL:HG23	1:A:137:THR:CG2	2.12	0.80
1:B:297:ASP:OD1	1:B:300:LYS:HE2	1.81	0.80
1:B:170:ASN:ND2	1:B:172:GLN:H	1.78	0.79
1:A:134:LYS:HE3	1:A:331:LEU:CD2	2.13	0.79
1:A:374:VAL:HG22	1:A:374:VAL:O	1.83	0.79
1:A:149:THR:OG1	1:A:150:PRO:CD	2.30	0.78
1:B:394:MET:HA	1:B:394:MET:CE	2.13	0.78
1:A:108:ILE:HD13	1:A:315:LEU:HD12	1.65	0.77
1:B:356:ALA:O	1:B:360:THR:HG22	1.85	0.77
1:A:229:VAL:HG13	1:A:282:VAL:HG23	1.67	0.77
1:A:444:THR:O	1:A:448:LYS:HG2	1.83	0.77
1:A:321:PRO:O	1:B:172:GLN:NE2	2.17	0.77
1:A:98:VAL:CG2	1:A:137:THR:HG22	2.14	0.77
1:B:158:LEU:HD12	1:B:158:LEU:O	1.85	0.77
1:B:43:VAL:HG13	1:B:48:PRO:HD2	1.67	0.76
1:B:160:PHE:HB3	1:B:161:PRO:HD3	1.66	0.76
1:A:405:PRO:O	1:A:405:PRO:HD2	1.85	0.76
1:A:406:ASN:C	1:A:406:ASN:ND2	2.39	0.75
1:A:92:ARG:HB2	1:A:92:ARG:NH1	2.00	0.75
1:B:284:THR:HB	1:B:287:GLU:HG3	1.66	0.75
1:A:223:ASN:ND2	1:A:225:ASP:H	1.84	0.75
1:B:394:MET:HA	1:B:394:MET:HE3	1.67	0.75
1:B:98:VAL:HG23	1:B:137:THR:CG2	2.17	0.75
1:B:279:TYR:CE1	1:B:311:PRO:HG3	2.22	0.74
1:B:384:ASN:C	1:B:384:ASN:HD22	1.87	0.74
1:A:294:ASN:ND2	1:A:296:PHE:H	1.85	0.74
1:B:147:ASN:HB2	2:B:507:HEM:HAC	1.68	0.74
1:A:173:THR:HG23	1:A:175:LEU:HD12	1.69	0.74
1:A:297:ASP:OD1	1:A:300:LYS:HE2	1.88	0.74
1:A:238:ASP:OD1	1:A:314:LYS:NZ	2.13	0.73
1:B:371:GLN:HE22	1:B:393:MET:H	1.37	0.72
1:A:446:TYR:HA	1:A:450:LEU:CD2	2.19	0.72
1:B:450:LEU:CD2	1:B:455:ARG:HG2	2.19	0.72
1:B:79:GLY:O	1:B:80:ALA:HB2	1.88	0.72
1:A:446:TYR:HA	1:A:450:LEU:HD21	1.70	0.72
1:B:220:LYS:HE3	1:B:420:HIS:CD2	2.25	0.72
1:A:77:GLY:O	1:A:324:TYR:OH	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ARG:O	1:A:223:ASN:HB3	1.90	0.71
1:A:79:GLY:O	1:A:80:ALA:HB2	1.89	0.71
1:B:223:ASN:ND2	1:B:225:ASP:H	1.88	0.71
1:A:209:ARG:HG2	1:A:274:PRO:HB3	1.73	0.71
1:A:155:ARG:NH2	1:A:438:ASN:ND2	2.05	0.71
1:A:220:LYS:CE	1:A:420:HIS:CD2	2.74	0.71
1:B:410:ALA:HB1	1:B:411:PRO:HD2	1.72	0.71
1:B:360:THR:HG21	2:B:507:HEM:HMA3	1.73	0.71
1:A:361:HIS:NE2	2:A:507:HEM:O2A	2.24	0.70
1:A:322:VAL:CA	1:B:172:GLN:NE2	2.52	0.70
1:A:358:PRO:O	1:A:362:ARG:HD2	1.91	0.70
2:B:507:HEM:HAD1	4:B:518:HOH:O	1.89	0.70
1:A:170:ASN:HD22	1:A:173:THR:H	1.40	0.70
1:A:173:THR:HG22	1:A:175:LEU:H	1.57	0.70
1:A:173:THR:CG2	1:A:175:LEU:CD1	2.66	0.69
1:B:18:ARG:O	1:B:21:GLN:NE2	2.24	0.69
1:A:371:GLN:NE2	1:A:393:MET:HB2	2.05	0.69
1:B:306:ASP:HB3	1:B:307:TYR:CE2	2.28	0.69
1:B:98:VAL:CG2	1:B:137:THR:CG2	2.71	0.69
1:B:173:THR:CG2	1:B:175:LEU:HG	2.20	0.69
1:B:447:LEU:HB2	1:B:448:LYS:HD3	1.75	0.69
1:B:189:PRO:C	1:B:191:SER:H	1.95	0.69
1:A:94:SER:HB2	1:A:221:LEU:HD22	1.74	0.69
1:A:466:LEU:HD12	1:A:466:LEU:O	1.92	0.69
1:A:177:ASP:HB3	1:A:180:MET:CE	2.23	0.69
1:B:476:LYS:O	1:B:477:ALA:C	2.31	0.69
1:A:453:GLU:OE1	1:A:456:LYS:HE2	1.92	0.68
1:A:496:LEU:O	1:A:500:ASN:HB2	1.93	0.68
1:B:90:ILE:CD1	1:B:312:VAL:HG13	2.23	0.68
1:A:36:ASP:HB3	1:B:430:ARG:HD3	1.75	0.68
1:A:263:ASP:O	1:A:264:LEU:C	2.32	0.68
1:A:152:PHE:CB	1:A:298:LEU:HD13	2.24	0.68
1:A:383:ALA:HB1	1:A:411:PRO:CG	2.24	0.68
1:A:85:GLU:HA	1:A:104:LYS:O	1.94	0.68
1:B:65:ARG:HG3	1:B:65:ARG:HH11	1.59	0.68
1:A:90:ILE:O	1:A:93:TYR:HB2	1.93	0.68
1:B:456:LYS:HB3	1:B:491:ARG:HH12	1.58	0.67
1:A:406:ASN:HD22	1:A:408:PHE:H	1.39	0.67
1:B:173:THR:HG22	1:B:175:LEU:CG	2.24	0.67
1:A:177:ASP:HB3	1:A:180:MET:HE2	1.77	0.67
1:A:367:PRO:CG	1:A:390:PRO:HG2	2.13	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:LYS:HG2	1:B:222:VAL:O	1.94	0.67
1:B:384:ASN:ND2	1:B:386:GLN:H	1.91	0.67
1:B:98:VAL:HG23	1:B:137:THR:HB	1.76	0.67
1:B:406:ASN:HD22	1:B:408:PHE:N	1.93	0.67
1:B:15:LYS:HE2	4:B:522:HOH:O	1.95	0.67
1:B:179:ASP:O	1:B:183:ASP:CB	2.42	0.66
1:B:104:LYS:NZ	1:B:138:GLU:OE1	2.23	0.66
1:A:484:VAL:CG2	1:A:488:TYR:HD1	2.09	0.66
1:B:18:ARG:HD3	1:B:21:GLN:HG3	1.77	0.66
1:B:275:SER:HA	1:B:315:LEU:O	1.94	0.66
1:A:126:ARG:O	1:A:127:ASP:HB2	1.96	0.66
1:A:90:ILE:HD13	1:A:312:VAL:HG13	1.77	0.66
1:A:43:VAL:HG13	1:A:48:PRO:HD2	1.78	0.66
1:A:118:GLU:OE2	1:A:169:ARG:NE	2.21	0.66
1:A:281:GLN:HG2	1:A:307:TYR:O	1.95	0.65
1:A:17:GLN:HG2	1:A:17:GLN:O	1.96	0.65
1:A:179:ASP:O	1:A:183:ASP:HB2	1.96	0.65
1:A:183:ASP:O	1:A:187:LEU:HB2	1.95	0.65
1:B:374:VAL:O	1:B:374:VAL:HG22	1.94	0.65
1:A:360:THR:HB	1:B:64:ASP:HB3	1.79	0.65
1:B:169:ARG:NH1	1:B:174:HIS:O	2.26	0.65
1:B:63:PHE:C	1:B:65:ARG:H	1.99	0.65
1:A:300:LYS:NZ	4:A:530:HOH:O	2.29	0.65
1:B:170:ASN:HD22	1:B:172:GLN:N	1.90	0.65
1:B:445:PHE:O	1:B:449:VAL:HB	1.97	0.65
1:A:428:VAL:HG13	1:B:50:LEU:CD1	2.26	0.65
1:B:279:TYR:HE1	1:B:311:PRO:HG3	1.59	0.65
1:A:172:GLN:NE2	1:B:322:VAL:HA	2.12	0.64
1:B:402:ASN:C	1:B:402:ASN:HD22	2.00	0.64
1:A:304:HIS:HD2	1:A:309:LEU:HD21	1.62	0.64
1:A:463:ALA:O	1:A:467:LYS:HB3	1.97	0.64
1:A:236:LYS:HG3	1:A:279:TYR:CE2	2.33	0.64
1:A:458:LEU:HD11	1:A:462:ILE:HD11	1.79	0.64
1:A:98:VAL:CG2	1:A:137:THR:CG2	2.74	0.64
1:B:223:ASN:HD22	1:B:223:ASN:C	2.01	0.64
1:A:172:GLN:HG3	1:B:322:VAL:O	1.98	0.63
1:B:51:VAL:O	1:B:51:VAL:CG1	2.47	0.63
1:B:142:TRP:HB2	1:B:339:PRO:CD	2.27	0.63
1:B:43:VAL:O	1:B:47:GLY:HA3	1.99	0.63
1:A:342:ILE:O	1:A:343:GLU:HB2	1.98	0.63
1:A:172:GLN:HE21	1:B:322:VAL:HA	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:VAL:CG2	1:B:137:THR:HG22	2.29	0.62
1:A:110:VAL:HA	1:A:132:ALA:O	1.99	0.62
1:A:453:GLU:OE1	1:A:456:LYS:CE	2.48	0.62
1:B:74:HIS:CE1	1:B:115:VAL:HG22	2.35	0.62
1:A:220:LYS:CE	1:A:420:HIS:HD2	2.09	0.62
1:B:191:SER:O	1:B:195:VAL:HG23	2.00	0.62
1:B:173:THR:HG21	1:B:175:LEU:HD12	1.82	0.61
1:B:284:THR:HG22	1:B:286:SER:HB2	1.81	0.61
1:B:192:LEU:HD22	1:B:484:VAL:HG11	1.82	0.61
1:B:307:TYR:CD2	1:B:307:TYR:N	2.68	0.61
1:B:458:LEU:CD1	1:B:462:ILE:CD1	2.79	0.61
1:A:100:GLU:HG3	1:A:100:GLU:O	2.01	0.61
1:A:484:VAL:HG22	1:A:488:TYR:HD1	1.66	0.61
1:A:100:GLU:CG	1:A:100:GLU:O	2.48	0.60
1:A:74:HIS:O	1:A:111:ARG:NH2	2.32	0.60
1:A:131:PHE:C	1:A:131:PHE:HD1	2.03	0.60
1:A:471:LEU:HD22	1:A:474:GLN:HE22	1.63	0.60
1:B:17:GLN:HG2	1:B:17:GLN:O	2.00	0.60
1:B:189:PRO:C	1:B:191:SER:N	2.50	0.60
1:A:471:LEU:HD21	1:A:500:ASN:OD1	2.01	0.60
1:A:95:LYS:HG2	1:A:222:VAL:O	2.02	0.60
1:A:152:PHE:HB2	1:A:298:LEU:HD13	1.83	0.60
1:A:275:SER:HA	1:A:315:LEU:O	2.02	0.60
1:B:478:VAL:HG11	1:B:493:GLN:OE1	2.01	0.60
1:A:284:THR:HG22	1:A:286:SER:H	1.66	0.59
1:A:147:ASN:CB	2:A:507:HEM:HAC	2.31	0.59
1:B:458:LEU:CD1	1:B:462:ILE:HD11	2.32	0.59
1:A:385:TYR:OH	1:A:411:PRO:O	2.18	0.59
1:B:385:TYR:OH	1:B:411:PRO:O	2.20	0.59
1:A:236:LYS:HG3	1:A:279:TYR:HE2	1.67	0.59
1:A:160:PHE:HB3	1:A:161:PRO:HD3	1.84	0.59
1:B:470:GLN:OE1	1:B:472:PHE:HE2	1.85	0.59
1:A:268:ILE:HG23	1:A:318:ASN:HA	1.85	0.59
1:A:152:PHE:HB3	1:A:298:LEU:HD13	1.84	0.59
1:B:192:LEU:HD22	1:B:484:VAL:CG1	2.33	0.59
1:B:51:VAL:O	1:B:51:VAL:HG13	2.03	0.59
1:A:125:VAL:O	1:A:129:ARG:NH1	2.32	0.59
1:A:371:GLN:NE2	1:A:393:MET:H	2.01	0.58
1:A:9:ASP:HB3	1:A:13:HIS:CE1	2.38	0.58
1:A:471:LEU:HD22	1:A:474:GLN:CD	2.23	0.58
1:A:4:ARG:HD3	1:A:9:ASP:OD1	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:VAL:HG13	1:B:50:LEU:HD12	1.85	0.58
1:B:156:ASP:OD2	1:B:158:LEU:HB2	2.02	0.58
1:A:131:PHE:C	1:A:131:PHE:CD1	2.75	0.58
1:A:147:ASN:CG	2:A:507:HEM:HAC	2.23	0.58
1:A:173:THR:HG23	1:A:175:LEU:CD1	2.34	0.57
1:B:125:VAL:O	1:B:129:ARG:NH2	2.35	0.57
1:B:21:GLN:O	1:B:22:LYS:CB	2.52	0.57
1:A:98:VAL:HG23	1:A:137:THR:HB	1.86	0.57
1:A:435:ASN:C	1:A:436:ASP:O	2.42	0.57
1:B:371:GLN:NE2	1:B:393:MET:H	2.01	0.57
1:B:458:LEU:HD12	1:B:462:ILE:CD1	2.33	0.57
1:B:98:VAL:HG23	1:B:137:THR:HG21	1.87	0.57
1:A:154:ILE:HG13	1:A:349:MET:CE	2.34	0.57
1:B:453:GLU:O	1:B:456:LYS:HG2	2.05	0.57
1:B:466:LEU:HD12	1:B:466:LEU:O	2.04	0.57
1:B:89:ASP:OD1	1:B:89:ASP:C	2.39	0.56
2:B:507:HEM:HMB1	2:B:507:HEM:HBB2	1.88	0.56
1:A:175:LEU:HD22	1:B:262:ARG:NH2	2.20	0.56
1:A:439:VAL:O	1:A:442:VAL:N	2.38	0.56
1:A:348:LYS:CE	4:A:549:HOH:O	2.54	0.56
1:B:304:HIS:HE1	3:B:508:NDP:O3B	1.89	0.56
1:B:73:VAL:O	1:B:74:HIS:HB2	2.06	0.56
1:A:453:GLU:OE1	1:A:456:LYS:NZ	2.38	0.56
1:A:60:MET:CE	1:A:63:PHE:HD2	2.18	0.56
1:A:238:ASP:CG	1:A:314:LYS:HZ2	2.05	0.56
1:A:356:ALA:O	1:A:360:THR:HG22	2.06	0.56
1:A:237:THR:HG21	1:A:240:GLY:O	2.07	0.55
1:B:131:PHE:HD1	1:B:131:PHE:C	2.09	0.55
1:B:157:ALA:HB2	2:B:507:HEM:HBB1	1.89	0.55
1:B:274:PRO:HB2	1:B:276:TRP:CZ3	2.41	0.55
1:B:334:ASP:O	1:B:337:ASN:HB2	2.06	0.55
1:B:410:ALA:HB1	1:B:411:PRO:CD	2.36	0.55
1:B:456:LYS:CB	1:B:491:ARG:HH12	2.18	0.55
1:A:147:ASN:HB2	2:A:507:HEM:HAC	1.87	0.55
1:A:374:VAL:CG2	1:A:374:VAL:O	2.53	0.55
1:B:284:THR:CG2	1:B:286:SER:HB2	2.35	0.55
1:B:301:VAL:HG22	1:B:441:GLN:OE1	2.05	0.55
1:A:266:ASN:O	1:A:267:ALA:O	2.25	0.55
1:A:487:GLU:HG2	1:A:491:ARG:HD2	1.88	0.55
1:B:372:ILE:O	1:B:373:PRO:C	2.45	0.55
1:B:485:HIS:CD2	1:B:486:PRO:HD2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:PHE:O	1:B:65:ARG:N	2.39	0.55
1:A:157:ALA:CB	2:A:507:HEM:HBB1	2.37	0.55
1:A:447:LEU:CB	1:A:448:LYS:HD2	2.37	0.54
1:B:453:GLU:HA	1:B:453:GLU:OE2	2.06	0.54
1:B:65:ARG:NH1	1:B:65:ARG:HG3	2.21	0.54
1:A:345:SER:HB2	1:A:346:PRO:CD	2.37	0.54
1:A:73:VAL:O	1:A:74:HIS:HB2	2.07	0.54
1:A:239:GLN:H	1:A:239:GLN:NE2	2.05	0.54
1:A:200:SER:O	1:A:203:GLY:N	2.40	0.54
1:A:189:PRO:C	1:A:191:SER:H	2.10	0.54
1:A:245:SER:OG	1:A:248:ASP:HB2	2.07	0.54
1:B:229:VAL:HG11	1:B:282:VAL:HG23	1.89	0.54
1:A:229:VAL:HG13	1:A:282:VAL:CG2	2.36	0.54
1:B:212:ASP:OD1	1:B:237:THR:HG22	2.08	0.54
1:A:4:ARG:CD	1:A:9:ASP:OD1	2.56	0.54
1:B:63:PHE:C	1:B:65:ARG:N	2.61	0.54
1:A:178:PRO:O	1:A:182:TRP:HB2	2.08	0.53
1:A:98:VAL:HG23	1:A:137:THR:HG22	1.81	0.53
1:A:406:ASN:O	1:A:406:ASN:ND2	2.42	0.53
1:A:371:GLN:HE22	1:A:393:MET:H	1.57	0.53
1:B:188:ARG:O	1:B:191:SER:HB3	2.07	0.53
1:B:291:PHE:CE1	1:B:293:PHE:HB2	2.44	0.53
1:B:331:LEU:HD13	1:B:333:PHE:CZ	2.44	0.53
1:A:179:ASP:O	1:A:183:ASP:N	2.33	0.53
1:A:487:GLU:CG	1:A:491:ARG:HD2	2.37	0.53
1:A:74:HIS:HA	1:A:114:THR:O	2.08	0.53
1:B:189:PRO:HB2	1:B:192:LEU:CD1	2.39	0.53
1:B:229:VAL:CG1	1:B:282:VAL:CG2	2.82	0.53
1:B:384:ASN:C	1:B:384:ASN:ND2	2.61	0.53
1:A:82:GLY:HA3	1:A:316:VAL:O	2.08	0.53
1:A:142:TRP:HA	1:A:337:ASN:O	2.09	0.53
1:A:38:LEU:HA	1:B:159:LEU:HD22	1.91	0.53
1:A:405:PRO:CD	1:A:405:PRO:O	2.55	0.53
1:A:444:THR:CA	1:A:448:LYS:HD3	2.28	0.53
1:A:92:ARG:O	1:A:223:ASN:CB	2.57	0.53
1:B:383:ALA:HB1	1:B:411:PRO:HG3	1.90	0.53
1:A:155:ARG:NE	1:A:433:SER:O	2.29	0.53
1:A:276:TRP:HZ3	1:A:317:LEU:HD22	1.74	0.52
1:B:447:LEU:HB2	1:B:448:LYS:CD	2.39	0.52
1:B:57:THR:O	1:B:61:ALA:HB2	2.09	0.52
1:A:400:ALA:O	1:A:401:PRO:C	2.47	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:GLY:O	1:B:80:ALA:CB	2.57	0.52
1:B:21:GLN:O	1:B:22:LYS:HB3	2.10	0.52
1:B:245:SER:OG	1:B:248:ASP:HB2	2.10	0.52
1:A:294:ASN:HD22	1:A:295:PRO:N	2.07	0.52
1:A:406:ASN:OD1	1:A:410:ALA:HB3	2.10	0.52
1:A:430:ARG:HD3	1:B:36:ASP:HB3	1.92	0.52
1:B:110:VAL:HG21	1:B:317:LEU:HD11	1.92	0.52
1:B:458:LEU:HD11	1:B:462:ILE:CD1	2.40	0.52
1:B:136:TYR:HB3	4:B:531:HOH:O	2.09	0.52
1:B:148:ASN:HD22	1:B:148:ASN:H	1.58	0.52
1:B:384:ASN:HD22	1:B:385:TYR:N	2.08	0.52
1:B:415:PRO:C	1:B:417:ALA:H	2.14	0.52
1:B:439:VAL:O	1:B:440:THR:C	2.48	0.52
1:B:60:MET:CE	1:B:64:ASP:OD2	2.58	0.52
1:A:342:ILE:O	1:A:343:GLU:CB	2.56	0.51
1:B:131:PHE:CD1	1:B:131:PHE:C	2.84	0.51
1:B:236:LYS:O	1:B:276:TRP:HA	2.10	0.51
1:A:74:HIS:CE1	1:A:115:VAL:HG22	2.46	0.51
1:B:392:CYS:SG	1:B:396:ASN:HB2	2.51	0.51
1:A:276:TRP:CZ3	1:A:317:LEU:HD22	2.45	0.51
1:B:129:ARG:H	1:B:148:ASN:ND2	2.09	0.51
1:B:84:PHE:O	1:B:105:ARG:HA	2.11	0.51
1:B:402:ASN:C	1:B:402:ASN:ND2	2.64	0.51
1:B:54:VAL:O	1:B:54:VAL:HG23	2.10	0.51
1:A:458:LEU:HD12	1:A:462:ILE:HG13	1.92	0.51
1:B:394:MET:HA	1:B:394:MET:HE2	1.91	0.51
1:A:150:PRO:HD2	1:A:151:ILE:H	1.76	0.51
1:B:147:ASN:CB	2:B:507:HEM:HAC	2.38	0.51
1:B:493:GLN:O	1:B:494:ALA:C	2.48	0.50
1:B:177:ASP:CB	1:B:180:MET:CE	2.85	0.50
1:B:300:LYS:NZ	1:B:437:ASP:O	2.43	0.50
1:A:406:ASN:HD22	1:A:408:PHE:N	2.09	0.50
1:A:471:LEU:CD2	1:A:474:GLN:HE22	2.25	0.50
1:B:189:PRO:HB2	1:B:192:LEU:HD12	1.93	0.50
1:A:458:LEU:CD1	1:A:462:ILE:HD11	2.41	0.50
1:A:46:ARG:HD3	1:B:294:ASN:ND2	2.26	0.50
1:A:235:TYR:HA	1:A:277:THR:O	2.12	0.50
1:A:93:TYR:HB3	1:A:221:LEU:HD13	1.94	0.50
1:B:152:PHE:HB3	1:B:298:LEU:HD13	1.94	0.50
1:B:470:GLN:OE1	1:B:472:PHE:CE2	2.65	0.50
1:B:18:ARG:HH11	1:B:18:ARG:HG2	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:458:LEU:CD1	1:B:462:ILE:HD12	2.41	0.50
1:A:86:VAL:N	1:A:104:LYS:O	2.43	0.50
1:A:294:ASN:C	1:A:294:ASN:HD22	2.15	0.50
1:A:309:LEU:HD12	4:A:517:HOH:O	2.11	0.50
1:B:90:ILE:CD1	1:B:312:VAL:CG1	2.89	0.50
1:B:406:ASN:C	1:B:406:ASN:ND2	2.65	0.50
1:A:90:ILE:HG21	1:A:312:VAL:HG22	1.94	0.49
1:B:236:LYS:HG3	1:B:279:TYR:CE2	2.47	0.49
1:A:170:ASN:ND2	1:A:172:GLN:H	2.10	0.49
1:A:118:GLU:HG3	1:B:120:GLY:CA	2.43	0.49
1:A:154:ILE:HG13	1:A:349:MET:HE2	1.94	0.49
1:A:54:VAL:HA	1:A:57:THR:HG23	1.93	0.49
1:A:155:ARG:HH22	1:A:438:ASN:HD21	0.53	0.49
1:A:463:ALA:HA	1:A:466:LEU:HB3	1.94	0.49
1:B:9:ASP:OD1	1:B:12:LYS:NZ	2.45	0.49
1:B:173:THR:CG2	1:B:175:LEU:CG	2.86	0.49
1:B:223:ASN:ND2	1:B:225:ASP:N	2.59	0.49
1:A:430:ARG:NH2	1:B:53:ASP:OD2	2.45	0.49
1:B:57:THR:O	1:B:61:ALA:CB	2.60	0.49
1:B:306:ASP:O	1:B:308:PRO:HD3	2.13	0.49
1:A:189:PRO:C	1:A:191:SER:N	2.66	0.49
1:A:487:GLU:HG2	1:A:491:ARG:CD	2.42	0.49
1:B:155:ARG:NH2	1:B:438:ASN:ND2	2.13	0.49
1:A:142:TRP:HB2	1:A:339:PRO:HD3	1.93	0.49
1:B:129:ARG:HG2	4:B:542:HOH:O	2.13	0.49
1:B:72:VAL:HG13	1:B:73:VAL:HG22	1.95	0.49
1:B:178:PRO:O	1:B:182:TRP:HB2	2.12	0.49
1:B:294:ASN:HD21	1:B:296:PHE:HD2	1.61	0.49
1:A:449:VAL:O	1:A:449:VAL:HG12	2.12	0.49
1:A:435:ASN:O	1:A:436:ASP:O	2.31	0.48
1:A:487:GLU:O	1:A:491:ARG:CG	2.44	0.48
1:B:19:ALA:C	1:B:21:GLN:H	2.16	0.48
1:B:394:MET:CA	1:B:394:MET:CE	2.84	0.48
1:A:81:PHE:CD1	1:A:81:PHE:N	2.80	0.48
1:B:229:VAL:HG11	1:B:282:VAL:CG2	2.43	0.48
1:A:84:PHE:O	1:A:105:ARG:HA	2.13	0.48
1:A:357:TYR:CZ	2:A:507:HEM:NA	2.81	0.48
1:A:447:LEU:HB2	1:A:448:LYS:CD	2.44	0.48
1:B:361:HIS:NE2	2:B:507:HEM:O2A	2.46	0.48
1:A:236:LYS:O	1:A:276:TRP:HA	2.14	0.48
1:B:386:GLN:O	1:B:387:ARG:NH1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:VAL:HG21	1:A:137:THR:HG22	1.93	0.48
1:A:371:GLN:HE22	1:A:393:MET:N	2.11	0.48
1:A:478:VAL:O	1:A:482:SER:HB2	2.14	0.48
1:A:283:MET:HB3	1:A:302:TRP:CH2	2.49	0.48
1:B:297:ASP:OD2	1:B:299:THR:OG1	2.31	0.48
1:B:441:GLN:O	1:B:444:THR:HG23	2.14	0.47
1:A:98:VAL:HG23	1:A:137:THR:CB	2.45	0.47
1:B:444:THR:HB	1:B:448:LYS:HZ3	1.79	0.47
1:A:223:ASN:ND2	1:A:223:ASN:C	2.56	0.47
1:B:406:ASN:C	1:B:406:ASN:HD22	2.18	0.47
1:A:223:ASN:ND2	1:A:225:ASP:N	2.57	0.47
1:A:471:LEU:CD2	1:A:474:GLN:NE2	2.64	0.47
1:A:60:MET:HE3	1:A:63:PHE:HD2	1.78	0.47
1:B:138:GLU:N	1:B:138:GLU:OE2	2.44	0.47
1:B:293:PHE:O	1:B:295:PRO:HD3	2.15	0.47
1:A:134:LYS:HE3	1:A:331:LEU:HD23	1.93	0.47
1:A:201:ASP:C	1:A:203:GLY:H	2.14	0.47
1:A:418:LEU:HA	1:A:418:LEU:HD23	1.78	0.47
1:B:98:VAL:CG2	1:B:137:THR:HG21	2.44	0.47
1:B:159:LEU:HD11	1:B:188:ARG:CZ	2.44	0.47
1:B:487:GLU:O	1:B:491:ARG:HG3	2.14	0.47
1:A:18:ARG:O	1:A:21:GLN:NE2	2.47	0.47
1:A:40:SER:HB3	1:A:49:LEU:HD13	1.97	0.47
1:B:135:PHE:CD1	1:B:142:TRP:CE3	3.02	0.47
1:A:64:ASP:HB3	1:B:360:THR:HB	1.97	0.47
1:B:209:ARG:HB2	4:B:541:HOH:O	2.14	0.47
1:B:218:THR:HA	1:B:231:CYS:O	2.15	0.47
1:B:71:ARG:HD2	1:B:111:ARG:NH2	2.30	0.47
1:B:149:THR:HG23	1:B:151:ILE:O	2.15	0.47
1:B:145:VAL:HG22	1:B:333:PHE:HB3	1.97	0.47
1:B:384:ASN:HD22	1:B:386:GLN:H	1.62	0.47
1:A:93:TYR:CZ	1:A:282:VAL:HG11	2.50	0.47
1:A:294:ASN:ND2	1:A:294:ASN:C	2.69	0.46
1:A:324:TYR:O	1:A:325:PHE:C	2.54	0.46
1:B:127:ASP:C	1:B:128:PRO:O	2.52	0.46
1:B:89:ASP:O	1:B:89:ASP:OD1	2.32	0.46
1:A:217:HIS:HB2	1:A:219:PHE:CZ	2.50	0.46
1:A:59:GLU:HB2	4:A:515:HOH:O	2.14	0.46
1:A:168:LYS:HE3	1:B:67:ARG:NH2	2.30	0.46
1:A:172:GLN:NE2	1:B:321:PRO:O	2.46	0.46
1:B:177:ASP:HA	1:B:178:PRO:HD3	1.70	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:458:LEU:HD11	1:B:462:ILE:HD11	1.97	0.46
1:A:304:HIS:CD2	1:A:309:LEU:HD21	2.47	0.46
1:B:284:THR:HG22	1:B:286:SER:N	2.21	0.46
1:B:191:SER:O	1:B:195:VAL:CG2	2.63	0.46
1:B:19:ALA:C	1:B:21:GLN:N	2.69	0.46
1:A:112:PHE:CD2	1:A:208:HIS:HB3	2.51	0.46
1:A:293:PHE:O	1:A:295:PRO:HD3	2.16	0.46
1:B:209:ARG:HH11	1:B:209:ARG:HD3	1.45	0.46
1:B:400:ALA:O	1:B:401:PRO:C	2.54	0.46
1:A:5:ASP:OD2	1:A:7:ALA:HB3	2.15	0.46
1:B:437:ASP:OD2	1:B:437:ASP:C	2.55	0.46
1:B:447:LEU:O	1:B:455:ARG:NH2	2.49	0.46
1:A:53:ASP:C	1:A:55:VAL:H	2.19	0.46
1:A:77:GLY:HA3	1:A:112:PHE:O	2.15	0.46
1:B:475:LYS:HA	1:B:475:LYS:HD2	1.67	0.46
1:A:372:ILE:O	1:A:373:PRO:C	2.54	0.45
1:A:141:ASN:OD1	1:A:377:PRO:HA	2.16	0.45
1:A:282:VAL:CG2	1:A:283:MET:N	2.78	0.45
1:A:360:THR:HG21	2:A:507:HEM:HMA3	1.98	0.45
1:A:43:VAL:O	1:A:47:GLY:HA3	2.16	0.45
1:A:97:LYS:O	1:A:100:GLU:HB3	2.16	0.45
1:B:134:LYS:HE3	1:B:331:LEU:CD2	2.46	0.45
1:B:351:GLN:HA	1:B:354:LEU:HD22	1.97	0.45
1:A:147:ASN:ND2	2:A:507:HEM:C3C	2.84	0.45
1:A:342:ILE:HG22	1:A:343:GLU:H	1.82	0.45
1:A:384:ASN:ND2	1:A:386:GLN:H	2.14	0.45
1:B:467:LYS:HE2	1:B:468:ASP:OD2	2.17	0.45
1:B:22:LYS:HD3	1:B:22:LYS:HA	1.61	0.45
1:B:364:ARG:HH21	1:B:364:ARG:HD2	1.35	0.45
1:B:177:ASP:OD1	1:B:179:ASP:HB2	2.17	0.45
1:B:223:ASN:ND2	1:B:223:ASN:C	2.69	0.45
1:A:118:GLU:H	1:A:118:GLU:HG2	1.16	0.45
1:B:450:LEU:HD11	1:B:458:LEU:HD22	1.99	0.45
1:A:343:GLU:HA	1:A:344:PRO:HD3	1.94	0.45
1:A:157:ALA:HB2	2:A:507:HEM:HBB1	1.98	0.45
1:B:239:GLN:OE1	1:B:274:PRO:HA	2.17	0.45
1:A:266:ASN:O	1:A:267:ALA:C	2.54	0.45
1:A:322:VAL:CA	1:B:172:GLN:HE21	2.28	0.45
1:A:439:VAL:HG23	1:A:443:ARG:HH11	1.82	0.45
1:B:206:ASP:HA	1:B:244:LEU:HG	1.99	0.45
1:B:4:ARG:NH1	1:B:9:ASP:OD1	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:GLY:O	1:A:80:ALA:CB	2.59	0.45
1:A:134:LYS:HE3	1:A:331:LEU:HD22	1.99	0.44
1:A:108:ILE:CD1	1:A:315:LEU:HD12	2.42	0.44
1:A:357:TYR:CB	1:A:358:PRO:CD	2.96	0.44
1:A:51:VAL:O	1:A:51:VAL:CG1	2.65	0.44
1:B:110:VAL:HA	1:B:132:ALA:O	2.16	0.44
1:B:158:LEU:HD13	1:B:158:LEU:HA	1.70	0.44
1:B:293:PHE:O	1:B:295:PRO:CD	2.65	0.44
1:B:487:GLU:CG	1:B:491:ARG:HD2	2.46	0.44
1:B:5:ASP:HA	1:B:6:PRO:HD3	1.80	0.44
1:A:326:ALA:HA	1:A:330:GLN:HE21	1.82	0.44
1:A:72:VAL:HG12	2:A:507:HEM:HMA1	1.99	0.44
1:A:127:ASP:C	1:A:128:PRO:O	2.52	0.44
1:A:92:ARG:HG3	1:A:92:ARG:H	1.56	0.44
1:B:135:PHE:CE1	1:B:142:TRP:CZ3	3.05	0.44
1:B:220:LYS:HD2	1:B:228:ALA:HB1	1.98	0.44
1:B:458:LEU:HD12	1:B:462:ILE:HD11	1.98	0.44
1:B:157:ALA:CB	2:B:507:HEM:CBB	2.95	0.44
1:A:322:VAL:HA	1:B:172:GLN:HE21	1.68	0.44
1:A:406:ASN:HD22	1:A:407:SER:N	2.14	0.44
1:A:39:ASN:ND2	1:B:432:ASN:HA	2.33	0.44
1:A:449:VAL:CG1	1:A:449:VAL:O	2.64	0.44
1:A:84:PHE:HA	1:A:314:LYS:O	2.18	0.44
1:B:95:LYS:HG2	1:B:95:LYS:H	1.47	0.44
1:A:173:THR:HG22	1:A:175:LEU:N	2.28	0.44
1:A:177:ASP:CG	1:A:180:MET:HG3	2.38	0.44
1:A:360:THR:HB	1:B:64:ASP:CB	2.48	0.44
2:A:507:HEM:CBB	2:A:507:HEM:CMB	2.92	0.44
1:B:98:VAL:HG23	1:B:137:THR:CB	2.45	0.44
1:A:282:VAL:HG23	1:A:283:MET:N	2.31	0.43
1:A:182:TRP:HB3	1:A:473:ILE:CG2	2.48	0.43
1:B:177:ASP:CB	1:B:180:MET:HE2	2.48	0.43
1:B:239:GLN:HB2	1:B:239:GLN:HE21	1.53	0.43
1:B:92:ARG:HD2	1:B:93:TYR:CE1	2.53	0.43
1:B:299:THR:C	1:B:300:LYS:HG2	2.37	0.43
1:A:284:THR:CG2	1:A:286:SER:H	2.30	0.43
1:A:353:ARG:O	1:A:354:LEU:C	2.56	0.43
1:A:439:VAL:CG2	1:A:443:ARG:NH1	2.81	0.43
1:A:458:LEU:HD12	1:A:458:LEU:C	2.38	0.43
1:A:9:ASP:O	1:A:12:LYS:HB3	2.17	0.43
1:A:430:ARG:HH11	1:A:430:ARG:HD2	1.20	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:LEU:HD11	1:A:500:ASN:OD1	2.18	0.43
1:A:91:THR:HA	1:A:94:SER:O	2.19	0.43
1:B:182:TRP:O	1:B:183:ASP:C	2.55	0.43
1:A:150:PRO:CD	1:A:151:ILE:H	2.31	0.43
1:A:99:PHE:CE1	1:A:312:VAL:HG11	2.53	0.43
1:B:448:LYS:H	1:B:448:LYS:HG2	1.50	0.43
1:A:206:ASP:HA	1:A:244:LEU:HG	2.01	0.43
1:A:79:GLY:HA2	1:A:110:VAL:O	2.18	0.43
1:A:147:ASN:HB2	2:A:507:HEM:CAC	2.47	0.43
1:A:154:ILE:HG13	1:A:349:MET:HE1	2.01	0.43
1:B:236:LYS:HB3	1:B:236:LYS:HE2	1.70	0.43
1:B:484:VAL:HG22	1:B:488:TYR:HD1	1.84	0.43
1:A:172:GLN:HE21	1:B:322:VAL:CA	2.29	0.43
1:A:381:ARG:HD3	1:A:381:ARG:HH11	1.60	0.43
1:B:387:ARG:HA	1:B:396:ASN:HD21	1.84	0.43
1:A:170:ASN:HD21	1:B:10:GLN:NE2	2.17	0.42
1:A:342:ILE:HG22	1:A:343:GLU:N	2.34	0.42
1:A:444:THR:O	1:A:445:PHE:C	2.57	0.42
1:A:447:LEU:HB2	1:A:448:LYS:HD2	2.00	0.42
1:B:221:LEU:O	1:B:228:ALA:HA	2.19	0.42
1:B:236:LYS:HG2	1:B:236:LYS:H	1.67	0.42
1:B:394:MET:CA	1:B:394:MET:HE3	2.42	0.42
1:B:479:LYS:HB3	1:B:479:LYS:HE2	1.46	0.42
1:B:78:ALA:O	1:B:111:ARG:HA	2.19	0.42
1:A:251:ARG:O	1:A:255:GLU:HB2	2.18	0.42
1:A:387:ARG:HD3	1:A:387:ARG:HH11	1.67	0.42
1:B:3:ASN:HB3	1:B:4:ARG:H	1.70	0.42
1:B:157:ALA:HB2	2:B:507:HEM:CBB	2.49	0.42
1:B:354:LEU:HD12	1:B:354:LEU:HA	1.68	0.42
1:A:337:ASN:HD22	1:A:337:ASN:HA	1.57	0.42
1:B:294:ASN:HA	1:B:295:PRO:HD2	1.75	0.42
1:B:449:VAL:HG21	3:B:508:NDP:C4D	2.49	0.42
1:A:147:ASN:ND2	2:A:507:HEM:CAC	2.83	0.42
1:B:304:HIS:CE1	3:B:508:NDP:O3B	2.71	0.42
1:A:118:GLU:OE2	1:A:169:ARG:NH2	2.50	0.42
1:A:170:ASN:HA	1:A:171:PRO:HD3	1.85	0.42
1:A:50:LEU:HD12	1:B:428:VAL:HG13	2.01	0.42
1:B:170:ASN:HA	1:B:171:PRO:HD3	1.82	0.42
1:B:18:ARG:HH11	1:B:18:ARG:CG	2.32	0.42
1:B:306:ASP:CB	1:B:307:TYR:CE2	3.02	0.42
1:B:471:LEU:O	1:B:472:PHE:C	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:GLU:OE2	1:A:456:LYS:HG2	2.20	0.42
1:B:332:ALA:HB1	1:B:361:HIS:CE1	2.55	0.42
1:A:388:ASP:H	1:A:396:ASN:HD21	1.68	0.41
1:B:429:GLN:HE21	1:B:429:GLN:HB2	1.34	0.41
1:B:177:ASP:HB3	1:B:180:MET:HE2	1.94	0.41
1:B:402:ASN:HD22	1:B:403:TYR:N	2.18	0.41
1:A:77:GLY:CA	1:A:112:PHE:O	2.69	0.41
1:A:329:GLU:HA	1:A:329:GLU:OE2	2.20	0.41
1:A:87:THR:OG1	1:A:88:HIS:ND1	2.51	0.41
1:A:89:ASP:OD1	1:A:89:ASP:C	2.57	0.41
1:B:9:ASP:HB3	1:B:13:HIS:CE1	2.56	0.41
1:B:194:GLN:O	1:B:198:LEU:N	2.44	0.41
1:B:275:SER:HB3	1:B:316:VAL:HG22	2.02	0.41
1:B:439:VAL:O	1:B:440:THR:O	2.38	0.41
1:B:453:GLU:OE2	1:B:453:GLU:CA	2.66	0.41
1:A:134:LYS:HE2	1:A:134:LYS:HB2	1.56	0.41
1:A:496:LEU:HA	1:A:496:LEU:HD23	1.99	0.41
1:A:127:ASP:HA	1:A:128:PRO:HD3	1.93	0.41
1:A:135:PHE:CD1	1:A:142:TRP:CE3	3.08	0.41
1:A:148:ASN:N	1:A:148:ASN:ND2	2.46	0.41
1:A:237:THR:CG2	1:A:240:GLY:O	2.68	0.41
1:B:50:LEU:HA	1:B:50:LEU:HD23	1.85	0.41
1:A:443:ARG:HB2	1:A:443:ARG:HE	1.49	0.41
1:A:19:ALA:C	1:A:21:GLN:H	2.24	0.41
1:A:456:LYS:HG3	1:A:460:GLU:OE1	2.20	0.41
1:A:267:ALA:O	1:A:268:ILE:C	2.59	0.41
1:A:298:LEU:HA	1:A:298:LEU:HD23	1.66	0.41
1:A:239:GLN:CD	1:A:239:GLN:N	2.74	0.41
1:A:145:VAL:HG22	1:A:333:PHE:HB3	2.02	0.41
1:A:439:VAL:CG2	1:A:443:ARG:HH11	2.34	0.41
1:A:439:VAL:O	1:A:440:THR:C	2.58	0.41
1:A:39:ASN:HA	1:B:156:ASP:OD1	2.21	0.41
1:A:484:VAL:HG21	1:A:488:TYR:HD1	1.84	0.41
1:A:120:GLY:HA2	1:B:118:GLU:HG3	2.03	0.40
1:B:98:VAL:HG21	1:B:137:THR:HG22	2.03	0.40
1:B:222:VAL:HG21	1:B:343:GLU:OE2	2.21	0.40
1:A:14:TRP:CZ3	1:A:18:ARG:HD2	2.56	0.40
1:A:221:LEU:HG	1:A:231:CYS:SG	2.62	0.40
1:A:274:PRO:HG2	1:A:317:LEU:HB2	2.02	0.40
1:A:154:ILE:O	1:A:349:MET:HE2	2.21	0.40
1:B:134:LYS:HE2	1:B:134:LYS:HB2	1.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:ARG:CZ	1:B:175:LEU:HD13	2.51	0.40
1:B:213:GLY:HA3	1:B:235:TYR:CE1	2.56	0.40
1:B:5:ASP:OD1	1:B:5:ASP:N	2.53	0.40
1:A:170:ASN:HD22	1:A:172:GLN:H	1.69	0.40
1:A:334:ASP:O	1:A:337:ASN:HB2	2.21	0.40
1:A:451:ASN:O	1:A:455:ARG:HG3	2.22	0.40
1:B:84:PHE:HA	1:B:314:LYS:O	2.21	0.40
1:A:295:PRO:HD2	1:B:46:ARG:NH2	2.36	0.40
1:A:354:LEU:HA	1:A:354:LEU:HD12	1.71	0.40
1:A:357:TYR:HB2	1:A:358:PRO:CD	2.51	0.40
1:A:471:LEU:HD21	1:A:500:ASN:HD21	1.87	0.40
1:B:160:PHE:HB3	1:B:161:PRO:CD	2.45	0.40

All (3) 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]	1.78	0.42
1:A:10:GLN:NE2	4:A:541:HOH:O[6_556]	1.86	0.34
1:A:183:ASP:OD1	1:B:407:SER:OG[6_556]	2.12	0.08

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	496/506 (98%)	418 (84%)	64 (13%)	14 (3%)	5	7
1	B	496/506 (98%)	425 (86%)	63 (13%)	8 (2%)	9	17
All	All	992/1012 (98%)	843 (85%)	127 (13%)	22 (2%)	6	10

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	242	LYS
1	A	267	ALA
1	A	373	PRO
1	A	440	THR
1	A	451	ASN
1	A	54	VAL
1	A	101	HIS
1	A	268	ILE
1	B	54	VAL
1	B	64	ASP
1	B	242	LYS
1	B	440	THR
1	A	128	PRO
1	A	340	PRO
1	B	267	ALA
1	A	22	LYS
1	A	64	ASP
1	B	80	ALA
1	A	436	ASP
1	B	22	LYS
1	B	401	PRO
1	A	485	HIS

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	430/437 (98%)	351 (82%)	79 (18%)	1	2
1	B	430/437 (98%)	351 (82%)	79 (18%)	1	2
All	All	860/874 (98%)	702 (82%)	158 (18%)	1	2

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	10	GLN

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Mol	Chain	Res	Type
1	A	11	MET
1	A	13	HIS
1	A	18	ARG
1	A	21	GLN
1	A	26	LEU
1	A	37	LYS
1	A	40	SER
1	A	43	VAL
1	A	51	VAL
1	A	55	VAL
1	A	57	THR
1	A	67	ARG
1	A	72	VAL
1	A	89	ASP
1	A	92	ARG
1	A	100	GLU
1	A	102	ILE
1	A	118	GLU
1	A	129	ARG
1	A	131	PHE
1	A	137	THR
1	A	148	ASN
1	A	155	ARG
1	A	158	LEU
1	A	159	LEU
1	A	204	ILE
1	A	220	LYS
1	A	223	ASN
1	A	229	VAL
1	A	235	TYR
1	A	236	LYS
1	A	239	GLN
1	A	242	LYS
1	A	255	GLU
1	A	261	LEU
1	A	263	ASP
1	A	264	LEU
1	A	282	VAL
1	A	286	SER
1	A	290	ILE
1	A	294	ASN
1	A	298	LEU

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Mol	Chain	Res	Type
1	A	304	HIS
1	A	311	PRO
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	373	PRO
1	A	384	ASN
1	A	386	GLN
1	A	393	MET
1	A	394	MET
1	A	396	ASN
1	A	402	ASN
1	A	406	ASN
1	A	413	HIS
1	A	439	VAL
1	A	443	ARG
1	A	444	THR
1	A	448	LYS
1	A	450	LEU
1	A	452	GLU
1	A	456	LYS
1	A	458	LEU
1	A	471	LEU
1	A	475	LYS
1	A	482	SER
1	A	484	VAL
1	A	488	TYR
1	A	498	LYS
1	A	500	ASN
1	B	4	ARG
1	B	10	GLN
1	B	12	LYS
1	B	18	ARG
1	B	21	GLN
1	B	37	LYS
1	B	40	SER

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Mol	Chain	Res	Type
1	B	43	VAL
1	B	48	PRO
1	B	51	VAL
1	B	57	THR
1	B	71	ARG
1	B	73	VAL
1	B	76	LYS
1	B	89	ASP
1	B	91	THR
1	B	92	ARG
1	B	95	LYS
1	B	102	ILE
1	B	118	GLU
1	B	131	PHE
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	170	ASN
1	B	172	GLN
1	B	192	LEU
1	B	220	LYS
1	B	223	ASN
1	B	229	VAL
1	B	235	TYR
1	B	236	LYS
1	B	239	GLN
1	B	244	LEU
1	B	246	VAL
1	B	247	GLU
1	B	264	LEU
1	B	272	ASN
1	B	290	ILE
1	B	294	ASN
1	B	298	LEU
1	B	315	LEU
1	B	317	LEU
1	B	318	ASN

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Mol	Chain	Res	Type
1	B	331	LEU
1	B	335	PRO
1	B	337	ASN
1	B	339	PRO
1	B	354	LEU
1	B	355	PHE
1	B	365	LEU
1	B	372	ILE
1	B	379	ARG
1	B	384	ASN
1	B	386	GLN
1	B	392	CYS
1	B	394	MET
1	B	402	ASN
1	B	405	PRO
1	B	406	ASN
1	B	407	SER
1	B	413	HIS
1	B	414	GLN
1	B	415	PRO
1	B	444	THR
1	B	448	LYS
1	B	450	LEU
1	B	458	LEU
1	B	471	LEU
1	B	475	LYS
1	B	479	LYS
1	B	488	TYR
1	B	498	LYS
1	B	500	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	10	GLN
1	A	13	HIS
1	A	17	GLN
1	A	21	GLN
1	A	39	ASN
1	A	148	ASN
1	A	170	ASN

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Mol	Chain	Res	Type
1	A	172	GLN
1	A	223	ASN
1	A	234	HIS
1	A	272	ASN
1	A	281	GLN
1	A	294	ASN
1	A	304	HIS
1	A	330	GLN
1	A	337	ASN
1	A	368	ASN
1	A	371	GLN
1	A	384	ASN
1	A	396	ASN
1	A	397	GLN
1	A	406	ASN
1	A	420	HIS
1	A	429	GLN
1	A	438	ASN
1	A	474	GLN
1	A	485	HIS
1	B	10	GLN
1	B	17	GLN
1	B	21	GLN
1	B	148	ASN
1	B	170	ASN
1	B	172	GLN
1	B	223	ASN
1	B	234	HIS
1	B	272	ASN
1	B	281	GLN
1	B	294	ASN
1	B	304	HIS
1	B	323	ASN
1	B	337	ASN
1	B	368	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

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Mol	Chain	Res	Type
1	B	420	HIS
1	B	429	GLN
1	B	438	ASN
1	B	474	GLN
1	B	485	HIS

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 carbohydrates 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	$\# Z > 2$
3	NDP	B	508	-	45,52,52	2.54	11 (24%)	53,80,80	2.20	12 (22%)
2	HEM	B	507	1	27,50,50	1.71	6 (22%)	17,82,82	2.35	8 (47%)
2	HEM	A	507	1	27,50,50	1.86	9 (33%)	17,82,82	3.18	8 (47%)
3	NDP	A	508	-	45,52,52	2.52	11 (24%)	53,80,80	2.20	12 (22%)

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	-	1/1/14/17	3/30/77/77	0/5/5/5
2	HEM	B	507	1	-	0/6/54/54	-
2	HEM	A	507	1	-	0/6/54/54	-
3	NDP	A	508	-	1/1/14/17	3/30/77/77	0/5/5/5

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	508	NDP	O4B-C1B	9.69	1.54	1.41
3	A	508	NDP	O4B-C1B	9.65	1.54	1.41
3	B	508	NDP	P2B-O2B	8.71	1.75	1.59
3	A	508	NDP	P2B-O2B	8.61	1.75	1.59
3	B	508	NDP	O3B-C3B	-5.10	1.31	1.43
3	A	508	NDP	O3B-C3B	-5.05	1.31	1.43
3	B	508	NDP	C4N-C3N	-4.47	1.41	1.49
3	A	508	NDP	C4N-C3N	-4.42	1.41	1.49
2	A	507	HEM	C3B-C2B	-4.16	1.34	1.40
2	B	507	HEM	C3B-C2B	-4.05	1.34	1.40
3	B	508	NDP	C4N-C5N	-3.82	1.38	1.48
3	A	508	NDP	C4N-C5N	-3.81	1.38	1.48
2	A	507	HEM	C3C-CAC	3.64	1.55	1.47
3	B	508	NDP	C7N-C3N	3.51	1.56	1.48
3	A	508	NDP	C7N-C3N	3.49	1.56	1.48
2	A	507	HEM	C3C-C2C	-3.31	1.35	1.40
2	B	507	HEM	CAA-C2A	3.13	1.56	1.52
2	A	507	HEM	C3B-CAB	2.89	1.53	1.47
3	B	508	NDP	C6N-C5N	2.60	1.38	1.33
3	A	508	NDP	C6N-C5N	2.60	1.38	1.33
2	B	507	HEM	CMA-C3A	2.60	1.57	1.51
2	A	507	HEM	C1C-C2C	-2.49	1.36	1.42
2	B	507	HEM	C3B-CAB	2.46	1.52	1.47
2	B	507	HEM	C3C-C2C	-2.45	1.37	1.40
2	A	507	HEM	CMA-C3A	2.42	1.56	1.51
2	A	507	HEM	C1A-NA	2.29	1.40	1.36
2	A	507	HEM	C4B-NB	2.25	1.40	1.36
3	A	508	NDP	O2B-C2B	2.13	1.51	1.44
3	B	508	NDP	C2A-N1A	2.13	1.37	1.33
3	A	508	NDP	C2A-N1A	2.13	1.37	1.33
2	B	507	HEM	C2A-C3A	-2.11	1.31	1.37
3	B	508	NDP	PA-O2A	-2.10	1.45	1.55
3	A	508	NDP	PA-O2A	-2.09	1.45	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	508	NDP	O2B-C2B	2.08	1.51	1.44
3	A	508	NDP	PN-O2N	-2.07	1.45	1.55
3	B	508	NDP	PN-O2N	-2.06	1.45	1.55
2	A	507	HEM	CMB-C2B	2.03	1.56	1.51

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	508	NDP	O3B-C3B-C4B	9.48	138.46	111.05
3	B	508	NDP	O3B-C3B-C4B	9.46	138.41	111.05
2	A	507	HEM	CAA-CBA-CGA	9.27	128.23	112.67
2	B	507	HEM	CMC-C2C-C3C	6.43	136.71	124.68
3	A	508	NDP	O4B-C1B-C2B	-6.36	95.55	106.59
3	B	508	NDP	O4B-C1B-C2B	-6.34	95.59	106.59
2	A	507	HEM	CMC-C2C-C3C	5.18	134.38	124.68
3	A	508	NDP	O2X-P2B-O2B	4.74	127.21	105.99
3	B	508	NDP	O2X-P2B-O2B	4.73	127.19	105.99
2	A	507	HEM	CBA-CAA-C2A	3.73	119.37	112.49
2	A	507	HEM	CMB-C2B-C3B	3.62	131.45	124.68
3	A	508	NDP	O3X-P2B-O2B	-3.49	90.35	105.99
3	B	508	NDP	O3X-P2B-O2B	-3.48	90.40	105.99
2	B	507	HEM	CMD-C2D-C1D	-3.26	123.45	128.46
3	B	508	NDP	O3B-C3B-C2B	3.18	120.19	111.17
3	A	508	NDP	O3B-C3B-C2B	3.16	120.14	111.17
3	B	508	NDP	C5A-C6A-N6A	3.04	124.97	120.35
3	A	508	NDP	C5A-C6A-N6A	2.99	124.90	120.35
2	B	507	HEM	CMB-C2B-C3B	2.79	129.90	124.68
3	B	508	NDP	C3N-C2N-N1N	-2.62	119.36	123.10
3	A	508	NDP	O2B-C2B-C3B	-2.62	102.19	111.68
3	B	508	NDP	O2B-C2B-C3B	-2.62	102.20	111.68
2	A	507	HEM	CMA-C3A-C4A	-2.57	124.52	128.46
3	A	508	NDP	C3N-C2N-N1N	-2.56	119.44	123.10
3	A	508	NDP	C3D-C2D-C1D	2.51	106.20	101.43
3	B	508	NDP	C3D-C2D-C1D	2.51	106.20	101.43
2	B	507	HEM	CAA-C2A-C3A	2.51	134.47	127.25
3	B	508	NDP	C1D-N1N-C2N	-2.45	117.03	121.11
2	B	507	HEM	CMD-C2D-C3D	2.44	129.54	124.94
3	A	508	NDP	C1D-N1N-C2N	-2.43	117.06	121.11
3	A	508	NDP	O2B-C2B-C1B	-2.22	102.12	110.10
3	B	508	NDP	O2B-C2B-C1B	-2.21	102.14	110.10
2	B	507	HEM	CAD-CBD-CGD	-2.20	108.99	112.67
2	B	507	HEM	CBD-CAD-C3D	2.17	116.47	112.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	508	NDP	O3D-C3D-C4D	-2.14	104.86	111.05
3	A	508	NDP	O3D-C3D-C4D	-2.12	104.91	111.05
2	A	507	HEM	CMD-C2D-C1D	-2.11	125.23	128.46
2	A	507	HEM	CAD-CBD-CGD	-2.11	109.14	112.67
2	B	507	HEM	C3C-C4C-NC	-2.07	107.03	110.94
2	A	507	HEM	C3C-C4C-NC	-2.02	107.13	110.94

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	508	NDP	C3B
3	A	508	NDP	C3B

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	508	NDP	O4B-C4B-C5B-O5B
3	A	508	NDP	O4B-C4B-C5B-O5B
3	B	508	NDP	PN-O3-PA-O2A
3	A	508	NDP	PN-O3-PA-O2A
3	B	508	NDP	O4D-C1D-N1N-C6N
3	A	508	NDP	O4D-C1D-N1N-C6N

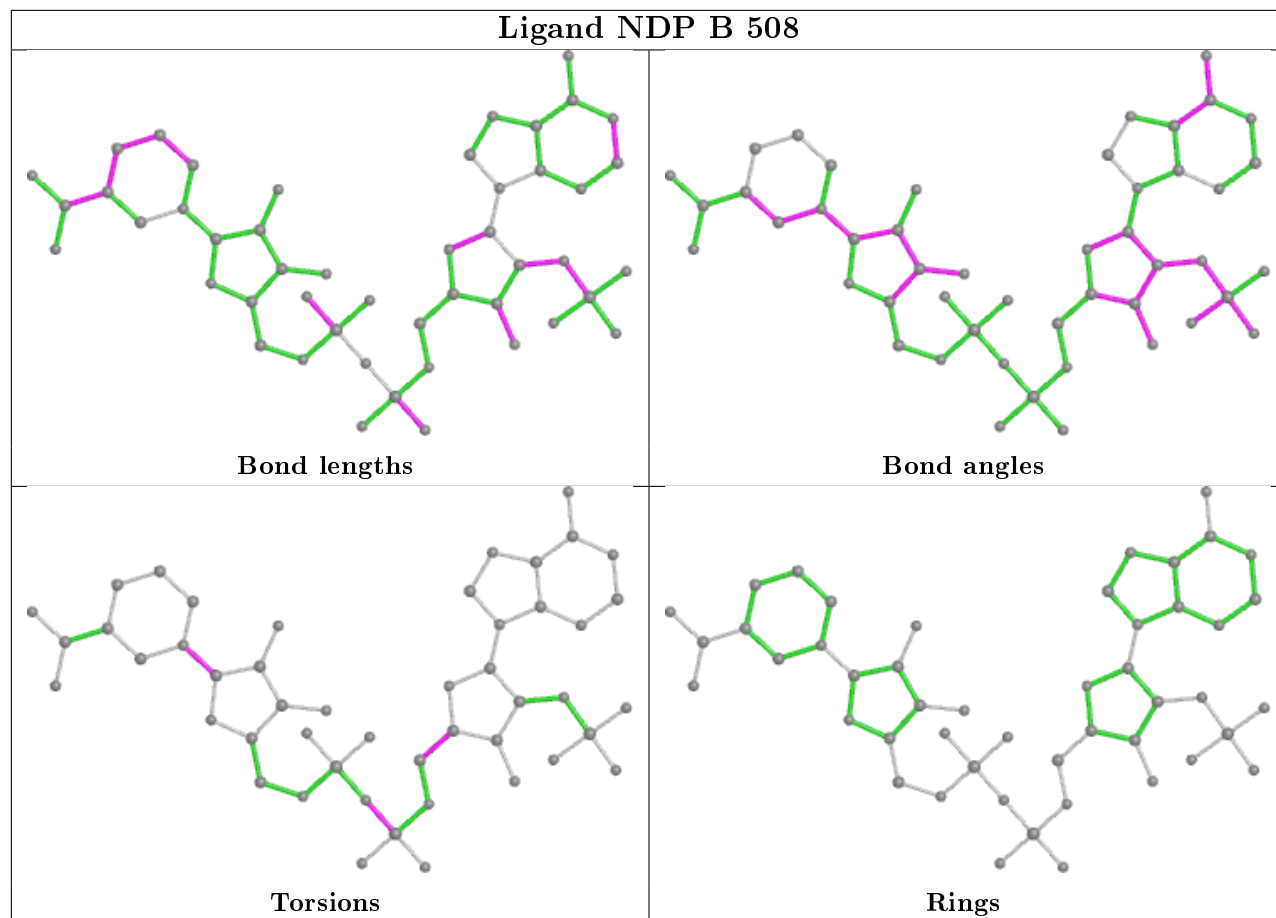
There are no ring outliers.

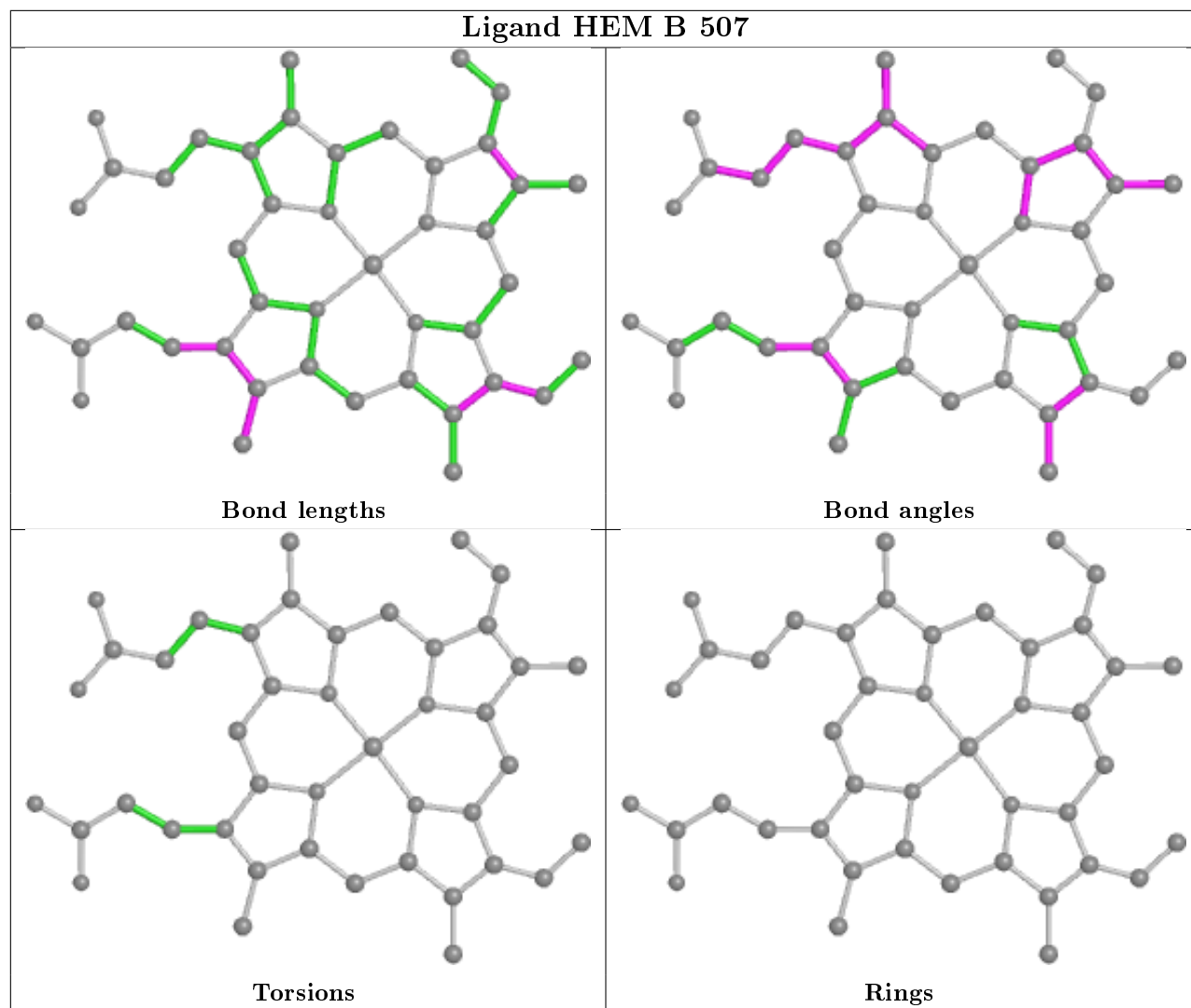
3 monomers are involved in 27 short contacts:

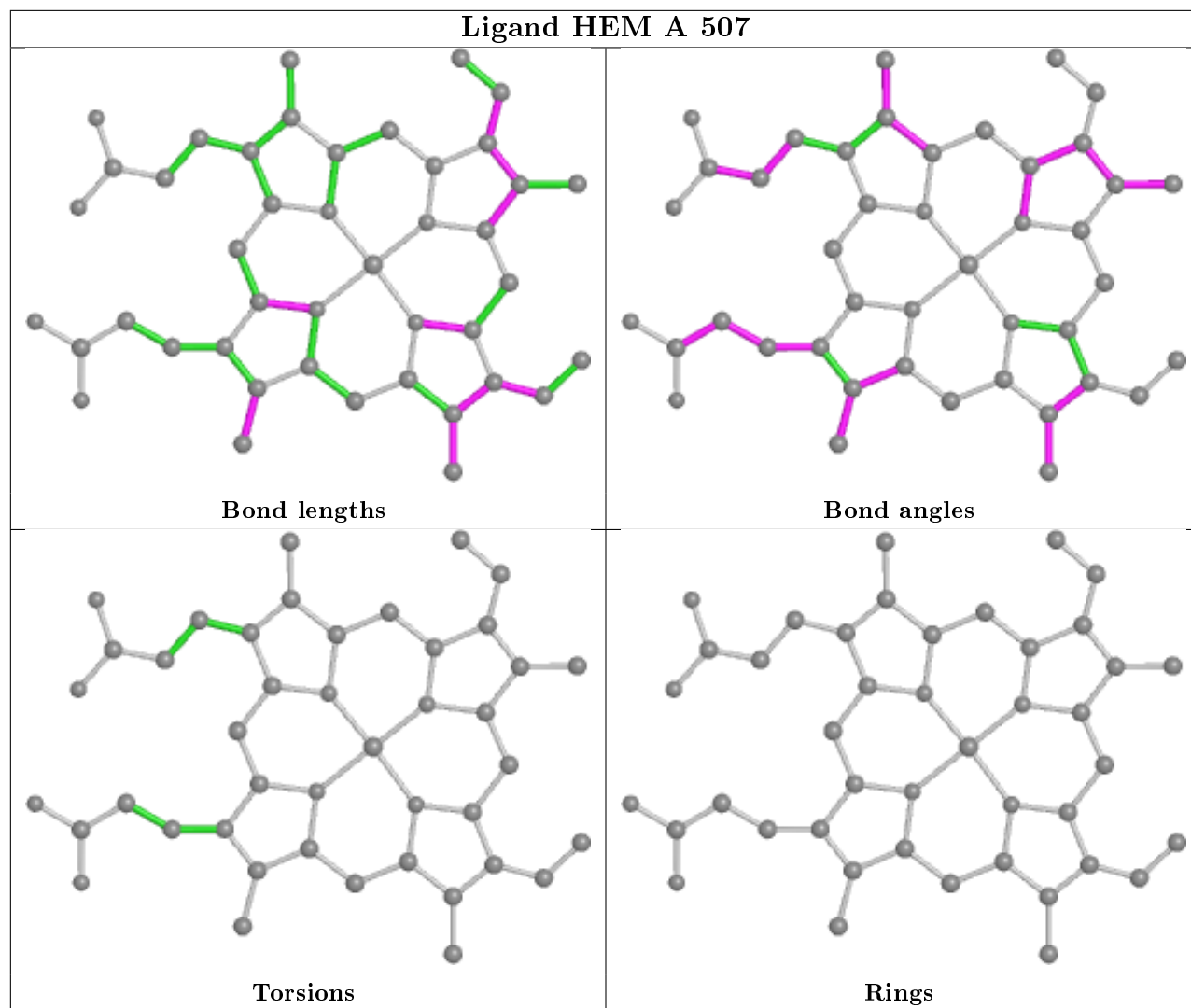
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	508	NDP	3	0
2	B	507	HEM	9	0
2	A	507	HEM	15	0

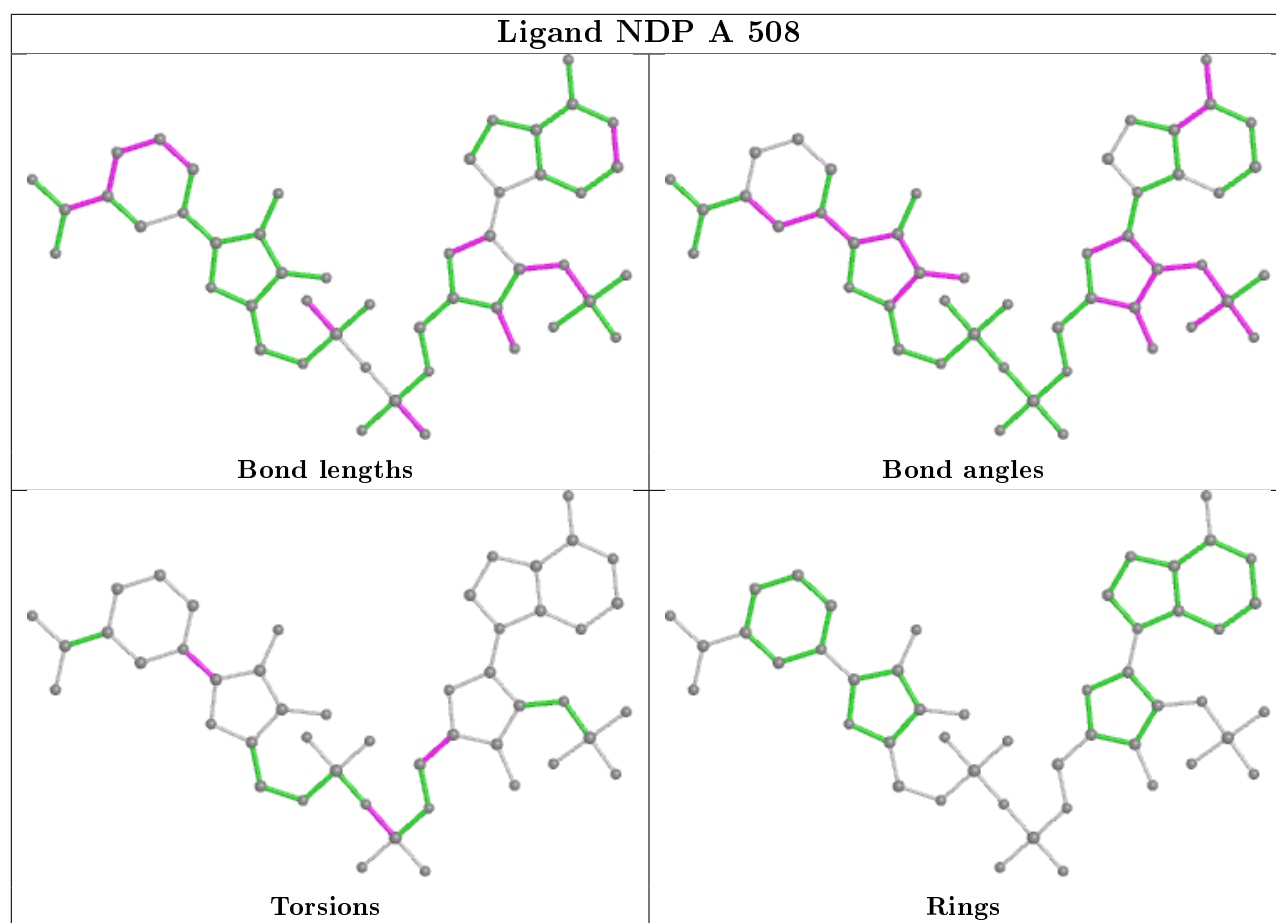
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 [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.