Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2024 – 03:08 PM EDT

PDB ID	:	2VAO
Title	:	STRUCTURE OF THE OCTAMERIC FLAVOENZYME VANILLYL-ALCOHOL OXIDASE IN COMPLEX WITH ISOEUGENOL
Authors	:	Mattevi, A.
Deposited on	:	1997-04-10
Resolution	:	2.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

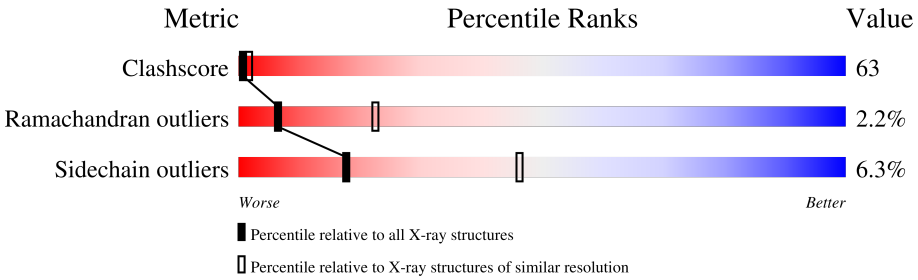
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	560	23% 56% 18%
1	B	560	24% 55% 18%

2 Entry composition

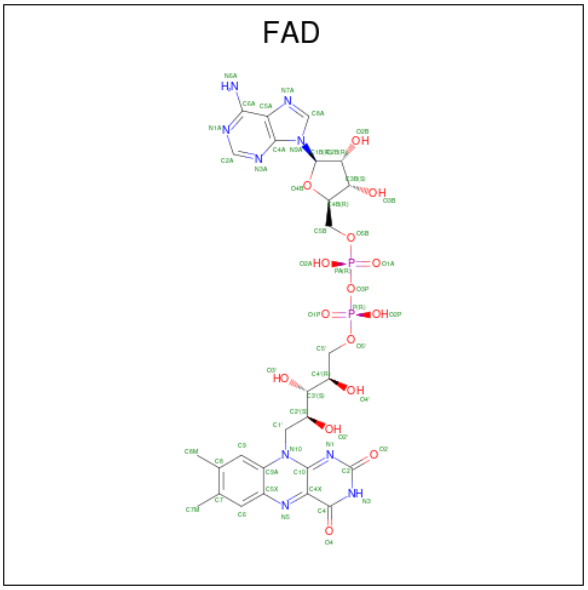
There are 4 unique types of molecules in this entry. The entry contains 8948 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 VANILLYL-ALCOHOL OXIDASE.

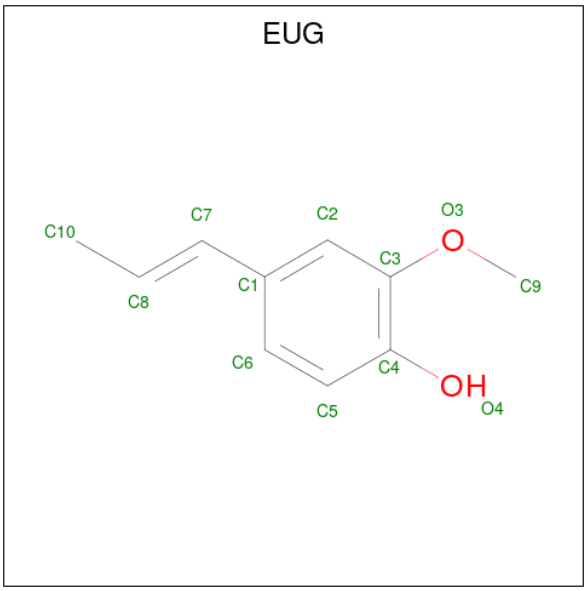
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	51	0	0
			4391	2817	751	799	24			
1	B	555	Total	C	N	O	S	51	0	0
			4391	2817	751	799	24			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is 2-methoxy-4-[(1E)-prop-1-en-1-yl]phenol (three-letter code: EUG) (formula: $C_{10}H_{12}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 11 9 2	0	0
3	B	1	Total C O 11 9 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	14	Total O 14 14	0	0
4	B	24	Total O 24 24	0	0

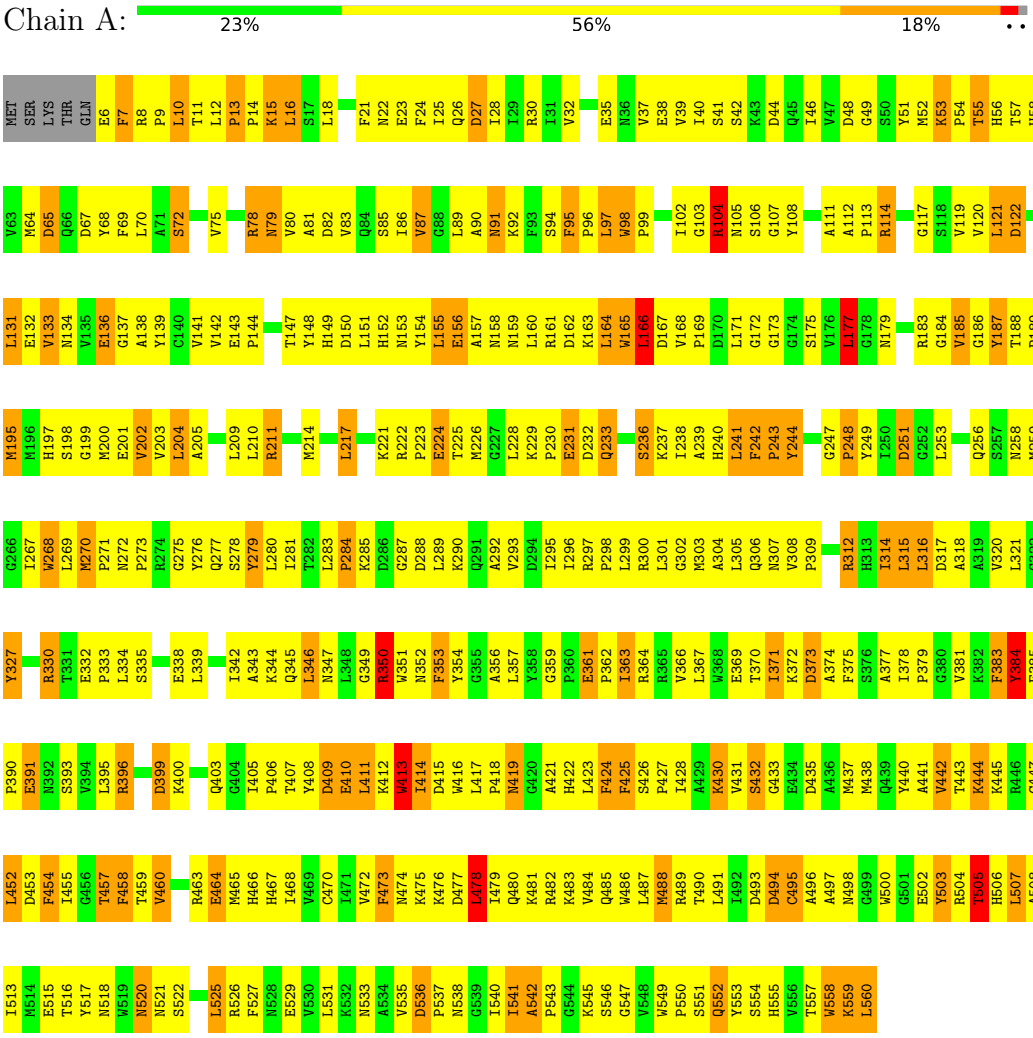
3 Residue-property plots (i)

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.

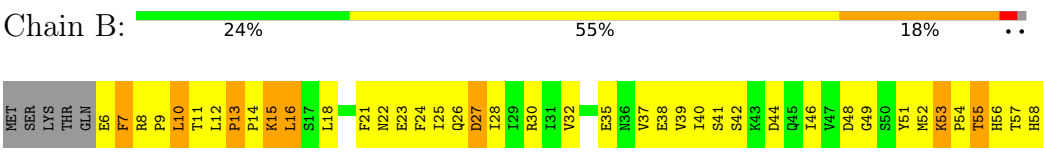
• Molecule 1: VANILLYL-ALCOHOL OXIDASE

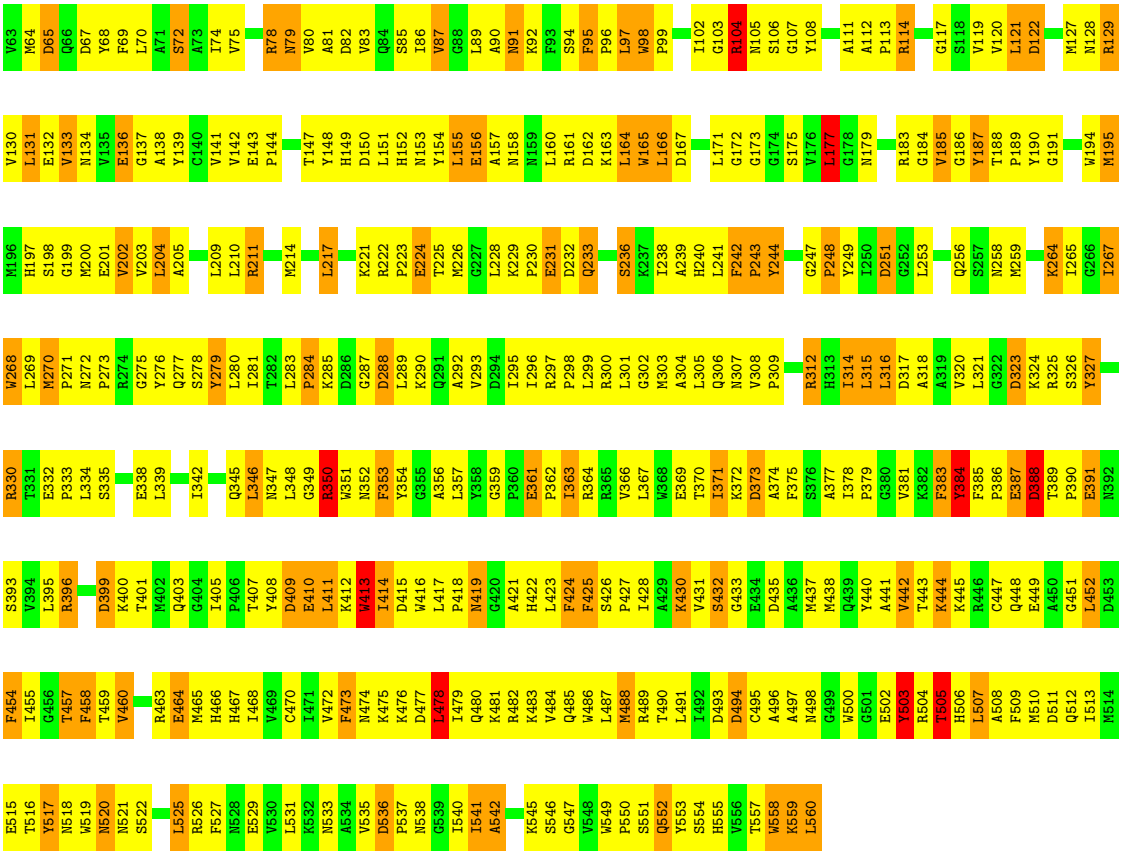
Chain A:



• Molecule 1: VANILLYL-ALCOHOL OXIDASE

Chain B:




V63 M64 D65 Q66 D67 Y68 F69 L70 A71 S72 A73 I74 V75 R78 N79 V80 A81 D82 V83 Q84 S85 I86 V87 G88 L89 A90 N91 K92 F93 S94 F95 P96 L97 W98 P99 I102 G103 R104 N105 S106 G107 Y108 A111 A112 P113 R114 G117 S118 V119 V120 L121 D122 M127 N128 R129
V130 L131 E132 V133 N134 V135 E136 G137 A138 Y139 C140 V141 V142 E143 P144 T147 Y148 H149 D150 L151 H152 N153 Y154 L155 E156 A157 N158 N159 L160 R161 D162 K163 L164 W165 L166 D167 L171 G172 G173 G174 S175 V176 L177 G178 N179 R183 G184 V185 G186 Y187 T188 P189 Y190 G191 W194 M195
M196 H197 S198 G199 M200 E201 V202 V203 L204 A205 L209 L210 R211 M214 L217 K221 R222 P223 E224 T225 M226 G227 L228 K229 P230 E231 D232 Q233 S236 K237 I238 A239 H240 L241 F242 P243 Y244 G247 P248 Y249 I250 D251 G252 L253 Q256 S257 N258 M259 K264 I265 G266 I267
W268 L269 M270 P271 N272 P273 R274 G275 Y276 Q277 S278 Y279 L280 I281 T282 L283 P284 K285 D286 G287 D288 L289 K290 Q291 A292 V293 D294 I295 I296 R297 P298 L299 R300 L301 G302 M303 A304 L305 Q306 N307 V308 P309 R312 H313 I314 L315 L316 D317 A318 A319 V320 L321 G322 D323 K324 R325 S326 Y327
R330 T331 E332 P333 L334 S335 E338 L339 I342 Q345 L346 N347 L348 G349 R350 W351 N352 F353 Y354 G355 A356 L357 Y358 G359 P360 E361 P362 I363 R364 H365 V366 L367 W368 E369 T370 I371 K372 D373 A374 F375 S376 A377 I378 P379 G380 V381 K382 F383 Y384 F385 P386 E387 D388 T389 P390 E391 N392
S393 V394 L395 R396 D399 K400 T401 M402 Q403 G404 I405 P406 T407 Y408 D409 E410 L411 K412 W413 I414 D415 W416 L417 P418 N419 G420 A421 H422 L423 F424 F425 S426 P427 I428 A429 K430 V431 S432 G433 E434 D435 A436 M437 M438 Q439 Y440 A441 V442 T443 K444 K445 R446 C447 Q448 E449 A450 G451 L452 D453
F454 I455 G456 T457 F458 T459 V460 R463 E464 M465 H466 H467 I468 V469 C470 I471 V472 F473 N474 K475 K476 D477 L478 I479 Q480 K481 R482 K483 V484 Q485 W486 L487 M488 R489 T490 L491 I492 D493 D494 C495 A496 A497 N498 G499 W500 G501 E502 Y503 R504 T505 H506 L507 A508 F509 M510 D511 Q512 I513 M514
E515 T516 Y517 N518 W519 N520 N521 S522 L525 R526 F527 N528 E529 V530 L531 K532 N533 A534 V535 D536 P537 N538 G539 I540 I541 A542 K545 S546 G547 V548 W549 P550 S551 Q552 Y553 S554 H555 V556 T557 W558 K559 L560

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	128.38Å 128.38Å 130.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80	Depositor
% Data completeness (in resolution range)	90.6 (30.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
Refinement program	TNT 5E	Depositor
R, R_{free}	0.214 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8948	wwPDB-VP
Average B, all atoms (Å^2)	26.0	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: FAD, EUG

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	0.81	3/4511 (0.1%)	1.88	127/6131 (2.1%)
1	B	0.81	2/4511 (0.0%)	1.88	128/6131 (2.1%)
All	All	0.81	5/9022 (0.1%)	1.88	255/12262 (2.1%)

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

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	268	TRP	CB-CG	-5.99	1.39	1.50
1	B	156	GLU	CG-CD	5.97	1.60	1.51
1	B	268	TRP	CB-CG	-5.95	1.39	1.50
1	A	156	GLU	CG-CD	5.94	1.60	1.51
1	A	244	TYR	CB-CG	-5.03	1.44	1.51

All (255) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	560	LEU	CB-CG-CD2	-12.85	89.15	111.00
1	A	560	LEU	CB-CG-CD2	-12.83	89.19	111.00
1	B	16	LEU	CA-CB-CG	-11.58	88.66	115.30
1	A	16	LEU	CA-CB-CG	-11.56	88.70	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	495	CYS	CA-CB-SG	-11.13	93.97	114.00
1	A	495	CYS	CA-CB-SG	-11.12	93.98	114.00
1	A	177	LEU	CA-CB-CG	10.64	139.78	115.30
1	B	177	LEU	CA-CB-CG	10.63	139.74	115.30
1	B	505	THR	CB-CA-C	-10.48	83.30	111.60
1	A	505	THR	CB-CA-C	-10.48	83.31	111.60
1	A	411	LEU	CB-CA-C	-10.15	90.91	110.20
1	B	411	LEU	CB-CA-C	-10.15	90.92	110.20
1	A	122	ASP	CB-CG-OD1	10.10	127.39	118.30
1	B	122	ASP	CB-CG-OD1	10.07	127.37	118.30
1	A	366	VAL	CB-CA-C	-9.83	92.73	111.40
1	B	366	VAL	CB-CA-C	-9.81	92.75	111.40
1	B	452	LEU	CA-CB-CG	-9.61	93.19	115.30
1	A	452	LEU	CA-CB-CG	-9.60	93.21	115.30
1	A	202	VAL	CB-CA-C	-8.86	94.56	111.40
1	B	202	VAL	CB-CA-C	-8.86	94.56	111.40
1	A	316	LEU	CB-CG-CD2	-8.80	96.04	111.00
1	B	316	LEU	CB-CG-CD2	-8.77	96.08	111.00
1	B	460	VAL	CB-CA-C	8.74	128.02	111.40
1	A	460	VAL	CB-CA-C	8.72	127.96	111.40
1	B	97	LEU	CA-CB-CG	-8.52	95.70	115.30
1	A	97	LEU	CA-CB-CG	-8.51	95.73	115.30
1	A	129	ARG	N-CA-C	8.35	133.53	111.00
1	B	129	ARG	N-CA-C	8.34	133.51	111.00
1	B	518	ASN	N-CA-C	8.16	133.04	111.00
1	A	518	ASN	N-CA-C	8.15	133.01	111.00
1	B	457	THR	CB-CA-C	-8.01	89.97	111.60
1	A	457	THR	CB-CA-C	-8.01	89.98	111.60
1	B	242	PHE	C-N-CD	-7.86	103.32	120.60
1	A	242	PHE	C-N-CD	-7.85	103.34	120.60
1	B	142	VAL	CB-CA-C	-7.56	97.03	111.40
1	A	142	VAL	CB-CA-C	-7.54	97.08	111.40
1	B	244	TYR	CB-CA-C	-7.51	95.38	110.40
1	A	244	TYR	CB-CA-C	-7.49	95.42	110.40
1	B	473	PHE	N-CA-C	-7.44	90.92	111.00
1	A	473	PHE	N-CA-C	-7.42	90.95	111.00
1	B	558	TRP	N-CA-C	7.42	131.03	111.00
1	A	558	TRP	N-CA-C	7.40	130.97	111.00
1	A	162	ASP	CB-CA-C	7.38	125.17	110.40
1	B	162	ASP	CB-CA-C	7.38	125.17	110.40
1	A	195	MET	CA-CB-CG	-7.37	100.78	113.30
1	B	195	MET	CA-CB-CG	-7.37	100.77	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	350	ARG	NE-CZ-NH2	-7.31	116.65	120.30
1	A	432	SER	N-CA-CB	7.30	121.45	110.50
1	B	155	LEU	CA-CB-CG	-7.29	98.52	115.30
1	A	155	LEU	CA-CB-CG	-7.29	98.54	115.30
1	B	432	SER	N-CA-CB	7.29	121.43	110.50
1	A	350	ARG	NE-CZ-NH2	-7.27	116.66	120.30
1	B	419	ASN	N-CA-C	-7.15	91.70	111.00
1	A	121	LEU	CA-CB-CG	-7.15	98.86	115.30
1	B	121	LEU	CA-CB-CG	-7.15	98.86	115.30
1	A	44	ASP	CB-CA-C	7.14	124.67	110.40
1	A	327	TYR	CA-CB-CG	7.14	126.96	113.40
1	B	72	SER	N-CA-C	-7.14	91.73	111.00
1	A	419	ASN	N-CA-C	-7.13	91.74	111.00
1	B	44	ASP	CB-CA-C	7.12	124.65	110.40
1	A	511	ASP	CB-CG-OD1	-7.12	111.89	118.30
1	A	53	LYS	N-CA-CB	7.12	123.41	110.60
1	A	72	SER	N-CA-C	-7.12	91.79	111.00
1	B	327	TYR	CA-CB-CG	7.11	126.91	113.40
1	B	187	TYR	N-CA-C	7.09	130.16	111.00
1	B	53	LYS	N-CA-CB	7.09	123.36	110.60
1	A	187	TYR	N-CA-C	7.08	130.11	111.00
1	B	430	LYS	CB-CA-C	-7.05	96.29	110.40
1	B	511	ASP	CB-CG-OD1	-7.04	111.96	118.30
1	A	430	LYS	CB-CA-C	-7.03	96.33	110.40
1	A	268	TRP	CB-CA-C	-6.98	96.44	110.40
1	B	268	TRP	CB-CA-C	-6.97	96.45	110.40
1	B	131	LEU	CA-CB-CG	-6.97	99.27	115.30
1	B	114	ARG	CB-CG-CD	6.96	129.68	111.60
1	A	114	ARG	CB-CG-CD	6.95	129.68	111.60
1	A	131	LEU	CA-CB-CG	-6.95	99.32	115.30
1	A	330	ARG	N-CA-CB	-6.67	98.60	110.60
1	B	330	ARG	N-CA-CB	-6.65	98.62	110.60
1	B	267	ILE	CB-CA-C	-6.60	98.40	111.60
1	B	306	GLN	N-CA-C	6.59	128.80	111.00
1	A	267	ILE	CB-CA-C	-6.59	98.42	111.60
1	A	306	GLN	N-CA-C	6.59	128.79	111.00
1	B	371	ILE	CG1-CB-CG2	6.57	125.85	111.40
1	A	371	ILE	CG1-CB-CG2	6.57	125.84	111.40
1	A	494	ASP	CB-CA-C	-6.55	97.29	110.40
1	B	363	ILE	CB-CA-C	6.54	124.69	111.60
1	A	363	ILE	CB-CA-C	6.54	124.68	111.60
1	B	478	LEU	CB-CA-C	-6.54	97.77	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	494	ASP	CB-CA-C	-6.53	97.33	110.40
1	A	478	LEU	CB-CA-C	-6.53	97.80	110.20
1	B	130	VAL	N-CA-C	-6.50	93.46	111.00
1	A	130	VAL	N-CA-C	-6.49	93.47	111.00
1	B	241	LEU	CB-CA-C	-6.48	97.89	110.20
1	A	241	LEU	CB-CA-C	-6.47	97.90	110.20
1	A	414	ILE	CG1-CB-CG2	6.47	125.64	111.40
1	B	414	ILE	CG1-CB-CG2	6.47	125.64	111.40
1	A	62	HIS	N-CA-C	6.41	128.29	111.00
1	B	62	HIS	N-CA-C	6.38	128.22	111.00
1	B	87	VAL	CB-CA-C	-6.35	99.34	111.40
1	A	87	VAL	CB-CA-C	-6.34	99.35	111.40
1	A	164	LEU	N-CA-C	6.26	127.89	111.00
1	A	476	LYS	CB-CA-C	6.26	122.91	110.40
1	B	476	LYS	CB-CA-C	6.25	122.91	110.40
1	B	164	LEU	N-CA-C	6.25	127.88	111.00
1	A	384	TYR	CA-CB-CG	6.22	125.22	113.40
1	A	410	GLU	N-CA-C	6.21	127.78	111.00
1	B	384	TYR	CA-CB-CG	6.21	125.21	113.40
1	B	410	GLU	N-CA-C	6.19	127.70	111.00
1	A	396	ARG	CG-CD-NE	-6.18	98.81	111.80
1	B	396	ARG	CG-CD-NE	-6.17	98.85	111.80
1	A	185	VAL	CB-CA-C	-6.16	99.70	111.40
1	A	67	ASP	N-CA-CB	-6.15	99.53	110.60
1	B	67	ASP	N-CA-CB	-6.15	99.53	110.60
1	B	185	VAL	CB-CA-C	-6.15	99.72	111.40
1	A	304	ALA	N-CA-C	-6.14	94.43	111.00
1	B	304	ALA	N-CA-C	-6.14	94.43	111.00
1	A	541	ILE	CB-CA-C	-6.11	99.37	111.60
1	B	166	LEU	CB-CG-CD1	6.10	121.37	111.00
1	B	541	ILE	CB-CA-C	-6.09	99.42	111.60
1	A	166	LEU	CB-CG-CD1	6.08	121.34	111.00
1	A	155	LEU	CB-CA-C	-6.06	98.68	110.20
1	B	387	GLU	N-CA-CB	-6.05	99.70	110.60
1	A	452	LEU	N-CA-C	6.05	127.34	111.00
1	B	155	LEU	CB-CA-C	-6.05	98.70	110.20
1	A	387	GLU	N-CA-CB	-6.04	99.72	110.60
1	B	452	LEU	N-CA-C	6.04	127.31	111.00
1	B	425	PHE	CB-CA-C	6.04	122.48	110.40
1	A	425	PHE	CB-CA-C	6.03	122.46	110.40
1	B	231	GLU	CA-CB-CG	-6.01	100.17	113.40
1	A	231	GLU	CA-CB-CG	-6.01	100.19	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	442	VAL	CB-CA-C	-5.97	100.06	111.40
1	B	312	ARG	CB-CG-CD	-5.96	96.10	111.60
1	A	312	ARG	CB-CG-CD	-5.96	96.10	111.60
1	A	442	VAL	CB-CA-C	-5.96	100.08	111.40
1	A	10	LEU	CB-CA-C	-5.95	98.89	110.20
1	B	10	LEU	CB-CA-C	-5.95	98.90	110.20
1	B	473	PHE	CA-C-N	-5.88	104.26	117.20
1	A	473	PHE	CA-C-N	-5.88	104.27	117.20
1	B	525	LEU	CA-CB-CG	-5.87	101.79	115.30
1	A	525	LEU	CA-CB-CG	-5.86	101.83	115.30
1	B	312	ARG	N-CA-C	5.85	126.80	111.00
1	A	312	ARG	N-CA-C	5.85	126.78	111.00
1	B	177	LEU	CB-CA-C	5.84	121.30	110.20
1	B	204	LEU	CA-CB-CG	-5.84	101.86	115.30
1	A	177	LEU	CB-CA-C	5.83	121.28	110.20
1	B	301	LEU	CB-CG-CD1	5.83	120.92	111.00
1	A	204	LEU	CA-CB-CG	-5.83	101.90	115.30
1	A	301	LEU	CB-CG-CD1	5.83	120.90	111.00
1	A	228	LEU	CB-CG-CD2	-5.81	101.12	111.00
1	A	458	PHE	CB-CA-C	-5.80	98.79	110.40
1	B	228	LEU	CB-CG-CD2	-5.80	101.14	111.00
1	B	413	TRP	CA-CB-CG	5.79	124.69	113.70
1	B	458	PHE	CB-CA-C	-5.78	98.84	110.40
1	B	388	ASP	CB-CG-OD1	-5.78	113.10	118.30
1	A	413	TRP	CA-CB-CG	5.76	124.65	113.70
1	A	444	LYS	N-CA-CB	-5.76	100.23	110.60
1	B	444	LYS	N-CA-CB	-5.76	100.23	110.60
1	A	388	ASP	CB-CG-OD1	-5.75	113.12	118.30
1	B	323	ASP	CB-CG-OD1	-5.75	113.13	118.30
1	A	323	ASP	CB-CG-OD1	-5.72	113.15	118.30
1	B	432	SER	N-CA-C	-5.70	95.60	111.00
1	A	432	SER	N-CA-C	-5.69	95.63	111.00
1	B	350	ARG	N-CA-C	-5.67	95.68	111.00
1	A	350	ARG	N-CA-C	-5.67	95.69	111.00
1	A	536	ASP	C-N-CD	-5.67	108.12	120.60
1	B	536	ASP	C-N-CD	-5.66	108.15	120.60
1	A	49	GLY	N-CA-C	5.65	127.23	113.10
1	B	49	GLY	N-CA-C	5.64	127.21	113.10
1	A	270	MET	CA-CB-CG	-5.64	103.71	113.30
1	B	384	TYR	CB-CA-C	-5.64	99.12	110.40
1	A	259	MET	CA-CB-CG	-5.64	103.72	113.30
1	A	384	TYR	CB-CA-C	-5.64	99.13	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	270	MET	CA-CB-CG	-5.62	103.74	113.30
1	B	259	MET	CA-CB-CG	-5.62	103.75	113.30
1	A	511	ASP	CB-CG-OD2	5.60	123.34	118.30
1	B	211	ARG	NE-CZ-NH1	-5.59	117.50	120.30
1	A	211	ARG	NE-CZ-NH1	-5.59	117.50	120.30
1	B	315	LEU	CB-CG-CD2	-5.59	101.50	111.00
1	A	315	LEU	CB-CG-CD2	-5.59	101.50	111.00
1	A	383	PHE	N-CA-C	5.57	126.05	111.00
1	B	217	LEU	N-CA-C	-5.57	95.97	111.00
1	B	383	PHE	N-CA-C	5.57	126.03	111.00
1	A	217	LEU	N-CA-C	-5.56	96.00	111.00
1	A	129	ARG	CB-CA-C	-5.55	99.30	110.40
1	B	233	GLN	N-CA-CB	-5.55	100.62	110.60
1	A	233	GLN	N-CA-CB	-5.54	100.62	110.60
1	B	129	ARG	CB-CA-C	-5.54	99.32	110.40
1	A	98	TRP	CA-CB-CG	-5.53	103.19	113.70
1	A	165	TRP	N-CA-C	5.53	125.94	111.00
1	B	98	TRP	CA-CB-CG	-5.52	103.21	113.70
1	B	165	TRP	N-CA-C	5.50	125.86	111.00
1	B	384	TYR	N-CA-C	5.49	125.82	111.00
1	A	384	TYR	N-CA-C	5.49	125.81	111.00
1	B	511	ASP	CB-CG-OD2	5.48	123.23	118.30
1	A	558	TRP	CA-CB-CG	-5.46	103.33	113.70
1	B	558	TRP	CA-CB-CG	-5.45	103.34	113.70
1	A	504	ARG	NE-CZ-NH2	5.44	123.02	120.30
1	B	104	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	B	430	LYS	CB-CG-CD	-5.43	97.48	111.60
1	A	430	LYS	CB-CG-CD	-5.42	97.50	111.60
1	A	104	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	264	LYS	CB-CA-C	-5.40	99.60	110.40
1	B	264	LYS	CB-CA-C	-5.38	99.63	110.40
1	B	204	LEU	CB-CA-C	-5.37	99.99	110.20
1	A	204	LEU	CB-CA-C	-5.37	100.00	110.20
1	A	7	PHE	N-CA-C	5.35	125.44	111.00
1	A	204	LEU	CB-CG-CD2	-5.35	101.91	111.00
1	A	236	SER	N-CA-CB	-5.35	102.48	110.50
1	B	7	PHE	N-CA-C	5.33	125.41	111.00
1	B	204	LEU	CB-CG-CD2	-5.33	101.94	111.00
1	B	504	ARG	NE-CZ-NH2	5.33	122.97	120.30
1	B	454	PHE	N-CA-C	-5.32	96.63	111.00
1	A	454	PHE	N-CA-C	-5.31	96.67	111.00
1	B	236	SER	N-CA-CB	-5.31	102.54	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	452	LEU	CB-CA-C	-5.29	100.14	110.20
1	B	452	LEU	CB-CA-C	-5.29	100.16	110.20
1	A	507	LEU	CB-CA-C	-5.26	100.21	110.20
1	B	279	TYR	CB-CG-CD1	-5.25	117.85	121.00
1	B	507	LEU	CB-CA-C	-5.23	100.27	110.20
1	A	279	TYR	CB-CG-CD1	-5.20	117.88	121.00
1	B	560	LEU	CB-CG-CD1	5.19	119.83	111.00
1	A	560	LEU	CB-CG-CD1	5.19	119.82	111.00
1	B	346	LEU	N-CA-C	5.18	124.98	111.00
1	B	11	THR	CB-CA-C	-5.16	97.66	111.60
1	A	346	LEU	N-CA-C	5.16	124.94	111.00
1	A	11	THR	CB-CA-C	-5.15	97.69	111.60
1	B	13	PRO	N-CA-C	-5.15	98.70	112.10
1	A	55	THR	N-CA-CB	5.14	120.07	110.30
1	A	211	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	A	13	PRO	N-CA-C	-5.13	98.75	112.10
1	B	399	ASP	CB-CG-OD2	5.13	122.92	118.30
1	B	55	THR	N-CA-CB	5.12	120.03	110.30
1	B	503	TYR	CB-CG-CD1	5.12	124.07	121.00
1	B	211	ARG	NE-CZ-NH2	5.11	122.86	120.30
1	B	133	VAL	N-CA-C	-5.10	97.22	111.00
1	A	121	LEU	CB-CG-CD1	-5.10	102.34	111.00
1	A	133	VAL	N-CA-C	-5.10	97.24	111.00
1	B	121	LEU	CB-CG-CD1	-5.09	102.34	111.00
1	A	353	PHE	N-CA-C	5.08	124.72	111.00
1	B	353	PHE	N-CA-C	5.08	124.71	111.00
1	A	399	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	503	TYR	CB-CG-CD1	5.07	124.04	121.00
1	B	424	PHE	CB-CA-C	-5.06	100.28	110.40
1	A	424	PHE	CB-CA-C	-5.06	100.29	110.40
1	A	156	GLU	OE1-CD-OE2	-5.05	117.24	123.30
1	A	453	ASP	CB-CG-OD1	-5.04	113.76	118.30
1	B	209	LEU	CB-CG-CD2	-5.04	102.43	111.00
1	B	15	LYS	N-CA-CB	-5.04	101.53	110.60
1	A	15	LYS	N-CA-CB	-5.04	101.54	110.60
1	A	209	LEU	CB-CG-CD2	-5.03	102.45	111.00
1	B	165	TRP	CA-C-N	-5.02	106.15	117.20
1	B	156	GLU	OE1-CD-OE2	-5.02	117.28	123.30
1	B	288	ASP	CB-CA-C	5.01	120.42	110.40
1	B	401	THR	CB-CA-C	5.01	125.12	111.60
1	A	165	TRP	CA-C-N	-5.00	106.19	117.20

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	363	ILE	CA
1	A	410	GLU	CA
1	B	363	ILE	CA
1	B	410	GLU	CA

There are no planarity outliers.

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	4391	0	4330	550	0
1	B	4391	0	4330	552	0
2	A	53	0	31	17	0
2	B	53	0	31	18	0
3	A	11	0	7	4	0
3	B	11	0	7	5	0
4	A	14	0	0	2	0
4	B	24	0	0	0	0
All	All	8948	0	8736	1088	0

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 63.

All (1088) 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:422:HIS:NE2	2:B:600:FAD:HM81	1.45	1.12
1:A:422:HIS:NE2	2:A:600:FAD:HM82	1.42	1.10
2:B:600:FAD:H51A	2:B:600:FAD:H8A	1.27	1.08
1:A:422:HIS:NE2	2:A:600:FAD:HM81	1.45	1.08
2:A:600:FAD:H8A	2:A:600:FAD:H51A	1.27	1.08
1:B:422:HIS:NE2	2:B:600:FAD:HM82	1.42	1.08
1:B:550:PRO:HB2	1:B:552:GLN:HE21	1.18	1.08
1:A:253:LEU:HD21	1:B:253:LEU:HD21	1.31	1.07
1:B:177:LEU:HD22	1:B:265:ILE:HG22	1.35	1.07
1:A:177:LEU:HD22	1:A:265:ILE:HG22	1.35	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:PRO:HB2	1:A:552:GLN:HE21	1.18	1.05
1:B:361:GLU:N	1:B:364:ARG:HH21	1.57	1.02
1:A:422:HIS:CE1	2:A:600:FAD:HM81	1.95	1.01
1:A:361:GLU:N	1:A:364:ARG:HH21	1.57	1.01
1:B:422:HIS:CE1	2:B:600:FAD:HM81	1.95	1.00
1:A:422:HIS:CE1	2:A:600:FAD:C8M	2.46	0.99
1:B:422:HIS:CE1	2:B:600:FAD:C8M	2.46	0.98
1:A:133:VAL:HG21	1:A:154:TYR:CE1	2.00	0.97
1:B:133:VAL:HG21	1:B:154:TYR:CE1	2.00	0.97
1:A:422:HIS:CD2	2:A:600:FAD:HM82	2.02	0.94
1:B:422:HIS:CD2	2:B:600:FAD:HM82	2.02	0.93
1:B:78:ARG:HD3	1:B:82:ASP:OD2	1.69	0.93
1:B:40:ILE:HD11	1:B:57:THR:HG22	1.50	0.92
1:A:478:LEU:HD12	1:A:478:LEU:H	1.35	0.92
1:A:40:ILE:HD11	1:A:57:THR:HG22	1.50	0.91
1:A:78:ARG:HD3	1:A:82:ASP:OD2	1.69	0.91
1:B:419:ASN:O	1:B:474:ASN:HA	1.71	0.90
1:A:419:ASN:O	1:A:474:ASN:HA	1.71	0.90
1:B:478:LEU:HD12	1:B:478:LEU:H	1.35	0.90
1:B:56:HIS:HA	1:B:111:ALA:CB	2.03	0.89
1:A:91:ASN:ND2	1:A:538:ASN:HD22	1.71	0.88
1:A:300:ARG:HH21	1:A:308:VAL:HA	1.37	0.88
1:B:205:ALA:HA	1:B:541:ILE:HD11	1.56	0.88
1:A:205:ALA:HA	1:A:541:ILE:HD11	1.55	0.88
1:A:56:HIS:HA	1:A:111:ALA:CB	2.03	0.87
1:B:91:ASN:ND2	1:B:538:ASN:HD22	1.71	0.87
1:B:555:HIS:CG	1:B:559:LYS:HE3	2.09	0.87
1:A:443:THR:HA	1:A:491:LEU:HD21	1.57	0.86
1:A:555:HIS:CG	1:A:559:LYS:HE3	2.09	0.86
1:B:443:THR:HA	1:B:491:LEU:HD21	1.57	0.86
1:B:300:ARG:HH21	1:B:308:VAL:HA	1.37	0.86
1:A:457:THR:HG22	1:A:458:PHE:H	1.39	0.85
1:B:423:LEU:HD21	1:B:488:MET:HG3	1.57	0.85
1:B:457:THR:HG22	1:B:458:PHE:H	1.39	0.84
1:A:423:LEU:HD21	1:A:488:MET:HG3	1.57	0.84
2:A:600:FAD:H8A	2:A:600:FAD:C5B	2.08	0.84
1:A:431:VAL:HG22	1:A:465:MET:HG3	1.60	0.83
1:A:425:PHE:HB2	1:A:488:MET:CE	2.09	0.83
1:B:550:PRO:HB2	1:B:552:GLN:NE2	1.94	0.82
2:B:600:FAD:H8A	2:B:600:FAD:C5B	2.08	0.82
1:A:40:ILE:CD1	1:A:57:THR:HG22	2.10	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:550:PRO:CB	1:B:552:GLN:HE21	1.93	0.81
1:A:247:GLY:O	1:B:183:ARG:NH2	2.12	0.81
1:B:431:VAL:HG22	1:B:465:MET:HG3	1.60	0.81
1:B:425:PHE:HB2	1:B:488:MET:CE	2.09	0.81
1:A:459:THR:OG1	1:A:466:HIS:HB2	1.81	0.81
1:A:505:THR:HG22	1:A:506:HIS:H	1.45	0.81
1:A:156:GLU:HG3	1:A:161:ARG:CZ	2.10	0.80
1:A:550:PRO:CB	1:A:552:GLN:HE21	1.94	0.80
1:B:40:ILE:CD1	1:B:57:THR:HG22	2.10	0.80
1:B:505:THR:HG22	1:B:506:HIS:H	1.45	0.80
1:A:275:GLY:HA3	1:A:359:GLY:O	1.81	0.80
1:A:295:ILE:O	1:A:298:PRO:HD2	1.81	0.80
1:B:156:GLU:HG3	1:B:161:ARG:CZ	2.11	0.80
1:B:277:GLN:HB3	1:B:357:LEU:HD12	1.62	0.80
1:A:277:GLN:HB3	1:A:357:LEU:HD12	1.62	0.80
1:B:295:ILE:O	1:B:298:PRO:HD2	1.81	0.80
1:B:459:THR:OG1	1:B:466:HIS:HB2	1.81	0.80
1:A:550:PRO:HB2	1:A:552:GLN:NE2	1.94	0.79
2:A:600:FAD:H51A	2:A:600:FAD:C8A	2.11	0.79
1:B:10:LEU:HD11	1:B:42:SER:HA	1.64	0.79
1:A:57:THR:O	1:A:70:LEU:HD12	1.83	0.79
1:A:378:ILE:O	1:A:381:VAL:HB	1.83	0.79
1:B:361:GLU:O	1:B:361:GLU:HG3	1.77	0.79
1:B:275:GLY:HA3	1:B:359:GLY:O	1.81	0.79
1:B:414:ILE:HD11	2:B:600:FAD:HM71	1.64	0.79
1:A:94:SER:HA	1:A:540:ILE:HD11	1.66	0.78
1:B:57:THR:O	1:B:70:LEU:HD12	1.83	0.78
1:B:378:ILE:O	1:B:381:VAL:HB	1.83	0.78
1:B:48:ASP:OD1	1:B:60:PRO:HA	1.84	0.78
1:A:377:ALA:O	1:A:379:PRO:HD3	1.84	0.78
1:A:414:ILE:HD11	2:A:600:FAD:HM71	1.64	0.78
1:A:132:GLU:HG2	1:A:133:VAL:N	1.99	0.78
1:A:10:LEU:HD11	1:A:42:SER:HA	1.64	0.77
1:A:85:SER:O	1:A:89:LEU:HD13	1.85	0.77
1:A:479:ILE:O	1:A:483:LYS:HG3	1.84	0.77
1:B:377:ALA:O	1:B:379:PRO:HD3	1.84	0.77
1:B:134:ASN:OD1	1:B:137:GLY:N	2.17	0.77
1:A:361:GLU:O	1:A:361:GLU:HG3	1.77	0.77
1:B:132:GLU:HG2	1:B:133:VAL:N	1.99	0.77
1:A:32:VAL:HA	1:A:78:ARG:HD2	1.67	0.77
1:B:56:HIS:HA	1:B:111:ALA:HB1	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:479:ILE:O	1:B:483:LYS:HG3	1.84	0.77
1:A:507:LEU:HD23	1:A:510:MET:HE3	1.67	0.77
1:B:85:SER:O	1:B:89:LEU:HD13	1.85	0.77
2:B:600:FAD:H51A	2:B:600:FAD:C8A	2.11	0.76
1:A:357:LEU:HB3	1:A:364:ARG:HG2	1.66	0.76
1:A:48:ASP:OD1	1:A:60:PRO:HA	1.84	0.76
1:A:102:ILE:HG12	1:A:175:SER:HB2	1.68	0.76
1:B:357:LEU:HB3	1:B:364:ARG:HG2	1.66	0.76
1:A:425:PHE:HB2	1:A:488:MET:HE1	1.66	0.76
1:B:94:SER:HA	1:B:540:ILE:HD11	1.66	0.76
1:A:56:HIS:HA	1:A:111:ALA:HB1	1.66	0.76
1:B:507:LEU:HD23	1:B:510:MET:HE3	1.68	0.75
1:A:134:ASN:OD1	1:A:137:GLY:N	2.17	0.75
1:A:183:ARG:NH2	1:B:247:GLY:O	2.20	0.75
1:A:443:THR:HA	1:A:491:LEU:CD2	2.17	0.75
1:B:32:VAL:HA	1:B:78:ARG:HD2	1.67	0.75
1:B:443:THR:HA	1:B:491:LEU:CD2	2.17	0.75
1:A:248:PRO:HD3	1:B:256:GLN:O	1.87	0.74
1:A:423:LEU:HD21	1:A:488:MET:CG	2.16	0.74
1:A:244:TYR:OH	1:B:195:MET:HG3	1.86	0.74
1:B:423:LEU:HD21	1:B:488:MET:CG	2.16	0.74
1:A:79:ASN:HD21	1:A:81:ALA:HB3	1.52	0.74
1:A:527:PHE:CE2	1:A:531:LEU:HD11	2.23	0.74
1:B:79:ASN:HD21	1:B:81:ALA:HB3	1.52	0.74
1:B:527:PHE:CE2	1:B:531:LEU:HD11	2.23	0.74
2:B:600:FAD:N5	3:B:601:EUG:H7	2.02	0.74
2:A:600:FAD:N5	3:A:601:EUG:H7	2.02	0.74
1:B:385:PHE:HB3	1:B:386:PRO:HD2	1.70	0.74
1:A:284:PRO:HD2	1:A:288:ASP:OD2	1.87	0.73
1:B:361:GLU:N	1:B:364:ARG:NH2	2.36	0.73
1:B:507:LEU:HA	1:B:510:MET:CE	2.18	0.73
1:B:284:PRO:HD2	1:B:288:ASP:OD2	1.87	0.73
1:A:244:TYR:CD2	1:B:183:ARG:HD2	2.23	0.73
1:B:419:ASN:H	1:B:474:ASN:ND2	1.86	0.73
1:B:102:ILE:HG12	1:B:175:SER:HB2	1.68	0.73
1:A:339:LEU:HD12	1:A:350:ARG:CZ	2.19	0.73
1:A:205:ALA:CA	1:A:541:ILE:HD11	2.19	0.73
1:A:507:LEU:HA	1:A:510:MET:CE	2.18	0.73
1:A:487:LEU:HD11	1:A:491:LEU:HD11	1.70	0.73
1:B:102:ILE:CG1	1:B:175:SER:HB2	2.19	0.73
1:A:102:ILE:CG1	1:A:175:SER:HB2	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:ASN:H	1:A:474:ASN:ND2	1.86	0.72
1:B:52:MET:O	1:B:53:LYS:HG3	1.90	0.72
1:A:187:TYR:O	1:A:307:ASN:HB2	1.89	0.72
1:B:187:TYR:O	1:B:307:ASN:HB2	1.89	0.72
1:A:487:LEU:HG	1:A:491:LEU:HD12	1.72	0.72
1:B:96:PRO:O	1:B:97:LEU:HD23	1.89	0.72
1:B:425:PHE:CZ	1:B:427:PRO:HG3	2.25	0.72
1:A:418:PRO:HD2	1:A:474:ASN:HD22	1.53	0.72
1:B:312:ARG:HH22	1:B:410:GLU:CD	1.93	0.72
1:B:223:PRO:HG2	1:B:224:GLU:OE2	1.89	0.72
1:B:418:PRO:HD2	1:B:474:ASN:HD22	1.53	0.72
1:B:487:LEU:HD11	1:B:491:LEU:HD11	1.71	0.72
1:A:425:PHE:CZ	1:A:427:PRO:HG3	2.25	0.72
1:B:339:LEU:HD12	1:B:350:ARG:CZ	2.19	0.72
1:A:223:PRO:HG2	1:A:224:GLU:OE2	1.89	0.71
1:A:550:PRO:HG2	1:A:553:TYR:CD1	2.26	0.71
1:B:205:ALA:CA	1:B:541:ILE:HD11	2.19	0.71
1:B:13:PRO:HG2	1:B:16:LEU:HB2	1.72	0.71
1:A:183:ARG:HD2	1:B:244:TYR:CD2	2.26	0.71
2:B:600:FAD:C5X	3:B:601:EUG:H7	2.21	0.71
1:B:217:LEU:O	1:B:236:SER:HB2	1.91	0.71
1:A:52:MET:O	1:A:53:LYS:HG3	1.90	0.71
1:A:96:PRO:O	1:A:97:LEU:HD23	1.89	0.71
1:A:217:LEU:O	1:A:236:SER:HB2	1.91	0.71
1:A:238:ILE:HG21	1:B:428:ILE:HG21	1.72	0.71
1:A:299:LEU:HB2	1:A:305:LEU:HD12	1.72	0.71
1:A:385:PHE:HB3	1:A:386:PRO:HD2	1.70	0.71
1:B:18:LEU:HD12	1:B:21:PHE:HB3	1.73	0.71
1:B:309:PRO:HG2	1:B:460:VAL:HB	1.73	0.71
2:A:600:FAD:C5X	3:A:601:EUG:H7	2.21	0.71
1:B:55:THR:HG21	1:B:58:HIS:CE1	2.26	0.71
1:B:61:HIS:ND1	1:B:422:HIS:ND1	2.39	0.71
1:A:21:PHE:O	1:A:25:ILE:HG22	1.91	0.70
1:A:309:PRO:HG2	1:A:460:VAL:HB	1.73	0.70
1:B:200:MET:HE1	1:B:251:ASP:HB3	1.73	0.70
1:B:487:LEU:HG	1:B:491:LEU:HD12	1.72	0.70
1:B:21:PHE:O	1:B:25:ILE:HG22	1.91	0.70
1:B:391:GLU:HA	1:B:396:ARG:HD2	1.73	0.70
1:B:550:PRO:HG2	1:B:553:TYR:CD1	2.26	0.70
1:B:292:ALA:O	1:B:296:ILE:HG13	1.91	0.70
1:A:312:ARG:HH22	1:A:410:GLU:CD	1.93	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:LEU:HB2	1:B:305:LEU:HD12	1.72	0.70
1:A:391:GLU:HA	1:A:396:ARG:HD2	1.73	0.70
1:B:507:LEU:HA	1:B:510:MET:HE3	1.73	0.70
1:A:61:HIS:ND1	1:A:422:HIS:ND1	2.39	0.69
1:B:422:HIS:CE1	2:B:600:FAD:HM82	2.21	0.69
1:A:292:ALA:O	1:A:296:ILE:HG13	1.91	0.69
1:A:361:GLU:N	1:A:364:ARG:NH2	2.35	0.69
1:A:13:PRO:HG2	1:A:16:LEU:HB2	1.72	0.69
1:A:59:ASP:N	1:A:112:ALA:HB2	2.07	0.69
1:A:419:ASN:N	1:A:474:ASN:ND2	2.40	0.69
1:B:59:ASP:N	1:B:112:ALA:HB2	2.07	0.69
1:A:55:THR:HG21	1:A:58:HIS:CE1	2.26	0.69
1:B:214:MET:HB2	1:B:239:ALA:HA	1.74	0.69
1:A:164:LEU:HD23	1:A:271:PRO:HA	1.74	0.69
1:B:426:SER:N	1:B:427:PRO:HD3	2.08	0.69
1:B:464:GLU:HG2	1:B:465:MET:N	2.08	0.69
1:A:18:LEU:HD12	1:A:21:PHE:HB3	1.73	0.69
1:A:195:MET:HG3	1:B:244:TYR:OH	1.93	0.68
1:B:419:ASN:N	1:B:474:ASN:ND2	2.40	0.68
1:A:222:ARG:HB2	1:A:223:PRO:HD2	1.74	0.68
1:A:297:ARG:HB3	1:A:298:PRO:HD3	1.75	0.68
1:B:494:ASP:O	1:B:498:ASN:ND2	2.26	0.68
1:A:61:HIS:CE1	1:A:422:HIS:HD1	2.11	0.68
1:A:200:MET:HE1	1:A:251:ASP:HB3	1.74	0.68
1:A:464:GLU:HG2	1:A:465:MET:N	2.08	0.68
1:B:48:ASP:OD1	1:B:58:HIS:NE2	2.24	0.68
1:B:61:HIS:CE1	1:B:422:HIS:HD1	2.11	0.68
1:B:502:GLU:N	1:B:502:GLU:OE1	2.26	0.68
1:B:222:ARG:HB2	1:B:223:PRO:HD2	1.74	0.68
1:B:297:ARG:HB3	1:B:298:PRO:HD3	1.75	0.68
1:B:316:LEU:O	1:B:320:VAL:HG23	1.94	0.68
1:A:214:MET:HB2	1:A:239:ALA:HA	1.74	0.68
1:A:427:PRO:HD2	1:A:467:HIS:O	1.93	0.68
1:B:164:LEU:HD23	1:B:271:PRO:HA	1.74	0.68
1:B:427:PRO:HD2	1:B:467:HIS:O	1.93	0.68
1:A:316:LEU:O	1:A:320:VAL:HG23	1.94	0.68
1:A:494:ASP:O	1:A:498:ASN:ND2	2.26	0.68
1:A:502:GLU:N	1:A:502:GLU:OE1	2.26	0.68
1:A:324:LYS:HA	1:A:416:TRP:CH2	2.29	0.68
1:B:112:ALA:O	1:B:507:LEU:HD11	1.94	0.67
1:A:506:HIS:CE1	1:A:508:ALA:H	2.13	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:THR:O	1:A:150:ASP:HB2	1.95	0.67
1:A:200:MET:CE	1:A:251:ASP:HB3	2.25	0.67
1:A:426:SER:N	1:A:427:PRO:HD3	2.08	0.67
1:B:147:THR:O	1:B:150:ASP:HB2	1.95	0.67
1:B:324:LYS:HA	1:B:416:TRP:CH2	2.29	0.67
1:B:425:PHE:HB2	1:B:488:MET:HE1	1.75	0.67
1:A:112:ALA:O	1:A:507:LEU:HD11	1.94	0.67
1:A:507:LEU:HA	1:A:510:MET:HE3	1.74	0.67
1:B:9:PRO:HG3	1:B:21:PHE:CZ	2.30	0.67
1:B:425:PHE:HB2	1:B:488:MET:HE3	1.77	0.67
1:A:522:SER:O	1:A:526:ARG:HG2	1.95	0.66
1:B:152:HIS:CE1	1:B:161:ARG:HH21	2.13	0.66
1:A:238:ILE:HG21	1:B:428:ILE:CG2	2.25	0.66
1:B:205:ALA:HB2	1:B:541:ILE:HD12	1.77	0.66
1:B:295:ILE:HD12	1:B:378:ILE:HD11	1.77	0.66
1:B:486:TRP:O	1:B:490:THR:OG1	2.14	0.66
1:B:506:HIS:CE1	1:B:508:ALA:H	2.12	0.66
1:B:522:SER:O	1:B:526:ARG:HG2	1.95	0.66
1:A:9:PRO:HG3	1:A:21:PHE:CZ	2.30	0.66
1:A:95:PHE:HD1	1:A:96:PRO:CD	2.09	0.66
1:A:457:THR:CG2	1:A:458:PHE:H	2.01	0.66
1:B:351:TRP:O	1:B:352:ASN:ND2	2.29	0.66
1:A:422:HIS:CE1	2:A:600:FAD:HM82	2.21	0.66
1:B:200:MET:CE	1:B:251:ASP:HB3	2.25	0.66
1:B:95:PHE:HD1	1:B:96:PRO:CD	2.09	0.66
1:B:95:PHE:O	1:B:540:ILE:HD12	1.96	0.66
1:B:270:MET:CG	1:B:271:PRO:HD2	2.26	0.66
1:B:283:LEU:HB2	1:B:351:TRP:HB2	1.78	0.66
1:A:205:ALA:HB2	1:A:541:ILE:HD12	1.77	0.65
1:A:486:TRP:O	1:A:490:THR:OG1	2.14	0.65
1:A:479:ILE:HG22	1:A:483:LYS:CE	2.27	0.65
1:B:289:LEU:HD23	1:B:437:MET:SD	2.37	0.65
1:A:95:PHE:O	1:A:540:ILE:HD12	1.96	0.65
1:A:270:MET:CG	1:A:271:PRO:HD2	2.26	0.65
1:A:152:HIS:CE1	1:A:161:ARG:HH21	2.13	0.65
1:A:289:LEU:HD23	1:A:437:MET:SD	2.37	0.65
1:A:479:ILE:HG22	1:A:483:LYS:HE3	1.77	0.65
1:A:295:ILE:HD12	1:A:378:ILE:HD11	1.77	0.65
1:A:351:TRP:O	1:A:352:ASN:ND2	2.29	0.65
1:B:149:HIS:O	1:B:153:ASN:ND2	2.29	0.65
1:B:425:PHE:C	1:B:427:PRO:HD3	2.17	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:GLU:CD	1:A:224:GLU:H	2.01	0.65
1:B:224:GLU:CD	1:B:224:GLU:H	2.01	0.64
1:A:312:ARG:NH2	1:A:410:GLU:OE2	2.30	0.64
1:A:555:HIS:CB	1:A:559:LYS:HE3	2.27	0.64
1:B:312:ARG:NH2	1:B:410:GLU:OE2	2.30	0.64
1:B:479:ILE:HG22	1:B:483:LYS:CE	2.27	0.64
1:A:425:PHE:CD1	1:A:488:MET:HE1	2.33	0.64
1:B:91:ASN:HD22	1:B:538:ASN:HD22	1.45	0.64
1:A:95:PHE:HD1	1:A:96:PRO:N	1.96	0.64
1:A:108:TYR:O	1:A:506:HIS:HA	1.98	0.64
1:A:283:LEU:HB2	1:A:351:TRP:HB2	1.78	0.64
1:B:506:HIS:ND1	1:B:508:ALA:N	2.39	0.64
1:B:550:PRO:HG2	1:B:553:TYR:HD1	1.62	0.64
1:B:95:PHE:HD1	1:B:96:PRO:N	1.96	0.64
1:B:151:LEU:HD12	1:B:151:LEU:O	1.98	0.64
1:B:555:HIS:CB	1:B:559:LYS:HE3	2.27	0.64
1:A:91:ASN:HD22	1:A:538:ASN:HD22	1.45	0.64
1:A:149:HIS:O	1:A:153:ASN:ND2	2.30	0.63
1:A:269:LEU:O	1:B:463:ARG:NH2	2.31	0.63
1:A:425:PHE:C	1:A:427:PRO:HD3	2.17	0.63
1:A:555:HIS:HB3	1:A:559:LYS:HE3	1.80	0.63
1:B:309:PRO:HB2	1:B:353:PHE:CE1	2.33	0.63
1:B:479:ILE:HG22	1:B:483:LYS:HE3	1.77	0.63
1:A:309:PRO:HB2	1:A:353:PHE:CE1	2.33	0.63
1:B:349:GLY:H	1:B:352:ASN:HD21	1.47	0.63
1:B:425:PHE:CD1	1:B:488:MET:HE1	2.32	0.63
1:B:411:LEU:O	1:B:414:ILE:HB	1.99	0.63
1:A:48:ASP:OD1	1:A:58:HIS:NE2	2.24	0.63
1:A:151:LEU:HD12	1:A:151:LEU:O	1.98	0.63
1:A:559:LYS:O	1:A:560:LEU:HG	1.99	0.63
1:B:393:SER:OG	1:B:396:ARG:HG3	1.99	0.63
1:A:197:HIS:HB2	1:A:265:ILE:HD11	1.81	0.63
1:A:349:GLY:H	1:A:352:ASN:HD21	1.47	0.63
1:A:185:VAL:HG12	1:A:186:GLY:N	2.15	0.62
1:B:79:ASN:HD22	1:B:81:ALA:H	1.46	0.62
1:A:79:ASN:HD22	1:A:81:ALA:H	1.46	0.62
1:A:256:GLN:O	1:B:248:PRO:HD3	1.98	0.62
1:A:393:SER:OG	1:A:396:ARG:HG3	1.99	0.62
1:B:555:HIS:HB3	1:B:559:LYS:HE3	1.80	0.62
1:B:108:TYR:O	1:B:506:HIS:HA	1.98	0.62
1:A:411:LEU:O	1:A:414:ILE:HB	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:LYS:HA	1:B:416:TRP:CZ3	2.34	0.62
1:B:559:LYS:O	1:B:560:LEU:HG	1.99	0.62
1:B:10:LEU:HD11	1:B:42:SER:CA	2.30	0.62
1:B:24:PHE:CE1	1:B:28:ILE:HD12	2.34	0.62
1:B:280:LEU:HB2	1:B:395:LEU:HD13	1.81	0.62
1:A:24:PHE:CE1	1:A:28:ILE:HD12	2.34	0.62
1:A:148:TYR:HB2	1:A:172:GLY:O	2.00	0.62
1:B:167:ASP:OD1	1:B:186:GLY:HA3	2.00	0.62
1:A:315:LEU:HA	1:A:318:ALA:HB3	1.82	0.62
1:A:550:PRO:HG2	1:A:553:TYR:HD1	1.62	0.62
1:B:13:PRO:HG3	1:B:95:PHE:CE1	2.35	0.62
1:B:148:TYR:HB2	1:B:172:GLY:O	2.00	0.62
1:B:197:HIS:HB2	1:B:265:ILE:HD11	1.81	0.62
1:A:280:LEU:HB2	1:A:395:LEU:HD13	1.81	0.61
1:A:506:HIS:ND1	1:A:508:ALA:N	2.39	0.61
1:B:6:GLU:N	1:B:39:VAL:HG21	2.15	0.61
1:B:189:PRO:HA	1:B:307:ASN:HA	1.82	0.61
1:A:13:PRO:HG3	1:A:95:PHE:CE1	2.35	0.61
1:A:485:GLN:O	1:A:489:ARG:HG3	2.00	0.61
1:B:285:LYS:O	1:B:288:ASP:HB2	2.00	0.61
1:A:6:GLU:N	1:A:39:VAL:HG21	2.15	0.61
1:B:485:GLN:O	1:B:489:ARG:HG3	2.00	0.61
1:A:167:ASP:OD1	1:A:186:GLY:HA3	2.00	0.61
1:A:189:PRO:HA	1:A:307:ASN:HA	1.82	0.61
1:A:505:THR:HG22	1:A:506:HIS:N	2.15	0.61
1:B:61:HIS:CE1	1:B:422:HIS:ND1	2.69	0.61
1:B:149:HIS:O	1:B:152:HIS:HB3	2.01	0.61
1:B:505:THR:HG22	1:B:506:HIS:N	2.15	0.61
1:A:10:LEU:HD11	1:A:42:SER:CA	2.30	0.61
1:A:61:HIS:CE1	1:A:422:HIS:ND1	2.69	0.61
1:A:285:LYS:O	1:A:288:ASP:HB2	2.00	0.61
1:A:316:LEU:HD11	1:A:413:TRP:NE1	2.16	0.61
1:B:185:VAL:HG12	1:B:186:GLY:N	2.15	0.61
1:B:416:TRP:HA	1:B:416:TRP:CE3	2.36	0.61
1:A:39:VAL:HG12	1:A:40:ILE:H	1.66	0.61
1:A:230:PRO:HA	1:A:233:GLN:CD	2.21	0.61
1:A:324:LYS:HA	1:A:416:TRP:CZ3	2.34	0.61
1:A:426:SER:O	1:A:502:GLU:HA	2.01	0.61
1:B:230:PRO:HA	1:B:233:GLN:CD	2.21	0.60
1:B:315:LEU:HA	1:B:318:ALA:HB3	1.82	0.60
1:B:39:VAL:HG12	1:B:40:ILE:H	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:LEU:HD11	1:B:413:TRP:NE1	2.16	0.60
1:A:24:PHE:CD2	1:A:95:PHE:HD2	2.20	0.60
1:B:82:ASP:O	1:B:86:ILE:HG13	2.01	0.60
1:B:129:ARG:HB2	1:B:131:LEU:HD21	1.83	0.60
1:A:136:GLU:CD	1:A:136:GLU:H	2.05	0.60
1:A:149:HIS:O	1:A:152:HIS:HB3	2.01	0.60
1:A:549:TRP:CZ2	1:A:558:TRP:HB3	2.37	0.60
1:A:445:LYS:O	1:A:449:GLU:HG3	2.02	0.60
1:B:24:PHE:CD2	1:B:95:PHE:HD2	2.20	0.60
1:B:37:VAL:HG12	1:B:38:GLU:N	2.17	0.60
1:B:549:TRP:CZ2	1:B:558:TRP:HB3	2.37	0.60
1:B:426:SER:O	1:B:502:GLU:HA	2.01	0.60
1:A:37:VAL:HG12	1:A:38:GLU:N	2.17	0.59
1:A:478:LEU:H	1:A:478:LEU:CD1	2.12	0.59
1:B:96:PRO:C	1:B:97:LEU:HD23	2.22	0.59
1:B:445:LYS:O	1:B:449:GLU:HG3	2.02	0.59
1:A:96:PRO:C	1:A:97:LEU:HD23	2.22	0.59
1:A:129:ARG:HB2	1:A:131:LEU:HD21	1.83	0.59
1:A:425:PHE:CB	1:A:488:MET:HE1	2.32	0.59
1:A:554:SER:HB3	1:A:557:THR:HB	1.84	0.59
1:A:82:ASP:O	1:A:86:ILE:HG13	2.01	0.59
1:A:242:PHE:CD1	1:A:243:PRO:HD2	2.37	0.59
1:A:416:TRP:HA	1:A:416:TRP:CE3	2.36	0.59
1:A:39:VAL:HG12	1:A:40:ILE:N	2.17	0.59
1:A:430:LYS:O	1:A:465:MET:HE2	2.03	0.59
1:B:136:GLU:H	1:B:136:GLU:CD	2.05	0.59
1:A:299:LEU:HB2	1:A:305:LEU:CD1	2.33	0.59
1:B:430:LYS:O	1:B:465:MET:HE2	2.02	0.59
1:A:243:PRO:HD2	1:A:244:TYR:H	1.68	0.59
1:B:242:PHE:CD1	1:B:243:PRO:HD2	2.37	0.59
1:B:283:LEU:HD12	1:B:351:TRP:HB3	1.85	0.58
1:A:332:GLU:CB	1:A:333:PRO:HD2	2.33	0.58
1:B:243:PRO:HD2	1:B:244:TYR:H	1.68	0.58
1:B:554:SER:HB3	1:B:557:THR:HB	1.84	0.58
1:A:230:PRO:HD2	1:A:231:GLU:H	1.68	0.58
1:A:411:LEU:HA	1:A:414:ILE:HD12	1.86	0.58
1:B:154:TYR:HD1	1:B:155:LEU:HD23	1.68	0.58
1:B:222:ARG:CB	1:B:223:PRO:HD2	2.30	0.58
1:B:299:LEU:HB2	1:B:305:LEU:CD1	2.33	0.58
1:A:525:LEU:HD12	1:A:525:LEU:O	2.04	0.58
1:B:230:PRO:HD2	1:B:231:GLU:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:475:LYS:O	1:B:481:LYS:HD2	2.04	0.58
1:B:272:ASN:OD1	1:B:273:PRO:HD2	2.04	0.58
1:A:154:TYR:HD1	1:A:155:LEU:HD23	1.68	0.58
1:B:35:GLU:HA	1:B:35:GLU:OE1	2.04	0.58
1:B:51:TYR:CZ	1:B:104:ARG:HD3	2.39	0.58
1:B:332:GLU:CB	1:B:333:PRO:HD2	2.33	0.58
1:A:272:ASN:OD1	1:A:273:PRO:HD2	2.04	0.57
1:A:475:LYS:O	1:A:481:LYS:HD2	2.04	0.57
1:A:24:PHE:CE1	1:A:28:ILE:CD1	2.87	0.57
1:A:51:TYR:CZ	1:A:104:ARG:HD3	2.39	0.57
1:A:61:HIS:CE1	1:A:422:HIS:CE1	2.93	0.57
1:B:13:PRO:HD3	1:B:117:GLY:O	2.04	0.57
1:A:65:ASP:N	1:A:65:ASP:OD1	2.37	0.57
1:B:39:VAL:HG12	1:B:40:ILE:N	2.17	0.57
1:A:283:LEU:HD12	1:A:351:TRP:HB3	1.85	0.57
1:B:83:VAL:O	1:B:87:VAL:HG23	2.04	0.57
1:A:13:PRO:HD3	1:A:117:GLY:O	2.04	0.57
1:B:411:LEU:HA	1:B:414:ILE:HD12	1.86	0.57
1:B:24:PHE:CE1	1:B:28:ILE:CD1	2.88	0.57
1:B:393:SER:O	1:B:396:ARG:HB2	2.05	0.57
1:B:421:ALA:O	1:B:472:VAL:HA	2.05	0.57
1:A:83:VAL:O	1:A:87:VAL:HG23	2.04	0.57
1:A:332:GLU:CG	1:A:333:PRO:HD2	2.35	0.57
1:A:425:PHE:HB2	1:A:488:MET:HE3	1.86	0.57
1:A:222:ARG:CB	1:A:223:PRO:HD2	2.30	0.56
1:A:280:LEU:O	1:A:280:LEU:HG	2.05	0.56
1:B:165:TRP:HB2	1:B:270:MET:O	2.05	0.56
1:B:525:LEU:HD12	1:B:525:LEU:O	2.04	0.56
1:A:48:ASP:HA	1:A:58:HIS:CE1	2.40	0.56
1:A:165:TRP:HB2	1:A:270:MET:O	2.05	0.56
1:A:393:SER:O	1:A:396:ARG:HB2	2.05	0.56
1:A:421:ALA:O	1:A:472:VAL:HA	2.05	0.56
1:A:448:GLN:O	1:A:451:GLY:N	2.33	0.56
1:B:444:LYS:O	1:B:447:CYS:N	2.39	0.56
1:A:35:GLU:OE1	1:A:35:GLU:HA	2.04	0.56
1:B:48:ASP:HA	1:B:58:HIS:CE1	2.40	0.56
1:B:61:HIS:CE1	1:B:422:HIS:CE1	2.93	0.56
1:B:332:GLU:CG	1:B:333:PRO:HD2	2.35	0.56
1:B:389:THR:HB	1:B:390:PRO:HD2	1.86	0.56
1:B:418:PRO:HB2	1:B:474:ASN:ND2	2.21	0.56
1:B:478:LEU:H	1:B:478:LEU:CD1	2.12	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:PRO:O	1:A:226:MET:HG2	2.06	0.56
1:A:389:THR:HB	1:A:390:PRO:CD	2.36	0.56
1:A:156:GLU:C	1:A:158:ASN:H	2.09	0.56
1:B:389:THR:HB	1:B:390:PRO:CD	2.36	0.56
1:A:237:LYS:NZ	1:B:500:TRP:CZ2	2.73	0.56
1:A:389:THR:HB	1:A:390:PRO:HD2	1.86	0.56
1:A:400:LYS:HB3	1:A:405:ILE:HB	1.87	0.56
1:B:223:PRO:O	1:B:226:MET:HG2	2.06	0.56
1:A:10:LEU:HD13	1:A:40:ILE:O	2.06	0.56
1:A:545:LYS:HG3	1:A:546:SER:N	2.20	0.56
1:A:27:ASP:N	1:A:27:ASP:OD1	2.39	0.56
1:B:156:GLU:C	1:B:158:ASN:H	2.09	0.56
1:B:201:GLU:HG2	1:B:202:VAL:N	2.19	0.56
1:B:229:LYS:HB3	1:B:230:PRO:CD	2.36	0.56
1:A:444:LYS:O	1:A:447:CYS:N	2.39	0.56
1:A:494:ASP:O	1:A:497:ALA:HB3	2.06	0.56
1:B:10:LEU:HD13	1:B:40:ILE:O	2.06	0.56
1:B:280:LEU:O	1:B:280:LEU:HG	2.05	0.56
1:A:270:MET:HG3	1:A:271:PRO:HD2	1.87	0.55
1:B:59:ASP:O	1:B:62:HIS:HB3	2.07	0.55
1:B:65:ASP:OD1	1:B:65:ASP:N	2.37	0.55
1:B:494:ASP:O	1:B:497:ALA:HB3	2.06	0.55
1:B:555:HIS:HB3	1:B:559:LYS:CE	2.37	0.55
1:A:201:GLU:HG2	1:A:202:VAL:N	2.20	0.55
1:B:270:MET:HG3	1:B:271:PRO:HD2	1.87	0.55
1:B:425:PHE:CE2	1:B:427:PRO:HG3	2.41	0.55
1:A:59:ASP:O	1:A:62:HIS:HB3	2.07	0.55
1:A:425:PHE:CE2	1:A:427:PRO:HG3	2.41	0.55
1:B:143:GLU:HB3	1:B:144:PRO:HD2	1.89	0.55
1:A:549:TRP:CH2	1:A:558:TRP:HB3	2.42	0.55
1:B:164:LEU:C	1:B:165:TRP:HD1	2.10	0.55
1:B:403:GLN:HG3	1:B:405:ILE:HG13	1.89	0.55
1:B:545:LYS:HG3	1:B:546:SER:N	2.20	0.55
1:A:418:PRO:HB2	1:A:474:ASN:ND2	2.21	0.55
1:B:276:TYR:OH	1:B:399:ASP:O	2.19	0.55
1:A:229:LYS:HB3	1:A:230:PRO:CD	2.36	0.55
1:B:549:TRP:CH2	1:B:558:TRP:HB3	2.42	0.55
1:A:75:VAL:O	1:A:122:ASP:N	2.37	0.55
1:A:361:GLU:N	1:A:362:PRO:HD2	2.22	0.55
1:A:18:LEU:HD12	1:A:18:LEU:O	2.07	0.55
1:A:270:MET:HG2	1:A:271:PRO:HD2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:ASP:O	1:A:321:LEU:HG	2.08	0.54
1:A:463:ARG:NH2	1:B:269:LEU:O	2.40	0.54
1:B:270:MET:HG2	1:B:271:PRO:HD2	1.88	0.54
1:A:422:HIS:CD2	1:A:424:PHE:CZ	2.95	0.54
1:A:554:SER:HB3	1:A:557:THR:CB	2.37	0.54
1:B:97:LEU:CD2	1:B:119:VAL:HB	2.37	0.54
1:B:505:THR:CG2	1:B:506:HIS:N	2.71	0.54
1:A:555:HIS:HB3	1:A:559:LYS:CE	2.37	0.54
1:B:312:ARG:NH1	1:B:317:ASP:OD1	2.40	0.54
1:B:422:HIS:CD2	1:B:424:PHE:CZ	2.95	0.54
1:A:9:PRO:HG3	1:A:21:PHE:CE2	2.42	0.54
1:B:89:LEU:N	1:B:89:LEU:CD1	2.71	0.54
1:B:361:GLU:N	1:B:362:PRO:HD2	2.22	0.54
1:B:400:LYS:HB3	1:B:405:ILE:HB	1.87	0.54
1:B:478:LEU:O	1:B:482:ARG:HG3	2.08	0.54
1:A:7:PHE:HB3	1:A:8:ARG:HG3	1.89	0.54
1:A:164:LEU:C	1:A:165:TRP:HD1	2.10	0.54
1:A:229:LYS:O	1:A:233:GLN:HG3	2.08	0.54
1:B:7:PHE:HB3	1:B:8:ARG:HG3	1.89	0.54
1:B:9:PRO:HG3	1:B:21:PHE:CE2	2.42	0.54
1:B:312:ARG:HD2	1:B:354:TYR:CE1	2.43	0.54
1:B:506:HIS:ND1	1:B:507:LEU:N	2.56	0.54
1:A:143:GLU:HB3	1:A:144:PRO:HD2	1.89	0.54
1:B:503:TYR:OH	3:B:601:EUG:O4	2.15	0.54
1:A:312:ARG:HD2	1:A:354:TYR:CE1	2.43	0.54
1:A:506:HIS:ND1	1:A:507:LEU:N	2.56	0.54
1:B:217:LEU:C	1:B:217:LEU:HD13	2.28	0.54
1:B:229:LYS:O	1:B:233:GLN:HG3	2.08	0.54
1:B:317:ASP:O	1:B:321:LEU:HG	2.08	0.54
1:B:533:ASN:OD1	1:B:552:GLN:NE2	2.41	0.54
1:A:97:LEU:CD2	1:A:119:VAL:HB	2.37	0.54
1:B:221:LYS:O	1:B:222:ARG:HB3	2.08	0.54
1:A:505:THR:CG2	1:A:506:HIS:N	2.71	0.54
1:A:388:ASP:OD1	1:A:388:ASP:N	2.41	0.54
1:B:18:LEU:HD12	1:B:18:LEU:O	2.07	0.54
1:A:296:ILE:HG21	1:A:460:VAL:HG11	1.90	0.53
1:B:388:ASP:N	1:B:388:ASP:OD1	2.41	0.53
1:A:221:LYS:O	1:A:222:ARG:HB3	2.08	0.53
1:A:403:GLN:HG3	1:A:405:ILE:HG13	1.89	0.53
1:B:554:SER:HB3	1:B:557:THR:CB	2.37	0.53
1:A:79:ASN:ND2	1:A:81:ALA:H	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:GLU:OE2	1:A:466:HIS:ND1	2.41	0.53
1:A:533:ASN:OD1	1:A:552:GLN:NE2	2.41	0.53
1:A:205:ALA:CB	1:A:536:ASP:HB2	2.39	0.53
1:A:217:LEU:HD13	1:A:217:LEU:C	2.28	0.53
1:A:478:LEU:O	1:A:482:ARG:HG3	2.08	0.53
1:B:27:ASP:OD1	1:B:27:ASP:N	2.39	0.53
1:B:194:TRP:O	1:B:197:HIS:CD2	2.62	0.53
1:A:89:LEU:N	1:A:89:LEU:CD1	2.71	0.53
1:A:136:GLU:OE1	1:A:136:GLU:N	2.34	0.53
1:B:23:GLU:O	1:B:27:ASP:OD1	2.27	0.53
1:B:422:HIS:NE2	2:B:600:FAD:C8	2.64	0.53
1:B:422:HIS:HD2	1:B:424:PHE:CZ	2.27	0.53
1:A:7:PHE:HA	1:A:22:ASN:OD1	2.09	0.53
1:A:23:GLU:O	1:A:27:ASP:OD1	2.27	0.53
1:A:495:CYS:HB2	4:A:605:HOH:O	2.07	0.53
1:A:509:PHE:O	1:A:513:ILE:HG13	2.09	0.53
1:B:205:ALA:CB	1:B:536:ASP:HB2	2.39	0.53
1:A:194:TRP:O	1:A:197:HIS:CD2	2.62	0.53
1:A:422:HIS:HD2	1:A:424:PHE:CZ	2.27	0.53
1:B:390:PRO:O	1:B:393:SER:HB3	2.09	0.53
1:B:509:PHE:O	1:B:513:ILE:HG13	2.09	0.53
1:A:390:PRO:O	1:A:393:SER:HB3	2.09	0.53
1:B:79:ASN:ND2	1:B:81:ALA:H	2.06	0.53
1:A:160:LEU:O	1:A:163:LYS:N	2.37	0.53
1:A:419:ASN:O	1:A:475:LYS:N	2.38	0.53
1:A:472:VAL:HG12	1:A:473:PHE:N	2.24	0.53
1:B:62:HIS:O	1:B:62:HIS:ND1	2.39	0.53
1:B:194:TRP:O	1:B:197:HIS:HD2	1.91	0.53
1:A:165:TRP:N	1:A:270:MET:O	2.39	0.52
1:A:247:GLY:HA2	1:B:546:SER:OG	2.09	0.52
1:B:7:PHE:HA	1:B:22:ASN:OD1	2.09	0.52
1:B:349:GLY:N	1:B:352:ASN:HD21	2.07	0.52
1:B:419:ASN:O	1:B:475:LYS:N	2.38	0.52
1:A:55:THR:HG21	1:A:58:HIS:ND1	2.25	0.52
1:A:62:HIS:O	1:A:62:HIS:ND1	2.39	0.52
1:A:194:TRP:O	1:A:197:HIS:HD2	1.91	0.52
1:A:349:GLY:N	1:A:352:ASN:HD21	2.07	0.52
1:B:383:PHE:C	1:B:384:TYR:CD1	2.82	0.52
1:B:457:THR:CG2	1:B:458:PHE:H	2.01	0.52
1:B:464:GLU:OE2	1:B:466:HIS:ND1	2.41	0.52
1:B:165:TRP:N	1:B:270:MET:O	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:ILE:HG21	1:B:460:VAL:HG11	1.90	0.52
1:A:369:GLU:O	1:A:373:ASP:HB3	2.10	0.52
1:B:369:GLU:O	1:B:373:ASP:HB3	2.10	0.52
1:A:383:PHE:C	1:A:384:TYR:CD1	2.82	0.52
1:A:507:LEU:HA	1:A:510:MET:HE2	1.92	0.52
1:B:371:ILE:O	1:B:374:ALA:HB3	2.10	0.52
1:B:243:PRO:CD	1:B:244:TYR:H	2.23	0.52
1:A:243:PRO:CD	1:A:244:TYR:H	2.23	0.52
1:A:312:ARG:NH1	1:A:317:ASP:OD1	2.40	0.52
1:A:371:ILE:O	1:A:374:ALA:HB3	2.10	0.52
1:B:156:GLU:O	1:B:158:ASN:N	2.43	0.52
1:B:55:THR:HG21	1:B:58:HIS:ND1	2.25	0.52
1:A:132:GLU:HG2	1:A:133:VAL:H	1.75	0.51
1:A:323:ASP:OD1	1:A:326:SER:HB3	2.10	0.51
1:B:515:GLU:OE1	1:B:515:GLU:HA	2.11	0.51
1:B:323:ASP:OD1	1:B:326:SER:HB3	2.10	0.51
1:A:409:ASP:HA	1:A:412:LYS:HE3	1.92	0.51
1:A:505:THR:HG21	1:A:509:PHE:HB2	1.91	0.51
1:B:472:VAL:HG12	1:B:473:PHE:N	2.24	0.51
1:B:442:VAL:O	1:B:445:LYS:HB3	2.11	0.51
1:B:200:MET:O	1:B:211:ARG:HA	2.11	0.51
1:B:409:ASP:N	1:B:409:ASP:OD1	2.44	0.51
1:B:433:GLY:O	1:B:437:MET:HB2	2.11	0.51
1:A:411:LEU:HA	1:A:414:ILE:CD1	2.41	0.51
1:A:533:ASN:HD21	1:A:551:SER:H	1.59	0.51
1:B:95:PHE:CD1	1:B:96:PRO:CD	2.94	0.51
1:B:300:ARG:NH2	1:B:308:VAL:HA	2.18	0.51
1:B:418:PRO:CD	1:B:474:ASN:HD22	2.22	0.51
1:B:505:THR:HG21	1:B:509:PHE:HB2	1.91	0.51
1:A:425:PHE:CE1	1:A:502:GLU:CG	2.94	0.51
1:A:433:GLY:O	1:A:437:MET:HB2	2.11	0.51
1:A:484:VAL:O	1:A:487:LEU:HB3	2.11	0.51
1:B:107:GLY:HA2	1:B:422:HIS:O	2.11	0.51
1:B:136:GLU:OE1	1:B:136:GLU:N	2.34	0.51
1:B:289:LEU:HB2	1:B:351:TRP:NE1	2.26	0.51
1:B:409:ASP:HA	1:B:412:LYS:HE3	1.92	0.51
1:B:425:PHE:CE1	1:B:502:GLU:CG	2.94	0.51
1:B:507:LEU:HA	1:B:510:MET:HE2	1.93	0.51
1:A:156:GLU:O	1:A:158:ASN:N	2.43	0.50
1:A:277:GLN:O	1:A:357:LEU:N	2.29	0.50
1:A:133:VAL:HG21	1:A:154:TYR:CZ	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:LEU:HB2	1:A:351:TRP:NE1	2.26	0.50
1:A:351:TRP:HA	1:A:351:TRP:CE3	2.47	0.50
1:A:409:ASP:OD1	1:A:409:ASP:N	2.44	0.50
1:A:300:ARG:HE	1:A:309:PRO:HD2	1.76	0.50
1:A:442:VAL:O	1:A:445:LYS:HB3	2.11	0.50
1:B:533:ASN:HD21	1:B:551:SER:H	1.59	0.50
1:A:223:PRO:HG2	1:A:224:GLU:CD	2.32	0.50
1:A:371:ILE:O	1:A:374:ALA:N	2.44	0.50
1:B:179:ASN:OD1	1:B:184:GLY:HA3	2.11	0.50
1:A:22:ASN:HA	1:A:25:ILE:HG22	1.94	0.50
1:A:144:PRO:HA	1:A:177:LEU:HG	1.93	0.50
1:B:28:ILE:O	1:B:32:VAL:HG22	2.12	0.50
1:B:411:LEU:HA	1:B:414:ILE:CD1	2.41	0.50
1:B:448:GLN:O	1:B:451:GLY:N	2.33	0.50
1:A:24:PHE:CE2	1:A:95:PHE:CD2	3.00	0.50
1:A:349:GLY:CA	1:A:352:ASN:HD21	2.25	0.50
1:A:385:PHE:HB2	1:A:387:GLU:OE1	2.11	0.50
1:B:24:PHE:CE2	1:B:95:PHE:CD2	3.00	0.50
1:B:277:GLN:O	1:B:357:LEU:N	2.29	0.50
1:A:200:MET:O	1:A:211:ARG:HA	2.11	0.50
1:B:75:VAL:O	1:B:122:ASP:N	2.37	0.50
1:B:324:LYS:HE2	1:B:334:LEU:HD21	1.94	0.50
1:B:351:TRP:CE3	1:B:351:TRP:HA	2.47	0.50
1:B:371:ILE:O	1:B:374:ALA:N	2.44	0.50
1:B:425:PHE:CB	1:B:488:MET:HE1	2.40	0.50
1:B:51:TYR:CE1	1:B:171:LEU:HD13	2.47	0.50
1:A:425:PHE:HE1	1:A:502:GLU:CG	2.25	0.50
1:B:144:PRO:HA	1:B:177:LEU:HG	1.93	0.50
1:B:385:PHE:HB2	1:B:387:GLU:OE1	2.11	0.50
1:B:484:VAL:O	1:B:487:LEU:HB3	2.11	0.50
1:A:107:GLY:HA2	1:A:422:HIS:O	2.11	0.49
1:A:179:ASN:OD1	1:A:184:GLY:HA3	2.11	0.49
1:B:205:ALA:HB2	1:B:541:ILE:CD1	2.42	0.49
1:B:223:PRO:HG2	1:B:224:GLU:CD	2.32	0.49
1:A:205:ALA:HB2	1:A:541:ILE:CD1	2.42	0.49
1:B:132:GLU:HG2	1:B:133:VAL:H	1.75	0.49
1:B:155:LEU:O	1:B:160:LEU:N	2.40	0.49
1:B:279:TYR:HB3	1:B:385:PHE:CE1	2.47	0.49
1:A:152:HIS:CE1	1:A:161:ARG:NH2	2.79	0.49
1:A:279:TYR:HB3	1:A:385:PHE:CE1	2.47	0.49
1:B:58:HIS:C	1:B:112:ALA:HB2	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:GLU:HA	1:A:515:GLU:OE1	2.11	0.49
1:A:51:TYR:CE1	1:A:171:LEU:HD13	2.47	0.49
1:B:133:VAL:HG21	1:B:154:TYR:CZ	2.44	0.49
1:B:297:ARG:HB3	1:B:298:PRO:CD	2.42	0.49
1:B:349:GLY:CA	1:B:352:ASN:HD21	2.25	0.49
1:B:22:ASN:HA	1:B:25:ILE:HG22	1.94	0.49
1:A:28:ILE:O	1:A:32:VAL:HG22	2.12	0.49
1:A:428:ILE:HG21	1:B:238:ILE:HG21	1.93	0.49
1:B:217:LEU:HA	1:B:217:LEU:HD22	1.41	0.49
1:B:454:PHE:CD1	1:B:455:ILE:N	2.81	0.49
1:B:103:GLY:C	1:B:105:ASN:H	2.16	0.49
1:B:309:PRO:HB2	1:B:353:PHE:HE1	1.78	0.49
1:A:58:HIS:C	1:A:112:ALA:HB2	2.32	0.49
1:A:244:TYR:CD1	1:A:244:TYR:N	2.77	0.49
1:A:526:ARG:NH1	1:A:529:GLU:OE1	2.46	0.49
1:B:186:GLY:O	1:B:191:GLY:HA3	2.13	0.49
1:B:300:ARG:HE	1:B:309:PRO:HD2	1.76	0.49
1:B:526:ARG:NH1	1:B:529:GLU:OE1	2.46	0.49
1:A:324:LYS:HE2	1:A:334:LEU:HD21	1.94	0.49
1:A:243:PRO:CD	1:A:244:TYR:N	2.76	0.48
1:A:361:GLU:CA	1:A:364:ARG:NH2	2.76	0.48
1:A:454:PHE:CD1	1:A:455:ILE:N	2.81	0.48
1:A:478:LEU:HB2	1:A:479:ILE:HD12	1.95	0.48
1:B:147:THR:HG23	1:B:150:ASP:OD2	2.13	0.48
1:B:425:PHE:HE1	1:B:502:GLU:CG	2.25	0.48
1:A:103:GLY:C	1:A:105:ASN:H	2.16	0.48
1:A:186:GLY:O	1:A:191:GLY:HA3	2.13	0.48
1:A:190:TYR:CE1	1:A:270:MET:HG3	2.48	0.48
1:A:321:LEU:HD12	1:A:346:LEU:CD2	2.43	0.48
1:A:422:HIS:NE2	2:A:600:FAD:C8	2.64	0.48
1:B:149:HIS:C	1:B:153:ASN:HD22	2.17	0.48
1:B:323:ASP:OD1	1:B:323:ASP:N	2.46	0.48
1:A:6:GLU:N	1:A:39:VAL:CG2	2.76	0.48
1:A:147:THR:HG23	1:A:150:ASP:OD2	2.13	0.48
1:A:229:LYS:O	1:A:232:ASP:N	2.43	0.48
1:A:270:MET:HA	1:A:271:PRO:HD3	1.72	0.48
1:B:167:ASP:OD2	1:B:191:GLY:N	2.47	0.48
1:B:321:LEU:HD12	1:B:346:LEU:CD2	2.43	0.48
1:B:361:GLU:CA	1:B:364:ARG:NH2	2.76	0.48
1:A:87:VAL:O	1:A:91:ASN:N	2.44	0.48
1:A:238:ILE:HD13	1:A:238:ILE:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:ASN:O	1:B:160:LEU:HG	2.13	0.48
1:B:160:LEU:O	1:B:163:LYS:N	2.37	0.48
1:A:69:PHE:HB3	1:A:113:PRO:O	2.14	0.48
1:A:324:LYS:CE	1:A:334:LEU:HD21	2.44	0.48
1:A:463:ARG:HH21	1:B:138:ALA:CB	2.27	0.48
1:B:6:GLU:N	1:B:39:VAL:CG2	2.76	0.48
1:B:148:TYR:O	1:B:152:HIS:N	2.45	0.48
1:B:244:TYR:N	1:B:244:TYR:CD1	2.77	0.48
1:B:422:HIS:CD2	2:B:600:FAD:C8M	2.73	0.48
1:A:158:ASN:O	1:A:160:LEU:HG	2.13	0.48
1:B:190:TYR:CE1	1:B:270:MET:HG3	2.48	0.48
1:A:149:HIS:C	1:A:153:ASN:HD22	2.17	0.48
1:A:472:VAL:HG12	1:A:473:PHE:H	1.79	0.48
1:A:53:LYS:HA	1:A:54:PRO:HD3	1.70	0.48
1:A:496:ALA:N	4:A:605:HOH:O	2.46	0.48
1:B:87:VAL:O	1:B:91:ASN:N	2.44	0.48
1:B:108:TYR:HD1	1:B:505:THR:C	2.17	0.48
1:B:279:TYR:CD2	1:B:280:LEU:N	2.82	0.48
1:B:478:LEU:HB2	1:B:479:ILE:HD12	1.95	0.48
1:A:148:TYR:O	1:A:152:HIS:N	2.44	0.47
1:A:167:ASP:OD2	1:A:191:GLY:N	2.47	0.47
1:A:201:GLU:HA	1:A:210:LEU:O	2.14	0.47
1:A:217:LEU:HB2	1:B:517:TYR:CE1	2.50	0.47
1:A:268:TRP:O	1:A:269:LEU:HD23	2.13	0.47
1:B:24:PHE:CD2	1:B:95:PHE:CD2	3.01	0.47
1:B:201:GLU:HA	1:B:210:LEU:O	2.14	0.47
1:B:383:PHE:N	1:B:383:PHE:CD1	2.82	0.47
1:B:484:VAL:O	1:B:488:MET:N	2.31	0.47
1:B:99:PRO:HA	1:B:121:LEU:HB3	1.97	0.47
1:B:243:PRO:CD	1:B:244:TYR:N	2.76	0.47
1:B:268:TRP:O	1:B:269:LEU:HD23	2.14	0.47
1:A:9:PRO:HA	1:A:40:ILE:O	2.15	0.47
1:B:59:ASP:HA	1:B:60:PRO:HD2	1.67	0.47
1:B:324:LYS:CE	1:B:334:LEU:HD21	2.43	0.47
1:B:468:ILE:HG22	1:B:470:CYS:SG	2.54	0.47
1:A:95:PHE:CD1	1:A:96:PRO:CD	2.94	0.47
1:A:99:PRO:HA	1:A:121:LEU:HB3	1.96	0.47
1:A:108:TYR:HD1	1:A:505:THR:C	2.17	0.47
1:A:61:HIS:N	1:A:61:HIS:CD2	2.82	0.47
1:A:160:LEU:HA	1:A:160:LEU:HD23	1.72	0.47
1:A:283:LEU:HA	1:A:284:PRO:HD3	1.65	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:ARG:NH2	1:A:308:VAL:HA	2.18	0.47
1:A:383:PHE:CD1	1:A:383:PHE:N	2.82	0.47
1:A:8:ARG:O	1:A:41:SER:HA	2.15	0.47
1:A:244:TYR:HH	1:B:195:MET:HG3	1.79	0.47
1:A:494:ASP:O	1:A:497:ALA:N	2.48	0.47
1:B:148:TYR:O	1:B:151:LEU:N	2.48	0.47
1:A:204:LEU:HA	1:A:204:LEU:HD23	1.65	0.47
1:A:279:TYR:CD2	1:A:280:LEU:N	2.82	0.47
1:A:290:LYS:HG3	1:A:433:GLY:HA3	1.97	0.47
1:A:489:ARG:NE	1:A:512:GLN:OE1	2.46	0.47
1:B:8:ARG:O	1:B:41:SER:HA	2.15	0.47
1:B:37:VAL:CG1	1:B:38:GLU:N	2.78	0.47
1:B:69:PHE:HB3	1:B:113:PRO:O	2.14	0.47
1:B:229:LYS:O	1:B:232:ASP:N	2.43	0.47
1:B:238:ILE:N	1:B:238:ILE:HD13	2.28	0.47
1:A:24:PHE:CD2	1:A:95:PHE:CD2	3.01	0.47
1:A:323:ASP:OD1	1:A:323:ASP:N	2.46	0.47
1:A:327:TYR:HB3	1:A:342:ILE:HD11	1.97	0.47
1:A:418:PRO:CD	1:A:474:ASN:HD22	2.22	0.47
1:A:468:ILE:HG22	1:A:470:CYS:SG	2.54	0.47
1:A:520:ASN:O	1:A:521:ASN:HB2	2.15	0.47
1:B:152:HIS:CE1	1:B:161:ARG:NH2	2.80	0.47
1:A:342:ILE:HA	1:A:345:GLN:HG3	1.97	0.47
1:A:14:PRO:C	1:A:16:LEU:N	2.69	0.47
1:A:79:ASN:ND2	1:A:81:ALA:N	2.63	0.47
1:B:290:LYS:HG3	1:B:433:GLY:HA3	1.97	0.47
1:B:472:VAL:HG12	1:B:473:PHE:H	1.79	0.47
1:B:494:ASP:C	1:B:498:ASN:HD22	2.18	0.47
1:A:242:PHE:HA	1:A:243:PRO:HD3	1.49	0.46
1:B:99:PRO:HD3	1:B:542:ALA:HB2	1.97	0.46
1:B:314:ILE:HB	1:B:350:ARG:O	2.15	0.46
1:B:441:ALA:O	1:B:444:LYS:HB3	2.15	0.46
1:A:143:GLU:HB3	1:A:144:PRO:CD	2.45	0.46
1:A:173:GLY:N	1:A:408:TYR:HE1	2.13	0.46
1:A:222:ARG:HG2	1:A:225:THR:OG1	2.16	0.46
1:B:79:ASN:HD22	1:B:81:ALA:N	2.14	0.46
1:A:148:TYR:O	1:A:151:LEU:N	2.48	0.46
1:B:189:PRO:CA	1:B:307:ASN:HA	2.45	0.46
1:B:278:SER:HA	1:B:356:ALA:HA	1.97	0.46
1:B:361:GLU:N	1:B:362:PRO:CD	2.78	0.46
1:B:494:ASP:O	1:B:497:ALA:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:LEU:O	1:A:160:LEU:N	2.40	0.46
1:A:276:TYR:OH	1:A:399:ASP:O	2.19	0.46
1:A:367:LEU:O	1:A:370:THR:HB	2.15	0.46
1:A:416:TRP:HA	1:A:416:TRP:HE3	1.79	0.46
1:B:8:ARG:HA	1:B:9:PRO:HD3	1.78	0.46
1:B:541:ILE:O	1:B:541:ILE:HG22	2.16	0.46
1:A:21:PHE:CE2	1:A:25:ILE:HG21	2.50	0.46
1:A:297:ARG:HB3	1:A:298:PRO:CD	2.43	0.46
1:A:321:LEU:HD12	1:A:346:LEU:HD23	1.97	0.46
1:A:425:PHE:CG	1:A:488:MET:HE1	2.50	0.46
1:B:21:PHE:CE2	1:B:25:ILE:HG21	2.50	0.46
1:B:399:ASP:O	1:B:403:GLN:HG2	2.15	0.46
1:A:399:ASP:O	1:A:403:GLN:HG2	2.15	0.46
1:A:413:TRP:CZ2	2:A:600:FAD:HM72	2.51	0.46
1:A:505:THR:OG1	1:A:513:ILE:HD12	2.16	0.46
1:B:61:HIS:N	1:B:61:HIS:CD2	2.82	0.46
1:B:137:GLY:O	1:B:138:ALA:HB3	2.16	0.46
1:B:321:LEU:HD12	1:B:346:LEU:HD23	1.96	0.46
1:B:428:ILE:HD13	1:B:428:ILE:HA	1.62	0.46
1:B:79:ASN:ND2	1:B:81:ALA:N	2.63	0.46
1:A:99:PRO:HD3	1:A:542:ALA:HB2	1.97	0.46
1:A:217:LEU:HA	1:A:217:LEU:HD22	1.41	0.46
1:A:309:PRO:HB2	1:A:353:PHE:HE1	1.78	0.46
1:A:484:VAL:O	1:A:488:MET:N	2.31	0.46
1:B:222:ARG:HG2	1:B:225:THR:OG1	2.16	0.46
1:B:533:ASN:HD21	1:B:551:SER:N	2.14	0.46
1:A:139:TYR:CD1	1:A:139:TYR:C	2.90	0.46
1:A:332:GLU:CB	1:A:333:PRO:CD	2.94	0.46
1:B:327:TYR:HB3	1:B:342:ILE:HD11	1.97	0.46
1:A:164:LEU:C	1:A:165:TRP:CD1	2.89	0.46
1:A:441:ALA:O	1:A:444:LYS:HB3	2.15	0.46
1:B:173:GLY:N	1:B:408:TYR:HE1	2.13	0.46
1:B:280:LEU:HD12	1:B:281:ILE:N	2.31	0.46
1:B:367:LEU:O	1:B:370:THR:HB	2.15	0.46
1:B:560:LEU:HA	1:B:560:LEU:HD23	1.50	0.46
1:A:37:VAL:CG1	1:A:38:GLU:N	2.78	0.45
1:A:137:GLY:O	1:A:138:ALA:HB3	2.16	0.45
1:A:230:PRO:HD2	1:A:231:GLU:HG2	1.99	0.45
1:A:425:PHE:CE1	1:A:502:GLU:HG3	2.52	0.45
1:A:428:ILE:CG2	1:B:238:ILE:HG21	2.46	0.45
1:A:533:ASN:HD21	1:A:551:SER:N	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:489:ARG:NE	1:B:512:GLN:OE1	2.46	0.45
1:A:189:PRO:CA	1:A:307:ASN:HA	2.45	0.45
1:B:9:PRO:HA	1:B:40:ILE:O	2.15	0.45
1:B:143:GLU:HB3	1:B:144:PRO:CD	2.45	0.45
1:B:342:ILE:HA	1:B:345:GLN:HG3	1.97	0.45
1:B:424:PHE:HD2	1:B:468:ILE:HG23	1.82	0.45
1:A:141:VAL:HG21	1:A:240:HIS:CE1	2.52	0.45
1:A:361:GLU:N	1:A:362:PRO:CD	2.78	0.45
1:B:141:VAL:HG21	1:B:240:HIS:CE1	2.52	0.45
1:B:425:PHE:CE1	1:B:502:GLU:HG3	2.52	0.45
1:A:14:PRO:HB2	1:A:15:LYS:HE3	1.99	0.45
1:A:16:LEU:HD12	1:A:16:LEU:HA	1.51	0.45
1:A:278:SER:HA	1:A:356:ALA:HA	1.97	0.45
1:A:280:LEU:HD12	1:A:281:ILE:N	2.31	0.45
1:A:314:ILE:HB	1:A:350:ARG:O	2.15	0.45
1:B:243:PRO:CG	1:B:244:TYR:N	2.79	0.45
1:B:416:TRP:HA	1:B:416:TRP:HE3	1.79	0.45
1:B:164:LEU:C	1:B:165:TRP:CD1	2.89	0.45
1:A:243:PRO:CG	1:A:244:TYR:N	2.79	0.45
1:A:487:LEU:HD11	1:A:491:LEU:CD1	2.44	0.45
1:B:139:TYR:CD1	1:B:139:TYR:C	2.90	0.45
1:B:413:TRP:CZ2	2:B:600:FAD:HM72	2.51	0.45
1:B:424:PHE:CE2	3:B:601:EUG:H6	2.51	0.45
1:A:56:HIS:O	1:A:111:ALA:HB1	2.17	0.45
1:B:25:ILE:HD12	1:B:25:ILE:HA	1.78	0.45
1:B:267:ILE:O	1:B:267:ILE:HG22	2.10	0.45
1:B:269:LEU:HD23	1:B:269:LEU:HA	1.81	0.45
1:A:112:ALA:HA	1:A:113:PRO:HD3	1.69	0.45
1:A:149:HIS:HB2	1:A:408:TYR:OH	2.17	0.45
1:A:284:PRO:HG2	1:A:379:PRO:O	2.17	0.45
1:A:287:GLY:HA2	1:A:437:MET:CE	2.47	0.45
1:A:424:PHE:CE2	3:A:601:EUG:H6	2.51	0.45
1:A:487:LEU:CD1	1:A:491:LEU:CD1	2.95	0.45
1:A:513:ILE:HA	1:A:516:THR:HG23	1.98	0.45
1:B:56:HIS:O	1:B:111:ALA:HB1	2.17	0.45
1:B:487:LEU:CD1	1:B:491:LEU:CD1	2.95	0.45
1:A:10:LEU:HD11	1:A:41:SER:C	2.37	0.45
1:A:79:ASN:HD22	1:A:81:ALA:N	2.14	0.45
1:A:171:LEU:HD21	2:A:600:FAD:HM73	1.99	0.45
1:A:263:THR:H	1:A:263:THR:HG1	1.46	0.45
1:A:405:ILE:HA	1:A:406:PRO:HD2	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:HIS:HB2	1:B:408:TYR:OH	2.17	0.45
1:B:204:LEU:HD23	1:B:204:LEU:HA	1.65	0.45
1:B:287:GLY:HA2	1:B:437:MET:CE	2.47	0.45
1:B:293:VAL:C	1:B:295:ILE:N	2.68	0.45
1:B:348:LEU:HA	1:B:348:LEU:HD23	1.69	0.45
1:B:438:MET:O	1:B:442:VAL:HG23	2.17	0.45
1:B:505:THR:OG1	1:B:513:ILE:HD12	2.16	0.45
1:B:513:ILE:HA	1:B:516:THR:HG23	1.98	0.45
1:B:520:ASN:O	1:B:521:ASN:HB2	2.15	0.45
1:B:550:PRO:HB2	1:B:552:GLN:HG2	1.99	0.45
1:A:185:VAL:CG1	1:A:186:GLY:N	2.80	0.44
1:B:10:LEU:HD11	1:B:41:SER:C	2.37	0.44
1:B:171:LEU:HD21	2:B:600:FAD:HM73	1.99	0.44
1:A:89:LEU:N	1:A:89:LEU:HD12	2.33	0.44
1:A:339:LEU:O	1:A:342:ILE:N	2.51	0.44
1:B:40:ILE:O	1:B:40:ILE:HG22	2.18	0.44
1:B:230:PRO:HD2	1:B:231:GLU:OE2	2.18	0.44
1:B:267:ILE:HD13	1:B:267:ILE:HA	1.57	0.44
1:B:279:TYR:O	1:B:395:LEU:HD11	2.17	0.44
1:B:287:GLY:HA2	1:B:437:MET:HE2	1.99	0.44
1:B:385:PHE:HA	1:B:386:PRO:HD3	1.68	0.44
1:A:151:LEU:HD12	1:A:151:LEU:C	2.37	0.44
1:A:155:LEU:HD23	1:A:155:LEU:HA	1.63	0.44
1:A:279:TYR:O	1:A:395:LEU:HD11	2.17	0.44
1:A:283:LEU:HD12	1:A:351:TRP:CB	2.47	0.44
1:A:372:LYS:HA	1:A:383:PHE:CE2	2.52	0.44
1:B:14:PRO:C	1:B:16:LEU:N	2.68	0.44
1:B:53:LYS:HA	1:B:54:PRO:HD3	1.70	0.44
1:B:72:SER:HB3	1:B:117:GLY:O	2.17	0.44
1:B:89:LEU:O	1:B:92:LYS:N	2.51	0.44
1:B:230:PRO:HD2	1:B:231:GLU:HG2	1.98	0.44
1:B:283:LEU:HA	1:B:284:PRO:HD3	1.65	0.44
1:B:372:LYS:HA	1:B:383:PHE:CE2	2.52	0.44
1:A:214:MET:CB	1:A:239:ALA:HA	2.46	0.44
1:B:97:LEU:O	1:B:542:ALA:HA	2.17	0.44
1:B:284:PRO:HG2	1:B:379:PRO:O	2.17	0.44
1:B:487:LEU:CD1	1:B:491:LEU:HD11	2.44	0.44
1:A:541:ILE:O	1:A:541:ILE:HG22	2.16	0.44
1:B:188:THR:HB	1:B:189:PRO:HD2	1.99	0.44
1:B:387:GLU:H	1:B:387:GLU:HG3	1.22	0.44
1:A:97:LEU:HD23	1:A:97:LEU:HA	1.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:PHE:HD2	1:A:468:ILE:HG23	1.82	0.44
1:A:438:MET:O	1:A:442:VAL:HG23	2.17	0.44
1:B:72:SER:HB3	1:B:117:GLY:HA2	1.99	0.44
1:A:72:SER:HB3	1:A:117:GLY:HA2	1.99	0.44
1:A:90:ALA:HB2	1:A:97:LEU:HD11	2.00	0.44
1:A:332:GLU:HB3	1:A:333:PRO:HD2	1.98	0.44
1:B:89:LEU:N	1:B:89:LEU:HD12	2.33	0.44
1:B:270:MET:HA	1:B:271:PRO:HD3	1.72	0.44
1:B:283:LEU:HD12	1:B:351:TRP:CB	2.48	0.44
1:B:487:LEU:HD11	1:B:491:LEU:CD1	2.44	0.44
1:A:535:VAL:C	1:A:537:PRO:HD3	2.38	0.44
1:A:545:LYS:C	1:A:547:GLY:N	2.71	0.44
1:A:550:PRO:HB2	1:A:552:GLN:HG2	1.99	0.44
1:B:332:GLU:HB3	1:B:333:PRO:HD2	1.98	0.44
1:B:535:VAL:C	1:B:537:PRO:HD3	2.38	0.44
1:A:80:VAL:O	1:A:83:VAL:HB	2.17	0.44
1:A:97:LEU:O	1:A:542:ALA:HA	2.17	0.44
1:A:330:ARG:HH22	1:A:335:SER:HB3	1.83	0.44
1:A:378:ILE:HA	1:A:379:PRO:HD2	1.83	0.44
1:A:389:THR:CB	1:A:390:PRO:CD	2.95	0.44
1:B:102:ILE:HG13	1:B:175:SER:HB2	1.99	0.44
1:A:72:SER:HB3	1:A:117:GLY:C	2.39	0.43
1:A:177:LEU:HD22	1:A:265:ILE:CG2	2.26	0.43
1:A:546:SER:OG	1:B:247:GLY:HA2	2.17	0.43
1:B:16:LEU:HD12	1:B:16:LEU:HA	1.51	0.43
1:B:90:ALA:HB2	1:B:97:LEU:HD11	2.00	0.43
1:A:494:ASP:C	1:A:498:ASN:HD22	2.18	0.43
1:A:552:GLN:CD	1:A:552:GLN:H	2.22	0.43
1:B:23:GLU:O	1:B:26:GLN:N	2.51	0.43
1:B:80:VAL:O	1:B:83:VAL:HB	2.17	0.43
1:B:330:ARG:HH22	1:B:335:SER:HB3	1.83	0.43
1:B:339:LEU:O	1:B:342:ILE:N	2.51	0.43
1:A:27:ASP:O	1:A:30:ARG:HB3	2.18	0.43
1:A:72:SER:HB3	1:A:117:GLY:O	2.17	0.43
1:A:346:LEU:O	1:A:347:ASN:HB2	2.19	0.43
1:A:487:LEU:CD1	1:A:491:LEU:HD11	2.44	0.43
1:B:27:ASP:O	1:B:30:ARG:HB3	2.18	0.43
1:B:72:SER:HB3	1:B:117:GLY:C	2.39	0.43
1:B:272:ASN:HA	1:B:273:PRO:HD3	1.64	0.43
1:B:432:SER:OG	1:B:435:ASP:HB2	2.19	0.43
1:A:417:LEU:HD22	1:A:473:PHE:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:PRO:O	1:A:552:GLN:NE2	2.51	0.43
1:A:560:LEU:HA	1:A:560:LEU:HD23	1.50	0.43
1:B:440:TYR:O	1:B:444:LYS:HB2	2.19	0.43
1:A:58:HIS:HA	1:A:112:ALA:HB2	2.01	0.43
1:A:188:THR:HB	1:A:189:PRO:CD	2.49	0.43
1:A:323:ASP:OD2	1:A:325:ARG:HB3	2.18	0.43
1:B:14:PRO:HB2	1:B:15:LYS:HE3	1.99	0.43
1:B:545:LYS:C	1:B:547:GLY:N	2.71	0.43
1:A:10:LEU:N	1:A:10:LEU:HD12	2.34	0.43
1:A:134:ASN:HB3	1:A:139:TYR:CZ	2.54	0.43
1:A:230:PRO:HD2	1:A:231:GLU:OE2	2.18	0.43
1:A:428:ILE:HD13	1:A:428:ILE:HA	1.62	0.43
1:B:417:LEU:HD22	1:B:473:PHE:HA	2.00	0.43
1:B:537:PRO:O	1:B:552:GLN:NE2	2.52	0.43
1:A:89:LEU:O	1:A:92:LYS:N	2.51	0.43
1:A:188:THR:HB	1:A:189:PRO:HD2	1.99	0.43
1:A:241:LEU:HB3	1:B:463:ARG:O	2.19	0.43
1:B:56:HIS:HA	1:B:111:ALA:HB2	1.97	0.43
1:B:464:GLU:CG	1:B:465:MET:N	2.80	0.43
1:B:536:ASP:HA	1:B:537:PRO:HD3	1.34	0.43
1:A:418:PRO:HB2	1:A:474:ASN:HD21	1.84	0.43
1:A:452:LEU:HD23	1:A:452:LEU:HA	1.18	0.43
1:A:40:ILE:O	1:A:40:ILE:HG22	2.17	0.43
1:A:98:TRP:CD2	1:A:113:PRO:HA	2.54	0.43
1:B:188:THR:HB	1:B:189:PRO:CD	2.49	0.43
1:B:395:LEU:HD12	1:B:395:LEU:HA	1.93	0.43
2:B:600:FAD:N1	2:B:600:FAD:O3'	2.28	0.43
1:A:51:TYR:CE1	1:A:104:ARG:HD3	2.54	0.42
1:A:233:GLN:HG3	1:A:233:GLN:H	1.32	0.42
1:B:14:PRO:CB	1:B:15:LYS:HE3	2.49	0.42
1:B:323:ASP:OD2	1:B:325:ARG:HB3	2.18	0.42
1:B:413:TRP:C	1:B:413:TRP:HE3	2.22	0.42
1:B:425:PHE:CG	1:B:488:MET:HE1	2.54	0.42
1:A:177:LEU:CD2	1:A:265:ILE:HG22	2.26	0.42
1:B:134:ASN:HB3	1:B:139:TYR:CZ	2.54	0.42
1:B:332:GLU:HB3	1:B:333:PRO:CD	2.50	0.42
1:B:335:SER:OG	1:B:338:GLU:N	2.42	0.42
1:B:346:LEU:O	1:B:347:ASN:HB2	2.19	0.42
1:B:386:PRO:N	1:B:395:LEU:HD23	2.34	0.42
1:B:413:TRP:C	1:B:415:ASP:N	2.72	0.42
1:A:14:PRO:CB	1:A:15:LYS:HE3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:TYR:CE1	1:A:251:ASP:CG	2.93	0.42
1:A:312:ARG:O	1:A:352:ASN:N	2.53	0.42
1:B:552:GLN:CD	1:B:552:GLN:H	2.22	0.42
1:A:104:ARG:C	1:A:106:SER:H	2.23	0.42
1:A:386:PRO:N	1:A:395:LEU:HD23	2.34	0.42
1:A:413:TRP:C	1:A:415:ASP:N	2.72	0.42
1:B:505:THR:CG2	1:B:513:ILE:HD12	2.50	0.42
1:A:440:TYR:O	1:A:444:LYS:HB2	2.19	0.42
1:A:463:ARG:NH2	1:B:138:ALA:HB3	2.34	0.42
1:B:104:ARG:C	1:B:106:SER:H	2.23	0.42
1:B:152:HIS:CE1	1:B:156:GLU:OE1	2.73	0.42
1:B:177:LEU:HD22	1:B:265:ILE:CG2	2.26	0.42
1:B:330:ARG:CZ	1:B:338:GLU:OE1	2.68	0.42
1:A:200:MET:CE	1:A:251:ASP:CB	2.97	0.42
1:A:413:TRP:C	1:A:413:TRP:HE3	2.22	0.42
1:B:102:ILE:HA	1:B:102:ILE:HD13	1.87	0.42
1:B:324:LYS:N	1:B:416:TRP:CE3	2.88	0.42
1:B:454:PHE:CD1	1:B:454:PHE:C	2.93	0.42
1:A:156:GLU:O	1:A:159:ASN:N	2.43	0.42
1:A:293:VAL:C	1:A:295:ILE:N	2.68	0.42
1:A:295:ILE:HD12	1:A:378:ILE:CD1	2.48	0.42
1:B:10:LEU:N	1:B:10:LEU:HD12	2.33	0.42
1:B:58:HIS:HA	1:B:112:ALA:HB2	2.01	0.42
1:B:98:TRP:CD2	1:B:113:PRO:HA	2.54	0.42
1:B:108:TYR:CD1	1:B:505:THR:C	2.93	0.42
1:A:23:GLU:O	1:A:26:GLN:N	2.51	0.42
1:A:296:ILE:HG13	1:A:296:ILE:H	1.57	0.42
1:A:432:SER:OG	1:A:435:ASP:HB2	2.19	0.42
2:A:600:FAD:C4	3:A:601:EUG:C2	2.97	0.42
1:B:332:GLU:CB	1:B:333:PRO:CD	2.94	0.42
1:A:58:HIS:CA	1:A:112:ALA:HB2	2.50	0.42
1:B:202:VAL:HG12	1:B:203:VAL:N	2.34	0.42
1:B:249:TYR:CE1	1:B:251:ASP:CG	2.93	0.42
1:B:299:LEU:HB3	1:B:305:LEU:HG	2.02	0.42
2:B:600:FAD:C4	3:B:601:EUG:C2	2.97	0.42
1:A:324:LYS:N	1:A:416:TRP:CE3	2.88	0.42
1:B:418:PRO:HB2	1:B:474:ASN:HD21	1.84	0.42
1:B:493:ASP:O	1:B:496:ALA:HB3	2.20	0.42
1:A:12:LEU:HD13	1:A:16:LEU:O	2.20	0.41
1:A:201:GLU:HB3	1:A:264:LYS:HB2	2.02	0.41
1:A:332:GLU:HB3	1:A:333:PRO:CD	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:THR:CG2	1:A:513:ILE:HD12	2.50	0.41
1:B:229:LYS:CB	1:B:230:PRO:CD	2.98	0.41
1:B:242:PHE:HA	1:B:243:PRO:HD3	1.49	0.41
1:B:479:ILE:C	1:B:483:LYS:HE3	2.40	0.41
1:A:422:HIS:HD1	1:A:422:HIS:H	1.68	0.41
1:A:463:ARG:HH21	1:B:138:ALA:HB3	1.85	0.41
1:A:479:ILE:C	1:A:483:LYS:HE3	2.40	0.41
1:B:367:LEU:O	1:B:370:THR:N	2.53	0.41
1:B:411:LEU:O	1:B:414:ILE:N	2.46	0.41
1:B:422:HIS:HD1	1:B:422:HIS:H	1.68	0.41
1:B:536:ASP:N	1:B:537:PRO:HD3	2.26	0.41
1:B:185:VAL:CG1	1:B:186:GLY:N	2.80	0.41
1:B:378:ILE:HA	1:B:379:PRO:HD2	1.83	0.41
1:A:168:VAL:HA	1:A:169:PRO:HD3	1.75	0.41
1:A:454:PHE:CD1	1:A:454:PHE:C	2.93	0.41
1:A:493:ASP:O	1:A:496:ALA:HB3	2.20	0.41
1:B:10:LEU:HD11	1:B:42:SER:N	2.35	0.41
1:B:68:TYR:CD1	1:B:68:TYR:C	2.94	0.41
1:B:278:SER:OG	1:B:399:ASP:OD2	2.30	0.41
1:A:10:LEU:HD11	1:A:42:SER:N	2.35	0.41
1:A:108:TYR:CD1	1:A:505:THR:C	2.93	0.41
1:A:152:HIS:CE1	1:A:156:GLU:OE1	2.73	0.41
1:A:330:ARG:CZ	1:A:338:GLU:OE1	2.68	0.41
1:A:363:ILE:HG12	1:B:363:ILE:HG12	2.02	0.41
1:A:411:LEU:O	1:A:414:ILE:N	2.46	0.41
1:A:535:VAL:CG1	1:B:531:LEU:HD21	2.50	0.41
1:B:12:LEU:HD13	1:B:16:LEU:O	2.20	0.41
1:B:60:PRO:C	1:B:62:HIS:H	2.24	0.41
1:B:151:LEU:HD12	1:B:151:LEU:HA	1.75	0.41
1:B:160:LEU:HD23	1:B:160:LEU:HA	1.72	0.41
1:A:139:TYR:HA	1:A:269:LEU:H	1.86	0.41
1:A:202:VAL:HG12	1:A:203:VAL:N	2.34	0.41
1:A:367:LEU:O	1:A:370:THR:N	2.53	0.41
1:B:281:ILE:HG21	1:B:375:PHE:CD2	2.56	0.41
1:B:385:PHE:O	1:B:388:ASP:N	2.54	0.41
1:A:385:PHE:HA	1:A:386:PRO:HD3	1.68	0.41
1:B:58:HIS:CA	1:B:112:ALA:HB2	2.50	0.41
1:B:112:ALA:HA	1:B:113:PRO:HD3	1.69	0.41
1:B:164:LEU:O	1:B:165:TRP:HD1	2.04	0.41
1:B:201:GLU:HB3	1:B:264:LYS:HB2	2.02	0.41
1:B:316:LEU:HD11	1:B:413:TRP:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:LEU:HD23	1:B:452:LEU:HA	1.18	0.41
1:A:316:LEU:HD11	1:A:413:TRP:CE2	2.55	0.41
1:A:387:GLU:H	1:A:387:GLU:HG3	1.22	0.41
1:B:39:VAL:CG1	1:B:40:ILE:N	2.84	0.41
1:B:51:TYR:CE1	1:B:104:ARG:HD3	2.54	0.41
1:A:59:ASP:HA	1:A:60:PRO:HD2	1.67	0.41
1:A:60:PRO:C	1:A:62:HIS:H	2.24	0.41
1:A:230:PRO:O	1:B:519:TRP:HZ2	2.02	0.41
1:A:281:ILE:HG21	1:A:375:PHE:CD2	2.56	0.41
1:A:409:ASP:O	1:A:412:LYS:HG3	2.21	0.41
1:A:505:THR:CG2	1:A:513:ILE:CD1	2.99	0.41
1:A:540:ILE:HD13	1:A:540:ILE:HA	1.71	0.41
1:A:542:ALA:HA	1:A:543:PRO:HD2	1.78	0.41
1:B:74:ILE:HG22	1:B:75:VAL:N	2.35	0.41
1:B:156:GLU:C	1:B:158:ASN:N	2.74	0.41
1:B:258:ASN:HB3	1:B:542:ALA:O	2.21	0.41
1:B:283:LEU:O	1:B:349:GLY:CA	2.69	0.41
1:B:444:LYS:HB3	1:B:445:LYS:H	1.66	0.41
1:A:164:LEU:O	1:A:165:TRP:HD1	2.04	0.41
1:A:283:LEU:O	1:A:349:GLY:CA	2.69	0.41
1:A:419:ASN:C	1:A:474:ASN:HA	2.39	0.41
1:A:495:CYS:HA	1:A:500:TRP:HE3	1.86	0.41
1:B:139:TYR:HA	1:B:269:LEU:H	1.86	0.41
1:B:200:MET:CE	1:B:251:ASP:CB	2.97	0.41
1:B:312:ARG:O	1:B:352:ASN:N	2.53	0.41
1:B:330:ARG:NH1	1:B:338:GLU:OE1	2.54	0.41
1:A:166:LEU:HD23	1:A:166:LEU:HA	1.82	0.40
1:B:214:MET:CB	1:B:239:ALA:HA	2.46	0.40
1:A:68:TYR:CD1	1:A:68:TYR:C	2.94	0.40
1:A:104:ARG:N	2:A:600:FAD:O2P	2.55	0.40
1:A:339:LEU:O	1:A:343:ALA:N	2.49	0.40
1:A:279:TYR:HB2	1:A:280:LEU:H	1.60	0.40
1:A:302:GLY:O	1:A:303:MET:HB2	2.21	0.40
1:A:330:ARG:NH1	1:A:338:GLU:OE1	2.54	0.40
1:B:129:ARG:HB2	1:B:131:LEU:CD2	2.51	0.40
1:B:198:SER:O	1:B:240:HIS:HD2	2.04	0.40
1:A:198:SER:O	1:A:240:HIS:HD2	2.04	0.40
1:A:258:ASN:HB3	1:A:542:ALA:O	2.21	0.40
1:A:385:PHE:O	1:A:388:ASP:N	2.54	0.40
1:B:302:GLY:O	1:B:303:MET:HB2	2.21	0.40
1:B:400:LYS:O	1:B:403:GLN:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:ASN:C	1:B:474:ASN:HA	2.39	0.40
1:B:477:ASP:OD2	1:B:480:GLN:HB2	2.21	0.40
1:A:10:LEU:CD1	1:A:41:SER:C	2.90	0.40
1:A:24:PHE:CE1	1:A:28:ILE:HD11	2.56	0.40
1:A:119:VAL:HG12	1:A:120:VAL:N	2.37	0.40
1:A:154:TYR:CD1	1:A:154:TYR:C	2.95	0.40
1:A:344:LYS:C	1:A:346:LEU:N	2.75	0.40
1:A:385:PHE:CB	1:A:386:PRO:CD	2.97	0.40
1:A:477:ASP:OD2	1:A:480:GLN:HB2	2.21	0.40
1:B:119:VAL:HG12	1:B:120:VAL:N	2.37	0.40
1:B:314:ILE:HG23	1:B:315:LEU:N	2.36	0.40
1:B:502:GLU:N	1:B:502:GLU:CD	2.75	0.40

There are no symmetry-related clashes.

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	553/560 (99%)	472 (85%)	69 (12%)	12 (2%)	6 22
1	B	553/560 (99%)	472 (85%)	69 (12%)	12 (2%)	6 22
All	All	1106/1120 (99%)	944 (85%)	138 (12%)	24 (2%)	6 22

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	ILE
1	A	559	LYS
1	B	46	ILE
1	B	559	LYS
1	A	157	ALA
1	B	157	ALA

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Mol	Chain	Res	Type
1	A	391	GLU
1	A	517	TYR
1	B	391	GLU
1	B	517	TYR
1	A	127	MET
1	A	166	LEU
1	B	127	MET
1	B	166	LEU
1	A	104	ARG
1	A	388	ASP
1	B	104	ARG
1	B	388	ASP
1	A	199	GLY
1	A	284	PRO
1	B	199	GLY
1	B	284	PRO
1	A	542	ALA
1	B	542	ALA

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	475/482 (98%)	445 (94%)	30 (6%)	18	46
1	B	475/482 (98%)	445 (94%)	30 (6%)	18	46
All	All	950/964 (98%)	890 (94%)	60 (6%)	18	46

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ASP
1	A	64	MET
1	A	65	ASP
1	A	78	ARG
1	A	79	ASN

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Mol	Chain	Res	Type
1	A	91	ASN
1	A	95	PHE
1	A	114	ARG
1	A	128	ASN
1	A	136	GLU
1	A	177	LEU
1	A	224	GLU
1	A	243	PRO
1	A	248	PRO
1	A	251	ASP
1	A	314	ILE
1	A	350	ARG
1	A	361	GLU
1	A	373	ASP
1	A	384	TYR
1	A	407	THR
1	A	409	ASP
1	A	413	TRP
1	A	464	GLU
1	A	478	LEU
1	A	488	MET
1	A	503	TYR
1	A	505	THR
1	A	520	ASN
1	A	552	GLN
1	B	27	ASP
1	B	64	MET
1	B	65	ASP
1	B	78	ARG
1	B	79	ASN
1	B	91	ASN
1	B	95	PHE
1	B	114	ARG
1	B	128	ASN
1	B	136	GLU
1	B	177	LEU
1	B	224	GLU
1	B	243	PRO
1	B	248	PRO
1	B	251	ASP
1	B	314	ILE
1	B	350	ARG

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Mol	Chain	Res	Type
1	B	361	GLU
1	B	373	ASP
1	B	384	TYR
1	B	407	THR
1	B	409	ASP
1	B	413	TRP
1	B	464	GLU
1	B	478	LEU
1	B	488	MET
1	B	503	TYR
1	B	505	THR
1	B	520	ASN
1	B	552	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	ASN
1	A	91	ASN
1	A	152	HIS
1	A	153	ASN
1	A	197	HIS
1	A	240	HIS
1	A	352	ASN
1	A	403	GLN
1	A	467	HIS
1	A	474	ASN
1	A	485	GLN
1	A	520	ASN
1	A	528	ASN
1	A	533	ASN
1	A	552	GLN
1	B	79	ASN
1	B	91	ASN
1	B	152	HIS
1	B	153	ASN
1	B	197	HIS
1	B	240	HIS
1	B	352	ASN
1	B	403	GLN
1	B	474	ASN
1	B	485	GLN

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Mol	Chain	Res	Type
1	B	520	ASN
1	B	528	ASN
1	B	533	ASN
1	B	552	GLN

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	EUG	B	601	-	11,11,12	0.45	0	14,14,15	1.52	2 (14%)
3	EUG	A	601	-	11,11,12	0.45	0	14,14,15	1.51	2 (14%)
2	FAD	A	600	1	53,58,58	0.90	4 (7%)	68,89,89	0.99	4 (5%)
2	FAD	B	600	1	53,58,58	0.89	4 (7%)	68,89,89	1.00	4 (5%)

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	EUG	B	601	-	-	4/4/4/5	0/1/1/1
3	EUG	A	601	-	-	4/4/4/5	0/1/1/1
2	FAD	A	600	1	-	10/30/50/50	0/6/6/6
2	FAD	B	600	1	-	10/30/50/50	0/6/6/6

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	FAD	C5X-N5	-2.56	1.34	1.39
2	B	600	FAD	C5X-N5	-2.53	1.34	1.39
2	B	600	FAD	O5B-C5B	-2.41	1.35	1.44
2	A	600	FAD	O5B-C5B	-2.39	1.35	1.44
2	B	600	FAD	C4X-N5	2.06	1.34	1.30
2	A	600	FAD	C9A-N10	-2.05	1.37	1.41
2	A	600	FAD	C4X-N5	2.04	1.34	1.30
2	B	600	FAD	C9A-N10	-2.03	1.37	1.41

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	601	EUG	O3-C3-C4	4.01	120.38	114.57
3	A	601	EUG	O3-C3-C4	3.98	120.33	114.57
2	B	600	FAD	PA-O5B-C5B	2.48	136.23	121.68
2	A	600	FAD	PA-O5B-C5B	2.47	136.17	121.68
2	B	600	FAD	C5A-C6A-N6A	2.38	123.97	120.35
3	B	601	EUG	C9-O3-C3	2.37	121.11	117.53
3	A	601	EUG	C9-O3-C3	2.36	121.10	117.53
2	A	600	FAD	C5A-C6A-N6A	2.35	123.93	120.35
2	A	600	FAD	C4-N3-C2	-2.29	121.42	125.64
2	B	600	FAD	C4-N3-C2	-2.28	121.43	125.64
2	B	600	FAD	C4X-C10-N10	2.10	119.55	116.48
2	A	600	FAD	C4X-C10-N10	2.05	119.48	116.48

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	FAD	C5B-O5B-PA-O3P
2	A	600	FAD	C5'-O5'-P-O1P
2	B	600	FAD	C5B-O5B-PA-O3P
2	B	600	FAD	C5'-O5'-P-O1P

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Mol	Chain	Res	Type	Atoms
3	A	601	EUG	C6-C1-C7-C8
3	B	601	EUG	C6-C1-C7-C8
2	A	600	FAD	O4B-C4B-C5B-O5B
2	B	600	FAD	O4B-C4B-C5B-O5B
3	A	601	EUG	C2-C1-C7-C8
3	B	601	EUG	C2-C1-C7-C8
3	A	601	EUG	C2-C3-O3-C9
3	B	601	EUG	C2-C3-O3-C9
2	A	600	FAD	C4'-C5'-O5'-P
2	B	600	FAD	C4'-C5'-O5'-P
2	A	600	FAD	O4'-C4'-C5'-O5'
2	B	600	FAD	O4'-C4'-C5'-O5'
3	A	601	EUG	C4-C3-O3-C9
3	B	601	EUG	C4-C3-O3-C9
2	A	600	FAD	C3'-C4'-C5'-O5'
2	B	600	FAD	C3'-C4'-C5'-O5'
2	A	600	FAD	C5'-O5'-P-O3P
2	B	600	FAD	C5'-O5'-P-O3P
2	A	600	FAD	C5B-O5B-PA-O1A
2	A	600	FAD	C5'-O5'-P-O2P
2	B	600	FAD	C5B-O5B-PA-O1A
2	B	600	FAD	C5'-O5'-P-O2P
2	A	600	FAD	C1'-C2'-C3'-O3'
2	B	600	FAD	C1'-C2'-C3'-O3'

There are no ring outliers.

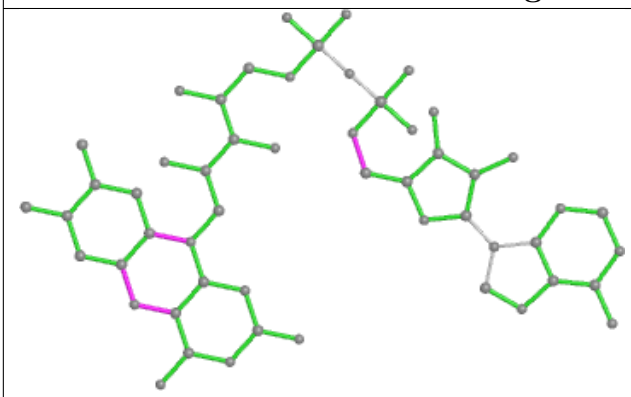
4 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	EUG	5	0
3	A	601	EUG	4	0
2	A	600	FAD	17	0
2	B	600	FAD	18	0

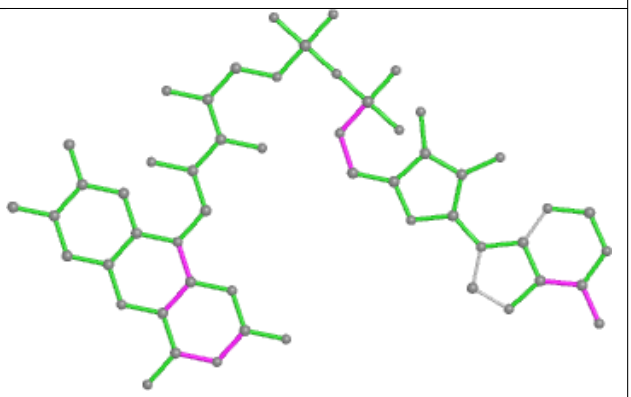
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

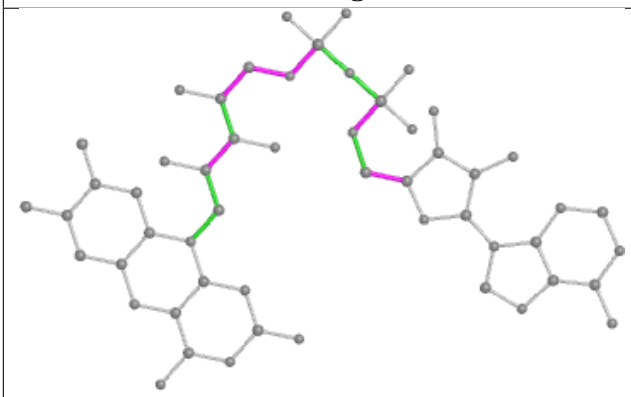
Ligand FAD A 600



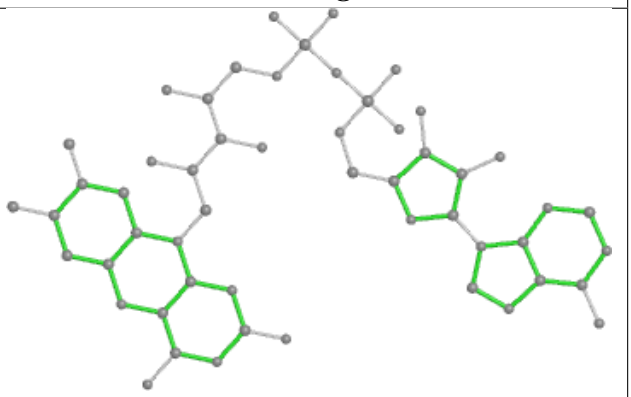
Bond lengths



Bond angles

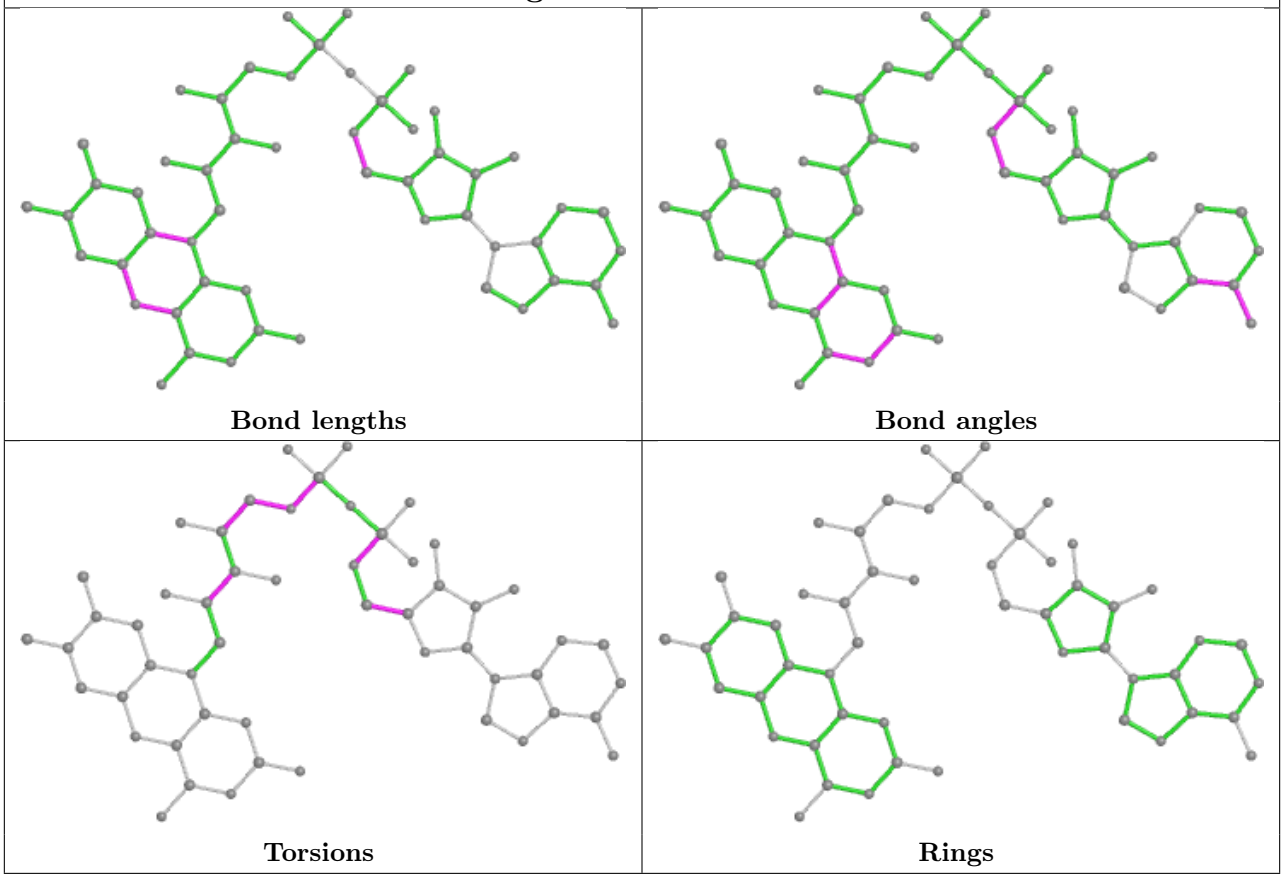


Torsions



Rings

Ligand FAD B 600



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.