Full wwPDB X-ray Structure Validation Report ⓘ

Sep 18, 2023 – 02:14 PM EDT

PDB ID	:	7CAT
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:

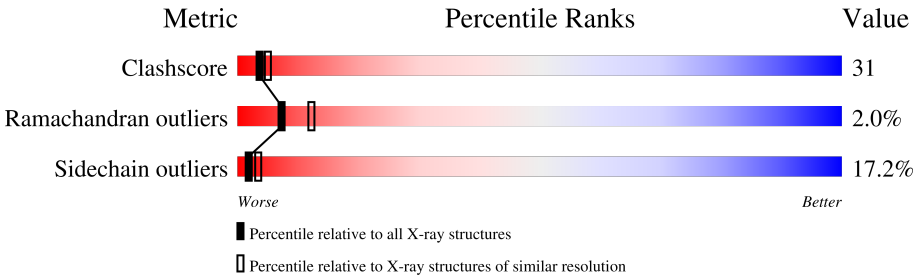
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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	40% 38% 18%
1	B	506	39% 38% 19%

2 Entry composition

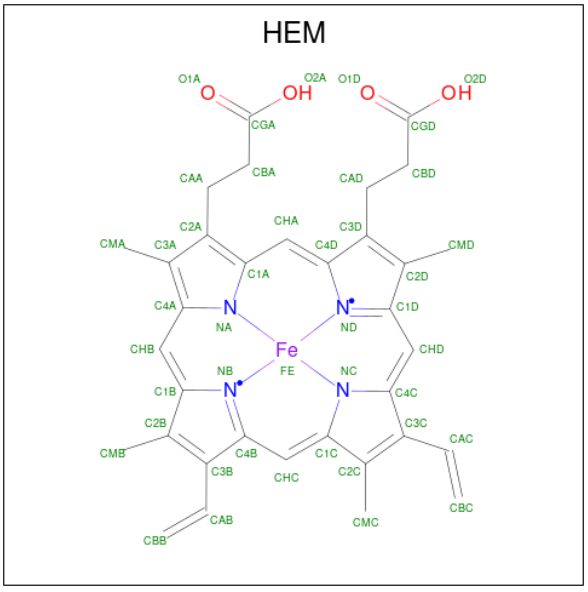
There are 4 unique types of molecules in this entry. The entry contains 8298 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CATALASE.

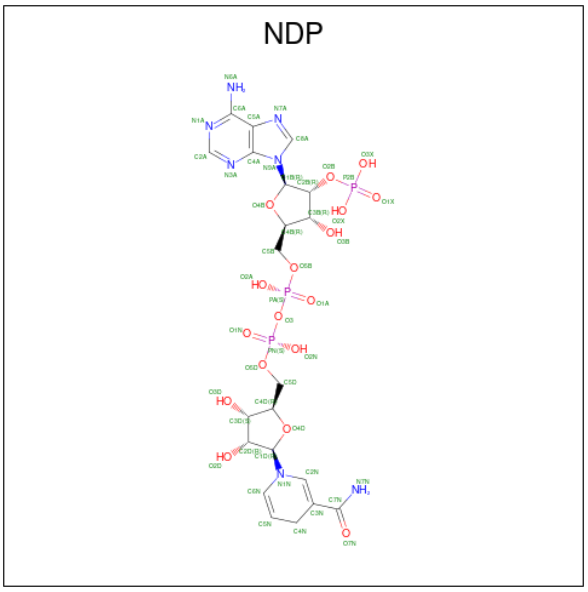
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	0	0	0
			4008	2543	714	737	14			
1	B	498	Total	C	N	O	S	0	0	0
			4008	2543	714	737	14			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (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	50	Total	O	0	0
			50	50		
4	B	50	Total	O	0	0
			50	50		

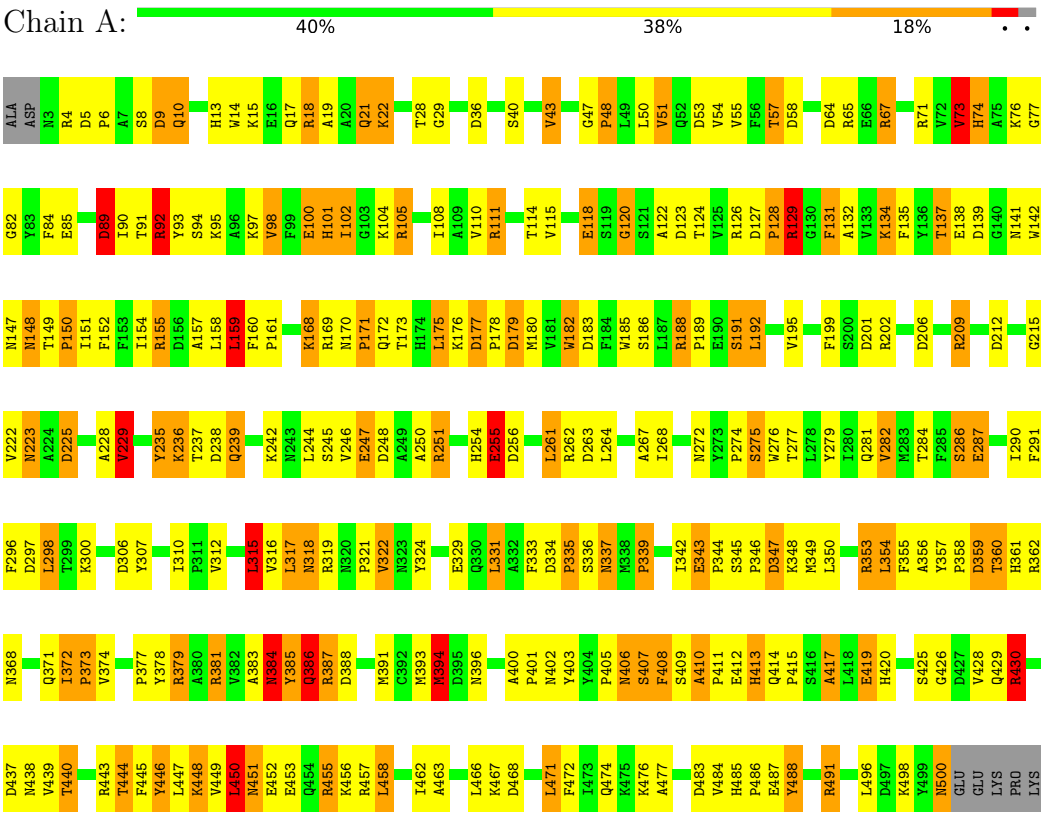
3 Residue-property plots (i)

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.

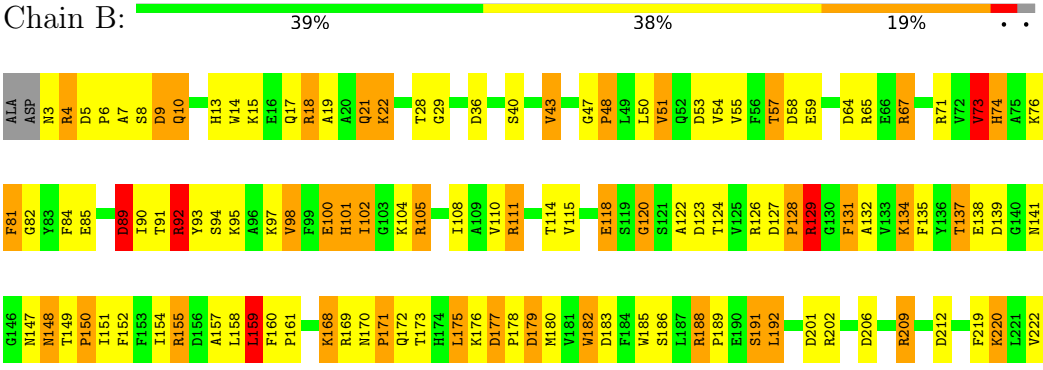
• Molecule 1: CATALASE

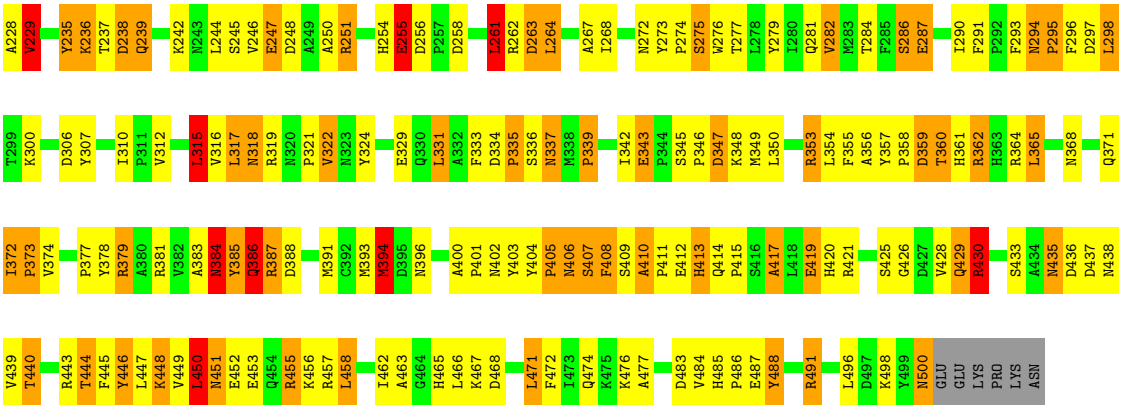
Chain A:



• Molecule 1: CATALASE

Chain B:




A228 V229 Y235 K236 T237 D238 Q239 K242 N243 L244 S245 V246 E247 D248 A249 A250 R251 H254 E255 D256 P257 D258 L261 R262 D263 L264 A267 I268 N272 Y273 P274 S275 W276 T277 L278 Y279 I280 Q281 V282 M283 T284 F285 S286 E287 I290 F291 P292 F293 N294 P295 F296 D297 L298
T299 K300 D306 Y307 I310 P311 V312 L315 V316 L317 N318 R319 N320 P321 V322 N323 Y324 E329 Q330 L331 A332 F333 D334 P335 S336 N337 M338 P339 I342 E343 P344 S345 P346 D347 K348 M349 L350 R353 L354 F355 A356 Y357 P358 D359 T360 H361 R362 H363 R364 L365 N368 Q371
I372 P373 V374 P377 Y378 R379 A380 R381 V382 A383 N384 Y385 Q386 R387 D388 M391 C392 M393 M394 D395 N396 A400 P401 N402 Y403 Y404 P405 N406 S407 F408 S409 A410 P411 E412 H413 Q414 P415 S416 A417 L418 E419 H420 R421 S425 G426 D427 V428 Q429 R430 S433 A434 N435 D436 D437 N438
V439 T440 R443 T444 F445 Y446 L447 K448 V449 L450 N451 E452 E453 Q454 R455 K456 R457 L458 I462 A463 G464 H465 L466 K467 D468 L471 F472 I473 Q474 K475 K476 A477 D483 V484 H485 P486 E487 Y488 R491 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}	0.212 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8298	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.45	15/4128 (0.4%)	2.14	148/5607 (2.6%)
1	B	1.45	16/4128 (0.4%)	2.14	147/5607 (2.6%)
All	All	1.45	31/8256 (0.4%)	2.14	295/11214 (2.6%)

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

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

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	336	SER	CB-OG	-7.37	1.32	1.42
1	A	336	SER	CB-OG	-7.28	1.32	1.42
1	A	364	ARG	NE-CZ	6.69	1.41	1.33
1	B	364	ARG	NE-CZ	6.67	1.41	1.33
1	A	171	PRO	N-CD	6.43	1.56	1.47
1	B	171	PRO	N-CD	6.41	1.56	1.47
1	B	134	LYS	CE-NZ	6.19	1.64	1.49
1	A	134	LYS	CE-NZ	6.13	1.64	1.49
1	B	286	SER	CB-OG	5.96	1.50	1.42
1	A	286	SER	CB-OG	5.94	1.50	1.42
1	A	426	GLY	N-CA	5.89	1.54	1.46
1	B	426	GLY	N-CA	5.84	1.54	1.46
1	B	100	GLU	CD-OE2	-5.74	1.19	1.25
1	A	100	GLU	CD-OE2	-5.71	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	360	THR	C-O	5.50	1.33	1.23
1	B	360	THR	C-O	5.48	1.33	1.23
1	A	409	SER	CB-OG	5.42	1.49	1.42
1	B	409	SER	CB-OG	5.36	1.49	1.42
1	B	120	GLY	N-CA	5.26	1.53	1.46
1	A	120	GLY	N-CA	5.24	1.53	1.46
1	B	29	GLY	N-CA	5.20	1.53	1.46
1	A	29	GLY	N-CA	5.17	1.53	1.46
1	B	151	ILE	N-CA	5.15	1.56	1.46
1	A	185	TRP	C-O	5.13	1.33	1.23
1	A	151	ILE	N-CA	5.13	1.56	1.46
1	A	191	SER	CA-CB	5.12	1.60	1.52
1	B	185	TRP	C-O	5.08	1.32	1.23
1	B	191	SER	CA-CB	5.07	1.60	1.52
1	A	94	SER	CA-CB	5.05	1.60	1.52
1	B	94	SER	CA-CB	5.04	1.60	1.52
1	B	67	ARG	CD-NE	-5.01	1.38	1.46

All (295) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	67	ARG	CD-NE-CZ	21.63	153.88	123.60
1	A	67	ARG	CD-NE-CZ	21.59	153.82	123.60
1	A	92	ARG	NE-CZ-NH1	18.39	129.49	120.30
1	B	92	ARG	NE-CZ-NH1	18.36	129.48	120.30
1	B	261	LEU	CA-CB-CG	16.87	154.11	115.30
1	A	261	LEU	CA-CB-CG	16.84	154.04	115.30
1	A	111	ARG	NE-CZ-NH1	15.89	128.25	120.30
1	B	111	ARG	NE-CZ-NH1	15.89	128.25	120.30
1	B	359	ASP	CB-CG-OD2	-14.14	105.58	118.30
1	A	359	ASP	CB-CG-OD2	-14.09	105.62	118.30
1	B	353	ARG	NE-CZ-NH2	-13.25	113.67	120.30
1	A	353	ARG	NE-CZ-NH2	-13.25	113.68	120.30
1	B	362	ARG	NE-CZ-NH1	13.21	126.91	120.30
1	A	362	ARG	NE-CZ-NH1	13.17	126.88	120.30
1	A	430	ARG	NE-CZ-NH1	-13.06	113.77	120.30
1	B	430	ARG	NE-CZ-NH1	-13.06	113.77	120.30
1	B	457	ARG	NE-CZ-NH1	13.03	126.82	120.30
1	A	457	ARG	NE-CZ-NH1	12.96	126.78	120.30
1	B	343	GLU	CA-CB-CG	12.56	141.04	113.40
1	A	343	GLU	CA-CB-CG	12.55	141.02	113.40
1	A	111	ARG	CD-NE-CZ	12.08	140.51	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	111	ARG	CD-NE-CZ	12.06	140.48	123.60
1	B	89	ASP	CB-CG-OD1	-11.84	107.64	118.30
1	A	89	ASP	CB-CG-OD1	-11.79	107.69	118.30
1	B	111	ARG	NE-CZ-NH2	-11.75	114.42	120.30
1	A	111	ARG	NE-CZ-NH2	-11.71	114.45	120.30
1	A	362	ARG	NE-CZ-NH2	-11.58	114.51	120.30
1	B	362	ARG	NE-CZ-NH2	-11.58	114.51	120.30
1	A	359	ASP	CB-CG-OD1	10.91	128.12	118.30
1	B	359	ASP	CB-CG-OD1	10.89	128.10	118.30
1	A	379	ARG	NE-CZ-NH1	10.85	125.73	120.30
1	B	379	ARG	NE-CZ-NH1	10.84	125.72	120.30
1	A	71	ARG	CD-NE-CZ	10.62	138.46	123.60
1	B	71	ARG	CD-NE-CZ	10.60	138.44	123.60
1	A	159	LEU	CA-CB-CG	10.60	139.67	115.30
1	B	159	LEU	CA-CB-CG	10.57	139.62	115.30
1	B	188	ARG	NE-CZ-NH1	-10.41	115.09	120.30
1	A	364	ARG	CD-NE-CZ	-10.38	109.07	123.60
1	B	364	ARG	CD-NE-CZ	-10.35	109.12	123.60
1	A	188	ARG	NE-CZ-NH1	-10.34	115.13	120.30
1	A	388	ASP	CB-CG-OD2	9.96	127.26	118.30
1	B	388	ASP	CB-CG-OD2	9.92	127.23	118.30
1	A	410	ALA	CB-CA-C	9.82	124.83	110.10
1	B	410	ALA	CB-CA-C	9.80	124.81	110.10
1	A	437	ASP	CB-CG-OD1	9.79	127.11	118.30
1	B	437	ASP	CB-CG-OD1	9.73	127.06	118.30
1	A	443	ARG	CD-NE-CZ	9.36	136.70	123.60
1	B	443	ARG	CD-NE-CZ	9.35	136.69	123.60
1	B	188	ARG	NE-CZ-NH2	8.84	124.72	120.30
1	A	225	ASP	CB-CG-OD2	-8.77	110.41	118.30
1	A	188	ARG	NE-CZ-NH2	8.73	124.66	120.30
1	B	225	ASP	CB-CG-OD2	-8.72	110.45	118.30
1	A	335	PRO	C-N-CA	8.68	143.39	121.70
1	B	335	PRO	C-N-CA	8.67	143.38	121.70
1	B	58	ASP	CB-CG-OD2	-8.59	110.57	118.30
1	A	58	ASP	CB-CG-OD2	-8.57	110.59	118.30
1	B	134	LYS	CD-CE-NZ	-8.31	92.59	111.70
1	A	134	LYS	CD-CE-NZ	-8.27	92.68	111.70
1	A	247	GLU	CA-CB-CG	8.19	131.42	113.40
1	B	247	GLU	CA-CB-CG	8.19	131.42	113.40
1	B	129	ARG	NE-CZ-NH2	8.15	124.37	120.30
1	A	129	ARG	NE-CZ-NH2	8.14	124.37	120.30
1	A	378	TYR	CB-CG-CD1	8.12	125.87	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	378	TYR	CB-CG-CD1	8.12	125.87	121.00
1	B	329	GLU	OE1-CD-OE2	7.94	132.83	123.30
1	B	450	LEU	CB-CA-C	7.92	125.25	110.20
1	A	329	GLU	OE1-CD-OE2	7.92	132.80	123.30
1	A	450	LEU	CB-CA-C	7.90	125.22	110.20
1	A	92	ARG	NH1-CZ-NH2	-7.71	110.92	119.40
1	B	378	TYR	CB-CG-CD2	-7.67	116.39	121.00
1	A	263	ASP	CB-CG-OD1	7.67	125.20	118.30
1	B	92	ARG	NH1-CZ-NH2	-7.67	110.97	119.40
1	B	263	ASP	CB-CG-OD1	7.67	125.20	118.30
1	B	457	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	A	378	TYR	CB-CG-CD2	-7.61	116.43	121.00
1	A	457	ARG	NE-CZ-NH2	-7.52	116.54	120.30
1	A	381	ARG	NE-CZ-NH1	-7.49	116.56	120.30
1	B	256	ASP	CB-CG-OD1	7.48	125.03	118.30
1	A	256	ASP	CB-CG-OD1	7.47	125.03	118.30
1	B	381	ARG	NE-CZ-NH1	-7.47	116.57	120.30
1	B	225	ASP	CB-CG-OD1	7.38	124.94	118.30
1	A	168	LYS	CA-CB-CG	7.35	129.58	113.40
1	B	168	LYS	CA-CB-CG	7.34	129.54	113.40
1	A	225	ASP	CB-CG-OD1	7.33	124.90	118.30
1	B	201	ASP	CB-CG-OD2	-7.31	111.72	118.30
1	A	386	GLN	CA-CB-CG	7.31	129.47	113.40
1	B	386	GLN	CA-CB-CG	7.29	129.45	113.40
1	A	472	PHE	CA-CB-CG	7.27	131.35	113.90
1	A	129	ARG	CD-NE-CZ	-7.26	113.44	123.60
1	A	388	ASP	CB-CG-OD1	-7.25	111.77	118.30
1	B	472	PHE	CA-CB-CG	7.25	131.31	113.90
1	B	129	ARG	CD-NE-CZ	-7.25	113.45	123.60
1	B	388	ASP	CB-CG-OD1	-7.23	111.80	118.30
1	A	201	ASP	CB-CG-OD2	-7.21	111.81	118.30
1	B	387	ARG	NE-CZ-NH2	7.17	123.88	120.30
1	B	206	ASP	CB-CG-OD2	7.12	124.71	118.30
1	A	387	ARG	NE-CZ-NH2	7.12	123.86	120.30
1	A	206	ASP	CB-CG-OD2	7.11	124.70	118.30
1	B	126	ARG	CA-CB-CG	7.09	128.99	113.40
1	A	126	ARG	CA-CB-CG	7.07	128.96	113.40
1	A	74	HIS	C-N-CA	6.94	139.04	121.70
1	B	74	HIS	C-N-CA	6.93	139.04	121.70
1	B	71	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	B	386	GLN	CB-CG-CD	6.87	129.46	111.60
1	A	386	GLN	CB-CG-CD	6.87	129.45	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	71	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	B	169	ARG	CD-NE-CZ	6.84	133.18	123.60
1	A	169	ARG	CD-NE-CZ	6.81	133.14	123.60
1	B	407	SER	CA-C-O	-6.81	105.80	120.10
1	A	139	ASP	CA-CB-CG	6.80	128.36	113.40
1	A	407	SER	CA-C-O	-6.80	105.82	120.10
1	B	139	ASP	CA-CB-CG	6.79	128.33	113.40
1	A	457	ARG	CD-NE-CZ	6.67	132.94	123.60
1	A	244	LEU	CA-CB-CG	6.65	130.60	115.30
1	B	244	LEU	CA-CB-CG	6.63	130.54	115.30
1	A	202	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	B	202	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	B	457	ARG	CD-NE-CZ	6.60	132.84	123.60
1	B	365	LEU	CA-CB-CG	6.59	130.45	115.30
1	A	365	LEU	CA-CB-CG	6.58	130.44	115.30
1	B	177	ASP	N-CA-CB	-6.56	98.79	110.60
1	A	28	THR	CA-C-N	6.54	129.29	116.20
1	A	177	ASP	N-CA-CB	-6.54	98.82	110.60
1	B	28	THR	CA-C-N	6.53	129.27	116.20
1	B	429	GLN	CA-CB-CG	6.53	127.77	113.40
1	A	429	GLN	CA-CB-CG	6.52	127.74	113.40
1	A	412	GLU	CA-CB-CG	6.50	127.69	113.40
1	B	412	GLU	CA-CB-CG	6.49	127.69	113.40
1	A	435	ASN	CB-CA-C	6.47	123.34	110.40
1	A	9	ASP	CB-CG-OD1	6.46	124.11	118.30
1	B	435	ASN	CB-CA-C	6.44	123.28	110.40
1	B	9	ASP	CB-CG-OD1	6.44	124.09	118.30
1	B	384	ASN	CB-CA-C	6.42	123.24	110.40
1	A	384	ASN	CB-CA-C	6.41	123.22	110.40
1	A	417	ALA	CB-CA-C	6.38	119.67	110.10
1	B	417	ALA	CB-CA-C	6.37	119.65	110.10
1	A	126	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	A	385	TYR	CB-CA-C	6.33	123.05	110.40
1	A	343	GLU	CB-CA-C	6.31	123.03	110.40
1	B	343	GLU	CB-CA-C	6.30	122.99	110.40
1	B	126	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	B	385	TYR	CB-CA-C	6.28	122.97	110.40
1	B	177	ASP	CB-CG-OD1	-6.28	112.65	118.30
1	A	336	SER	CA-CB-OG	6.25	128.07	111.20
1	B	336	SER	CA-CB-OG	6.25	128.06	111.20
1	A	177	ASP	CB-CG-OD1	-6.19	112.73	118.30
1	B	182	TRP	CB-CA-C	6.15	122.71	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	182	TRP	CB-CA-C	6.15	122.71	110.40
1	A	425	SER	C-N-CA	-6.12	109.45	122.30
1	A	123	ASP	CB-CG-OD1	6.11	123.80	118.30
1	B	446	TYR	CB-CG-CD2	6.10	124.66	121.00
1	B	425	SER	C-N-CA	-6.10	109.49	122.30
1	A	364	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	A	254	HIS	CA-CB-CG	6.08	123.94	113.60
1	B	364	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	A	446	TYR	CB-CG-CD2	6.06	124.64	121.00
1	B	254	HIS	CA-CB-CG	6.06	123.90	113.60
1	B	28	THR	CA-C-O	-6.05	107.39	120.10
1	A	28	THR	CA-C-O	-6.04	107.41	120.10
1	B	123	ASP	CB-CG-OD1	6.03	123.73	118.30
1	A	138	GLU	OE1-CD-OE2	-6.03	116.07	123.30
1	A	318	ASN	N-CA-CB	-6.03	99.75	110.60
1	A	262	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	B	318	ASN	N-CA-CB	-6.01	99.78	110.60
1	B	138	GLU	OE1-CD-OE2	-6.00	116.10	123.30
1	A	81	PHE	N-CA-CB	-5.95	99.89	110.60
1	B	262	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	B	81	PHE	N-CA-CB	-5.91	99.96	110.60
1	A	179	ASP	CB-CG-OD2	5.90	123.61	118.30
1	A	491	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	B	247	GLU	CG-CD-OE2	-5.87	106.56	118.30
1	B	275	SER	C-N-CA	5.85	136.33	121.70
1	A	247	GLU	CG-CD-OE2	-5.85	106.60	118.30
1	B	179	ASP	CB-CG-OD2	5.84	123.55	118.30
1	A	275	SER	C-N-CA	5.83	136.28	121.70
1	B	379	ARG	CA-CB-CG	5.83	126.22	113.40
1	A	319	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	A	379	ARG	CA-CB-CG	5.82	126.21	113.40
1	A	343	GLU	CG-CD-OE1	5.81	129.92	118.30
1	B	343	GLU	CG-CD-OE1	5.81	129.91	118.30
1	A	295	PRO	N-CD-CG	-5.80	94.50	103.20
1	B	295	PRO	N-CD-CG	-5.80	94.50	103.20
1	B	319	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	B	368	ASN	CA-C-O	-5.78	107.96	120.10
1	A	67	ARG	CA-CB-CG	5.78	126.11	113.40
1	B	491	ARG	NE-CZ-NH2	-5.77	117.41	120.30
1	A	368	ASN	CA-C-O	-5.77	107.98	120.10
1	A	343	GLU	OE1-CD-OE2	-5.77	116.38	123.30
1	B	450	LEU	CA-CB-CG	5.76	128.56	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	450	LEU	CA-CB-CG	5.76	128.55	115.30
1	B	67	ARG	CA-CB-CG	5.76	126.07	113.40
1	B	343	GLU	OE1-CD-OE2	-5.73	116.42	123.30
1	A	129	ARG	NE-CZ-NH1	-5.71	117.44	120.30
1	B	129	ARG	NE-CZ-NH1	-5.70	117.45	120.30
1	A	318	ASN	CB-CA-C	5.70	121.79	110.40
1	B	318	ASN	CB-CA-C	5.69	121.78	110.40
1	B	408	PHE	C-N-CA	5.68	135.91	121.70
1	A	408	PHE	C-N-CA	5.67	135.88	121.70
1	B	209	ARG	CD-NE-CZ	-5.67	115.66	123.60
1	A	413	HIS	N-CA-CB	5.67	120.80	110.60
1	B	122	ALA	CB-CA-C	5.66	118.59	110.10
1	B	413	HIS	N-CA-CB	5.66	120.79	110.60
1	A	209	ARG	CD-NE-CZ	-5.65	115.69	123.60
1	B	168	LYS	N-CA-CB	5.63	120.74	110.60
1	A	29	GLY	O-C-N	-5.63	113.63	123.20
1	B	281	GLN	CG-CD-OE1	5.63	132.86	121.60
1	A	255	GLU	CA-CB-CG	5.62	125.77	113.40
1	A	71	ARG	NH1-CZ-NH2	-5.62	113.22	119.40
1	B	29	GLY	O-C-N	-5.61	113.66	123.20
1	B	255	GLU	CA-CB-CG	5.61	125.75	113.40
1	A	122	ALA	CB-CA-C	5.61	118.52	110.10
1	A	364	ARG	NE-CZ-NH1	-5.61	117.50	120.30
1	A	281	GLN	CG-CD-OE1	5.61	132.81	121.60
1	B	71	ARG	NH1-CZ-NH2	-5.60	113.24	119.40
1	A	168	LYS	N-CA-CB	5.60	120.67	110.60
1	A	263	ASP	CB-CA-C	5.59	121.57	110.40
1	B	263	ASP	CB-CA-C	5.59	121.58	110.40
1	A	319	ARG	CD-NE-CZ	-5.57	115.80	123.60
1	B	250	ALA	CB-CA-C	5.57	118.45	110.10
1	B	319	ARG	CD-NE-CZ	-5.57	115.81	123.60
1	A	250	ALA	CB-CA-C	5.56	118.43	110.10
1	B	57	THR	CB-CA-C	5.55	126.58	111.60
1	A	57	THR	CB-CA-C	5.53	126.53	111.60
1	B	201	ASP	CB-CG-OD1	5.52	123.27	118.30
1	B	175	LEU	CA-CB-CG	5.52	127.99	115.30
1	A	175	LEU	CA-CB-CG	5.50	127.95	115.30
1	B	225	ASP	CA-C-O	-5.50	108.55	120.10
1	B	364	ARG	NE-CZ-NH1	-5.49	117.56	120.30
1	A	225	ASP	CA-C-O	-5.48	108.60	120.10
1	A	201	ASP	CB-CG-OD1	5.46	123.22	118.30
1	B	73	VAL	CA-CB-CG1	5.46	119.08	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	251	ARG	CA-CB-CG	5.42	125.33	113.40
1	A	73	VAL	CA-CB-CG1	5.41	119.02	110.90
1	A	251	ARG	CA-CB-CG	5.40	125.29	113.40
1	A	89	ASP	CB-CA-C	5.40	121.20	110.40
1	B	89	ASP	CB-CA-C	5.39	121.18	110.40
1	A	329	GLU	CG-CD-OE2	-5.39	107.52	118.30
1	B	329	GLU	CG-CD-OE2	-5.38	107.54	118.30
1	B	238	ASP	CB-CG-OD1	5.37	123.14	118.30
1	B	102	ILE	O-C-N	5.37	132.33	123.20
1	A	102	ILE	O-C-N	5.35	132.30	123.20
1	A	322	VAL	CB-CA-C	5.35	121.56	111.40
1	B	322	VAL	CB-CA-C	5.33	121.53	111.40
1	B	92	ARG	C-N-CA	5.33	135.01	121.70
1	B	229	VAL	N-CA-CB	-5.33	99.78	111.50
1	A	229	VAL	N-CA-CB	-5.32	99.80	111.50
1	A	123	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	A	67	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	238	ASP	CB-CG-OD1	5.30	123.07	118.30
1	A	242	LYS	O-C-N	5.30	131.17	122.70
1	A	92	ARG	C-N-CA	5.29	134.94	121.70
1	B	242	LYS	O-C-N	5.27	131.13	122.70
1	B	123	ASP	CB-CG-OD2	-5.26	113.56	118.30
1	A	126	ARG	O-C-N	5.25	131.10	122.70
1	A	364	ARG	NH1-CZ-NH2	5.23	125.16	119.40
1	B	105	ARG	CB-CA-C	-5.23	99.94	110.40
1	A	105	ARG	CB-CA-C	-5.22	99.95	110.40
1	B	67	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	B	412	GLU	CB-CA-C	-5.21	99.97	110.40
1	A	53	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	A	261	LEU	N-CA-CB	5.20	120.80	110.40
1	B	191	SER	C-N-CA	5.20	134.69	121.70
1	B	261	LEU	N-CA-CB	5.20	120.79	110.40
1	A	412	GLU	CB-CA-C	-5.19	100.01	110.40
1	B	126	ARG	O-C-N	5.19	131.00	122.70
1	A	191	SER	C-N-CA	5.19	134.67	121.70
1	B	455	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	A	98	VAL	CA-CB-CG1	5.19	118.68	110.90
1	B	98	VAL	CA-CB-CG1	5.17	118.66	110.90
1	B	364	ARG	NH1-CZ-NH2	5.17	125.09	119.40
1	B	419	GLU	CA-CB-CG	5.15	124.74	113.40
1	A	419	GLU	CA-CB-CG	5.15	124.74	113.40
1	B	53	ASP	CB-CG-OD2	-5.15	113.66	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	315	LEU	CA-CB-CG	5.14	127.12	115.30
1	B	315	LEU	CA-CB-CG	5.13	127.11	115.30
1	A	403	TYR	CB-CG-CD1	-5.13	117.92	121.00
1	B	219	PHE	CB-CA-C	5.12	120.64	110.40
1	A	455	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	B	403	TYR	CB-CG-CD1	-5.11	117.93	121.00
1	A	219	PHE	CB-CA-C	5.11	120.62	110.40
1	A	55	VAL	CA-CB-CG1	5.09	118.54	110.90
1	B	247	GLU	CG-CD-OE1	5.09	128.48	118.30
1	B	255	GLU	CG-CD-OE1	5.09	128.47	118.30
1	A	255	GLU	CG-CD-OE1	5.08	128.47	118.30
1	A	247	GLU	CG-CD-OE1	5.08	128.46	118.30
1	A	192	LEU	CB-CG-CD1	-5.07	102.38	111.00
1	A	483	ASP	CB-CG-OD1	5.07	122.86	118.30
1	B	55	VAL	CA-CB-CG1	5.07	118.50	110.90
1	B	483	ASP	CB-CG-OD1	5.06	122.86	118.30
1	B	192	LEU	CB-CG-CD1	-5.06	102.40	111.00
1	B	169	ARG	CB-CA-C	-5.05	100.29	110.40
1	A	347	ASP	CB-CG-OD2	5.04	122.84	118.30
1	A	169	ARG	CB-CA-C	-5.03	100.33	110.40
1	B	347	ASP	CB-CG-OD2	5.03	122.83	118.30
1	A	215	GLY	C-N-CA	5.00	134.21	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

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

5.2 Too-close contacts (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	262	3
1	B	4008	0	3830	259	3
2	A	43	0	30	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	43	0	30	11	0
3	A	48	0	26	3	0
3	B	48	0	26	3	0
4	A	50	0	0	4	1
4	B	50	0	0	3	1
All	All	8298	0	7772	502	4

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 31.

All (502) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:ARG:NH2	1:B:438:ASN:HD21	1.22	1.35
1:A:155:ARG:NH2	1:A:438:ASN:HD21	1.22	1.34
1:A:155:ARG:HH22	1:A:438:ASN:ND2	1.22	1.33
1:B:155:ARG:HH22	1:B:438:ASN:ND2	1.22	1.32
1:A:177:ASP:HB3	1:A:180:MET:HE2	1.35	1.07
1:A:322:VAL:HA	1:B:172:GLN:NE2	1.79	0.98
1:A:384:ASN:C	1:A:384:ASN:HD22	1.66	0.97
1:A:172:GLN:NE2	1:B:322:VAL:HA	1.79	0.96
1:A:172:GLN:HE21	1:B:322:VAL:HA	1.29	0.96
1:A:444:THR:O	1:A:448:LYS:HG2	1.66	0.95
1:A:322:VAL:HA	1:B:172:GLN:HE21	1.30	0.95
1:B:177:ASP:HB3	1:B:180:MET:HE2	1.48	0.95
1:B:444:THR:O	1:B:448:LYS:HG2	1.66	0.95
1:A:173:THR:HG21	1:A:175:LEU:HD12	1.49	0.94
1:B:173:THR:HG21	1:B:175:LEU:HD12	1.49	0.94
1:B:384:ASN:C	1:B:384:ASN:HD22	1.66	0.91
1:A:406:ASN:HD22	1:A:408:PHE:H	1.20	0.89
1:A:406:ASN:ND2	1:A:408:PHE:H	1.71	0.89
1:B:148:ASN:H	1:B:148:ASN:HD22	1.20	0.88
1:A:220:LYS:HE3	1:A:420:HIS:CD2	2.09	0.87
1:B:220:LYS:HE3	1:B:420:HIS:CD2	2.09	0.87
1:B:406:ASN:ND2	1:B:408:PHE:H	1.71	0.87
1:B:406:ASN:HD22	1:B:408:PHE:H	1.20	0.86
1:A:177:ASP:HB3	1:A:180:MET:CE	2.05	0.86
1:A:229:VAL:HG13	1:A:282:VAL:HG23	1.57	0.86
1:B:177:ASP:HB3	1:B:180:MET:CE	2.05	0.85
1:A:148:ASN:HD22	1:A:148:ASN:H	1.20	0.85
1:A:189:PRO:O	1:A:192:LEU:HD12	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:PRO:O	1:B:192:LEU:HD12	1.76	0.85
1:B:229:VAL:HG13	1:B:282:VAL:HG23	1.57	0.84
1:A:90:ILE:HD13	1:A:312:VAL:HG13	1.58	0.83
1:B:90:ILE:HD13	1:B:312:VAL:HG13	1.58	0.83
1:B:179:ASP:O	1:B:183:ASP:HB2	1.82	0.80
1:B:142:TRP:HB2	1:B:339:PRO:HD3	1.65	0.79
1:A:179:ASP:O	1:A:183:ASP:HB2	1.82	0.78
1:A:142:TRP:HB2	1:A:339:PRO:HD3	1.65	0.78
1:A:487:GLU:O	1:A:491:ARG:HG3	1.84	0.78
1:A:384:ASN:HD22	1:A:385:TYR:N	1.82	0.77
1:B:384:ASN:HD22	1:B:385:TYR:N	1.82	0.77
1:B:487:GLU:O	1:B:491:ARG:HG3	1.83	0.77
1:B:173:THR:CG2	1:B:175:LEU:HD12	2.15	0.76
1:A:458:LEU:CD1	1:A:462:ILE:HD11	2.16	0.76
1:A:173:THR:CG2	1:A:175:LEU:HD12	2.15	0.76
1:A:251:ARG:O	1:A:255:GLU:HB2	1.86	0.75
1:B:17:GLN:O	1:B:17:GLN:HG2	1.86	0.75
1:B:458:LEU:CD1	1:B:462:ILE:HD11	2.16	0.75
1:A:17:GLN:O	1:A:17:GLN:HG2	1.85	0.75
1:A:451:ASN:O	1:A:455:ARG:HG3	1.87	0.74
1:B:98:VAL:HG23	1:B:137:THR:CG2	2.17	0.74
1:B:79:GLY:O	1:B:80:ALA:HB2	1.88	0.74
1:A:98:VAL:HG23	1:A:137:THR:HB	1.68	0.74
1:B:251:ARG:O	1:B:255:GLU:HB2	1.86	0.74
1:B:74:HIS:O	1:B:111:ARG:NH2	2.20	0.74
1:B:98:VAL:HG23	1:B:137:THR:HB	1.68	0.73
1:A:284:THR:HG22	1:A:286:SER:H	1.53	0.73
1:B:170:ASN:ND2	1:B:172:GLN:H	1.87	0.73
1:B:284:THR:HG22	1:B:286:SER:H	1.53	0.73
1:B:451:ASN:O	1:B:455:ARG:HG3	1.87	0.73
1:B:384:ASN:C	1:B:384:ASN:ND2	2.42	0.73
1:A:98:VAL:HG23	1:A:137:THR:CG2	2.17	0.73
1:A:79:GLY:O	1:A:80:ALA:HB2	1.88	0.73
1:A:170:ASN:ND2	1:A:172:GLN:H	1.87	0.73
1:B:496:LEU:O	1:B:500:ASN:HB2	1.89	0.73
1:A:384:ASN:C	1:A:384:ASN:ND2	2.41	0.73
1:B:297:ASP:OD1	1:B:300:LYS:HE2	1.89	0.73
1:A:108:ILE:HD13	1:A:315:LEU:HD12	1.69	0.72
1:B:458:LEU:O	1:B:462:ILE:HG13	1.90	0.72
1:A:297:ASP:OD1	1:A:300:LYS:HE2	1.89	0.72
1:B:108:ILE:HD13	1:B:315:LEU:HD12	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:458:LEU:O	1:B:458:LEU:HD12	1.90	0.71
1:A:458:LEU:O	1:A:462:ILE:HG13	1.90	0.71
1:A:458:LEU:O	1:A:458:LEU:HD12	1.90	0.71
1:A:496:LEU:O	1:A:500:ASN:HB2	1.89	0.71
1:B:223:ASN:ND2	1:B:225:ASP:H	1.88	0.71
1:A:74:HIS:O	1:A:111:ARG:NH2	2.20	0.71
1:A:223:ASN:C	1:A:223:ASN:HD22	1.94	0.70
1:B:134:LYS:HE3	1:B:331:LEU:CD2	2.21	0.70
1:A:223:ASN:ND2	1:A:225:ASP:H	1.88	0.70
1:A:134:LYS:HE3	1:A:331:LEU:CD2	2.21	0.70
1:A:446:TYR:HA	1:A:450:LEU:HD22	1.74	0.70
1:A:170:ASN:HD22	1:A:172:GLN:H	1.40	0.70
1:B:223:ASN:C	1:B:223:ASN:HD22	1.94	0.70
1:B:446:TYR:HA	1:B:450:LEU:HD22	1.74	0.70
1:B:383:ALA:HB1	1:B:411:PRO:HG3	1.73	0.69
1:B:170:ASN:HD22	1:B:172:GLN:H	1.39	0.69
1:A:383:ALA:HB1	1:A:411:PRO:HG3	1.73	0.69
1:B:155:ARG:NH2	1:B:438:ASN:ND2	2.02	0.68
1:A:172:GLN:HE21	1:B:322:VAL:CA	2.05	0.68
1:A:275:SER:HA	1:A:315:LEU:O	1.94	0.68
1:B:447:LEU:HB2	1:B:448:LYS:HD3	1.76	0.68
1:A:284:THR:HB	1:A:287:GLU:HG3	1.75	0.68
1:B:275:SER:HA	1:B:315:LEU:O	1.93	0.68
1:B:458:LEU:HD11	1:B:462:ILE:HD11	1.76	0.67
1:A:322:VAL:CA	1:B:172:GLN:HE21	2.05	0.67
1:A:458:LEU:HD11	1:A:462:ILE:HD11	1.77	0.67
1:B:43:VAL:HG13	1:B:48:PRO:HD2	1.77	0.67
1:B:284:THR:HB	1:B:287:GLU:HG3	1.75	0.67
1:A:374:VAL:O	1:A:374:VAL:HG22	1.95	0.67
1:A:447:LEU:HB2	1:A:448:LYS:HD3	1.76	0.66
1:A:43:VAL:HG13	1:A:48:PRO:HD2	1.77	0.66
1:A:149:THR:OG1	1:A:150:PRO:HD2	1.96	0.66
1:B:149:THR:OG1	1:B:150:PRO:HD2	1.95	0.66
1:B:374:VAL:HG22	1:B:374:VAL:O	1.95	0.66
1:B:342:ILE:O	1:B:343:GLU:HB2	1.95	0.66
1:A:92:ARG:O	1:A:223:ASN:HB3	1.96	0.65
1:B:43:VAL:O	1:B:47:GLY:HA3	1.96	0.65
1:B:467:LYS:HE2	1:B:468:ASP:OD2	1.96	0.65
1:A:155:ARG:NH2	1:A:438:ASN:ND2	2.02	0.65
2:B:507:HEM:HMB2	2:B:507:HEM:HBB2	1.79	0.65
1:B:148:ASN:HD22	1:B:148:ASN:N	1.94	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:LYS:CE	4:A:551:HOH:O	2.45	0.65
1:B:98:VAL:CG2	1:B:137:THR:HG22	2.27	0.65
1:A:98:VAL:CG2	1:A:137:THR:HG22	2.27	0.65
1:A:487:GLU:CG	1:A:491:ARG:HD2	2.27	0.65
1:A:371:GLN:NE2	1:A:393:MET:H	1.95	0.64
1:A:467:LYS:HE2	1:A:468:ASP:OD2	1.96	0.64
1:A:148:ASN:HD22	1:A:148:ASN:N	1.94	0.64
2:A:507:HEM:HBB2	2:A:507:HEM:HMB2	1.79	0.64
1:A:342:ILE:O	1:A:343:GLU:HB2	1.95	0.64
1:B:98:VAL:CG2	1:B:137:THR:CG2	2.76	0.64
1:A:371:GLN:HE22	1:A:393:MET:H	1.45	0.64
1:B:92:ARG:O	1:B:223:ASN:HB3	1.96	0.64
1:B:371:GLN:NE2	1:B:393:MET:H	1.95	0.64
1:A:43:VAL:O	1:A:47:GLY:HA3	1.96	0.64
1:B:186:SER:O	1:B:476:LYS:NZ	2.27	0.64
1:B:487:GLU:CG	1:B:491:ARG:HD2	2.27	0.64
1:B:348:LYS:CE	4:B:509:HOH:O	2.45	0.64
1:B:371:GLN:HE22	1:B:393:MET:H	1.44	0.64
1:B:371:GLN:HE21	1:B:393:MET:HB2	1.64	0.63
1:A:371:GLN:HE21	1:A:393:MET:HB2	1.64	0.63
1:A:98:VAL:CG2	1:A:137:THR:CG2	2.76	0.63
1:B:458:LEU:CD1	1:B:462:ILE:CD1	2.77	0.63
1:B:466:LEU:HD12	1:B:466:LEU:O	1.99	0.63
1:A:131:PHE:C	1:A:131:PHE:HD1	2.03	0.63
1:A:385:TYR:OH	1:A:411:PRO:O	2.16	0.62
1:A:466:LEU:HD12	1:A:466:LEU:O	1.99	0.62
1:A:458:LEU:CD1	1:A:462:ILE:CD1	2.77	0.62
1:B:100:GLU:O	1:B:101:HIS:HB3	2.00	0.62
1:A:100:GLU:O	1:A:101:HIS:HB3	2.00	0.61
1:A:471:LEU:HD21	1:A:500:ASN:OD1	2.00	0.61
1:B:131:PHE:HD1	1:B:131:PHE:C	2.03	0.61
1:A:18:ARG:O	1:A:21:GLN:NE2	2.32	0.61
1:A:229:VAL:CG1	1:A:282:VAL:HG23	2.30	0.61
1:B:18:ARG:O	1:B:21:GLN:NE2	2.32	0.61
1:B:410:ALA:HB1	1:B:411:PRO:HD2	1.82	0.61
1:B:471:LEU:HD21	1:B:500:ASN:OD1	2.00	0.61
1:A:410:ALA:HB1	1:A:411:PRO:HD2	1.82	0.61
1:A:90:ILE:CD1	1:A:312:VAL:HG13	2.30	0.61
1:B:406:ASN:HD22	1:B:408:PHE:N	1.96	0.60
1:B:471:LEU:HD22	1:B:474:GLN:NE2	2.16	0.60
1:A:173:THR:HG22	1:A:175:LEU:HG	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:PHE:HB3	1:A:298:LEU:HD13	1.84	0.60
1:A:73:VAL:O	1:A:74:HIS:HB2	2.01	0.60
1:B:152:PHE:HB3	1:B:298:LEU:HD13	1.84	0.60
1:B:384:ASN:ND2	1:B:386:GLN:H	2.00	0.60
1:A:110:VAL:HG21	1:A:317:LEU:HD11	1.84	0.60
1:A:186:SER:O	1:A:476:LYS:NZ	2.27	0.60
1:B:245:SER:OG	1:B:248:ASP:HB2	2.01	0.60
1:B:385:TYR:OH	1:B:411:PRO:O	2.16	0.60
1:B:453:GLU:HA	1:B:453:GLU:OE2	2.01	0.60
1:B:73:VAL:O	1:B:74:HIS:HB2	2.01	0.60
1:B:90:ILE:CD1	1:B:312:VAL:HG13	2.30	0.60
1:A:471:LEU:HD22	1:A:474:GLN:NE2	2.16	0.60
1:B:229:VAL:CG1	1:B:282:VAL:HG23	2.30	0.60
1:B:458:LEU:HD11	1:B:462:ILE:CD1	2.32	0.60
1:A:245:SER:OG	1:A:248:ASP:HB2	2.01	0.59
1:A:360:THR:HG21	2:A:507:HEM:HMA3	1.83	0.59
1:A:209:ARG:HG2	1:A:274:PRO:HB3	1.83	0.59
1:A:372:ILE:O	1:A:373:PRO:C	2.41	0.59
1:A:458:LEU:HD11	1:A:462:ILE:CD1	2.32	0.59
1:B:131:PHE:C	1:B:131:PHE:CD1	2.76	0.59
1:A:453:GLU:OE2	1:A:453:GLU:HA	2.01	0.59
1:A:131:PHE:C	1:A:131:PHE:CD1	2.76	0.59
1:B:110:VAL:HG21	1:B:317:LEU:HD11	1.84	0.58
1:A:110:VAL:HA	1:A:132:ALA:O	2.03	0.58
1:B:173:THR:HG22	1:B:175:LEU:HG	1.83	0.58
1:B:372:ILE:O	1:B:373:PRO:C	2.41	0.58
1:B:209:ARG:HG2	1:B:274:PRO:HB3	1.83	0.58
1:A:384:ASN:ND2	1:A:386:GLN:H	2.00	0.58
1:A:406:ASN:HD22	1:A:406:ASN:C	2.07	0.58
1:A:406:ASN:HD22	1:A:408:PHE:N	1.96	0.58
1:B:360:THR:HG21	2:B:507:HEM:HMA3	1.83	0.58
1:B:110:VAL:HA	1:B:132:ALA:O	2.03	0.57
1:B:406:ASN:ND2	1:B:406:ASN:C	2.58	0.57
1:B:356:ALA:O	1:B:360:THR:HG22	2.04	0.57
1:B:134:LYS:HE3	1:B:331:LEU:HD22	1.86	0.57
1:B:406:ASN:HD22	1:B:406:ASN:C	2.07	0.57
1:A:487:GLU:HG2	1:A:491:ARG:HD2	1.87	0.57
1:B:487:GLU:HG2	1:B:491:ARG:HD2	1.87	0.57
1:A:356:ALA:O	1:A:360:THR:HG22	2.04	0.57
1:A:406:ASN:ND2	1:A:406:ASN:C	2.57	0.57
1:A:173:THR:CG2	1:A:175:LEU:CD1	2.82	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:TRP:HB2	1:A:339:PRO:CD	2.35	0.56
1:B:182:TRP:HE1	1:B:465:HIS:HD1	1.54	0.56
1:A:64:ASP:HB3	1:B:360:THR:HB	1.88	0.56
1:B:173:THR:CG2	1:B:175:LEU:CD1	2.82	0.56
1:A:134:LYS:HE3	1:A:331:LEU:HD22	1.86	0.56
1:A:236:LYS:HG3	1:A:279:TYR:CE2	2.40	0.56
1:A:294:ASN:ND2	1:A:296:PHE:H	2.03	0.56
1:B:236:LYS:HG3	1:B:279:TYR:CE2	2.41	0.55
1:B:100:GLU:O	1:B:100:GLU:CG	2.55	0.55
1:B:294:ASN:ND2	1:B:296:PHE:H	2.03	0.55
1:A:192:LEU:HD22	1:A:484:VAL:HG11	1.89	0.55
1:A:147:ASN:CG	2:A:507:HEM:HAC	2.27	0.55
1:B:142:TRP:HB2	1:B:339:PRO:CD	2.35	0.55
1:A:446:TYR:HA	1:A:450:LEU:CD2	2.36	0.55
1:B:446:TYR:HA	1:B:450:LEU:CD2	2.36	0.55
1:A:360:THR:HB	1:B:64:ASP:HB3	1.87	0.55
1:B:160:PHE:HB3	1:B:161:PRO:HD3	1.89	0.55
1:B:446:TYR:CE2	1:B:455:ARG:HD3	2.43	0.55
1:A:147:ASN:ND2	2:A:507:HEM:HAC	2.22	0.54
1:A:361:HIS:NE2	2:A:507:HEM:O2A	2.40	0.54
1:B:189:PRO:C	1:B:191:SER:H	2.10	0.54
1:B:306:ASP:HB3	1:B:307:TYR:CE2	2.43	0.54
1:A:463:ALA:O	1:A:467:LYS:HB3	2.07	0.54
1:A:485:HIS:CD2	1:A:486:PRO:HD2	2.43	0.54
1:B:147:ASN:CG	2:B:507:HEM:HAC	2.27	0.54
1:B:463:ALA:O	1:B:467:LYS:HB3	2.07	0.54
1:A:306:ASP:HB3	1:A:307:TYR:CE2	2.43	0.54
1:B:51:VAL:O	1:B:51:VAL:CG1	2.55	0.54
1:B:179:ASP:O	1:B:183:ASP:CB	2.52	0.54
1:B:192:LEU:HD22	1:B:484:VAL:HG11	1.89	0.54
1:B:361:HIS:NE2	2:B:507:HEM:O2A	2.40	0.54
1:A:476:LYS:O	1:A:477:ALA:C	2.46	0.54
1:B:77:GLY:O	1:B:324:TYR:OH	2.19	0.54
1:B:173:THR:HG22	1:B:175:LEU:CG	2.38	0.54
1:A:100:GLU:O	1:A:100:GLU:CG	2.55	0.54
1:A:170:ASN:HD22	1:A:173:THR:H	1.56	0.54
1:B:147:ASN:ND2	2:B:507:HEM:HAC	2.22	0.54
1:A:446:TYR:CE2	1:A:455:ARG:HD3	2.42	0.53
1:A:453:GLU:OE2	1:A:453:GLU:CA	2.55	0.53
1:A:173:THR:HG22	1:A:175:LEU:CG	2.38	0.53
1:B:212:ASP:OD1	1:B:237:THR:HG22	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:PHE:HB3	1:A:161:PRO:HD3	1.89	0.53
1:A:189:PRO:C	1:A:191:SER:H	2.10	0.53
1:B:485:HIS:CD2	1:B:486:PRO:HD2	2.43	0.53
1:A:51:VAL:O	1:A:51:VAL:CG1	2.55	0.53
1:A:179:ASP:O	1:A:183:ASP:CB	2.52	0.53
1:A:95:LYS:HG2	1:A:222:VAL:O	2.09	0.53
1:A:155:ARG:NE	1:A:433:SER:O	2.35	0.53
1:A:282:VAL:HG12	1:A:310:ILE:CD1	2.39	0.53
1:B:95:LYS:HG2	1:B:222:VAL:O	2.09	0.52
1:B:282:VAL:HG12	1:B:310:ILE:CD1	2.39	0.52
1:A:212:ASP:OD1	1:A:237:THR:HG22	2.09	0.52
1:B:476:LYS:O	1:B:477:ALA:C	2.46	0.52
1:B:453:GLU:OE2	1:B:453:GLU:CA	2.55	0.52
1:A:148:ASN:H	1:A:148:ASN:ND2	1.98	0.52
1:B:148:ASN:H	1:B:148:ASN:ND2	1.98	0.52
1:A:157:ALA:HB2	2:A:507:HEM:HBB1	1.91	0.52
1:B:170:ASN:HD22	1:B:173:THR:H	1.56	0.52
1:A:172:GLN:NE2	1:B:321:PRO:O	2.43	0.52
1:A:36:ASP:HB3	1:B:430:ARG:HD3	1.92	0.52
1:A:50:LEU:HD12	1:B:428:VAL:HG13	1.92	0.52
1:A:170:ASN:HD22	1:A:172:GLN:N	2.07	0.52
1:A:321:PRO:O	1:B:172:GLN:NE2	2.43	0.52
1:A:428:VAL:HG13	1:B:50:LEU:HD12	1.92	0.52
1:B:85:GLU:HA	1:B:104:LYS:O	2.10	0.52
1:A:189:PRO:C	1:A:191:SER:N	2.63	0.51
1:A:85:GLU:HA	1:A:104:LYS:O	2.10	0.51
1:B:386:GLN:O	1:B:387:ARG:NH1	2.43	0.51
1:A:155:ARG:HD2	1:A:433:SER:HB2	1.92	0.51
1:B:157:ALA:HB2	2:B:507:HEM:HBB1	1.91	0.51
1:A:430:ARG:HD3	1:B:36:ASP:HB3	1.92	0.51
1:B:155:ARG:HD2	1:B:433:SER:HB2	1.92	0.51
1:A:178:PRO:O	1:A:182:TRP:HB2	2.10	0.50
1:A:220:LYS:CE	1:A:420:HIS:CD2	2.90	0.50
1:B:178:PRO:O	1:B:182:TRP:HB2	2.10	0.50
1:A:82:GLY:HA3	1:A:316:VAL:O	2.12	0.50
1:A:386:GLN:O	1:A:387:ARG:NH1	2.43	0.50
1:A:179:ASP:O	1:A:183:ASP:N	2.42	0.50
1:B:82:GLY:HA3	1:B:316:VAL:O	2.12	0.50
1:B:189:PRO:C	1:B:191:SER:N	2.63	0.50
1:A:223:ASN:C	1:A:223:ASN:ND2	2.64	0.50
1:B:179:ASP:O	1:B:183:ASP:N	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:ASP:C	1:B:128:PRO:O	2.48	0.50
1:B:155:ARG:NE	1:B:433:SER:O	2.35	0.50
1:B:98:VAL:HG23	1:B:137:THR:CB	2.41	0.50
1:A:236:LYS:O	1:A:276:TRP:HA	2.12	0.49
1:B:170:ASN:HD22	1:B:172:GLN:N	2.07	0.49
1:B:345:SER:HB2	1:B:346:PRO:CD	2.43	0.49
1:B:276:TRP:HZ3	1:B:317:LEU:HD22	1.77	0.49
1:B:236:LYS:O	1:B:276:TRP:HA	2.12	0.49
1:B:334:ASP:O	1:B:337:ASN:HB2	2.13	0.49
1:A:236:LYS:HG3	1:A:279:TYR:HE2	1.78	0.49
1:A:394:MET:HE3	1:A:394:MET:HA	1.94	0.49
1:B:129:ARG:H	1:B:148:ASN:ND2	2.10	0.49
1:B:223:ASN:ND2	1:B:223:ASN:C	2.64	0.49
1:B:394:MET:HE3	1:B:394:MET:HA	1.95	0.49
1:B:223:ASN:ND2	1:B:225:ASP:N	2.59	0.49
1:A:51:VAL:O	1:A:51:VAL:HG13	2.13	0.49
1:A:141:ASN:OD1	1:A:377:PRO:HA	2.13	0.49
1:A:173:THR:CG2	1:A:175:LEU:CG	2.91	0.49
1:A:334:ASP:O	1:A:337:ASN:HB2	2.13	0.49
1:B:141:ASN:OD1	1:B:377:PRO:HA	2.13	0.49
1:A:331:LEU:HD13	1:A:333:PHE:CZ	2.48	0.48
1:A:345:SER:HB2	1:A:346:PRO:CD	2.42	0.48
1:A:9:ASP:HB3	1:A:13:HIS:CE1	2.49	0.48
1:B:51:VAL:O	1:B:51:VAL:HG13	2.13	0.48
1:B:458:LEU:HD12	1:B:462:ILE:CD1	2.43	0.48
1:A:129:ARG:H	1:A:148:ASN:ND2	2.10	0.48
1:A:239:GLN:OE1	1:A:275:SER:N	2.38	0.48
1:A:276:TRP:HZ3	1:A:317:LEU:HD22	1.77	0.48
1:B:173:THR:CG2	1:B:175:LEU:CG	2.91	0.48
1:A:192:LEU:HD22	1:A:484:VAL:CG1	2.43	0.48
1:B:192:LEU:HD22	1:B:484:VAL:CG1	2.43	0.48
1:B:239:GLN:OE1	1:B:275:SER:N	2.38	0.48
1:A:458:LEU:HD12	1:A:462:ILE:CD1	2.43	0.48
1:A:127:ASP:C	1:A:128:PRO:O	2.48	0.48
1:B:9:ASP:HB3	1:B:13:HIS:CE1	2.49	0.48
1:B:134:LYS:HE2	1:B:134:LYS:HB2	1.57	0.48
1:B:157:ALA:CB	2:B:507:HEM:HBB1	2.44	0.48
1:B:74:HIS:CE1	1:B:115:VAL:HG22	2.49	0.47
1:A:77:GLY:O	1:A:324:TYR:OH	2.19	0.47
1:A:449:VAL:HG21	3:A:508:NDP:O4D	2.14	0.47
1:A:74:HIS:CE1	1:A:115:VAL:HG22	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:LEU:HD13	1:B:333:PHE:CZ	2.48	0.47
1:B:449:VAL:HG21	3:B:508:NDP:O4D	2.14	0.47
1:B:236:LYS:HG3	1:B:279:TYR:HE2	1.78	0.47
1:A:147:ASN:HB2	2:A:507:HEM:HAC	1.97	0.47
1:A:157:ALA:CB	2:A:507:HEM:HBB1	2.44	0.47
1:A:400:ALA:O	1:A:401:PRO:C	2.52	0.47
1:B:173:THR:CG2	1:B:175:LEU:HG	2.44	0.47
1:A:98:VAL:HG23	1:A:137:THR:CB	2.41	0.47
1:B:400:ALA:O	1:B:401:PRO:C	2.52	0.47
1:A:223:ASN:ND2	1:A:225:ASP:N	2.59	0.47
1:B:484:VAL:HG22	1:B:488:TYR:HD1	1.80	0.47
1:B:108:ILE:O	1:B:108:ILE:HG13	2.15	0.47
1:A:100:GLU:O	1:A:100:GLU:HG3	2.15	0.46
1:B:220:LYS:CE	1:B:420:HIS:CD2	2.90	0.46
1:A:239:GLN:OE1	1:A:274:PRO:HA	2.15	0.46
1:A:291:PHE:CE1	1:A:293:PHE:HB2	2.51	0.46
1:A:134:LYS:HB2	1:A:134:LYS:HE2	1.57	0.46
1:A:159:LEU:HD11	1:A:188:ARG:CZ	2.46	0.46
1:B:357:TYR:N	1:B:358:PRO:HD2	2.29	0.46
1:B:374:VAL:O	1:B:374:VAL:CG2	2.63	0.46
1:A:90:ILE:CD1	1:A:312:VAL:CG1	2.94	0.46
1:B:22:LYS:HD3	1:B:22:LYS:HA	1.77	0.46
1:B:90:ILE:CD1	1:B:312:VAL:CG1	2.94	0.46
1:B:100:GLU:O	1:B:100:GLU:HG3	2.15	0.46
1:B:154:ILE:HG13	1:B:349:MET:HE2	1.97	0.46
1:B:170:ASN:HA	1:B:171:PRO:HD3	1.87	0.46
1:B:15:LYS:HE2	4:B:522:HOH:O	2.15	0.46
1:B:135:PHE:CD1	1:B:142:TRP:CE3	3.04	0.46
1:B:239:GLN:OE1	1:B:274:PRO:HA	2.15	0.46
1:A:15:LYS:HE2	4:A:514:HOH:O	2.15	0.46
1:A:90:ILE:HD13	1:A:312:VAL:CG1	2.38	0.46
1:A:348:LYS:HE2	4:A:551:HOH:O	2.13	0.46
1:A:391:MET:HB3	1:A:391:MET:HE3	1.81	0.46
1:B:149:THR:OG1	1:B:150:PRO:CD	2.64	0.46
1:A:357:TYR:N	1:A:358:PRO:HD2	2.29	0.46
1:B:5:ASP:O	1:B:8:SER:HB2	2.16	0.46
1:B:90:ILE:HD13	1:B:312:VAL:CG1	2.38	0.46
1:B:276:TRP:CZ3	1:B:317:LEU:HD22	2.51	0.46
1:A:5:ASP:O	1:A:8:SER:HB2	2.16	0.46
1:A:276:TRP:CZ3	1:A:317:LEU:HD22	2.51	0.46
1:A:371:GLN:HE22	1:A:393:MET:N	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:PHE:CD1	1:B:81:PHE:N	2.84	0.46
1:B:147:ASN:HB2	2:B:507:HEM:HAC	1.97	0.46
1:B:159:LEU:HD11	1:B:188:ARG:CZ	2.46	0.46
1:B:177:ASP:HA	1:B:178:PRO:HD3	1.85	0.46
1:A:50:LEU:HA	1:A:50:LEU:HD23	1.63	0.45
1:A:173:THR:CG2	1:A:175:LEU:HG	2.44	0.45
1:A:357:TYR:H	1:A:358:PRO:HD2	1.81	0.45
1:A:135:PHE:CD1	1:A:142:TRP:CE3	3.04	0.45
1:A:188:ARG:O	1:A:191:SER:HB3	2.16	0.45
1:A:484:VAL:HG22	1:A:488:TYR:HD1	1.80	0.45
1:B:357:TYR:H	1:B:358:PRO:HD2	1.82	0.45
1:A:142:TRP:HA	1:A:337:ASN:O	2.16	0.45
1:B:79:GLY:O	1:B:80:ALA:CB	2.58	0.45
1:B:188:ARG:O	1:B:191:SER:HB3	2.16	0.45
1:B:435:ASN:C	1:B:436:ASP:O	2.55	0.45
1:B:487:GLU:HG2	1:B:491:ARG:CD	2.46	0.45
1:A:81:PHE:CD1	1:A:81:PHE:N	2.84	0.45
1:B:142:TRP:HA	1:B:337:ASN:O	2.16	0.45
1:B:439:VAL:O	1:B:440:THR:C	2.55	0.45
1:A:487:GLU:HG2	1:A:491:ARG:CD	2.46	0.45
1:B:429:GLN:HE21	1:B:429:GLN:HB2	1.60	0.45
1:A:453:GLU:O	1:A:456:LYS:HG2	2.17	0.45
1:B:98:VAL:HG21	1:B:137:THR:HG22	1.99	0.45
1:B:331:LEU:HD13	1:B:333:PHE:CE2	2.52	0.45
1:A:98:VAL:HG21	1:A:137:THR:HG22	1.99	0.45
1:A:228:ALA:HB2	1:A:420:HIS:CE1	2.52	0.45
1:A:97:LYS:O	1:A:100:GLU:HB3	2.17	0.45
1:B:282:VAL:HG12	1:B:310:ILE:HD12	1.99	0.45
1:B:371:GLN:HE22	1:B:393:MET:N	2.13	0.44
1:B:453:GLU:O	1:B:456:LYS:HG2	2.17	0.44
1:B:291:PHE:CE1	1:B:293:PHE:HB2	2.51	0.44
1:A:484:VAL:HG23	1:A:484:VAL:O	2.18	0.44
1:B:97:LYS:O	1:B:100:GLU:HB3	2.17	0.44
1:B:430:ARG:HH11	1:B:430:ARG:HD2	1.58	0.44
1:A:209:ARG:HH11	1:A:209:ARG:HD3	1.63	0.44
1:A:439:VAL:O	1:A:440:THR:C	2.55	0.44
1:A:79:GLY:O	1:A:80:ALA:CB	2.58	0.44
1:A:236:LYS:HB3	1:A:236:LYS:HE2	1.46	0.44
1:A:331:LEU:HD13	1:A:333:PHE:CE2	2.52	0.44
1:A:381:ARG:HH11	1:A:381:ARG:HD3	1.59	0.44
1:B:147:ASN:CB	2:B:507:HEM:HAC	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:VAL:HG21	3:B:508:NDP:C4D	2.48	0.44
1:A:282:VAL:HG12	1:A:310:ILE:HD12	1.99	0.43
1:A:354:LEU:HD12	1:A:354:LEU:HA	1.63	0.43
1:B:145:VAL:HG22	1:B:333:PHE:HB3	2.00	0.43
1:B:148:ASN:N	1:B:148:ASN:ND2	2.63	0.43
1:A:19:ALA:C	1:A:21:GLN:H	2.22	0.43
1:A:145:VAL:HG22	1:A:333:PHE:HB3	2.00	0.43
1:B:228:ALA:HB2	1:B:420:HIS:CE1	2.52	0.43
1:B:484:VAL:O	1:B:484:VAL:HG23	2.18	0.43
1:A:449:VAL:HG21	3:A:508:NDP:C4D	2.47	0.43
1:A:108:ILE:O	1:A:108:ILE:HG13	2.15	0.43
1:A:84:PHE:O	1:A:105:ARG:HA	2.19	0.43
1:A:147:ASN:CB	2:A:507:HEM:HAC	2.48	0.43
1:B:50:LEU:HA	1:B:50:LEU:HD23	1.63	0.43
1:B:236:LYS:HE2	1:B:236:LYS:HB3	1.46	0.43
1:B:360:THR:HG21	2:B:507:HEM:CMA	2.47	0.43
1:A:92:ARG:H	1:A:92:ARG:HG3	1.62	0.43
1:A:134:LYS:HG3	1:A:143:ASP:OD2	2.19	0.43
1:A:157:ALA:CB	2:A:507:HEM:CBB	2.97	0.43
1:A:293:PHE:O	1:A:295:PRO:CD	2.67	0.43
1:B:134:LYS:HG3	1:B:143:ASP:OD2	2.18	0.43
1:B:238:ASP:OD1	1:B:275:SER:OG	2.26	0.43
1:B:293:PHE:O	1:B:295:PRO:CD	2.67	0.43
1:B:19:ALA:C	1:B:21:GLN:H	2.22	0.43
1:A:360:THR:HG21	2:A:507:HEM:CMA	2.47	0.43
1:A:435:ASN:C	1:A:436:ASP:O	2.55	0.43
1:B:84:PHE:O	1:B:105:ARG:HA	2.19	0.43
1:B:445:PHE:O	1:B:449:VAL:HB	2.19	0.43
1:A:22:LYS:HD3	1:A:22:LYS:HA	1.77	0.42
1:B:89:ASP:C	1:B:89:ASP:OD1	2.56	0.42
1:B:110:VAL:CG2	1:B:317:LEU:HD11	2.48	0.42
1:A:149:THR:OG1	1:A:150:PRO:CD	2.64	0.42
1:A:343:GLU:HA	1:A:344:PRO:HD3	1.96	0.42
1:A:374:VAL:O	1:A:374:VAL:CG2	2.63	0.42
1:B:157:ALA:CB	2:B:507:HEM:CBB	2.97	0.42
1:A:152:PHE:CB	1:A:298:LEU:HD13	2.49	0.42
1:A:189:PRO:O	1:A:192:LEU:HB2	2.20	0.42
1:A:298:LEU:HD12	1:A:349:MET:HG3	2.02	0.42
1:A:337:ASN:HD22	1:A:337:ASN:HA	1.67	0.42
1:B:90:ILE:O	1:B:93:TYR:HB2	2.20	0.42
3:B:508:NDP:C6N	3:B:508:NDP:H4B	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ASP:C	1:A:89:ASP:OD1	2.56	0.42
1:A:347:ASP:HB3	1:A:350:LEU:HB3	2.02	0.42
1:B:349:MET:O	1:B:353:ARG:HG3	2.20	0.42
1:A:177:ASP:HA	1:A:178:PRO:HD3	1.85	0.42
1:A:120:GLY:H	1:B:120:GLY:H	1.68	0.42
1:A:410:ALA:HB1	1:A:411:PRO:CD	2.50	0.42
1:B:3:ASN:HB3	1:B:4:ARG:H	1.67	0.42
1:A:118:GLU:H	1:A:118:GLU:HG2	1.04	0.42
1:A:445:PHE:O	1:A:449:VAL:HB	2.19	0.42
3:A:508:NDP:C6N	3:A:508:NDP:H4B	2.50	0.41
1:B:6:PRO:O	1:B:7:ALA:C	2.58	0.41
1:B:189:PRO:O	1:B:192:LEU:HB2	2.20	0.41
1:B:391:MET:HB3	1:B:391:MET:HE3	1.81	0.41
1:A:90:ILE:O	1:A:93:TYR:HB2	2.20	0.41
1:A:284:THR:CG2	1:A:286:SER:H	2.28	0.41
1:A:485:HIS:HA	1:A:486:PRO:HD2	1.83	0.41
1:A:135:PHE:CE1	1:A:142:TRP:CZ3	3.09	0.41
1:B:298:LEU:HD12	1:B:349:MET:HG3	2.02	0.41
1:B:421:ARG:HE	1:B:421:ARG:HB3	1.60	0.41
1:A:98:VAL:HG23	1:A:137:THR:HG21	2.01	0.41
1:A:110:VAL:CG2	1:A:317:LEU:HD11	2.48	0.41
1:A:349:MET:O	1:A:353:ARG:HG3	2.20	0.41
1:A:415:PRO:C	1:A:417:ALA:H	2.23	0.41
1:B:14:TRP:CZ3	1:B:18:ARG:HD2	2.56	0.41
1:B:293:PHE:O	1:B:295:PRO:HD3	2.20	0.41
1:B:307:TYR:N	1:B:307:TYR:CD2	2.88	0.41
1:A:14:TRP:CZ3	1:A:18:ARG:HD2	2.56	0.41
1:A:65:ARG:HH12	1:B:359:ASP:CG	2.24	0.41
1:A:67:ARG:NH2	1:B:168:LYS:HE3	2.35	0.41
1:A:359:ASP:CG	1:B:65:ARG:HH12	2.24	0.41
1:B:404:TYR:HA	1:B:405:PRO:HA	1.93	0.41
1:A:371:GLN:NE2	1:A:393:MET:HB2	2.33	0.41
1:B:118:GLU:H	1:B:118:GLU:HG2	1.04	0.41
1:B:235:TYR:HA	1:B:277:THR:O	2.21	0.41
1:B:415:PRO:C	1:B:417:ALA:H	2.23	0.41
1:A:209:ARG:HB2	4:A:533:HOH:O	2.21	0.41
1:A:293:PHE:O	1:A:295:PRO:HD3	2.20	0.41
1:B:135:PHE:CE1	1:B:142:TRP:CZ3	3.09	0.41
1:A:118:GLU:HG3	1:B:120:GLY:CA	2.51	0.41
1:A:168:LYS:HE3	1:B:67:ARG:NH2	2.35	0.41
1:A:195:VAL:O	1:A:199:PHE:HD1	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:TYR:N	1:A:307:TYR:CD2	2.88	0.41
1:B:263:ASP:O	1:B:264:LEU:C	2.59	0.41
1:B:273:TYR:HA	1:B:274:PRO:HD2	1.95	0.41
1:A:5:ASP:HA	1:A:6:PRO:HD3	1.88	0.41
1:A:394:MET:HE2	1:A:394:MET:HB3	1.97	0.41
1:B:258:ASP:O	1:B:261:LEU:N	2.53	0.41
1:B:347:ASP:HB3	1:B:350:LEU:HB3	2.02	0.40
1:B:358:PRO:O	1:B:362:ARG:HD2	2.22	0.40
1:A:64:ASP:OD1	1:B:359:ASP:OD2	2.39	0.40
1:A:92:ARG:O	1:A:223:ASN:CB	2.68	0.40
1:A:235:TYR:HA	1:A:277:THR:O	2.21	0.40
1:B:114:THR:HG22	1:B:129:ARG:HD2	2.04	0.40
1:A:120:GLY:CA	1:B:118:GLU:HG3	2.51	0.40
1:A:154:ILE:HG13	1:A:349:MET:CE	2.51	0.40
1:A:170:ASN:HA	1:A:171:PRO:HD3	1.87	0.40
1:A:353:ARG:O	1:A:354:LEU:C	2.59	0.40
1:B:177:ASP:HB3	1:B:180:MET:HE1	1.96	0.40
1:B:410:ALA:HB1	1:B:411:PRO:CD	2.50	0.40
1:A:114:THR:HG22	1:A:129:ARG:HD2	2.03	0.40
1:B:59:GLU:HB2	4:B:524:HOH:O	2.21	0.40
1:A:294:ASN:HA	1:A:295:PRO:HD2	1.77	0.40
1:A:359:ASP:OD2	1:B:64:ASP:OD1	2.39	0.40
1:B:294:ASN:C	1:B:294:ASN:HD22	2.25	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:GLU:OE2	1:B:430:ARG:NH1[6_556]	1.98	0.22
1:A:430:ARG:NH1	1:B:419:GLU:OE2[6_556]	1.98	0.22
1:B:10:GLN:NE2	4:B:551:HOH:O[6_556]	2.13	0.07
1:A:10:GLN:NE2	4:A:543:HOH:O[6_556]	2.14	0.06

5.3 Torsion angles (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%)	434 (88%)	52 (10%)	10 (2%)	7 12
1	B	496/506 (98%)	434 (88%)	52 (10%)	10 (2%)	7 12
All	All	992/1012 (98%)	868 (88%)	104 (10%)	20 (2%)	7 12

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	267	ALA
1	B	267	ALA
1	A	54	VAL
1	A	440	THR
1	B	54	VAL
1	B	440	THR
1	A	451	ASN
1	B	451	ASN
1	A	101	HIS
1	A	268	ILE
1	A	373	PRO
1	B	101	HIS
1	B	268	ILE
1	B	373	PRO
1	A	22	LYS
1	A	394	MET
1	B	22	LYS
1	B	394	MET
1	A	128	PRO
1	B	128	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	430/437 (98%)	356 (83%)	74 (17%)	2 3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	430/437 (98%)	356 (83%)	74 (17%)	2 3
All	All	860/874 (98%)	712 (83%)	148 (17%)	2 3

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	10	GLN
1	A	18	ARG
1	A	21	GLN
1	A	40	SER
1	A	43	VAL
1	A	48	PRO
1	A	51	VAL
1	A	57	THR
1	A	73	VAL
1	A	76	LYS
1	A	89	ASP
1	A	91	THR
1	A	92	ARG
1	A	102	ILE
1	A	118	GLU
1	A	124	THR
1	A	129	ARG
1	A	131	PHE
1	A	137	THR
1	A	148	ASN
1	A	150	PRO
1	A	155	ARG
1	A	158	LEU
1	A	159	LEU
1	A	176	LYS
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	246	VAL
1	A	247	GLU
1	A	255	GLU
1	A	261	LEU

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Mol	Chain	Res	Type
1	A	264	LEU
1	A	272	ASN
1	A	282	VAL
1	A	287	GLU
1	A	290	ILE
1	A	294	ASN
1	A	298	LEU
1	A	315	LEU
1	A	317	LEU
1	A	318	ASN
1	A	331	LEU
1	A	335	PRO
1	A	337	ASN
1	A	339	PRO
1	A	354	LEU
1	A	355	PHE
1	A	365	LEU
1	A	372	ILE
1	A	379	ARG
1	A	384	ASN
1	A	386	GLN
1	A	394	MET
1	A	396	ASN
1	A	402	ASN
1	A	405	PRO
1	A	406	ASN
1	A	407	SER
1	A	413	HIS
1	A	414	GLN
1	A	444	THR
1	A	448	LYS
1	A	450	LEU
1	A	452	GLU
1	A	458	LEU
1	A	471	LEU
1	A	488	TYR
1	A	498	LYS
1	A	500	ASN
1	B	4	ARG
1	B	10	GLN
1	B	18	ARG
1	B	21	GLN

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Mol	Chain	Res	Type
1	B	40	SER
1	B	43	VAL
1	B	48	PRO
1	B	51	VAL
1	B	57	THR
1	B	73	VAL
1	B	76	LYS
1	B	89	ASP
1	B	91	THR
1	B	92	ARG
1	B	102	ILE
1	B	118	GLU
1	B	124	THR
1	B	129	ARG
1	B	131	PHE
1	B	137	THR
1	B	148	ASN
1	B	150	PRO
1	B	155	ARG
1	B	158	LEU
1	B	159	LEU
1	B	176	LYS
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	246	VAL
1	B	247	GLU
1	B	255	GLU
1	B	261	LEU
1	B	264	LEU
1	B	272	ASN
1	B	282	VAL
1	B	287	GLU
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	394	MET
1	B	396	ASN
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	444	THR
1	B	448	LYS
1	B	450	LEU
1	B	452	GLU
1	B	458	LEU
1	B	471	LEU
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 (59) 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
1	A	172	GLN
1	A	223	ASN

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Mol	Chain	Res	Type
1	A	234	HIS
1	A	272	ASN
1	A	281	GLN
1	A	294	ASN
1	A	323	ASN
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	402	ASN
1	A	406	ASN
1	A	414	GLN
1	A	420	HIS
1	A	429	GLN
1	A	438	ASN
1	A	474	GLN
1	A	485	HIS
1	B	3	ASN
1	B	10	GLN
1	B	17	GLN
1	B	21	GLN
1	B	39	ASN
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	323	ASN
1	B	330	GLN
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

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Mol	Chain	Res	Type
1	B	406	ASN
1	B	414	GLN
1	B	420	HIS
1	B	429	GLN
1	B	438	ASN
1	B	474	GLN
1	B	485	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HEM	A	507	1	41,50,50	1.33	4 (9%)	45,82,82	1.53	8 (17%)
3	NDP	A	508	-	45,52,52	1.77	9 (20%)	53,80,80	1.58	7 (13%)
3	NDP	B	508	-	45,52,52	1.76	9 (20%)	53,80,80	1.57	7 (13%)
2	HEM	B	507	1	41,50,50	1.35	4 (9%)	45,82,82	1.53	8 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	507	1	-	2/12/54/54	-
3	NDP	A	508	-	-	4/30/77/77	0/5/5/5
3	NDP	B	508	-	-	4/30/77/77	0/5/5/5
2	HEM	B	507	1	-	2/12/54/54	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	508	NDP	O4B-C1B	5.76	1.49	1.41
3	B	508	NDP	O4B-C1B	5.71	1.49	1.41
3	A	508	NDP	C4N-C3N	-4.44	1.41	1.49
3	B	508	NDP	C4N-C3N	-4.42	1.41	1.49
3	A	508	NDP	P2B-O2B	4.21	1.67	1.59
3	B	508	NDP	P2B-O2B	4.15	1.67	1.59
3	B	508	NDP	C4N-C5N	-3.95	1.38	1.48
3	A	508	NDP	C4N-C5N	-3.94	1.38	1.48
2	B	507	HEM	C3C-C2C	-3.74	1.35	1.40
2	A	507	HEM	C3C-C2C	-3.68	1.35	1.40
3	A	508	NDP	C7N-C3N	3.52	1.56	1.48
3	B	508	NDP	C7N-C3N	3.50	1.56	1.48
2	B	507	HEM	C3C-CAC	3.04	1.54	1.47
2	A	507	HEM	C3C-CAC	2.98	1.53	1.47
3	A	508	NDP	C6N-C5N	2.54	1.37	1.33
3	B	508	NDP	C6N-C5N	2.50	1.37	1.33
2	A	507	HEM	CAB-C3B	2.33	1.53	1.47
2	B	507	HEM	CAB-C3B	2.32	1.53	1.47
3	B	508	NDP	PA-O2A	-2.11	1.45	1.55
3	B	508	NDP	C2A-N1A	2.11	1.37	1.33
3	A	508	NDP	PA-O2A	-2.10	1.45	1.55
3	A	508	NDP	C2A-N1A	2.09	1.37	1.33
2	A	507	HEM	C3B-C2B	-2.07	1.33	1.37
2	B	507	HEM	C3B-C2B	-2.05	1.33	1.37
3	A	508	NDP	PN-O2N	-2.04	1.45	1.55
3	B	508	NDP	PN-O2N	-2.03	1.45	1.55

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	508	NDP	O2X-P2B-O2B	4.95	128.15	105.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	508	NDP	O2X-P2B-O2B	4.94	128.15	105.99
2	B	507	HEM	O2D-CGD-O1D	3.89	133.01	123.30
2	A	507	HEM	O2D-CGD-O1D	3.89	133.00	123.30
3	A	508	NDP	PN-O3-PA	3.80	145.88	132.83
3	B	508	NDP	PN-O3-PA	3.79	145.84	132.83
3	A	508	NDP	O3X-P2B-O2B	-3.72	89.31	105.99
3	B	508	NDP	O3X-P2B-O2B	-3.72	89.33	105.99
2	A	507	HEM	CMC-C2C-C3C	3.37	130.98	124.68
2	B	507	HEM	CMC-C2C-C3C	3.35	130.95	124.68
3	A	508	NDP	O4B-C1B-C2B	-3.16	101.10	106.59
3	B	508	NDP	O4B-C1B-C2B	-3.16	101.10	106.59
3	A	508	NDP	C5A-C6A-N6A	3.02	124.94	120.35
3	B	508	NDP	C5A-C6A-N6A	2.97	124.87	120.35
2	B	507	HEM	CMA-C3A-C4A	-2.87	124.06	128.46
2	A	507	HEM	CMA-C3A-C4A	-2.83	124.11	128.46
2	B	507	HEM	O1D-CGD-CBD	-2.82	114.01	123.08
2	A	507	HEM	O1D-CGD-CBD	-2.82	114.02	123.08
2	A	507	HEM	CBA-CAA-C2A	2.81	117.42	112.62
2	B	507	HEM	CBA-CAA-C2A	2.79	117.39	112.62
2	B	507	HEM	O1A-CGA-CBA	-2.61	114.70	123.08
2	A	507	HEM	O1A-CGA-CBA	-2.59	114.77	123.08
3	A	508	NDP	C3N-C2N-N1N	-2.54	119.47	123.10
3	B	508	NDP	C3N-C2N-N1N	-2.48	119.56	123.10
2	B	507	HEM	C4C-CHD-C1D	2.11	125.34	122.56
3	A	508	NDP	C1D-N1N-C2N	-2.07	117.66	121.11
3	B	508	NDP	C1D-N1N-C2N	-2.04	117.71	121.11
2	A	507	HEM	C4C-CHD-C1D	2.04	125.25	122.56
2	A	507	HEM	CHC-C4B-C3B	2.03	127.68	124.57
2	B	507	HEM	CHC-C4B-C3B	2.02	127.66	124.57

There are no chirality outliers.

All (12) 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
3	A	508	NDP	PN-O3-PA-O1A
3	B	508	NDP	PN-O3-PA-O1A

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Mol	Chain	Res	Type	Atoms
2	B	507	HEM	CAD-CBD-CGD-O2D
2	A	507	HEM	CAD-CBD-CGD-O2D
2	B	507	HEM	CAD-CBD-CGD-O1D
2	A	507	HEM	CAD-CBD-CGD-O1D

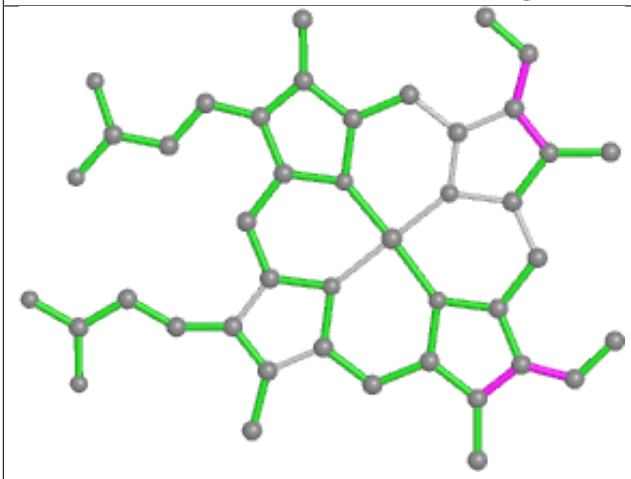
There are no ring outliers.

4 monomers are involved in 28 short contacts:

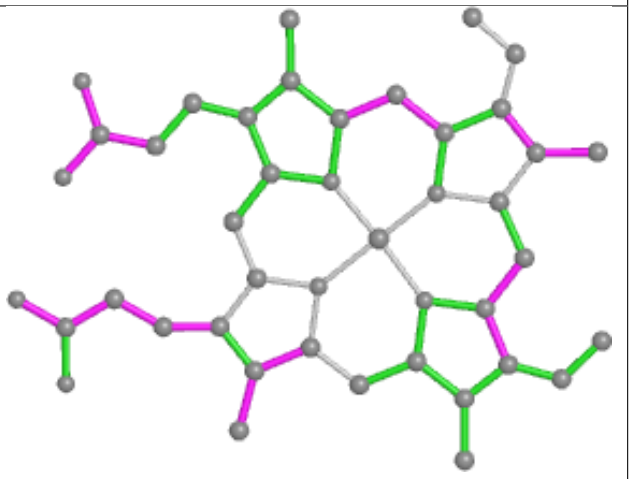
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	507	HEM	11	0
3	A	508	NDP	3	0
3	B	508	NDP	3	0
2	B	507	HEM	11	0

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.

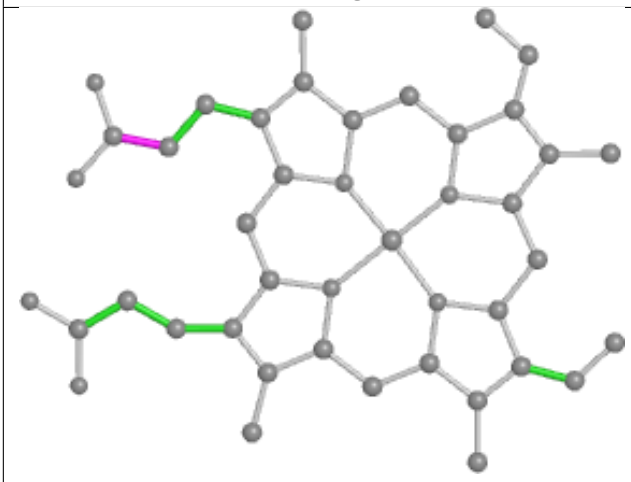
Ligand HEM A 507



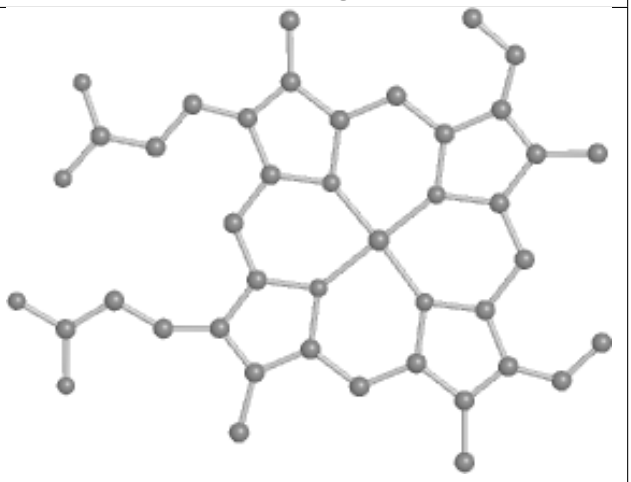
Bond lengths



Bond angles

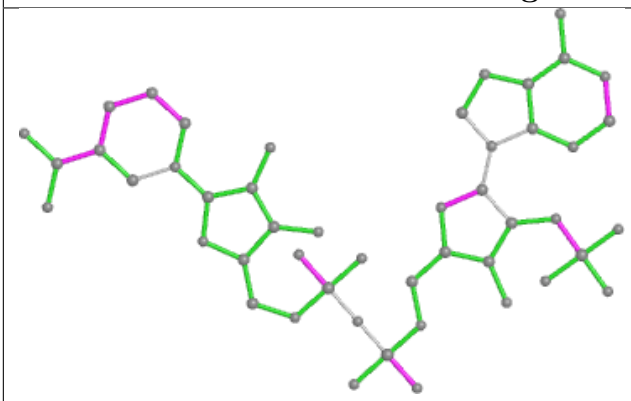


Torsions

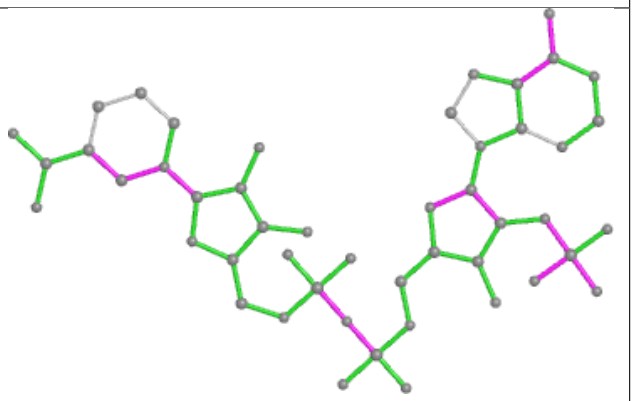


Rings

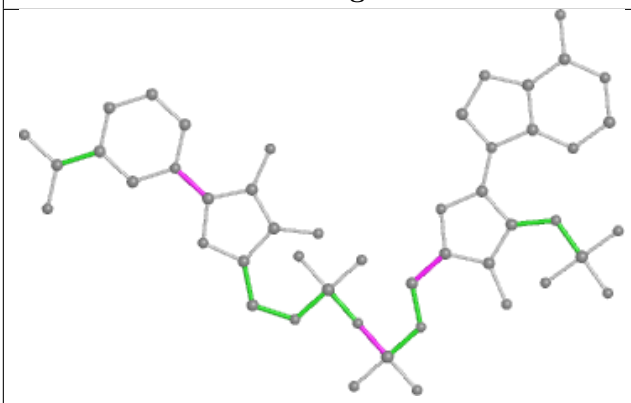
Ligand NDP A 508



Bond lengths



Bond angles



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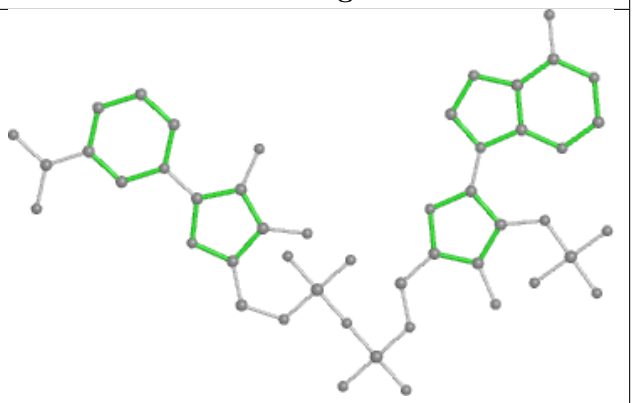
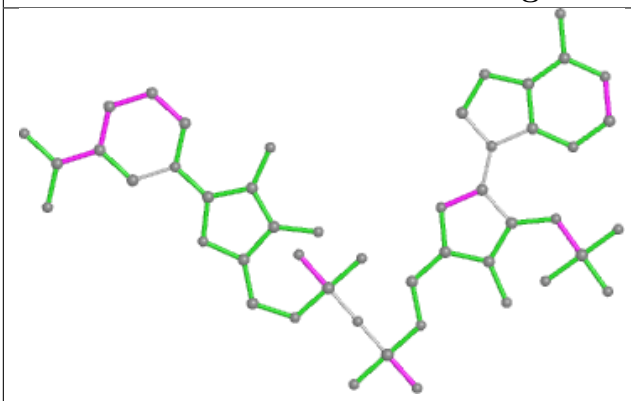
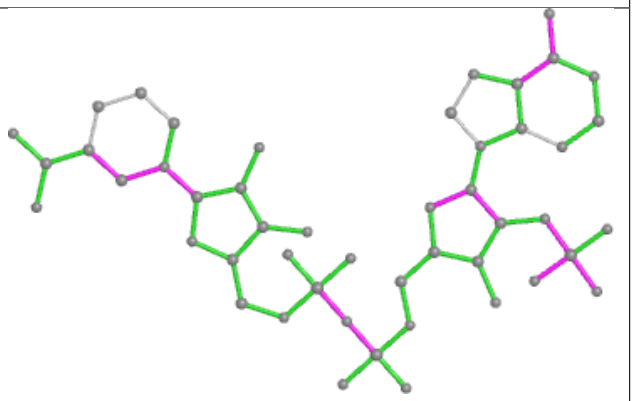


Rings

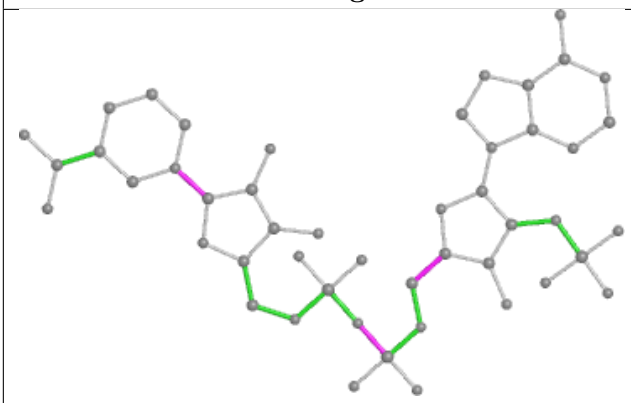
Ligand NDP B 508



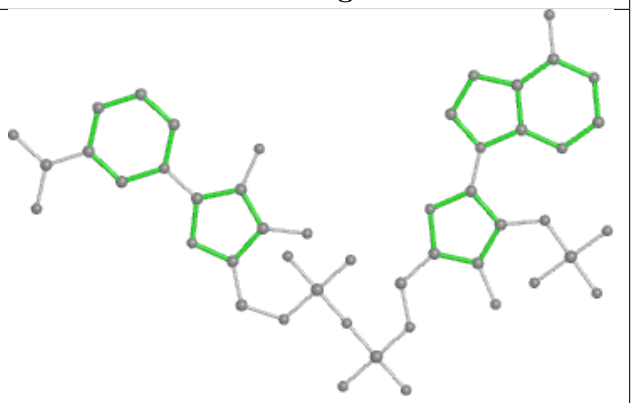
Bond lengths



Bond angles

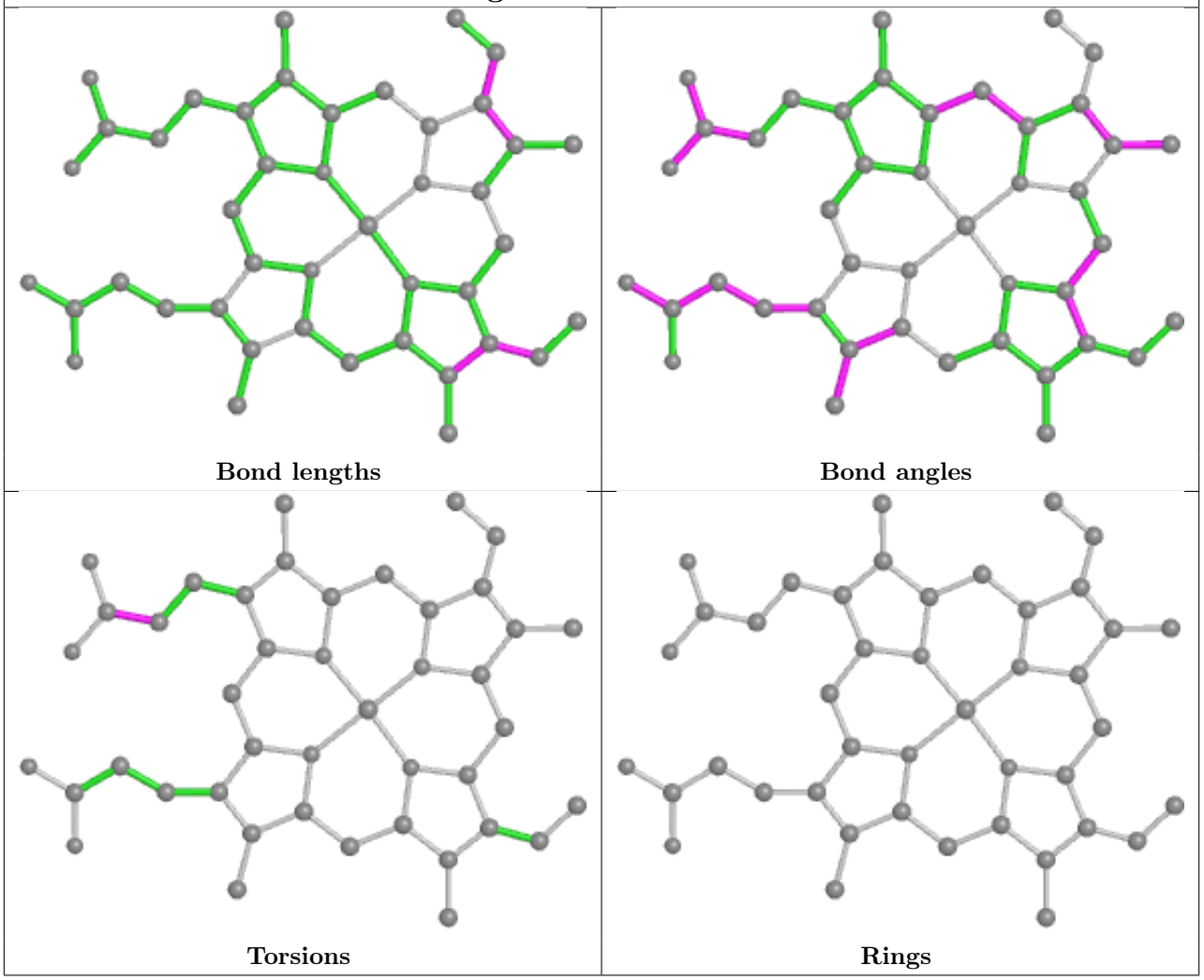


Torsions



Rings

Ligand HEM B 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.