



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 11:57 am BST

PDB ID : 4E0V
Title : Structure of L-amino acid oxidase from the B. jararacussu venom
Authors : Ullah, A.; Souza, T.A.C.B.; Betzel, C.; Murakami, M.T.; Arni, R.K.
Deposited on : 2012-03-05
Resolution : 3.10 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 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) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

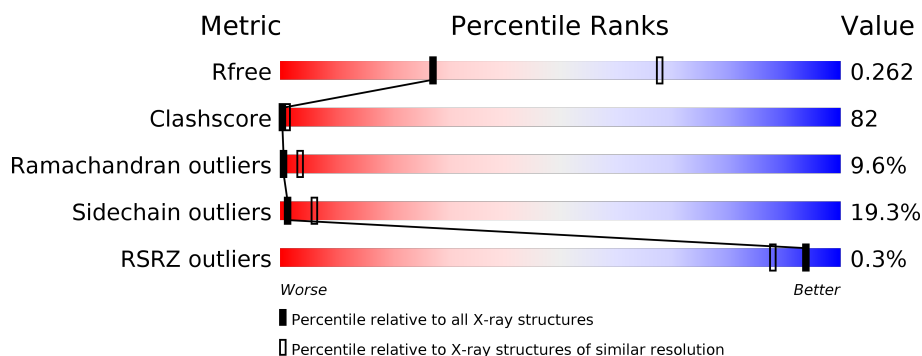
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

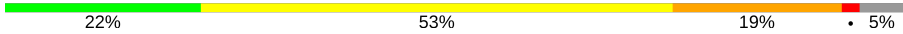
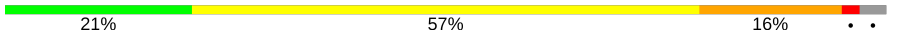
The reported resolution of this entry is 3.10 Å.

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))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 ≥ 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	497	
1	B	497	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FAD	A	501	-	-	X	-

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 7726 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 L-amino-acid oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	474	Total	C	N	O	S	0	0	0
			3771	2398	637	722	14			
1	B	480	Total	C	N	O	S	0	0	0
			3833	2432	653	734	14			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

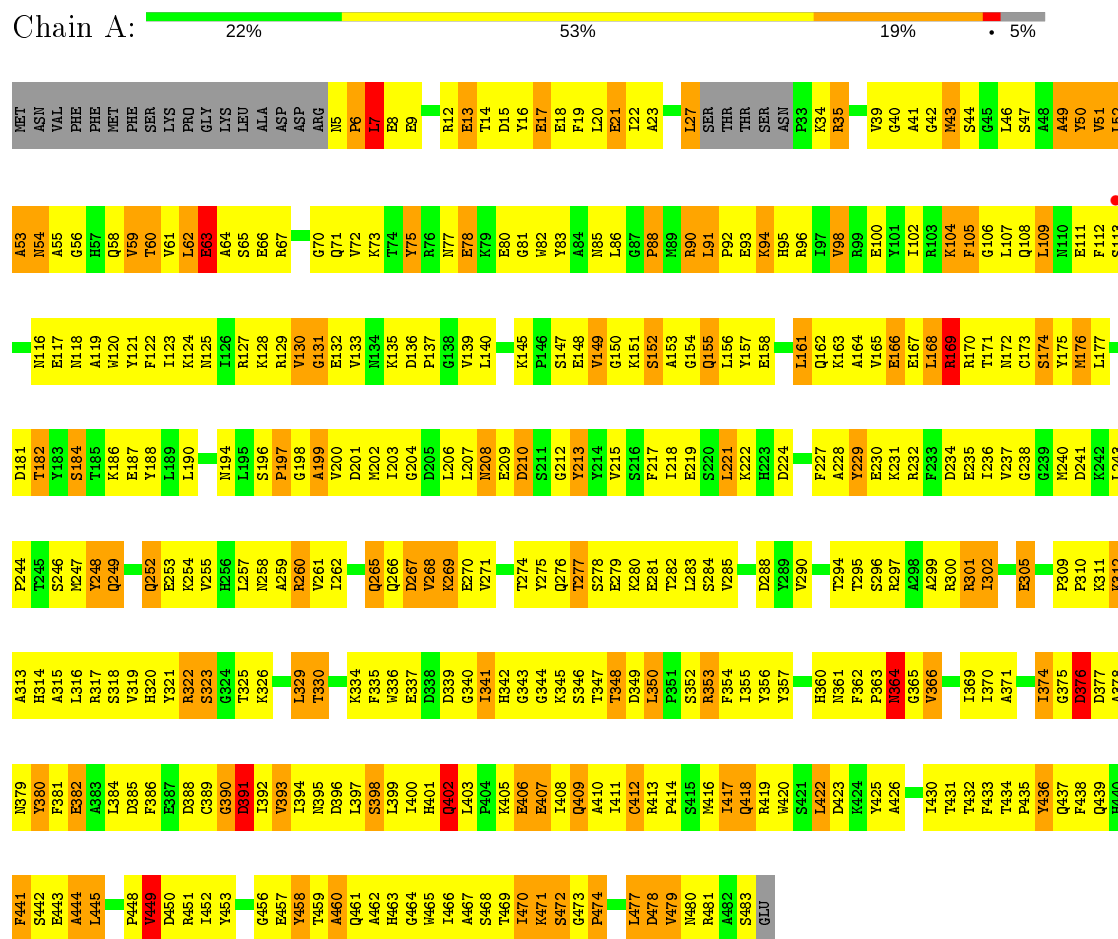
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total 7	O 7	0	0
3	B	9	Total 9	O 9	0	0

3 Residue-property plots

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

- Molecule 1: L-amino-acid oxidase



F433	A371	P307	P244	N178	N116
T434	Y372	L308	T245	K179	E117
P435	G373	P309	S246	Y180	N118
Y436	I374	P310	M247	D181	A119
Q437	G375	K311	Y248	T182	W120
F438	D376	K312	Q249	Y183	Y121
Q439	D377	A313	A250	F122	F122
H440	A378	H314	I251	K186	I123
F441	N379	A315	Q252	K187	K124
S442	Y380	L316	E253	Y188	N125
	F381		K254	L189	I126
	E382	V319	V255	L190	R127
L445	A383	H320		K191	K128
T446	L384	Y321	N256	E192	R129
A447	D385	R322	A259		V130
P448	F386	S323	R260	S196	G131
D450	E387	G324	V261	P197	E132
R451	D388	T325	I262	G198	V133
I452		K326	K263	A199	M134
Y453	D391	I327	I264	V200	K135
F454	I392	F328	Q265	D201	D136
A455	V393	L329	Q266	M202	P137
G456	I394	T330	D267	I203	G138
E457	N395	G331	V268	G204	V139
Y458	D396	T332	K269	D205	L140
T459	L397	K332	E270	L206	D141
A460	S398	K333	Y271	L207	Y142
Q461	L399	F335	T272	N208	P143
A462	I400	W336	W273	E209	V144
H463	H401	E337	T274	D210	K145
G464	Q402	D338	Y275	S211	P146
H465	L403	D339	Q276	G212	S147
I466	P404	G340	T277	Y213	E148
A467	K405	I341	S278	Y214	V149
S468	E406		E279	V215	G150
T469	E407	K345	K280	K151	K151
I470	I408	S346	E281	S152	S152
K471	Q409	T347	T282	I217	A153
S472	A410	T348	L283		
G473	I411	D349	S284	L221	L156
P474	C412	L350	V285	K222	Y157
E475	R413	P351	T286	H223	
G476		S352	A287	D224	
L477	M416	R353	D288	D225	S160
D478	I417	F354	Y289	I226	L161
V479	Q418	I355	V290		Q162
Y480	R419	Y356	I291	Y229	K163
R481	W420	Y357	V292	E230	A164
A482	S421	P358	C293	V165	V165
	L422	N359	T294	K231	E166
SER	D423	H360	T295	R232	E167
GLU	K424	N361	S296	F233	L168
	Y425		R297	D234	R169
	A426	N364	A298	E235	R170
	M427	G365	A299	I236	T171
	G428	V366	R300	V237	N172
	G429	G367	R301		C173
	I430	V368	I302		S174
	T431	I369	K303	M240	Y175
	T432	I370		K242	M176

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.39Å 72.19Å 101.53Å 90.00° 90.90° 90.00°	Depositor
Resolution (Å)	29.02 – 3.10 28.79 – 3.10	Depositor EDS
% Data completeness (in resolution range)	95.1 (29.02-3.10) 94.7 (28.79-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 3.11Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.181 , 0.259 0.188 , 0.262	Depositor DCC
R_{free} test set	852 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	50.9	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 73.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7726	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: 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	0.67	1/3856 (0.0%)	0.80	0/5218
1	B	0.61	0/3920	0.76	0/5305
All	All	0.64	1/7776 (0.0%)	0.78	0/10523

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	88	PRO	N-CD	11.01	1.63	1.47

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	62	LEU	Peptide
1	A	63	GLU	Peptide
1	B	449	VAL	Peptide

5.2 Too-close contacts ⓘ

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	3771	0	3678	591	1
1	B	3833	0	3747	655	1
2	A	53	0	31	29	0
2	B	53	0	31	18	0
3	A	7	0	0	0	0
3	B	9	0	0	1	0
All	All	7726	0	7487	1242	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 82.

All (1242) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:ASP:HB3	1:A:19:PHE:CE2	1.54	1.42
1:B:315:ALA:O	1:B:319:VAL:HG23	1.24	1.35
1:A:92:PRO:HG2	1:A:95:HIS:ND1	1.39	1.34
1:B:473:GLY:HA2	1:B:475:GLU:OE1	1.18	1.30
1:A:269:LYS:C	1:A:269:LYS:HE3	1.56	1.26
1:A:265:GLN:HB2	1:A:305:GLU:OE1	1.19	1.25
1:B:97:ILE:CG2	1:B:470:ILE:HD11	1.66	1.24
1:A:6:PRO:HG3	1:A:229:TYR:CE1	1.72	1.23
1:A:472:SER:C	1:A:474:PRO:HD3	1.61	1.17
1:A:98:VAL:HG12	1:A:467:ALA:HB2	1.24	1.17
1:A:269:LYS:O	1:A:269:LYS:CE	1.94	1.16
1:B:90:ARG:HG2	1:B:91:LEU:H	1.04	1.16
1:A:269:LYS:HE3	1:A:269:LYS:O	1.45	1.15
1:B:466:ILE:H	2:B:501:FAD:HM81	1.02	1.14
1:B:204:GLY:HA2	1:B:209:GLU:HB3	1.14	1.12
1:B:395:ASN:OD1	1:B:405:LYS:CD	1.97	1.12
1:B:90:ARG:CD	1:B:233:PHE:CD2	2.32	1.11
1:B:301:ARG:HH21	1:B:427:MET:CE	1.63	1.11
1:A:63:GLU:CB	2:A:501:FAD:H2A	1.81	1.10
1:B:197:PRO:O	1:B:200:VAL:HG22	1.49	1.10
1:B:3:ASP:N	1:B:229:TYR:CD2	2.20	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:473:GLY:CA	1:B:475:GLU:OE1	1.99	1.09
1:A:63:GLU:CA	2:A:501:FAD:H2A	1.81	1.09
1:B:278:SER:HB2	1:B:281:GLU:OE1	1.53	1.09
1:A:61:VAL:HB	1:A:255:VAL:HG22	1.25	1.08
1:A:430:ILE:HD11	1:A:464:GLY:CA	1.82	1.08
1:A:472:SER:C	1:A:474:PRO:CD	2.22	1.08
2:A:501:FAD:H2B	2:A:501:FAD:N3A	1.37	1.07
1:A:305:GLU:HG2	1:A:305:GLU:O	1.50	1.07
1:B:157:TYR:O	1:B:160:SER:HB3	1.54	1.07
1:B:245:THR:O	1:B:249:GLN:HG3	1.54	1.07
1:B:121:TYR:CE2	1:B:133:VAL:HG21	1.88	1.07
1:A:472:SER:CA	1:A:474:PRO:HD3	1.85	1.07
1:B:61:VAL:HB	1:B:255:VAL:HG22	1.36	1.06
1:B:27:LEU:O	1:B:28:SER:HB2	1.52	1.06
1:B:77:ASN:ND2	1:B:80:GLU:HG3	1.69	1.05
1:B:97:ILE:HG21	1:B:470:ILE:HD11	1.10	1.05
1:A:153:ALA:HB2	1:A:202:MET:HE2	1.35	1.04
1:B:348:THR:HG22	1:B:353:ARG:O	1.56	1.04
1:B:386:PHE:C	1:B:387:GLU:HG3	1.74	1.04
1:B:90:ARG:HD3	1:B:233:PHE:CD2	1.93	1.04
1:A:63:GLU:HB2	2:A:501:FAD:H2A	1.39	1.03
1:A:92:PRO:CG	1:A:95:HIS:ND1	2.21	1.03
1:B:293:CYS:SG	1:B:455:ALA:HB3	1.99	1.03
1:A:430:ILE:HD11	1:A:464:GLY:HA3	1.03	1.02
1:B:181:ASP:HB2	1:B:218:ILE:HD11	1.03	1.02
1:B:280:LYS:O	1:B:281:GLU:CG	2.06	1.02
1:A:6:PRO:HG3	1:A:229:TYR:CZ	1.94	1.02
1:B:271:VAL:HG11	1:B:290:VAL:HG23	1.39	1.02
1:A:271:VAL:HG11	1:A:290:VAL:HG21	1.41	1.01
1:B:395:ASN:OD1	1:B:405:LYS:HD3	1.59	1.01
1:A:63:GLU:CB	2:A:501:FAD:C2A	2.39	1.01
1:A:176:MET:HG3	1:A:177:LEU:N	1.74	1.01
1:B:278:SER:CB	1:B:281:GLU:OE1	2.08	1.01
1:B:301:ARG:HH21	1:B:427:MET:HE1	1.21	1.00
1:B:280:LYS:O	1:B:281:GLU:HG3	1.62	1.00
1:A:401:HIS:O	1:A:402:GLN:HB2	1.59	1.00
1:A:168:LEU:HD23	1:A:168:LEU:C	1.82	0.99
1:B:470:ILE:HD12	1:B:471:LYS:N	1.77	0.99
1:B:181:ASP:CB	1:B:218:ILE:HD11	1.91	0.99
1:B:480:ASN:O	1:B:482:ALA:N	1.93	0.99
1:A:181:ASP:OD2	1:A:438:PHE:HB2	1.60	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:MET:HG3	1:B:470:ILE:CG2	1.92	0.99
1:A:279:GLU:H	1:A:280:LYS:HA	1.27	0.99
1:A:15:ASP:CB	1:A:19:PHE:HE2	1.74	0.98
1:A:322:ARG:CZ	1:A:374:ILE:HD11	1.92	0.98
1:B:43:MET:HA	1:B:43:MET:CE	1.91	0.98
1:B:280:LYS:C	1:B:281:GLU:HG3	1.83	0.98
1:A:265:GLN:CB	1:A:305:GLU:OE1	2.12	0.97
1:A:63:GLU:HB2	2:A:501:FAD:C2A	1.93	0.97
1:B:395:ASN:OD1	1:B:405:LYS:HD2	1.62	0.97
1:B:404:PRO:HB2	1:B:407:GLU:HG3	1.42	0.97
1:B:71:GLN:NE2	2:B:501:FAD:O1A	1.98	0.97
1:A:269:LYS:C	1:A:269:LYS:CE	2.32	0.96
1:A:430:ILE:CD1	1:A:464:GLY:HA3	1.96	0.96
1:B:116:ASN:O	1:B:118:ASN:N	1.96	0.96
1:A:267:ASP:OD1	1:A:269:LYS:N	1.98	0.96
1:A:15:ASP:CB	1:A:19:PHE:CE2	2.46	0.95
1:B:3:ASP:N	1:B:229:TYR:CG	2.35	0.95
1:B:312:LYS:NZ	1:B:447:ALA:O	2.00	0.95
1:A:277:THR:HG21	1:A:283:LEU:HD13	1.47	0.95
1:B:322:ARG:HH11	1:B:432:THR:CG2	1.80	0.94
1:B:475:GLU:O	1:B:479:VAL:HG23	1.67	0.94
1:A:406:GLU:HA	1:A:409:GLN:HE21	1.30	0.94
1:B:3:ASP:N	1:B:229:TYR:HB3	1.82	0.94
1:B:90:ARG:HG2	1:B:91:LEU:N	1.73	0.94
1:A:15:ASP:HB3	1:A:19:PHE:CD2	2.01	0.94
1:A:172:ASN:OD1	1:A:173:CYS:N	2.00	0.93
1:B:43:MET:HG3	1:B:470:ILE:HG22	1.49	0.93
1:B:479:VAL:O	1:B:482:ALA:HB2	1.67	0.93
1:B:322:ARG:NH1	1:B:432:THR:HG21	1.83	0.93
1:A:111:GLU:CD	1:A:232:ARG:HG3	1.89	0.93
1:A:301:ARG:HG2	1:B:380:TYR:OH	1.67	0.93
1:A:406:GLU:N	1:A:406:GLU:OE2	2.02	0.92
1:A:471:LYS:O	1:A:474:PRO:HD3	1.68	0.92
1:B:386:PHE:O	1:B:387:GLU:HG3	1.69	0.92
1:A:181:ASP:HB2	1:A:218:ILE:HD11	1.49	0.92
1:B:396:ASP:O	1:B:400:ILE:HD12	1.68	0.92
1:B:97:ILE:HG21	1:B:470:ILE:CD1	2.00	0.92
1:A:265:GLN:HE21	1:A:305:GLU:CD	1.72	0.92
1:A:322:ARG:HG3	1:A:322:ARG:HH11	1.34	0.91
1:B:181:ASP:HB2	1:B:218:ILE:CD1	1.99	0.91
1:B:315:ALA:O	1:B:319:VAL:CG2	2.18	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:LEU:HB3	1:A:244:PRO:HD3	1.52	0.91
1:B:279:GLU:O	1:B:280:LYS:HG2	1.71	0.91
2:A:501:FAD:N3A	2:A:501:FAD:C2B	2.30	0.91
1:B:472:SER:C	1:B:474:PRO:HD2	1.91	0.90
1:A:265:GLN:NE2	1:A:305:GLU:CD	2.24	0.90
1:A:363:PRO:O	1:A:364:ASN:HB3	1.71	0.90
1:A:269:LYS:HE3	1:A:270:GLU:CA	2.02	0.89
1:B:466:ILE:N	2:B:501:FAD:HM81	1.86	0.89
1:B:77:ASN:ND2	1:B:80:GLU:CG	2.35	0.89
1:B:132:GLU:OE2	1:B:139:VAL:HG11	1.71	0.89
1:B:111:GLU:OE1	1:B:232:ARG:HG3	1.72	0.89
1:B:358:PRO:HD3	1:B:368:VAL:O	1.71	0.89
1:B:328:PHE:HD1	1:B:416:MET:O	1.55	0.89
1:A:217:PHE:CZ	1:A:221:LEU:HD21	2.08	0.88
1:B:473:GLY:HA2	1:B:475:GLU:CD	1.92	0.88
1:A:317:ARG:NH1	1:B:210:ASP:OD1	2.06	0.88
1:A:271:VAL:HG11	1:A:290:VAL:CG2	2.04	0.88
1:B:77:ASN:HD22	1:B:80:GLU:CG	1.85	0.88
1:A:63:GLU:N	2:A:501:FAD:H2A	1.89	0.87
1:B:90:ARG:CD	1:B:233:PHE:CE2	2.57	0.87
1:A:166:GLU:C	1:A:167:GLU:CD	2.33	0.87
1:A:478:ASP:O	1:A:481:ARG:HG2	1.74	0.87
1:B:98:VAL:O	1:B:102:ILE:HG12	1.75	0.87
1:B:90:ARG:HD2	1:B:233:PHE:CE2	2.10	0.86
1:A:181:ASP:HB2	1:A:218:ILE:CD1	2.03	0.86
1:A:168:LEU:CD2	1:A:169:ARG:N	2.38	0.86
1:B:204:GLY:HA2	1:B:209:GLU:CB	2.03	0.86
1:B:136:ASP:OD1	1:B:138:GLY:N	2.07	0.86
1:A:323:SER:O	1:A:375:GLY:N	2.08	0.86
1:A:166:GLU:O	1:A:167:GLU:CD	2.14	0.86
1:A:153:ALA:HB2	1:A:202:MET:CE	2.04	0.86
1:A:330:THR:HG22	1:A:330:THR:O	1.75	0.86
1:A:380:TYR:CD2	1:A:380:TYR:O	2.28	0.86
1:B:264:ILE:HG12	1:B:273:VAL:HG12	1.56	0.86
1:B:322:ARG:HH11	1:B:432:THR:HG21	1.39	0.85
1:A:277:THR:O	1:A:280:LYS:CB	2.23	0.85
1:B:146:PRO:C	1:B:148:GLU:H	1.78	0.85
1:B:102:ILE:HA	1:B:107:LEU:HD12	1.56	0.85
1:A:121:TYR:CD2	1:A:133:VAL:HG21	2.10	0.85
1:B:471:LYS:O	1:B:474:PRO:HD3	1.74	0.85
1:B:130:VAL:O	1:B:131:GLY:C	2.15	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:ILE:HG12	1:B:273:VAL:CG1	2.07	0.85
1:A:117:GLU:HA	1:A:130:VAL:HG22	1.58	0.84
1:B:168:LEU:HB2	1:B:176:MET:SD	2.16	0.84
1:A:315:ALA:HB1	1:A:445:LEU:HD11	1.58	0.84
1:A:269:LYS:HE3	1:A:270:GLU:N	1.91	0.84
1:A:279:GLU:N	1:A:280:LYS:HA	1.82	0.84
1:A:204:GLY:HA2	1:A:209:GLU:HB2	1.60	0.84
1:B:277:THR:OG1	1:B:281:GLU:HB2	1.77	0.84
1:A:120:TRP:CZ2	1:A:129:ARG:NH2	2.45	0.84
1:A:315:ALA:O	1:A:319:VAL:HG12	1.77	0.83
1:A:112:PHE:O	1:A:112:PHE:CD1	2.30	0.83
1:B:376:ASP:O	1:B:379:ASN:HB2	1.78	0.83
1:B:456:GLY:H	1:B:459:THR:CG2	1.90	0.83
1:B:48:ALA:HB1	1:B:475:GLU:HG3	1.58	0.83
1:A:471:LYS:O	1:A:474:PRO:CD	2.27	0.83
1:B:348:THR:CG2	1:B:353:ARG:O	2.26	0.83
1:B:434:THR:HB	1:B:435:PRO:HD3	1.60	0.83
1:B:441:PHE:O	1:B:445:LEU:HD12	1.78	0.83
1:A:15:ASP:HB3	1:A:19:PHE:HE2	1.03	0.83
1:A:63:GLU:CA	2:A:501:FAD:C2A	2.56	0.83
1:B:43:MET:HA	1:B:43:MET:HE3	1.60	0.83
1:B:121:TYR:CE1	1:B:347:THR:HG23	2.14	0.83
1:B:271:VAL:HG11	1:B:290:VAL:CG2	2.09	0.82
1:A:168:LEU:CD2	1:A:168:LEU:C	2.48	0.82
1:A:176:MET:HG3	1:A:177:LEU:H	1.43	0.82
1:B:14:THR:O	1:B:17:GLU:OE1	1.96	0.82
1:B:62:LEU:HD22	1:B:259:ALA:HB1	1.60	0.82
1:A:158:GLU:HA	1:A:161:LEU:HD22	1.62	0.82
1:B:453:TYR:CE1	1:B:478:ASP:HB3	2.15	0.82
1:B:480:ASN:C	1:B:482:ALA:N	2.31	0.82
1:A:322:ARG:NE	1:A:374:ILE:HD11	1.93	0.82
1:A:473:GLY:N	1:A:474:PRO:HD3	1.95	0.82
1:A:208:ASN:HD21	1:A:374:ILE:HG21	1.44	0.81
1:B:108:GLN:NE2	1:B:109:LEU:N	2.27	0.81
1:A:77:ASN:HD22	1:A:80:GLU:HB2	1.46	0.81
1:B:301:ARG:HH21	1:B:427:MET:HE2	1.45	0.81
1:A:181:ASP:CB	1:A:218:ILE:HD11	2.11	0.81
1:A:364:ASN:HD21	1:A:366:VAL:H	1.29	0.81
1:B:62:LEU:CD2	1:B:259:ALA:HB1	2.11	0.81
1:B:20:LEU:O	1:B:24:LYS:HG2	1.81	0.81
1:B:3:ASP:N	1:B:229:TYR:CB	2.44	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:470:ILE:HD12	1:B:470:ILE:C	2.02	0.80
1:B:301:ARG:NH2	1:B:427:MET:HE1	1.96	0.80
1:B:97:ILE:HG22	1:B:470:ILE:HD11	1.61	0.80
1:A:459:THR:O	1:A:460:ALA:O	1.99	0.80
1:A:51:VAL:HG12	1:A:52:LEU:N	1.96	0.80
1:A:269:LYS:HE2	1:A:270:GLU:HB3	1.62	0.79
1:A:430:ILE:CD1	1:A:464:GLY:CA	2.57	0.79
1:A:202:MET:HE2	1:A:206:LEU:HD12	1.64	0.79
1:B:90:ARG:HD2	1:B:233:PHE:CD2	2.13	0.79
1:B:74:THR:HG23	1:B:84:ALA:O	1.81	0.79
1:A:170:ARG:HG3	1:A:171:THR:CG2	2.13	0.79
1:A:181:ASP:CB	1:A:218:ILE:CD1	2.61	0.79
1:B:279:GLU:O	1:B:280:LYS:CG	2.31	0.79
1:B:283:LEU:HD12	1:B:283:LEU:N	1.98	0.78
1:A:322:ARG:NH1	1:A:322:ARG:HG3	1.97	0.78
1:B:114:GLN:O	1:B:345:LYS:HE3	1.82	0.78
1:B:475:GLU:HG2	1:B:476:GLY:N	1.98	0.78
1:A:433:PHE:HE2	1:A:442:SER:HG	1.30	0.78
1:A:364:ASN:HD22	1:A:365:GLY:N	1.80	0.78
1:B:186:LYS:HA	1:B:189:LEU:HB2	1.66	0.78
1:B:97:ILE:CG2	1:B:470:ILE:CD1	2.56	0.78
1:A:145:LYS:HB3	1:A:148:GLU:HG3	1.65	0.78
1:A:168:LEU:HD22	1:A:169:ARG:N	1.99	0.78
1:B:7:LEU:HD21	1:B:161:LEU:HD22	1.65	0.78
1:A:336:TRP:O	1:A:341:ILE:HB	1.83	0.78
1:B:90:ARG:HD3	1:B:233:PHE:CE2	2.19	0.78
1:A:127:ARG:NH2	1:A:401:HIS:O	2.17	0.77
1:B:19:PHE:CE1	1:B:474:PRO:HB3	2.19	0.77
1:A:19:PHE:O	1:A:20:LEU:C	2.22	0.77
1:B:327:ILE:HG23	1:B:417:ILE:CD1	2.15	0.77
1:B:43:MET:HG2	1:B:466:ILE:HG23	1.66	0.77
1:A:329:LEU:CD1	1:A:414:PRO:HA	2.14	0.77
1:B:66:GLU:OE2	1:B:258:ASN:ND2	2.16	0.77
1:A:269:LYS:O	1:A:269:LYS:CD	2.33	0.77
1:A:265:GLN:HG3	1:A:266:GLN:N	1.98	0.76
1:B:153:ALA:H	1:B:202:MET:HE2	1.47	0.76
1:A:54:ASN:C	1:A:56:GLY:H	1.88	0.76
1:B:167:GLU:OE1	1:B:179:LYS:HE2	1.86	0.76
1:B:457:GLU:OE2	2:B:501:FAD:O2P	2.03	0.76
1:B:333:LYS:O	1:B:335:PHE:N	2.19	0.76
1:B:456:GLY:H	1:B:459:THR:HG23	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:THR:HG23	1:A:281:GLU:O	1.85	0.76
1:A:98:VAL:CG1	1:A:467:ALA:HB2	2.12	0.76
1:A:265:GLN:HG3	1:A:266:GLN:H	1.51	0.75
1:B:130:VAL:O	1:B:133:VAL:N	2.20	0.75
1:B:438:PHE:O	1:B:442:SER:OG	2.05	0.75
1:B:403:LEU:HD23	1:B:407:GLU:OE1	1.85	0.75
1:B:480:ASN:O	1:B:481:ARG:C	2.23	0.75
1:B:145:LYS:O	1:B:148:GLU:HB2	1.85	0.75
1:A:70:GLY:HA3	2:A:501:FAD:O2A	1.86	0.75
1:A:145:LYS:HB2	1:A:148:GLU:OE1	1.86	0.75
1:B:157:TYR:O	1:B:160:SER:CB	2.34	0.75
1:B:167:GLU:O	1:B:171:THR:HG23	1.87	0.75
1:B:114:GLN:O	1:B:345:LYS:CE	2.34	0.75
1:A:43:MET:CE	1:A:247:MET:HE3	2.16	0.74
1:A:7:LEU:C	1:A:9:GLU:H	1.91	0.74
1:B:404:PRO:CB	1:B:407:GLU:HG3	2.17	0.74
1:B:471:LYS:O	1:B:474:PRO:CD	2.36	0.74
1:B:10:CYS:O	1:B:11:PHE:HB2	1.87	0.74
1:A:329:LEU:HD13	1:A:414:PRO:HA	1.69	0.74
1:A:67:ARG:O	2:A:501:FAD:N7A	2.20	0.74
1:A:71:GLN:HG3	2:A:501:FAD:O1A	1.88	0.74
1:B:329:LEU:N	1:B:329:LEU:HD12	2.01	0.74
1:A:128:LYS:HD2	1:A:132:GLU:OE2	1.88	0.74
1:B:115:GLU:O	1:B:116:ASN:HB3	1.87	0.74
1:B:357:TYR:HA	1:B:369:ILE:HG22	1.70	0.74
1:A:269:LYS:C	1:A:269:LYS:CD	2.56	0.73
1:A:274:THR:HA	1:A:284:SER:HA	1.69	0.73
1:A:186:LYS:HG2	1:A:190:LEU:HD12	1.69	0.73
1:A:61:VAL:CB	1:A:255:VAL:HG22	2.14	0.73
1:A:248:TYR:CD2	1:A:249:GLN:N	2.56	0.73
1:A:269:LYS:CE	1:A:270:GLU:HB3	2.18	0.73
1:A:435:PRO:O	1:A:436:TYR:HB2	1.87	0.73
1:B:294:THR:OG1	1:B:299:ALA:HB2	1.88	0.73
1:B:419:ARG:HD2	1:B:422:LEU:HD12	1.70	0.73
1:A:436:TYR:HB3	1:B:186:LYS:HZ1	1.52	0.73
1:B:121:TYR:CE1	1:B:347:THR:CG2	2.71	0.73
1:A:120:TRP:CZ2	1:A:129:ARG:NE	2.57	0.73
1:A:170:ARG:HG3	1:A:171:THR:HG23	1.69	0.73
1:B:453:TYR:CE1	1:B:478:ASP:CB	2.71	0.72
1:A:472:SER:C	1:A:474:PRO:HD2	2.08	0.72
1:B:348:THR:HG23	1:B:353:ARG:HA	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:PHE:O	1:B:387:GLU:CG	2.37	0.72
1:A:120:TRP:CE2	1:A:129:ARG:NH2	2.54	0.72
1:A:364:ASN:ND2	1:A:365:GLY:N	2.37	0.72
1:A:167:GLU:HA	1:A:170:ARG:HB3	1.69	0.72
1:B:100:GLU:OE2	1:B:103:ARG:NH2	2.21	0.72
1:A:166:GLU:C	1:A:167:GLU:OE1	2.28	0.72
1:A:197:PRO:O	1:A:200:VAL:HB	1.90	0.72
1:A:39:VAL:O	1:A:39:VAL:HG12	1.88	0.72
1:A:72:VAL:HG22	1:A:88:PRO:HG2	1.72	0.72
1:A:277:THR:CG2	1:A:283:LEU:HD13	2.19	0.72
1:A:406:GLU:HA	1:A:409:GLN:NE2	2.04	0.72
1:B:111:GLU:OE1	1:B:232:ARG:CG	2.37	0.72
1:A:364:ASN:ND2	1:A:366:VAL:H	1.87	0.72
1:B:479:VAL:O	1:B:482:ALA:CB	2.38	0.72
1:A:376:ASP:O	1:A:379:ASN:HB2	1.90	0.72
1:B:74:THR:HB	1:B:241:ASP:OD2	1.89	0.72
1:B:404:PRO:HD2	1:B:407:GLU:OE1	1.90	0.71
1:B:196:SER:O	1:B:200:VAL:HG13	1.89	0.71
1:A:171:THR:O	1:A:172:ASN:HB2	1.89	0.71
1:B:302:ILE:HG22	1:B:303:LYS:N	2.04	0.71
1:B:153:ALA:H	1:B:202:MET:CE	2.03	0.71
1:B:395:ASN:CG	1:B:405:LYS:HD2	2.10	0.71
1:A:262:ILE:O	1:A:302:ILE:HG22	1.91	0.71
1:B:165:VAL:C	1:B:167:GLU:H	1.94	0.71
1:B:353:ARG:NH2	1:B:354:PHE:CE2	2.58	0.71
1:A:337:GLU:C	1:A:339:ASP:H	1.93	0.71
1:B:88:PRO:HA	2:B:501:FAD:C5X	2.20	0.71
1:A:472:SER:HA	1:A:474:PRO:HD3	1.69	0.70
1:B:146:PRO:O	1:B:148:GLU:N	2.23	0.70
1:B:108:GLN:NE2	1:B:109:LEU:H	1.88	0.70
1:B:16:TYR:CZ	1:B:97:ILE:HG13	2.27	0.70
1:B:473:GLY:N	1:B:474:PRO:HD2	2.05	0.70
1:A:277:THR:O	1:A:280:LYS:HB3	1.91	0.70
1:A:314:HIS:CG	1:A:441:PHE:HZ	2.10	0.70
1:A:73:LYS:O	1:A:86:LEU:HB2	1.91	0.70
1:B:97:ILE:HD12	1:B:471:LYS:HB2	1.72	0.70
1:B:114:GLN:HG2	1:B:115:GLU:HG2	1.74	0.70
1:A:109:LEU:H	1:A:109:LEU:HD12	1.56	0.70
1:A:350:LEU:N	1:A:350:LEU:CD2	2.55	0.70
1:B:480:ASN:C	1:B:482:ALA:H	1.93	0.70
1:A:181:ASP:CA	1:A:218:ILE:HD11	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:LYS:HG2	1:A:336:TRP:CZ2	2.27	0.70
1:B:207:LEU:HD13	1:B:209:GLU:OE1	1.89	0.70
1:B:212:GLY:O	1:B:215:VAL:HG22	1.92	0.70
1:B:279:GLU:O	1:B:280:LYS:CB	2.39	0.70
1:A:277:THR:O	1:A:280:LYS:HA	1.91	0.70
1:A:363:PRO:O	1:A:364:ASN:CB	2.40	0.70
1:B:251:ILE:C	1:B:253:GLU:N	2.45	0.70
1:B:328:PHE:N	1:B:328:PHE:CD1	2.60	0.70
1:B:77:ASN:HD22	1:B:80:GLU:CD	1.95	0.69
1:B:355:ILE:N	1:B:355:ILE:HD13	2.05	0.69
1:B:98:VAL:HG23	1:B:467:ALA:HB2	1.74	0.69
1:B:146:PRO:C	1:B:148:GLU:N	2.43	0.69
1:A:105:PHE:CD1	1:A:246:SER:HB3	2.27	0.69
1:A:168:LEU:HD23	1:A:169:ARG:N	2.05	0.69
1:A:472:SER:CA	1:A:474:PRO:CD	2.63	0.69
1:B:204:GLY:CA	1:B:209:GLU:HB3	2.09	0.69
1:B:21:GLU:O	1:B:25:ASN:N	2.15	0.69
1:B:280:LYS:O	1:B:281:GLU:CB	2.41	0.69
1:B:301:ARG:NH2	1:B:427:MET:CE	2.48	0.69
1:B:280:LYS:O	1:B:281:GLU:OE1	2.11	0.69
1:B:335:PHE:HE2	1:B:412:CYS:SG	2.15	0.69
1:B:322:ARG:NH1	1:B:432:THR:CG2	2.49	0.69
1:B:434:THR:HB	1:B:435:PRO:CD	2.22	0.69
1:A:279:GLU:N	1:A:280:LYS:CA	2.54	0.69
1:A:472:SER:HA	1:A:474:PRO:CD	2.23	0.69
1:B:261:VAL:O	1:B:302:ILE:HG12	1.93	0.69
1:B:302:ILE:CG2	1:B:303:LYS:N	2.56	0.69
1:B:326:LYS:HB3	1:B:370:ILE:CG2	2.23	0.69
1:B:172:ASN:H	1:B:175:TYR:HD2	1.40	0.68
1:B:5:ASN:ND2	1:B:224:ASP:OD2	2.26	0.68
1:B:70:GLY:C	1:B:72:VAL:H	1.96	0.68
1:A:300:ARG:HG3	1:A:316:LEU:HB3	1.75	0.68
1:B:230:GLU:OE2	1:B:230:GLU:HA	1.92	0.68
1:A:282:THR:HG23	1:A:282:THR:O	1.94	0.68
1:B:322:ARG:O	1:B:429:GLY:HA3	1.93	0.68
1:B:434:THR:O	1:B:437:GLN:HG3	1.94	0.68
1:B:328:PHE:CD1	1:B:416:MET:O	2.44	0.68
1:B:9:GLU:O	1:B:12:ARG:HB3	1.93	0.68
1:A:148:GLU:O	1:A:151:LYS:CG	2.42	0.68
1:B:77:ASN:HD21	1:B:80:GLU:HG3	1.52	0.68
1:B:80:GLU:HB2	1:B:82:TRP:CD1	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:PRO:CG	1:A:229:TYR:CE1	2.66	0.67
1:B:43:MET:HG3	1:B:470:ILE:HG23	1.76	0.67
1:B:5:ASN:O	1:B:6:PRO:C	2.33	0.67
1:B:278:SER:O	1:B:280:LYS:N	2.28	0.67
1:A:46:LEU:HB3	1:A:247:MET:SD	2.33	0.67
1:A:394:ILE:HG23	1:A:408:ILE:HG21	1.76	0.67
1:B:162:GLN:HG3	1:B:163:LYS:H	1.60	0.67
1:B:207:LEU:O	1:B:208:ASN:O	2.12	0.67
1:B:30:THR:O	1:B:30:THR:HG23	1.93	0.67
1:B:403:LEU:CD2	1:B:407:GLU:OE1	2.42	0.67
1:A:336:TRP:HD1	1:A:341:ILE:HG22	1.59	0.67
1:A:477:LEU:HG	1:A:478:ASP:N	2.09	0.67
1:B:243:LEU:HB3	1:B:244:PRO:HD3	1.76	0.67
1:A:210:ASP:C	1:A:210:ASP:OD2	2.33	0.67
1:B:353:ARG:NH2	1:B:354:PHE:CZ	2.62	0.67
1:A:43:MET:CE	1:A:247:MET:CE	2.72	0.67
1:A:184:SER:O	1:A:187:GLU:HB3	1.95	0.66
1:A:86:LEU:HD21	1:A:416:MET:HE3	1.78	0.66
1:B:90:ARG:CG	1:B:233:PHE:CD2	2.78	0.66
1:B:73:LYS:CG	1:B:86:LEU:HD12	2.25	0.66
1:A:85:ASN:HD21	1:A:240:MET:H	1.42	0.66
1:B:62:LEU:CD2	1:B:259:ALA:CB	2.73	0.66
1:A:469:THR:O	1:A:472:SER:N	2.27	0.66
1:B:170:ARG:O	1:B:171:THR:CG2	2.42	0.66
1:A:71:GLN:NE2	2:A:501:FAD:O1A	2.28	0.66
1:B:165:VAL:O	1:B:167:GLU:N	2.27	0.66
1:B:472:SER:CA	1:B:474:PRO:HD2	2.25	0.66
1:A:312:LYS:O	1:A:316:LEU:HG	1.95	0.66
1:B:352:SER:HB3	1:B:355:ILE:HD11	1.77	0.66
1:B:405:LYS:C	1:B:407:GLU:H	1.99	0.66
1:A:315:ALA:HB1	1:A:445:LEU:CD1	2.24	0.66
1:B:406:GLU:HA	1:B:409:GLN:HE21	1.61	0.66
1:A:236:ILE:H	1:A:240:MET:CE	2.09	0.66
1:A:379:ASN:C	1:A:381:PHE:H	1.99	0.66
1:B:327:ILE:HG23	1:B:417:ILE:HD13	1.76	0.66
1:A:129:ARG:NH2	1:A:339:ASP:OD2	2.29	0.66
1:A:312:LYS:HD3	1:A:444:ALA:O	1.95	0.66
1:A:269:LYS:HD2	1:A:269:LYS:O	1.95	0.66
1:A:319:VAL:HA	1:A:437:GLN:HE22	1.61	0.66
1:B:116:ASN:HD21	1:B:341:ILE:HG23	1.60	0.66
1:A:164:ALA:HB2	1:A:188:TYR:OH	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:VAL:O	1:A:452:ILE:HB	1.95	0.65
1:A:49:ALA:O	1:A:50:TYR:C	2.34	0.65
1:B:24:LYS:HE3	1:B:100:GLU:OE1	1.96	0.65
1:B:353:ARG:CZ	1:B:354:PHE:CE2	2.80	0.65
1:A:322:ARG:CG	1:A:322:ARG:HH11	2.08	0.65
1:A:51:VAL:O	1:A:53:ALA:N	2.29	0.65
1:A:5:ASN:HB2	1:A:6:PRO:HD3	1.77	0.65
1:B:102:ILE:HA	1:B:107:LEU:CD1	2.25	0.65
1:B:211:SER:HB3	1:B:377:ASP:OD2	1.96	0.65
1:B:170:ARG:O	1:B:171:THR:HG22	1.96	0.65
1:B:417:ILE:O	1:B:417:ILE:CG2	2.44	0.65
1:A:379:ASN:O	1:A:381:PHE:N	2.30	0.65
1:B:471:LYS:C	1:B:473:GLY:H	2.00	0.65
1:A:277:THR:O	1:A:280:LYS:CA	2.44	0.65
1:A:472:SER:O	1:A:474:PRO:HD2	1.95	0.65
1:B:114:GLN:O	1:B:345:LYS:NZ	2.28	0.65
1:B:277:THR:O	1:B:278:SER:OG	2.13	0.65
1:B:277:THR:OG1	1:B:281:GLU:CB	2.45	0.65
1:A:63:GLU:HB2	2:A:501:FAD:N3A	2.12	0.65
1:A:92:PRO:CG	1:A:95:HIS:CE1	2.80	0.65
1:B:405:LYS:O	1:B:407:GLU:N	2.30	0.65
1:B:457:GLU:HB3	2:B:501:FAD:O2P	1.97	0.65
1:B:327:ILE:HG12	1:B:417:ILE:HD11	1.79	0.64
1:A:230:GLU:OE2	1:A:231:LYS:N	2.23	0.64
1:B:453:TYR:CZ	1:B:478:ASP:HB3	2.32	0.64
1:B:74:THR:HG23	1:B:84:ALA:C	2.18	0.64
1:B:59:VAL:O	1:B:254:LYS:HD2	1.96	0.64
1:A:166:GLU:HB3	1:A:167:GLU:OE2	1.97	0.64
1:B:262:ILE:HG13	1:B:274:THR:HG22	1.79	0.64
1:A:120:TRP:CZ2	1:A:129:ARG:CZ	2.80	0.64
1:A:217:PHE:CE1	1:A:221:LEU:HD21	2.32	0.64
1:B:74:THR:HA	1:B:84:ALA:O	1.98	0.64
1:A:375:GLY:O	1:A:378:ALA:N	2.31	0.64
1:B:309:PRO:HD3	1:B:449:VAL:HG11	1.80	0.64
1:A:236:ILE:H	1:A:240:MET:HE2	1.62	0.63
1:A:436:TYR:HB3	1:B:186:LYS:NZ	2.13	0.63
1:A:436:TYR:CB	1:B:186:LYS:NZ	2.61	0.63
1:B:108:GLN:O	1:B:237:VAL:HG23	1.97	0.63
1:A:436:TYR:CB	1:B:186:LYS:HZ1	2.12	0.63
1:A:170:ARG:CG	1:A:171:THR:HG23	2.29	0.63
1:B:144:VAL:HB	1:B:148:GLU:OE1	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:VAL:CB	1:B:255:VAL:HG22	2.20	0.63
1:B:36:VAL:HG22	1:B:289:TYR:HB2	1.80	0.63
1:B:251:ILE:C	1:B:253:GLU:H	2.01	0.63
1:B:121:TYR:CD1	1:B:347:THR:HG23	2.34	0.63
1:B:348:THR:OG1	1:B:350:LEU:HB2	1.98	0.63
1:B:479:VAL:O	1:B:482:ALA:CA	2.47	0.62
1:A:201:ASP:O	1:A:202:MET:C	2.38	0.62
1:B:395:ASN:H	1:B:395:ASN:HD22	1.47	0.62
1:A:90:ARG:C	1:A:91:LEU:HG	2.19	0.62
1:B:187:GLU:HG2	1:B:191:LYS:HD3	1.81	0.62
1:B:95:HIS:O	1:B:97:ILE:N	2.32	0.62
1:A:111:GLU:OE1	1:A:232:ARG:CD	2.48	0.62
1:B:88:PRO:HA	2:B:501:FAD:N5	2.15	0.62
1:B:9:GLU:O	1:B:12:ARG:CB	2.47	0.62
1:B:103:ARG:HH11	1:B:103:ARG:HG2	1.64	0.62
1:B:187:GLU:O	1:B:188:TYR:C	2.35	0.62
1:B:291:ILE:HG22	1:B:293:CYS:SG	2.40	0.62
1:B:395:ASN:O	1:B:397:LEU:N	2.32	0.62
1:B:399:LEU:HD12	1:B:399:LEU:N	2.14	0.62
1:B:397:LEU:O	1:B:398:SER:C	2.36	0.62
1:A:252:GLN:HG2	1:A:253:GLU:N	2.15	0.62
1:A:314:HIS:CG	1:A:441:PHE:CZ	2.87	0.62
1:A:236:ILE:HG13	1:A:240:MET:CE	2.30	0.62
1:A:314:HIS:CD2	1:A:441:PHE:HZ	2.18	0.62
1:A:364:ASN:HD22	1:A:365:GLY:H	1.45	0.62
1:A:320:HIS:H	1:A:437:GLN:HE22	1.47	0.62
1:B:152:SER:O	1:B:153:ALA:C	2.38	0.62
1:B:348:THR:HG23	1:B:353:ARG:CA	2.30	0.62
1:A:111:GLU:OE2	1:A:232:ARG:HG3	1.99	0.61
1:B:117:GLU:HA	1:B:130:VAL:HB	1.81	0.61
1:A:102:ILE:HG23	1:A:107:LEU:HB2	1.82	0.61
1:B:266:GLN:NE2	1:B:452:ILE:HG13	2.14	0.61
1:B:121:TYR:CE2	1:B:133:VAL:CG2	2.75	0.61
1:B:327:ILE:HG23	1:B:417:ILE:HD11	1.83	0.61
1:A:119:ALA:O	1:A:129:ARG:HA	2.00	0.61
1:B:163:LYS:CD	1:B:192:GLU:HA	2.30	0.61
1:B:473:GLY:N	1:B:474:PRO:CD	2.64	0.61
1:B:440:HIS:HD2	1:B:440:HIS:O	1.83	0.61
1:A:41:ALA:C	1:A:42:GLY:O	2.38	0.61
1:A:320:HIS:H	1:A:437:GLN:NE2	1.99	0.61
1:A:406:GLU:O	1:A:407:GLU:C	2.39	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:MET:HE2	1:A:247:MET:CE	2.31	0.61
1:A:63:GLU:C	2:A:501:FAD:C2A	2.69	0.61
1:B:186:LYS:HE2	1:B:190:LEU:HD11	1.83	0.61
1:B:268:VAL:CG1	1:B:269:LYS:N	2.64	0.61
1:B:393:VAL:O	1:B:397:LEU:HG	2.01	0.61
1:B:5:ASN:HB2	1:B:229:TYR:HE1	1.66	0.61
1:A:117:GLU:HA	1:A:130:VAL:CG2	2.30	0.60
1:B:251:ILE:O	1:B:253:GLU:N	2.34	0.60
1:B:473:GLY:CA	1:B:475:GLU:CD	2.60	0.60
1:B:62:LEU:HD23	1:B:259:ALA:CB	2.31	0.60
1:B:19:PHE:CZ	1:B:474:PRO:HB3	2.37	0.60
1:B:48:ALA:HB2	1:B:475:GLU:CD	2.21	0.60
1:A:353:ARG:HG3	1:A:354:PHE:CE2	2.36	0.60
1:A:360:HIS:NE2	1:A:362:PHE:CZ	2.69	0.60
1:B:97:ILE:CD1	1:B:471:LYS:HB2	2.30	0.60
1:A:208:ASN:C	1:A:208:ASN:HD22	2.04	0.60
1:A:375:GLY:O	1:A:377:ASP:N	2.34	0.60
1:B:120:TRP:CZ3	1:B:129:ARG:HG3	2.36	0.60
1:B:90:ARG:O	2:B:501:FAD:HM73	2.01	0.60
1:A:347:THR:HG23	1:A:354:PHE:CE1	2.36	0.60
1:A:54:ASN:C	1:A:56:GLY:N	2.55	0.60
1:B:11:PHE:CE1	1:B:222:LYS:HE2	2.36	0.60
1:B:396:ASP:O	1:B:400:ILE:CD1	2.46	0.60
1:A:161:LEU:O	1:A:164:ALA:N	2.35	0.60
1:A:315:ALA:CB	1:A:445:LEU:HD11	2.31	0.60
1:B:5:ASN:HB2	1:B:229:TYR:CE1	2.36	0.60
1:A:198:GLY:C	1:A:200:VAL:N	2.52	0.60
1:A:269:LYS:NZ	1:A:269:LYS:O	2.34	0.60
1:A:311:LYS:HB3	1:A:444:ALA:CB	2.32	0.60
1:B:101:TYR:O	1:B:105:PHE:N	2.31	0.60
1:B:268:VAL:HG13	1:B:269:LYS:N	2.16	0.60
1:A:148:GLU:O	1:A:151:LYS:HG3	2.00	0.59
1:A:166:GLU:O	1:A:167:GLU:OE2	2.19	0.59
1:A:417:ILE:HG12	1:A:418:GLN:N	2.16	0.59
1:A:51:VAL:O	1:A:52:LEU:C	2.39	0.59
1:B:358:PRO:CD	1:B:368:VAL:O	2.48	0.59
1:B:27:LEU:HD11	1:B:51:VAL:HG23	1.83	0.59
1:B:70:GLY:O	1:B:72:VAL:N	2.35	0.59
1:A:350:LEU:N	1:A:350:LEU:HD23	2.17	0.59
1:A:305:GLU:CG	1:A:305:GLU:O	2.34	0.59
1:A:319:VAL:HA	1:A:437:GLN:NE2	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:LEU:O	1:A:9:GLU:N	2.27	0.59
1:B:138:GLY:O	1:B:140:LEU:N	2.35	0.59
1:A:265:GLN:HB2	1:A:305:GLU:CD	2.18	0.59
1:A:315:ALA:C	1:A:317:ARG:N	2.55	0.59
1:B:417:ILE:HG22	1:B:417:ILE:O	2.02	0.59
1:A:165:VAL:C	1:A:167:GLU:H	2.06	0.59
1:A:170:ARG:HG3	1:A:171:THR:HG22	1.84	0.59
1:B:72:VAL:HG22	1:B:88:PRO:HG2	1.85	0.59
1:A:269:LYS:HE3	1:A:270:GLU:HA	1.81	0.59
1:A:397:LEU:O	1:A:401:HIS:HB2	2.03	0.59
1:A:65:SER:OG	2:A:501:FAD:N7A	2.35	0.59
1:B:11:PHE:HZ	1:B:218:ILE:HB	1.68	0.59
1:B:136:ASP:OD1	1:B:138:GLY:CA	2.51	0.59
1:B:3:ASP:CA	1:B:229:TYR:HB3	2.33	0.59
1:A:145:LYS:HB2	1:A:148:GLU:CD	2.23	0.59
1:A:6:PRO:HB3	1:A:229:TYR:OH	2.02	0.59
1:A:44:SER:HB3	1:A:469:THR:HG22	1.83	0.59
1:A:109:LEU:HA	1:A:237:VAL:H	1.68	0.59
1:A:162:GLN:HG3	1:A:162:GLN:O	2.02	0.59
1:A:18:GLU:O	1:A:21:GLU:HB3	2.03	0.59
1:A:320:HIS:CE1	1:A:321:TYR:O	2.56	0.59
1:A:63:GLU:CB	2:A:501:FAD:N3A	2.66	0.59
1:B:475:GLU:HG2	1:B:476:GLY:H	1.66	0.59
1:A:172:ASN:O	1:A:176:MET:HB3	2.02	0.58
1:A:181:ASP:CG	1:A:438:PHE:HB2	2.22	0.58
1:A:224:ASP:HA	1:A:227:PHE:HB2	1.85	0.58
1:A:269:LYS:NZ	1:A:288:ASP:OD1	2.36	0.58
1:A:401:HIS:O	1:A:402:GLN:CB	2.44	0.58
1:A:384:LEU:HD21	1:B:427:MET:HE2	1.85	0.58
1:A:120:TRP:NE1	1:A:129:ARG:NH2	2.49	0.58
1:A:78:GLU:N	1:A:78:GLU:OE2	2.35	0.58
1:B:386:PHE:C	1:B:388:ASP:H	2.07	0.58
1:B:232:ARG:NH2	1:B:234:ASP:OD2	2.37	0.58
1:B:248:TYR:O	1:B:252:GLN:N	2.36	0.58
1:B:267:ASP:N	1:B:267:ASP:OD1	2.34	0.58
1:B:283:LEU:CD1	1:B:283:LEU:N	2.66	0.58
1:B:337:GLU:C	1:B:339:ASP:N	2.57	0.58
1:B:350:LEU:CB	1:B:351:PRO:HD2	2.32	0.58
1:A:181:ASP:CA	1:A:218:ILE:CD1	2.81	0.58
1:B:120:TRP:CH2	1:B:129:ARG:HG3	2.38	0.58
1:A:267:ASP:OD1	1:A:268:VAL:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:TYR:H	1:A:458:TYR:HD2	1.50	0.58
1:A:139:VAL:HG23	1:A:140:LEU:HG	1.85	0.58
1:A:64:ALA:HB2	1:A:260:ARG:N	2.19	0.58
1:A:265:GLN:CG	1:A:266:GLN:N	2.67	0.58
1:A:271:VAL:HG11	1:A:452:ILE:HD11	1.85	0.58
1:B:329:LEU:H	1:B:329:LEU:HD12	1.65	0.58
1:A:130:VAL:CG2	1:A:131:GLY:N	2.66	0.57
1:A:299:ALA:O	1:A:300:ARG:C	2.41	0.57
1:A:473:GLY:N	1:A:474:PRO:CD	2.60	0.57
1:A:7:LEU:C	1:A:9:GLU:N	2.58	0.57
1:B:14:THR:O	1:B:17:GLU:CD	2.42	0.57
1:B:391:ASP:CG	1:B:392:ILE:N	2.57	0.57
1:A:43:MET:SD	1:A:244:PRO:HG3	2.44	0.57
1:A:385:ASP:O	1:A:386:PHE:C	2.39	0.57
1:B:473:GLY:C	1:B:475:GLU:OE1	2.42	0.57
1:A:236:ILE:HG13	1:A:240:MET:HE1	1.85	0.57
1:A:290:VAL:HB	1:A:452:ILE:HD12	1.85	0.57
1:A:344:GLY:O	1:A:357:TYR:HD2	1.88	0.57
1:B:10:CYS:SG	1:B:168:LEU:HD13	2.44	0.57
1:B:280:LYS:O	1:B:281:GLU:CD	2.42	0.57
1:B:90:ARG:CG	1:B:91:LEU:N	2.56	0.57
1:B:146:PRO:O	1:B:149:VAL:HG22	2.04	0.57
1:B:210:ASP:C	1:B:212:GLY:H	2.08	0.57
1:B:325:THR:O	1:B:372:TYR:HD1	1.88	0.57
1:A:208:ASN:O	1:A:208:ASN:ND2	2.37	0.57
1:B:165:VAL:C	1:B:167:GLU:N	2.56	0.57
1:B:315:ALA:C	1:B:319:VAL:HG23	2.18	0.57
1:B:73:LYS:HD2	1:B:86:LEU:HD12	1.86	0.57
1:A:111:GLU:OE1	1:A:232:ARG:HD2	2.05	0.57
1:A:295:THR:HB	1:A:321:TYR:OH	2.04	0.57
1:A:409:GLN:O	1:A:412:CYS:N	2.33	0.57
1:A:158:GLU:HA	1:A:161:LEU:CD2	2.33	0.57
1:B:103:ARG:NH1	1:B:103:ARG:HG2	2.18	0.57
1:B:77:ASN:ND2	1:B:80:GLU:CD	2.58	0.57
1:A:409:GLN:O	1:A:411:ILE:N	2.37	0.57
1:B:387:GLU:O	1:B:391:ASP:HB3	2.05	0.57
1:B:93:GLU:HG3	1:B:232:ARG:NH1	2.19	0.57
1:A:323:SER:CB	1:A:379:ASN:HD21	2.17	0.56
1:B:456:GLY:H	1:B:459:THR:HG21	1.68	0.56
1:B:70:GLY:C	1:B:72:VAL:N	2.57	0.56
1:A:105:PHE:CD2	1:A:105:PHE:N	2.73	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:ASN:CB	1:A:6:PRO:HD3	2.35	0.56
1:B:322:ARG:CZ	1:B:432:THR:HG21	2.35	0.56
1:B:98:VAL:CG2	1:B:467:ALA:HB2	2.35	0.56
1:A:375:GLY:O	1:A:376:ASP:C	2.44	0.56
1:A:329:LEU:CD2	1:A:393:VAL:HG11	2.34	0.56
1:B:48:ALA:CB	1:B:475:GLU:HG3	2.30	0.56
1:A:243:LEU:HB3	1:A:244:PRO:CD	2.31	0.56
1:B:197:PRO:O	1:B:200:VAL:CG2	2.39	0.56
1:B:457:GLU:O	1:B:460:ALA:CB	2.54	0.56
1:A:111:GLU:HB2	1:A:232:ARG:HE	1.70	0.56
1:B:434:THR:CB	1:B:435:PRO:CD	2.84	0.56
1:B:465:TRP:HE3	2:B:501:FAD:HM82	1.69	0.56
1:B:93:GLU:OE1	1:B:232:ARG:NH1	2.39	0.56
1:A:7:LEU:C	1:A:7:LEU:HD12	2.26	0.56
1:B:241:ASP:C	1:B:244:PRO:HD2	2.26	0.56
1:B:7:LEU:HD13	1:B:176:MET:HE3	1.87	0.56
1:B:27:LEU:HD11	1:B:51:VAL:CG2	2.36	0.56
1:A:135:LYS:HE3	1:A:135:LYS:HA	1.87	0.55
1:A:334:LYS:HB3	1:A:337:GLU:HG3	1.88	0.55
1:B:353:ARG:CZ	1:B:354:PHE:HE2	2.18	0.55
1:A:92:PRO:HG3	1:A:95:HIS:CE1	2.40	0.55
1:B:168:LEU:HD12	1:B:168:LEU:O	2.06	0.55
1:B:95:HIS:HE1	1:B:226:ILE:HD13	1.71	0.55
1:A:261:VAL:HG12	1:A:262:ILE:N	2.21	0.55
1:A:437:GLN:O	1:A:441:PHE:HB2	2.07	0.55
1:B:140:LEU:O	1:B:142:TYR:N	2.40	0.55
1:B:162:GLN:O	1:B:165:VAL:N	2.29	0.55
1:B:208:ASN:HD22	1:B:209:GLU:N	2.05	0.55
1:A:448:PRO:O	1:A:449:VAL:HG13	2.06	0.55
1:A:50:TYR:O	1:A:53:ALA:HB3	2.06	0.55
1:A:95:HIS:HB3	1:A:98:VAL:CG1	2.37	0.55
1:B:187:GLU:HG2	1:B:191:LYS:CD	2.37	0.55
1:A:61:VAL:HG12	1:A:62:LEU:N	2.22	0.55
1:B:105:PHE:HB2	1:B:107:LEU:HD11	1.87	0.55
1:B:279:GLU:O	1:B:280:LYS:HB3	2.06	0.55
1:B:366:VAL:HG23	1:B:367:GLY:N	2.20	0.55
1:B:457:GLU:O	1:B:460:ALA:HB2	2.07	0.55
1:A:130:VAL:HG22	1:A:131:GLY:H	1.71	0.55
1:A:6:PRO:HD2	1:A:7:LEU:H	1.71	0.55
1:B:203:ILE:O	1:B:207:LEU:CD1	2.55	0.55
1:B:350:LEU:HB3	1:B:351:PRO:HD2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:PHE:CE1	1:A:221:LEU:CD2	2.90	0.55
1:A:405:LYS:O	1:A:408:ILE:HB	2.06	0.55
1:B:16:TYR:OH	1:B:97:ILE:HG13	2.07	0.55
1:A:228:ALA:O	1:A:229:TYR:CG	2.60	0.54
1:B:115:GLU:O	1:B:116:ASN:CB	2.53	0.54
1:B:405:LYS:C	1:B:407:GLU:N	2.60	0.54
1:A:152:SER:N	1:A:155:GLN:HE21	2.06	0.54
1:B:136:ASP:OD1	1:B:138:GLY:HA3	2.07	0.54
1:B:385:ASP:O	1:B:388:ASP:HB2	2.08	0.54
1:B:470:ILE:HD12	1:B:471:LYS:CA	2.37	0.54
1:A:105:PHE:CD1	1:A:246:SER:CB	2.90	0.54
1:B:291:ILE:HD13	1:B:475:GLU:HB2	1.89	0.54
1:A:121:TYR:HD2	1:A:133:VAL:HG21	1.68	0.54
1:A:203:ILE:HG22	1:A:209:GLU:HG3	1.90	0.54
1:A:417:ILE:CG1	1:A:418:GLN:N	2.70	0.54
1:A:430:ILE:CD1	1:A:464:GLY:HA2	2.34	0.54
1:B:113:SER:N	1:B:359:ASN:HD21	2.04	0.54
1:A:108:GLN:CD	1:A:237:VAL:HG21	2.27	0.54
1:A:471:LYS:C	1:A:474:PRO:HD3	2.25	0.54
1:A:51:VAL:HG12	1:A:52:LEU:H	1.68	0.54
1:B:445:LEU:HD22	1:B:458:TYR:CD2	2.43	0.54
1:B:7:LEU:CD1	1:B:176:MET:HE3	2.38	0.54
1:B:10:CYS:SG	1:B:168:LEU:CD1	2.95	0.54
1:B:197:PRO:C	1:B:200:VAL:HG22	2.25	0.54
1:B:249:GLN:O	1:B:252:GLN:HB3	2.07	0.54
1:B:282:THR:CA	1:B:283:LEU:HD12	2.38	0.54
1:A:109:LEU:N	1:A:109:LEU:HD12	2.17	0.54
1:B:266:GLN:OE1	1:B:451:ARG:HB3	2.07	0.54
1:A:72:VAL:HG11	1:A:244:PRO:CG	2.38	0.54
1:A:315:ALA:CB	1:A:445:LEU:CD1	2.86	0.54
1:B:148:GLU:O	1:B:149:VAL:C	2.46	0.54
1:B:169:ARG:HD2	1:B:169:ARG:O	2.08	0.54
1:B:80:GLU:CB	1:B:82:TRP:HD1	2.20	0.54
1:A:54:ASN:O	1:A:56:GLY:N	2.42	0.53
1:B:182:THR:OG1	1:B:182:THR:O	2.22	0.53
1:B:248:TYR:C	1:B:248:TYR:CD2	2.80	0.53
1:B:440:HIS:O	1:B:440:HIS:CD2	2.62	0.53
1:A:43:MET:HE2	1:A:247:MET:HE1	1.89	0.53
1:B:191:LYS:O	1:B:192:GLU:OE2	2.26	0.53
1:B:282:THR:C	1:B:283:LEU:HD12	2.28	0.53
1:B:80:GLU:CB	1:B:82:TRP:CD1	2.92	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:VAL:HG21	1:A:290:VAL:HG23	1.90	0.53
1:A:392:ILE:O	1:A:393:VAL:C	2.47	0.53
1:A:419:ARG:HB2	1:A:422:LEU:HD23	1.91	0.53
1:B:11:PHE:HE1	1:B:222:LYS:HE2	1.73	0.53
1:B:30:THR:O	1:B:31:SER:C	2.46	0.53
1:B:348:THR:CG2	1:B:353:ARG:C	2.77	0.53
1:B:471:LYS:O	1:B:471:LYS:CG	2.57	0.53
1:B:386:PHE:O	1:B:388:ASP:N	2.35	0.53
1:B:80:GLU:OE1	1:B:82:TRP:NE1	2.42	0.53
1:A:130:VAL:O	1:A:133:VAL:N	2.42	0.53
1:A:154:GLY:O	1:A:157:TYR:HB3	2.08	0.53
1:B:153:ALA:N	1:B:202:MET:HE2	2.20	0.53
1:B:113:SER:H	1:B:359:ASN:ND2	2.05	0.53
1:B:395:ASN:C	1:B:397:LEU:N	2.62	0.53
1:B:80:GLU:HB2	1:B:82:TRP:HD1	1.73	0.53
1:A:13:GLU:HB3	1:A:461:GLN:NE2	2.24	0.53
1:B:123:ILE:O	1:B:124:LYS:HB2	2.08	0.53
1:A:232:ARG:NH2	1:A:234:ASP:OD1	2.42	0.53
1:B:144:VAL:HG12	1:B:196:SER:OG	2.08	0.53
1:A:313:ALA:C	1:A:315:ALA:N	2.61	0.53
1:B:163:LYS:HD3	1:B:192:GLU:HA	1.91	0.53
1:A:44:SER:HB3	1:A:469:THR:CG2	2.38	0.52
1:B:85:ASN:HB3	1:B:88:PRO:O	2.08	0.52
1:B:99:ARG:O	1:B:103:ARG:N	2.37	0.52
1:A:257:LEU:O	1:A:258:ASN:HB2	2.09	0.52
1:A:290:VAL:HB	1:A:452:ILE:CD1	2.40	0.52
1:A:380:TYR:CG	1:A:380:TYR:O	2.62	0.52
1:A:176:MET:CG	1:A:177:LEU:N	2.58	0.52
1:A:352:SER:OG	1:A:393:VAL:HA	2.09	0.52
1:A:399:LEU:O	1:A:402:GLN:HG2	2.08	0.52
1:B:136:ASP:O	1:B:139:VAL:HG22	2.09	0.52
1:A:168:LEU:HD22	1:A:169:ARG:H	1.71	0.52
1:B:352:SER:O	1:B:354:PHE:N	2.42	0.52
1:B:71:GLN:HE21	2:B:501:FAD:PA	2.25	0.52
1:B:162:GLN:HG3	1:B:163:LYS:N	2.24	0.52
1:B:337:GLU:C	1:B:339:ASP:H	2.13	0.52
1:A:59:VAL:HG23	1:A:60:THR:N	2.23	0.52
1:A:362:PHE:O	1:A:364:ASN:ND2	2.42	0.52
1:A:42:GLY:HA3	2:A:501:FAD:O3P	2.10	0.52
1:A:450:ASP:O	1:A:453:TYR:HE2	1.92	0.52
1:B:127:ARG:O	1:B:128:LYS:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:ASP:OD2	1:B:19:PHE:HE2	1.93	0.52
1:B:473:GLY:C	1:B:475:GLU:CD	2.68	0.52
1:A:269:LYS:C	1:A:269:LYS:HD2	2.31	0.52
1:A:323:SER:O	1:A:375:GLY:CA	2.58	0.52
1:A:477:LEU:O	1:A:480:ASN:N	2.40	0.52
1:B:113:SER:H	1:B:359:ASN:HD21	1.57	0.52
1:B:7:LEU:CD1	1:B:176:MET:CE	2.87	0.52
1:A:111:GLU:CD	1:A:232:ARG:CG	2.71	0.52
1:A:241:ASP:C	1:A:244:PRO:HD2	2.30	0.52
1:A:275:TYR:N	1:A:283:LEU:O	2.39	0.52
1:A:388:ASP:O	1:A:391:ASP:HB2	2.10	0.52
1:A:44:SER:O	1:A:47:SER:HB2	2.10	0.52
1:A:172:ASN:CG	1:A:173:CYS:N	2.62	0.52
1:B:418:GLN:HA	1:B:418:GLN:NE2	2.24	0.52
1:B:475:GLU:CG	1:B:476:GLY:N	2.71	0.52
1:A:433:PHE:HE2	1:A:442:SER:OG	1.93	0.51
1:B:353:ARG:NH2	1:B:354:PHE:HE2	2.04	0.51
1:A:181:ASP:N	1:A:218:ILE:HD11	2.26	0.51
1:A:17:GLU:O	1:A:18:GLU:C	2.49	0.51
1:A:364:ASN:C	1:A:364:ASN:ND2	2.61	0.51
1:B:375:GLY:O	1:B:376:ASP:C	2.49	0.51
1:A:120:TRP:CH2	1:A:129:ARG:NE	2.77	0.51
1:A:61:VAL:CG1	1:A:62:LEU:N	2.74	0.51
1:B:21:GLU:HA	1:B:24:LYS:CG	2.40	0.51
1:B:395:ASN:N	1:B:395:ASN:HD22	2.07	0.51
1:A:118:ASN:ND2	1:A:340:GLY:O	2.44	0.51
1:B:74:THR:OG1	1:B:85:ASN:ND2	2.44	0.51
1:A:262:ILE:C	1:A:302:ILE:HG22	2.31	0.51
1:B:326:LYS:HB3	1:B:370:ILE:HG21	1.92	0.51
1:B:381:PHE:O	1:B:383:ALA:N	2.43	0.51
1:A:311:LYS:HB3	1:A:444:ALA:HB1	1.92	0.51
1:A:61:VAL:O	1:A:62:LEU:HD23	2.10	0.51
1:A:94:LYS:O	1:A:94:LYS:HG3	2.11	0.51
1:B:181:ASP:O	1:B:181:ASP:OD1	2.28	0.51
1:A:155:GLN:HG2	1:A:156:LEU:N	2.24	0.51
1:A:198:GLY:O	1:A:199:ALA:C	2.46	0.51
1:A:86:LEU:HD21	1:A:416:MET:CE	2.40	0.51
1:B:92:PRO:HG3	1:B:233:PHE:HE2	1.75	0.51
1:B:35:ARG:O	1:B:288:ASP:HB2	2.10	0.51
1:A:269:LYS:HE3	1:A:270:GLU:CB	2.40	0.51
1:A:270:GLU:OE1	1:A:271:VAL:C	2.50	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:LEU:N	1:A:27:LEU:HD23	2.26	0.51
1:A:337:GLU:C	1:A:339:ASP:N	2.63	0.51
1:A:329:LEU:CD1	1:A:414:PRO:CA	2.85	0.51
1:A:461:GLN:O	1:A:462:ALA:HB2	2.10	0.51
1:A:479:VAL:CG1	1:A:480:ASN:N	2.72	0.51
1:A:479:VAL:HG12	1:A:480:ASN:N	2.26	0.51
1:B:121:TYR:CD2	1:B:133:VAL:HG11	2.45	0.51
1:B:335:PHE:CE2	1:B:412:CYS:SG	3.00	0.51
1:B:438:PHE:C	1:B:442:SER:HG	2.10	0.51
1:A:241:ASP:C	1:A:241:ASP:OD1	2.49	0.51
1:B:157:TYR:CZ	1:B:224:ASP:HB2	2.46	0.51
1:B:433:PHE:CD2	1:B:437:GLN:HB3	2.46	0.51
1:A:122:PHE:O	1:A:348:THR:HA	2.10	0.50
1:A:124:LYS:O	1:A:125:ASN:HB2	2.11	0.50
1:A:15:ASP:CB	1:A:19:PHE:CD2	2.85	0.50
1:A:207:LEU:O	1:A:208:ASN:HB3	2.11	0.50
1:A:72:VAL:CG1	1:A:244:PRO:HG2	2.40	0.50
1:B:243:LEU:HB3	1:B:244:PRO:CD	2.40	0.50
1:B:300:ARG:HD2	1:B:316:LEU:O	2.11	0.50
1:B:310:PRO:O	1:B:313:ALA:HB3	2.11	0.50
1:B:471:LYS:C	1:B:473:GLY:N	2.63	0.50
1:B:473:GLY:CA	1:B:475:GLU:OE2	2.59	0.50
1:A:119:ALA:HB3	1:A:130:VAL:CG1	2.42	0.50
1:B:136:ASP:C	1:B:138:GLY:N	2.62	0.50
1:B:457:GLU:H	1:B:457:GLU:CD	2.15	0.50
1:B:73:LYS:CD	1:B:86:LEU:HD12	2.41	0.50
1:A:315:ALA:C	1:A:317:ARG:H	2.13	0.50
1:A:374:ILE:O	1:A:377:ASP:HB2	2.12	0.50
1:A:158:GLU:CA	1:A:161:LEU:HD22	2.36	0.50
1:A:181:ASP:OD1	1:A:218:ILE:HD12	2.10	0.50
1:A:269:LYS:CE	1:A:270:GLU:CB	2.89	0.50
1:A:266:GLN:HA	1:A:271:VAL:HA	1.92	0.50
2:B:501:FAD:O2'	2:B:501:FAD:O4'	2.28	0.50
1:A:72:VAL:HG11	1:A:244:PRO:HG2	1.94	0.50
1:B:260:ARG:O	1:B:275:TYR:HA	2.12	0.50
1:A:236:ILE:HD12	1:A:240:MET:HA	1.93	0.50
1:B:157:TYR:OH	1:B:224:ASP:HB2	2.12	0.50
1:B:408:ILE:HA	1:B:411:ILE:CG1	2.42	0.50
1:B:430:ILE:O	1:B:431:THR:C	2.50	0.50
1:A:157:TYR:CD2	1:A:157:TYR:C	2.84	0.50
1:A:259:ALA:HA	1:A:276:GLN:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:LEU:H	1:A:350:LEU:HD23	1.77	0.50
1:A:59:VAL:CG2	1:A:60:THR:N	2.75	0.50
1:A:75:TYR:O	1:A:83:TYR:HA	2.11	0.49
1:B:353:ARG:HB3	1:B:354:PHE:HD2	1.77	0.49
1:A:119:ALA:HB3	1:A:130:VAL:HG11	1.94	0.49
1:A:196:SER:O	1:A:200:VAL:HG23	2.12	0.49
1:A:21:GLU:O	1:A:23:ALA:N	2.46	0.49
1:A:353:ARG:HG3	1:A:354:PHE:CD2	2.48	0.49
1:A:232:ARG:NH1	1:A:234:ASP:OD2	2.44	0.49
1:A:241:ASP:O	1:A:244:PRO:HD2	2.12	0.49
1:A:64:ALA:HB2	1:A:260:ARG:CA	2.42	0.49
1:A:334:LYS:O	1:A:336:TRP:N	2.46	0.49
1:A:77:ASN:O	1:A:81:GLY:HA2	2.12	0.49
1:B:264:ILE:HG21	1:B:452:ILE:HD13	1.94	0.49
1:B:273:VAL:O	1:B:284:SER:HA	2.12	0.49
1:B:385:ASP:O	1:B:386:PHE:O	2.30	0.49
1:B:418:GLN:HA	1:B:418:GLN:HE21	1.77	0.49
1:A:167:GLU:OE1	1:A:167:GLU:N	2.46	0.49
1:A:173:CYS:O	1:A:174:SER:C	2.50	0.49
1:A:380:TYR:HE1	1:B:297:ARG:O	1.94	0.49
1:B:86:LEU:HD21	1:B:416:MET:HE3	1.95	0.49
1:B:83:TYR:CD1	1:B:84:ALA:N	2.80	0.49
1:A:369:ILE:HG22	1:A:370:ILE:N	2.28	0.49
1:A:309:PRO:HB3	1:A:310:PRO:HD2	1.93	0.49
1:B:408:ILE:HA	1:B:411:ILE:HD11	1.95	0.49
1:A:477:LEU:HD23	1:A:478:ASP:OD1	2.13	0.49
1:A:313:ALA:O	1:A:314:HIS:C	2.51	0.49
1:B:148:GLU:O	1:B:150:GLY:N	2.46	0.49
1:A:271:VAL:CG1	1:A:290:VAL:HG21	2.29	0.49
1:A:433:PHE:CE1	1:A:463:HIS:CE1	3.00	0.49
1:B:88:PRO:HA	2:B:501:FAD:C6	2.42	0.49
1:A:469:THR:O	1:A:470:ILE:C	2.50	0.49
1:A:70:GLY:H	2:A:501:FAD:H8A	1.78	0.49
1:B:3:ASP:HB2	1:B:229:TYR:HB3	1.94	0.49
1:A:163:LYS:O	1:A:167:GLU:OE1	2.30	0.48
1:A:265:GLN:NE2	1:A:305:GLU:CG	2.75	0.48
1:A:329:LEU:HD12	1:A:414:PRO:CA	2.43	0.48
1:B:63:GLU:OE2	1:B:65:SER:HB3	2.13	0.48
1:B:113:SER:N	1:B:359:ASN:ND2	2.61	0.48
1:B:353:ARG:HB3	1:B:354:PHE:CD2	2.48	0.48
1:B:434:THR:O	1:B:437:GLN:CG	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:ASP:HA	1:A:218:ILE:CD1	2.42	0.48
1:A:443:GLU:O	1:A:445:LEU:N	2.46	0.48
1:B:241:ASP:O	1:B:244:PRO:HG2	2.14	0.48
1:B:391:ASP:O	1:B:392:ILE:C	2.52	0.48
1:B:420:TRP:C	1:B:422:LEU:H	2.16	0.48
1:B:480:ASN:O	1:B:482:ALA:CB	2.61	0.48
1:A:355:ILE:HA	1:A:370:ILE:O	2.14	0.48
1:A:389:CYS:O	1:A:390:GLY:C	2.51	0.48
1:B:163:LYS:HD3	1:B:192:GLU:HB3	1.95	0.48
1:B:278:SER:CA	1:B:281:GLU:OE1	2.61	0.48
1:B:404:PRO:HB2	1:B:407:GLU:CG	2.29	0.48
1:B:441:PHE:O	1:B:445:LEU:HB2	2.13	0.48
1:B:470:ILE:CD1	1:B:470:ILE:C	2.73	0.48
1:B:474:PRO:O	1:B:475:GLU:C	2.49	0.48
1:A:43:MET:HE3	1:A:247:MET:CE	2.43	0.48
1:A:458:TYR:N	1:A:458:TYR:CD2	2.82	0.48
1:B:328:PHE:HD1	1:B:328:PHE:H	1.59	0.48
1:B:189:LEU:HD23	1:B:189:LEU:HA	1.67	0.48
1:B:210:ASP:O	1:B:212:GLY:N	2.45	0.48
1:B:294:THR:HG1	1:B:299:ALA:HB2	1.78	0.48
1:B:395:ASN:C	1:B:397:LEU:H	2.16	0.48
1:B:424:LYS:HB3	1:B:424:LYS:HE2	1.57	0.48
1:A:139:VAL:HG23	1:A:140:LEU:N	2.27	0.48
1:A:148:GLU:O	1:A:151:LYS:HG2	2.13	0.48
1:A:7:LEU:C	1:A:7:LEU:CD1	2.81	0.48
1:B:162:GLN:O	1:B:163:LYS:C	2.51	0.48
1:B:43:MET:HB3	1:B:469:THR:HG22	1.95	0.48
1:A:21:GLU:HA	1:A:21:GLU:OE1	2.12	0.48
1:A:379:ASN:C	1:A:381:PHE:N	2.65	0.48
1:A:471:LYS:O	1:A:473:GLY:N	2.46	0.48
1:B:119:ALA:O	1:B:130:VAL:HG23	2.13	0.48
1:B:329:LEU:N	1:B:329:LEU:CD1	2.71	0.48
1:B:99:ARG:HA	1:B:102:ILE:HG13	1.95	0.48
1:A:174:SER:O	1:A:175:TYR:C	2.52	0.48
1:A:393:VAL:O	1:A:396:ASP:N	2.40	0.48
1:A:462:ALA:HB3	1:A:468:SER:OG	2.14	0.48
1:B:404:PRO:O	1:B:407:GLU:HB2	2.14	0.48
1:B:430:ILE:O	1:B:432:THR:OG1	2.32	0.48
1:A:364:ASN:OD1	1:A:366:VAL:HG13	2.14	0.48
1:A:329:LEU:HD12	1:A:414:PRO:HA	1.92	0.48
1:B:153:ALA:N	1:B:202:MET:CE	2.75	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:LEU:O	1:B:218:ILE:HD13	2.14	0.48
1:B:348:THR:HG22	1:B:353:ARG:C	2.30	0.48
1:B:399:LEU:O	1:B:400:ILE:C	2.52	0.48
1:B:176:MET:HG2	1:B:177:LEU:N	2.28	0.47
1:B:202:MET:O	1:B:203:ILE:C	2.50	0.47
1:B:326:LYS:HE2	1:B:372:TYR:CG	2.49	0.47
1:B:358:PRO:HG3	1:B:368:VAL:O	2.14	0.47
1:B:403:LEU:HD23	1:B:404:PRO:HD2	1.95	0.47
1:A:137:PRO:HG2	1:A:150:GLY:HA2	1.96	0.47
1:A:460:ALA:CB	1:A:468:SER:O	2.63	0.47
1:A:176:MET:O	1:A:177:LEU:C	2.51	0.47
1:B:109:LEU:HD22	1:B:234:ASP:HB3	1.96	0.47
1:B:28:SER:O	1:B:29:THR:C	2.50	0.47
1:B:348:THR:OG1	1:B:350:LEU:N	2.45	0.47
1:B:301:ARG:NH2	1:B:427:MET:HE2	2.20	0.47
1:A:477:LEU:HG	1:A:478:ASP:OD1	2.14	0.47
1:B:441:PHE:O	1:B:445:LEU:CD1	2.57	0.47
1:B:20:LEU:HD11	1:B:96:ARG:HD2	1.96	0.47
1:A:294:THR:HG22	2:A:501:FAD:O3B	2.14	0.47
1:A:50:TYR:O	1:A:51:VAL:O	2.31	0.47
1:A:243:LEU:CB	1:A:244:PRO:HD3	2.35	0.47
1:A:348:THR:OG1	1:A:349:ASP:N	2.47	0.47
1:A:460:ALA:HB1	1:A:468:SER:O	2.15	0.47
1:B:127:ARG:C	1:B:128:LYS:HG2	2.35	0.47
1:B:161:LEU:O	1:B:164:ALA:HB3	2.14	0.47
1:A:130:VAL:O	1:A:132:GLU:N	2.48	0.47
1:A:261:VAL:CG1	1:A:262:ILE:N	2.77	0.47
1:A:348:THR:OG1	1:A:350:LEU:HD23	2.14	0.47
1:A:320:HIS:N	1:A:437:GLN:HE22	2.11	0.47
1:A:477:LEU:CD2	1:A:478:ASP:OD1	2.62	0.47
1:B:131:GLY:O	1:B:135:LYS:HG3	2.15	0.47
1:B:208:ASN:HD22	1:B:208:ASN:C	2.17	0.47
1:B:90:ARG:HD3	1:B:233:PHE:CG	2.46	0.47
1:A:236:ILE:HG13	1:A:240:MET:SD	2.54	0.47
1:B:243:LEU:N	1:B:244:PRO:HD2	2.30	0.47
1:B:291:ILE:HD13	1:B:475:GLU:HG3	1.95	0.47
1:B:357:TYR:CD1	1:B:369:ILE:HG21	2.50	0.47
1:B:408:ILE:HA	1:B:411:ILE:HG13	1.96	0.47
1:A:186:LYS:HG2	1:A:190:LEU:CD1	2.43	0.47
1:A:389:CYS:O	1:A:390:GLY:O	2.32	0.47
1:A:438:PHE:HA	1:A:442:SER:OG	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:LEU:C	1:B:168:LEU:HD12	2.35	0.47
1:A:181:ASP:CB	1:A:218:ILE:HD12	2.42	0.47
1:A:222:LYS:CE	1:A:461:GLN:O	2.63	0.47
1:B:77:ASN:O	1:B:81:GLY:N	2.47	0.47
1:A:389:CYS:O	1:A:393:VAL:HG23	2.14	0.47
1:A:53:ALA:O	1:A:56:GLY:N	2.47	0.47
1:B:39:VAL:HG22	1:B:261:VAL:HG21	1.95	0.47
1:B:433:PHE:H	1:B:433:PHE:HD1	1.63	0.47
1:B:48:ALA:HB1	1:B:475:GLU:CG	2.37	0.47
1:A:277:THR:O	1:A:280:LYS:HB2	2.13	0.46
1:A:314:HIS:HB3	1:A:441:PHE:HE2	1.80	0.46
1:A:40:GLY:N	1:A:62:LEU:O	2.48	0.46
1:A:49:ALA:O	1:A:53:ALA:N	2.32	0.46
1:B:120:TRP:O	1:B:346:SER:HB2	2.16	0.46
1:B:48:ALA:CB	1:B:475:GLU:CD	2.83	0.46
1:B:296:SER:HB3	1:B:321:TYR:HE1	1.78	0.46
1:B:453:TYR:OH	1:B:478:ASP:HB3	2.16	0.46
1:B:312:LYS:HE2	1:B:454:PHE:CD1	2.50	0.46
1:B:456:GLY:N	1:B:459:THR:HG23	2.24	0.46
1:A:112:PHE:O	1:A:113:SER:C	2.53	0.46
1:A:280:LYS:HB3	1:A:280:LYS:HE2	1.68	0.46
1:A:325:THR:CG2	1:A:326:LYS:N	2.78	0.46
1:A:451:ARG:HH11	1:A:451:ARG:HG2	1.79	0.46
1:B:108:GLN:NE2	1:B:109:LEU:O	2.47	0.46
1:B:399:LEU:CD1	1:B:399:LEU:N	2.78	0.46
1:B:466:ILE:HG13	2:B:501:FAD:C9	2.45	0.46
1:B:111:GLU:OE1	1:B:232:ARG:HD2	2.15	0.46
1:B:111:GLU:HG3	1:B:233:PHE:O	2.15	0.46
1:B:433:PHE:HB3	1:B:437:GLN:HB2	1.98	0.46
1:B:65:SER:OG	1:B:66:GLU:N	2.49	0.46
1:A:188:TYR:C	1:A:188:TYR:CD2	2.89	0.46
1:B:15:ASP:C	1:B:15:ASP:OD1	2.53	0.46
1:B:170:ARG:O	1:B:171:THR:HG23	2.16	0.46
1:A:112:PHE:O	1:A:112:PHE:CG	2.62	0.46
1:A:6:PRO:CG	1:A:229:TYR:CZ	2.83	0.46
1:B:122:PHE:CE2	1:B:125:ASN:HA	2.51	0.46
1:B:230:GLU:OE2	1:B:230:GLU:CA	2.61	0.46
1:B:448:PRO:C	1:B:450:ASP:HA	2.36	0.46
1:B:74:THR:CA	1:B:84:ALA:O	2.63	0.46
1:B:83:TYR:HD1	1:B:84:ALA:N	2.13	0.46
1:A:130:VAL:O	1:A:131:GLY:C	2.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:SER:H	1:A:155:GLN:NE2	2.14	0.46
1:B:337:GLU:HA	1:B:341:ILE:H	1.81	0.46
1:A:212:GLY:O	1:A:215:VAL:HG22	2.16	0.46
1:A:392:ILE:HG22	1:A:393:VAL:N	2.31	0.46
1:A:94:LYS:CG	1:A:94:LYS:O	2.63	0.46
1:B:105:PHE:HB2	1:B:107:LEU:CD1	2.46	0.46
1:B:473:GLY:O	1:B:475:GLU:OE2	2.33	0.46
1:B:73:LYS:HE2	1:B:73:LYS:HB3	1.79	0.46
1:A:277:THR:C	1:A:279:GLU:H	2.20	0.45
1:B:102:ILE:CA	1:B:107:LEU:HD12	2.37	0.45
1:B:214:TYR:CE1	1:B:215:VAL:HG12	2.51	0.45
1:A:166:GLU:O	1:A:167:GLU:CG	2.64	0.45
1:A:228:ALA:O	1:A:229:TYR:CD1	2.70	0.45
1:A:261:VAL:HG12	1:A:302:ILE:HG21	1.97	0.45
1:B:121:TYR:CD2	1:B:133:VAL:HG21	2.45	0.45
1:B:353:ARG:NH2	1:B:354:PHE:HZ	2.12	0.45
1:B:352:SER:OG	1:B:393:VAL:HA	2.16	0.45
1:A:111:GLU:OE1	1:A:232:ARG:NE	2.49	0.45
1:A:466:ILE:O	1:A:470:ILE:HG13	2.16	0.45
1:A:6:PRO:CD	1:A:7:LEU:H	2.28	0.45
1:B:101:TYR:HD1	1:B:105:PHE:CE2	2.34	0.45
1:B:170:ARG:C	1:B:171:THR:HG23	2.37	0.45
1:B:278:SER:OG	1:B:281:GLU:OE1	2.34	0.45
1:B:311:LYS:HB3	1:B:311:LYS:HE3	1.62	0.45
1:A:152:SER:HB2	1:A:155:GLN:HB3	1.98	0.45
1:A:43:MET:CE	1:A:247:MET:HE1	2.45	0.45
1:A:300:ARG:HG3	1:A:316:LEU:CB	2.43	0.45
1:A:95:HIS:O	1:A:98:VAL:CG1	2.64	0.45
1:A:319:VAL:HG13	1:A:319:VAL:O	2.17	0.45
1:B:15:ASP:O	1:B:16:TYR:C	2.55	0.45
1:B:278:SER:N	1:B:281:GLU:OE1	2.49	0.45
1:A:165:VAL:C	1:A:167:GLU:N	2.69	0.45
1:A:71:GLN:HA	1:A:420:TRP:CH2	2.52	0.45
1:B:278:SER:O	1:B:280:LYS:O	2.35	0.45
1:B:395:ASN:ND2	1:B:395:ASN:N	2.65	0.45
1:A:279:GLU:OE1	1:A:279:GLU:O	2.34	0.45
1:A:323:SER:CB	1:A:379:ASN:ND2	2.79	0.45
1:A:95:HIS:O	1:A:98:VAL:HG12	2.17	0.45
1:B:453:TYR:CE1	1:B:478:ASP:HB2	2.51	0.45
1:A:345:LYS:HA	1:A:355:ILE:O	2.17	0.45
1:A:360:HIS:CD2	1:A:362:PHE:CZ	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:ASN:OD1	1:A:361:ASN:N	2.50	0.45
1:A:399:LEU:O	1:A:400:ILE:C	2.56	0.45
1:B:405:LYS:HE3	1:B:405:LYS:HB3	1.42	0.45
1:B:92:PRO:O	1:B:93:GLU:C	2.54	0.45
1:B:97:ILE:HG22	1:B:470:ILE:CD1	2.37	0.45
1:A:269:LYS:CE	1:A:270:GLU:CA	2.87	0.45
1:A:260:ARG:HH21	1:A:425:TYR:HE1	1.64	0.45
1:B:35:ARG:NH2	1:B:270:GLU:OE2	2.49	0.45
1:B:322:ARG:HH11	1:B:432:THR:HG23	1.73	0.45
1:B:350:LEU:HD23	1:B:396:ASP:CG	2.37	0.45
1:B:27:LEU:HD12	1:B:51:VAL:O	2.17	0.45
1:A:145:LYS:CB	1:A:148:GLU:OE1	2.62	0.45
1:A:459:THR:O	1:A:460:ALA:C	2.55	0.45
1:B:379:ASN:O	1:B:381:PHE:N	2.50	0.45
1:B:5:ASN:O	1:B:8:GLU:OE1	2.35	0.45
1:A:132:GLU:O	1:A:133:VAL:C	2.55	0.44
1:A:313:ALA:O	1:A:315:ALA:N	2.50	0.44
1:A:337:GLU:HB3	1:A:342:HIS:CE1	2.53	0.44
1:A:398:SER:O	1:A:402:GLN:HA	2.18	0.44
1:A:449:VAL:HA	1:A:450:ASP:OD1	2.18	0.44
1:B:176:MET:O	1:B:179:LYS:N	2.51	0.44
1:B:356:TYR:O	1:B:369:ILE:HG22	2.17	0.44
1:B:386:PHE:C	1:B:388:ASP:N	2.71	0.44
1:A:312:LYS:HE3	1:A:444:ALA:HB1	2.00	0.44
1:B:377:ASP:O	1:B:380:TYR:HB3	2.17	0.44
1:B:466:ILE:HG13	2:B:501:FAD:C8M	2.47	0.44
1:A:311:LYS:HB2	1:A:312:LYS:HE3	1.98	0.44
1:B:456:GLY:HA3	1:B:458:TYR:CE1	2.53	0.44
1:A:120:TRP:CZ3	1:A:129:ARG:HG2	2.52	0.44
1:A:182:THR:HB	1:A:436:TYR:OH	2.18	0.44
1:A:236:ILE:H	1:A:240:MET:HE1	1.82	0.44
1:A:296:SER:O	1:A:299:ALA:HB3	2.17	0.44
1:A:388:ASP:N	1:A:388:ASP:OD1	2.49	0.44
1:B:53:ALA:HA	1:B:59:VAL:HG13	1.98	0.44
1:A:158:GLU:O	1:A:161:LEU:HD22	2.18	0.44
1:A:235:GLU:HA	1:A:240:MET:CE	2.48	0.44
1:B:170:ARG:C	1:B:171:THR:CG2	2.86	0.44
1:B:3:ASP:CB	1:B:229:TYR:HB3	2.48	0.44
1:B:236:ILE:HG13	1:B:240:MET:SD	2.57	0.44
1:B:309:PRO:HA	1:B:310:PRO:HD3	1.75	0.44
1:A:300:ARG:HH21	1:B:351:PRO:HD3	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:ASP:HA	1:B:379:ASN:OD1	2.18	0.44
1:B:374:ILE:HA	1:B:378:ALA:HB2	1.99	0.44
1:B:445:LEU:HD22	1:B:458:TYR:HD2	1.82	0.44
1:A:202:MET:HE2	1:A:206:LEU:CD1	2.42	0.44
1:A:209:GLU:O	1:A:212:GLY:N	2.48	0.44
1:A:374:ILE:O	1:A:375:GLY:C	2.56	0.44
1:A:434:THR:O	1:A:437:GLN:HG3	2.17	0.44
1:B:124:LYS:NZ	1:B:142:TYR:HA	2.32	0.44
1:B:85:ASN:OD1	1:B:240:MET:HG2	2.17	0.44
1:B:273:VAL:HG23	1:B:285:VAL:HG23	2.00	0.44
1:B:286:THR:O	1:B:286:THR:OG1	2.30	0.44
1:B:433:PHE:CD1	1:B:433:PHE:N	2.86	0.44
1:B:46:LEU:O	1:B:47:SER:C	2.55	0.44
1:A:116:ASN:ND2	1:A:342:HIS:O	2.51	0.44
1:A:267:ASP:C	1:A:267:ASP:OD1	2.56	0.44
1:A:294:THR:HA	2:A:501:FAD:H51A	2.00	0.44
1:A:66:GLU:O	1:A:257:LEU:HD13	2.18	0.44
1:A:9:GLU:O	1:A:12:ARG:HG2	2.18	0.44
1:B:350:LEU:CG	1:B:351:PRO:HD2	2.47	0.44
1:B:327:ILE:CG1	1:B:417:ILE:HD11	2.48	0.44
1:A:181:ASP:OD2	1:A:438:PHE:CB	2.49	0.44
1:A:51:VAL:C	1:A:53:ALA:N	2.71	0.44
1:B:172:ASN:O	1:B:173:CYS:C	2.57	0.44
1:B:327:ILE:HB	1:B:371:ALA:HB3	1.98	0.44
1:B:266:GLN:HE22	1:B:452:ILE:HG13	1.83	0.44
1:B:97:ILE:HD12	1:B:471:LYS:HD3	2.00	0.44
1:B:214:TYR:CD1	1:B:214:TYR:C	2.91	0.43
1:B:280:LYS:HE2	1:B:280:LYS:HB2	1.54	0.43
1:B:326:LYS:HG2	1:B:372:TYR:CD1	2.53	0.43
1:B:251:ILE:O	1:B:252:GLN:C	2.56	0.43
1:B:3:ASP:N	1:B:229:TYR:HD2	2.01	0.43
1:B:433:PHE:CE1	1:B:463:HIS:NE2	2.86	0.43
1:A:354:PHE:O	1:A:371:ALA:HA	2.18	0.43
1:A:63:GLU:HB3	2:A:501:FAD:C2A	2.42	0.43
1:B:180:TYR:HA	1:B:183:TYR:HD2	1.83	0.43
1:B:163:LYS:HD2	1:B:192:GLU:O	2.19	0.43
1:B:260:ARG:O	1:B:262:ILE:HG23	2.18	0.43
1:B:262:ILE:HD11	1:B:274:THR:HG21	2.00	0.43
1:A:315:ALA:O	1:A:317:ARG:N	2.51	0.43
1:B:101:TYR:O	1:B:102:ILE:C	2.56	0.43
1:B:24:LYS:HB3	1:B:24:LYS:HE3	1.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:GLY:HA2	2:B:501:FAD:O3B	2.18	0.43
1:B:7:LEU:HD13	1:B:176:MET:CE	2.49	0.43
1:B:74:THR:CG2	1:B:84:ALA:O	2.60	0.43
1:A:246:SER:C	1:A:248:TYR:N	2.71	0.43
1:B:210:ASP:C	1:B:212:GLY:N	2.71	0.43
1:B:280:LYS:O	1:B:280:LYS:HG3	2.18	0.43
1:B:327:ILE:HA	1:B:417:ILE:CD1	2.48	0.43
1:B:348:THR:CG2	1:B:353:ARG:CA	2.97	0.43
1:B:53:ALA:HA	1:B:59:VAL:CG1	2.49	0.43
1:B:63:GLU:HA	1:B:63:GLU:OE1	2.19	0.43
1:A:170:ARG:HG3	1:A:171:THR:N	2.32	0.43
1:B:130:VAL:O	1:B:131:GLY:O	2.35	0.43
1:B:277:THR:C	1:B:278:SER:HG	2.16	0.43
1:B:449:VAL:N	1:B:450:ASP:HA	2.34	0.43
1:A:128:LYS:HA	1:A:128:LYS:HD3	1.79	0.43
1:A:334:LYS:HE3	1:A:334:LYS:HB2	1.79	0.43
1:A:91:LEU:HA	1:A:92:PRO:HD2	1.86	0.43
1:B:104:LYS:HB2	1:B:104:LYS:HE3	1.70	0.43
1:B:149:VAL:O	1:B:149:VAL:HG23	2.19	0.43
1:B:353:ARG:NE	1:B:354:PHE:HE2	2.16	0.43
1:A:267:ASP:CG	1:A:268:VAL:N	2.73	0.43
1:A:456:GLY:O	1:A:457:GLU:C	2.57	0.43
1:A:59:VAL:HG13	1:A:254:LYS:HD3	2.01	0.43
1:B:43:MET:O	1:B:44:SER:C	2.56	0.43
1:A:315:ALA:O	1:A:316:LEU:C	2.55	0.42
1:A:296:SER:HB3	1:A:458:TYR:CD1	2.54	0.42
1:B:245:THR:HG22	1:B:249:GLN:NE2	2.33	0.42
1:B:279:GLU:C	1:B:280:LYS:CG	2.87	0.42
1:B:330:THR:HG22	1:B:368:VAL:HG22	2.00	0.42
1:A:329:LEU:CD2	1:A:393:VAL:CG1	2.96	0.42
1:A:71:GLN:CG	2:A:501:FAD:O1A	2.63	0.42
1:B:217:PHE:CG	1:B:217:PHE:O	2.71	0.42
1:B:280:LYS:HB2	3:B:607:HOH:O	2.18	0.42
1:A:469:THR:HG21	2:A:501:FAD:H5'2	2.01	0.42
1:B:326:LYS:HE2	1:B:372:TYR:CD2	2.54	0.42
1:B:7:LEU:HD23	1:B:7:LEU:H	1.83	0.42
1:B:83:TYR:C	1:B:83:TYR:CD1	2.93	0.42
1:A:423:ASP:HB3	1:A:426:ALA:HB3	2.00	0.42
1:B:98:VAL:HG12	1:B:102:ILE:HD11	2.01	0.42
1:B:114:GLN:C	1:B:115:GLU:CG	2.88	0.42
1:B:307:PRO:O	1:B:308:LEU:C	2.56	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:MET:HB3	1:B:44:SER:H	1.72	0.42
1:A:300:ARG:NH1	1:A:317:ARG:HB2	2.35	0.42
1:B:110:ASN:HB3	1:B:235:GLU:HG2	2.00	0.42
1:A:436:TYR:HB2	1:B:186:LYS:HZ3	1.82	0.42
1:B:3:ASP:HA	1:B:4:ARG:HA	1.70	0.42
1:A:198:GLY:C	1:A:200:VAL:H	2.22	0.42
1:A:47:SER:OG	1:A:470:ILE:HG23	2.18	0.42
1:B:114:GLN:C	1:B:115:GLU:HG2	2.39	0.42
1:B:146:PRO:HA	1:B:149:VAL:HG13	2.00	0.42
1:B:350:LEU:CB	1:B:351:PRO:CD	2.96	0.42
1:A:124:LYS:O	1:A:125:ASN:CB	2.67	0.42
1:A:181:ASP:HA	1:A:218:ILE:HD12	2.01	0.42
1:B:433:PHE:N	1:B:433:PHE:HD1	2.16	0.42
1:A:149:VAL:O	1:A:149:VAL:CG1	2.63	0.42
1:A:237:VAL:CG1	1:A:238:GLY:N	2.83	0.42
1:A:71:GLN:OE1	2:A:501:FAD:HM81	2.20	0.42
1:B:123:ILE:O	1:B:123:ILE:HG22	2.19	0.42
1:B:162:GLN:O	1:B:164:ALA:N	2.53	0.42
1:B:353:ARG:HD2	1:B:353:ARG:HA	1.87	0.42
2:B:501:FAD:O5'	2:B:501:FAD:O2A	2.37	0.42
1:A:16:TYR:O	1:A:20:LEU:N	2.41	0.42
1:A:17:GLU:O	1:A:19:PHE:N	2.52	0.42
1:A:80:GLU:HB3	1:A:82:TRP:CD1	2.54	0.42
1:A:162:GLN:HA	1:A:165:VAL:HG22	2.01	0.42
1:A:237:VAL:HG12	1:A:238:GLY:N	2.35	0.42
1:B:262:ILE:CG1	1:B:274:THR:HG22	2.49	0.42
1:A:152:SER:H	1:A:155:GLN:HE21	1.65	0.41
1:A:7:LEU:O	1:A:7:LEU:CD1	2.68	0.41
1:B:445:LEU:HD22	1:B:458:TYR:CE2	2.55	0.41
1:A:85:ASN:ND2	1:A:240:MET:H	2.14	0.41
1:B:296:SER:HB3	1:B:321:TYR:CE1	2.54	0.41
1:B:417:ILE:HD12	1:B:417:ILE:HA	1.60	0.41
1:B:437:GLN:NE2	1:B:441:PHE:HD2	2.18	0.41
2:B:501:FAD:H9	2:B:501:FAD:H2'	2.01	0.41
1:B:34:LYS:H	1:B:57:HIS:HD1	1.68	0.41
1:A:106:GLY:O	1:A:107:LEU:HD23	2.21	0.41
1:A:136:ASP:C	1:A:136:ASP:OD1	2.58	0.41
1:A:390:GLY:O	1:A:391:ASP:C	2.58	0.41
1:B:27:LEU:O	1:B:28:SER:CB	2.38	0.41
1:B:336:TRP:O	1:B:341:ILE:HB	2.20	0.41
1:B:90:ARG:HG3	1:B:233:PHE:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:LYS:HB3	1:A:148:GLU:CG	2.44	0.41
1:A:165:VAL:O	1:A:167:GLU:N	2.53	0.41
1:A:219:GLU:HA	1:A:219:GLU:OE1	2.19	0.41
1:A:356:TYR:HB2	1:A:370:ILE:HB	2.02	0.41
1:A:409:GLN:HB2	1:A:409:GLN:HE21	1.64	0.41
1:A:409:GLN:C	1:A:411:ILE:N	2.74	0.41
1:B:395:ASN:O	1:B:396:ASP:C	2.58	0.41
1:B:327:ILE:HA	1:B:417:ILE:HD12	2.02	0.41
1:B:43:MET:CE	1:B:43:MET:CA	2.81	0.41
1:B:479:VAL:O	1:B:482:ALA:N	2.53	0.41
1:A:203:ILE:O	1:A:207:LEU:HB2	2.20	0.41
1:A:154:GLY:HA2	1:A:207:LEU:HD21	2.02	0.41
1:A:431:THR:C	1:A:432:THR:OG1	2.58	0.41
1:A:94:LYS:HZ3	1:A:94:LYS:HG3	1.70	0.41
1:B:475:GLU:CG	1:B:476:GLY:H	2.30	0.41
1:B:114:GLN:O	1:B:114:GLN:CG	2.69	0.41
1:B:48:ALA:CB	1:B:475:GLU:CG	2.97	0.41
1:A:104:LYS:HB3	1:A:105:PHE:CD2	2.55	0.41
1:A:137:PRO:O	1:A:139:VAL:N	2.53	0.41
1:A:381:PHE:O	1:A:382:GLU:C	2.58	0.41
2:A:501:FAD:HO3A	2:A:501:FAD:HO2A	1.60	0.41
1:A:85:ASN:HD22	1:A:85:ASN:HA	1.71	0.41
1:B:16:TYR:O	1:B:17:GLU:C	2.59	0.41
1:B:337:GLU:C	1:B:340:GLY:H	2.23	0.41
1:B:87:GLY:O	2:B:501:FAD:O4	2.39	0.41
1:A:90:ARG:HA	1:A:234:ASP:O	2.21	0.41
1:A:64:ALA:HA	1:A:259:ALA:H	1.86	0.41
1:A:309:PRO:CB	1:A:310:PRO:HD2	2.50	0.41
1:B:136:ASP:O	1:B:137:PRO:C	2.58	0.41
1:B:19:PHE:O	1:B:23:ALA:N	2.43	0.41
1:B:20:LEU:O	1:B:23:ALA:HB3	2.20	0.41
1:A:175:TYR:O	1:A:176:MET:C	2.57	0.41
1:A:88:PRO:HA	2:A:501:FAD:N5	2.36	0.41
1:A:168:LEU:O	1:A:168:LEU:HD23	2.14	0.41
1:A:71:GLN:HG3	2:A:501:FAD:PA	2.60	0.41
1:B:114:GLN:O	1:B:115:GLU:CB	2.67	0.41
1:B:187:GLU:OE2	1:B:191:LYS:NZ	2.48	0.41
1:B:196:SER:O	1:B:199:ALA:HB3	2.21	0.41
1:B:406:GLU:HG2	1:B:406:GLU:H	1.67	0.41
1:A:66:GLU:O	1:A:67:ARG:HB2	2.21	0.41
1:B:136:ASP:C	1:B:136:ASP:OD1	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:471:LYS:O	1:B:474:PRO:HD2	2.18	0.41
1:A:300:ARG:HH11	1:A:317:ARG:HA	1.86	0.40
1:B:162:GLN:C	1:B:164:ALA:N	2.73	0.40
1:B:21:GLU:HA	1:B:21:GLU:OE1	2.21	0.40
1:B:334:LYS:H	1:B:334:LYS:HG3	1.58	0.40
1:A:105:PHE:HD2	1:A:105:PHE:N	2.19	0.40
1:A:213:TYR:HA	1:A:213:TYR:HD1	1.72	0.40
1:A:246:SER:O	1:A:247:MET:C	2.59	0.40
1:A:296:SER:O	1:A:297:ARG:C	2.59	0.40
1:A:433:PHE:CD1	1:A:433:PHE:N	2.88	0.40
1:A:459:THR:OG1	1:A:460:ALA:N	2.54	0.40
1:B:10:CYS:SG	1:B:168:LEU:HD11	2.61	0.40
1:A:350:LEU:N	1:A:350:LEU:HD22	2.33	0.40
1:A:471:LYS:C	1:A:473:GLY:N	2.75	0.40
1:A:465:TRP:HA	2:A:501:FAD:N1	2.37	0.40
1:A:5:ASN:N	1:A:6:PRO:CD	2.84	0.40
1:B:123:ILE:HG13	1:B:349:ASP:HB3	2.04	0.40
1:B:404:PRO:HD2	1:B:407:GLU:CD	2.41	0.40
1:A:222:LYS:HE3	1:A:461:GLN:O	2.22	0.40
1:B:121:TYR:CE1	1:B:206:LEU:HD22	2.57	0.40
1:B:260:ARG:HH21	1:B:301:ARG:NH2	2.20	0.40
1:B:322:ARG:HB2	1:B:322:ARG:HE	1.76	0.40
1:B:442:SER:O	1:B:445:LEU:N	2.49	0.40
1:A:35:ARG:HA	1:A:58:GLN:HB2	2.03	0.40
1:A:471:LYS:O	1:A:474:PRO:N	2.54	0.40
1:B:111:GLU:OE1	1:B:232:ARG:CD	2.68	0.40
1:B:138:GLY:C	1:B:140:LEU:H	2.24	0.40
1:B:381:PHE:O	1:B:382:GLU:C	2.60	0.40
1:B:408:ILE:HA	1:B:411:ILE:CD1	2.52	0.40
1:B:264:ILE:CG2	1:B:452:ILE:HD13	2.52	0.40
1:B:65:SER:HA	1:B:425:TYR:CZ	2.56	0.40
1:B:73:LYS:HG2	1:B:86:LEU:HD12	2.01	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:104:LYS:O	1:B:387:GLU:OE2[2_545]	2.06	0.14

5.3 Torsion angles

5.3.1 Protein backbone

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	470/497 (95%)	326 (69%)	96 (20%)	48 (10%)	0	3
1	B	478/497 (96%)	357 (75%)	78 (16%)	43 (9%)	1	4
All	All	948/994 (95%)	683 (72%)	174 (18%)	91 (10%)	0	3

All (91) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	GLU
1	A	51	VAL
1	A	53	ALA
1	A	96	ARG
1	A	278	SER
1	A	335	PHE
1	A	402	GLN
1	A	460	ALA
1	A	477	LEU
1	B	28	SER
1	B	43	MET
1	B	96	ARG
1	B	116	ASN
1	B	117	GLU
1	B	139	VAL
1	B	141	ASP
1	B	147	SER
1	B	149	VAL
1	B	166	GLU
1	B	208	ASN
1	B	209	GLU
1	B	279	GLU
1	B	280	LYS
1	B	281	GLU
1	B	334	LYS

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Mol	Chain	Res	Type
1	B	353	ARG
1	B	386	PHE
1	B	481	ARG
1	A	6	PRO
1	A	7	LEU
1	A	17	GLU
1	A	21	GLU
1	A	22	ILE
1	A	52	LEU
1	A	55	ALA
1	A	166	GLU
1	A	249	GLN
1	A	301	ARG
1	A	343	GLY
1	A	364	ASN
1	A	376	ASP
1	A	380	TYR
1	A	390	GLY
1	A	391	ASP
1	A	410	ALA
1	A	444	ALA
1	A	449	VAL
1	B	47	SER
1	B	102	ILE
1	B	131	GLY
1	B	203	ILE
1	B	252	GLN
1	B	361	ASN
1	B	380	TYR
1	B	382	GLU
1	B	402	GLN
1	B	406	GLU
1	A	50	TYR
1	A	131	GLY
1	A	174	SER
1	A	199	ALA
1	A	229	TYR
1	A	353	ARG
1	A	436	TYR
1	B	44	SER
1	B	115	GLU
1	B	246	SER

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Mol	Chain	Res	Type
1	B	364	ASN
1	B	396	ASP
1	A	34	LYS
1	A	49	ALA
1	A	169	ARG
1	A	472	SER
1	A	474	PRO
1	B	71	GLN
1	B	95	HIS
1	B	480	ASN
1	A	248	TYR
1	B	177	LEU
1	B	211	SER
1	B	376	ASP
1	A	221	LEU
1	A	478	ASP
1	B	392	ILE
1	A	197	PRO
1	B	261	VAL
1	B	319	VAL
1	A	393	VAL
1	A	470	ILE
1	A	366	VAL
1	A	417	ILE

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	403/427 (94%)	322 (80%)	81 (20%)	1	5
1	B	412/427 (96%)	336 (82%)	76 (18%)	1	7
All	All	815/854 (95%)	658 (81%)	157 (19%)	1	6

All (157) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	13	GLU
1	A	14	THR
1	A	27	LEU
1	A	35	ARG
1	A	43	MET
1	A	54	ASN
1	A	59	VAL
1	A	60	THR
1	A	63	GLU
1	A	75	TYR
1	A	78	GLU
1	A	90	ARG
1	A	91	LEU
1	A	93	GLU
1	A	94	LYS
1	A	98	VAL
1	A	100	GLU
1	A	104	LYS
1	A	105	PHE
1	A	109	LEU
1	A	123	ILE
1	A	130	VAL
1	A	147	SER
1	A	149	VAL
1	A	152	SER
1	A	155	GLN
1	A	161	LEU
1	A	168	LEU
1	A	169	ARG
1	A	176	MET
1	A	182	THR
1	A	184	SER
1	A	194	ASN
1	A	208	ASN
1	A	210	ASP
1	A	213	TYR
1	A	252	GLN
1	A	260	ARG
1	A	265	GLN
1	A	267	ASP
1	A	268	VAL
1	A	269	LYS

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Mol	Chain	Res	Type
1	A	277	THR
1	A	285	VAL
1	A	302	ILE
1	A	305	GLU
1	A	312	LYS
1	A	318	SER
1	A	322	ARG
1	A	323	SER
1	A	329	LEU
1	A	330	THR
1	A	341	ILE
1	A	346	SER
1	A	348	THR
1	A	350	LEU
1	A	364	ASN
1	A	374	ILE
1	A	376	ASP
1	A	382	GLU
1	A	391	ASP
1	A	395	ASN
1	A	398	SER
1	A	402	GLN
1	A	403	LEU
1	A	406	GLU
1	A	407	GLU
1	A	409	GLN
1	A	412	CYS
1	A	413	ARG
1	A	418	GLN
1	A	422	LEU
1	A	439	GLN
1	A	441	PHE
1	A	445	LEU
1	A	449	VAL
1	A	458	TYR
1	A	471	LYS
1	A	479	VAL
1	A	483	SER
1	B	3	ASP
1	B	9	GLU
1	B	14	THR
1	B	24	LYS

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Mol	Chain	Res	Type
1	B	28	SER
1	B	32	ASN
1	B	35	ARG
1	B	43	MET
1	B	44	SER
1	B	52	LEU
1	B	61	VAL
1	B	66	GLU
1	B	67	ARG
1	B	79	LYS
1	B	90	ARG
1	B	91	LEU
1	B	95	HIS
1	B	107	LEU
1	B	108	GLN
1	B	115	GLU
1	B	123	ILE
1	B	144	VAL
1	B	156	LEU
1	B	163	LYS
1	B	167	GLU
1	B	168	LEU
1	B	174	SER
1	B	179	LYS
1	B	182	THR
1	B	196	SER
1	B	207	LEU
1	B	208	ASN
1	B	209	GLU
1	B	213	TYR
1	B	218	ILE
1	B	221	LEU
1	B	224	ASP
1	B	225	ASP
1	B	246	SER
1	B	248	TYR
1	B	251	ILE
1	B	260	ARG
1	B	273	VAL
1	B	279	GLU
1	B	280	LYS
1	B	282	THR

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Mol	Chain	Res	Type
1	B	283	LEU
1	B	284	SER
1	B	285	VAL
1	B	286	THR
1	B	303	LYS
1	B	322	ARG
1	B	323	SER
1	B	328	PHE
1	B	329	LEU
1	B	332	THR
1	B	337	GLU
1	B	347	THR
1	B	348	THR
1	B	369	ILE
1	B	386	PHE
1	B	387	GLU
1	B	391	ASP
1	B	395	ASN
1	B	398	SER
1	B	402	GLN
1	B	411	ILE
1	B	413	ARG
1	B	417	ILE
1	B	427	MET
1	B	437	GLN
1	B	461	GLN
1	B	463	HIS
1	B	472	SER
1	B	478	ASP
1	B	480	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	ASN
1	A	85	ASN
1	A	155	GLN
1	A	208	ASN
1	A	256	HIS
1	A	258	ASN
1	A	265	GLN
1	A	276	GLN

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Mol	Chain	Res	Type
1	A	342	HIS
1	A	359	ASN
1	A	364	ASN
1	A	379	ASN
1	A	401	HIS
1	A	402	GLN
1	A	409	GLN
1	A	418	GLN
1	A	437	GLN
1	B	77	ASN
1	B	85	ASN
1	B	95	HIS
1	B	108	GLN
1	B	194	ASN
1	B	208	ASN
1	B	249	GLN
1	B	276	GLN
1	B	359	ASN
1	B	360	HIS
1	B	364	ASN
1	B	379	ASN
1	B	402	GLN
1	B	409	GLN
1	B	418	GLN
1	B	437	GLN
1	B	440	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

2 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	501	-	51,58,58	1.36	6 (11%)	60,89,89	1.93	16 (26%)
2	FAD	B	501	-	51,58,58	1.39	7 (13%)	60,89,89	1.62	11 (18%)

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	501	-	-	16/30/50/50	0/6/6/6
2	FAD	B	501	-	-	14/30/50/50	0/6/6/6

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	FAD	C10-N1	4.66	1.39	1.33
2	B	501	FAD	C2A-N3A	3.94	1.38	1.32
2	A	501	FAD	C1'-N10	3.85	1.52	1.48
2	A	501	FAD	C4X-N5	3.50	1.38	1.33
2	A	501	FAD	C6-C5X	-3.29	1.36	1.41
2	A	501	FAD	C10-N1	3.27	1.37	1.33
2	B	501	FAD	C1'-N10	3.24	1.51	1.48
2	B	501	FAD	C4-N3	3.14	1.38	1.33
2	A	501	FAD	C2A-N3A	3.06	1.37	1.32
2	A	501	FAD	C4-N3	2.66	1.37	1.33
2	B	501	FAD	C4X-N5	2.11	1.36	1.33
2	B	501	FAD	O4B-C4B	-2.09	1.40	1.45
2	B	501	FAD	C2A-N1A	2.01	1.37	1.33

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	FAD	N3A-C2A-N1A	-6.33	118.78	128.68
2	B	501	FAD	N3A-C2A-N1A	-5.64	119.87	128.68
2	A	501	FAD	C4-N3-C2	5.37	119.68	115.14
2	B	501	FAD	C1'-N10-C9A	4.40	121.75	118.29
2	A	501	FAD	C1B-N9A-C4A	-4.15	119.36	126.64
2	B	501	FAD	C4-N3-C2	3.85	118.39	115.14
2	A	501	FAD	C5X-C9A-N10	3.64	120.36	117.72
2	A	501	FAD	N6A-C6A-N1A	-3.42	111.48	118.57
2	A	501	FAD	C5A-C6A-N6A	-3.34	115.28	120.35
2	B	501	FAD	P-O3P-PA	-3.23	121.74	132.83
2	B	501	FAD	O5B-C5B-C4B	-3.21	97.94	108.99
2	B	501	FAD	C4X-N5-C5X	3.00	119.77	116.77
2	A	501	FAD	C2B-C3B-C4B	-2.90	97.00	102.64
2	A	501	FAD	C9A-N10-C10	-2.87	118.15	121.91
2	A	501	FAD	C1'-N10-C10	2.72	120.85	118.41
2	B	501	FAD	O3'-C3'-C4'	-2.67	102.36	108.81
2	B	501	FAD	O4B-C4B-C3B	2.62	110.31	105.11
2	B	501	FAD	C5X-C9A-N10	2.51	119.54	117.72
2	A	501	FAD	O2'-C2'-C1'	2.46	115.52	109.59
2	A	501	FAD	C4X-C4-N3	-2.44	120.09	123.43
2	B	501	FAD	C9A-N10-C10	-2.36	118.81	121.91
2	B	501	FAD	C3B-C2B-C1B	2.33	104.49	100.98
2	A	501	FAD	C10-C4X-N5	-2.23	119.72	121.26
2	A	501	FAD	C7M-C7-C6	-2.19	115.10	120.34
2	A	501	FAD	O4B-C4B-C5B	2.09	116.25	109.37
2	A	501	FAD	C4A-C5A-N7A	-2.06	107.25	109.40
2	A	501	FAD	O4'-C4'-C5'	-2.06	105.29	109.92

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	FAD	C5B-O5B-PA-O3P
2	A	501	FAD	N10-C1'-C2'-O2'
2	A	501	FAD	N10-C1'-C2'-C3'
2	A	501	FAD	C2'-C3'-C4'-O4'
2	A	501	FAD	C2'-C3'-C4'-C5'
2	A	501	FAD	O3'-C3'-C4'-O4'
2	A	501	FAD	O3'-C3'-C4'-C5'
2	A	501	FAD	O4'-C4'-C5'-O5'
2	A	501	FAD	C5'-O5'-P-O1P
2	A	501	FAD	C5'-O5'-P-O2P
2	A	501	FAD	C5'-O5'-P-O3P

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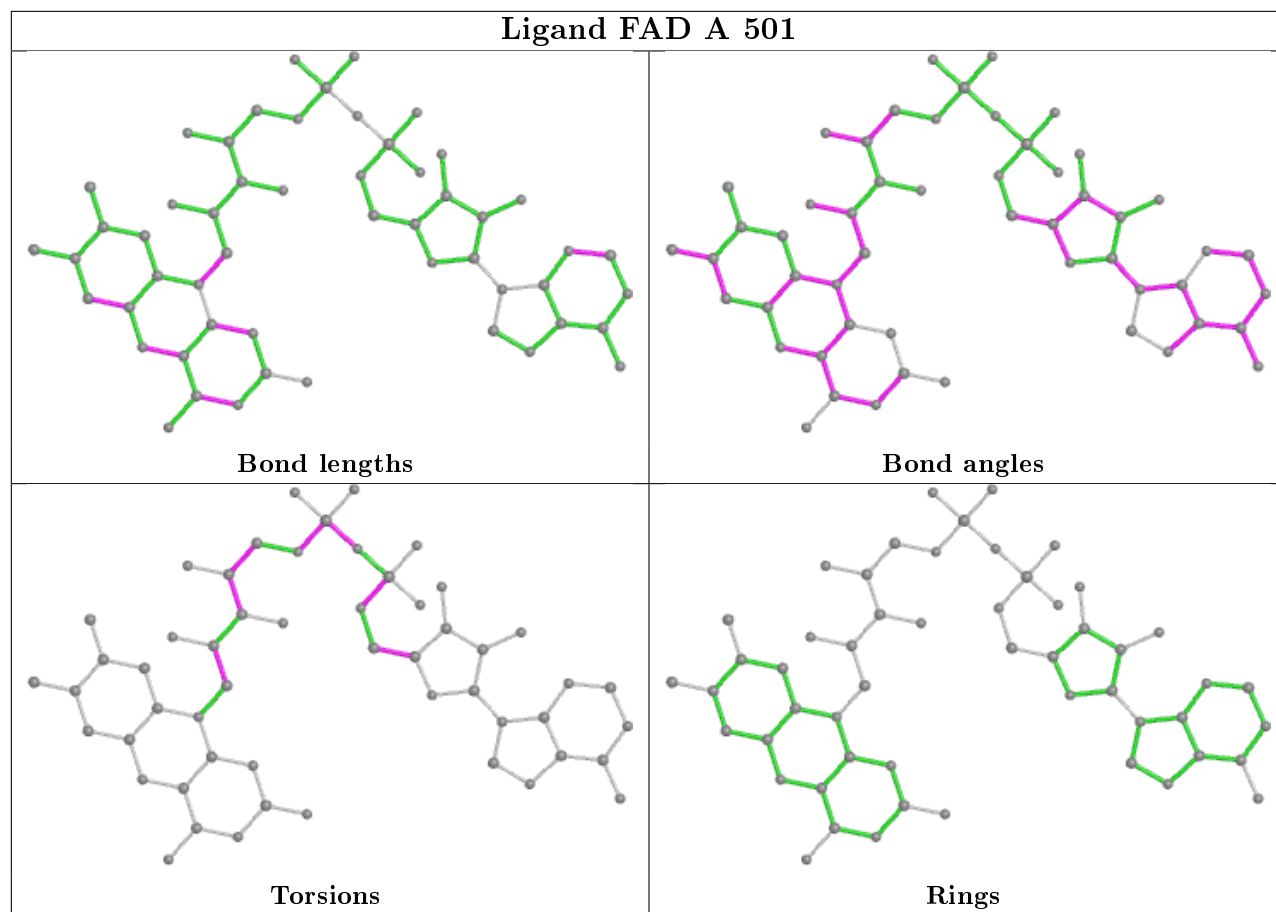
Mol	Chain	Res	Type	Atoms
2	B	501	FAD	O4B-C4B-C5B-O5B
2	B	501	FAD	C2'-C1'-N10-C10
2	B	501	FAD	C2'-C3'-C4'-O4'
2	B	501	FAD	C2'-C3'-C4'-C5'
2	B	501	FAD	O3'-C3'-C4'-O4'
2	B	501	FAD	O3'-C3'-C4'-C5'
2	B	501	FAD	C5'-O5'-P-O1P
2	B	501	FAD	C5'-O5'-P-O2P
2	B	501	FAD	C3B-C4B-C5B-O5B
2	A	501	FAD	PA-O3P-P-O5'
2	B	501	FAD	PA-O3P-P-O5'
2	B	501	FAD	C5'-O5'-P-O3P
2	A	501	FAD	C3B-C4B-C5B-O5B
2	A	501	FAD	C5B-O5B-PA-O2A
2	B	501	FAD	P-O3P-PA-O1A
2	B	501	FAD	P-O3P-PA-O2A
2	B	501	FAD	PA-O3P-P-O2P
2	A	501	FAD	C5B-O5B-PA-O1A
2	A	501	FAD	C3'-C4'-C5'-O5'

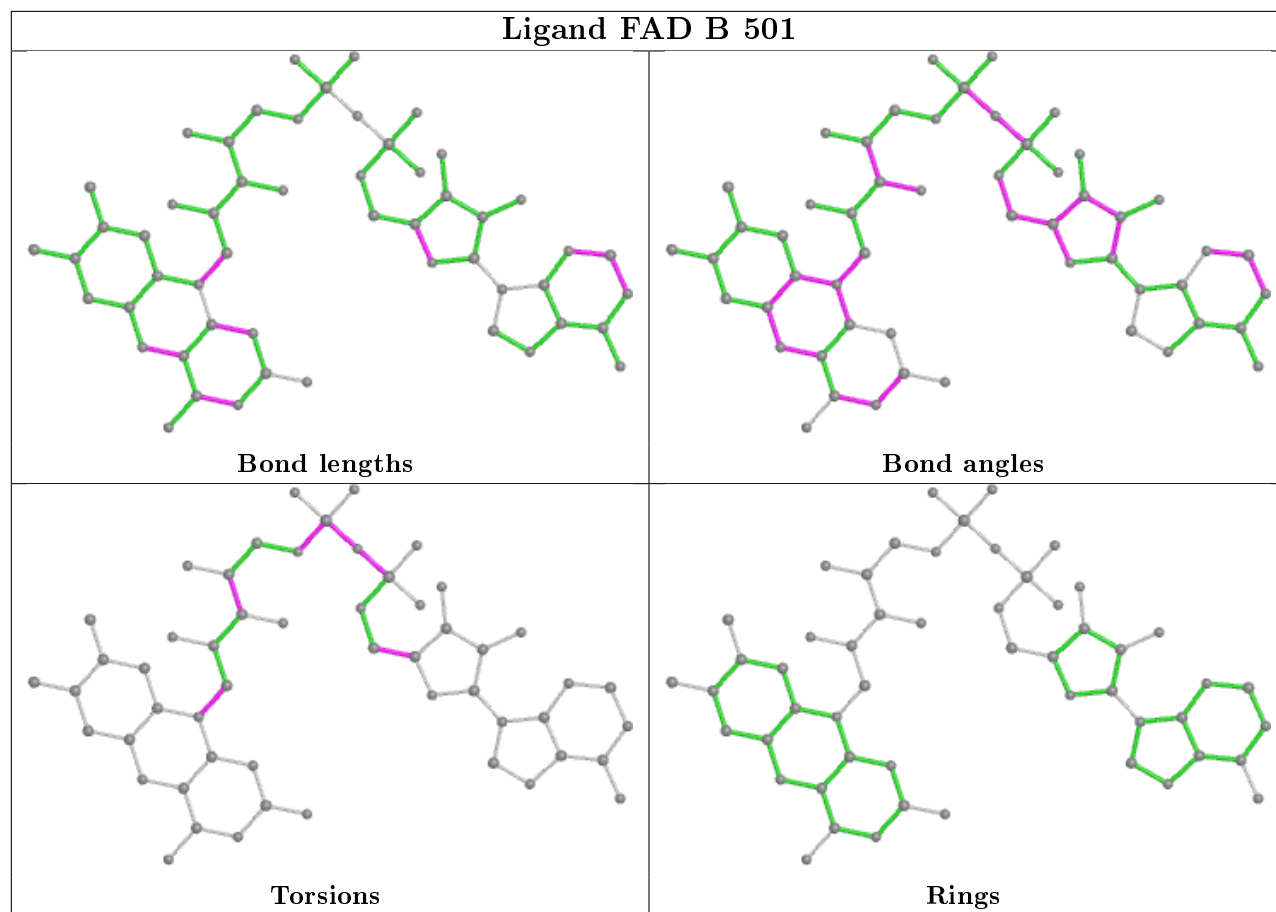
There are no ring outliers.

2 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	FAD	29	0
2	B	501	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	474/497 (95%)	-0.53	1 (0%) 95 90	18, 30, 44, 53	11 (2%)
1	B	480/497 (96%)	-0.49	2 (0%) 92 84	14, 31, 49, 63	16 (3%)
All	All	954/994 (95%)	-0.51	3 (0%) 94 88	14, 30, 45, 63	27 (2%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	113	SER	2.3
1	B	3	ASP	2.0
1	B	9	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

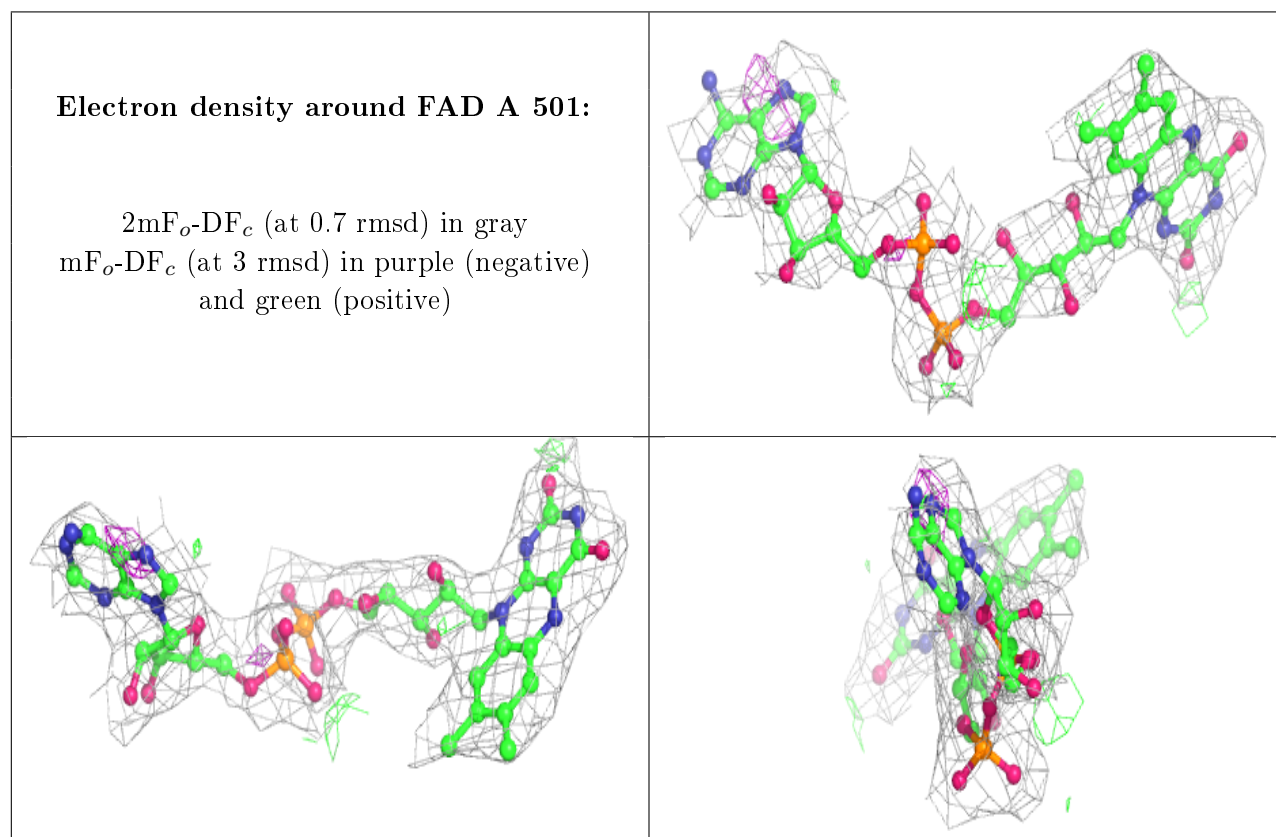
There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

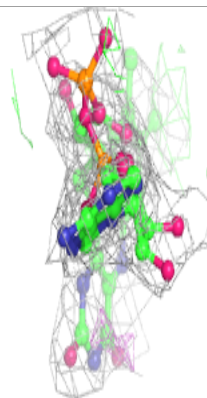
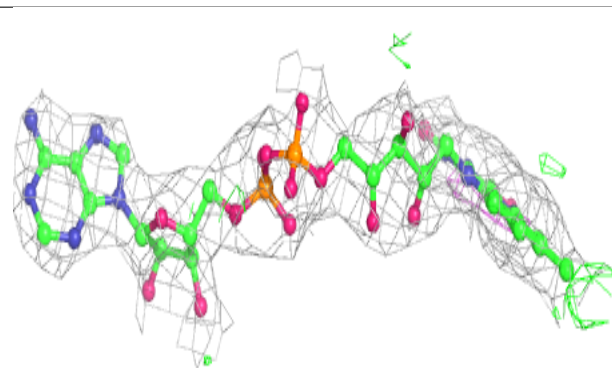
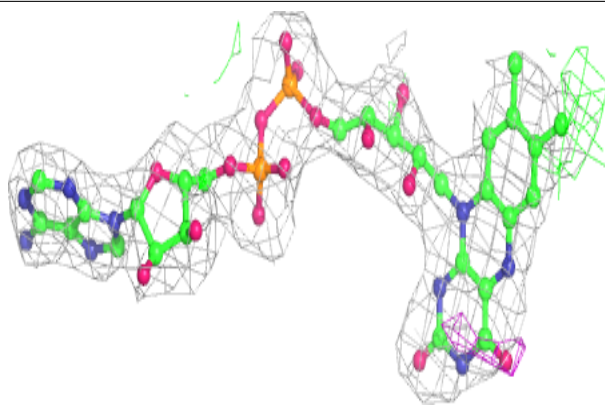
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FAD	A	501	53/53	0.94	0.18	8,19,39,40	0
2	FAD	B	501	53/53	0.95	0.16	13,25,28,32	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around FAD B 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.