



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 04:21 pm BST

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](mailto: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.

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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)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

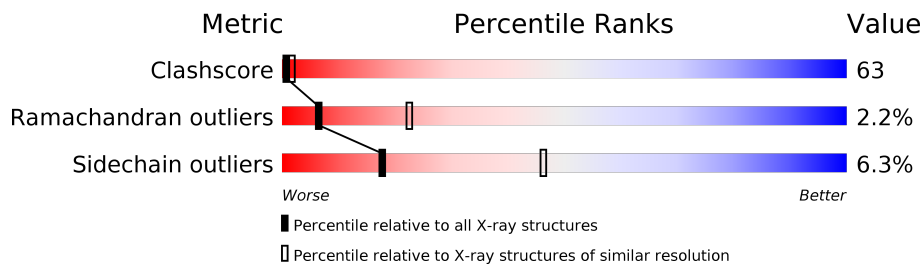
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	560	
1	B	560	

## 2 Entry composition [i](#)

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.

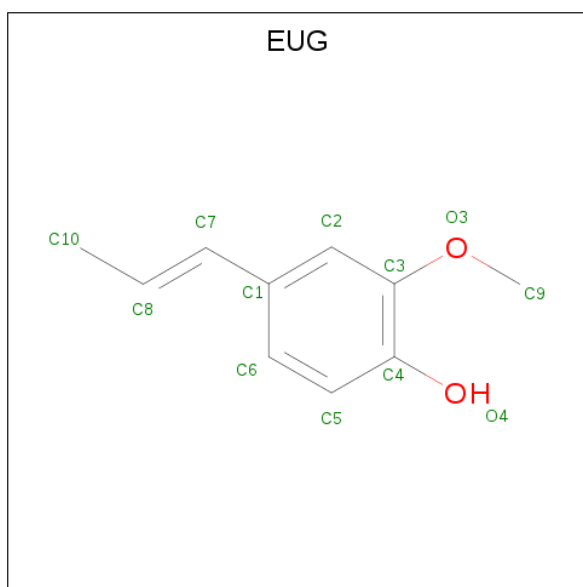
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	555	4391	2817	751	799	24	51	0	0
1	B	555	4391	2817	751	799	24	51	0	0

- 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
			Total	C	N	O	P		
2	A	1	53	27	9	15	2	0	0
2	B	1	53	27	9	15	2	0	0

- 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.

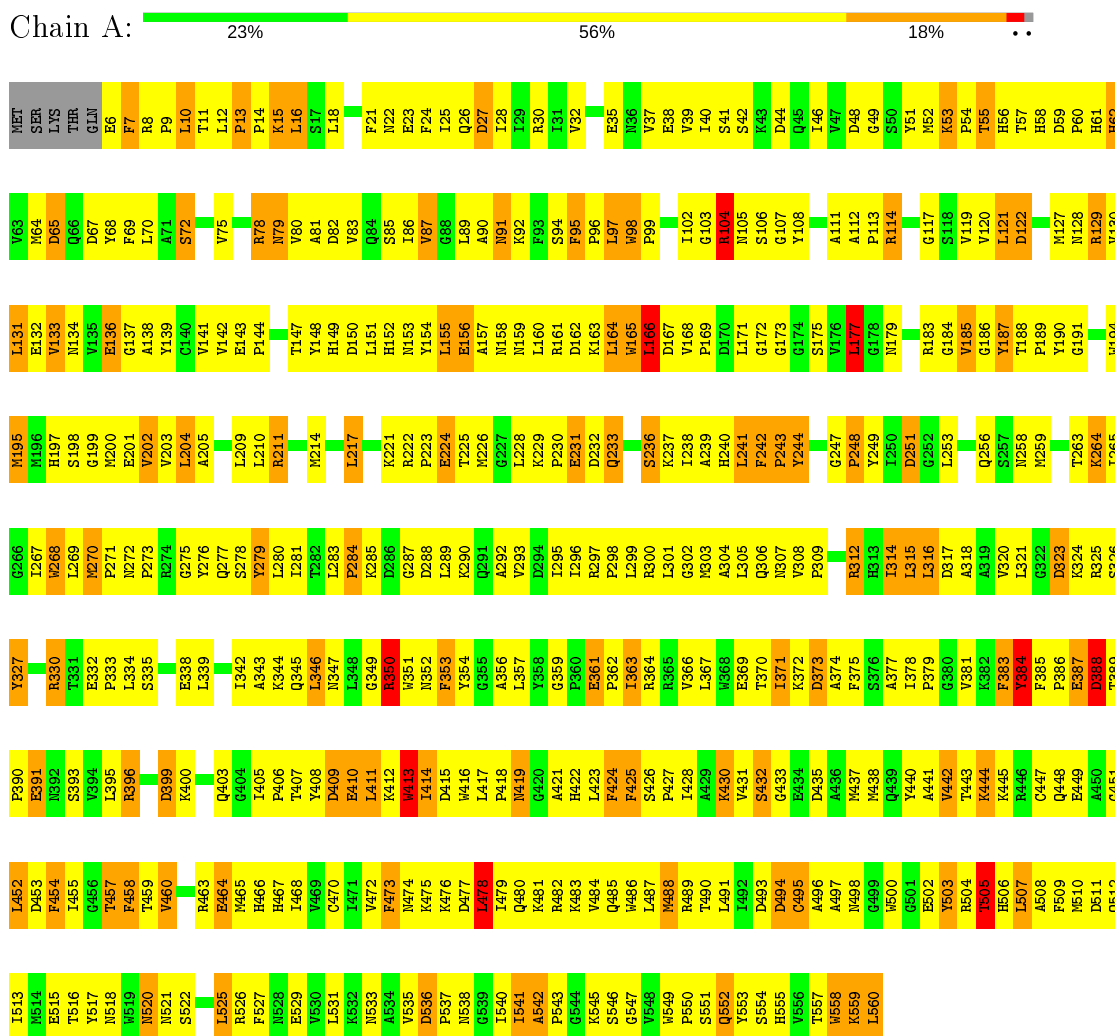
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	14	Total O 14 14	0	0
4	B	24	Total O 24 24	0	0

### 3 Residue-property plots [\(i\)](#)

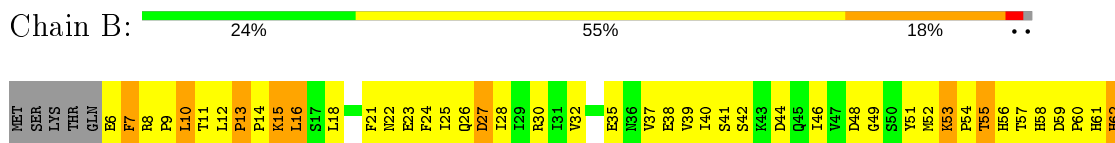
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

- Molecule 1: VANILLYL-ALCOHOL OXIDASE



- Molecule 1: VANILLYL-ALCOHOL OXIDASE



E515	F454	S393	R330	W268	X196	V130	M63
T516	I485	Y394	T331	L269	H197	L431	M64
Y517	G456	L395	E332	M270	S198	E132	Q66
N518	T457	R396	P333	P271	G199	V133	D66
W519	F458	L334	L334	M272	M201	M134	D67
N520	T459	S335	S335	P273	E200	V135	Y68
N521	V460	K400	E336	G274	V202	E136	F69
S522	R463	T401	L339	G275	V203	G137	L70
L525	E464	H402	L342	Y276	L204	A138	A71
R526	N465	Q403	T342	Q277	A205	Y139	S72
N527	H466	G404	I342	S278	L209	C140	A73
F528	H467	I405	Q345	Y279	L210	V141	I74
N529	H468	F406	L346	L280	R211	V142	V75
W530	V469	T407	L347	I281	M214	E143	V75
L531	C470	D408	N347	T282	M214	P144	R78
N532	I471	D409	L348	L283	L217	T147	N79
N533	V472	E410	G349	P284	K285	Y148	V80
A534	F473	L411	R350	K285	D286	D82	A81
W535	M474	K412	W351	G287	G287	D150	D82
D536	K475	W413	N352	D288	K221	V83	V83
P537	K476	I414	F353	L289	R222	Q84	Q84
N538	D477	D415	Y354	L289	P223	S85	S85
G539	L478	W416	G355	K290	E224	I86	I86
I540	I479	L417	A356	Q291	T225	W87	W87
I541	Q480	P418	L357	A292	M226	L155	G88
A542	R481	M419	W356	V293	G227	E156	L89
K545	R482	G420	G359	D294	L228	A157	A90
S546	K483	A421	P360	I295	K229	M158	N91
G547	V484	H422	E361	I296	P230	N159	K92
W548	K485	L423	P362	R297	E231	L160	F93
W549	W486	F424	I363	P298	D232	R161	S94
M549	L487	F425	R364	L299	Q233	K162	F95
P550	M488	S426	R365	R300	S236	K163	P96
S551	R489	P427	V366	L301	K237	L164	L97
Y552	T490	I428	L367	G302	I238	W165	W98
S554	L491	K430	W368	M303	A239	L166	P99
H555	I492	V431	T370	L305	R240	D167	P99
W556	D493	S432	I371	Q306	F242	L171	I102
T557	D494	G433	K372	N307	P243	G172	G103
W558	A495	F434	D373	V308	Y244	G173	R104
K559	A497	A436	F375	P309	G247	G174	N105
L560	M498	M437	S376	R312	P246	S175	S106
	G499	M438	A377	H313	Y249	W176	G107
	W500	Q439	I378	I314	I250	L177	Y108
	G501	Y440	P379	L315	D251	G178	A111
	E502	A441	G380	L316	G252	N179	A112
	Y503	V442	V381	D317	L253	R183	P113
	R504	T443	K382	A318	Q256	V184	R114
	T505	K444	F383	A319	S257	V185	G117
	H506	K445	Y384	V320	N258	G186	S118
	L507	R446	F385	L321	M259	T187	V119
	A508	C447	P386	G322	K264	Y188	V120
	F509	Q448	E387	D323	I265	P189	L121
	M510	E449	D388	K324	G266	Y190	D122
	D511	A450	T389	R325	I267	G191	G191
	Q512	G451	P390	S326		W194	M127
	I513	L452	E391	Y327		M128	N128
	N514	D453	N392			R129	R129

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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.	Xtrriage
Total number of atoms	8948	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EUG, FAD

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(°)	Ideal(°)
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(°)	Ideal(°)
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(°)	Ideal(°)
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(°)	Ideal(°)
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(°)	Ideal(°)
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(°)	Ideal(°)
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(°)	Ideal(°)
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:H8A	2:B:600:FAD:H51A	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:H	1:A:478:LEU:HD12	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:555:HIS:CG	1:B:559:LYS:HE3	2.09	0.87
1:B:91:ASN:ND2	1:B:538:ASN:HD22	1.71	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:C5B	2:B:600:FAD:H8A	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:505:THR:HG22	1:B:506:HIS:H	1.45	0.80
1:B:40:ILE:CD1	1:B:57:THR:HG22	2.10	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:C8A	2:A:600:FAD:H51A	2.11	0.79
1:B:10:LEU:HD11	1:B:42:SER:HA	1.64	0.79
1:A:378:ILE:O	1:A:381:VAL:HB	1.83	0.79
1:A:57:THR:O	1:A:70:LEU:HD12	1.83	0.79
1:B:361:GLU:HG3	1:B:361:GLU:O	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:378:ILE:O	1:B:381:VAL:HB	1.83	0.78
1:B:57:THR:O	1:B:70:LEU:HD12	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:479:ILE:O	1:A:483:LYS:HG3	1.84	0.77
1:A:85:SER:O	1:A:89:LEU:HD13	1.85	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:HG3	1:A:361:GLU:O	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:C8A	2:B:600:FAD:H51A	2.11	0.76
1:A:357:LEU:HB3	1:A:364:ARG:HG2	1.66	0.76
1:A:102:ILE:HG12	1:A:175:SER:HB2	1.68	0.76
1:A:48:ASP:OD1	1:A:60:PRO:HA	1.84	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:423:LEU:HD21	1:A:488:MET:CG	2.16	0.74
1:A:248:PRO:HD3	1:B:256:GLN:O	1.87	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:527:PHE:CE2	1:A:531:LEU:HD11	2.23	0.74
1:A:79:ASN:HD21	1:A: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
1:B:79:ASN:HD21	1:B:81:ALA:HB3	1.52	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:425:PHE:CZ	1:B:427:PRO:HG3	2.25	0.72
1:B:96:PRO:O	1:B:97:LEU:HD23	1.89	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: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:A:96:PRO:O	1:A:97:LEU:HD23	1.89	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:59:ASP:N	1:A:112:ALA:HB2	2.07	0.69
1:A:13:PRO:HG2	1:A:16:LEU:HB2	1.72	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:200:MET:HE1	1:A:251:ASP:HB3	1.74	0.68
1:A:61:HIS:CE1	1:A:422:HIS:HD1	2.11	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:502:GLU:N	1:B:502:GLU:OE1	2.26	0.68
1:B:61:HIS:CE1	1:B:422:HIS:HD1	2.11	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:351:TRP:O	1:A:352:ASN:ND2	2.29	0.65
1:A:295:ILE:HD12	1:A:378:ILE:HD11	1.77	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:H	1:A:224:GLU:CD	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:151:LEU:O	1:B:151:LEU:HD12	1.98	0.64
1:B:555:HIS:CB	1:B:559:LYS:HE3	2.27	0.64
1:B:95:PHE:HD1	1:B:96:PRO:N	1.96	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:151:LEU:HD12	1:A:151:LEU:O	1.98	0.63
1:A:48:ASP:OD1	1:A:58:HIS:NE2	2.24	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:256:GLN:O	1:B:248:PRO:HD3	1.98	0.62
1:A:79:ASN:HD22	1:A:81:ALA:H	1.46	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:280:LEU:HB2	1:B:395:LEU:HD13	1.81	0.62
1:B:24:PHE:CE1	1:B:28:ILE:HD12	2.34	0.62
1:A:148:TYR:HB2	1:A:172:GLY:O	2.00	0.62
1:A:24:PHE:CE1	1:A:28:ILE:HD12	2.34	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: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:B:13:PRO:HG3	1:B:95:PHE:CE1	2.35	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:189:PRO:HA	1:B:307:ASN:HA	1.82	0.61
1:B:6:GLU:N	1:B:39:VAL:HG21	2.15	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:149:HIS:O	1:B:152:HIS:HB3	2.01	0.61
1:B:61:HIS:CE1	1:B:422:HIS:ND1	2.69	0.61
1:B:505:THR:HG22	1:B:506:HIS:N	2.15	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: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:B:185:VAL:HG12	1:B:186:GLY:N	2.15	0.61
1:B:416:TRP:CE3	1:B:416:TRP:HA	2.36	0.61
1:A:230:PRO:HA	1:A:233:GLN:CD	2.21	0.61
1:A:39:VAL:HG12	1:A:40:ILE:H	1.66	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:H	1:A:136:GLU:CD	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: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:24:PHE:CD2	1:B:95:PHE:HD2	2.20	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:445:LYS:O	1:B:449:GLU:HG3	2.02	0.59
1:B:96:PRO:C	1:B:97:LEU:HD23	2.22	0.59
1:A:129:ARG:HB2	1:A:131:LEU:HD21	1.83	0.59
1:A:96:PRO:C	1:A:97:LEU:HD23	2.22	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:242:PHE:CD1	1:A:243:PRO:HD2	2.37	0.59
1:A:416:TRP:CE3	1:A:416:TRP:HA	2.36	0.59
1:A:82:ASP:O	1:A:86:ILE:HG13	2.01	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:O	1:A:525:LEU:HD12	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: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:B:35:GLU:HA	1:B:35:GLU:OE1	2.04	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:51:TYR:CZ	1:A:104:ARG:HD3	2.39	0.57
1:A:24:PHE:CE1	1:A:28:ILE:CD1	2.87	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: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:83:VAL:O	1:A:87:VAL:HG23	2.04	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:O	1:B:525:LEU:HD12	2.04	0.56
1:A:165:TRP:HB2	1:A:270:MET:O	2.05	0.56
1:A:448:GLN:O	1:A:451:GLY:N	2.33	0.56
1:A:48:ASP:HA	1:A:58:HIS:CE1	2.40	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: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: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:61:HIS:CE1	1:B:422:HIS:CE1	2.93	0.56
1:B:478:LEU:CD1	1:B:478:LEU:H	2.12	0.56
1:B:48:ASP:HA	1:B:58:HIS:CE1	2.40	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:OD1	1:A:27:ASP:N	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:HG	1:B:280:LEU:O	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: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:B:65:ASP:OD1	1:B:65:ASP:N	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:425:PHE:CE2	1:A:427:PRO:HG3	2.41	0.55
1:A:59:ASP:O	1:A:62:HIS:HB3	2.07	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:361:GLU:N	1:A:362:PRO:HD2	2.22	0.55
1:A:75:VAL:O	1:A:122:ASP:N	2.37	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: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:B:89:LEU:CD1	1:B:89:LEU:N	2.71	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:A:7:PHE:HB3	1:A:8:ARG:HG3	1.89	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: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: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:HD13	1:B:217:LEU:C	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:464:GLU:OE2	1:A:466:HIS:ND1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ASN:ND2	1:A:81:ALA:H	2.06	0.53
1:A:533:ASN:OD1	1:A:552:GLN:NE2	2.41	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:A:205:ALA:CB	1:A:536:ASP:HB2	2.39	0.53
1:B:194:TRP:O	1:B:197:HIS:CD2	2.62	0.53
1:B:27:ASP:OD1	1:B:27:ASP:N	2.39	0.53
1:A:136:GLU:OE1	1:A:136:GLU:N	2.34	0.53
1:A:89:LEU:N	1:A:89:LEU:CD1	2.71	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: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:A:7:PHE:HA	1:A:22:ASN:OD1	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:194:TRP:O	1:B:197:HIS:HD2	1.91	0.53
1:B:62:HIS:O	1:B:62:HIS:ND1	2.39	0.53
1:A:247:GLY:HA2	1:B:546:SER:OG	2.09	0.52
1:A:165:TRP:N	1:A:270:MET:O	2.39	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: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: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: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:OD1	1:B:409:ASP:N	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: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:B:95:PHE:CD1	1:B:96:PRO:CD	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:A:425:PHE:CE1	1:A:502:GLU:CG	2.94	0.51
1:B:136:GLU:N	1:B:136:GLU:OE1	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:107:GLY:HA2	1:B:422:HIS:O	2.11	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:CE3	1:A:351:TRP:HA	2.47	0.50
1:A:409:ASP:N	1:A:409:ASP:OD1	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:144:PRO:HA	1:A:177:LEU:HG	1.93	0.50
1:A:22:ASN:HA	1:A:25:ILE:HG22	1.94	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:277:GLN:O	1:B:357:LEU:N	2.29	0.50
1:B:24:PHE:CE2	1:B:95:PHE:CD2	3.00	0.50
1:A:200:MET:O	1:A:211:ARG:HA	2.11	0.50
1:B:324:LYS:HE2	1:B:334:LEU:HD21	1.94	0.50
1:B:351:TRP:HA	1:B:351:TRP:CE3	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:75:VAL:O	1:B:122:ASP:N	2.37	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:179:ASN:OD1	1:A:184:GLY:HA3	2.11	0.49
1:A:107:GLY:HA2	1:A:422:HIS:O	2.11	0.49
1:B:223:PRO:HG2	1:B:224:GLU:CD	2.32	0.49
1:B:205:ALA:HB2	1:B:541:ILE:CD1	2.42	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:HD22	1:B:217:LEU:HA	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:N	1:B:323:ASP:OD1	2.46	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:6:GLU:N	1:A:39:VAL:CG2	2.76	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:238:ILE:N	1:A:238:ILE:HD13	2.28	0.48
1:A:87:VAL:O	1:A:91:ASN:N	2.44	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: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:6:GLU:N	1:B:39:VAL:CG2	2.76	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:496:ALA:N	4:A:605:HOH:O	2.46	0.48
1:A:53:LYS:HA	1:A:54:PRO:HD3	1.70	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:B:108:TYR:HD1	1:B:505:THR:C	2.17	0.48
1:B:87:VAL:O	1:B:91:ASN:N	2.44	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:201:GLU:HA	1:B:210:LEU:O	2.14	0.47
1:B:24:PHE:CD2	1:B:95:PHE:CD2	3.01	0.47
1:B:383:PHE:CD1	1:B:383:PHE:N	2.82	0.47
1:B:484:VAL:O	1:B:488:MET:N	2.31	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:B:99:PRO:HA	1:B:121:LEU:HB3	1.97	0.47
1:A:9:PRO:HA	1:A:40:ILE:O	2.15	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:B:59:ASP:HA	1:B:60:PRO:HD2	1.67	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:95:PHE:CD1	1:A:96:PRO:CD	2.94	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
1:A:300:ARG:NH2	1:A:308:VAL:HA	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:PHE:N	1:A:383:PHE:CD1	2.82	0.47
1:A:61:HIS:N	1:A:61:HIS:CD2	2.82	0.47
1:A:494:ASP:O	1:A:497:ALA:N	2.48	0.47
1:A:8:ARG:O	1:A:41:SER:HA	2.15	0.47
1:B:148:TYR:O	1:B:151:LEU:N	2.48	0.47
1:A:244:TYR:HH	1:B:195:MET:HG3	1.79	0.47
1:A:204:LEU:HD23	1:A:204:LEU:HA	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:B:69:PHE:HB3	1:B:113:PRO:O	2.14	0.47
1:B:37:VAL:CG1	1:B:38:GLU:N	2.78	0.47
1:A:489:ARG:NE	1:A:512:GLN:OE1	2.46	0.47
1:B:229:LYS:O	1:B:232:ASP:N	2.43	0.47
1:B:238:ILE:HD13	1:B:238:ILE:N	2.28	0.47
1:B:8:ARG:O	1:B:41:SER:HA	2.15	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:468:ILE:HG22	1:A:470:CYS:SG	2.54	0.47
1:A:418:PRO:CD	1:A:474:ASN:HD22	2.22	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: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:B:99:PRO:HD3	1:B:542:ALA:HB2	1.97	0.46
1:A:143:GLU:HB3	1:A:144:PRO:CD	2.45	0.46
1:A:222:ARG:HG2	1:A:225:THR:OG1	2.16	0.46
1:A:173:GLY:N	1:A:408:TYR:HE1	2.13	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:278:SER:HA	1:B:356:ALA:HA	1.97	0.46
1:B:189:PRO:CA	1:B:307:ASN:HA	2.45	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:367:LEU:O	1:A:370:THR:HB	2.15	0.46
1:A:276:TYR:OH	1:A:399:ASP:O	2.19	0.46
1:A:416:TRP:HE3	1:A:416:TRP:HA	1.79	0.46
1:B:541:ILE:O	1:B:541:ILE:HG22	2.16	0.46
1:B:8:ARG:HA	1:B:9:PRO:HD3	1.78	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: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:61:HIS:CD2	1:B:61:HIS:N	2.82	0.46
1:B:79:ASN:ND2	1:B:81:ALA:N	2.63	0.46
1:A:217:LEU:HD22	1:A:217:LEU:HA	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:A:99:PRO:HD3	1:A:542:ALA:HB2	1.97	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:HD23	1:B:560:LEU:HA	1.50	0.46
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:37:VAL:CG1	1:A:38:GLU:N	2.78	0.45
1:A:425:PHE:CE1	1:A:502:GLU:HG3	2.52	0.45
1:A:533:ASN:HD21	1:A:551:SER:N	2.14	0.45
1:A:428:ILE:CG2	1:B:238:ILE:HG21	2.46	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: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:9:PRO:HA	1:B:40:ILE:O	2.15	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:HA	1:A:16:LEU:HD12	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:HE3	1:B:416:TRP:HA	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:HG22	1:B:267:ILE:O	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:424:PHE:CE2	3:A:601:EUG:H6	2.51	0.45
1:A:287:GLY:HA2	1:A:437:MET:CE	2.47	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:487:LEU:CD1	1:B:491:LEU:CD1	2.95	0.45
1:B:56:HIS:O	1:B:111:ALA:HB1	2.17	0.45
1:A:10:LEU:HD11	1:A:41:SER:C	2.37	0.45
1:A:263:THR:HG1	1:A:263:THR:H	1.46	0.45
1:A:405:ILE:HA	1:A:406:PRO:HD2	1.79	0.45
1:A:171:LEU:HD21	2:A:600:FAD:HM73	1.99	0.45
1:A:79:ASN:HD22	1:A:81:ALA:N	2.14	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:293:VAL:C	1:B:295:ILE:N	2.68	0.45
1:B:348:LEU:HD23	1:B:348:LEU:HA	1.69	0.45
1:B:287:GLY:HA2	1:B:437:MET:CE	2.47	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:339:LEU:O	1:A:342:ILE:N	2.51	0.44
1:A:89:LEU:N	1:A:89:LEU:HD12	2.33	0.44
1:B:230:PRO:HD2	1:B:231:GLU:OE2	2.18	0.44
1:B:267:ILE:HA	1:B:267:ILE:HD13	1.57	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:B:279:TYR:O	1:B:395:LEU:HD11	2.17	0.44
1:B:40:ILE:O	1:B:40:ILE:HG22	2.18	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: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:A:279:TYR:O	1:A:395:LEU:HD11	2.17	0.44
1:B:14:PRO:C	1:B:16:LEU:N	2.68	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: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:A:214:MET:CB	1:A:239:ALA:HA	2.46	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:B:97:LEU:O	1:B:542:ALA:HA	2.17	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:HG3	1:B:387:GLU:H	1.22	0.44
1:A:438:MET:O	1:A:442:VAL:HG23	2.17	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:97:LEU:HD23	1:A:97:LEU:HA	1.48	0.44
1:B:72:SER:HB3	1:B:117:GLY:HA2	1.99	0.44
1:A:332:GLU:HB3	1:A:333:PRO:HD2	1.98	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: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:B:89:LEU:HD12	1:B:89:LEU:N	2.33	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: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: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:B:102:ILE:HG13	1:B:175:SER:HB2	1.99	0.44
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:A:72:SER:HB3	1:A:117:GLY:C	2.39	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: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:B:80:VAL:O	1:B:83:VAL:HB	2.17	0.43
1:A:27:ASP:O	1:A:30:ARG:HB3	2.18	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:A:72:SER:HB3	1:A:117:GLY:O	2.17	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:27:ASP:O	1:B:30:ARG:HB3	2.18	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: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:A:58:HIS:HA	1:A:112:ALA:HB2	2.01	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:HD12	1:A:10:LEU:N	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:HA	1:A:428:ILE:HD13	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:188:THR:HB	1:A:189:PRO:HD2	1.99	0.43
1:A:89:LEU:O	1:A:92:LYS:N	2.51	0.43
1:A:241:LEU:HB3	1:B:463:ARG:O	2.19	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:B:56:HIS:HA	1:B:111:ALA:HB2	1.97	0.43
1:A:452:LEU:HA	1:A:452:LEU:HD23	1.18	0.43
1:A:418:PRO:HB2	1:A:474:ASN:HD21	1.84	0.43
1:A:40:ILE:HG22	1:A:40:ILE:O	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:HE3	1:B:413:TRP:C	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:H	1:B:552:GLN:CD	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:B:104:ARG:C	1:B:106:SER:H	2.23	0.42
1:A:463:ARG:NH2	1:B:138:ALA:HB3	2.34	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:HD13	1:B:102:ILE:HA	1.87	0.42
1:B:324:LYS:N	1:B:416:TRP:CE3	2.88	0.42
1:B:454:PHE:C	1:B:454:PHE:CD1	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: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:B:58:HIS:HA	1:B:112:ALA:HB2	2.01	0.42
1:A:23:GLU:O	1:A:26:GLN:N	2.51	0.42
1:A:296:ILE:H	1:A:296:ILE:HG13	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:H	1:B:422:HIS:HD1	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:278:SER:OG	1:B:399:ASP:OD2	2.30	0.41
1:B:68:TYR:CD1	1:B:68:TYR:C	2.94	0.41
1:A:10:LEU:HD11	1:A:42:SER:N	2.35	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:108:TYR:CD1	1:A:505:THR:C	2.93	0.41
1:B:12:LEU:HD13	1:B:16:LEU:O	2.20	0.41
1:B:151:LEU:HA	1:B:151:LEU:HD12	1.75	0.41
1:B:160:LEU:HA	1:B:160:LEU:HD23	1.72	0.41
1:A:535:VAL:CG1	1:B:531:LEU:HD21	2.50	0.41
1:B:60:PRO:C	1:B:62:HIS:H	2.24	0.41
1:A:202:VAL:HG12	1:A:203:VAL:N	2.34	0.41
1:A:139:TYR:HA	1:A:269:LEU:H	1.86	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:HG3	1:A:387:GLU:H	1.22	0.41
1:B:51:TYR:CE1	1:B:104:ARG:HD3	2.54	0.41
1:B:39:VAL:CG1	1:B:40:ILE:N	2.84	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:HA	1:A:540:ILE:HD13	1.71	0.41
1:A:542:ALA:HA	1:A:543:PRO:HD2	1.78	0.41
1:A:59:ASP:HA	1:A:60:PRO:HD2	1.67	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: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:60:PRO:C	1:A:62:HIS:H	2.24	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:B:74:ILE:HG22	1:B:75:VAL:N	2.35	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:200:MET:CE	1:B:251:ASP:CB	2.97	0.41
1:B:139:TYR:HA	1:B:269:LEU:H	1.86	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:HA	1:A:166:LEU:HD23	1.82	0.40
1:B:214:MET:CB	1:B:239:ALA:HA	2.46	0.40
1:A:339:LEU:O	1:A:343:ALA:N	2.49	0.40
1:A:104:ARG:N	2:A:600:FAD:O2P	2.55	0.40
1:A:68:TYR:CD1	1:A:68:TYR:C	2.94	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:385:PHE:O	1:A:388:ASP:N	2.54	0.40
1:A:258:ASN:HB3	1:A:542:ALA:O	2.21	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: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:24:PHE:CE1	1:A:28:ILE:HD11	2.56	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:10:LEU:CD1	1:A:41:SER:C	2.90	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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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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

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

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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 [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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	FAD	A	600	1	51,58,58	1.12	4 (7%)	60,89,89	1.63	6 (10%)
3	EUG	A	601	-	11,11,12	0.45	0	14,14,15	1.51	2 (14%)
3	EUG	B	601	-	11,11,12	0.45	0	14,14,15	1.52	2 (14%)
2	FAD	B	600	1	51,58,58	1.12	4 (7%)	60,89,89	1.63	6 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	600	1	-	10/30/50/50	0/6/6/6
3	EUG	A	601	-	-	4/4/4/5	0/1/1/1
3	EUG	B	601	-	-	4/4/4/5	0/1/1/1
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	C4-N3	3.68	1.39	1.33
2	B	600	FAD	C4-N3	3.64	1.39	1.33
2	B	600	FAD	C4X-C10	3.59	1.42	1.38
2	A	600	FAD	C4X-C10	3.55	1.42	1.38
2	B	600	FAD	C2-N1	-2.93	1.32	1.38
2	A	600	FAD	C2-N1	-2.90	1.32	1.38
2	B	600	FAD	O5B-C5B	-2.41	1.35	1.44
2	A	600	FAD	O5B-C5B	-2.39	1.35	1.44

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	FAD	C4-N3-C2	7.45	121.43	115.14
2	A	600	FAD	C4-N3-C2	7.44	121.42	115.14
2	A	600	FAD	C4X-C4-N3	-5.53	115.87	123.43
2	B	600	FAD	C4X-C4-N3	-5.51	115.90	123.43
2	B	600	FAD	C1'-N10-C9A	4.24	121.63	118.29
2	A	600	FAD	C1'-N10-C9A	4.23	121.62	118.29
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	C6-C5X-N5	-2.72	116.05	119.05
2	A	600	FAD	C6-C5X-N5	-2.71	116.07	119.05
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

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
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.

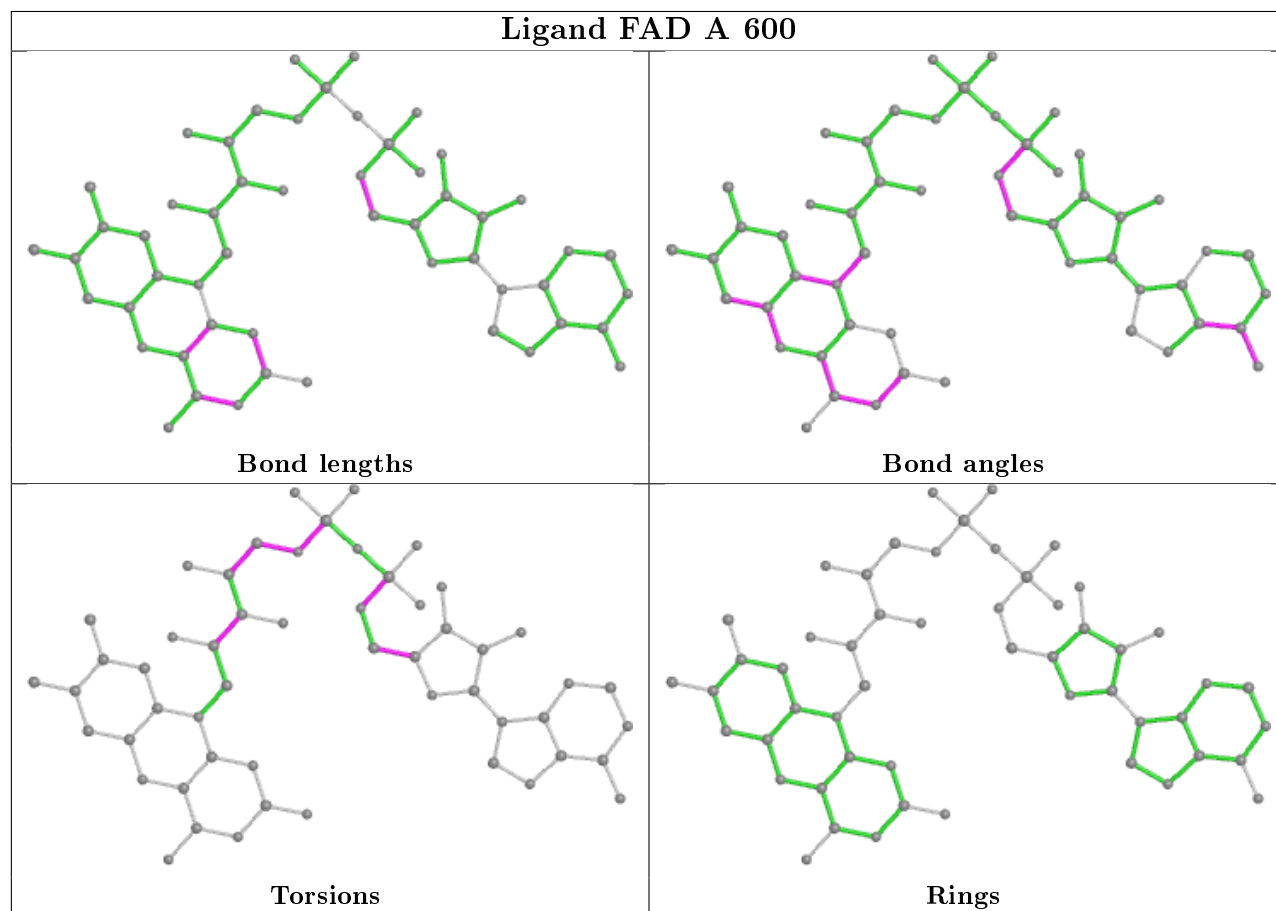
4 monomers are involved in 38 short contacts:

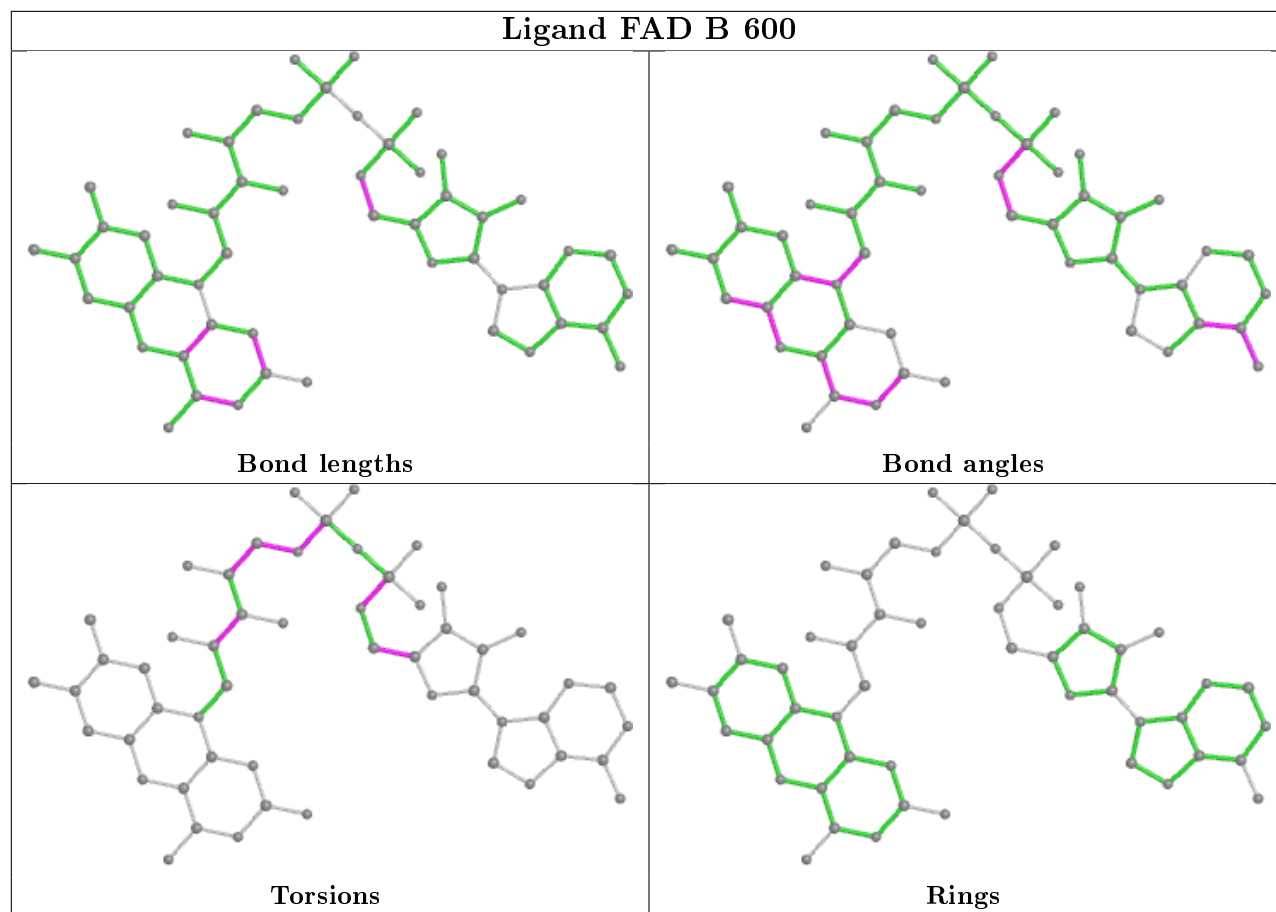
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	FAD	17	0
3	A	601	EUG	4	0
3	B	601	EUG	5	0
2	B	600	FAD	18	0

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.



Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.