Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2024 – 09:34 PM EDT

PDB ID	:	1VAO
Title	:	STRUCTURE OF THE OCTAMERIC FLAVOENZYME VANILLYL-ALCOHOL OXIDASE
Authors	:	Mattevi, A.
Deposited on	:	1997-04-10
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:

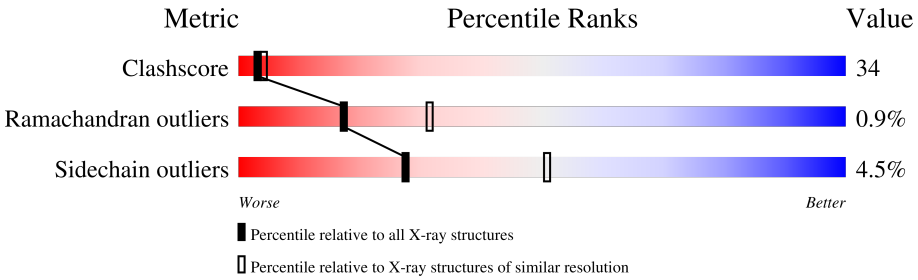
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

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	560	47% 41% 8%
1	B	560	48% 40% 8%

2 Entry composition

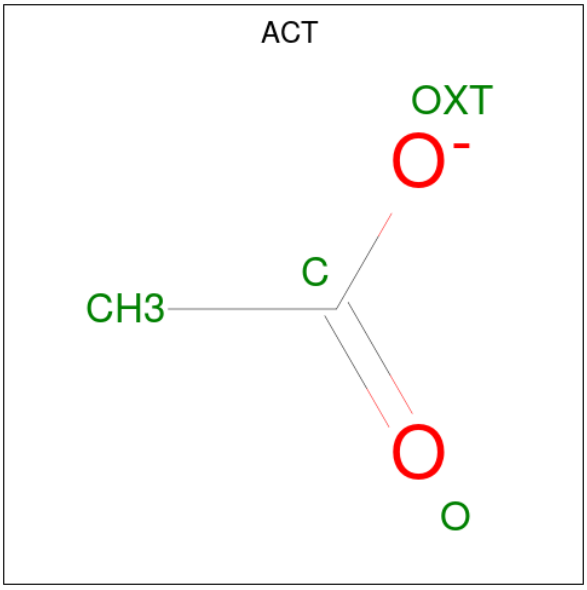
There are 5 unique types of molecules in this entry. The entry contains 9134 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	550	Total	C	N	O	S	36	0	0
			4351	2793	744	790	24			
1	B	550	Total	C	N	O	S	36	0	0
			4351	2793	744	790	24			

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

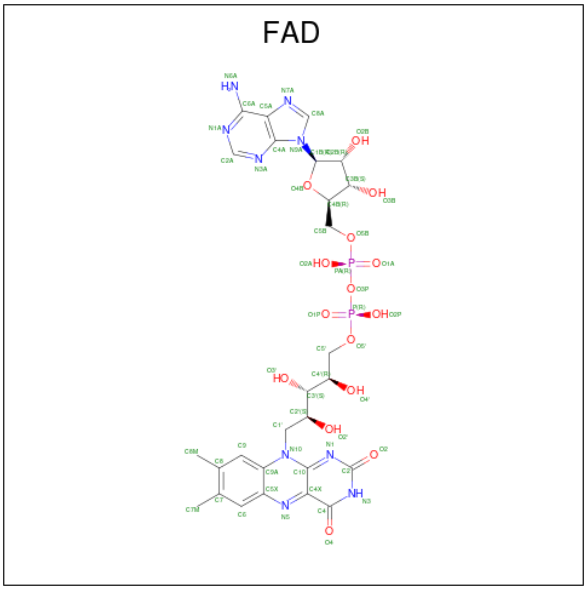


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	166	Total O 166 166	0	0
5	B	150	Total O 150 150	0	0

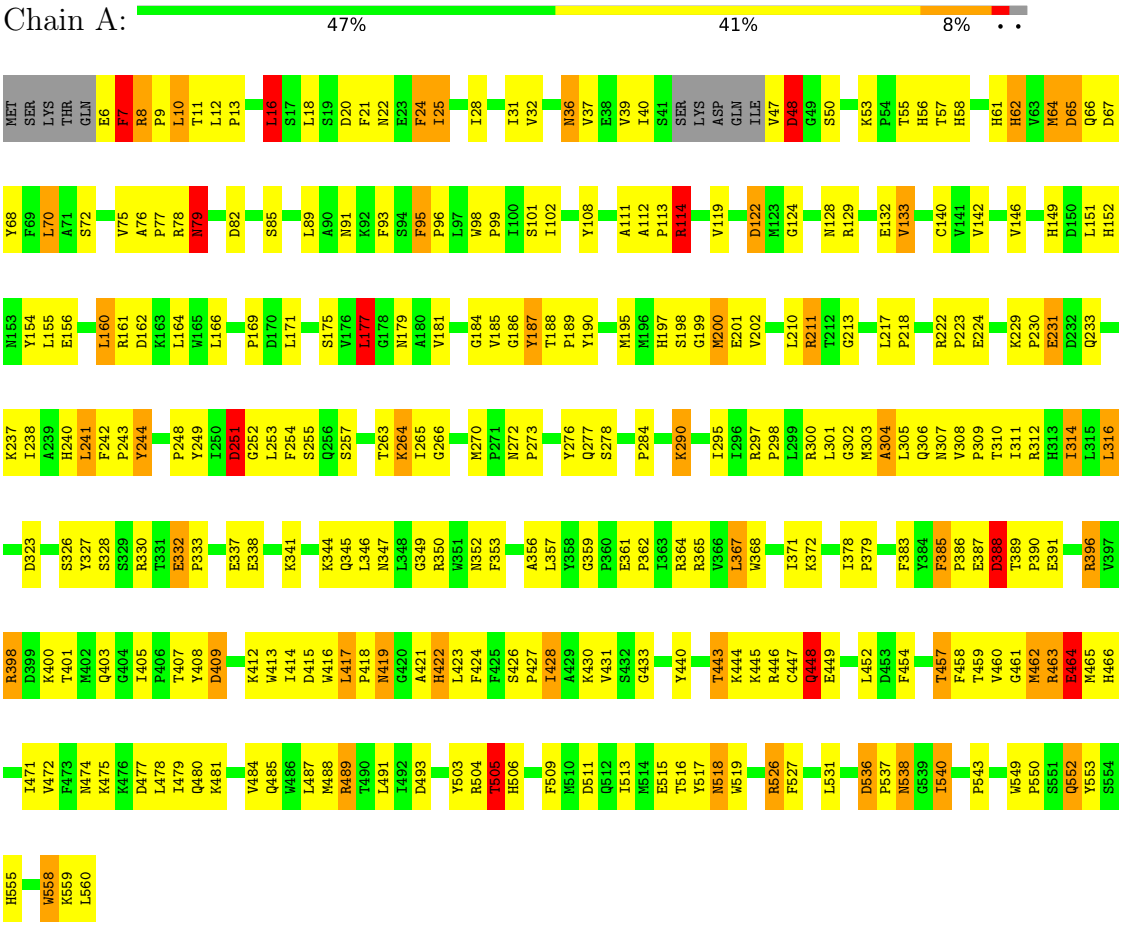
3 Residue-property plots (i)

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.

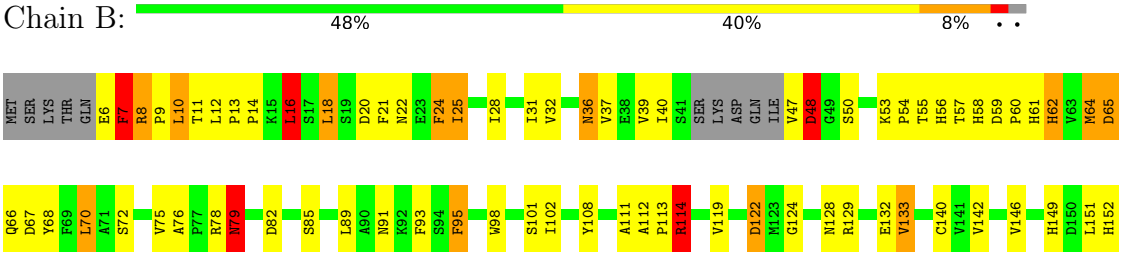
• Molecule 1: VANILLYL-ALCOHOL OXIDASE

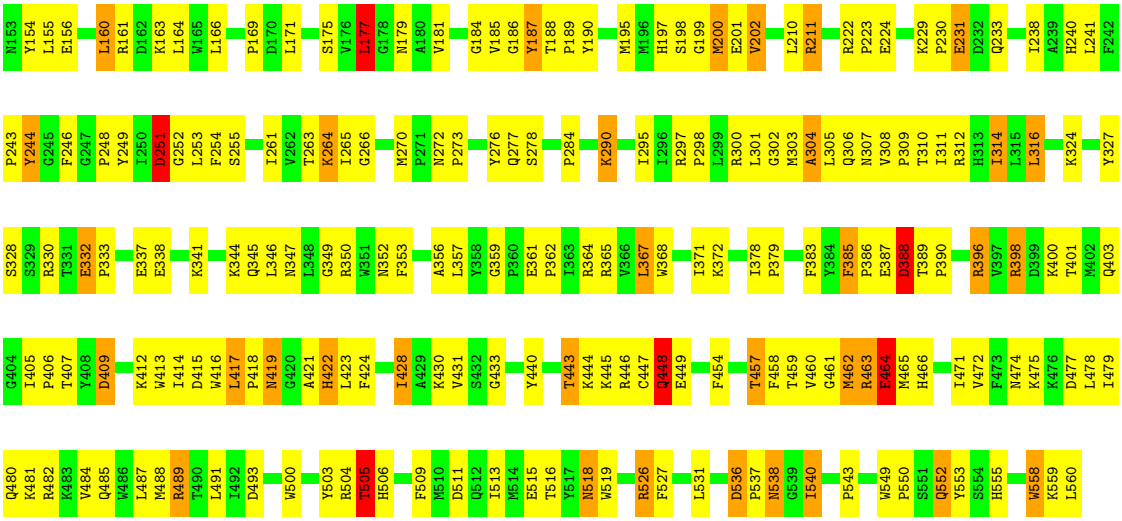
Chain A:



• Molecule 1: VANILLYL-ALCOHOL OXIDASE

Chain B:




N153 Y154 L155 E156 L160 R161 D162 K163 L164 W165 L166 P169 D170 L171 S175 V176 L177 G178 N179 A180 V181 G184 V185 G186 Y187 T188 P189 Y190 M195 M196 H197 S198 G199 M200 E201 V202 L210 R211 R222 P223 E224 K229 P230 E231 D232 Q233 I238 A239 H240 L241 F242
P243 Y244 G245 F246 G247 P248 Y249 I250 D251 G252 L253 F254 S255 I261 V262 T263 K264 I265 G266 M270 P271 N272 P273 Y276 Q277 S278 P284 K290 I295 I296 R297 P298 L299 R300 L301 G302 M303 A304 L305 Q306 N307 V308 P309 T310 I311 R312 H313 I314 L315 L316 K324 Y327
S328 S329 R330 T331 E332 P333 E337 E338 K341 K344 Q345 L346 N347 L348 G349 R350 W351 N352 F353 A356 L357 Y358 G359 P360 E361 P362 I363 R364 R365 V366 L367 W368 I371 K372 I378 P379 F383 Y384 F385 P386 E387 D388 T389 P390 R396 V397 R398 D399 K400 T401 M402 Q403
G404 I405 P406 T407 Y408 D409 K412 W413 I414 D415 W416 L417 P418 N419 G420 A421 H422 L423 F424 I428 A429 K430 V431 S432 G433 Y440 T443 K444 K445 R446 C447 Q448 E449 F454 T457 F458 T459 V460 G461 M462 R463 E464 M465 H466 I471 V472 F473 N474 K475 K476 D477 L478 I479
Q480 K481 R482 K483 V484 Q485 W486 L487 M488 R489 T490 L491 I492 D493 W500 Y503 R504 T505 H506 F509 M510 D511 Q512 I513 N514 E515 T516 Y517 N518 W519 R526 F527 L531 D536 P537 N538 G539 I540 P543 W549 P550 S551 Q552 Y553 S554 H555 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	130.24Å 130.24Å 133.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50	Depositor
% Data completeness (in resolution range)	98.9 (30.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.88	Depositor
Refinement program	TNT 5E	Depositor
R, R_{free}	0.220 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9134	wwPDB-VP
Average B, all atoms (Å^2)	24.0	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, CL, ACT

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	0.76	3/4470 (0.1%)	1.68	89/6075 (1.5%)
1	B	0.76	3/4470 (0.1%)	1.68	89/6075 (1.5%)
All	All	0.76	6/8940 (0.1%)	1.68	178/12150 (1.5%)

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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	7	PHE	CE1-CZ	7.54	1.51	1.37
1	B	7	PHE	CE1-CZ	7.50	1.51	1.37
1	A	7	PHE	CD1-CE1	7.35	1.53	1.39
1	B	7	PHE	CD1-CE1	7.35	1.53	1.39
1	A	7	PHE	CD2-CE2	6.36	1.51	1.39
1	B	7	PHE	CD2-CE2	6.34	1.51	1.39

All (178) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	526	ARG	NE-CZ-NH2	-19.95	110.33	120.30
1	A	526	ARG	NE-CZ-NH2	-19.88	110.36	120.30
1	B	526	ARG	NE-CZ-NH1	13.88	127.24	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	526	ARG	NE-CZ-NH1	13.87	127.23	120.30
1	A	489	ARG	NE-CZ-NH1	12.01	126.31	120.30
1	B	489	ARG	NE-CZ-NH1	11.88	126.24	120.30
1	A	7	PHE	CB-CG-CD1	11.24	128.67	120.80
1	B	7	PHE	CB-CG-CD1	11.23	128.66	120.80
1	B	128	ASN	CB-CA-C	-10.13	90.14	110.40
1	A	128	ASN	CB-CA-C	-10.12	90.15	110.40
1	B	526	ARG	CG-CD-NE	-9.51	91.83	111.80
1	A	526	ARG	CG-CD-NE	-9.50	91.86	111.80
1	B	200	MET	CG-SD-CE	-9.06	85.70	100.20
1	A	200	MET	CG-SD-CE	-9.05	85.71	100.20
1	B	464	GLU	N-CA-CB	-8.84	94.69	110.60
1	A	464	GLU	N-CA-CB	-8.81	94.73	110.60
1	B	7	PHE	CB-CG-CD2	-8.78	114.65	120.80
1	A	7	PHE	CB-CG-CD2	-8.77	114.66	120.80
1	A	536	ASP	C-N-CD	-8.63	101.62	120.60
1	B	536	ASP	C-N-CD	-8.62	101.63	120.60
1	B	7	PHE	N-CA-C	8.55	134.09	111.00
1	A	7	PHE	N-CA-C	8.54	134.06	111.00
1	A	489	ARG	NE-CZ-NH2	-8.43	116.09	120.30
1	B	489	ARG	NE-CZ-NH2	-8.38	116.11	120.30
1	A	202	VAL	CB-CA-C	-8.35	95.53	111.40
1	B	202	VAL	CB-CA-C	-8.35	95.54	111.40
1	B	129	ARG	N-CA-C	8.30	133.40	111.00
1	A	129	ARG	N-CA-C	8.29	133.38	111.00
1	B	505	THR	CB-CA-C	-8.18	89.52	111.60
1	A	505	THR	CB-CA-C	-8.17	89.55	111.60
1	A	388	ASP	CB-CG-OD1	-8.10	111.01	118.30
1	B	388	ASP	CB-CG-OD1	-8.07	111.04	118.30
1	A	419	ASN	N-CA-C	-8.02	89.35	111.00
1	B	419	ASN	N-CA-C	-8.00	89.40	111.00
1	B	187	TYR	N-CA-C	7.80	132.06	111.00
1	A	187	TYR	N-CA-C	7.79	132.03	111.00
1	A	396	ARG	NE-CZ-NH2	-7.59	116.50	120.30
1	B	396	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	B	122	ASP	N-CA-CB	7.11	123.39	110.60
1	A	122	ASP	N-CA-CB	7.10	123.38	110.60
1	A	160	LEU	CB-CG-CD2	-7.09	98.94	111.00
1	B	160	LEU	CB-CG-CD2	-7.09	98.94	111.00
1	B	114	ARG	CB-CG-CD	7.07	129.99	111.60
1	A	114	ARG	CB-CG-CD	7.06	129.96	111.60
1	B	446	ARG	NE-CZ-NH1	-7.02	116.79	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	25	ILE	CB-CA-C	7.02	125.64	111.60
1	A	446	ARG	NE-CZ-NH1	-7.00	116.80	120.30
1	B	25	ILE	CB-CA-C	7.00	125.59	111.60
1	B	448	GLN	CB-CA-C	6.94	124.28	110.40
1	A	448	GLN	CB-CA-C	6.92	124.24	110.40
1	A	18	LEU	CA-CB-CG	-6.91	99.40	115.30
1	B	18	LEU	CA-CB-CG	-6.90	99.44	115.30
1	A	463	ARG	N-CA-CB	-6.85	98.27	110.60
1	B	463	ARG	N-CA-CB	-6.85	98.27	110.60
1	A	518	ASN	N-CA-C	6.80	129.35	111.00
1	B	518	ASN	N-CA-C	6.79	129.34	111.00
1	A	428	ILE	CG1-CB-CG2	-6.77	96.51	111.40
1	B	428	ILE	CG1-CB-CG2	-6.76	96.52	111.40
1	A	457	THR	CB-CA-C	-6.73	93.44	111.60
1	B	457	THR	CB-CA-C	-6.73	93.44	111.60
1	A	430	LYS	CB-CG-CD	-6.57	94.51	111.60
1	B	430	LYS	CB-CG-CD	-6.57	94.53	111.60
1	B	540	ILE	CB-CA-C	-6.56	98.49	111.60
1	A	540	ILE	CB-CA-C	-6.51	98.57	111.60
1	A	177	LEU	CA-CB-CG	6.42	130.08	115.30
1	B	177	LEU	CA-CB-CG	6.42	130.05	115.30
1	A	558	TRP	N-CA-C	6.40	128.28	111.00
1	B	558	TRP	N-CA-C	6.39	128.25	111.00
1	B	241	LEU	CB-CG-CD2	6.24	121.60	111.00
1	A	241	LEU	CB-CG-CD2	6.22	121.57	111.00
1	A	304	ALA	N-CA-C	-6.14	94.42	111.00
1	B	251	ASP	CB-CG-OD1	6.13	123.82	118.30
1	A	526	ARG	CD-NE-CZ	6.13	132.18	123.60
1	B	487	LEU	CB-CG-CD2	-6.13	100.58	111.00
1	B	177	LEU	CB-CA-C	6.13	121.84	110.20
1	A	430	LYS	CD-CE-NZ	-6.12	97.61	111.70
1	B	304	ALA	N-CA-C	-6.12	94.47	111.00
1	B	430	LYS	CD-CE-NZ	-6.12	97.62	111.70
1	A	177	LEU	CB-CA-C	6.12	121.83	110.20
1	A	487	LEU	CB-CG-CD2	-6.11	100.61	111.00
1	B	526	ARG	CD-NE-CZ	6.11	132.15	123.60
1	B	36	ASN	CB-CA-C	6.08	122.57	110.40
1	A	251	ASP	CB-CG-OD1	6.08	123.77	118.30
1	A	211	ARG	CB-CG-CD	6.08	127.40	111.60
1	B	211	ARG	CB-CG-CD	6.08	127.40	111.60
1	A	36	ASN	CB-CA-C	6.07	122.53	110.40
1	B	388	ASP	CB-CG-OD2	6.02	123.72	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	62	HIS	N-CA-C	6.02	127.25	111.00
1	A	367	LEU	CA-CB-CG	-6.01	101.46	115.30
1	B	367	LEU	CA-CB-CG	-6.01	101.48	115.30
1	A	62	HIS	N-CA-C	6.00	127.20	111.00
1	A	388	ASP	CB-CG-OD2	5.98	123.68	118.30
1	B	297	ARG	N-CA-C	5.97	127.13	111.00
1	A	297	ARG	N-CA-C	5.97	127.11	111.00
1	A	8	ARG	CB-CA-C	-5.96	98.47	110.40
1	B	8	ARG	CB-CA-C	-5.93	98.53	110.40
1	A	24	PHE	N-CA-CB	-5.92	99.94	110.60
1	B	24	PHE	N-CA-CB	-5.92	99.95	110.60
1	A	171	LEU	CB-CG-CD2	-5.91	100.96	111.00
1	B	171	LEU	CB-CG-CD2	-5.90	100.98	111.00
1	B	398	ARG	NE-CZ-NH1	5.87	123.24	120.30
1	A	398	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	A	462	MET	CA-CB-CG	5.83	123.21	113.30
1	A	493	ASP	CB-CG-OD1	5.80	123.52	118.30
1	B	462	MET	CA-CB-CG	5.79	123.14	113.30
1	B	290	LYS	CD-CE-NZ	5.77	124.97	111.70
1	A	290	LYS	CD-CE-NZ	5.75	124.94	111.70
1	B	493	ASP	CB-CG-OD1	5.75	123.47	118.30
1	B	48	ASP	C-N-CA	-5.74	110.25	122.30
1	A	48	ASP	C-N-CA	-5.72	110.28	122.30
1	B	164	LEU	CB-CA-C	-5.69	99.39	110.20
1	A	164	LEU	CB-CA-C	-5.65	99.46	110.20
1	A	79	ASN	N-CA-CB	-5.65	100.43	110.60
1	B	211	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	B	79	ASN	N-CA-CB	-5.64	100.44	110.60
1	B	244	TYR	N-CA-C	5.64	126.22	111.00
1	A	244	TYR	N-CA-C	5.63	126.21	111.00
1	A	211	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	B	264	LYS	CB-CA-C	-5.57	99.26	110.40
1	A	264	LYS	CB-CA-C	-5.56	99.28	110.40
1	B	312	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	B	16	LEU	CB-CG-CD1	5.54	120.42	111.00
1	A	89	LEU	CB-CG-CD2	-5.54	101.59	111.00
1	A	16	LEU	CB-CG-CD1	5.53	120.40	111.00
1	B	89	LEU	CB-CG-CD2	-5.51	101.63	111.00
1	B	133	VAL	N-CA-C	-5.50	96.14	111.00
1	A	133	VAL	N-CA-C	-5.50	96.15	111.00
1	A	415	ASP	N-CA-C	5.50	125.84	111.00
1	B	415	ASP	N-CA-C	5.49	125.82	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	312	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	A	417	LEU	CB-CG-CD2	5.45	120.27	111.00
1	B	417	LEU	CB-CG-CD2	5.45	120.26	111.00
1	A	421	ALA	N-CA-C	-5.42	96.36	111.00
1	B	10	LEU	CB-CG-CD1	-5.41	101.81	111.00
1	B	421	ALA	N-CA-C	-5.41	96.41	111.00
1	A	16	LEU	CA-CB-CG	5.40	127.71	115.30
1	B	16	LEU	CA-CB-CG	5.40	127.72	115.30
1	B	443	THR	CB-CA-C	-5.40	97.03	111.60
1	A	443	THR	CB-CA-C	-5.39	97.04	111.60
1	A	10	LEU	CB-CG-CD1	-5.39	101.84	111.00
1	A	32	VAL	N-CA-C	5.37	125.50	111.00
1	B	32	VAL	N-CA-C	5.36	125.48	111.00
1	B	560	LEU	N-CA-C	-5.32	96.65	111.00
1	A	560	LEU	N-CA-C	-5.30	96.70	111.00
1	A	396	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	B	493	ASP	CB-CG-OD2	-5.25	113.58	118.30
1	B	251	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	B	396	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	B	316	LEU	CB-CG-CD2	-5.22	102.13	111.00
1	A	316	LEU	CB-CG-CD2	-5.21	102.13	111.00
1	A	461	GLY	N-CA-C	-5.19	100.12	113.10
1	A	493	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	B	461	GLY	N-CA-C	-5.19	100.13	113.10
1	A	251	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	B	114	ARG	CG-CD-NE	5.14	122.59	111.80
1	A	114	ARG	CG-CD-NE	5.13	122.57	111.80
1	A	332	GLU	N-CA-CB	5.12	119.82	110.60
1	A	290	LYS	CB-CG-CD	5.12	124.92	111.60
1	B	70	LEU	CA-CB-CG	5.12	127.08	115.30
1	B	306	GLN	N-CA-C	5.12	124.83	111.00
1	A	249	TYR	CB-CA-C	5.11	120.63	110.40
1	A	70	LEU	CA-CB-CG	5.11	127.06	115.30
1	B	290	LYS	CB-CG-CD	5.11	124.89	111.60
1	A	290	LYS	CA-CB-CG	-5.11	102.16	113.40
1	B	332	GLU	N-CA-CB	5.11	119.80	110.60
1	B	290	LYS	CA-CB-CG	-5.11	102.17	113.40
1	A	306	GLN	N-CA-C	5.10	124.77	111.00
1	B	249	TYR	CB-CA-C	5.10	120.59	110.40
1	A	385	PHE	N-CA-C	-5.09	97.26	111.00
1	B	385	PHE	N-CA-C	-5.08	97.28	111.00
1	B	211	ARG	CB-CA-C	5.07	120.54	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	171	LEU	CA-CB-CG	-5.06	103.66	115.30
1	A	231	GLU	CA-CB-CG	-5.06	102.27	113.40
1	B	231	GLU	CA-CB-CG	-5.06	102.27	113.40
1	A	211	ARG	CB-CA-C	5.05	120.50	110.40
1	B	171	LEU	CA-CB-CG	-5.05	103.68	115.30
1	B	538	ASN	CB-CA-C	-5.02	100.36	110.40
1	A	538	ASN	CB-CA-C	-5.02	100.36	110.40

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	7	PHE	CA
1	A	332	GLU	CA
1	B	7	PHE	CA
1	B	332	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	4351	0	4288	307	1
1	B	4351	0	4288	286	0
2	A	4	0	3	0	0
2	B	4	0	3	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	53	0	29	6	0
4	B	53	0	29	5	0
5	A	166	0	0	19	0
5	B	150	0	0	11	0
All	All	9134	0	8640	580	1

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 34.

All (580) 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)
4:B:600:FAD:H51A	4:B:600:FAD:H8A	1.22	1.16
4:A:600:FAD:H8A	4:A:600:FAD:H51A	1.23	1.11
1:A:253:LEU:HD21	1:B:253:LEU:HD21	1.11	1.07
1:A:211:ARG:HG3	1:B:519:TRP:CZ3	1.99	0.98
1:B:555:HIS:HB3	1:B:559:LYS:HE3	1.46	0.97
1:A:91:ASN:HD22	1:A:538:ASN:ND2	1.62	0.97
1:A:555:HIS:HB3	1:A:559:LYS:HE3	1.46	0.97
1:B:91:ASN:HD22	1:B:538:ASN:ND2	1.62	0.96
1:B:91:ASN:ND2	1:B:538:ASN:HD22	1.66	0.94
1:A:519:TRP:CZ3	1:B:211:ARG:HG3	2.03	0.93
1:A:91:ASN:ND2	1:A:538:ASN:HD22	1.66	0.91
1:A:448:GLN:HE21	1:A:448:GLN:N	1.70	0.89
1:B:448:GLN:N	1:B:448:GLN:HE21	1.70	0.89
1:A:550:PRO:HB2	1:A:552:GLN:HE21	1.39	0.87
1:A:505:THR:HG22	1:A:506:HIS:H	1.37	0.87
1:B:550:PRO:HB2	1:B:552:GLN:HE21	1.39	0.87
1:B:505:THR:HG22	1:B:506:HIS:H	1.37	0.86
1:A:91:ASN:HD22	1:A:538:ASN:HD22	0.88	0.85
1:A:445:LYS:HE2	1:A:449:GLU:OE2	1.76	0.85
1:A:341:LYS:O	1:A:344:LYS:HG2	1.77	0.85
4:A:600:FAD:H51A	4:A:600:FAD:C8A	2.06	0.85
1:B:445:LYS:HE2	1:B:449:GLU:OE2	1.76	0.84
1:A:538:ASN:CB	1:A:540:ILE:HD11	2.08	0.84
1:A:78:ARG:HD3	1:A:82:ASP:OD2	1.78	0.84
1:A:414:ILE:HD11	4:A:600:FAD:HM71	1.56	0.84
1:A:550:PRO:HG2	1:A:553:TYR:CD1	2.13	0.84
1:B:538:ASN:CB	1:B:540:ILE:HD11	2.08	0.84
1:B:91:ASN:HD22	1:B:538:ASN:HD22	0.88	0.84
1:B:550:PRO:HG2	1:B:553:TYR:CD1	2.13	0.84
1:B:414:ILE:HD11	4:B:600:FAD:HM71	1.56	0.83
4:B:600:FAD:H51A	4:B:600:FAD:C8A	2.06	0.83
1:B:78:ARG:HD3	1:B:82:ASP:OD2	1.78	0.83
1:B:341:LYS:O	1:B:344:LYS:HG2	1.77	0.83
1:A:349:GLY:H	1:A:352:ASN:HD21	1.27	0.81
1:A:550:PRO:CB	1:A:552:GLN:HE21	1.93	0.80
1:B:349:GLY:H	1:B:352:ASN:HD21	1.27	0.80
1:B:550:PRO:CB	1:B:552:GLN:HE21	1.93	0.80
1:A:538:ASN:HB2	1:A:540:ILE:HD11	1.63	0.79
1:B:538:ASN:HB2	1:B:540:ILE:HD11	1.63	0.79
1:A:253:LEU:CD2	1:B:253:LEU:HD21	2.05	0.78
1:A:187:TYR:O	1:A:307:ASN:HB2	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:TYR:O	1:B:307:ASN:HB2	1.83	0.77
1:B:350:ARG:HD2	5:B:694:HOH:O	1.85	0.77
1:A:361:GLU:HB3	1:A:362:PRO:HD3	1.67	0.77
1:A:385:PHE:HB3	1:A:386:PRO:HD2	1.66	0.77
1:B:21:PHE:O	1:B:25:ILE:HG22	1.86	0.76
1:B:385:PHE:HB3	1:B:386:PRO:HD2	1.66	0.76
1:B:516:THR:HG21	5:B:731:HOH:O	1.84	0.76
1:B:304:ALA:HB2	5:B:631:HOH:O	1.86	0.76
1:B:341:LYS:O	1:B:345:GLN:HG3	1.86	0.76
1:B:361:GLU:HB3	1:B:362:PRO:HD3	1.67	0.76
1:A:341:LYS:O	1:A:345:GLN:HG3	1.86	0.76
1:B:482:ARG:HD2	5:B:655:HOH:O	1.86	0.76
1:A:21:PHE:O	1:A:25:ILE:HG22	1.86	0.75
1:B:419:ASN:O	1:B:474:ASN:HA	1.86	0.75
1:A:79:ASN:ND2	1:A:82:ASP:H	1.85	0.74
1:A:478:LEU:HD12	1:A:478:LEU:H	1.53	0.74
1:B:416:TRP:C	1:B:417:LEU:HD23	2.08	0.74
1:A:416:TRP:C	1:A:417:LEU:HD23	2.08	0.74
4:B:600:FAD:H8A	4:B:600:FAD:C5B	2.11	0.74
1:A:515:GLU:HB2	5:A:765:HOH:O	1.87	0.74
1:A:409:ASP:HA	1:A:412:LYS:HE3	1.69	0.74
1:A:419:ASN:O	1:A:474:ASN:HA	1.87	0.74
1:B:79:ASN:ND2	1:B:82:ASP:H	1.85	0.73
1:B:230:PRO:HA	1:B:233:GLN:HG3	1.70	0.73
1:B:409:ASP:HA	1:B:412:LYS:HE3	1.69	0.73
1:B:478:LEU:HD12	1:B:478:LEU:H	1.53	0.72
1:A:91:ASN:ND2	1:A:538:ASN:ND2	2.31	0.72
4:A:600:FAD:H8A	4:A:600:FAD:C5B	2.11	0.72
1:A:516:THR:HG21	5:A:709:HOH:O	1.88	0.72
1:B:114:ARG:NH2	5:B:638:HOH:O	2.23	0.72
1:A:230:PRO:HA	1:A:233:GLN:HG3	1.70	0.72
1:A:253:LEU:HD21	1:B:253:LEU:CD2	2.05	0.72
1:A:314:ILE:HD13	1:A:314:ILE:O	1.91	0.71
1:A:244:TYR:OH	1:B:195:MET:HG2	1.90	0.71
1:B:389:THR:HB	1:B:390:PRO:HD2	1.72	0.71
1:A:37:VAL:HG13	1:A:75:VAL:HG22	1.72	0.70
1:B:314:ILE:HD13	1:B:314:ILE:O	1.91	0.70
1:A:389:THR:HB	1:A:390:PRO:HD2	1.72	0.70
1:B:37:VAL:HG13	1:B:75:VAL:HG22	1.72	0.70
1:B:31:ILE:HD13	1:B:85:SER:HB3	1.74	0.70
1:A:31:ILE:HD13	1:A:85:SER:HB3	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:463:ARG:HD2	5:B:725:HOH:O	1.92	0.70
1:B:156:GLU:HB2	1:B:161:ARG:NH2	2.07	0.69
1:B:132:GLU:HG2	1:B:133:VAL:N	2.08	0.69
1:A:156:GLU:HB2	1:A:161:ARG:NH2	2.07	0.69
1:B:210:LEU:HD23	1:B:211:ARG:N	2.08	0.69
1:A:210:LEU:HD23	1:A:211:ARG:N	2.08	0.68
1:A:96:PRO:HG3	5:A:746:HOH:O	1.94	0.68
1:A:550:PRO:HG2	1:A:553:TYR:HD1	1.58	0.68
1:A:132:GLU:HG2	1:A:133:VAL:N	2.08	0.67
1:A:538:ASN:HB3	1:A:540:ILE:HD11	1.75	0.67
1:A:162:ASP:HB2	5:A:727:HOH:O	1.95	0.67
1:A:195:MET:HG2	1:B:244:TYR:OH	1.94	0.67
1:B:163:LYS:HG2	5:B:726:HOH:O	1.93	0.67
1:B:513:ILE:O	1:B:516:THR:HB	1.95	0.67
1:B:538:ASN:HB3	1:B:540:ILE:HD11	1.75	0.67
1:A:513:ILE:O	1:A:516:THR:HB	1.95	0.67
1:B:91:ASN:ND2	1:B:538:ASN:ND2	2.31	0.67
1:B:133:VAL:HG21	1:B:154:TYR:CE2	2.30	0.66
1:A:423:LEU:HD21	1:A:488:MET:HG3	1.78	0.66
1:B:142:VAL:CG2	1:B:146:VAL:HB	2.26	0.66
1:A:133:VAL:HG21	1:A:154:TYR:CE2	2.30	0.66
1:A:142:VAL:CG2	1:A:146:VAL:HB	2.25	0.66
1:B:550:PRO:HG2	1:B:553:TYR:HD1	1.58	0.66
1:B:156:GLU:HB2	1:B:161:ARG:NE	2.10	0.66
1:B:423:LEU:HD21	1:B:488:MET:HG3	1.78	0.66
1:A:505:THR:HG21	1:A:513:ILE:HD12	1.78	0.66
1:A:222:ARG:HG3	1:A:224:GLU:OE1	1.96	0.65
1:A:156:GLU:HB2	1:A:161:ARG:NE	2.11	0.65
1:B:349:GLY:N	1:B:352:ASN:HD21	1.94	0.65
1:A:330:ARG:NH1	1:A:338:GLU:OE1	2.30	0.65
1:B:330:ARG:NH1	1:B:338:GLU:OE1	2.30	0.65
1:A:50:SER:OG	1:A:53:LYS:N	2.29	0.65
1:A:379:PRO:HG3	5:A:668:HOH:O	1.97	0.64
1:B:505:THR:HG21	1:B:513:ILE:HD12	1.78	0.64
1:B:222:ARG:HG3	1:B:224:GLU:OE1	1.97	0.64
1:B:505:THR:HG22	1:B:506:HIS:N	2.11	0.64
1:A:99:PRO:HD2	5:A:642:HOH:O	1.97	0.64
1:A:505:THR:HG22	1:A:506:HIS:N	2.11	0.64
1:A:478:LEU:HD12	1:A:478:LEU:N	2.12	0.64
1:B:464:GLU:OE2	1:B:466:HIS:ND1	2.30	0.64
1:A:464:GLU:OE2	1:A:466:HIS:ND1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:GLY:N	1:A:352:ASN:HD21	1.94	0.64
1:A:543:PRO:HB3	1:A:550:PRO:HG3	1.80	0.64
1:B:550:PRO:HB2	1:B:552:GLN:HG2	1.80	0.63
1:B:65:ASP:OD1	1:B:65:ASP:N	2.31	0.63
1:B:478:LEU:HD12	1:B:478:LEU:N	2.12	0.63
1:B:50:SER:OG	1:B:53:LYS:N	2.30	0.63
1:A:156:GLU:HB2	1:A:161:ARG:CZ	2.29	0.63
1:A:300:ARG:NH2	1:A:460:VAL:O	2.32	0.63
1:B:156:GLU:HB2	1:B:161:ARG:CZ	2.29	0.62
1:A:550:PRO:HB2	1:A:552:GLN:HG2	1.80	0.62
1:B:300:ARG:NH2	1:B:460:VAL:O	2.32	0.62
1:B:337:GLU:O	1:B:341:LYS:HG3	1.99	0.62
1:A:95:PHE:CE1	1:A:119:VAL:HG23	2.34	0.62
1:B:95:PHE:CE1	1:B:119:VAL:HG23	2.34	0.62
1:B:543:PRO:HB3	1:B:550:PRO:HG3	1.80	0.62
1:B:310:THR:HG22	1:B:459:THR:HG22	1.82	0.62
1:A:337:GLU:O	1:A:341:LYS:HG3	2.00	0.62
1:A:211:ARG:HG3	1:B:519:TRP:CE3	2.34	0.61
1:A:310:THR:HG22	1:A:459:THR:HG22	1.82	0.61
1:B:478:LEU:H	1:B:478:LEU:CD1	2.14	0.61
1:B:79:ASN:C	1:B:79:ASN:HD22	2.04	0.61
1:A:156:GLU:OE1	1:A:161:ARG:NH2	2.34	0.61
1:A:243:PRO:HD2	1:A:244:TYR:H	1.65	0.61
1:B:156:GLU:OE1	1:B:161:ARG:NH2	2.34	0.61
1:B:243:PRO:HD2	1:B:244:TYR:H	1.65	0.60
1:A:79:ASN:C	1:A:79:ASN:HD22	2.04	0.60
1:B:361:GLU:HB3	1:B:362:PRO:CD	2.31	0.60
1:A:478:LEU:H	1:A:478:LEU:CD1	2.13	0.60
1:B:505:THR:HG21	1:B:509:PHE:HB2	1.83	0.60
1:A:238:ILE:HG12	5:A:689:HOH:O	2.02	0.59
1:A:316:LEU:HD11	1:A:413:TRP:CD1	2.38	0.59
1:A:505:THR:HG21	1:A:509:PHE:HB2	1.83	0.59
1:B:13:PRO:HG3	1:B:95:PHE:CE1	2.37	0.59
1:B:409:ASP:HA	1:B:412:LYS:CE	2.33	0.59
1:A:479:ILE:HD12	1:A:479:ILE:N	2.18	0.59
1:B:316:LEU:HD11	1:B:413:TRP:CD1	2.38	0.59
1:A:361:GLU:HB3	1:A:362:PRO:CD	2.31	0.59
1:B:224:GLU:CD	1:B:224:GLU:H	2.06	0.59
1:A:58:HIS:HA	1:A:112:ALA:HB2	1.85	0.59
1:B:479:ILE:N	1:B:479:ILE:HD12	2.18	0.59
1:A:24:PHE:O	1:A:28:ILE:HG13	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:ASN:HA	1:B:25:ILE:HG22	1.85	0.58
1:A:65:ASP:N	1:A:65:ASP:OD1	2.31	0.58
1:A:224:GLU:CD	1:A:224:GLU:H	2.06	0.58
1:A:98:TRP:CD2	1:A:113:PRO:HA	2.38	0.58
1:B:24:PHE:O	1:B:28:ILE:HG13	2.02	0.58
1:B:98:TRP:CD2	1:B:113:PRO:HA	2.38	0.58
1:A:189:PRO:HA	1:A:307:ASN:HA	1.85	0.58
1:B:152:HIS:CE1	1:B:161:ARG:NH2	2.72	0.58
1:A:13:PRO:HG3	1:A:95:PHE:CE1	2.38	0.58
1:A:152:HIS:CE1	1:A:161:ARG:NH2	2.72	0.58
1:B:189:PRO:HA	1:B:307:ASN:HA	1.85	0.58
1:A:409:ASP:HA	1:A:412:LYS:CE	2.33	0.58
1:A:417:LEU:HD23	1:A:417:LEU:N	2.19	0.58
1:A:238:ILE:HD13	1:A:238:ILE:N	2.18	0.57
1:B:238:ILE:N	1:B:238:ILE:HD13	2.18	0.57
1:B:477:ASP:O	1:B:481:LYS:HG3	2.03	0.57
1:A:22:ASN:HA	1:A:25:ILE:HG22	1.86	0.57
1:A:156:GLU:HB2	1:A:161:ARG:HH21	1.68	0.57
1:A:477:ASP:O	1:A:481:LYS:HG3	2.03	0.57
5:A:724:HOH:O	1:B:519:TRP:HE3	1.86	0.57
1:B:47:VAL:HG13	1:B:66:GLN:HE22	1.70	0.57
1:B:56:HIS:HA	1:B:111:ALA:CB	2.34	0.57
1:B:149:HIS:O	1:B:152:HIS:HB3	2.05	0.57
1:A:56:HIS:HA	1:A:111:ALA:CB	2.34	0.57
1:B:58:HIS:HA	1:B:112:ALA:HB2	1.85	0.57
1:B:550:PRO:HB2	1:B:552:GLN:NE2	2.16	0.57
1:A:149:HIS:O	1:A:152:HIS:HB3	2.05	0.56
1:A:361:GLU:O	1:A:365:ARG:HB2	2.05	0.56
1:B:79:ASN:HD21	1:B:82:ASP:H	1.54	0.56
1:A:417:LEU:HB3	1:A:418:PRO:CD	2.35	0.56
1:B:40:ILE:HD11	1:B:57:THR:HG22	1.88	0.56
1:B:417:LEU:HB3	1:B:418:PRO:CD	2.35	0.56
1:A:156:GLU:HB2	1:A:161:ARG:HE	1.70	0.56
1:B:156:GLU:HB2	1:B:161:ARG:HH21	1.68	0.56
1:B:361:GLU:O	1:B:365:ARG:HB2	2.05	0.56
1:B:543:PRO:HB3	1:B:550:PRO:CG	2.36	0.56
1:A:338:GLU:HB3	5:A:670:HOH:O	2.04	0.56
1:A:133:VAL:HG21	1:A:154:TYR:HE2	1.69	0.56
1:A:543:PRO:HB3	1:A:550:PRO:CG	2.36	0.56
1:B:61:HIS:CE1	1:B:422:HIS:HD1	2.24	0.56
1:A:79:ASN:HD21	1:A:82:ASP:H	1.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:LEU:HD23	1:A:210:LEU:C	2.26	0.56
1:A:519:TRP:CH2	1:B:211:ARG:HG3	2.40	0.56
1:B:156:GLU:HB2	1:B:161:ARG:HE	1.70	0.56
1:B:61:HIS:ND1	1:B:422:HIS:ND1	2.51	0.55
1:B:133:VAL:HG21	1:B:154:TYR:HE2	1.69	0.55
1:A:47:VAL:HG13	1:A:66:GLN:HE22	1.70	0.55
1:B:409:ASP:N	1:B:409:ASP:OD1	2.39	0.55
1:B:388:ASP:N	1:B:388:ASP:OD1	2.37	0.55
1:A:238:ILE:O	1:A:238:ILE:HG22	2.07	0.55
1:A:505:THR:CG2	1:A:513:ILE:HD12	2.37	0.55
1:B:210:LEU:HD23	1:B:210:LEU:C	2.26	0.55
1:A:40:ILE:HD11	1:A:57:THR:HG22	1.88	0.55
1:B:349:GLY:H	1:B:352:ASN:ND2	2.02	0.55
1:A:200:MET:HB3	1:A:265:ILE:HG13	1.89	0.54
1:A:409:ASP:OD1	1:A:409:ASP:N	2.39	0.54
1:A:489:ARG:NH2	5:A:630:HOH:O	2.40	0.54
1:B:417:LEU:HD23	1:B:417:LEU:N	2.19	0.54
1:A:36:ASN:HB3	1:A:76:ALA:O	2.08	0.54
1:A:550:PRO:HB2	1:A:552:GLN:NE2	2.16	0.54
1:A:9:PRO:HG3	1:A:21:PHE:CZ	2.42	0.54
1:A:349:GLY:H	1:A:352:ASN:ND2	2.02	0.54
1:B:151:LEU:HD23	1:B:166:LEU:HD22	1.89	0.54
1:A:24:PHE:CE1	1:A:28:ILE:HD11	2.43	0.54
1:A:388:ASP:OD1	1:A:388:ASP:N	2.37	0.54
1:B:505:THR:CG2	1:B:513:ILE:HD12	2.37	0.54
1:A:300:ARG:HH21	1:A:308:VAL:HA	1.72	0.54
1:B:9:PRO:HG3	1:B:21:PHE:CZ	2.43	0.54
1:B:24:PHE:CE1	1:B:28:ILE:HD11	2.43	0.54
1:B:238:ILE:HG22	1:B:238:ILE:O	2.06	0.54
1:B:272:ASN:OD1	1:B:273:PRO:HD2	2.08	0.54
1:A:300:ARG:NH2	1:A:308:VAL:HA	2.23	0.54
1:B:300:ARG:HH21	1:B:308:VAL:HA	1.72	0.53
1:B:537:PRO:HD2	1:B:538:ASN:H	1.73	0.53
1:A:11:THR:O	1:A:72:SER:HB3	2.08	0.53
1:A:61:HIS:CE1	1:A:422:HIS:HD1	2.24	0.53
1:A:229:LYS:HD2	1:A:231:GLU:OE2	2.08	0.53
1:B:11:THR:O	1:B:72:SER:HB3	2.08	0.53
1:B:36:ASN:HB3	1:B:76:ALA:O	2.08	0.53
1:A:272:ASN:OD1	1:A:273:PRO:HD2	2.08	0.53
1:B:229:LYS:HD2	1:B:231:GLU:OE2	2.07	0.53
1:B:398:ARG:HA	1:B:401:THR:HB	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:MET:HB3	1:B:265:ILE:HG13	1.89	0.53
1:B:284:PRO:HG2	1:B:379:PRO:O	2.09	0.53
1:A:61:HIS:CE1	1:A:422:HIS:ND1	2.77	0.53
1:A:479:ILE:H	1:A:479:ILE:CD1	2.21	0.53
1:B:400:LYS:HB3	1:B:405:ILE:HB	1.90	0.53
1:B:478:LEU:HD21	5:B:664:HOH:O	2.09	0.53
1:B:422:HIS:CD2	1:B:424:PHE:CZ	2.97	0.53
1:A:422:HIS:CD2	1:A:424:PHE:CZ	2.97	0.53
1:B:479:ILE:H	1:B:479:ILE:CD1	2.21	0.53
1:A:398:ARG:HA	1:A:401:THR:HB	1.91	0.52
1:A:485:GLN:O	1:A:489:ARG:HG3	2.09	0.52
1:A:537:PRO:HD2	1:A:538:ASN:H	1.73	0.52
1:B:300:ARG:NH2	1:B:308:VAL:HA	2.23	0.52
1:A:188:THR:HG21	5:A:691:HOH:O	2.08	0.52
1:A:151:LEU:HD23	1:A:166:LEU:HD22	1.89	0.52
1:A:211:ARG:HG3	1:B:519:TRP:CH2	2.44	0.52
1:A:475:LYS:O	1:A:481:LYS:HD2	2.09	0.52
1:B:61:HIS:CE1	1:B:422:HIS:ND1	2.77	0.52
1:B:485:GLN:O	1:B:489:ARG:HG3	2.09	0.52
1:A:284:PRO:HG2	1:A:379:PRO:O	2.09	0.52
1:A:400:LYS:HB3	1:A:405:ILE:HB	1.91	0.52
1:B:447:CYS:HB2	1:B:448:GLN:HE22	1.75	0.52
1:A:61:HIS:ND1	1:A:422:HIS:ND1	2.51	0.52
1:B:133:VAL:CG2	1:B:154:TYR:CE2	2.93	0.52
1:B:515:GLU:O	1:B:518:ASN:ND2	2.43	0.52
1:B:475:LYS:O	1:B:481:LYS:HD2	2.09	0.51
1:A:515:GLU:O	1:A:518:ASN:ND2	2.43	0.51
1:A:16:LEU:HD13	1:A:20:ASP:HB2	1.93	0.51
1:A:447:CYS:HB2	1:A:448:GLN:HE22	1.75	0.51
1:B:21:PHE:CE2	1:B:25:ILE:HG21	2.45	0.51
1:A:133:VAL:CG2	1:A:154:TYR:CE2	2.93	0.51
1:A:552:GLN:CD	1:A:552:GLN:H	2.14	0.51
1:B:407:THR:HB	1:B:409:ASP:OD1	2.11	0.51
1:A:407:THR:HB	1:A:409:ASP:OD1	2.11	0.51
1:B:108:TYR:CZ	1:B:504:ARG:HG2	2.46	0.51
1:B:447:CYS:C	1:B:448:GLN:HE21	2.14	0.51
1:A:21:PHE:CE2	1:A:25:ILE:HG21	2.45	0.51
1:A:108:TYR:CZ	1:A:504:ARG:HG2	2.46	0.51
1:B:198:SER:O	1:B:240:HIS:HD2	1.94	0.51
1:A:198:SER:O	1:A:240:HIS:HD2	1.94	0.51
1:A:443:THR:HA	1:A:491:LEU:HD21	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:THR:HA	1:B:491:LEU:HD21	1.92	0.50
1:B:440:TYR:O	1:B:444:LYS:HB2	2.12	0.50
1:B:447:CYS:HB2	1:B:448:GLN:NE2	2.26	0.50
1:B:552:GLN:CD	1:B:552:GLN:H	2.14	0.50
1:A:350:ARG:HD2	5:A:729:HOH:O	2.11	0.50
1:B:16:LEU:HD13	1:B:20:ASP:HB2	1.93	0.50
1:A:555:HIS:CB	1:A:559:LYS:HE3	2.31	0.50
1:B:6:GLU:CB	1:B:39:VAL:HG21	2.41	0.50
1:B:200:MET:CE	1:B:251:ASP:HB3	2.42	0.50
1:A:6:GLU:CB	1:A:39:VAL:HG21	2.41	0.50
1:A:200:MET:CE	1:A:251:ASP:HB3	2.42	0.50
1:B:479:ILE:HD12	1:B:479:ILE:H	1.76	0.50
1:A:408:TYR:N	5:A:620:HOH:O	2.44	0.50
1:A:447:CYS:HB2	1:A:448:GLN:NE2	2.26	0.50
1:B:332:GLU:HB3	1:B:333:PRO:HD2	1.94	0.50
1:A:198:SER:HB3	1:A:240:HIS:HA	1.93	0.50
1:B:230:PRO:HA	1:B:233:GLN:CG	2.42	0.49
1:A:332:GLU:HB3	1:A:333:PRO:HD2	1.94	0.49
1:B:198:SER:HB3	1:B:240:HIS:HA	1.93	0.49
1:A:185:VAL:HG12	1:A:186:GLY:N	2.27	0.49
1:A:440:TYR:O	1:A:444:LYS:HB2	2.12	0.49
1:B:555:HIS:CB	1:B:559:LYS:HE3	2.31	0.49
1:B:132:GLU:CG	1:B:133:VAL:N	2.75	0.49
1:B:185:VAL:HG12	1:B:186:GLY:N	2.27	0.49
1:A:201:GLU:HG2	1:A:263:THR:OG1	2.13	0.49
1:A:447:CYS:C	1:A:448:GLN:HE21	2.14	0.49
1:B:526:ARG:HA	1:B:526:ARG:HD3	1.58	0.49
1:A:230:PRO:HA	1:A:233:GLN:CG	2.42	0.49
1:A:47:VAL:HG13	1:A:48:ASP:H	1.78	0.48
1:A:190:TYR:CE1	1:A:270:MET:HG3	2.48	0.48
1:A:350:ARG:HD3	1:A:350:ARG:HA	1.75	0.48
1:B:309:PRO:HG2	1:B:460:VAL:HB	1.94	0.48
1:B:457:THR:HG22	1:B:458:PHE:N	2.28	0.48
1:A:132:GLU:CG	1:A:133:VAL:N	2.75	0.48
1:A:457:THR:HG22	1:A:458:PHE:N	2.28	0.48
1:A:479:ILE:N	1:A:479:ILE:CD1	2.77	0.48
1:B:47:VAL:HG13	1:B:48:ASP:H	1.78	0.48
1:B:190:TYR:CE1	1:B:270:MET:HG3	2.48	0.48
1:A:295:ILE:O	1:A:298:PRO:HD2	2.14	0.48
1:A:368:TRP:NE1	1:A:372:LYS:HD2	2.29	0.48
1:A:237:LYS:HD2	1:B:500:TRP:NE1	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:PHE:C	1:B:8:ARG:HG3	2.32	0.48
1:A:479:ILE:HD12	1:A:479:ILE:H	1.76	0.47
1:B:67:ASP:HB2	1:B:70:LEU:HD22	1.97	0.47
1:A:390:PRO:O	1:A:396:ARG:HD2	2.14	0.47
1:A:391:GLU:N	5:A:677:HOH:O	2.26	0.47
1:B:229:LYS:HB3	1:B:231:GLU:OE2	2.14	0.47
1:A:309:PRO:HG2	1:A:460:VAL:HB	1.94	0.47
1:A:463:ARG:HD2	5:B:660:HOH:O	2.14	0.47
1:B:201:GLU:HG2	1:B:263:THR:OG1	2.13	0.47
1:B:295:ILE:O	1:B:298:PRO:HD2	2.14	0.47
1:B:368:TRP:NE1	1:B:372:LYS:HD2	2.29	0.47
1:A:67:ASP:HB2	1:A:70:LEU:HD22	1.96	0.47
1:A:538:ASN:HB2	1:A:540:ILE:CD1	2.39	0.47
1:B:55:THR:HG21	1:B:58:HIS:CE1	2.49	0.47
1:B:278:SER:HA	1:B:356:ALA:HA	1.96	0.47
1:A:527:PHE:CE2	1:A:531:LEU:HD11	2.50	0.47
1:B:433:GLY:N	5:B:622:HOH:O	2.47	0.47
1:A:55:THR:HG21	1:A:58:HIS:CE1	2.49	0.47
1:A:151:LEU:HD23	1:A:166:LEU:CD2	2.44	0.47
1:A:200:MET:HE1	1:A:251:ASP:HB3	1.96	0.47
1:A:218:PRO:HD2	5:A:685:HOH:O	2.15	0.47
1:A:276:TYR:CE1	1:A:356:ALA:HB1	2.49	0.47
1:A:423:LEU:O	1:A:471:ILE:HB	2.15	0.47
1:B:151:LEU:HD23	1:B:166:LEU:CD2	2.45	0.47
1:B:276:TYR:CE1	1:B:356:ALA:HB1	2.49	0.47
1:B:405:ILE:HA	1:B:406:PRO:HD2	1.56	0.47
1:A:300:ARG:HG3	1:A:462:MET:HA	1.97	0.47
1:B:346:LEU:O	1:B:347:ASN:HB2	2.15	0.47
1:A:114:ARG:NH1	1:A:511:ASP:OD2	2.47	0.47
1:A:316:LEU:HD11	1:A:413:TRP:NE1	2.30	0.47
1:B:390:PRO:O	1:B:396:ARG:HD2	2.14	0.47
1:B:423:LEU:O	1:B:471:ILE:HB	2.15	0.47
1:A:316:LEU:CD1	1:A:413:TRP:CD1	2.98	0.47
1:A:349:GLY:CA	1:A:352:ASN:HD21	2.28	0.47
1:A:536:ASP:N	1:A:537:PRO:HD3	2.16	0.47
1:B:350:ARG:HD3	1:B:350:ARG:HA	1.75	0.47
1:A:47:VAL:CG1	1:A:48:ASP:N	2.78	0.46
1:B:114:ARG:NH1	1:B:511:ASP:OD2	2.47	0.46
1:B:200:MET:HE1	1:B:251:ASP:HB3	1.96	0.46
1:A:257:SER:HA	5:A:683:HOH:O	2.15	0.46
1:A:359:GLY:O	1:A:364:ARG:NE	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:PHE:C	1:A:8:ARG:HG3	2.32	0.46
1:A:361:GLU:N	1:A:364:ARG:HH21	2.13	0.46
1:B:10:LEU:HD12	1:B:70:LEU:HD21	1.98	0.46
1:B:527:PHE:CE2	1:B:531:LEU:HD11	2.50	0.46
1:A:93:PHE:N	1:A:93:PHE:CD1	2.83	0.46
1:A:278:SER:HA	1:A:356:ALA:HA	1.96	0.46
1:A:307:ASN:OD1	1:A:307:ASN:N	2.47	0.46
1:B:47:VAL:CG1	1:B:48:ASP:N	2.78	0.46
1:B:316:LEU:CD1	1:B:413:TRP:CD1	2.98	0.46
1:A:79:ASN:ND2	1:A:79:ASN:C	2.69	0.46
1:B:277:GLN:O	1:B:357:LEU:N	2.41	0.46
1:B:361:GLU:N	1:B:364:ARG:HH21	2.13	0.46
1:A:412:LYS:H	1:A:412:LYS:HG3	1.37	0.46
1:A:132:GLU:O	1:A:140:CYS:HA	2.16	0.46
1:A:229:LYS:HB3	1:A:231:GLU:OE2	2.14	0.46
1:A:346:LEU:O	1:A:347:ASN:HB2	2.15	0.46
1:A:491:LEU:HA	1:A:491:LEU:HD23	1.78	0.46
1:B:79:ASN:ND2	1:B:79:ASN:C	2.69	0.46
1:B:300:ARG:HG3	1:B:462:MET:HA	1.97	0.46
1:B:416:TRP:HB3	1:B:472:VAL:HG21	1.98	0.46
1:B:540:ILE:HD13	1:B:540:ILE:N	2.31	0.46
1:A:295:ILE:HD12	1:A:378:ILE:HD11	1.97	0.46
1:A:526:ARG:HA	1:A:526:ARG:HD3	1.58	0.46
1:B:359:GLY:O	1:B:364:ARG:NE	2.48	0.46
1:B:540:ILE:HG23	1:B:540:ILE:HD12	1.63	0.46
1:A:22:ASN:HA	1:A:25:ILE:CG2	2.46	0.45
1:A:188:THR:HB	1:A:189:PRO:CD	2.46	0.45
1:B:349:GLY:CA	1:B:352:ASN:HD21	2.28	0.45
1:B:479:ILE:N	1:B:479:ILE:CD1	2.77	0.45
1:A:309:PRO:O	1:A:460:VAL:HG23	2.16	0.45
1:A:383:PHE:CD1	1:A:383:PHE:N	2.85	0.45
1:B:132:GLU:O	1:B:140:CYS:HA	2.16	0.45
1:B:309:PRO:O	1:B:460:VAL:HG23	2.16	0.45
1:B:553:TYR:HD2	1:B:558:TRP:CD1	2.34	0.45
1:B:188:THR:HB	1:B:189:PRO:CD	2.46	0.45
1:B:307:ASN:N	1:B:307:ASN:OD1	2.47	0.45
1:B:538:ASN:HB2	1:B:540:ILE:CD1	2.40	0.45
1:A:332:GLU:CB	1:A:333:PRO:HD2	2.47	0.45
1:B:197:HIS:HA	1:B:266:GLY:O	2.16	0.45
1:A:217:LEU:CD2	1:B:516:THR:HG23	2.47	0.45
1:A:416:TRP:HB3	1:A:472:VAL:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ASP:N	1:A:67:ASP:OD1	2.49	0.45
1:A:156:GLU:CD	1:A:161:ARG:NH2	2.70	0.45
1:A:367:LEU:O	1:A:371:ILE:HG13	2.17	0.45
1:A:454:PHE:CD1	1:A:454:PHE:C	2.90	0.45
1:B:316:LEU:HD11	1:B:413:TRP:NE1	2.30	0.45
1:A:65:ASP:O	1:A:68:TYR:HB2	2.17	0.45
1:B:295:ILE:HD12	1:B:378:ILE:HD11	1.97	0.45
1:B:409:ASP:HA	1:B:412:LYS:NZ	2.31	0.45
1:B:423:LEU:HD21	1:B:488:MET:CG	2.44	0.45
1:B:93:PHE:CD1	1:B:93:PHE:N	2.83	0.45
1:A:197:HIS:HA	1:A:266:GLY:O	2.17	0.45
1:A:409:ASP:HA	1:A:412:LYS:NZ	2.31	0.45
1:B:367:LEU:HD23	1:B:367:LEU:HA	1.66	0.45
1:B:383:PHE:CD1	1:B:383:PHE:N	2.84	0.45
1:A:62:HIS:O	1:A:62:HIS:ND1	2.50	0.45
1:A:132:GLU:HA	5:A:693:HOH:O	2.17	0.45
1:A:361:GLU:N	1:A:362:PRO:HD2	2.32	0.45
1:A:423:LEU:HD21	1:A:488:MET:CG	2.44	0.45
1:B:22:ASN:HA	1:B:25:ILE:CG2	2.46	0.45
1:B:324:LYS:NZ	1:B:332:GLU:O	2.40	0.45
1:B:332:GLU:CB	1:B:333:PRO:HD2	2.47	0.45
1:B:361:GLU:N	1:B:362:PRO:HD2	2.32	0.45
1:A:447:CYS:CB	1:A:448:GLN:NE2	2.81	0.44
1:A:505:THR:CG2	1:A:506:HIS:N	2.72	0.44
1:A:553:TYR:HD2	1:A:558:TRP:CD1	2.34	0.44
1:B:108:TYR:HD1	1:B:505:THR:C	2.20	0.44
1:B:151:LEU:CD2	1:B:166:LEU:HD21	2.48	0.44
1:B:155:LEU:HD22	1:B:160:LEU:HB2	1.99	0.44
1:A:426:SER:HA	1:A:427:PRO:HD2	1.63	0.44
1:B:102:ILE:CG1	1:B:175:SER:HB2	2.47	0.44
1:A:252:GLY:C	1:A:254:PHE:N	2.71	0.44
1:A:10:LEU:HD12	1:A:70:LEU:HD21	1.98	0.44
1:A:277:GLN:O	1:A:357:LEU:N	2.41	0.44
1:B:65:ASP:O	1:B:68:TYR:HB2	2.17	0.44
1:B:367:LEU:O	1:B:371:ILE:HG13	2.17	0.44
1:B:387:GLU:HA	1:B:387:GLU:OE1	2.17	0.44
1:A:519:TRP:CE3	1:B:211:ARG:HG3	2.49	0.44
1:A:540:ILE:N	1:A:540:ILE:HD13	2.31	0.44
1:B:62:HIS:O	1:B:62:HIS:ND1	2.50	0.44
1:B:156:GLU:CD	1:B:161:ARG:NH2	2.70	0.44
1:B:179:ASN:OD1	1:B:184:GLY:HA3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:454:PHE:CD1	1:B:454:PHE:C	2.90	0.44
1:A:480:GLN:O	1:A:484:VAL:HG23	2.18	0.44
1:A:549:TRP:CH2	1:A:558:TRP:HB3	2.53	0.44
1:A:102:ILE:CG1	1:A:175:SER:HB2	2.47	0.44
1:A:367:LEU:HD23	1:A:367:LEU:HA	1.66	0.44
1:A:428:ILE:HD12	1:A:428:ILE:HG23	1.60	0.44
1:A:443:THR:O	1:A:443:THR:HG22	2.18	0.44
1:A:290:LYS:HG3	1:A:433:GLY:HA3	2.00	0.44
1:A:387:GLU:OE1	1:A:387:GLU:HA	2.17	0.44
1:B:413:TRP:CZ2	4:B:600:FAD:HM72	2.53	0.44
1:A:151:LEU:CD2	1:A:166:LEU:HD21	2.48	0.44
1:A:179:ASN:OD1	1:A:184:GLY:HA3	2.17	0.44
1:B:344:LYS:HG3	1:B:345:GLN:N	2.33	0.44
1:B:480:GLN:O	1:B:484:VAL:HG23	2.18	0.44
1:A:37:VAL:HG13	1:A:75:VAL:CG2	2.46	0.43
1:A:108:TYR:HD1	1:A:505:THR:C	2.20	0.43
1:B:101:SER:O	1:B:124:GLY:HA3	2.17	0.43
1:A:101:SER:O	1:A:124:GLY:HA3	2.17	0.43
1:A:187:TYR:CD2	1:A:187:TYR:N	2.81	0.43
1:A:241:LEU:HB3	1:B:463:ARG:O	2.17	0.43
1:A:332:GLU:CB	1:A:333:PRO:CD	2.95	0.43
1:A:413:TRP:CZ2	4:A:600:FAD:HM72	2.53	0.43
1:B:61:HIS:CE1	1:B:422:HIS:CE1	3.06	0.43
1:A:540:ILE:HD12	1:A:540:ILE:HG23	1.63	0.43
1:B:447:CYS:CB	1:B:448:GLN:NE2	2.80	0.43
1:A:76:ALA:HA	1:A:77:PRO:HD2	1.69	0.43
1:A:155:LEU:HD22	1:A:160:LEU:HB2	1.99	0.43
1:A:452:LEU:HD23	1:A:452:LEU:HA	1.68	0.43
1:B:332:GLU:CB	1:B:333:PRO:CD	2.95	0.43
1:A:361:GLU:N	1:A:362:PRO:CD	2.80	0.43
1:B:201:GLU:OE1	1:B:211:ARG:HD3	2.18	0.43
1:A:431:VAL:HA	1:A:465:MET:HE2	2.01	0.43
1:A:9:PRO:HG3	1:A:21:PHE:CE2	2.54	0.43
1:A:12:LEU:HB3	1:A:13:PRO:HD2	2.01	0.43
1:A:160:LEU:HD23	1:A:160:LEU:HA	1.71	0.43
1:A:201:GLU:OE1	1:A:211:ARG:HD3	2.18	0.43
1:A:211:ARG:HD3	1:B:519:TRP:CH2	2.53	0.43
1:A:311:ILE:HG12	1:A:353:PHE:HD1	1.84	0.43
1:B:9:PRO:HG3	1:B:21:PHE:CE2	2.54	0.43
1:B:13:PRO:HG3	1:B:95:PHE:CZ	2.53	0.43
1:B:549:TRP:CH2	1:B:558:TRP:HB3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:PRO:HG3	1:A:95:PHE:CZ	2.53	0.43
1:B:252:GLY:C	1:B:254:PHE:N	2.71	0.43
1:A:403:GLN:HG3	1:A:405:ILE:HG13	2.00	0.43
1:A:222:ARG:HB2	1:A:223:PRO:HD2	2.01	0.43
1:B:290:LYS:HG3	1:B:433:GLY:HA3	2.00	0.43
1:B:555:HIS:O	1:B:559:LYS:HG3	2.19	0.43
1:A:222:ARG:HA	1:A:223:PRO:HD3	1.76	0.42
1:A:231:GLU:H	1:A:231:GLU:HG3	0.96	0.42
1:A:61:HIS:CE1	1:A:422:HIS:CE1	3.06	0.42
1:A:142:VAL:O	1:A:264:LYS:HA	2.19	0.42
1:A:344:LYS:HG3	1:A:345:GLN:N	2.33	0.42
1:A:361:GLU:HB2	1:A:364:ARG:NH2	2.34	0.42
1:B:14:PRO:HB2	5:B:749:HOH:O	2.19	0.42
1:B:142:VAL:O	1:B:264:LYS:HA	2.19	0.42
1:A:385:PHE:CB	1:A:386:PRO:HD2	2.38	0.42
1:A:188:THR:CB	1:A:189:PRO:CD	2.98	0.42
1:A:304:ALA:HA	1:A:367:LEU:HD22	2.01	0.42
1:B:62:HIS:O	1:B:481:LYS:HE3	2.19	0.42
1:B:156:GLU:CG	1:B:161:ARG:CZ	2.98	0.42
1:B:188:THR:CB	1:B:189:PRO:CD	2.98	0.42
1:B:302:GLY:C	1:B:303:MET:HG3	2.40	0.42
1:B:428:ILE:HG23	1:B:428:ILE:HD12	1.60	0.42
1:A:478:LEU:N	1:A:478:LEU:CD1	2.79	0.42
1:B:181:VAL:O	1:B:255:SER:HB2	2.20	0.42
1:B:361:GLU:HB2	1:B:364:ARG:NH2	2.34	0.42
1:B:443:THR:O	1:B:443:THR:HG22	2.18	0.42
1:A:108:TYR:CE1	1:A:504:ARG:HG2	2.54	0.42
1:A:177:LEU:HD22	1:A:265:ILE:HG22	2.01	0.42
1:A:181:VAL:O	1:A:255:SER:HB2	2.20	0.42
1:B:12:LEU:HB3	1:B:13:PRO:HD2	2.01	0.42
1:B:361:GLU:N	1:B:362:PRO:CD	2.80	0.42
1:B:108:TYR:CE1	1:B:504:ARG:HG2	2.54	0.42
1:A:62:HIS:O	1:A:481:LYS:HE3	2.19	0.42
1:A:242:PHE:HA	1:A:243:PRO:HD3	1.87	0.42
1:B:59:ASP:HA	1:B:60:PRO:HD2	1.93	0.42
1:B:222:ARG:HB2	1:B:223:PRO:HD2	2.01	0.42
1:B:243:PRO:CD	1:B:244:TYR:H	2.32	0.42
1:B:304:ALA:HA	1:B:367:LEU:HD22	2.01	0.42
1:B:311:ILE:HG12	1:B:353:PHE:HD1	1.83	0.42
1:B:491:LEU:HD23	1:B:491:LEU:HA	1.78	0.42
1:B:160:LEU:HD23	1:B:160:LEU:HA	1.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:GLN:HG3	1:B:405:ILE:HG13	2.00	0.42
1:A:16:LEU:CD1	1:A:21:PHE:N	2.83	0.42
1:A:156:GLU:CG	1:A:161:ARG:CZ	2.98	0.42
1:A:195:MET:CE	1:B:195:MET:CE	2.97	0.42
1:B:177:LEU:HD22	1:B:265:ILE:HG22	2.01	0.42
1:B:16:LEU:CD1	1:B:21:PHE:N	2.83	0.41
1:B:431:VAL:HA	1:B:465:MET:HE2	2.02	0.41
1:A:12:LEU:HA	1:A:13:PRO:HD3	1.73	0.41
1:A:237:LYS:HD2	1:B:500:TRP:CD1	2.56	0.41
1:A:302:GLY:C	1:A:303:MET:HG3	2.40	0.41
1:A:555:HIS:O	1:A:559:LYS:HG3	2.19	0.41
1:B:18:LEU:HD12	1:B:18:LEU:HA	1.48	0.41
1:B:416:TRP:O	1:B:417:LEU:HD23	2.19	0.41
1:A:217:LEU:CD2	1:B:516:THR:CG2	2.98	0.41
1:A:416:TRP:O	1:A:417:LEU:HD23	2.19	0.41
1:B:67:ASP:N	1:B:67:ASP:OD1	2.49	0.41
1:B:151:LEU:HG	1:B:166:LEU:HD21	2.03	0.41
1:B:252:GLY:C	1:B:254:PHE:H	2.24	0.41
1:A:156:GLU:CB	1:A:161:ARG:NE	2.80	0.41
1:A:553:TYR:HD2	1:A:558:TRP:NE1	2.19	0.41
1:B:156:GLU:CB	1:B:161:ARG:NE	2.79	0.41
1:B:536:ASP:N	1:B:537:PRO:HD3	2.16	0.41
1:A:64:MET:HG2	1:A:68:TYR:CD2	2.56	0.41
1:A:151:LEU:HG	1:A:166:LEU:HD21	2.03	0.41
1:A:185:VAL:CG1	1:A:186:GLY:N	2.84	0.41
1:A:213:GLY:HA3	5:A:717:HOH:O	2.20	0.41
1:A:323:ASP:OD1	1:A:326:SER:OG	2.29	0.41
1:A:517:TYR:CE1	1:B:246:PHE:CB	3.04	0.41
1:A:537:PRO:HD2	5:A:742:HOH:O	2.19	0.41
1:B:50:SER:O	1:B:54:PRO:N	2.54	0.41
1:B:305:LEU:HA	1:B:305:LEU:HD23	1.89	0.41
1:A:311:ILE:O	1:A:457:THR:HG23	2.21	0.41
1:B:12:LEU:HA	1:B:13:PRO:HD3	1.72	0.41
1:B:202:VAL:HA	1:B:261:ILE:O	2.21	0.41
1:A:177:LEU:HB2	1:A:265:ILE:CG2	2.52	0.40
1:A:305:LEU:HA	1:A:305:LEU:HD23	1.89	0.40
1:A:414:ILE:HD11	4:A:600:FAD:C7M	2.40	0.40
1:B:156:GLU:CB	1:B:161:ARG:CZ	2.99	0.40
1:B:6:GLU:CB	1:B:39:VAL:CG2	3.00	0.40
1:B:64:MET:HG2	1:B:68:TYR:CD2	2.56	0.40
1:B:417:LEU:N	1:B:417:LEU:CD2	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:VAL:HG22	1:A:66:GLN:HE22	1.87	0.40
1:A:151:LEU:CD2	1:A:166:LEU:CD2	2.99	0.40
1:A:252:GLY:C	1:A:254:PHE:H	2.24	0.40
1:A:272:ASN:HA	1:A:273:PRO:HD3	1.85	0.40
1:A:344:LYS:CG	1:A:345:GLN:N	2.85	0.40
1:A:243:PRO:CD	1:A:244:TYR:H	2.32	0.40

All (1) 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:330:ARG:NH2	1:A:330:ARG:NH2[2_765]	2.15	0.05

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	546/560 (98%)	503 (92%)	38 (7%)	5 (1%)	17	31
1	B	546/560 (98%)	503 (92%)	38 (7%)	5 (1%)	17	31
All	All	1092/1120 (98%)	1006 (92%)	76 (7%)	10 (1%)	17	31

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	ASP
1	B	48	ASP
1	A	199	GLY
1	A	388	ASP
1	B	199	GLY
1	B	388	ASP
1	A	327	TYR

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Mol	Chain	Res	Type
1	B	327	TYR
1	A	328	SER
1	B	328	SER

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	470/482 (98%)	449 (96%)	21 (4%)	27	51
1	B	470/482 (98%)	449 (96%)	21 (4%)	27	51
All	All	940/964 (98%)	898 (96%)	42 (4%)	27	51

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	PHE
1	A	16	LEU
1	A	64	MET
1	A	65	ASP
1	A	79	ASN
1	A	95	PHE
1	A	114	ARG
1	A	122	ASP
1	A	169	PRO
1	A	177	LEU
1	A	248	PRO
1	A	251	ASP
1	A	301	LEU
1	A	314	ILE
1	A	409	ASP
1	A	422	HIS
1	A	448	GLN
1	A	464	GLU
1	A	503	TYR
1	A	505	THR

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Mol	Chain	Res	Type
1	A	552	GLN
1	B	7	PHE
1	B	16	LEU
1	B	64	MET
1	B	65	ASP
1	B	79	ASN
1	B	95	PHE
1	B	114	ARG
1	B	122	ASP
1	B	169	PRO
1	B	177	LEU
1	B	248	PRO
1	B	251	ASP
1	B	301	LEU
1	B	314	ILE
1	B	409	ASP
1	B	422	HIS
1	B	448	GLN
1	B	464	GLU
1	B	503	TYR
1	B	505	THR
1	B	552	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	HIS
1	A	66	GLN
1	A	79	ASN
1	A	91	ASN
1	A	128	ASN
1	A	152	HIS
1	A	197	HIS
1	A	240	HIS
1	A	352	ASN
1	A	448	GLN
1	A	485	GLN
1	A	518	ASN
1	A	520	ASN
1	A	552	GLN
1	A	555	HIS
1	B	56	HIS

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Mol	Chain	Res	Type
1	B	66	GLN
1	B	79	ASN
1	B	91	ASN
1	B	128	ASN
1	B	152	HIS
1	B	197	HIS
1	B	240	HIS
1	B	352	ASN
1	B	448	GLN
1	B	485	GLN
1	B	518	ASN
1	B	520	ASN
1	B	552	GLN
1	B	555	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)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	ACT	B	601	-	3,3,3	1.01	0	3,3,3	0.89	0
4	FAD	B	600	1	53,58,58	0.95	3 (5%)	68,89,89	1.01	4 (5%)
2	ACT	A	601	-	3,3,3	1.00	0	3,3,3	0.89	0
4	FAD	A	600	1	53,58,58	0.96	3 (5%)	68,89,89	1.01	3 (4%)

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
4	FAD	B	600	1	-	6/30/50/50	0/6/6/6
4	FAD	A	600	1	-	6/30/50/50	0/6/6/6

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	600	FAD	O5B-C5B	-3.58	1.31	1.44
4	B	600	FAD	O5B-C5B	-3.57	1.31	1.44
4	A	600	FAD	C4X-N5	2.45	1.35	1.30
4	B	600	FAD	C4X-N5	2.45	1.35	1.30
4	B	600	FAD	C5X-N5	-2.14	1.35	1.39
4	A	600	FAD	C5X-N5	-2.13	1.35	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	600	FAD	C4-N3-C2	-2.26	121.46	125.64
4	A	600	FAD	C4-N3-C2	-2.23	121.53	125.64
4	B	600	FAD	O4B-C4B-C5B	-2.21	102.09	109.37
4	A	600	FAD	O4B-C4B-C5B	-2.21	102.12	109.37
4	A	600	FAD	C5A-C6A-N6A	2.11	123.55	120.35
4	B	600	FAD	C5A-C6A-N6A	2.10	123.55	120.35
4	B	600	FAD	O4B-C1B-C2B	-2.00	104.00	106.93

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	600	FAD	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
4	A	600	FAD	O4'-C4'-C5'-O5'
4	B	600	FAD	C3'-C4'-C5'-O5'
4	B	600	FAD	O4'-C4'-C5'-O5'
4	A	600	FAD	C4'-C5'-O5'-P
4	B	600	FAD	C4'-C5'-O5'-P
4	A	600	FAD	C2'-C3'-C4'-O4'
4	B	600	FAD	C2'-C3'-C4'-O4'
4	A	600	FAD	O4B-C4B-C5B-O5B
4	B	600	FAD	O4B-C4B-C5B-O5B
4	A	600	FAD	PA-O3P-P-O2P
4	B	600	FAD	PA-O3P-P-O2P

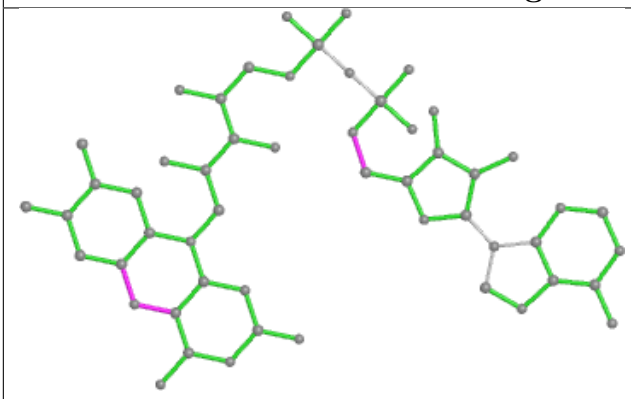
There are no ring outliers.

2 monomers are involved in 11 short contacts:

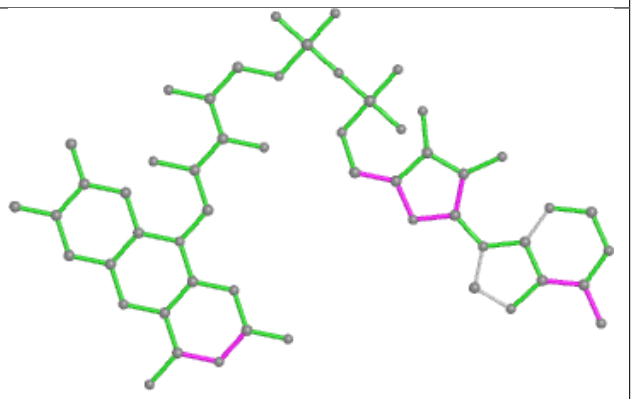
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	600	FAD	5	0
4	A	600	FAD	6	0

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.

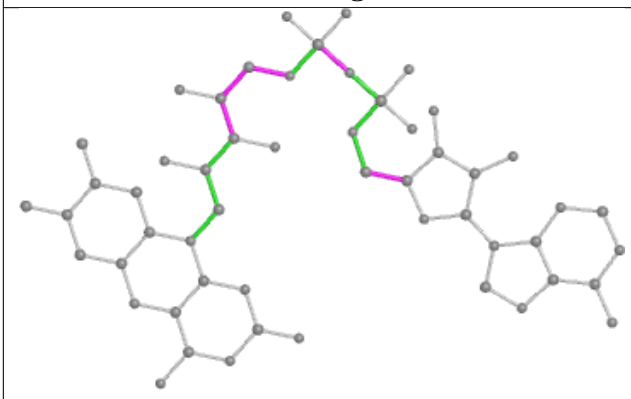
Ligand FAD B 600



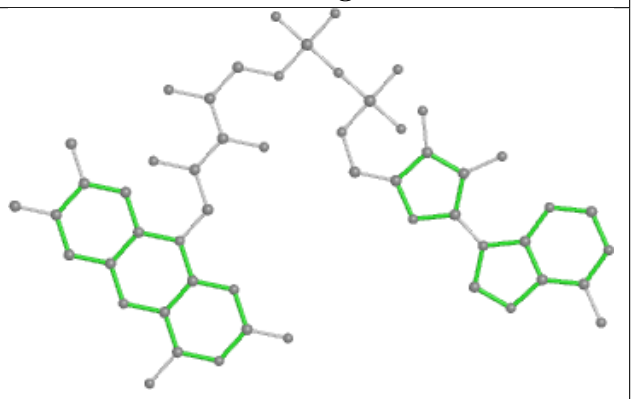
Bond lengths



Bond angles

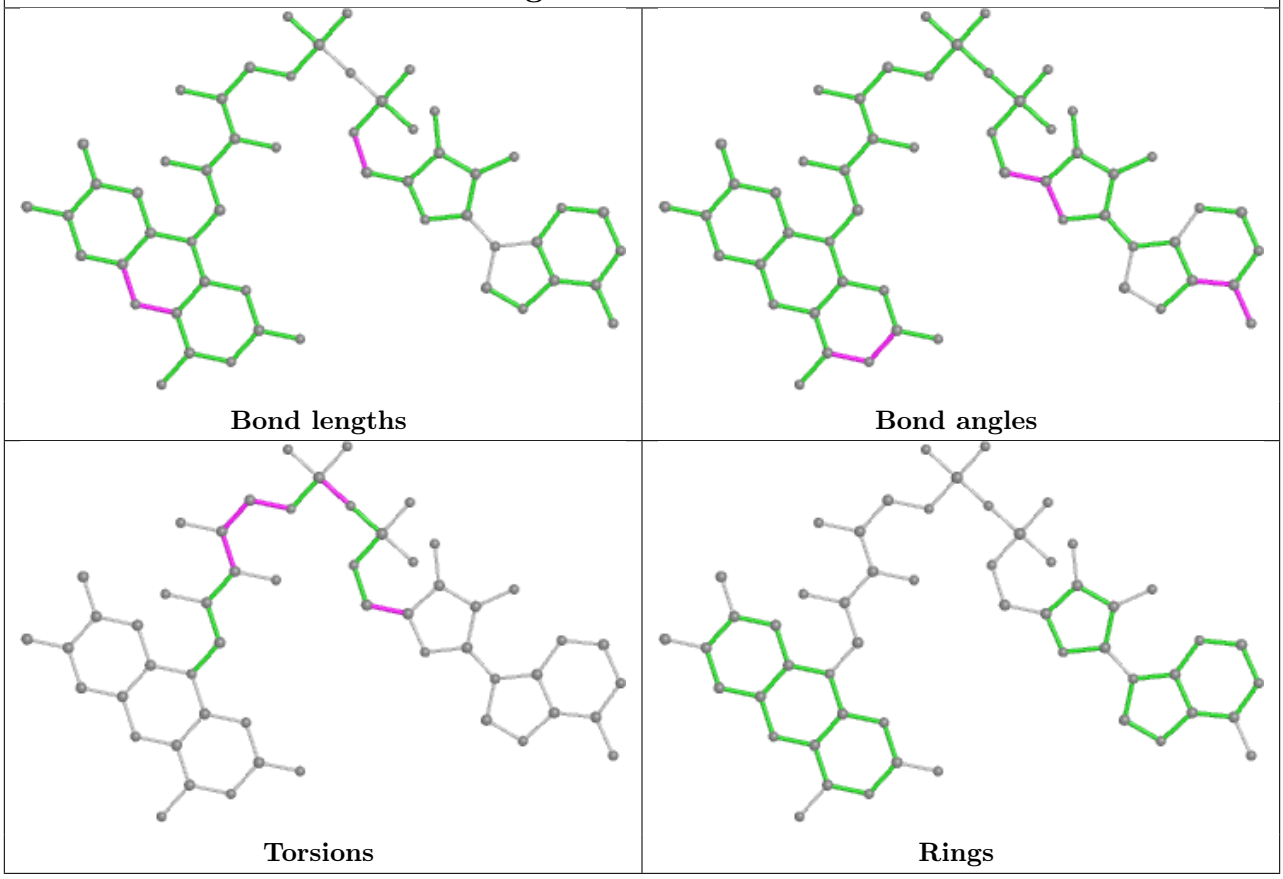


Torsions



Rings

Ligand FAD A 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.