Full wwPDB X-ray Structure Validation Report ⓘ

Sep 18, 2023 – 02:20 PM EDT

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 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:

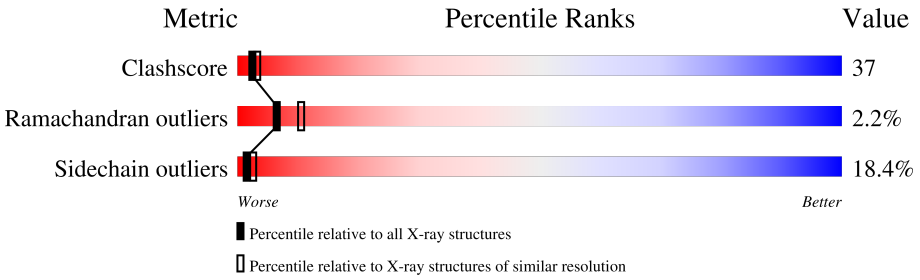
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	506	33% 38% 23% 5% •
1	B	506	36% 36% 21% 5% •

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	-	-	-

2 Entry composition

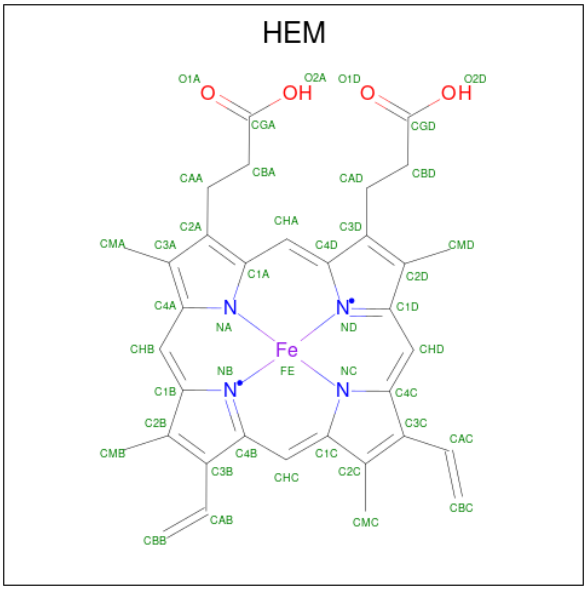
There are 4 unique types of molecules in this entry. The entry contains 8296 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

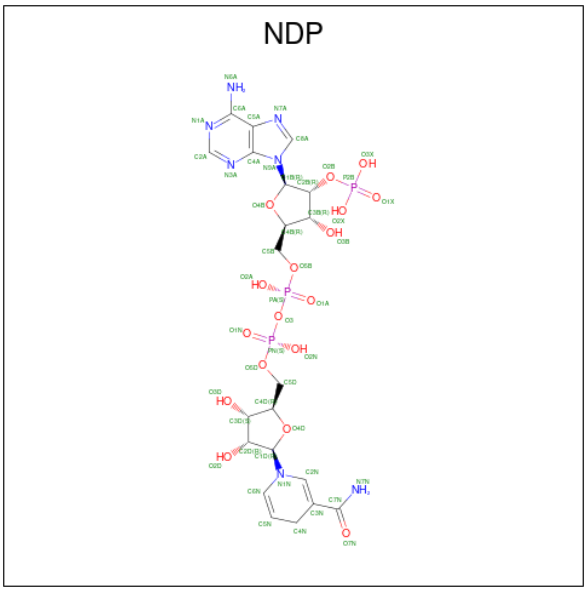
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	0	0	0
			4008	2543	714	737	14			
1	B	498	Total	C	N	O	S	0	0	0
			4008	2543	714	737	14			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: 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 (three-letter code: 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	48	Total	O	0	0
			48	48		
4	B	50	Total	O	0	0
			50	50		

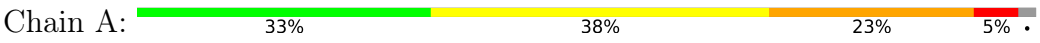
3 Residue-property plots (i)

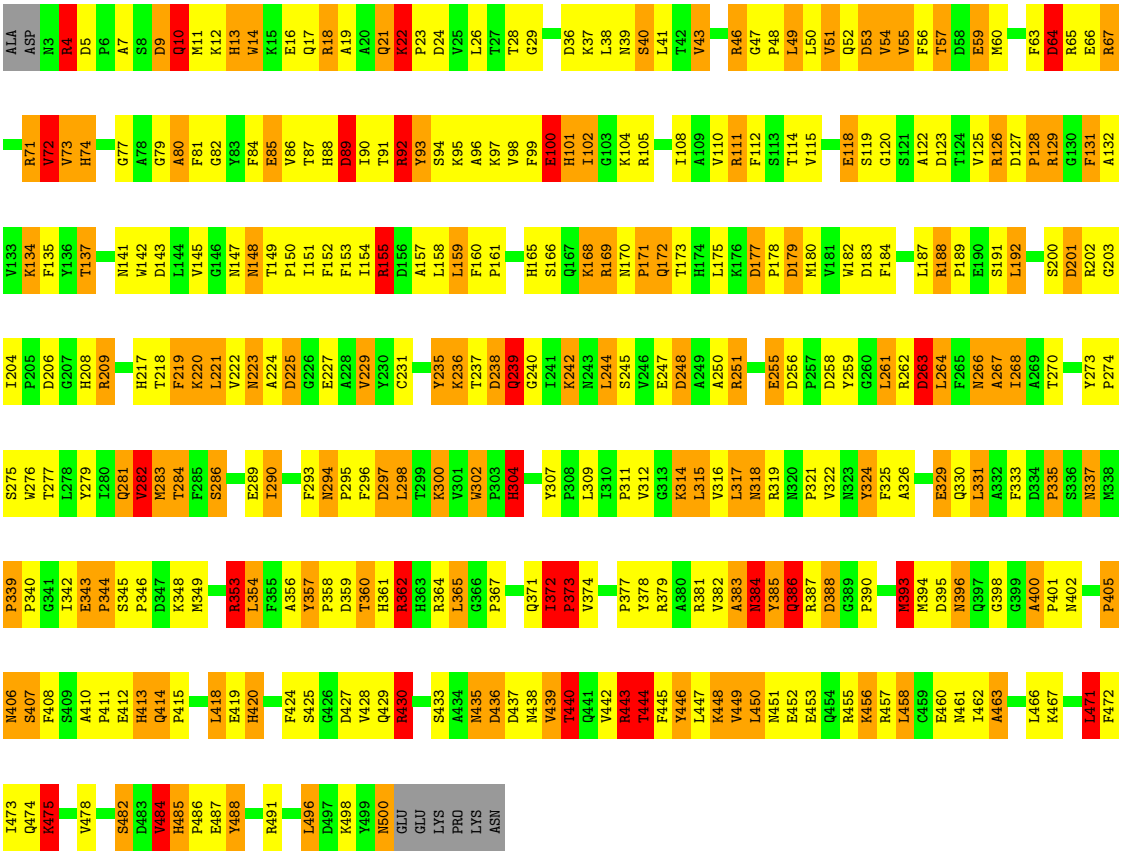
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

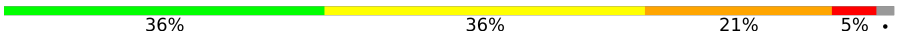
Chain A:

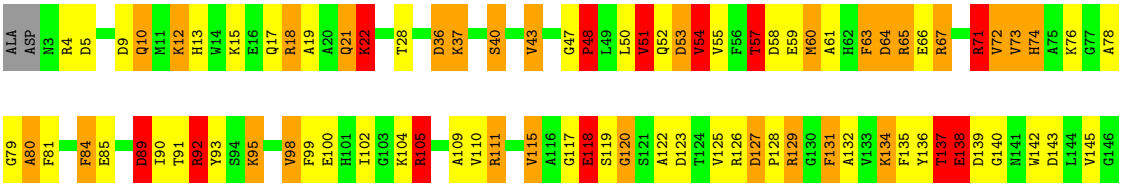


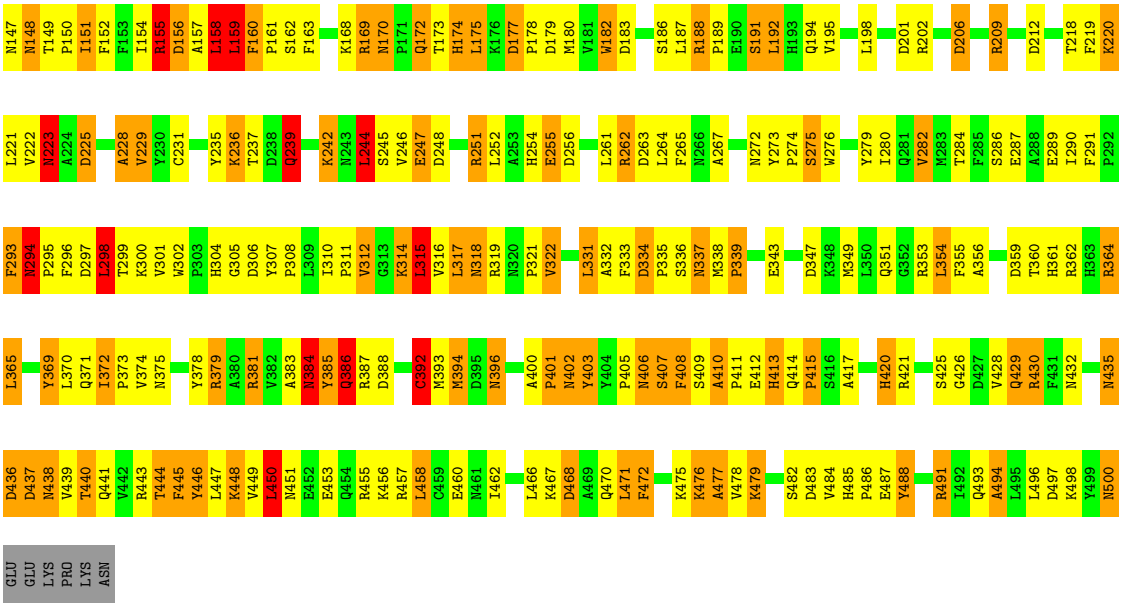


- Molecule 1: CATALASE

Chain B:






N147 N148 T149 P150 I151 F152 F153 I154 R155 D156 A157 L158 L159 F160 P161 S162 F163 K168 R169 N170 P171 Q172 T173 H174 L175 K176 D177 P178 D179 M180 V181 W182 D183 S186 L187 R188 P189 E190 S191 L192 H193 Q194 V195 L198 D201 R202 D206 R209 D212 T218 F219 K220
L221 V222 N223 A224 D225 A228 V229 Y230 C231 Y235 K236 T237 D238 Q239 K242 N243 L244 S245 V246 E247 D248 R251 L252 A253 H254 E255 D256 L261 R262 D263 L264 F265 N266 A267 N272 Y273 P274 S275 W276 Y279 I280 Q281 V282 M283 T284 F285 S286 E287 A288 E289 I290 F291 P292
F293 N294 P295 F296 D297 L298 T299 K300 V301 W302 P303 H304 G305 D306 Y307 P308 L309 I310 P311 V312 G313 K314 L315 V316 L317 N318 R319 N320 P321 V322 L331 A332 F333 D334 P335 S336 N337 M338 P339 E343 D347 K348 M349 L350 Q351 G352 R353 L354 F355 A356 D359 T360 H361 R362 H363 R364
L365 Y369 L370 Q371 I372 P373 V374 N375 Y378 R379 A380 R381 V382 A383 N384 Y385 Q386 R387 D388 C392 M393 M394 D395 N396 A400 P401 N402 Y403 Y404 P405 N406 S407 F408 S409 A410 P411 E412 H413 Q414 P415 S416 A417 H420 R421 S425 G426 D427 V428 Q429 R430 F431 N432 N435
D436 D437 N438 V439 T440 Q441 V442 R443 T444 F445 Y446 L447 K448 V449 L450 N451 E452 E453 Q454 R455 K456 R457 L458 C459 E460 N461 I462 L466 K467 D468 A469 Q470 L471 F472 K475 K476 A477 V478 K479 S482 D483 V484 H485 P486 E487 Y488 R491 I492 Q493 A494 L495 L496 D497 K498 Y499 N500
GLU GLU LYS PRO LYS ASN

4 Data and refinement statistics (i)

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}	0.191 , (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: NDP, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.53	22/4128 (0.5%)	2.37	193/5607 (3.4%)
1	B	1.57	21/4128 (0.5%)	2.42	233/5607 (4.2%)
All	All	1.55	43/8256 (0.5%)	2.39	426/11214 (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 (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	67	ARG	CD-NE	-6.84	1.34	1.46
1	A	343	GLU	N-CA	6.50	1.59	1.46
1	A	166	SER	CB-OG	6.44	1.50	1.42
1	B	100	GLU	CD-OE2	-6.35	1.18	1.25
1	B	119	SER	CB-OG	-6.28	1.34	1.42
1	A	59	GLU	CD-OE1	6.16	1.32	1.25
1	B	294	ASN	N-CA	6.08	1.58	1.46
1	A	364	ARG	NE-CZ	6.08	1.41	1.33
1	A	171	PRO	N-CD	6.04	1.56	1.47
1	B	261	LEU	CA-CB	-5.97	1.40	1.53
1	A	29	GLY	N-CA	5.96	1.54	1.46
1	A	360	THR	C-O	5.81	1.34	1.23
1	A	14	TRP	NE1-CE2	5.78	1.45	1.37
1	A	344	PRO	N-CD	5.78	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	305	GLY	N-CA	5.77	1.54	1.46
1	A	329	GLU	CA-CB	-5.74	1.41	1.53
1	A	353	ARG	CZ-NH2	5.71	1.40	1.33
1	A	300	LYS	C-O	5.68	1.34	1.23
1	B	129	ARG	CG-CD	-5.66	1.37	1.51
1	A	155	ARG	CZ-NH2	-5.55	1.25	1.33
1	B	409	SER	CB-OG	5.54	1.49	1.42
1	B	151	ILE	N-CA	5.50	1.57	1.46
1	B	426	GLY	N-CA	5.50	1.54	1.46
1	A	65	ARG	CZ-NH2	5.42	1.40	1.33
1	B	381	ARG	CZ-NH1	5.34	1.40	1.33
1	A	67	ARG	CG-CD	-5.27	1.38	1.51
1	B	48	PRO	N-CD	5.26	1.55	1.47
1	B	319	ARG	CZ-NH2	5.25	1.39	1.33
1	B	120	GLY	N-CA	5.22	1.53	1.46
1	A	85	GLU	CD-OE1	-5.21	1.20	1.25
1	B	336	SER	CB-OG	-5.20	1.35	1.42
1	B	118	GLU	CD-OE2	-5.18	1.20	1.25
1	B	28	THR	C-O	5.16	1.33	1.23
1	A	165	HIS	CG-CD2	-5.16	1.26	1.35
1	B	66	GLU	CD-OE1	-5.15	1.20	1.25
1	A	56	PHE	CE2-CZ	5.14	1.47	1.37
1	A	398	GLY	N-CA	5.10	1.53	1.46
1	B	162	SER	CB-OG	5.10	1.48	1.42
1	A	122	ALA	N-CA	5.06	1.56	1.46
1	A	400	ALA	CA-CB	5.04	1.63	1.52
1	B	40	SER	CB-OG	5.01	1.48	1.42
1	B	59	GLU	CG-CD	-5.01	1.44	1.51
1	B	289	GLU	CD-OE2	5.01	1.31	1.25

All (426) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	67	ARG	CD-NE-CZ	25.87	159.81	123.60
1	B	92	ARG	NE-CZ-NH1	23.31	131.96	120.30
1	B	126	ARG	NE-CZ-NH2	21.07	130.84	120.30
1	B	261	LEU	CA-CB-CG	20.41	162.25	115.30
1	A	362	ARG	NE-CZ-NH2	-20.39	110.11	120.30
1	A	111	ARG	NE-CZ-NH2	-20.23	110.19	120.30
1	A	353	ARG	NE-CZ-NH1	20.17	130.38	120.30
1	A	362	ARG	NE-CZ-NH1	20.04	130.32	120.30
1	A	169	ARG	NE-CZ-NH2	-19.70	110.45	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	353	ARG	NE-CZ-NH2	-19.60	110.50	120.30
1	A	430	ARG	NE-CZ-NH1	-18.76	110.92	120.30
1	A	169	ARG	NE-CZ-NH1	17.38	128.99	120.30
1	B	89	ASP	CB-CG-OD1	-17.00	103.00	118.30
1	A	111	ARG	NE-CZ-NH1	16.75	128.67	120.30
1	B	71	ARG	CD-NE-CZ	15.97	145.96	123.60
1	A	155	ARG	NE-CZ-NH1	-15.73	112.43	120.30
1	B	457	ARG	NE-CZ-NH1	15.23	127.92	120.30
1	B	188	ARG	NE-CZ-NH1	-15.11	112.75	120.30
1	B	457	ARG	NE-CZ-NH2	-14.47	113.06	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	14.08	127.34	120.30
1	B	364	ARG	NE-CZ-NH2	-13.19	113.70	120.30
1	B	225	ASP	CB-CG-OD1	13.14	130.12	118.30
1	B	111	ARG	NE-CZ-NH2	-13.11	113.74	120.30
1	A	261	LEU	CA-CB-CG	12.78	144.70	115.30
1	B	111	ARG	NE-CZ-NH1	12.72	126.66	120.30
1	B	188	ARG	NE-CZ-NH2	12.69	126.65	120.30
1	A	359	ASP	CB-CG-OD2	-12.66	106.91	118.30
1	B	381	ARG	NE-CZ-NH1	-12.52	114.04	120.30
1	B	155	ARG	NE-CZ-NH1	12.49	126.55	120.30
1	B	362	ARG	NE-CZ-NH1	12.24	126.42	120.30
1	B	437	ASP	CB-CG-OD1	12.24	129.32	118.30
1	A	359	ASP	CB-CG-OD1	12.01	129.11	118.30
1	B	159	LEU	CA-CB-CG	11.95	142.79	115.30
1	B	155	ARG	CD-NE-CZ	11.80	140.12	123.60
1	A	65	ARG	CD-NE-CZ	11.62	139.86	123.60
1	B	430	ARG	NE-CZ-NH2	11.49	126.05	120.30
1	B	92	ARG	NE-CZ-NH2	-11.14	114.73	120.30
1	B	138	GLU	OE1-CD-OE2	-10.98	110.13	123.30
1	B	129	ARG	NE-CZ-NH2	10.92	125.76	120.30
1	A	378	TYR	CB-CG-CD1	10.83	127.50	121.00
1	B	362	ARG	NE-CZ-NH2	-10.76	114.92	120.30
1	B	263	ASP	CB-CG-OD2	-10.60	108.76	118.30
1	A	9	ASP	CB-CG-OD1	10.45	127.70	118.30
1	B	225	ASP	CB-CG-OD2	-10.17	109.15	118.30
1	B	319	ARG	NE-CZ-NH2	-10.08	115.26	120.30
1	A	93	TYR	CB-CG-CD2	-10.03	114.98	121.00
1	A	143	ASP	CB-CG-OD2	-10.00	109.30	118.30
1	A	343	GLU	CA-CB-CG	10.00	135.40	113.40
1	A	188	ARG	NE-CZ-NH1	-9.98	115.31	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	36	ASP	CB-CG-OD1	9.83	127.14	118.30
1	A	455	ARG	NE-CZ-NH1	9.81	125.20	120.30
1	A	329	GLU	OE1-CD-OE2	9.72	134.96	123.30
1	B	65	ARG	NE-CZ-NH2	9.63	125.11	120.30
1	B	381	ARG	NE-CZ-NH2	9.50	125.05	120.30
1	A	251	ARG	NE-CZ-NH1	9.48	125.04	120.30
1	B	343	GLU	OE1-CD-OE2	-9.43	111.98	123.30
1	A	89	ASP	CB-CG-OD1	-9.40	109.84	118.30
1	B	169	ARG	NE-CZ-NH1	-9.37	115.62	120.30
1	B	262	ARG	NE-CZ-NH1	-9.34	115.63	120.30
1	A	155	ARG	CD-NE-CZ	-9.34	110.52	123.60
1	A	126	ARG	NE-CZ-NH1	9.31	124.96	120.30
1	A	378	TYR	CB-CG-CD2	-9.29	115.43	121.00
1	A	53	ASP	CB-CG-OD2	-9.14	110.07	118.30
1	B	359	ASP	CB-CG-OD2	-9.09	110.12	118.30
1	B	386	GLN	CB-CG-CD	9.08	135.21	111.60
1	A	455	ARG	NE-CZ-NH2	-9.02	115.79	120.30
1	A	364	ARG	CD-NE-CZ	-8.91	111.12	123.60
1	B	127	ASP	CB-CG-OD1	8.87	126.28	118.30
1	B	343	GLU	CA-CB-CG	8.83	132.82	113.40
1	B	81	PHE	CB-CG-CD1	-8.82	114.63	120.80
1	B	53	ASP	CB-CG-OD1	8.80	126.22	118.30
1	B	450	LEU	CB-CA-C	8.73	126.79	110.20
1	B	168	LYS	CA-CB-CG	8.72	132.59	113.40
1	A	335	PRO	C-N-CA	8.69	143.42	121.70
1	B	254	HIS	CA-CB-CG	8.65	128.31	113.60
1	B	386	GLN	CA-CB-CG	8.64	132.42	113.40
1	B	364	ARG	CD-NE-CZ	-8.62	111.53	123.60
1	A	251	ARG	CA-CB-CG	8.55	132.20	113.40
1	B	65	ARG	NE-CZ-NH1	-8.53	116.04	120.30
1	B	353	ARG	NE-CZ-NH2	-8.48	116.06	120.30
1	B	343	GLU	CG-CD-OE1	8.48	135.25	118.30
1	B	255	GLU	CA-CB-CG	8.44	131.97	113.40
1	B	59	GLU	OE1-CD-OE2	-8.44	113.17	123.30
1	B	429	GLN	CA-CB-CG	8.43	131.94	113.40
1	B	202	ARG	NE-CZ-NH2	-8.40	116.10	120.30
1	B	347	ASP	CB-CG-OD2	8.40	125.86	118.30
1	B	134	LYS	CD-CE-NZ	-8.33	92.54	111.70
1	B	472	PHE	CA-CB-CG	8.27	133.75	113.90
1	B	334	ASP	CB-CG-OD1	8.27	125.74	118.30
1	A	457	ARG	CD-NE-CZ	8.24	135.14	123.60
1	B	497	ASP	CB-CG-OD2	-8.22	110.91	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	497	ASP	CB-CG-OD1	8.20	125.68	118.30
1	B	89	ASP	OD1-CG-OD2	8.18	138.84	123.30
1	B	408	PHE	C-N-CA	8.16	142.10	121.70
1	B	175	LEU	CA-CB-CG	8.15	134.04	115.30
1	B	450	LEU	CA-CB-CG	8.14	134.02	115.30
1	B	201	ASP	CB-CG-OD2	-8.14	110.97	118.30
1	B	262	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	A	430	ARG	CD-NE-CZ	-8.11	112.25	123.60
1	A	71	ARG	NE-CZ-NH1	8.05	124.32	120.30
1	B	187	LEU	CB-CA-C	8.03	125.46	110.20
1	B	314	LYS	CA-CB-CG	7.97	130.94	113.40
1	B	123	ASP	CB-CG-OD2	-7.97	111.13	118.30
1	A	93	TYR	CB-CG-CD1	7.95	125.77	121.00
1	B	494	ALA	CB-CA-C	7.94	122.01	110.10
1	A	179	ASP	CA-CB-CG	7.92	130.82	113.40
1	B	67	ARG	NE-CZ-NH2	7.90	124.25	120.30
1	A	179	ASP	CB-CG-OD2	7.89	125.40	118.30
1	A	373	PRO	N-CA-CB	-7.89	93.83	103.30
1	A	412	GLU	CA-CB-CG	7.86	130.69	113.40
1	B	60	MET	CA-CB-CG	7.86	126.66	113.30
1	B	457	ARG	CD-NE-CZ	7.86	134.60	123.60
1	A	457	ARG	NE-CZ-NH1	7.82	124.21	120.30
1	B	468	ASP	CB-CG-OD1	7.82	125.33	118.30
1	A	159	LEU	CA-CB-CG	7.77	133.18	115.30
1	A	324	TYR	CB-CG-CD2	7.77	125.66	121.00
1	B	443	ARG	CD-NE-CZ	7.77	134.47	123.60
1	A	67	ARG	CA-CB-CG	7.74	130.43	113.40
1	B	206	ASP	CB-CG-OD2	7.71	125.24	118.30
1	A	388	ASP	CB-CG-OD1	-7.67	111.39	118.30
1	B	262	ARG	NH1-CZ-NH2	7.67	127.84	119.40
1	B	126	ARG	NE-CZ-NH1	-7.64	116.48	120.30
1	A	155	ARG	NE-CZ-NH2	7.62	124.11	120.30
1	A	201	ASP	CB-CG-OD2	-7.61	111.45	118.30
1	B	483	ASP	CB-CG-OD1	7.57	125.12	118.30
1	B	298	LEU	CA-CB-CG	7.55	132.66	115.30
1	B	436	ASP	CB-CG-OD2	7.54	125.09	118.30
1	B	378	TYR	CB-CG-CD1	7.52	125.51	121.00
1	A	365	LEU	CA-CB-CG	7.50	132.55	115.30
1	A	357	TYR	CB-CG-CD2	-7.46	116.53	121.00
1	B	169	ARG	NE-CZ-NH2	7.40	124.00	120.30
1	A	80	ALA	CB-CA-C	7.34	121.11	110.10
1	A	263	ASP	CB-CG-OD1	7.34	124.90	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	67	ARG	CG-CD-NE	7.32	127.16	111.80
1	B	67	ARG	NE-CZ-NH1	-7.31	116.64	120.30
1	A	123	ASP	CB-CG-OD1	7.31	124.88	118.30
1	B	247	GLU	CA-CB-CG	7.27	129.39	113.40
1	A	65	ARG	NE-CZ-NH1	7.23	123.92	120.30
1	B	129	ARG	NE-CZ-NH1	-7.22	116.69	120.30
1	B	275	SER	C-N-CA	7.21	139.71	121.70
1	B	111	ARG	CD-NE-CZ	7.18	133.65	123.60
1	B	105	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	B	343	GLU	N-CA-CB	-7.14	97.75	110.60
1	A	248	ASP	CB-CG-OD2	-7.11	111.90	118.30
1	B	256	ASP	CB-CG-OD1	7.09	124.68	118.30
1	A	256	ASP	CB-CG-OD1	7.07	124.66	118.30
1	A	364	ARG	NH1-CZ-NH2	7.06	127.16	119.40
1	A	92	ARG	NE-CZ-NH2	7.04	123.82	120.30
1	A	10	GLN	CB-CG-CD	7.04	129.90	111.60
1	A	343	GLU	CB-CA-C	7.03	124.46	110.40
1	A	188	ARG	CD-NE-CZ	-7.02	113.77	123.60
1	B	126	ARG	CA-CB-CG	7.01	128.81	113.40
1	A	353	ARG	CD-NE-CZ	6.97	133.36	123.60
1	B	251	ARG	NE-CZ-NH2	6.97	123.79	120.30
1	A	221	LEU	O-C-N	6.95	133.81	122.70
1	B	209	ARG	CD-NE-CZ	-6.93	113.90	123.60
1	B	261	LEU	O-C-N	6.92	133.77	122.70
1	A	435	ASN	CB-CA-C	6.91	124.22	110.40
1	A	16	GLU	OE1-CD-OE2	6.88	131.55	123.30
1	A	263	ASP	CA-CB-CG	6.88	128.53	113.40
1	A	437	ASP	CB-CG-OD1	6.86	124.47	118.30
1	B	483	ASP	CB-CG-OD2	-6.86	112.13	118.30
1	B	74	HIS	C-N-CA	6.84	138.81	121.70
1	B	89	ASP	CA-CB-CG	-6.84	98.35	113.40
1	A	122	ALA	CB-CA-C	6.82	120.34	110.10
1	A	446	TYR	CB-CG-CD2	6.81	125.08	121.00
1	A	238	ASP	CB-CG-OD2	6.80	124.42	118.30
1	A	28	THR	CA-C-N	6.77	129.74	116.20
1	B	334	ASP	OD1-CG-OD2	-6.77	110.44	123.30
1	B	255	GLU	OE1-CD-OE2	-6.73	115.23	123.30
1	B	51	VAL	C-N-CA	6.72	138.50	121.70
1	A	471	LEU	CB-CA-C	6.72	122.96	110.20
1	B	364	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	A	302	TRP	CA-CB-CG	6.71	126.45	113.70
1	A	259	TYR	CB-CG-CD1	-6.71	116.97	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	312	VAL	CA-CB-CG2	6.71	120.96	110.90
1	A	379	ARG	NE-CZ-NH2	-6.67	116.96	120.30
1	B	92	ARG	C-N-CA	6.65	138.33	121.70
1	A	335	PRO	CA-CB-CG	-6.65	91.37	104.00
1	B	381	ARG	CD-NE-CZ	-6.63	114.32	123.60
1	B	111	ARG	O-C-N	6.62	133.29	122.70
1	A	111	ARG	N-CA-CB	6.60	122.48	110.60
1	B	468	ASP	OD1-CG-OD2	-6.58	110.79	123.30
1	A	49	LEU	CA-CB-CG	6.57	130.42	115.30
1	B	98	VAL	CG1-CB-CG2	-6.57	100.39	110.90
1	A	290	ILE	CA-CB-CG2	6.54	123.98	110.90
1	B	89	ASP	CB-CA-C	6.49	123.37	110.40
1	B	81	PHE	CB-CG-CD2	6.48	125.34	120.80
1	A	4	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	A	134	LYS	CD-CE-NZ	-6.46	96.84	111.70
1	B	343	GLU	CB-CG-CD	6.46	131.65	114.20
1	A	319	ARG	CD-NE-CZ	-6.43	114.59	123.60
1	A	247	GLU	CG-CD-OE1	6.43	131.16	118.30
1	A	440	THR	CA-CB-CG2	6.42	121.39	112.40
1	B	385	TYR	CB-CA-C	6.42	123.25	110.40
1	A	282	VAL	CA-CB-CG1	6.42	120.53	110.90
1	B	177	ASP	CB-CG-OD1	-6.42	112.52	118.30
1	B	182	TRP	CB-CA-C	6.40	123.20	110.40
1	B	54	VAL	CA-CB-CG1	6.39	120.49	110.90
1	B	187	LEU	CA-CB-CG	6.39	130.00	115.30
1	A	405	PRO	CA-N-CD	-6.39	102.56	111.50
1	A	209	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	A	284	THR	OG1-CB-CG2	6.37	124.65	110.00
1	B	315	LEU	CA-CB-CG	6.36	129.93	115.30
1	B	84	PHE	CB-CG-CD1	-6.36	116.35	120.80
1	A	188	ARG	NE-CZ-NH2	6.32	123.46	120.30
1	A	250	ALA	CB-CA-C	6.31	119.57	110.10
1	B	247	GLU	CG-CD-OE2	-6.30	105.70	118.30
1	B	365	LEU	N-CA-CB	-6.29	97.82	110.40
1	A	395	ASP	CB-CG-OD2	-6.26	112.67	118.30
1	B	139	ASP	CB-CG-OD2	6.26	123.93	118.30
1	B	126	ARG	NH1-CZ-NH2	-6.26	112.52	119.40
1	B	252	LEU	CA-CB-CG	6.25	129.67	115.30
1	B	359	ASP	CB-CG-OD1	6.23	123.91	118.30
1	B	318	ASN	CB-CA-C	6.22	122.84	110.40
1	A	172	GLN	CA-CB-CG	-6.21	99.74	113.40
1	A	429	GLN	CA-CB-CG	6.19	127.02	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	468	ASP	CB-CG-OD2	6.19	123.87	118.30
1	A	143	ASP	O-C-N	6.19	132.61	122.70
1	B	379	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	B	370	LEU	C-N-CA	6.17	137.13	121.70
1	A	382	VAL	CG1-CB-CG2	6.16	120.76	110.90
1	A	4	ARG	CD-NE-CZ	6.14	132.20	123.60
1	A	251	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	B	117	GLY	C-N-CA	6.13	137.03	121.70
1	B	261	LEU	N-CA-CB	6.13	122.66	110.40
1	B	334	ASP	CB-CG-OD2	6.13	123.82	118.30
1	B	160	PHE	CB-CG-CD1	-6.12	116.52	120.80
1	A	379	ARG	CA-CB-CG	6.10	126.82	113.40
1	B	437	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	A	329	GLU	CG-CD-OE2	-6.10	106.10	118.30
1	B	322	VAL	CA-CB-CG1	6.09	120.04	110.90
1	B	85	GLU	OE1-CD-OE2	-6.09	115.99	123.30
1	B	347	ASP	OD1-CG-OD2	-6.07	111.77	123.30
1	B	421	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	A	71	ARG	CD-NE-CZ	6.05	132.07	123.60
1	A	387	ARG	CD-NE-CZ	-6.05	115.14	123.60
1	A	126	ARG	CA-CB-CG	6.04	126.70	113.40
1	B	477	ALA	N-CA-CB	6.04	118.56	110.10
1	A	177	ASP	N-CA-CB	-6.03	99.76	110.60
1	A	407	SER	CA-C-O	-6.01	107.47	120.10
1	B	28	THR	CA-C-O	-6.01	107.48	120.10
1	A	46	ARG	NE-CZ-NH1	-6.01	117.30	120.30
1	B	396	ASN	C-N-CA	5.99	136.67	121.70
1	B	115	VAL	CA-CB-CG1	5.99	119.88	110.90
1	A	202	ARG	NE-CZ-NH1	-5.97	117.31	120.30
1	A	244	LEU	CA-CB-CG	5.97	129.03	115.30
1	B	163	PHE	N-CA-CB	5.94	121.29	110.60
1	B	57	THR	CB-CA-C	5.92	127.59	111.60
1	B	122	ALA	CB-CA-C	5.92	118.98	110.10
1	A	496	LEU	CB-CA-C	5.91	121.44	110.20
1	B	63	PHE	CB-CG-CD2	-5.90	116.67	120.80
1	B	388	ASP	CB-CG-OD2	5.90	123.61	118.30
1	A	427	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	B	375	ASN	CB-CG-ND2	5.89	130.84	116.70
1	A	4	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	B	239	GLN	CG-CD-OE1	5.87	133.34	121.60
1	A	100	GLU	CG-CD-OE2	-5.87	106.56	118.30
1	A	192	LEU	CA-CB-CG	5.86	128.77	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	338	MET	O-C-N	5.86	132.22	121.10
1	A	263	ASP	CB-CA-C	5.85	122.11	110.40
1	A	219	PHE	CB-CA-C	5.85	122.09	110.40
1	A	9	ASP	CB-CA-C	5.83	122.07	110.40
1	B	58	ASP	CB-CG-OD1	5.83	123.54	118.30
1	B	244	LEU	CA-CB-CG	5.82	128.69	115.30
1	A	71	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	B	450	LEU	N-CA-CB	-5.82	98.77	110.40
1	A	443	ARG	NE-CZ-NH2	5.82	123.21	120.30
1	A	52	GLN	CA-CB-CG	5.81	126.19	113.40
1	B	289	GLU	CA-CB-CG	5.81	126.19	113.40
1	B	410	ALA	CB-CA-C	5.81	118.82	110.10
1	B	445	PHE	O-C-N	5.80	131.99	122.70
1	B	137	THR	CA-CB-CG2	5.80	120.52	112.40
1	B	52	GLN	CB-CA-C	-5.80	98.81	110.40
1	A	73	VAL	CA-CB-CG1	5.78	119.56	110.90
1	A	289	GLU	CG-CD-OE1	5.77	129.84	118.30
1	A	385	TYR	CB-CG-CD2	-5.76	117.54	121.00
1	B	177	ASP	N-CA-CB	-5.75	100.25	110.60
1	A	221	LEU	CA-C-O	-5.74	108.05	120.10
1	B	202	ARG	CG-CD-NE	-5.74	99.74	111.80
1	A	360	THR	N-CA-CB	-5.73	99.41	110.30
1	B	412	GLU	CB-CA-C	-5.72	98.95	110.40
1	B	71	ARG	CA-CB-CG	5.72	125.99	113.40
1	A	314	LYS	CD-CE-NZ	-5.72	98.55	111.70
1	A	385	TYR	CB-CG-CD1	5.70	124.42	121.00
1	A	270	THR	CA-CB-CG2	5.70	120.38	112.40
1	B	58	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	A	72	VAL	CA-CB-CG1	5.69	119.44	110.90
1	B	420	HIS	C-N-CA	5.69	135.93	121.70
1	B	413	HIS	N-CA-CB	5.68	120.82	110.60
1	B	273	TYR	CB-CG-CD2	-5.67	117.60	121.00
1	B	182	TRP	N-CA-CB	-5.66	100.41	110.60
1	B	435	ASN	CB-CA-C	5.66	121.71	110.40
1	B	446	TYR	CA-CB-CG	5.65	124.14	113.40
1	A	388	ASP	CB-CG-OD2	5.64	123.38	118.30
1	A	283	MET	CG-SD-CE	5.61	109.18	100.20
1	B	92	ARG	NH1-CZ-NH2	-5.60	113.24	119.40
1	B	168	LYS	N-CA-CB	5.60	120.68	110.60
1	B	123	ASP	CB-CG-OD1	5.60	123.34	118.30
1	B	282	VAL	CA-CB-CG1	5.59	119.29	110.90
1	A	386	GLN	CB-CG-CD	5.59	126.13	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	74	HIS	C-N-CA	5.59	135.67	121.70
1	B	74	HIS	CB-CA-C	-5.59	99.23	110.40
1	B	99	PHE	CA-CB-CG	5.59	127.31	113.90
1	B	71	ARG	CB-CG-CD	5.58	126.11	111.60
1	B	202	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	184	PHE	C-N-CA	5.58	135.64	121.70
1	A	393	MET	CB-CA-C	-5.57	99.26	110.40
1	A	259	TYR	CB-CG-CD2	5.56	124.33	121.00
1	B	71	ARG	NE-CZ-NH1	-5.53	117.53	120.30
1	B	129	ARG	CG-CD-NE	5.53	123.41	111.80
1	A	425	SER	CB-CA-C	-5.52	99.61	110.10
1	A	405	PRO	N-CD-CG	-5.51	94.93	103.20
1	A	484	VAL	CA-CB-CG1	5.51	119.16	110.90
1	A	384	ASN	CB-CA-C	5.51	121.41	110.40
1	A	266	ASN	CB-CA-C	5.50	121.41	110.40
1	B	408	PHE	O-C-N	-5.50	113.89	122.70
1	A	111	ARG	CD-NE-CZ	5.50	131.30	123.60
1	B	384	ASN	CB-CA-C	5.50	121.39	110.40
1	B	263	ASP	CB-CA-C	5.48	121.37	110.40
1	A	224	ALA	CA-C-O	-5.47	108.61	120.10
1	B	143	ASP	C-N-CA	5.46	135.36	121.70
1	B	187	LEU	CB-CG-CD1	5.46	120.28	111.00
1	A	270	THR	N-CA-CB	5.45	120.66	110.30
1	A	297	ASP	CB-CG-OD1	5.45	123.20	118.30
1	A	261	LEU	N-CA-CB	5.44	121.28	110.40
1	A	247	GLU	CG-CD-OE2	-5.44	107.43	118.30
1	A	372	ILE	CA-CB-CG1	5.44	121.33	111.00
1	A	324	TYR	CG-CD2-CE2	5.43	125.64	121.30
1	A	420	HIS	CA-CB-CG	5.43	122.83	113.60
1	B	66	GLU	OE1-CD-OE2	5.42	129.81	123.30
1	A	64	ASP	C-N-CA	5.42	135.25	121.70
1	B	127	ASP	OD1-CG-OD2	-5.42	113.00	123.30
1	A	357	TYR	CB-CG-CD1	5.41	124.25	121.00
1	B	126	ARG	CA-C-O	-5.41	108.73	120.10
1	A	444	THR	OG1-CB-CG2	5.41	122.44	110.00
1	B	55	VAL	CA-CB-CG1	5.40	118.99	110.90
1	B	338	MET	CA-C-O	-5.38	108.80	120.10
1	A	413	HIS	N-CA-CB	5.38	120.28	110.60
1	B	126	ARG	O-C-N	5.37	131.30	122.70
1	B	353	ARG	NH1-CZ-NH2	5.37	125.31	119.40
1	A	89	ASP	CB-CA-C	5.37	121.14	110.40
1	A	393	MET	CA-CB-CG	-5.37	104.17	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	293	PHE	CA-CB-CG	5.36	126.77	113.90
1	A	24	ASP	CB-CG-OD2	-5.35	113.48	118.30
1	A	304	HIS	N-CA-CB	5.35	120.23	110.60
1	A	29	GLY	O-C-N	-5.34	114.11	123.20
1	A	461	ASN	CA-CB-CG	5.34	125.16	113.40
1	A	52	GLN	N-CA-CB	5.34	120.22	110.60
1	A	247	GLU	CA-CB-CG	5.34	125.15	113.40
1	B	105	ARG	CB-CA-C	-5.32	99.76	110.40
1	B	430	ARG	NH1-CZ-NH2	-5.32	113.55	119.40
1	A	429	GLN	N-CA-CB	-5.31	101.04	110.60
1	B	392	CYS	CA-CB-SG	-5.31	104.45	114.00
1	A	418	LEU	CB-CA-C	5.30	120.27	110.20
1	A	225	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	B	72	VAL	CB-CA-C	5.28	121.43	111.40
1	B	460	GLU	CG-CD-OE2	-5.27	107.76	118.30
1	B	129	ARG	CB-CG-CD	5.26	125.28	111.60
1	B	472	PHE	CB-CG-CD2	5.26	124.48	120.80
1	B	191	SER	C-N-CA	5.25	134.84	121.70
1	B	219	PHE	CB-CA-C	5.25	120.91	110.40
1	A	381	ARG	N-CA-CB	5.25	120.05	110.60
1	B	302	TRP	N-CA-CB	5.25	120.05	110.60
1	A	119	SER	N-CA-CB	-5.23	102.65	110.50
1	B	209	ARG	NE-CZ-NH1	-5.23	117.68	120.30
1	A	153	PHE	O-C-N	5.22	131.05	122.70
1	B	66	GLU	C-N-CA	5.21	134.74	121.70
1	B	476	LYS	CB-CG-CD	5.21	125.15	111.60
1	B	251	ARG	CD-NE-CZ	-5.20	116.32	123.60
1	B	438	ASN	CA-C-O	-5.20	109.18	120.10
1	A	258	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	429	GLN	C-N-CA	5.19	134.68	121.70
1	A	227	GLU	OE1-CD-OE2	5.19	129.53	123.30
1	A	475	LYS	N-CA-CB	5.18	119.93	110.60
1	B	202	ARG	CD-NE-CZ	5.18	130.85	123.60
1	B	425	SER	C-N-CA	-5.18	111.43	122.30
1	A	414	GLN	CA-CB-CG	5.17	124.78	113.40
1	A	383	ALA	CB-CA-C	-5.17	102.35	110.10
1	B	139	ASP	CB-CG-OD1	-5.17	113.65	118.30
1	A	281	GLN	CA-CB-CG	5.16	124.76	113.40
1	B	436	ASP	CB-CA-C	5.16	120.73	110.40
1	B	318	ASN	N-CA-CB	-5.16	101.31	110.60
1	B	140	GLY	O-C-N	5.16	130.96	122.70
1	B	242	LYS	O-C-N	5.16	130.95	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	174	HIS	CA-CB-CG	-5.15	104.84	113.60
1	B	37	LYS	CB-CG-CD	5.15	124.99	111.60
1	B	109	ALA	CA-C-N	5.15	128.53	117.20
1	B	48	PRO	N-CA-CB	-5.15	96.94	102.60
1	B	228	ALA	C-N-CA	5.14	134.56	121.70
1	B	223	ASN	O-C-N	5.14	130.92	122.70
1	B	105	ARG	CD-NE-CZ	-5.13	116.41	123.60
1	B	28	THR	CA-C-N	5.13	126.46	116.20
1	A	239	GLN	CB-CG-CD	5.12	124.92	111.60
1	B	491	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	B	378	TYR	CB-CG-CD2	-5.12	117.93	121.00
1	A	102	ILE	CB-CA-C	-5.12	101.37	111.60
1	B	159	LEU	CB-CG-CD2	5.12	119.70	111.00
1	A	463	ALA	N-CA-CB	-5.11	102.94	110.10
1	A	318	ASN	N-CA-CB	-5.11	101.40	110.60
1	A	66	GLU	CG-CD-OE2	-5.11	108.08	118.30
1	B	158	LEU	C-N-CA	5.11	134.47	121.70
1	A	281	GLN	CG-CD-OE1	5.10	131.80	121.60
1	B	187	LEU	N-CA-CB	-5.09	100.22	110.40
1	B	403	TYR	CB-CG-CD1	-5.08	117.95	121.00
1	A	96	ALA	O-C-N	5.06	130.80	122.70
1	A	429	GLN	CB-CA-C	5.06	120.53	110.40
1	B	81	PHE	N-CA-CB	-5.06	101.49	110.60
1	A	22	LYS	N-CA-C	-5.05	97.35	111.00
1	B	322	VAL	CG1-CB-CG2	-5.05	102.81	110.90
1	B	169	ARG	CB-CA-C	-5.04	100.31	110.40
1	B	156	ASP	CB-CG-OD1	5.04	122.84	118.30
1	A	168	LYS	CA-CB-CG	5.04	124.48	113.40
1	A	424	PHE	O-C-N	5.03	130.75	122.70
1	B	482	SER	N-CA-CB	5.03	118.05	110.50
1	B	265	PHE	CB-CG-CD2	-5.03	117.28	120.80
1	A	218	THR	CA-CB-CG2	5.03	119.44	112.40
1	A	430	ARG	NE-CZ-NH2	5.02	122.81	120.30
1	A	143	ASP	CB-CG-OD1	5.02	122.82	118.30
1	A	449	VAL	O-C-N	5.02	130.73	122.70
1	A	41	LEU	CB-CG-CD2	-5.01	102.48	111.00
1	B	369	TYR	CB-CG-CD2	5.01	124.01	121.00
1	A	284	THR	N-CA-CB	-5.01	100.79	110.30
1	B	22	LYS	N-CA-C	-5.01	97.48	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	353	ARG	Sidechain
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 (i)

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	327	3
1	B	4008	0	3825	292	2
2	A	43	0	30	15	0
2	B	43	0	30	11	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	597	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 (597) 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	1.38
1:A:155:ARG:HH22	1:A:438:ASN:ND2	1.28	1.31
1:B:155:ARG:HH22	1:B:438:ASN:ND2	1.27	1.29
1:B:155:ARG:NH2	1:B:438:ASN:HD21	1.34	1.26
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	1.10
1:A:487:GLU:O	1:A:491:ARG:HG3	1.52	1.10
1:A:173:THR:CG2	1:A:175:LEU:HD12	1.84	1.08
1:B:444:THR:O	1:B:448:LYS:HG2	1.62	1.00
1:A:444:THR:HA	1:A:448:LYS:HD3	1.42	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:ASN:C	1:A:384:ASN:HD22	1.56	0.99
1:A:220:LYS:HE3	1:A:420:HIS:CD2	1.97	0.98
1:A:189:PRO:O	1:A:192:LEU:HD12	1.63	0.97
1:B:177:ASP:HB3	1:B:180:MET:HE3	1.44	0.97
1:B:170:ASN:HD22	1:B:172:GLN:H	1.12	0.96
1:A:471:LEU:HD22	1:A:474:GLN:NE2	1.79	0.96
1:A:371:GLN:HE21	1:A:393:MET:HB2	1.30	0.94
2:A:507:HEM:HBB2	2:A:507:HEM:HMB2	1.48	0.94
1:A:148:ASN:HD22	1:A:148:ASN:H	0.99	0.93
1:A:383:ALA:HB1	1:A:411:PRO:HG3	1.51	0.93
1:A:173:THR:HG21	1:A:175:LEU:HD12	1.46	0.93
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:142:TRP:HB2	1:B:339:PRO:HD3	1.52	0.92
1:B:406:ASN:HD22	1:B:408:PHE:H	1.18	0.91
1:A:322:VAL:HA	1:B:172:GLN:HE22	1.30	0.91
1:B:229:VAL:HG13	1:B:282:VAL:HG23	1.52	0.91
1:B:298:LEU:HD12	1:B:349:MET:HG3	1.53	0.91
1:B:189:PRO:O	1:B:192:LEU:HD12	1.72	0.88
1:B:229:VAL:CG1	1:B:282:VAL:HG23	2.03	0.88
1:B:177:ASP:HB3	1:B:180:MET:CE	2.04	0.88
1:A:92:ARG:HH11	1:A:92:ARG:HB2	1.40	0.87
1:A:384:ASN:HD22	1:A:385:TYR:N	1.72	0.87
1:A:220:LYS:HE3	1:A:420:HIS:HD2	1.37	0.87
1:B:284:THR:HG22	1:B:286:SER:H	1.40	0.85
1:B:179:ASP:O	1:B:183:ASP:HB2	1.75	0.85
1:A:406:ASN:ND2	1:A:408:PHE:H	1.75	0.85
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:B:406:ASN:ND2	1:B:408:PHE:H	1.74	0.84
1:B:90:ILE:HD13	1:B:312:VAL:HG13	1.60	0.84
1:B:251:ARG:O	1:B:255:GLU:HB2	1.77	0.84
1:A:485:HIS:CD2	1:A:486:PRO:HD2	2.14	0.83
1:A:458:LEU:O	1:A:462:ILE:HG13	1.76	0.83
1:B:74:HIS:O	1:B:111:ARG:NH2	2.11	0.82
1:A:406:ASN:C	1:A:406:ASN:HD22	1.83	0.82
1:B:394:MET:HE3	1:B:394:MET:HA	1.59	0.82
1:A:458:LEU:O	1:A:458:LEU:HD12	1.80	0.82
1:A:149:THR:OG1	1:A:150:PRO:HD2	1.79	0.81
1:A:148:ASN:HD22	1:A:148:ASN:N	1.78	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	0.80
1:B:170:ASN:ND2	1:B:172:GLN:H	1.78	0.80
1:B:297:ASP:OD1	1:B:300:LYS:HE2	1.81	0.80
1:A:223:ASN:C	1:A:223:ASN:HD22	1.82	0.79
1:A:149:THR:OG1	1:A:150:PRO:CD	2.30	0.79
2:A:507:HEM:HBB2	2:A:507:HEM:CMB	2.11	0.79
1:B:496:LEU:O	1:B:500:ASN:HB2	1.81	0.79
1:A:98:VAL:HG23	1:A:137:THR:CG2	2.12	0.79
1:A:134:LYS:HE3	1:A:331:LEU:CD2	2.13	0.78
1:A:444:THR:O	1:A:448:LYS:HG2	1.83	0.78
1:B:394:MET:HA	1:B:394:MET:CE	2.13	0.78
1:A:98:VAL:CG2	1:A:137:THR:HG22	2.14	0.77
1:A:177:ASP:HB3	1:A:180:MET:HE2	1.66	0.77
1:B:160:PHE:HB3	1:B:161:PRO:HD3	1.66	0.77
1:A:321:PRO:O	1:B:172:GLN:NE2	2.17	0.77
1:B:284:THR:HB	1:B:287:GLU:HG3	1.66	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:A:92:ARG:HB2	1:A:92:ARG:NH1	2.00	0.76
1:B:384:ASN:C	1:B:384:ASN:HD22	1.87	0.76
1:B:356:ALA:O	1:B:360:THR:HG22	1.85	0.76
1:A:374:VAL:O	1:A:374:VAL:HG22	1.83	0.76
1:A:108:ILE:HD13	1:A:315:LEU:HD12	1.65	0.75
1:B:147:ASN:HB2	2:B:507:HEM:HAC	1.68	0.75
1:A:229:VAL:HG13	1:A:282:VAL:HG23	1.67	0.75
1:A:294:ASN:ND2	1:A:296:PHE:H	1.85	0.75
1:A:148:ASN:H	1:A:148:ASN:ND2	1.79	0.75
1:A:238:ASP:OD1	1:A:314:LYS:NZ	2.13	0.74
1:A:223:ASN:ND2	1:A:225:ASP:H	1.84	0.74
1:B:79:GLY:O	1:B:80:ALA:HB2	1.88	0.74
1:A:405:PRO:HD2	1:A:405:PRO:O	1.85	0.74
1:B:98:VAL:HG23	1:B:137:THR:CG2	2.17	0.74
1:A:446:TYR:HA	1:A:450:LEU:HD21	1.70	0.73
1:B:279:TYR:CE1	1:B:311:PRO:HG3	2.22	0.73
1:A:297:ASP:OD1	1:A:300:LYS:HE2	1.88	0.73
1:A:79:GLY:O	1:A:80:ALA:HB2	1.88	0.73
1:A:173:THR:HG23	1:A:175:LEU:HD12	1.69	0.72
1:B:371:GLN:HE22	1:B:393:MET:H	1.37	0.72
2:B:507:HEM:HAD1	4:B:518:HOH:O	1.89	0.72
1:B:450:LEU:CD2	1:B:455:ARG:HG2	2.19	0.72
1:B:223:ASN:ND2	1:B:225:ASP:H	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:TYR:HA	1:A:450:LEU:CD2	2.19	0.72
1:A:406:ASN:ND2	1:A:406:ASN:C	2.39	0.72
1:A:92:ARG:O	1:A:223:ASN:HB3	1.90	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
1:B:173:THR:CG2	1:B:175:LEU:HG	2.20	0.71
1:A:371:GLN:NE2	1:A:393:MET:HB2	2.05	0.71
1:B:410:ALA:HB1	1:B:411:PRO:HD2	1.72	0.71
1:A:361:HIS:NE2	2:A:507:HEM:O2A	2.24	0.71
1:B:360:THR:HG21	2:B:507:HEM:HMA3	1.73	0.70
1:B:18:ARG:O	1:B:21:GLN:NE2	2.24	0.70
1:A:220:LYS:CE	1:A:420:HIS:CD2	2.74	0.70
1:A:170:ASN:HD22	1:A:173:THR:H	1.40	0.70
1:A:358:PRO:O	1:A:362:ARG:HD2	1.91	0.70
1:A:209:ARG:HG2	1:A:274:PRO:HB3	1.73	0.70
1:A:173:THR:CG2	1:A:175:LEU:CD1	2.66	0.69
1:A:466:LEU:HD12	1:A:466:LEU:O	1.92	0.69
1:B:98:VAL:CG2	1:B:137:THR:CG2	2.70	0.69
1:B:456:LYS:HB3	1:B:491:ARG:HH12	1.58	0.69
1:A:173:THR:HG22	1:A:175:LEU:H	1.57	0.69
1:B:169:ARG:NH1	1:B:174:HIS:O	2.26	0.69
1:B:90:ILE:CD1	1:B:312:VAL:HG13	2.23	0.68
1:B:306:ASP:HB3	1:B:307:TYR:CE2	2.27	0.68
1:A:94:SER:HB2	1:A:221:LEU:HD22	1.74	0.68
1:A:152:PHE:CB	1:A:298:LEU:HD13	2.23	0.68
1:A:496:LEU:O	1:A:500:ASN:HB2	1.93	0.68
1:B:384:ASN:ND2	1:B:386:GLN:H	1.91	0.68
1:A:90:ILE:O	1:A:93:TYR:HB2	1.93	0.68
1:A:263:ASP:O	1:A:264:LEU:C	2.32	0.68
1:A:453:GLU:OE1	1:A:456:LYS:HE2	1.92	0.68
1:A:85:GLU:HA	1:A:104:LYS:O	1.94	0.68
1:A:177:ASP:HB3	1:A:180:MET:CE	2.23	0.68
1:B:65:ARG:HG3	1:B:65:ARG:HH11	1.59	0.68
1:B:279:TYR:HE1	1:B:311:PRO:HG3	1.59	0.68
1:B:189:PRO:C	1:B:191:SER:H	1.95	0.68
1:A:383:ALA:HB1	1:A:411:PRO:CG	2.24	0.67
1:A:406:ASN:HD22	1:A:408:PHE:H	1.39	0.67
1:B:476:LYS:O	1:B:477:ALA:C	2.31	0.67
1:B:447:LEU:HB2	1:B:448:LYS:HD3	1.75	0.67
1:A:36:ASP:HB3	1:B:430:ARG:HD3	1.75	0.67
1:B:18:ARG:HD3	1:B:21:GLN:HG3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:LYS:NZ	1:B:138:GLU:OE1	2.23	0.67
1:A:322:VAL:CA	1:B:172:GLN:NE2	2.52	0.67
1:B:179:ASP:O	1:B:183:ASP:CB	2.42	0.67
1:A:281:GLN:HG2	1:A:307:TYR:O	1.95	0.67
1:B:98:VAL:HG23	1:B:137:THR:HB	1.76	0.67
1:B:15:LYS:HE2	4:B:522:HOH:O	1.95	0.66
1:B:63:PHE:C	1:B:65:ARG:H	1.99	0.66
1:B:95:LYS:HG2	1:B:222:VAL:O	1.94	0.66
1:B:275:SER:HA	1:B:315:LEU:O	1.94	0.66
1:A:118:GLU:OE2	1:A:169:ARG:NE	2.21	0.66
1:A:90:ILE:HD13	1:A:312:VAL:HG13	1.77	0.66
1:A:484:VAL:CG2	1:A:488:TYR:HD1	2.09	0.66
1:A:183:ASP:O	1:A:187:LEU:HB2	1.95	0.65
1:B:374:VAL:HG22	1:B:374:VAL:O	1.94	0.65
1:A:126:ARG:O	1:A:127:ASP:HB2	1.96	0.65
1:A:458:LEU:HD11	1:A:462:ILE:HD11	1.79	0.65
1:A:43:VAL:HG13	1:A:48:PRO:HD2	1.78	0.65
1:A:463:ALA:O	1:A:467:LYS:HB3	1.97	0.65
1:A:17:GLN:O	1:A:17:GLN:HG2	1.96	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	0.64
1:B:142:TRP:HB2	1:B:339:PRO:CD	2.27	0.64
1:A:172:GLN:NE2	1:B:322:VAL:HA	2.12	0.64
1:A:360:THR:HB	1:B:64:ASP:HB3	1.79	0.64
1:A:179:ASP:O	1:A:183:ASP:HB2	1.96	0.64
1:A:342:ILE:O	1:A:343:GLU:HB2	1.97	0.64
1:A:98:VAL:CG2	1:A:137:THR:CG2	2.74	0.63
1:B:173:THR:HG22	1:B:175:LEU:CG	2.24	0.63
1:B:402:ASN:C	1:B:402:ASN:HD22	2.00	0.63
1:A:236:LYS:HG3	1:A:279:TYR:CE2	2.33	0.63
1:A:304:HIS:HD2	1:A:309:LEU:HD21	1.62	0.63
1:B:170:ASN:HD22	1:B:172:GLN:N	1.90	0.63
1:B:189:PRO:C	1:B:191:SER:N	2.50	0.63
1:B:284:THR:HG22	1:B:286:SER:HB2	1.81	0.63
1:A:220:LYS:CE	1:A:420:HIS:HD2	2.09	0.63
1:B:223:ASN:C	1:B:223:ASN:HD22	2.01	0.63
1:A:172:GLN:HE21	1:B:322:VAL:HA	1.63	0.63
1:A:110:VAL:HA	1:A:132:ALA:O	1.99	0.62
1:A:172:GLN:HG3	1:B:322:VAL:O	1.98	0.62
1:B:173:THR:HG21	1:B:175:LEU:HD12	1.82	0.62
1:B:43:VAL:O	1:B:47:GLY:HA3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:PHE:C	1:A:131:PHE:HD1	2.03	0.62
1:B:191:SER:O	1:B:195:VAL:HG23	2.00	0.62
1:B:98:VAL:CG2	1:B:137:THR:HG22	2.29	0.62
1:B:74:HIS:CE1	1:B:115:VAL:HG22	2.35	0.61
1:A:300:LYS:NZ	4:A:530:HOH:O	2.29	0.61
1:A:453:GLU:OE1	1:A:456:LYS:CE	2.48	0.61
1:B:51:VAL:O	1:B:51:VAL:CG1	2.47	0.61
1:A:100:GLU:O	1:A:100:GLU:CG	2.48	0.61
1:A:100:GLU:O	1:A:100:GLU:HG3	2.01	0.61
1:B:17:GLN:O	1:B:17:GLN:HG2	2.00	0.61
1:B:406:ASN:HD22	1:B:408:PHE:N	1.93	0.60
1:B:458:LEU:CD1	1:B:462:ILE:CD1	2.79	0.60
1:B:478:VAL:HG11	1:B:493:GLN:OE1	2.01	0.60
1:B:192:LEU:HD22	1:B:484:VAL:HG11	1.82	0.60
1:A:147:ASN:CB	2:A:507:HEM:HAC	2.31	0.60
1:A:471:LEU:HD21	1:A:500:ASN:OD1	2.01	0.60
1:B:470:GLN:OE1	1:B:472:PHE:HE2	1.85	0.60
1:A:160:PHE:HB3	1:A:161:PRO:HD3	1.84	0.60
1:A:484:VAL:HG22	1:A:488:TYR:HD1	1.66	0.59
1:B:307:TYR:N	1:B:307:TYR:CD2	2.68	0.59
1:B:385:TYR:OH	1:B:411:PRO:O	2.20	0.59
1:A:95:LYS:HG2	1:A:222:VAL:O	2.02	0.59
1:A:155:ARG:NH2	1:A:438:ASN:ND2	2.05	0.59
1:A:284:THR:HG22	1:A:286:SER:H	1.66	0.59
1:A:152:PHE:HB3	1:A:298:LEU:HD13	1.84	0.59
1:B:371:GLN:NE2	1:B:393:MET:H	2.01	0.59
1:B:458:LEU:CD1	1:B:462:ILE:HD11	2.32	0.59
1:A:9:ASP:HB3	1:A:13:HIS:CE1	2.38	0.59
1:B:192:LEU:HD22	1:B:484:VAL:CG1	2.33	0.59
1:A:152:PHE:HB2	1:A:298:LEU:HD13	1.83	0.59
1:A:147:ASN:CG	2:A:507:HEM:HAC	2.23	0.58
1:A:238:ASP:CG	1:A:314:LYS:HZ2	2.05	0.58
1:A:275:SER:HA	1:A:315:LEU:O	2.02	0.58
1:A:131:PHE:C	1:A:131:PHE:CD1	2.75	0.58
1:B:156:ASP:OD2	1:B:158:LEU:HB2	2.02	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
1:A:268:ILE:HG23	1:A:318:ASN:HA	1.85	0.58
1:B:458:LEU:HD12	1:B:462:ILE:CD1	2.33	0.58
1:A:74:HIS:O	1:A:111:ARG:NH2	2.32	0.58
1:A:98:VAL:HG23	1:A:137:THR:HG22	1.81	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:LYS:HG3	1:A:279:TYR:HE2	1.67	0.57
1:A:385:TYR:OH	1:A:411:PRO:O	2.18	0.57
1:B:21:GLN:O	1:B:22:LYS:CB	2.53	0.57
1:B:51:VAL:O	1:B:51:VAL:HG13	2.03	0.57
1:A:371:GLN:NE2	1:A:393:MET:H	2.01	0.57
1:B:89:ASP:C	1:B:89:ASP:OD1	2.39	0.57
1:A:428:VAL:HG13	1:B:50:LEU:HD12	1.85	0.57
1:A:223:ASN:C	1:A:223:ASN:ND2	2.56	0.57
1:A:439:VAL:O	1:A:442:VAL:N	2.38	0.57
1:B:453:GLU:O	1:B:456:LYS:HG2	2.05	0.57
1:A:453:GLU:OE1	1:A:456:LYS:NZ	2.38	0.57
1:B:125:VAL:O	1:B:129:ARG:NH2	2.35	0.57
1:A:147:ASN:HB2	2:A:507:HEM:HAC	1.87	0.56
1:A:173:THR:HG23	1:A:175:LEU:CD1	2.34	0.56
1:A:175:LEU:HD22	1:B:262:ARG:NH2	2.20	0.56
1:A:374:VAL:O	1:A:374:VAL:CG2	2.53	0.56
1:B:284:THR:CG2	1:B:286:SER:HB2	2.35	0.56
1:A:154:ILE:HG13	1:A:349:MET:CE	2.34	0.56
1:A:367:PRO:CG	1:A:390:PRO:HG2	2.12	0.56
1:B:456:LYS:CB	1:B:491:ARG:HH12	2.18	0.56
1:B:466:LEU:HD12	1:B:466:LEU:O	2.04	0.56
1:A:60:MET:CE	1:A:63:PHE:HD2	2.19	0.56
1:A:348:LYS:CE	4:A:549:HOH:O	2.53	0.56
1:A:356:ALA:O	1:A:360:THR:HG22	2.06	0.56
1:A:98:VAL:HG23	1:A:137:THR:HB	1.86	0.56
1:B:301:VAL:HG22	1:B:441:GLN:OE1	2.05	0.56
1:A:435:ASN:C	1:A:436:ASP:O	2.42	0.56
1:B:63:PHE:O	1:B:65:ARG:N	2.39	0.56
1:A:487:GLU:HG2	1:A:491:ARG:HD2	1.88	0.55
1:A:229:VAL:HG13	1:A:282:VAL:CG2	2.36	0.55
1:A:266:ASN:O	1:A:267:ALA:O	2.25	0.55
1:B:334:ASP:O	1:B:337:ASN:HB2	2.06	0.55
1:A:471:LEU:HD22	1:A:474:GLN:HE22	1.63	0.55
1:B:73:VAL:O	1:B:74:HIS:HB2	2.06	0.55
1:B:394:MET:HE3	1:B:394:MET:CA	2.34	0.55
1:B:304:HIS:HE1	3:B:508:NDP:O3B	1.89	0.55
1:B:229:VAL:CG1	1:B:282:VAL:CG2	2.82	0.55
2:B:507:HEM:HMB1	2:B:507:HEM:HBB2	1.88	0.55
1:A:345:SER:HB2	1:A:346:PRO:CD	2.37	0.55
1:B:274:PRO:HB2	1:B:276:TRP:CZ3	2.41	0.55
1:A:239:GLN:NE2	1:A:239:GLN:H	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:VAL:HG23	1:B:137:THR:HG21	1.87	0.55
1:A:245:SER:OG	1:A:248:ASP:HB2	2.07	0.55
1:B:65:ARG:HG3	1:B:65:ARG:NH1	2.21	0.55
1:A:157:ALA:CB	2:A:507:HEM:HBB1	2.37	0.55
1:A:179:ASP:O	1:A:183:ASP:N	2.33	0.55
1:A:447:LEU:CB	1:A:448:LYS:HD2	2.37	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:A:73:VAL:O	1:A:74:HIS:HB2	2.07	0.54
1:A:237:THR:HG21	1:A:240:GLY:O	2.07	0.54
1:B:188:ARG:O	1:B:191:SER:HB3	2.07	0.54
1:B:410:ALA:HB1	1:B:411:PRO:CD	2.36	0.54
1:B:485:HIS:CD2	1:B:486:PRO:HD2	2.42	0.54
1:A:189:PRO:C	1:A:191:SER:H	2.10	0.54
1:B:147:ASN:CB	2:B:507:HEM:HAC	2.38	0.54
1:B:372:ILE:O	1:B:373:PRO:C	2.45	0.54
1:A:178:PRO:O	1:A:182:TRP:HB2	2.08	0.54
1:B:453:GLU:HA	1:B:453:GLU:OE2	2.06	0.54
1:A:74:HIS:HA	1:A:114:THR:O	2.08	0.54
1:B:384:ASN:C	1:B:384:ASN:ND2	2.61	0.54
1:A:487:GLU:CG	1:A:491:ARG:HD2	2.37	0.53
1:B:57:THR:O	1:B:61:ALA:HB2	2.09	0.53
1:A:82:GLY:HA3	1:A:316:VAL:O	2.08	0.53
1:A:125:VAL:O	1:A:129:ARG:NH1	2.32	0.53
1:A:154:ILE:HG13	1:A:349:MET:HE1	1.90	0.53
1:B:189:PRO:HB2	1:B:192:LEU:CD1	2.39	0.53
1:B:212:ASP:OD1	1:B:237:THR:HG22	2.08	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:4:ARG:CD	1:A:9:ASP:OD1	2.56	0.53
1:A:371:GLN:HE22	1:A:393:MET:H	1.57	0.53
1:B:229:VAL:HG11	1:B:282:VAL:HG23	1.89	0.53
1:B:63:PHE:C	1:B:65:ARG:N	2.61	0.53
1:B:383:ALA:HB1	1:B:411:PRO:HG3	1.90	0.53
1:A:276:TRP:HZ3	1:A:317:LEU:HD22	1.74	0.53
1:A:400:ALA:O	1:A:401:PRO:C	2.47	0.52
1:A:406:ASN:ND2	1:A:406:ASN:O	2.42	0.52
1:A:322:VAL:HA	1:B:172:GLN:HE21	1.68	0.52
1:B:155:ARG:NH2	1:B:438:ASN:ND2	2.13	0.52
1:A:294:ASN:HD22	1:A:295:PRO:N	2.07	0.52
1:B:54:VAL:HG23	1:B:54:VAL:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:TRP:HA	1:A:337:ASN:O	2.09	0.52
1:B:439:VAL:O	1:B:440:THR:C	2.48	0.52
1:A:92:ARG:O	1:A:223:ASN:CB	2.57	0.52
1:A:405:PRO:O	1:A:405:PRO:CD	2.55	0.52
1:A:200:SER:O	1:A:203:GLY:N	2.40	0.52
1:B:18:ARG:HG2	1:B:18:ARG:HH11	1.75	0.52
1:B:245:SER:OG	1:B:248:ASP:HB2	2.10	0.52
1:A:342:ILE:O	1:A:343:GLU:CB	2.56	0.52
1:A:458:LEU:HD12	1:A:462:ILE:HG13	1.92	0.52
1:B:21:GLN:O	1:B:22:LYS:HB3	2.10	0.52
1:B:60:MET:CE	1:B:64:ASP:OD2	2.58	0.52
1:B:136:TYR:HB3	4:B:531:HOH:O	2.09	0.52
1:A:38:LEU:HA	1:B:159:LEU:HD22	1.91	0.51
1:A:54:VAL:HA	1:A:57:THR:HG23	1.93	0.51
1:B:148:ASN:H	1:B:148:ASN:HD22	1.58	0.51
1:A:201:ASP:C	1:A:203:GLY:H	2.14	0.51
1:B:392:CYS:SG	1:B:396:ASN:HB2	2.51	0.51
1:B:458:LEU:HD11	1:B:462:ILE:CD1	2.40	0.51
1:B:236:LYS:O	1:B:276:TRP:HA	2.10	0.51
1:A:430:ARG:HD3	1:B:36:ASP:HB3	1.92	0.51
1:A:46:ARG:HD3	1:B:294:ASN:ND2	2.26	0.51
1:B:110:VAL:HG21	1:B:317:LEU:HD11	1.92	0.51
1:B:415:PRO:C	1:B:417:ALA:H	2.14	0.51
1:B:84:PHE:O	1:B:105:ARG:HA	2.11	0.51
1:B:129:ARG:H	1:B:148:ASN:ND2	2.09	0.51
1:B:447:LEU:HB2	1:B:448:LYS:CD	2.39	0.51
1:A:60:MET:HE3	1:A:63:PHE:HD2	1.75	0.50
1:A:150:PRO:HD2	1:A:151:ILE:H	1.76	0.50
1:B:90:ILE:CD1	1:B:312:VAL:CG1	2.89	0.50
1:A:142:TRP:HB2	1:A:339:PRO:HD3	1.93	0.50
1:A:406:ASN:OD1	1:A:410:ALA:HB3	2.10	0.50
1:B:493:GLN:O	1:B:494:ALA:C	2.48	0.50
1:A:74:HIS:CE1	1:A:115:VAL:HG22	2.46	0.50
1:A:276:TRP:CZ3	1:A:317:LEU:HD22	2.45	0.50
1:B:152:PHE:HB3	1:B:298:LEU:HD13	1.94	0.50
1:B:236:LYS:HG3	1:B:279:TYR:CE2	2.47	0.50
1:B:470:GLN:OE1	1:B:472:PHE:CE2	2.65	0.50
1:B:402:ASN:C	1:B:402:ASN:ND2	2.64	0.50
1:B:173:THR:CG2	1:B:175:LEU:CG	2.86	0.50
1:B:394:MET:CE	1:B:394:MET:CA	2.84	0.50
1:B:9:ASP:OD1	1:B:12:LYS:NZ	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:ASN:HD22	1:B:385:TYR:N	2.08	0.50
1:A:90:ILE:HG21	1:A:312:VAL:HG22	1.94	0.50
1:A:170:ASN:ND2	1:A:172:GLN:H	2.10	0.50
1:A:458:LEU:CD1	1:A:462:ILE:HD11	2.41	0.50
1:B:189:PRO:HB2	1:B:192:LEU:HD12	1.93	0.50
1:B:300:LYS:NZ	1:B:437:ASP:O	2.43	0.50
1:A:449:VAL:HG12	1:A:449:VAL:O	2.12	0.49
1:A:430:ARG:NH2	1:B:53:ASP:OD2	2.45	0.49
1:B:406:ASN:ND2	1:B:406:ASN:C	2.65	0.49
1:A:118:GLU:HG3	1:B:120:GLY:CA	2.43	0.49
1:A:294:ASN:HD22	1:A:294:ASN:C	2.15	0.49
1:A:309:LEU:HD12	4:A:517:HOH:O	2.11	0.49
1:A:406:ASN:HD22	1:A:408:PHE:N	2.09	0.49
1:B:131:PHE:C	1:B:131:PHE:CD1	2.84	0.49
1:A:235:TYR:HA	1:A:277:THR:O	2.12	0.49
1:B:57:THR:O	1:B:61:ALA:CB	2.60	0.49
1:A:81:PHE:CD1	1:A:81:PHE:N	2.80	0.49
1:B:306:ASP:O	1:B:308:PRO:HD3	2.13	0.49
1:A:487:GLU:HG2	1:A:491:ARG:CD	2.42	0.49
1:B:178:PRO:O	1:B:182:TRP:HB2	2.12	0.49
1:B:19:ALA:C	1:B:21:GLN:H	2.16	0.49
1:B:458:LEU:CD1	1:B:462:ILE:HD12	2.42	0.49
1:A:93:TYR:HB3	1:A:221:LEU:HD13	1.94	0.49
1:A:223:ASN:ND2	1:A:225:ASP:N	2.57	0.49
1:B:294:ASN:HD21	1:B:296:PHE:HD2	1.61	0.49
1:A:371:GLN:HE22	1:A:393:MET:N	2.11	0.48
1:A:18:ARG:O	1:A:21:GLN:NE2	2.47	0.48
1:A:134:LYS:HE3	1:A:331:LEU:HD23	1.94	0.48
1:A:471:LEU:CD2	1:A:474:GLN:HE22	2.25	0.48
1:A:471:LEU:CD2	1:A:474:GLN:NE2	2.64	0.48
1:A:463:ALA:HA	1:A:466:LEU:HB3	1.94	0.48
1:A:487:GLU:O	1:A:491:ARG:CG	2.44	0.48
1:B:229:VAL:HG11	1:B:282:VAL:CG2	2.43	0.48
1:B:361:HIS:NE2	2:B:507:HEM:O2A	2.46	0.48
1:A:86:VAL:N	1:A:104:LYS:O	2.43	0.48
1:A:98:VAL:HG21	1:A:137:THR:HG22	1.94	0.48
1:B:135:PHE:CD1	1:B:142:TRP:CE3	3.02	0.48
1:A:435:ASN:O	1:A:436:ASP:O	2.31	0.48
1:A:447:LEU:HB2	1:A:448:LYS:CD	2.44	0.48
1:B:177:ASP:CB	1:B:180:MET:CE	2.85	0.48
1:B:223:ASN:ND2	1:B:225:ASP:N	2.59	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:ASN:HD22	1:B:386:GLN:H	1.62	0.48
1:A:155:ARG:NE	1:A:433:SER:O	2.29	0.48
1:B:129:ARG:HG2	4:B:542:HOH:O	2.13	0.48
1:A:59:GLU:HB2	4:A:515:HOH:O	2.14	0.47
1:A:236:LYS:O	1:A:276:TRP:HA	2.14	0.47
1:B:441:GLN:O	1:B:444:THR:HG23	2.14	0.47
1:A:84:PHE:O	1:A:105:ARG:HA	2.13	0.47
1:B:487:GLU:O	1:B:491:ARG:HG3	2.14	0.47
1:A:283:MET:HB3	1:A:302:TRP:CH2	2.49	0.47
1:A:357:TYR:CZ	2:A:507:HEM:NA	2.82	0.47
1:A:189:PRO:C	1:A:191:SER:N	2.66	0.47
1:B:72:VAL:HG13	1:B:73:VAL:HG22	1.95	0.47
1:B:429:GLN:HE21	1:B:429:GLN:HB2	1.34	0.47
1:A:478:VAL:O	1:A:482:SER:HB2	2.14	0.47
1:A:40:SER:HB3	1:A:49:LEU:HD13	1.97	0.47
1:B:386:GLN:O	1:B:387:ARG:NH1	2.47	0.47
1:A:64:ASP:HB3	1:B:360:THR:HB	1.97	0.47
1:A:172:GLN:NE2	1:B:321:PRO:O	2.46	0.47
1:B:293:PHE:O	1:B:295:PRO:HD3	2.15	0.47
1:B:297:ASP:OD2	1:B:299:THR:OG1	2.31	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:284:THR:HG22	1:B:286:SER:N	2.21	0.47
1:A:5:ASP:OD2	1:A:7:ALA:HB3	2.15	0.47
1:A:217:HIS:HB2	1:A:219:PHE:CZ	2.50	0.47
1:A:93:TYR:CZ	1:A:282:VAL:HG11	2.50	0.46
1:A:127:ASP:C	1:A:128:PRO:O	2.52	0.46
1:B:351:GLN:HA	1:B:354:LEU:HD22	1.97	0.46
1:A:98:VAL:HG23	1:A:137:THR:CB	2.45	0.46
1:B:149:THR:HG23	1:B:151:ILE:O	2.15	0.46
1:B:298:LEU:HD12	1:B:349:MET:CG	2.37	0.46
1:B:134:LYS:HE3	1:B:331:LEU:CD2	2.46	0.46
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:89:ASP:OD1	1:B:89:ASP:O	2.32	0.46
1:B:145:VAL:HG22	1:B:333:PHE:HB3	1.97	0.46
1:B:209:ARG:HB2	4:B:541:HOH:O	2.14	0.46
1:B:209:ARG:HH11	1:B:209:ARG:HD3	1.45	0.46
1:B:236:LYS:HE2	1:B:236:LYS:HB3	1.70	0.46
1:B:400:ALA:O	1:B:401:PRO:C	2.54	0.46
1:A:43:VAL:O	1:A:47:GLY:HA3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:ASN:ND2	1:B:223:ASN:C	2.69	0.46
1:A:157:ALA:HB2	2:A:507:HEM:HBB1	1.98	0.46
1:A:444:THR:CA	1:A:448:LYS:HD3	2.28	0.46
1:B:406:ASN:HD22	1:B:406:ASN:C	2.18	0.46
1:A:384:ASN:ND2	1:A:386:GLN:H	2.14	0.46
1:B:218:THR:HA	1:B:231:CYS:O	2.15	0.46
1:B:444:THR:HB	1:B:448:LYS:HZ3	1.81	0.46
1:B:447:LEU:O	1:B:455:ARG:NH2	2.49	0.46
1:B:19:ALA:C	1:B:21:GLN:N	2.69	0.46
1:B:127:ASP:C	1:B:128:PRO:O	2.52	0.46
1:B:138:GLU:OE2	1:B:138:GLU:N	2.44	0.46
1:A:77:GLY:HA3	1:A:112:PHE:O	2.15	0.46
1:A:79:GLY:O	1:A:80:ALA:CB	2.59	0.46
1:A:372:ILE:O	1:A:373:PRO:C	2.54	0.46
1:A:293:PHE:O	1:A:295:PRO:HD3	2.16	0.46
1:B:79:GLY:O	1:B:80:ALA:CB	2.57	0.46
1:A:168:LYS:HE3	1:B:67:ARG:NH2	2.30	0.45
1:B:239:GLN:HE21	1:B:239:GLN:HB2	1.53	0.45
1:A:112:PHE:CD2	1:A:208:HIS:HB3	2.51	0.45
1:B:110:VAL:HA	1:B:132:ALA:O	2.17	0.45
1:B:294:ASN:HA	1:B:295:PRO:HD2	1.75	0.45
1:B:458:LEU:HD11	1:B:462:ILE:HD11	1.97	0.45
1:A:53:ASP:C	1:A:55:VAL:H	2.19	0.45
1:A:147:ASN:ND2	2:A:507:HEM:C3C	2.84	0.45
1:A:173:THR:HG22	1:A:175:LEU:N	2.28	0.45
1:A:266:ASN:O	1:A:267:ALA:C	2.54	0.45
1:A:360:THR:HG21	2:A:507:HEM:HMA3	1.98	0.45
1:B:437:ASP:OD2	1:B:437:ASP:C	2.55	0.45
1:A:418:LEU:HD23	1:A:418:LEU:HA	1.78	0.45
1:B:22:LYS:HA	1:B:22:LYS:HD3	1.61	0.45
1:B:220:LYS:HD2	1:B:228:ALA:HB1	1.99	0.45
1:A:141:ASN:OD1	1:A:377:PRO:HA	2.16	0.45
1:A:147:ASN:HB2	2:A:507:HEM:CAC	2.46	0.45
1:B:177:ASP:CB	1:B:180:MET:HE2	2.47	0.45
1:B:177:ASP:OD1	1:B:179:ASP:HB2	2.17	0.45
1:A:326:ALA:HA	1:A:330:GLN:HE21	1.81	0.45
1:A:406:ASN:HD22	1:A:407:SER:N	2.14	0.45
1:B:71:ARG:HD2	1:B:111:ARG:NH2	2.30	0.45
1:B:450:LEU:HD11	1:B:458:LEU:HD22	1.99	0.45
1:B:299:THR:C	1:B:300:LYS:HG2	2.37	0.45
1:B:467:LYS:HE2	1:B:468:ASP:OD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:VAL:CA	1:B:172:GLN:HE21	2.28	0.45
1:B:239:GLN:OE1	1:B:274:PRO:HA	2.17	0.45
1:A:282:VAL:HG23	1:A:283:MET:N	2.31	0.45
1:B:65:ARG:NH1	1:B:65:ARG:CG	2.76	0.45
1:B:177:ASP:HA	1:B:178:PRO:HD3	1.70	0.45
1:A:51:VAL:O	1:A:51:VAL:CG1	2.65	0.44
1:A:97:LYS:O	1:A:100:GLU:HB3	2.16	0.44
1:A:118:GLU:OE2	1:A:169:ARG:NH2	2.50	0.44
1:A:9:ASP:O	1:A:12:LYS:HB3	2.17	0.44
1:A:155:ARG:HH11	1:A:155:ARG:HD3	1.40	0.44
1:A:172:GLN:HE21	1:B:322:VAL:CA	2.29	0.44
1:A:251:ARG:O	1:A:255:GLU:HB2	2.17	0.44
1:A:414:GLN:HA	1:A:415:PRO:HD2	1.89	0.44
1:B:293:PHE:O	1:B:295:PRO:CD	2.65	0.44
1:A:342:ILE:HG22	1:A:343:GLU:H	1.82	0.44
1:A:471:LEU:HD11	1:A:500:ASN:OD1	2.18	0.44
1:A:357:TYR:CB	1:A:358:PRO:CD	2.96	0.44
1:B:191:SER:O	1:B:195:VAL:CG2	2.63	0.44
1:B:354:LEU:HD12	1:B:354:LEU:HA	1.68	0.44
1:B:487:GLU:CG	1:B:491:ARG:HD2	2.46	0.44
1:A:439:VAL:CG2	1:A:443:ARG:NH1	2.81	0.44
1:B:134:LYS:HE2	1:B:134:LYS:HB2	1.65	0.44
1:B:135:PHE:CE1	1:B:142:TRP:CZ3	3.05	0.44
1:A:439:VAL:HG23	1:A:443:ARG:HH11	1.82	0.44
1:B:182:TRP:O	1:B:183:ASP:C	2.55	0.44
1:B:206:ASP:HA	1:B:244:LEU:HG	1.99	0.44
1:A:108:ILE:CD1	1:A:315:LEU:HD12	2.42	0.44
1:A:353:ARG:O	1:A:354:LEU:C	2.56	0.44
1:A:447:LEU:HB2	1:A:448:LYS:HD2	2.00	0.44
2:A:507:HEM:CMB	2:A:507:HEM:CBB	2.92	0.44
1:B:262:ARG:HH11	1:B:262:ARG:HD3	1.58	0.44
1:B:381:ARG:HH11	1:B:381:ARG:HD3	1.46	0.44
1:A:72:VAL:HG12	2:A:507:HEM:HMA1	1.99	0.44
1:A:84:PHE:HA	1:A:314:LYS:O	2.18	0.44
1:A:449:VAL:O	1:A:449:VAL:CG1	2.64	0.44
1:B:229:VAL:HG13	1:B:282:VAL:CG2	2.37	0.44
1:B:186:SER:O	1:B:476:LYS:NZ	2.35	0.43
1:B:194:GLN:O	1:B:198:LEU:N	2.44	0.43
1:A:79:GLY:HA2	1:A:110:VAL:O	2.18	0.43
1:A:39:ASN:ND2	1:B:432:ASN:HA	2.33	0.43
1:A:282:VAL:CG2	1:A:283:MET:N	2.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:GLU:HA	1:A:344:PRO:HD3	1.94	0.43
1:A:99:PHE:CE1	1:A:312:VAL:HG11	2.53	0.43
1:A:170:ASN:HA	1:A:171:PRO:HD3	1.85	0.43
1:A:298:LEU:HD23	1:A:298:LEU:HA	1.66	0.43
1:B:98:VAL:HG23	1:B:137:THR:CB	2.45	0.43
1:B:157:ALA:CB	2:B:507:HEM:CBB	2.95	0.43
1:A:458:LEU:HD12	1:A:458:LEU:C	2.38	0.43
1:A:91:THR:HA	1:A:94:SER:O	2.19	0.43
1:A:444:THR:O	1:A:445:PHE:C	2.57	0.43
1:A:177:ASP:CG	1:A:180:MET:HG3	2.38	0.43
1:A:50:LEU:HD12	1:B:428:VAL:HG13	2.00	0.43
1:A:354:LEU:HD12	1:A:354:LEU:HA	1.71	0.43
1:B:78:ALA:O	1:B:111:ARG:HA	2.19	0.43
1:B:221:LEU:O	1:B:228:ALA:HA	2.19	0.43
1:A:182:TRP:HB3	1:A:473:ILE:CG2	2.48	0.43
1:B:92:ARG:HD2	1:B:93:TYR:CE1	2.54	0.43
1:B:449:VAL:HG21	3:B:508:NDP:C4D	2.49	0.43
1:A:187:LEU:HA	1:A:187:LEU:HD12	1.72	0.42
1:A:118:GLU:H	1:A:118:GLU:HG2	1.16	0.42
1:A:170:ASN:HD21	1:B:10:GLN:NE2	2.17	0.42
1:A:150:PRO:CD	1:A:151:ILE:H	2.31	0.42
1:A:337:ASN:HD22	1:A:337:ASN:HA	1.57	0.42
1:A:342:ILE:HG22	1:A:343:GLU:N	2.34	0.42
1:B:484:VAL:HG22	1:B:488:TYR:HD1	1.84	0.42
1:A:134:LYS:CE	1:A:331:LEU:CD2	2.92	0.42
1:B:157:ALA:HB2	2:B:507:HEM:CBB	2.49	0.42
1:B:304:HIS:CE1	3:B:508:NDP:O3B	2.71	0.42
1:B:453:GLU:OE2	1:B:453:GLU:CA	2.66	0.42
1:A:135:PHE:CD1	1:A:142:TRP:CE3	3.08	0.42
1:B:364:ARG:HH21	1:B:364:ARG:HD2	1.35	0.42
1:A:87:THR:OG1	1:A:88:HIS:ND1	2.51	0.42
1:A:90:ILE:HD13	1:A:312:VAL:CG1	2.48	0.42
1:B:332:ALA:HB1	1:B:361:HIS:CE1	2.55	0.42
1:B:471:LEU:O	1:B:472:PHE:C	2.58	0.42
1:A:92:ARG:H	1:A:92:ARG:HG3	1.56	0.42
1:A:453:GLU:OE2	1:A:456:LYS:HG2	2.20	0.42
1:B:402:ASN:HD22	1:B:403:TYR:N	2.18	0.42
1:A:89:ASP:C	1:A:89:ASP:OD1	2.57	0.42
1:A:304:HIS:CD2	1:A:309:LEU:HD21	2.47	0.42
1:B:5:ASP:OD1	1:B:5:ASP:N	2.53	0.42
1:B:236:LYS:H	1:B:236:LYS:HG2	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:479:LYS:HE2	1:B:479:LYS:HB3	1.46	0.42
1:B:485:HIS:HA	1:B:486:PRO:HD2	1.73	0.42
1:A:147:ASN:ND2	2:A:507:HEM:CAC	2.83	0.41
1:A:439:VAL:O	1:A:440:THR:C	2.58	0.41
1:B:387:ARG:HA	1:B:396:ASN:HD21	1.84	0.41
1:A:329:GLU:OE2	1:A:329:GLU:HA	2.20	0.41
1:A:496:LEU:HD23	1:A:496:LEU:HA	1.99	0.41
1:A:456:LYS:HG3	1:A:460:GLU:OE1	2.20	0.41
1:B:435:ASN:O	1:B:436:ASP:C	2.59	0.41
1:A:19:ALA:C	1:A:21:GLN:H	2.24	0.41
1:A:77:GLY:CA	1:A:112:PHE:O	2.69	0.41
1:A:237:THR:CG2	1:A:240:GLY:O	2.68	0.41
1:A:388:ASP:H	1:A:396:ASN:HD21	1.68	0.41
1:B:360:THR:HG21	2:B:507:HEM:CMA	2.47	0.41
1:B:393:MET:C	1:B:394:MET:O	2.58	0.41
1:A:188:ARG:O	1:A:191:SER:HB3	2.21	0.41
1:A:239:GLN:CD	1:A:239:GLN:N	2.74	0.41
1:B:439:VAL:O	1:B:440:THR:O	2.38	0.41
1:A:400:ALA:HA	1:A:401:PRO:HD3	1.98	0.41
1:B:189:PRO:O	1:B:192:LEU:HB2	2.21	0.41
1:A:154:ILE:O	1:A:349:MET:HE2	2.21	0.41
1:A:345:SER:CB	1:A:346:PRO:CD	2.98	0.41
1:A:170:ASN:HD22	1:A:172:GLN:H	1.69	0.41
1:A:206:ASP:HA	1:A:244:LEU:HG	2.01	0.41
1:A:284:THR:CG2	1:A:286:SER:H	2.30	0.41
1:A:145:VAL:HG22	1:A:333:PHE:HB3	2.02	0.41
1:A:294:ASN:HA	1:A:295:PRO:HD2	1.84	0.41
1:A:471:LEU:HD21	1:A:500:ASN:ND2	2.36	0.41
1:B:50:LEU:HD23	1:B:50:LEU:HA	1.85	0.41
1:B:118:GLU:H	1:B:118:GLU:HG2	1.02	0.41
1:B:280:ILE:O	1:B:280:ILE:HG13	2.21	0.41
1:B:448:LYS:HG2	1:B:448:LYS:H	1.50	0.41
1:A:221:LEU:HG	1:A:231:CYS:SG	2.61	0.41
1:B:9:ASP:HB3	1:B:13:HIS:CE1	2.56	0.41
1:B:394:MET:HA	1:B:394:MET:HE2	1.99	0.41
1:B:446:TYR:HA	1:B:450:LEU:HD22	2.03	0.41
1:A:14:TRP:CH2	1:A:18:ARG:HD2	2.56	0.40
1:A:273:TYR:N	1:A:273:TYR:CD2	2.83	0.40
1:B:84:PHE:HA	1:B:314:LYS:O	2.21	0.40
1:B:275:SER:HB3	1:B:316:VAL:HG22	2.02	0.40
2:B:507:HEM:HHA	2:B:507:HEM:HAA1	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:TRP:CZ3	1:A:18:ARG:HD2	2.57	0.40
1:A:439:VAL:CG2	1:A:443:ARG:HH11	2.34	0.40
1:A:120:GLY:HA2	1:B:118:GLU:HG3	2.03	0.40
1:A:274:PRO:HG2	1:A:317:LEU:HB2	2.02	0.40
1:A:440:THR:O	1:A:443:ARG:N	2.54	0.40
1:B:18:ARG:HH11	1:B:18:ARG:CG	2.32	0.40
1:B:158:LEU:HD13	1:B:158:LEU:HA	1.70	0.40
1:A:262:ARG:CZ	1:B:175:LEU:HD13	2.51	0.40
1:A:357:TYR:HB2	1:A:358:PRO:CD	2.51	0.40
1:A:22:LYS:HA	1:A:23:PRO:HD3	1.89	0.40
1:A:471:LEU:HD21	1:A:500:ASN:HD21	1.87	0.40
1:A:472:PHE:O	1:A:475:LYS:N	2.55	0.40
1:B:369:TYR:HA	1:B:372:ILE:HD13	2.04	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 (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%)	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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	10	GLN
1	A	17	GLN
1	A	21	GLN
1	A	39	ASN
1	A	148	ASN
1	A	170	ASN
1	A	172	GLN

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Mol	Chain	Res	Type
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	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
1	B	420	HIS
1	B	429	GLN

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Mol	Chain	Res	Type
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 monosaccharides 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	A	508	-	45,52,52	2.52	11 (24%)	53,80,80	2.20	12 (22%)
2	HEM	B	507	1	41,50,50	1.46	7 (17%)	45,82,82	2.14	12 (26%)
3	NDP	B	508	-	45,52,52	2.54	11 (24%)	53,80,80	2.20	12 (22%)
2	HEM	A	507	1	41,50,50	1.55	9 (21%)	45,82,82	2.45	18 (40%)

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	A	508	-	1/1/14/17	3/30/77/77	0/5/5/5
2	HEM	B	507	1	-	1/12/54/54	-
3	NDP	B	508	-	1/1/14/17	3/30/77/77	0/5/5/5
2	HEM	A	507	1	-	0/12/54/54	-

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	508	NDP	O4B-C1B	9.67	1.54	1.41
3	A	508	NDP	O4B-C1B	9.62	1.54	1.41
3	B	508	NDP	P2B-O2B	8.71	1.75	1.59
3	A	508	NDP	P2B-O2B	8.60	1.75	1.59
3	B	508	NDP	O3B-C3B	-5.10	1.31	1.43
3	A	508	NDP	O3B-C3B	-5.04	1.31	1.43
3	B	508	NDP	C4N-C3N	-4.48	1.41	1.49
3	A	508	NDP	C4N-C3N	-4.43	1.41	1.49
3	B	508	NDP	C4N-C5N	-3.83	1.38	1.48
3	A	508	NDP	C4N-C5N	-3.80	1.39	1.48
2	A	507	HEM	C3C-CAC	3.65	1.55	1.47
3	B	508	NDP	C7N-C3N	3.53	1.56	1.48
3	A	508	NDP	C7N-C3N	3.48	1.56	1.48
2	A	507	HEM	C3C-C2C	-3.30	1.35	1.40
2	B	507	HEM	CAA-C2A	3.10	1.56	1.52
2	B	507	HEM	O1A-CGA	2.90	1.31	1.22
2	B	507	HEM	CHB-C1B	2.86	1.42	1.35
2	A	507	HEM	CMB-C2B	2.64	1.56	1.50
2	B	507	HEM	CBD-CGD	2.62	1.56	1.50
3	B	508	NDP	C6N-C5N	2.61	1.38	1.33
3	A	508	NDP	C6N-C5N	2.59	1.38	1.33
2	B	507	HEM	CMA-C3A	2.59	1.57	1.51
2	A	507	HEM	C2C-C1C	-2.48	1.37	1.42
2	B	507	HEM	C3C-C2C	-2.45	1.37	1.40
2	A	507	HEM	CHA-C4D	2.44	1.41	1.35
2	A	507	HEM	CMA-C3A	2.40	1.56	1.51
2	A	507	HEM	CHB-C1B	2.39	1.41	1.35
2	A	507	HEM	CAB-C3B	2.33	1.53	1.47
2	A	507	HEM	C1A-NA	2.27	1.40	1.36
3	B	508	NDP	C2A-N1A	2.16	1.37	1.33
3	A	508	NDP	C2A-N1A	2.14	1.37	1.33
3	A	508	NDP	O2B-C2B	2.13	1.51	1.44
2	B	507	HEM	C2A-C3A	-2.10	1.31	1.37
3	B	508	NDP	PA-O2A	-2.08	1.45	1.55
3	A	508	NDP	PA-O2A	-2.08	1.45	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	508	NDP	O2B-C2B	2.07	1.51	1.44
3	A	508	NDP	PN-O2N	-2.06	1.45	1.55
3	B	508	NDP	PN-O2N	-2.05	1.45	1.55

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	508	NDP	O3B-C3B-C4B	9.48	138.46	111.05
3	B	508	NDP	O3B-C3B-C4B	9.46	138.40	111.05
2	A	507	HEM	C4B-CHC-C1C	6.55	131.21	122.56
2	B	507	HEM	CMC-C2C-C3C	6.41	136.67	124.68
3	A	508	NDP	O4B-C1B-C2B	-6.36	95.55	106.59
3	B	508	NDP	O4B-C1B-C2B	-6.33	95.61	106.59
2	B	507	HEM	C4B-CHC-C1C	5.55	129.88	122.56
2	A	507	HEM	C4C-CHD-C1D	5.46	129.76	122.56
2	A	507	HEM	CMC-C2C-C3C	5.19	134.40	124.68
2	A	507	HEM	CAA-CBA-CGA	5.18	128.27	113.76
2	B	507	HEM	O2D-CGD-O1D	4.90	135.51	123.30
3	B	508	NDP	O2X-P2B-O2B	4.73	127.21	105.99
3	A	508	NDP	O2X-P2B-O2B	4.72	127.16	105.99
2	B	507	HEM	C4C-CHD-C1D	4.48	128.47	122.56
2	A	507	HEM	O2A-CGA-O1A	-4.37	112.42	123.30
2	A	507	HEM	CBA-CAA-C2A	3.97	119.40	112.62
2	A	507	HEM	O2D-CGD-O1D	3.89	133.00	123.30
2	B	507	HEM	O1A-CGA-CBA	-3.55	111.69	123.08
2	A	507	HEM	O1D-CGD-CBD	-3.52	111.77	123.08
3	A	508	NDP	O3X-P2B-O2B	-3.49	90.34	105.99
3	B	508	NDP	O3X-P2B-O2B	-3.48	90.41	105.99
3	B	508	NDP	O3B-C3B-C2B	3.18	120.20	111.17
3	A	508	NDP	O3B-C3B-C2B	3.16	120.13	111.17
2	B	507	HEM	O1D-CGD-CBD	-3.13	113.03	123.08
3	B	508	NDP	C5A-C6A-N6A	3.03	124.96	120.35
3	A	508	NDP	C5A-C6A-N6A	3.02	124.94	120.35
2	A	507	HEM	O2A-CGA-CBA	3.00	123.68	114.03
2	B	507	HEM	O2A-CGA-O1A	2.92	130.57	123.30
3	B	508	NDP	C3N-C2N-N1N	-2.63	119.34	123.10
2	A	507	HEM	CHD-C1D-ND	-2.63	121.58	124.43
3	A	508	NDP	O2B-C2B-C3B	-2.61	102.22	111.68
3	B	508	NDP	O2B-C2B-C3B	-2.61	102.22	111.68
2	A	507	HEM	CMA-C3A-C4A	-2.57	124.52	128.46
3	A	508	NDP	C3N-C2N-N1N	-2.57	119.43	123.10
3	B	508	NDP	C3D-C2D-C1D	2.53	106.23	101.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	507	HEM	CAA-C2A-C3A	2.51	134.47	127.25
2	A	507	HEM	CHA-C4D-ND	2.51	127.48	124.38
3	A	508	NDP	C3D-C2D-C1D	2.51	106.19	101.43
2	A	507	HEM	C4B-C3B-C2B	2.45	109.06	107.11
3	A	508	NDP	C1D-N1N-C2N	-2.45	117.04	121.11
3	B	508	NDP	C1D-N1N-C2N	-2.43	117.06	121.11
2	A	507	HEM	CBB-CAB-C3B	-2.40	115.68	127.62
2	B	507	HEM	CHA-C4D-ND	2.39	127.34	124.38
2	B	507	HEM	C1B-NB-C4B	2.23	107.37	105.07
3	A	508	NDP	O2B-C2B-C1B	-2.22	102.10	110.10
3	B	508	NDP	O2B-C2B-C1B	-2.20	102.18	110.10
2	A	507	HEM	CMB-C2B-C1B	-2.17	121.73	125.04
3	B	508	NDP	O3D-C3D-C4D	-2.15	104.83	111.05
2	B	507	HEM	CAD-CBD-CGD	-2.15	108.97	113.60
3	A	508	NDP	O3D-C3D-C4D	-2.12	104.92	111.05
2	A	507	HEM	CHC-C4B-C3B	2.11	127.80	124.57
2	A	507	HEM	CAD-CBD-CGD	-2.09	109.11	113.60
2	B	507	HEM	C3C-C4C-NC	-2.07	107.04	110.94
2	A	507	HEM	C3C-C4C-NC	-2.03	107.11	110.94

All (2) chirality outliers are listed below:

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

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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
2	B	507	HEM	C2A-CAA-CBA-CGA

There are no ring outliers.

3 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	507	HEM	11	0

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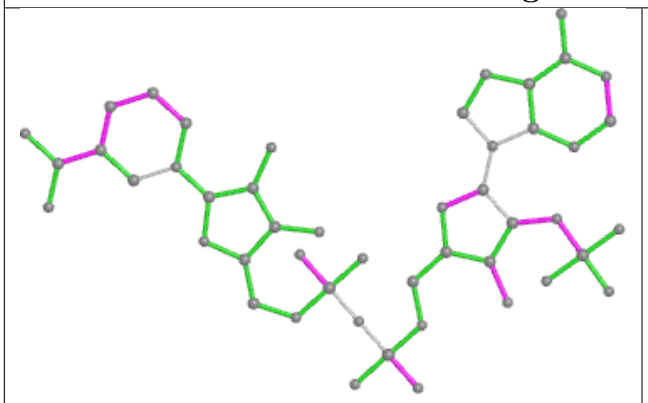
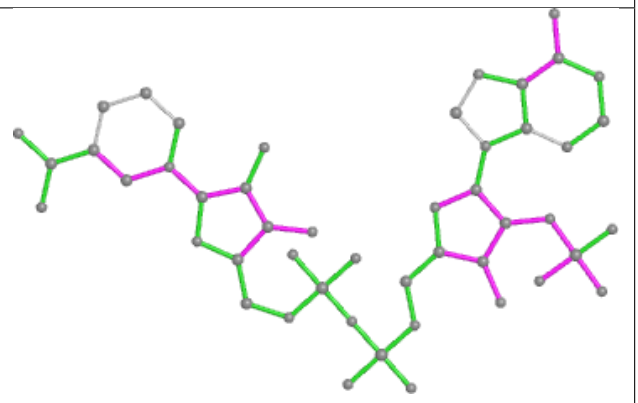
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	508	NDP	3	0
2	A	507	HEM	15	0

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 then 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.

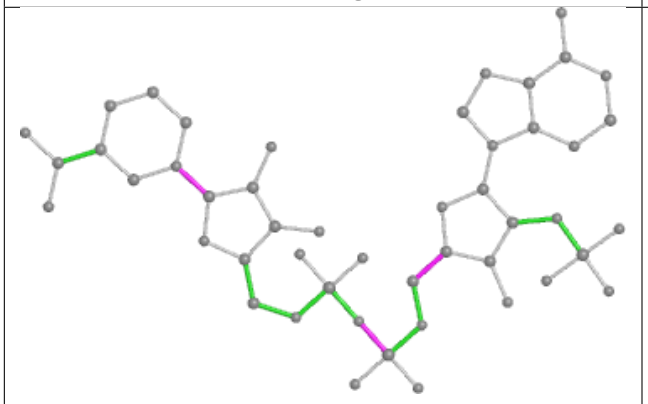
Ligand NDP A 508



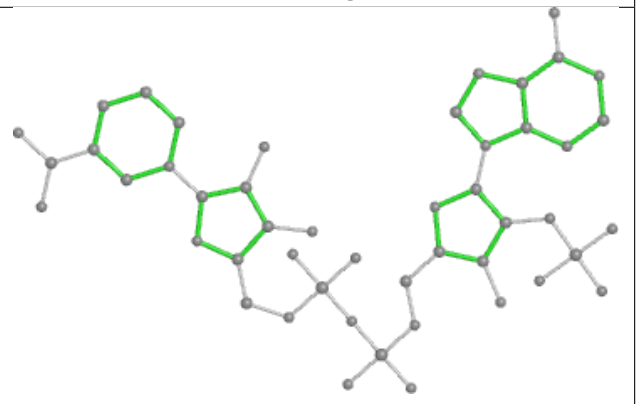
Bond lengths



Bond angles

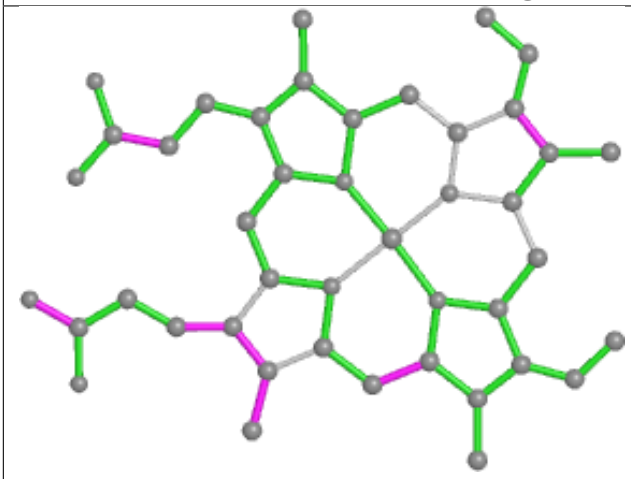


Torsions

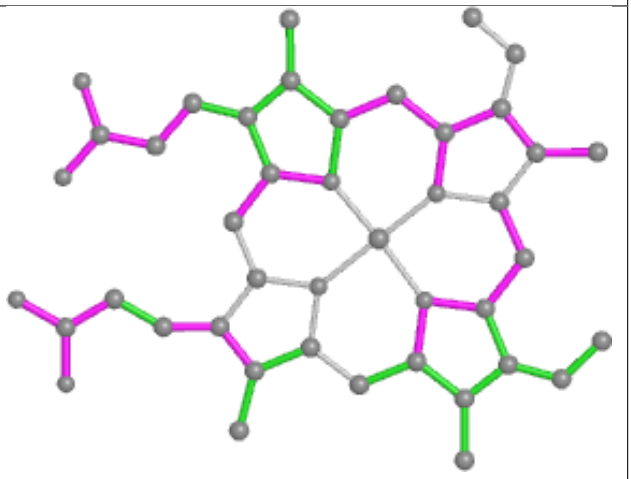


Rings

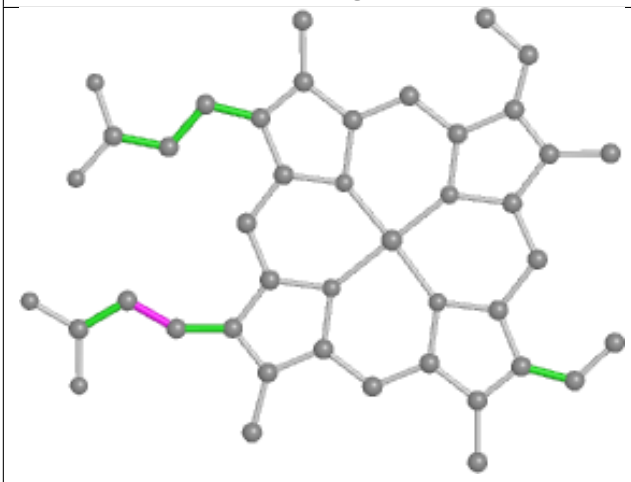
Ligand HEM B 507



Bond lengths



Bond angles



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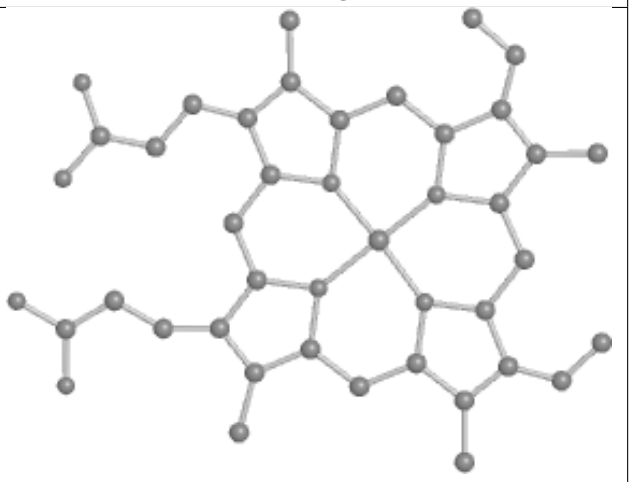
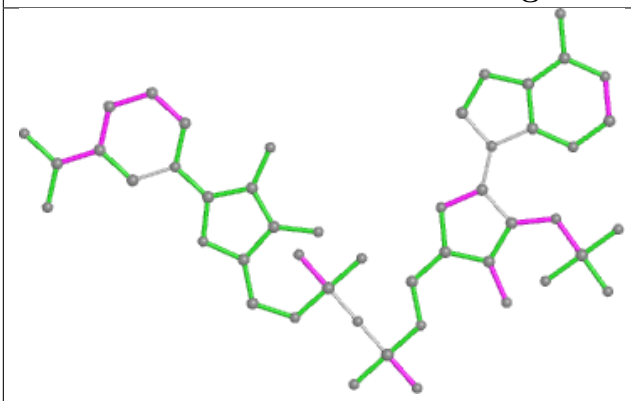
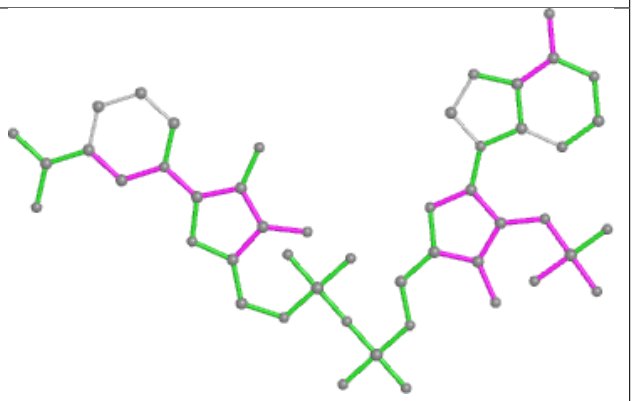


Rings

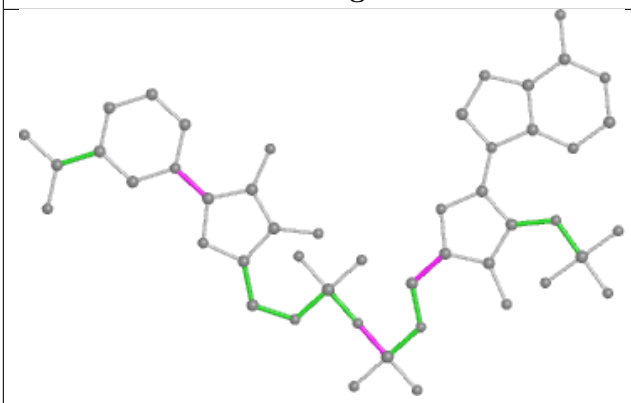
Ligand NDP B 508



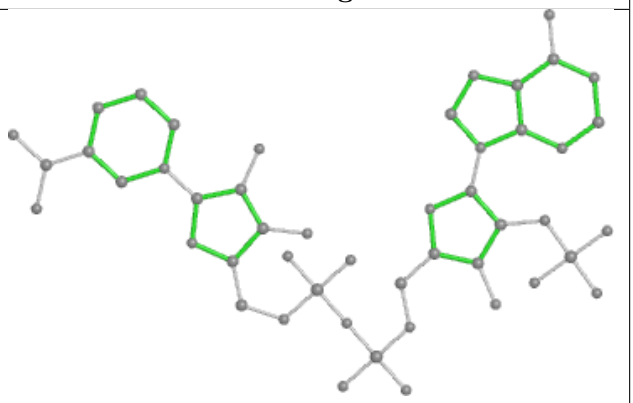
Bond lengths



Bond angles

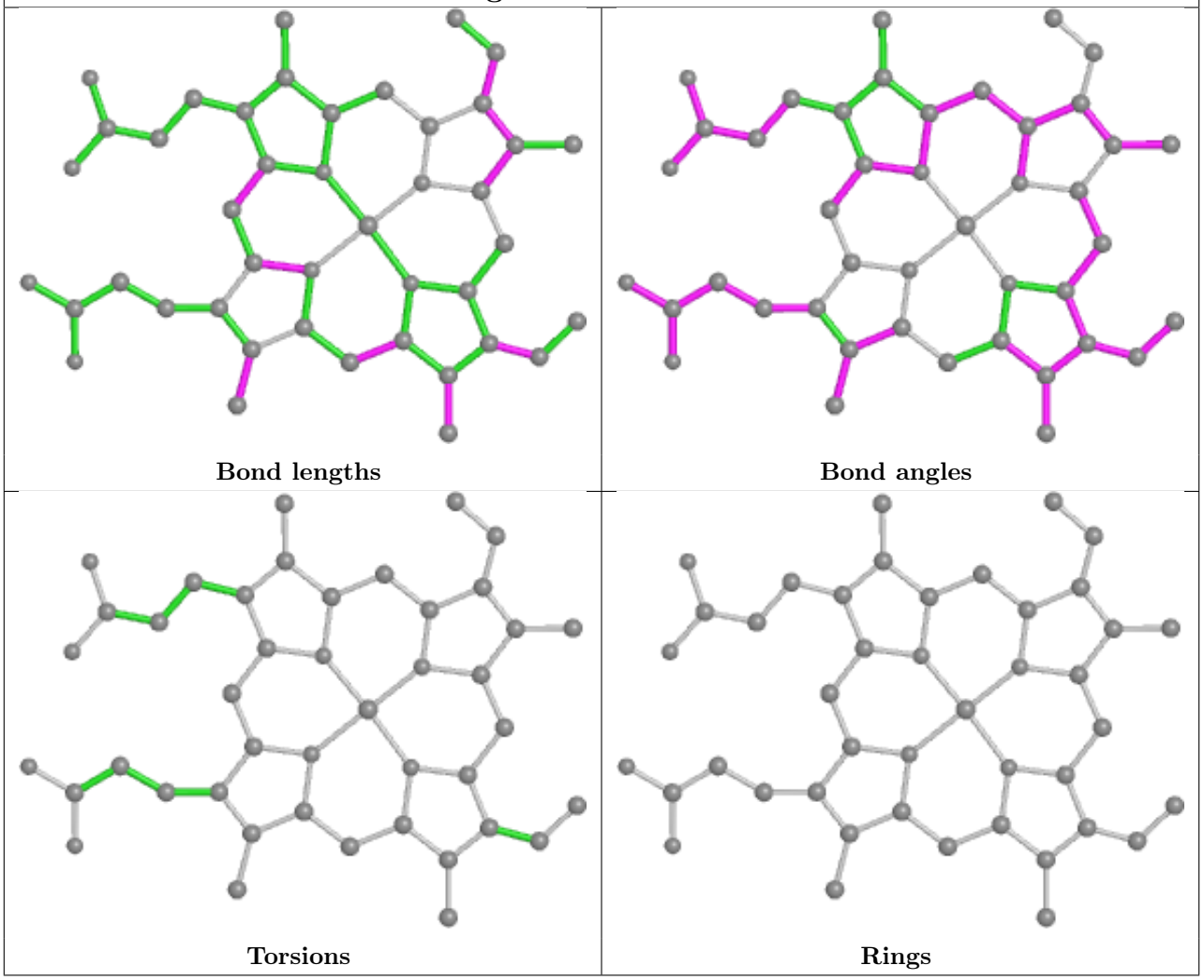


Torsions



Rings

Ligand HEM A 507



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.