



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:03 PM UTC

PDB ID : 4E0V / pdb_00004e0v
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

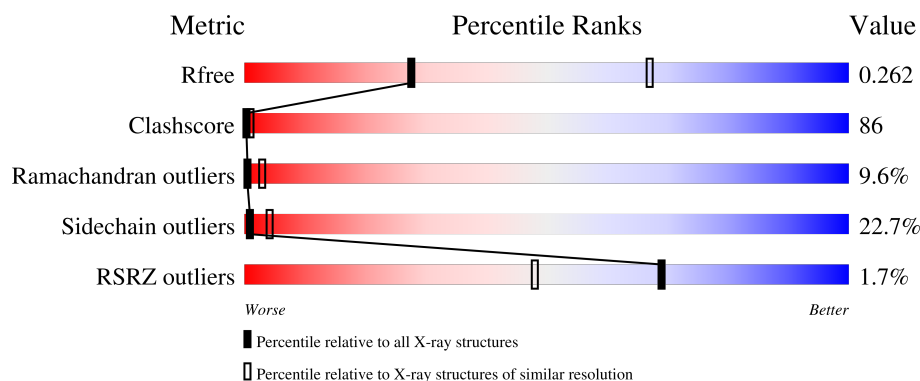
1 Overall quality at a glance

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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	18% 51% 24% 5%
1	B	497	18% 56% 21% 5%

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 [i](#)

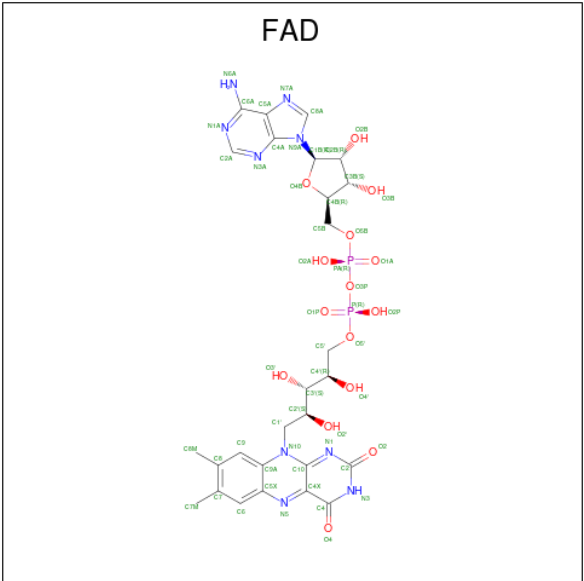
There are 3 unique types of molecules in this entry. The entry contains 7726 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).

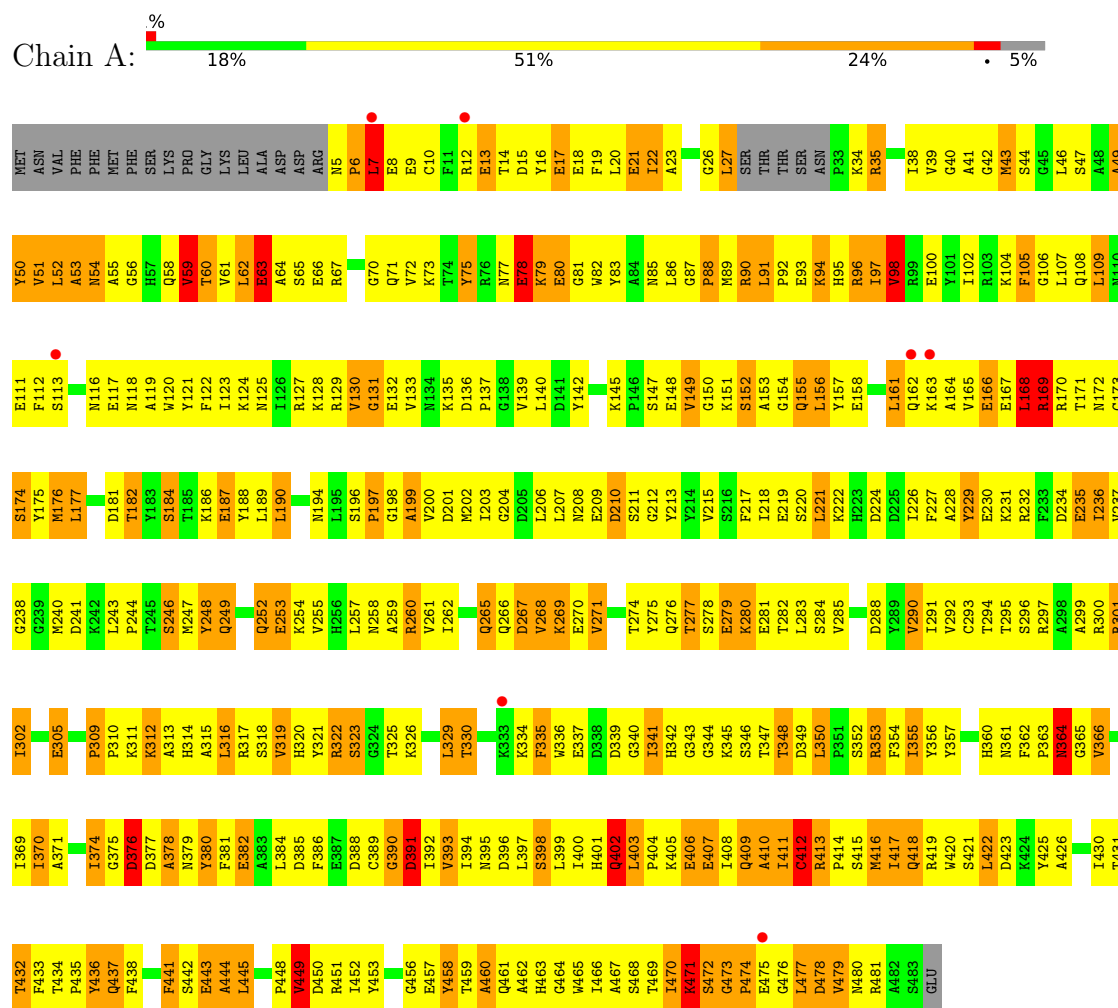


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total 7	O 7	0	0
3	B	9	Total 9	O 9	0	0

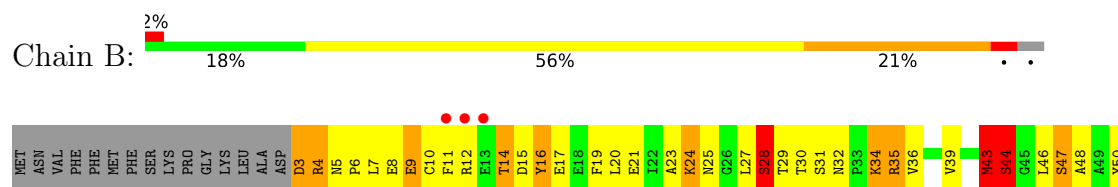
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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



• Molecule 1: L-amino-acid oxidase



M427	G428	G429	I430	T431	T432	F433	T434	P435	Y436	Q437	F438	Q439	H440	F441	S442	E443	A444	L445	T446	A447	P448	V449	D450	R451	I452	Y453	F454	A455	G456	E457	Y458	T459	A460	Q461	A462	H463	I466	A467	S468	T469	I470	K471	S472	G473	P474	E475	G476	L477	D478	V479	N480	R481	A482	SER	GLU					
G366	V366	G367	K303	F304	E305	P306	P307	L308	G373	I374	G375	D376	D377	A378	N379	Y380	F381	E382	A383	L384	D385	F386	E387	D388	C389	G390	D391	L392	V393	I394	N395	D396	L397	S398	L399	I400	H401	Q402	L403	P404	K405	E406	E407	I408	Q409	A410	I411	C412	M416	I417	Q418	R419	N420	S421	L422	D423	K424	Y425	A426	
R301	I302	D241	K303	F304	E305	P306	P307	L308	P309	P310	K311	D250	K312	A313	H314	A315	L316	V319	N258	A259	R260	V261	S323	G324	T325	K326	G327	L329	T330	C331	T332	K333	L334	P335	L396	E337	D338	D339	G340	I341	E281	T282	L283	S284	V285	T286	D288	P351	S352	V289	R353	I354	I355	Y356	W420	S421	N359	H360	N361	N364
L177	N178	K179	Y180	D181	T182	T183	Y183	T248	Q249	A250	L188	L189	Q252	L190	K191	E192	G193	N194	L195	S196	P197	G198	A199	D201	M202	L203	G204	D205	L206	L207	N208	E209	D210	S211	G212	Y213	Y214	V215	S216	F217	I218	E219	S220	L221	K222	H223	D224	I226	Y229	E230	K231	R232	F233	D234	E235	I236	V237			
V51	L52	A53	H57	G58	V59	T60	V61	L62	E63	A64	S65	E66	G70	Q71	V72	K73	T74	Y75	R76	N77	E78	K79	E80	G81	W82	Y83	A84	N85	L86	G87	P88	N89	R90	L91	P92	E93	K94	R95	R96	I97	V98	R99	E100	Y101	R102	R103	K104	F105	G106	L107	Q108	L109	N110	E111	F112	S113	Q114			
E115	N116	E117	N118	A119	W120	Y121	F122	I123	K124	N125	L126	R127	K128	E129	V130	G131	E132	V133	N134	K135	D136	P137	G138	V139	L140	D141	Y142	P143	V144	K145	P146	S147	E148	V149	G150	K151	S152	A153	L156	Y157	S160	L161	Q162	K163	A164	V165	E166	E167	L168	R169	R170	T171	N172	C173	S174	Y175	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 29.02 – 3.10	Depositor EDS
% Data completeness (in resolution range)	95.1 (29.02-3.10) 94.5 (29.02-3.10)	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	1721 reflections (9.77%)	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)	0.31 , 61.9	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

5.1 Standard geometry

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	0.83	2/3856 (0.1%)	1.18	30/5218 (0.6%)
1	B	0.76	0/3920	1.14	23/5305 (0.4%)
All	All	0.79	2/7776 (0.0%)	1.16	53/10523 (0.5%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	88	PRO	N-CD	11.08	1.63	1.47
1	A	291	ILE	CA-CB	-5.69	1.47	1.54

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	309	PRO	CA-C-N	9.54	131.77	119.84
1	A	309	PRO	C-N-CA	9.54	131.77	119.84
1	B	219	GLU	N-CA-C	-9.23	101.58	113.12
1	B	309	PRO	CA-C-N	8.20	127.77	119.24
1	B	309	PRO	C-N-CA	8.20	127.77	119.24
1	A	142	TYR	CA-C-N	-8.18	111.31	119.90
1	A	142	TYR	C-N-CA	-8.18	111.31	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	87	GLY	CA-C-N	8.16	128.21	119.89
1	B	87	GLY	C-N-CA	8.16	128.21	119.89
1	A	475	GLU	N-CA-C	-8.12	102.26	112.90
1	A	168	LEU	N-CA-C	-8.02	102.23	110.97
1	A	412	CYS	N-CA-C	7.68	122.28	108.69
1	A	476	GLY	N-CA-C	-7.11	104.04	112.64
1	A	87	GLY	CA-C-N	6.88	128.44	119.84
1	A	87	GLY	C-N-CA	6.88	128.44	119.84
1	B	34	LYS	N-CA-C	6.31	116.60	108.34
1	A	421	SER	N-CA-C	-6.17	104.85	112.38
1	A	413	ARG	CA-C-N	-6.15	113.44	119.78
1	A	413	ARG	C-N-CA	-6.15	113.44	119.78
1	A	97	ILE	CB-CA-C	-6.14	104.11	111.97
1	B	16	TYR	N-CA-C	-6.12	103.76	111.11
1	A	471	LYS	N-CA-C	-6.12	103.77	111.11
1	A	473	GLY	CA-C-N	6.07	127.42	119.84
1	A	473	GLY	C-N-CA	6.07	127.42	119.84
1	A	79	LYS	N-CA-C	-6.01	106.08	113.41
1	B	255	VAL	N-CA-C	5.93	117.12	108.58
1	A	211	SER	N-CA-C	-5.89	106.73	112.97
1	B	263	LYS	N-CA-C	5.85	117.30	108.46
1	B	192	GLU	N-CA-C	-5.83	105.05	114.09
1	A	316	LEU	N-CA-C	-5.83	104.76	112.34
1	B	187	GLU	N-CA-C	-5.80	104.59	111.03
1	B	309	PRO	O-C-N	5.71	123.94	121.31
1	A	236	ILE	CB-CA-C	-5.70	104.41	111.08
1	B	80	GLU	N-CA-C	-5.57	107.12	114.31
1	A	370	ILE	N-CA-C	5.56	116.79	107.18
1	A	78	GLU	N-CA-C	-5.46	106.97	113.97
1	A	98	VAL	N-CA-C	-5.39	105.24	110.42
1	B	388	ASP	N-CA-C	-5.36	105.47	112.23
1	B	61	VAL	N-CA-C	5.33	115.98	108.36
1	A	190	LEU	N-CA-C	5.28	117.94	111.82
1	B	434	THR	CA-C-N	-5.26	114.30	119.92
1	B	434	THR	C-N-CA	-5.26	114.30	119.92
1	A	378	ALA	N-CA-C	-5.24	104.82	111.11
1	B	300	ARG	N-CA-C	-5.23	105.66	111.36
1	B	124	LYS	N-CA-C	-5.22	106.22	112.58
1	A	59	VAL	N-CA-C	5.20	116.68	109.45
1	A	235	GLU	N-CA-C	-5.18	100.59	109.24
1	B	475	GLU	N-CA-C	-5.17	102.84	111.37
1	A	432	THR	N-CA-C	5.12	116.39	107.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	197	PRO	N-CA-C	-5.11	106.43	113.53
1	B	181	ASP	N-CA-C	-5.07	106.95	113.23
1	A	80	GLU	N-CA-C	-5.04	107.18	113.38
1	B	231	LYS	N-CA-C	-5.04	105.98	111.82

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	633	1
1	B	3833	0	3747	675	1
2	A	53	0	31	28	0
2	B	53	0	31	17	0
3	A	7	0	0	0	0
3	B	9	0	0	1	0
All	All	7726	0	7487	1302	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 86.

All (1302) 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:A:269:LYS:HE3	1:A:269:LYS:C	1.56	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:473:GLY:HA2	1:B:475:GLU:OE1	1.18	1.30
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	1.22
1:A:153:ALA:HB2	1:A:202:MET:HE2	1.17	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:A:472:SER:C	1:A:474:PRO:CD	2.22	1.13
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
1:B:43:MET:HE3	1:B:43:MET:HA	1.20	1.09
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
2:A:501:FAD:N3A	2:A:501:FAD:H2B	1.37	1.07
1:B:386:PHE:C	1:B:387:GLU:HG3	1.74	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:A:472:SER:CA	1:A:474:PRO:HD3	1.85	1.07
1:B:121:TYR:CE2	1:B:133:VAL:HG21	1.88	1.07
1:B:301:ARG:HH21	1:B:427:MET:HE1	1.14	1.06
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:B:348:THR:HG22	1:B:353:ARG:O	1.56	1.04
1:A:168:LEU:HD23	1:A:168:LEU:C	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:280:LYS:C	1:B:281:GLU:HG3	1.83	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:B:466:ILE:H	2:B:501:FAD:HM83	1.15	1.01
1:A:63:GLU:CB	2:A:501:FAD:C2A	2.39	1.01
1:A:269:LYS:C	1:A:269:LYS:CE	2.32	1.01
1:A:176:MET:HG3	1:A:177:LEU:N	1.74	1.01
1:B:153:ALA:H	1:B:202:MET:HE2	1.26	1.01
1:B:278:SER:CB	1:B:281:GLU:OE1	2.08	1.01
1:A:236:ILE:H	1:A:240:MET:HE2	1.22	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: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
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:7:LEU:CD1	1:B:176:MET:HE1	1.93	0.98
1:B:43:MET:HA	1:B:43:MET:CE	1.91	0.98
1:A:111:GLU:CD	1:A:232:ARG:HG3	1.89	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:265:GLN:HE21	1:A:305:GLU:CD	1.72	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:166:GLU:C	1:A:167:GLU:CD	2.33	0.96
1:A:267:ASP:OD1	1:A:269:LYS:N	1.98	0.96
1:B:312:LYS:NZ	1:B:447:ALA:O	2.00	0.95
1:A:15:ASP:CB	1:A:19:PHE:CE2	2.46	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:ASP:N	1:B:229:TYR:CG	2.35	0.95
1:B:472:SER:C	1:B:474:PRO:HD2	1.91	0.95
1:A:265:GLN:NE2	1:A:305:GLU:CD	2.24	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:301:ARG:HG2	1:B:380:TYR:OH	1.67	0.93
1:B:473:GLY:HA2	1:B:475:GLU:CD	1.92	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: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
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:A:166:GLU:O	1:A:167:GLU:CD	2.14	0.90
1:B:146:PRO:C	1:B:148:GLU:H	1.78	0.90
1:A:363:PRO:O	1:A:364:ASN:HB3	1.71	0.90
1:B:130:VAL:O	1:B:131:GLY:C	2.15	0.90
1:A:269:LYS:HE3	1:A:270:GLU:CA	2.02	0.89
1:B:77:ASN:ND2	1:B:80:GLU:CG	2.35	0.89
1:B:111:GLU:OE1	1:B:232:ARG:HG3	1.72	0.89
1:B:132:GLU:OE2	1:B:139:VAL:HG11	1.71	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:TRP:NE1	1:A:129:ARG:HH21	1.70	0.88
1:B:77:ASN:HD22	1:B:80:GLU:CG	1.85	0.88
1:A:168:LEU:C	1:A:168:LEU:CD2	2.48	0.87
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: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:480:ASN:C	1:B:482:ALA:N	2.31	0.86
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:330:THR:O	1:A:330:THR:HG22	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:301:ARG:NH2	1:B:427:MET:HE1	1.90	0.85
1:B:322:ARG:HH11	1:B:432:THR:HG21	1.39	0.85
1:A:153:ALA:HB2	1:A:202:MET:CE	2.04	0.85
1:A:277:THR:O	1:A:280:LYS:CB	2.23	0.85
1:B:102:ILE:HA	1:B:107:LEU:HD12	1.56	0.85
1:B:470:ILE:HD12	1:B:470:ILE:C	2.02	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: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:CD1	1:A:112:PHE:O	2.30	0.83
1:B:48:ALA:HB1	1:B:475:GLU:HG3	1.58	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:A:19:PHE:O	1:A:20:LEU:C	2.22	0.82
1:A:54:ASN:C	1:A:56:GLY:H	1.88	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: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:3:ASP:N	1:B:229:TYR:CB	2.44	0.81
1:B:20:LEU:O	1:B:24:LYS:HG2	1.81	0.81
1:B:97:ILE:HG22	1:B:470:ILE:HD11	1.61	0.80
1:B:480:ASN:O	1:B:481:ARG:C	2.23	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:7:LEU:C	1:A:9:GLU:H	1.91	0.79
1:B:74:THR:HG23	1:B:84:ALA:O	1.81	0.79
1:B:90:ARG:HD2	1:B:233:PHE:CD2	2.13	0.79
1:B:153:ALA:N	1:B:202:MET:HE2	1.98	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:A:472:SER:C	1:A:474:PRO:HD2	2.08	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:269:LYS:C	1:A:269:LYS:CD	2.56	0.78
1:A:322:ARG:HG3	1:A:322:ARG:NH1	1.97	0.78
1:B:114:GLN:O	1:B:345:LYS:HE3	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:475:GLU:HG2	1:B:476:GLY:N	1.98	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: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:A:166:GLU:C	1:A:167:GLU:OE1	2.28	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:167:GLU:OE1	1:B:179:LYS:HE2	1.86	0.76
1:B:466:ILE:N	2:B:501:FAD:HM83	1.98	0.76
1:B:457:GLU:OE2	2:B:501:FAD:O2P	2.03	0.76
1:B:7:LEU:HD13	1:B:176:MET:HE1	1.66	0.76
1:B:165:VAL:C	1:B:167:GLU:H	1.94	0.76
1:B:333:LYS:O	1:B:335:PHE:N	2.19	0.76
1:B:395:ASN:CG	1:B:405:LYS:HD2	2.10	0.76
1:A:43:MET:CE	1:A:247:MET:HE3	2.15	0.76
1:B:456:GLY:H	1:B:459:THR:HG23	1.51	0.76
1:A:98:VAL:CG1	1:A:467:ALA:HB2	2.12	0.76
1:A:277:THR:HG23	1:A:281:GLU:O	1.85	0.76
1:A:337:GLU:C	1:A:339:ASP:H	1.93	0.75
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:145:LYS:O	1:B:148:GLU:HB2	1.85	0.75
1:B:301:ARG:HH21	1:B:427:MET:HE2	1.52	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:466:ILE:H	2:B:501:FAD:C8M	1.97	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:GLN:O	1:B:345:LYS:CE	2.34	0.75
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:43:MET:HE3	1:B:43:MET:CA	2.10	0.74
1:B:77:ASN:HD22	1:B:80:GLU:CD	1.95	0.74
1:B:10:CYS:O	1:B:11:PHE:HB2	1.87	0.74
1:B:480:ASN:C	1:B:482:ALA:H	1.93	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:70:GLY:C	1:B:72:VAL:H	1.96	0.74
1:B:146:PRO:C	1:B:148:GLU:N	2.43	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:274:THR:HA	1:A:284:SER:HA	1.69	0.73
1:A:43:MET:HE3	1:A:247:MET:CE	2.18	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: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: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:A:435:PRO:O	1:A:436:TYR:HB2	1.87	0.72
1:B:453:TYR:CE1	1:B:478:ASP:CB	2.71	0.72
1:B:348:THR:HG23	1:B:353:ARG:HA	1.71	0.72
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:B:5:ASN:O	1:B:6:PRO:C	2.33	0.72
1:A:39:VAL:HG12	1:A:39:VAL:O	1.88	0.72
1:A:72:VAL:HG22	1:A:88:PRO:HG2	1.72	0.72
1:A:197:PRO:O	1:A:200:VAL:HB	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:210:ASP:OD2	1:A:210:ASP:C	2.33	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:A:262:ILE:O	1:A:302:ILE:HG22	1.91	0.71
1:B:353:ARG:NH2	1:B:354:PHE:CE2	2.58	0.71
1:B:88:PRO:HA	2:B:501:FAD:C5X	2.20	0.71
1:B:405:LYS:C	1:B:407:GLU:H	1.99	0.71
1:A:472:SER:HA	1:A:474:PRO:HD3	1.69	0.70
1:A:379:ASN:C	1:A:381:PHE:H	1.99	0.70
1:B:146:PRO:O	1:B:148:GLU:N	2.23	0.70
1:B:153:ALA:H	1:B:202:MET:CE	2.03	0.70
1:B:16:TYR:CZ	1:B:97:ILE:HG13	2.27	0.70
1:B:108:GLN:NE2	1:B:109:LEU:H	1.88	0.70
1:B:473:GLY:N	1:B:474:PRO:HD2	2.05	0.70
1:A:49:ALA:O	1:A:50:TYR:C	2.34	0.70
1:A:73:LYS:O	1:A:86:LEU:HB2	1.91	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: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:HD12	1:A:109:LEU:H	1.56	0.70
1:A:350:LEU:N	1:A:350:LEU:CD2	2.55	0.70
1:A:181:ASP:CA	1:A:218:ILE:HD11	2.22	0.70
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:328:PHE:N	1:B:328:PHE:CD1	2.60	0.70
1:B:98:VAL:HG23	1:B:467:ALA:HB2	1.74	0.69
1:B:355:ILE:N	1:B:355:ILE:HD13	2.05	0.69
1:A:89:MET:HE3	1:A:326:LYS:NZ	2.08	0.69
1:B:473:GLY:CA	1:B:475:GLU:CD	2.60	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:LEU:HD21	1:A:416:MET:HE1	1.74	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:471:LYS:C	1:B:473:GLY:H	2.00	0.69
1:B:21:GLU:O	1:B:25:ASN:N	2.15	0.69
1:B:74:THR:HG23	1:B:84:ALA:C	2.18	0.69
1:B:280:LYS:O	1:B:281:GLU:CB	2.41	0.69
1:B:280:LYS:O	1:B:281:GLU:OE1	2.11	0.69
1:B:322:ARG:NH1	1:B:432:THR:CG2	2.49	0.69
1:B:335:PHE:HE2	1:B:412:CYS:SG	2.15	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: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:436:TYR:HB3	1:B:186:LYS:HZ1	1.58	0.68
1:B:251:ILE:C	1:B:253:GLU:N	2.45	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
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: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:201:ASP:O	1:A:202:MET:C	2.38	0.67
1:A:394:ILE:HG23	1:A:408:ILE:HG21	1.76	0.67
1:B:30:THR:HG23	1:B:30:THR:O	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:LEU:CD2	1:B:407:GLU:OE1	2.42	0.67
1:A:90:ARG:C	1:A:91:LEU:HG	2.19	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:B:187:GLU:O	1:B:188:TYR:C	2.35	0.67
1:B:353:ARG:NH2	1:B:354:PHE:CZ	2.62	0.67
1:B:397:LEU:O	1:B:398:SER:C	2.36	0.67
1:A:184:SER:O	1:A:187:GLU:HB3	1.95	0.66
1:B:73:LYS:CG	1:B:86:LEU:HD12	2.25	0.66
1:B:90:ARG:CG	1:B:233:PHE:CD2	2.78	0.66
1:B:152:SER:O	1:B:153:ALA:C	2.38	0.66
1:A:43:MET:CE	1:A:247:MET:CE	2.72	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:A:312:LYS:O	1:A:316:LEU:HG	1.95	0.66
1:B:277:THR:O	1:B:278:SER:OG	2.13	0.66
1:B:352:SER:HB3	1:B:355:ILE:HD11	1.77	0.66
1:A:315:ALA:HB1	1:A:445:LEU:CD1	2.24	0.66
1:B:114:GLN:O	1:B:345:LYS:NZ	2.28	0.66
1:B:251:ILE:C	1:B:253:GLU:H	2.01	0.66
1:B:406:GLU:HA	1:B:409:GLN:HE21	1.61	0.66
1:A:41:ALA:C	1:A:42:GLY:O	2.38	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:O	1:A:269:LYS:HD2	1.95	0.66
1:A:319:VAL:HA	1:A:437:GLN:HE22	1.61	0.66
1:A:406:GLU:O	1:A:407:GLU:C	2.39	0.66
1:B:116:ASN:HD21	1:B:341:ILE:HG23	1.60	0.66
1:A:63:GLU:C	2:A:501:FAD:C2A	2.69	0.65
1:A:164:ALA:HB2	1:A:188:TYR:OH	1.96	0.65
1:A:449:VAL:O	1:A:452:ILE:HB	1.95	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:5:ASN:HB2	1:A:6:PRO:HD3	1.77	0.65
1:A:51:VAL:O	1:A:53:ALA:N	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:ARG:HH11	1:A:322:ARG:CG	2.08	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:B:472:SER:CA	1:B:474:PRO:HD2	2.25	0.65
1:A:379:ASN:O	1:A:381:PHE:N	2.30	0.65
1:B:48:ALA:HB2	1:B:475:GLU:CD	2.21	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: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:A:198:GLY:C	1:A:200:VAL:N	2.52	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:A:43:MET:HE3	1:A:247:MET:HE1	1.79	0.64
1:B:327:ILE:HG12	1:B:417:ILE:HD11	1.79	0.64
1:A:51:VAL:O	1:A:52:LEU:C	2.39	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: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:165:VAL:C	1:A:167:GLU:H	2.06	0.64
1:A:217:PHE:CE1	1:A:221:LEU:HD21	2.32	0.64
1:A:265:GLN:HB2	1:A:305:GLU:CD	2.18	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:145:LYS:HB2	1:A:148:GLU:CD	2.23	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:A:181:ASP:CG	1:A:438:PHE:HB2	2.22	0.63
1:A:208:ASN:C	1:A:208:ASN:HD22	2.04	0.63
1:B:108:GLN:O	1:B:237:VAL:HG23	1.97	0.63
1:B:386:PHE:C	1:B:388:ASP:H	2.07	0.63
1:A:170:ARG:CG	1:A:171:THR:HG23	2.29	0.63
1:B:36:VAL:HG22	1:B:289:TYR:HB2	1.80	0.63
1:B:61:VAL:CB	1:B:255:VAL:HG22	2.20	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:VAL:HB	1:B:148:GLU:OE1	1.98	0.63
1:B:315:ALA:C	1:B:319:VAL:HG23	2.18	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:B:395:ASN:HD22	1:B:395:ASN:H	1.47	0.62
1:B:95:HIS:O	1:B:97:ILE:N	2.32	0.62
1:B:187:GLU:HG2	1:B:191:LYS:HD3	1.81	0.62
1:A:7:LEU:C	1:A:9:GLU:N	2.58	0.62
1:A:111:GLU:OE1	1:A:232:ARG:CD	2.48	0.62
1:A:299:ALA:O	1:A:300:ARG:C	2.41	0.62
1:B:14:THR:O	1:B:17:GLU:CD	2.42	0.62
1:B:88:PRO:HA	2:B:501:FAD:N5	2.15	0.62
1:B:391:ASP:CG	1:B:392:ILE:N	2.57	0.62
1:A:385:ASP:O	1:A:386:PHE:C	2.39	0.62
1:B:9:GLU:O	1:B:12:ARG:CB	2.47	0.62
1:A:89:MET:HE3	1:A:326:LYS:HZ1	1.63	0.62
1:B:103:ARG:HG2	1:B:103:ARG:HH11	1.64	0.62
1:B:291:ILE:HG22	1:B:293:CYS:SG	2.40	0.62
1:B:473:GLY:C	1:B:475:GLU:OE1	2.42	0.62
1:B:280:LYS:O	1:B:281:GLU:CD	2.42	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:165:VAL:C	1:B:167:GLU:N	2.56	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:320:HIS:H	1:A:437:GLN:HE22	1.47	0.62
1:A:364:ASN:HD22	1:A:365:GLY:H	1.45	0.62
1:B:210:ASP:C	1:B:212:GLY:H	2.08	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:B:301:ARG:NH2	1:B:427:MET:CE	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:ASN:ND2	1:B:80:GLU:CD	2.58	0.61
1:B:473:GLY:N	1:B:474:PRO:CD	2.64	0.61
1:B:473:GLY:C	1:B:475:GLU:CD	2.68	0.61
1:B:440:HIS:HD2	1:B:440:HIS:O	1.83	0.61
1:A:320:HIS:H	1:A:437:GLN:NE2	1.99	0.61
1:A:375:GLY:O	1:A:376:ASP:C	2.44	0.61
1:A:471:LYS:C	1:A:474:PRO:HD3	2.25	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:19:PHE:CZ	1:B:474:PRO:HB3	2.37	0.60
1:B:62:LEU:HD23	1:B:259:ALA:CB	2.31	0.60
1:A:7:LEU:C	1:A:7:LEU:HD12	2.26	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:B:241:ASP:C	1:B:244:PRO:HD2	2.26	0.60
1:A:153:ALA:CB	1:A:202:MET:HE2	2.11	0.60
1:A:202:MET:HE2	1:A:206:LEU:HD12	1.83	0.60
1:A:375:GLY:O	1:A:377:ASP:N	2.34	0.60
1:B:70:GLY:C	1:B:72:VAL:N	2.57	0.60
1:B:120:TRP:CZ3	1:B:129:ARG:HG3	2.36	0.60
1:A:347:THR:HG23	1:A:354:PHE:CE1	2.36	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:B:405:LYS:C	1:B:407:GLU:N	2.60	0.60
1:A:269:LYS:O	1:A:269:LYS:NZ	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:7:LEU:O	1:A:9:GLU:N	2.27	0.59
1:A:305:GLU:O	1:A:305:GLU:CG	2.34	0.59
1:A:319:VAL:HA	1:A:437:GLN:NE2	2.17	0.59
1:B:138:GLY:O	1:B:140:LEU:N	2.35	0.59
1:B:417:ILE:O	1:B:417:ILE:HG22	2.02	0.59
1:A:170:ARG:HG3	1:A:171:THR:HG22	1.84	0.59
1:A:315:ALA:C	1:A:317:ARG:N	2.55	0.59
1:B:72:VAL:HG22	1:B:88:PRO:HG2	1.85	0.59
1:B:337:GLU:C	1:B:339:ASP:N	2.57	0.59
1:A:65:SER:OG	2:A:501:FAD:N7A	2.35	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:B:3:ASP:CA	1:B:229:TYR:HB3	2.33	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: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:18:GLU:O	1:A:21:GLU:HB3	2.03	0.59
1:A:63:GLU:CB	2:A:501:FAD:N3A	2.66	0.59
1:A:108:GLN:CD	1:A:237:VAL:HG21	2.27	0.59
1:A:109:LEU:HA	1:A:237:VAL:H	1.68	0.59
1:A:320:HIS:CE1	1:A:321:TYR:O	2.56	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: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:B:197:PRO:C	1:B:200:VAL:HG22	2.25	0.58
1:A:120:TRP:NE1	1:A:129:ARG:NH2	2.49	0.58
1:A:78:GLU:OE2	1:A:78:GLU:N	2.35	0.58
1:B:148:GLU:O	1:B:149:VAL:C	2.46	0.58
1:B:232:ARG:NH2	1:B:234:ASP:OD2	2.37	0.58
1:B:248:TYR:C	1:B:248:TYR:CD2	2.80	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:N	1:B:283:LEU:CD1	2.66	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ASP:OD1	1:A:268:VAL:N	2.37	0.58
1:A:392:ILE:O	1:A:393:VAL:C	2.47	0.58
1:A:458:TYR:H	1:A:458:TYR:HD2	1.50	0.58
1:B:282:THR:C	1:B:283:LEU:HD12	2.28	0.58
1:B:348:THR:CG2	1:B:353:ARG:C	2.77	0.58
1:A:64:ALA:HB2	1:A:260:ARG:N	2.19	0.58
1:A:139:VAL:HG23	1:A:140:LEU:HG	1.85	0.58
1:A:162:GLN:HG3	1:A:162:GLN:O	2.02	0.58
1:B:30:THR:O	1:B:31:SER:C	2.46	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:HD12	1:B:329:LEU:H	1.65	0.58
1:A:130:VAL:CG2	1:A:131:GLY:N	2.66	0.57
1:A:473:GLY:N	1:A:474:PRO:CD	2.60	0.57
1:A:43:MET:SD	1:A:244:PRO:HG3	2.44	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: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: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: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:HG2	1:B:103:ARG:NH1	2.18	0.57
1:A:315:ALA:C	1:A:317:ARG:H	2.13	0.57
1:A:409:GLN:O	1:A:411:ILE:N	2.37	0.57
1:B:93:GLU:HG3	1:B:232:ARG:NH1	2.19	0.57
1:B:387:GLU:O	1:B:391:ASP:HB3	2.05	0.57
1:A:323:SER:CB	1:A:379:ASN:HD21	2.17	0.56
1:A:384:LEU:HD21	1:B:427:MET:HE2	1.87	0.56
1:B:456:GLY:H	1:B:459:THR:HG21	1.68	0.56
1:A:5:ASN:CB	1:A:6:PRO:HD3	2.35	0.56
1:A:105:PHE:N	1:A:105:PHE:CD2	2.73	0.56
1:A:172:ASN:CG	1:A:173:CYS:H	2.07	0.56
1:A:172:ASN:CG	1:A:173:CYS:N	2.62	0.56
1:A:241:ASP:C	1:A:244:PRO:HD2	2.30	0.56
1:B:98:VAL:CG2	1:B:467:ALA:HB2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:ARG:CZ	1:B:432:THR:HG21	2.35	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:17:GLU:O	1:A:18:GLU:C	2.49	0.56
1:A:243:LEU:HB3	1:A:244:PRO:CD	2.31	0.56
1:A:364:ASN:ND2	1:A:364:ASN:C	2.61	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:B:471:LYS:C	1:B:473:GLY:N	2.63	0.56
1:A:111:GLU:CD	1:A:232:ARG:CG	2.71	0.56
1:A:111:GLU:HB2	1:A:232:ARG:HE	1.70	0.56
1:B:337:GLU:C	1:B:339:ASP:H	2.13	0.56
1:B:7:LEU:HD12	1:B:176:MET:HE1	1.85	0.56
1:B:93:GLU:OE1	1:B:232:ARG:NH1	2.39	0.56
1:B:434:THR:CB	1:B:435:PRO:CD	2.84	0.56
1:A:262:ILE:C	1:A:302:ILE:HG22	2.31	0.56
1:A:198:GLY:O	1:A:199:ALA:C	2.46	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:236:ILE:H	1:A:240:MET:CE	2.09	0.55
1:A:334:LYS:HB3	1:A:337:GLU:HG3	1.88	0.55
1:A:270:GLU:OE1	1:A:271:VAL:C	2.50	0.55
1:B:353:ARG:CZ	1:B:354:PHE:HE2	2.18	0.55
1:B:395:ASN:C	1:B:397:LEU:N	2.62	0.55
1:A:92:PRO:HG3	1:A:95:HIS:CE1	2.40	0.55
1:B:95:HIS:HE1	1:B:226:ILE:HD13	1.71	0.55
1:B:168:LEU:HD12	1:B:168:LEU:O	2.06	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:B:457:GLU:CD	1:B:457:GLU:H	2.15	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:A:448:PRO:O	1:A:449:VAL:HG13	2.06	0.55
1:B:187:GLU:HG2	1:B:191:LYS:CD	2.37	0.55
1:B:375:GLY:O	1:B:376:ASP:C	2.49	0.55
1:A:241:ASP:C	1:A:241:ASP:OD1	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:6:PRO:HD2	1:A:7:LEU:H	1.71	0.55
1:A:130:VAL:HG22	1:A:131:GLY: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
1:B:430:ILE:O	1:B:431:THR:C	2.50	0.55
1:A:157:TYR:C	1:A:157:TYR:CD2	2.84	0.55
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: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:A:44:SER:OG	2:A:501:FAD:O1P	2.21	0.54
1:A:54:ASN:C	1:A:56:GLY:N	2.55	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:51:VAL:HG12	1:A:52:LEU:H	1.68	0.54
1:A:173:CYS:O	1:A:174:SER:C	2.50	0.54
1:B:445:LEU:HD22	1:B:458:TYR:CD2	2.43	0.54
1:B:10:CYS:SG	1:B:168:LEU:CD1	2.95	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:HD12	1:A:109:LEU:N	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:313:ALA:O	1:A:314:HIS:C	2.51	0.54
1:A:315:ALA:CB	1:A:445:LEU:CD1	2.86	0.54
1:B:80:GLU:CB	1:B:82:TRP:HD1	2.20	0.54
1:B:169:ARG:HD2	1:B:169:ARG:O	2.08	0.54
1:A:54:ASN:O	1:A:56:GLY:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:THR:O	1:B:182:THR:OG1	2.22	0.53
1:A:7:LEU:C	1:A:7:LEU:CD1	2.81	0.53
1:A:469:THR:O	1:A:470:ILE:C	2.50	0.53
1:B:440:HIS:O	1:B:440:HIS:CD2	2.62	0.53
1:B:80:GLU:CB	1:B:82:TRP:CD1	2.92	0.53
1:B:191:LYS:O	1:B:192:GLU:OE2	2.26	0.53
1:A:271:VAL:HG21	1:A:290:VAL:HG23	1.90	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:471:LYS:O	1:B:471:LYS:CG	2.57	0.53
1:A:269:LYS:C	1:A:269:LYS:HD2	2.31	0.53
1:B:80:GLU:OE1	1:B:82:TRP:NE1	2.42	0.53
1:B:136:ASP:C	1:B:138:GLY:N	2.62	0.53
1:B:386:PHE:O	1:B:388:ASP:N	2.35	0.53
1:B:391:ASP:O	1:B:392:ILE:C	2.52	0.53
1:B:420:TRP:C	1:B:422:LEU:H	2.16	0.53
1:A:130:VAL:O	1:A:133:VAL:N	2.42	0.53
1:A:389:CYS:O	1:A:390:GLY:C	2.51	0.53
1:B:474:PRO:O	1:B:475:GLU:C	2.49	0.53
1:A:154:GLY:O	1:A:157:TYR:HB3	2.08	0.53
1:B:80:GLU:HB2	1:B:82:TRP:HD1	1.73	0.53
1:B:113:SER:H	1:B:359:ASN:ND2	2.05	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:B:395:ASN:C	1:B:397:LEU:H	2.16	0.53
1:A:232:ARG:NH2	1:A:234:ASP:OD1	2.42	0.53
1:A:313:ALA:C	1:A:315:ALA:N	2.61	0.53
1:B:144:VAL:HG12	1:B:196:SER:OG	2.08	0.53
1:B:162:GLN:O	1:B:163:LYS:C	2.51	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:A:174:SER:O	1:A:175:TYR:C	2.52	0.52
1:A:236:ILE:N	1:A:240:MET:HE2	2.07	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:O	1:A:380:TYR:CG	2.62	0.52
1:B:348:THR:HG22	1:B:353:ARG:C	2.30	0.52
1:B:399:LEU:O	1:B:400:ILE:C	2.52	0.52
1:B:470:ILE:CD1	1:B:470:ILE:C	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:202:MET:O	1:B:203:ILE:C	2.50	0.52
1:A:168:LEU:HD22	1:A:169:ARG:H	1.71	0.52
1:B:28:SER:O	1:B:29:THR:C	2.50	0.52
1:B:71:GLN:HE21	2:B:501:FAD:PA	2.25	0.52
1:B:352:SER:O	1:B:354:PHE:N	2.42	0.52
1:A:176:MET:O	1:A:177:LEU:C	2.51	0.52
1:B:162:GLN:HG3	1:B:163:LYS:N	2.24	0.52
1:A:59:VAL:HG23	1:A:60:THR:N	2.23	0.52
1:A:436:TYR:CB	1:B:186:LYS:HZ1	2.20	0.52
1:A:42:GLY:HA3	2:A:501:FAD:O3P	2.10	0.52
1:A:362:PHE:O	1:A:364:ASN:ND2	2.42	0.52
1:A:450:ASP:O	1:A:453:TYR:HE2	1.92	0.52
1:B:15:ASP:OD2	1:B:19:PHE:HE2	1.93	0.52
1:B:127:ARG:O	1:B:128:LYS:HG2	2.09	0.52
1:A:236:ILE:HG13	1:A:240:MET:HE2	1.90	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:127:ARG:C	1:B:128:LYS:HG2	2.35	0.52
1:A:44:SER:O	1:A:47:SER:HB2	2.10	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: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:168:LEU:HD12	1:B:168:LEU:C	2.35	0.51
1:B:208:ASN:HD22	1:B:208:ASN:C	2.17	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:61:VAL:CG1	1:A:62:LEU:N	2.74	0.51
1:A:120:TRP:CH2	1:A:129:ARG:NE	2.77	0.51
1:B:21:GLU:HA	1:B:24:LYS:CG	2.40	0.51
1:B:48:ALA:CB	1:B:475:GLU:CD	2.83	0.51
1:B:395:ASN:HD22	1:B:395:ASN:N	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:112:PHE:O	1:A:113:SER:C	2.53	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:311:LYS:HB3	1:A:444:ALA:HB1	1.92	0.51
1:B:181:ASP:O	1:B:181:ASP:OD1	2.28	0.51
1:A:86:LEU:HD21	1:A:416:MET:CE	2.40	0.51
1:A:155:GLN:HG2	1:A:156:LEU:N	2.24	0.51
1:A:436:TYR:CB	1:B:186:LYS:HZ3	2.24	0.51
1:B:35:ARG:O	1:B:288:ASP:HB2	2.10	0.51
1:B:92:PRO:HG3	1:B:233:PHE:HE2	1.75	0.51
1:B:448:PRO:C	1:B:450:ASP:HA	2.36	0.51
1:A:27:LEU:N	1:A:27:LEU:HD23	2.26	0.51
1:A:165:VAL:C	1:A:167:GLU:N	2.69	0.51
1:A:188:TYR:CD2	1:A:188:TYR:C	2.89	0.51
1:A:208:ASN:C	1:A:208:ASN:ND2	2.69	0.51
1:A:269:LYS:HE3	1:A:270:GLU:CB	2.40	0.51
1:A:329:LEU:CD1	1:A:414:PRO:CA	2.85	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:15:ASP:OD1	1:B:15:ASP:C	2.53	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:A:461:GLN:O	1:A:462:ALA:HB2	2.10	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:15:ASP:CB	1:A:19:PHE:CD2	2.85	0.50
1:A:72:VAL:CG1	1:A:244:PRO:HG2	2.40	0.50
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:207:LEU:O	1:A:208:ASN:HB3	2.11	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:A:119:ALA:HB3	1:A:130:VAL:CG1	2.42	0.50
1:A:130:VAL:O	1:A:131:GLY:C	2.53	0.50
1:B:73:LYS:CD	1:B:86:LEU:HD12	2.41	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:266:GLN:HA	1:A:271:VAL:HA	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:LYS:CE	1:A:270:GLU:CB	2.89	0.50
1:A:277:THR:C	1:A:279:GLU:H	2.20	0.50
2:B:501:FAD:O4'	2:B:501:FAD:O2'	2.28	0.50
1:A:72:VAL:HG11	1:A:244:PRO:HG2	1.94	0.50
1:B:170:ARG:C	1:B:171:THR:HG23	2.37	0.50
1:B:260:ARG:O	1:B:275:TYR:HA	2.12	0.50
1:A:43:MET:HE1	1:A:244:PRO:HA	1.94	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:473:GLY:CA	1:B:475:GLU:OE2	2.59	0.50
1:A:259:ALA:HA	1:A:276:GLN:O	2.11	0.50
1:A:436:TYR:HB2	1:B:186:LYS:HZ3	1.74	0.50
1:A:350:LEU:HD23	1:A:350:LEU:H	1.77	0.50
1:B:15:ASP:O	1:B:16:TYR:C	2.55	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:21:GLU:O	1:A:23:ALA:N	2.46	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:353:ARG:HG3	1:A:354:PHE:CD2	2.48	0.49
1:A:399:LEU:O	1:A:400:ILE:C	2.56	0.49
1:B:92:PRO:O	1:B:93:GLU:C	2.54	0.49
1:A:64:ALA:HB2	1:A:260:ARG:CA	2.42	0.49
1:A:77:ASN:O	1:A:81:GLY:HA2	2.12	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:334:LYS:O	1:A:336:TRP:N	2.46	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:350:LEU:HD23	1:B:396:ASP:CG	2.37	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:380:TYR:HE1	1:B:297:ARG:O	1.94	0.49
1:A:459:THR:O	1:A:460:ALA:C	2.55	0.49
1:B:83:TYR:CD1	1:B:84:ALA:N	2.80	0.49
1:A:132:GLU:O	1:A:133:VAL:C	2.55	0.49
1:A:369:ILE:HG22	1:A:370:ILE:N	2.28	0.49
1:B:386:PHE:C	1:B:388:ASP:N	2.71	0.49
1:A:309:PRO:HB3	1:A:310:PRO:HD2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:70:GLY:H	2:A:501:FAD:H8A	1.78	0.49
1:A:374:ILE:O	1:A:375:GLY:C	2.56	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:329:LEU:HD12	1:A:414:PRO:CA	2.43	0.48
1:B:46:LEU:O	1:B:47:SER:C	2.55	0.48
1:B:63:GLU:OE2	1:B:65:SER:HB3	2.13	0.48
1:B:170:ARG:C	1:B:171:THR:CG2	2.86	0.48
1:A:267:ASP:OD1	1:A:267:ASP:C	2.56	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
1:A:51:VAL:C	1:A:53:ALA:N	2.71	0.48
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:172:ASN:O	1:B:173:CYS:C	2.57	0.48
1:B:214:TYR:CD1	1:B:214:TYR:C	2.91	0.48
1:B:241:ASP:O	1:B:244:PRO:HG2	2.14	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: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:A:458:TYR:CD2	1:A:458:TYR:N	2.82	0.48
1:B:251:ILE:O	1:B:252:GLN:C	2.56	0.48
1:B:328:PHE:HD1	1:B:328:PHE:H	1.59	0.48
1:B:189:LEU:HA	1:B:189:LEU:HD23	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	1.77	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:265:GLN:NE2	1:A:305:GLU:CG	2.75	0.48
1:B:43:MET:HB3	1:B:469:THR:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:TYR:O	1:B:102:ILE:C	2.56	0.48
1:A:21:GLU:HA	1:A:21:GLU:OE1	2.12	0.48
1:A:471:LYS:O	1:A:473:GLY:N	2.46	0.48
1:B:99:ARG:HA	1:B:102:ILE:HG13	1.95	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: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:329:LEU:HD12	1:A:414:PRO:HA	1.92	0.48
1:A:364:ASN:OD1	1:A:366:VAL:HG13	2.14	0.48
1:B:177:LEU:O	1:B:218:ILE:HD13	2.14	0.48
1:B:176:MET:HG2	1:B:177:LEU:N	2.28	0.47
1:B:210:ASP:C	1:B:212:GLY:N	2.71	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:267:ASP:CG	1:A:268:VAL:N	2.73	0.47
1:A:460:ALA:CB	1:A:468:SER:O	2.63	0.47
1:B:43:MET:O	1:B:44:SER:C	2.56	0.47
1:B:109:LEU:HD22	1:B:234:ASP:HB3	1.96	0.47
1:B:348:THR:OG1	1:B:350:LEU:N	2.45	0.47
1:A:315:ALA:O	1:A:316:LEU:C	2.55	0.47
1:A:477:LEU:HG	1:A:478:ASP:OD1	2.14	0.47
1:B:20:LEU:HD11	1:B:96:ARG:HD2	1.96	0.47
1:B:279:GLU:C	1:B:280:LYS:CG	2.87	0.47
1:B:441:PHE:O	1:B:445:LEU:CD1	2.57	0.47
1:A:50:TYR:O	1:A:51:VAL:O	2.31	0.47
1:A:294:THR:HG22	2:A:501:FAD:O3B	2.14	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:83:TYR:CD1	1:B:83:TYR:C	2.93	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:148:GLU:OE1	1:A:196:SER:OG	2.30	0.47
1:A:236:ILE:HG13	1:A:240:MET:SD	2.54	0.47
1:A:261:VAL:CG1	1:A:262:ILE:N	2.77	0.47
1:A:320:HIS:N	1:A:437:GLN:HE22	2.11	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:THR:OG1	1:A:350:LEU:HD23	2.14	0.47
1:A:477:LEU:CD2	1:A:478:ASP:OD1	2.62	0.47
1:B:90:ARG:HD3	1:B:233:PHE:CG	2.46	0.47
1:B:131:GLY:O	1:B:135:LYS:HG3	2.15	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:307:PRO:O	1:B:308:LEU:C	2.56	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:B:475:GLU:C	1:B:479:VAL:HG23	2.39	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
1:B:114:GLN:C	1:B:115:GLU:HG2	2.39	0.47
1:A:181:ASP:CB	1:A:218:ILE:HD12	2.42	0.47
1:A:198:GLY:C	1:A:200:VAL:H	2.22	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:53:ALA:O	1:A:56:GLY:N	2.47	0.47
1:A:389:CYS:O	1:A:393:VAL:HG23	2.14	0.47
1:B:39:VAL:HG22	1:B:261:VAL:HG21	1.95	0.47
1:B:48:ALA:HB1	1:B:475:GLU:CG	2.37	0.47
1:B:114:GLN:C	1:B:115:GLU:CG	2.88	0.47
1:B:433:PHE:HD1	1:B:433:PHE:H	1.63	0.47
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: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:B:120:TRP:O	1:B:346:SER:HB2	2.16	0.46
1:B:296:SER:HB3	1:B:321:TYR:HE1	1.78	0.46
1:B:312:LYS:HE2	1:B:454:PHE:CD1	2.50	0.46
1:B:453:TYR:OH	1:B:478:ASP:HB3	2.16	0.46
1:B:456:GLY:N	1:B:459:THR:HG23	2.24	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:337:GLU:C	1:A:339:ASP:N	2.63	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:N	1:B:399:LEU:CD1	2.78	0.46
1:B:466:ILE:HG13	2:B:501:FAD:C9	2.45	0.46
1:A:202:MET:CE	1:A:206:LEU:HD12	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:SER:OG	1:B:66:GLU:N	2.49	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:A:136:ASP:C	1:A:136:ASP:OD1	2.58	0.46
1:A:390:GLY:O	1:A:391:ASP:C	2.58	0.46
1:B:395:ASN:O	1:B:396:ASP:C	2.58	0.46
1:A:456:GLY:O	1:A:457:GLU:C	2.57	0.46
1:B:170:ARG:O	1:B:171:THR:HG23	2.16	0.46
1:A:6:PRO:CG	1:A:229:TYR:CZ	2.83	0.46
1:A:112:PHE:O	1:A:112:PHE:CG	2.62	0.46
1:A:431:THR:C	1:A:432:THR:OG1	2.58	0.46
1:B:122:PHE:CE2	1:B:125:ASN:HA	2.51	0.46
1:B:16:TYR:O	1:B:17:GLU:C	2.59	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:B:230:GLU:OE2	1:B:230:GLU:CA	2.61	0.46
1:A:152:SER:H	1:A:155:GLN:NE2	2.14	0.46
1:A:409:GLN:C	1:A:411:ILE:N	2.74	0.46
1:B:136:ASP:O	1:B:137:PRO:C	2.58	0.46
1:B:337:GLU:C	1:B:340:GLY:H	2.23	0.46
1:B:337:GLU:HA	1:B:341:ILE:H	1.81	0.46
1:A:94:LYS:O	1:A:94:LYS:CG	2.63	0.46
1:A:175:TYR:O	1:A:176:MET:C	2.57	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:B:73:LYS:HE2	1:B:73:LYS:HB3	1.79	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: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:352:SER:OG	1:B:393:VAL:HA	2.16	0.45
1:B:353:ARG:NH2	1:B:354:PHE:HZ	2.12	0.45
1:A:6:PRO:CD	1:A:7:LEU:H	2.28	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:B:101:TYR:HD1	1:B:105:PHE:CE2	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:ASP:OD1	1:B:136:ASP:C	2.59	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:43:MET:HE2	1:A:243:LEU:HG	1.99	0.45
1:A:95:HIS:O	1:A:98:VAL:CG1	2.64	0.45
1:A:152:SER:HB2	1:A:155:GLN:HB3	1.98	0.45
1:A:300:ARG:HG3	1:A:316:LEU:CB	2.43	0.45
1:A:381:PHE:O	1:A:382:GLU:C	2.58	0.45
1:B:426:ALA:C	1:B:428:GLY:H	2.25	0.45
1:A:246:SER:O	1:A:247:MET:C	2.59	0.45
1:A:319:VAL:O	1:A:319:VAL:HG13	2.17	0.45
1:B:278:SER:N	1:B:281:GLU:OE1	2.49	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:N	1:B:395:ASN:ND2	2.65	0.45
1:B:404:PRO:HD2	1:B:407:GLU:CD	2.41	0.45
1:A:95:HIS:O	1:A:98:VAL:HG12	2.17	0.45
1:A:279:GLU:O	1:A:279:GLU:OE1	2.34	0.45
1:A:323:SER:CB	1:A:379:ASN:ND2	2.79	0.45
1:B:162:GLN:C	1:B:164:ALA:N	2.73	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
1:A:361:ASN:OD1	1:A:361:ASN:N	2.50	0.45
1:A:471:LYS:C	1:A:473:GLY:N	2.75	0.45
1:B:97:ILE:HG22	1:B:470:ILE:CD1	2.37	0.45
1:B:138:GLY:C	1:B:140:LEU:H	2.24	0.45
1:B:381:PHE:O	1:B:382:GLU:C	2.60	0.45
1:B:405:LYS:HB3	1:B:405:LYS:HE3	1.42	0.45
1:A:260:ARG:HH21	1:A:425:TYR:HE1	1.64	0.45
1:A:269:LYS:CE	1:A:270:GLU:CA	2.87	0.45
1:B:27:LEU:HD12	1:B:51:VAL:O	2.17	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:A:13:GLU:N	1:A:13:GLU:CD	2.75	0.45
1:A:145:LYS:CB	1:A:148:GLU:OE1	2.62	0.45
1:A:377:ASP:O	1:A:378:ALA:C	2.57	0.45
1:B:5:ASN:O	1:B:8:GLU:OE1	2.35	0.45
1:B:379:ASN:O	1:B:381:PHE:N	2.50	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:312:LYS:HE3	1:A:444:ALA:HB1	2.00	0.44
1:B:240:MET:C	1:B:242:LYS:N	2.74	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:59:VAL:CG2	1:A:60:THR:N	2.75	0.44
1:A:181:ASP:CG	1:A:218:ILE:HD12	2.42	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:296:SER:O	1:A:299:ALA:HB3	2.17	0.44
1:A:388:ASP:OD1	1:A:388:ASP:N	2.49	0.44
1:A:469:THR:C	1:A:471:LYS:N	2.73	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:A:246:SER:C	1:A:248:TYR:N	2.71	0.44
1:A:252:GLN:O	1:A:253:GLU:C	2.59	0.44
1:A:300:ARG:HH21	1:B:351:PRO:HD3	1.81	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:B:374:ILE:HA	1:B:378:ALA:HB2	1.99	0.44
1:B:376:ASP:HA	1:B:379:ASN:OD1	2.18	0.44
1:B:445:LEU:HD22	1:B:458:TYR:HD2	1.82	0.44
1:A:15:ASP:O	1:A:16:TYR:C	2.60	0.44
1:A:209:GLU:O	1:A:212:GLY:N	2.48	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:433:PHE:N	1:B:433:PHE:CD1	2.86	0.44
1:A:9:GLU:O	1:A:12:ARG:HG2	2.18	0.44
1:A:66:GLU:O	1:A:257:LEU:HD13	2.18	0.44
1:A:116:ASN:ND2	1:A:342:HIS:O	2.51	0.44
1:A:294:THR:HA	2:A:501:FAD:H51A	2.00	0.44
1:B:327:ILE:CG1	1:B:417:ILE:HD11	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:LEU:CG	1:B:351:PRO:HD2	2.47	0.44
1:A:181:ASP:OD2	1:A:438:PHE:CB	2.49	0.44
1:B:97:ILE:HD12	1:B:471:LYS:HD3	2.00	0.44
1:B:266:GLN:HE22	1:B:452:ILE:HG13	1.83	0.44
1:B:327:ILE:HB	1:B:371:ALA:HB3	1.98	0.44
1:A:119:ALA:C	1:A:130:VAL:HG13	2.43	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:A:267:ASP:C	1:A:269:LYS:N	2.76	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:63:GLU:HB3	2:A:501:FAD:C2A	2.42	0.43
1:A:109:LEU:HD22	1:A:234:ASP:CG	2.43	0.43
1:A:354:PHE:O	1:A:371:ALA:HA	2.18	0.43
1:B:163:LYS:HD2	1:B:192:GLU:O	2.19	0.43
1:B:180:TYR:HA	1:B:183:TYR:HD2	1.83	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:B:476:GLY:C	1:B:478:ASP:N	2.76	0.43
1:A:296:SER:O	1:A:297:ARG:C	2.59	0.43
1:A:315:ALA:O	1:A:317:ARG:N	2.51	0.43
1:B:24:LYS:HE3	1:B:24:LYS:HB3	1.62	0.43
1:B:70:GLY:HA2	2:B:501:FAD:O3B	2.18	0.43
1:B:74:THR:CG2	1:B:84:ALA:O	2.60	0.43
1:A:375:GLY:C	1:A:377:ASP:N	2.77	0.43
1:B:53:ALA:HA	1:B:59:VAL:CG1	2.49	0.43
1:B:63:GLU:OE1	1:B:63:GLU:HA	2.19	0.43
1:B:75:TYR:HB2	1:B:416:MET:HE2	2.00	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:A:170:ARG:HG3	1:A:171:THR:N	2.32	0.43
1:B:449:VAL:N	1:B:450:ASP:HA	2.34	0.43
1:B:245:THR:C	1:B:247:MET:N	2.77	0.43
1:A:404:PRO:O	1:A:405:LYS:C	2.62	0.43
1:B:280:LYS:O	1:B:280:LYS:HG3	2.18	0.43
1:A:91:LEU:HA	1:A:92:PRO:HD2	1.86	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:B:104:LYS:HE3	1:B:104:LYS:HB2	1.70	0.43
1:B:149:VAL:HG23	1:B:149:VAL:O	2.19	0.43
1:B:353:ARG:NE	1:B:354:PHE:HE2	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:VAL:HG13	1:A:254:LYS:HD3	2.01	0.43
1:B:48:ALA:C	1:B:50:TYR:N	2.76	0.43
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:277:THR:HG1	1:B:281:GLU:HB2	1.80	0.42
1:B:330:THR:HG22	1:B:368:VAL:HG22	2.00	0.42
1:A:71:GLN:CG	2:A:501:FAD:O1A	2.63	0.42
1:A:329:LEU:CD2	1:A:393:VAL:CG1	2.96	0.42
1:B:217:PHE:O	1:B:217:PHE:CG	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:7:LEU:HD23	1:B:7:LEU:H	1.83	0.42
1:B:326:LYS:HE2	1:B:372:TYR:CD2	2.54	0.42
1:A:43:MET:CE	1:A:247:MET:HE1	2.46	0.42
1:A:267:ASP:C	1:A:269:LYS:H	2.26	0.42
1:A:423:ASP:HB3	1:A:426:ALA:HB3	2.00	0.42
1:B:43:MET:HB3	1:B:44:SER:H	1.72	0.42
1:B:98:VAL:HG12	1:B:102:ILE:HD11	2.01	0.42
1:A:95:HIS:O	1:A:96:ARG:C	2.62	0.42
1:A:300:ARG:NH1	1:A:317:ARG:HB2	2.35	0.42
1:B:3:ASP:HA	1:B:4:ARG:HA	1.70	0.42
1:B:110:ASN:HB3	1:B:235:GLU:HG2	2.00	0.42
1:B:242:LYS:O	1:B:243:LEU:C	2.61	0.42
1:B:389:CYS:O	1:B:390:GLY:C	2.63	0.42
1:B:401:HIS:O	1:B:402:GLN:C	2.62	0.42
1:A:47:SER:OG	1:A:470:ILE:HG23	2.18	0.42
1:A:137:PRO:C	1:A:139:VAL:N	2.78	0.42
1:B:136:ASP:C	1:B:138:GLY:H	2.28	0.42
1:B:146:PRO:HA	1:B:149:VAL:HG13	2.00	0.42
1:B:201:ASP:O	1:B:205:ASP:CG	2.63	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:385:ASP:C	1:B:386:PHE:O	2.63	0.42
1:B:433:PHE:HD1	1:B:433:PHE:N	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: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:HA	1:B:353:ARG:HD2	1.87	0.42
2:B:501:FAD:O2A	2:B:501:FAD:O5'	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:26:GLY:C	1:A:27:LEU:CD2	2.93	0.42
1:A:80:GLU:HB3	1:A:82:TRP:CD1	2.54	0.42
1:A:97:ILE:O	1:A:98:VAL:C	2.62	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:A:409:GLN:O	1:A:410:ALA:C	2.63	0.42
1:B:262:ILE:CG1	1:B:274:THR:HG22	2.49	0.42
1:A:7:LEU:O	1:A:7:LEU:CD1	2.68	0.41
1:A:152:SER:H	1:A:155:GLN:HE21	1.65	0.41
1:A:224:ASP:C	1:A:226:ILE:N	2.77	0.41
1:A:403:LEU:O	1:A:404:PRO:C	2.61	0.41
1:A:443:GLU:C	1:A:445:LEU:N	2.78	0.41
1:B:5:ASN:OD1	1:B:5:ASN:C	2.63	0.41
1:B:442:SER:O	1:B:443:GLU:C	2.63	0.41
1:B:445:LEU:HD22	1:B:458:TYR:CE2	2.55	0.41
1:B:474:PRO:C	1:B:476:GLY:N	2.76	0.41
1:A:10:CYS:C	1:A:12:ARG:H	2.28	0.41
1:A:85:ASN:ND2	1:A:240:MET:H	2.14	0.41
1:A:188:TYR:O	1:A:189:LEU:C	2.58	0.41
1:A:220:SER:O	1:A:221:LEU:C	2.63	0.41
1:B:34:LYS:H	1:B:57:HIS:HD1	1.68	0.41
1:B:296:SER:HB3	1:B:321:TYR:CE1	2.54	0.41
1:B:379:ASN:O	1:B:380:TYR:C	2.63	0.41
1:B:417:ILE:HD12	1:B:417:ILE:HA	1.60	0.41
1:B:420:TRP:C	1:B:422:LEU:N	2.78	0.41
1:B:437:GLN:NE2	1:B:441:PHE:HD2	2.18	0.41
2:B:501:FAD:H2'	2:B:501:FAD:H9	2.01	0.41
1:A:106:GLY:O	1:A:107:LEU:HD23	2.21	0.41
1:B:27:LEU:O	1:B:28:SER:CB	2.38	0.41
1:B:90:ARG:HG3	1:B:233:PHE:HB3	2.01	0.41
1:B:336:TRP:O	1:B:341:ILE:HB	2.20	0.41
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:OE1	1:A:219:GLU:HA	2.19	0.41
1:A:356:TYR:HB2	1:A:370:ILE:HB	2.02	0.41
1:A:409:GLN:HE21	1:A:409:GLN:HB2	1.64	0.41
1:B:43:MET:CE	1:B:43:MET:CA	2.81	0.41
1:B:327:ILE:HA	1:B:417:ILE:HD12	2.02	0.41
1:B:479:VAL:O	1:B:482:ALA:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:LYS:HG3	1:A:94:LYS:HZ3	1.70	0.41
1:A:154:GLY:HA2	1:A:207:LEU:HD21	2.02	0.41
1:A:203:ILE:O	1:A:207:LEU:HB2	2.20	0.41
1:A:431:THR:C	1:A:432:THR:HG1	2.28	0.41
1:B:475:GLU:CG	1:B:476:GLY:H	2.30	0.41
1:A:129:ARG:HH22	1:A:339:ASP:CG	2.26	0.41
1:B:48:ALA:CB	1:B:475:GLU:CG	2.97	0.41
1:B:114:GLN:O	1:B:114:GLN:CG	2.69	0.41
1:A:85:ASN:HD22	1:A:85:ASN:HA	1.71	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:B:87:GLY:O	2:B:501:FAD:O4	2.39	0.41
1:B:160:SER:C	1:B:162:GLN:H	2.29	0.41
1:A:17:GLU:C	1:A:19:PHE:N	2.79	0.41
1:A:64:ALA:HA	1:A:259:ALA:H	1.86	0.41
1:A:90:ARG:HA	1:A:234:ASP:O	2.21	0.41
1:A:309:PRO:CB	1:A:310:PRO:HD2	2.50	0.41
1:A:378:ALA:O	1:A:379:ASN:C	2.63	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:B:193:GLY:O	1:B:194:ASN:C	2.61	0.41
1:B:305:GLU:HA	1:B:306:PRO:C	2.46	0.41
1:A:71:GLN:HG3	2:A:501:FAD:PA	2.60	0.41
1:A:88:PRO:HA	2:A:501:FAD:N5	2.36	0.41
1:A:168:LEU:HD23	1:A:168:LEU:O	2.14	0.41
1:A:379:ASN:C	1:A:381:PHE:N	2.65	0.41
1:A:470:ILE:O	1:A:471:LYS:C	2.63	0.41
1:B:196:SER:O	1:B:199:ALA:HB3	2.21	0.41
1:B:208:ASN:C	1:B:208:ASN:ND2	2.79	0.41
1:B:245:THR:C	1:B:249:GLN:HG3	2.38	0.41
1:B:406:GLU:H	1:B:406:GLU:HG2	1.67	0.41
1:A:66:GLU:O	1:A:67:ARG:HB2	2.21	0.41
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:86:LEU:HD21	1:B:416:MET:HE3	2.03	0.40
1:B:334:LYS:H	1:B:334:LYS:HG3	1.58	0.40
1:B:348:THR:C	1:B:350:LEU:H	2.29	0.40
1:A:16:TYR:O	1:A:17:GLU:C	2.64	0.40
1:A:75:TYR:CD2	1:A:75:TYR:C	2.99	0.40
1:A:105:PHE:N	1:A:105:PHE:HD2	2.19	0.40
1:A:137:PRO:C	1:A:139:VAL:H	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:TYR:HD1	1:A:213:TYR:HA	1.72	0.40
1:A:334:LYS:O	1:A:335:PHE:C	2.64	0.40
1:A:433:PHE:N	1:A:433:PHE:CD1	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:5:ASN:N	1:A:6:PRO:CD	2.84	0.40
1:A:350:LEU:N	1:A:350:LEU:HD22	2.33	0.40
1:A:465:TRP:HA	2:A:501:FAD:N1	2.37	0.40
1:B:114:GLN:O	1:B:115:GLU:CB	2.67	0.40
1:B:123:ILE:HG13	1:B:349:ASP:HB3	2.04	0.40
1:A:167:GLU:CD	1:A:167:GLU:N	2.78	0.40
1:A:222:LYS:HE3	1:A:461:GLN:O	2.22	0.40
1:A:391:ASP:O	1:A:392:ILE:C	2.65	0.40
1:B:10:CYS:C	1:B:12:ARG:H	2.29	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:HE	1:B:322:ARG:HB2	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: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
1:B:111:GLU:OE1	1:B:232:ARG:CD	2.68	0.40
1:B:207:LEU:O	1:B:208:ASN:C	2.64	0.40
1:B:240:MET:C	1:B:242:LYS:H	2.29	0.40
1:B:264:ILE:CG2	1:B:452:ILE:HD13	2.52	0.40
1:B:408:ILE:HA	1:B:411:ILE:CD1	2.52	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%)	0	3
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
1	B	353	ARG
1	B	386	PHE
1	B	481	ARG
1	A	6	PRO
1	A	7	LEU
1	A	17	GLU

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Mol	Chain	Res	Type
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
1	B	364	ASN
1	B	396	ASP
1	A	34	LYS
1	A	49	ALA
1	A	169	ARG
1	A	472	SER

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Mol	Chain	Res	Type
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%)	306 (76%)	97 (24%)	1	3
1	B	412/427 (96%)	324 (79%)	88 (21%)	1	5
All	All	815/854 (95%)	630 (77%)	185 (23%)	1	4

All (185) 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	22	ILE
1	A	27	LEU

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Mol	Chain	Res	Type
1	A	35	ARG
1	A	38	ILE
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	79	LYS
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	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	156	LEU
1	A	161	LEU
1	A	168	LEU
1	A	169	ARG
1	A	176	MET
1	A	177	LEU
1	A	182	THR
1	A	184	SER
1	A	187	GLU
1	A	194	ASN
1	A	210	ASP
1	A	246	SER
1	A	252	GLN
1	A	253	GLU
1	A	260	ARG
1	A	265	GLN
1	A	267	ASP
1	A	268	VAL

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Mol	Chain	Res	Type
1	A	269	LYS
1	A	271	VAL
1	A	277	THR
1	A	279	GLU
1	A	280	LYS
1	A	285	VAL
1	A	290	VAL
1	A	292	VAL
1	A	293	CYS
1	A	302	ILE
1	A	305	GLU
1	A	312	LYS
1	A	318	SER
1	A	319	VAL
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	355	ILE
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	411	ILE
1	A	412	CYS
1	A	413	ARG
1	A	415	SER
1	A	416	MET
1	A	418	GLN
1	A	422	LEU

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Mol	Chain	Res	Type
1	A	437	GLN
1	A	441	PHE
1	A	443	GLU
1	A	445	LEU
1	A	449	VAL
1	A	458	TYR
1	A	471	LYS
1	A	479	VAL
1	B	3	ASP
1	B	4	ARG
1	B	9	GLU
1	B	14	THR
1	B	24	LYS
1	B	28	SER
1	B	32	ASN
1	B	35	ARG
1	B	43	MET
1	B	44	SER
1	B	51	VAL
1	B	52	LEU
1	B	59	VAL
1	B	60	THR
1	B	61	VAL
1	B	66	GLU
1	B	79	LYS
1	B	90	ARG
1	B	91	LEU
1	B	95	HIS
1	B	98	VAL
1	B	102	ILE
1	B	107	LEU
1	B	108	GLN
1	B	115	GLU
1	B	123	ILE
1	B	129	ARG
1	B	144	VAL
1	B	156	LEU
1	B	167	GLU
1	B	168	LEU
1	B	174	SER
1	B	177	LEU
1	B	179	LYS

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Mol	Chain	Res	Type
1	B	182	THR
1	B	196	SER
1	B	207	LEU
1	B	213	TYR
1	B	218	ILE
1	B	221	LEU
1	B	224	ASP
1	B	225	ASP
1	B	226	ILE
1	B	246	SER
1	B	248	TYR
1	B	251	ILE
1	B	253	GLU
1	B	260	ARG
1	B	273	VAL
1	B	274	THR
1	B	279	GLU
1	B	280	LYS
1	B	282	THR
1	B	283	LEU
1	B	284	SER
1	B	285	VAL
1	B	286	THR
1	B	303	LYS
1	B	305	GLU
1	B	322	ARG
1	B	323	SER
1	B	328	PHE
1	B	329	LEU
1	B	330	THR
1	B	332	THR
1	B	337	GLU
1	B	347	THR
1	B	348	THR
1	B	350	LEU
1	B	355	ILE
1	B	366	VAL
1	B	369	ILE
1	B	386	PHE
1	B	387	GLU
1	B	391	ASP
1	B	395	ASN

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Mol	Chain	Res	Type
1	B	402	GLN
1	B	403	LEU
1	B	405	LYS
1	B	411	ILE
1	B	417	ILE
1	B	427	MET
1	B	437	GLN
1	B	461	GLN
1	B	463	HIS
1	B	468	SER
1	B	472	SER
1	B	480	ASN

Sometimes 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	114	GLN
1	A	155	GLN
1	A	208	ASN
1	A	258	ASN
1	A	265	GLN
1	A	276	GLN
1	A	342	HIS
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	266	GLN
1	B	276	GLN
1	B	359	ASN

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Mol	Chain	Res	Type
1	B	360	HIS
1	B	364	ASN
1	B	402	GLN
1	B	409	GLN
1	B	418	GLN
1	B	437	GLN
1	B	440	HIS
1	B	480	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	-	58,58,58	1.27	7 (12%)	85,89,89	2.18	28 (32%)
2	FAD	B	501	-	58,58,58	1.13	6 (10%)	85,89,89	1.71	17 (20%)

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	-	-	17/34/50/50	0/6/6/6
2	FAD	B	501	-	-	14/34/50/50	0/6/6/6

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	FAD	PA-O3P	3.98	1.63	1.59
2	A	501	FAD	C4X-N5	3.51	1.38	1.30
2	B	501	FAD	C10-N1	2.98	1.39	1.33
2	A	501	FAD	C8A-N7A	2.67	1.36	1.31
2	B	501	FAD	C4X-N5	2.59	1.36	1.30
2	B	501	FAD	C2A-N3A	2.54	1.38	1.33
2	B	501	FAD	P-O3P	2.54	1.62	1.59
2	A	501	FAD	P-O3P	2.46	1.62	1.59
2	A	501	FAD	C1'-C2'	2.31	1.55	1.52
2	A	501	FAD	C6-C5X	-2.14	1.36	1.40
2	A	501	FAD	C10-N1	2.10	1.37	1.33
2	B	501	FAD	O4B-C4B	-2.09	1.40	1.45
2	B	501	FAD	C2A-N1A	2.08	1.37	1.33

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	FAD	N3A-C2A-N1A	-6.48	118.78	128.58
2	B	501	FAD	N3A-C2A-N1A	-5.76	119.87	128.58
2	A	501	FAD	C4B-O4B-C1B	-5.56	97.18	109.47
2	A	501	FAD	N9A-C8A-N7A	-5.48	106.16	113.94
2	B	501	FAD	C5A-C4A-N3A	-4.48	120.55	126.72
2	B	501	FAD	C4-N3-C2	-4.08	118.39	125.64
2	A	501	FAD	O4B-C1B-N9A	4.07	115.91	108.09
2	A	501	FAD	O2P-P-O3P	4.05	118.23	107.27
2	B	501	FAD	N9A-C8A-N7A	-3.95	108.33	113.94
2	A	501	FAD	C5A-N7A-C8A	3.84	109.48	103.45
2	B	501	FAD	C2A-N3A-C4A	3.77	121.03	111.83
2	A	501	FAD	C4X-C10-N10	3.73	121.83	116.48
2	A	501	FAD	C4A-N9A-C8A	3.71	109.63	105.74
2	A	501	FAD	C2A-N3A-C4A	3.65	120.74	111.83
2	A	501	FAD	C5A-C4A-N3A	-3.50	121.90	126.72
2	A	501	FAD	C4-N3-C2	-3.36	119.68	125.64
2	B	501	FAD	C4X-C4-N3	3.33	121.72	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	FAD	C5A-N7A-C8A	3.28	108.61	103.45
2	B	501	FAD	O5B-C5B-C4B	-3.25	97.94	108.99
2	A	501	FAD	C5A-C6A-N6A	-3.23	115.28	123.29
2	A	501	FAD	C2B-C1B-N9A	-3.22	105.30	113.30
2	B	501	FAD	O4-C4-C4X	-3.19	118.11	126.53
2	B	501	FAD	N3A-C4A-N9A	3.17	132.55	127.17
2	A	501	FAD	C4A-N9A-C1B	-3.11	119.36	126.63
2	A	501	FAD	N6A-C6A-N1A	-3.10	111.48	118.38
2	A	501	FAD	C9-C9A-N10	-3.03	117.78	121.85
2	A	501	FAD	C4A-C5A-N7A	-2.92	107.25	110.58
2	A	501	FAD	C2B-C3B-C4B	-2.90	97.00	102.61
2	B	501	FAD	O3'-C3'-C4'	-2.89	102.36	108.93
2	A	501	FAD	O2A-PA-O3P	2.76	114.72	107.27
2	A	501	FAD	C4X-C4-N3	2.69	120.09	113.25
2	A	501	FAD	C5X-C9A-N10	2.64	120.36	117.97
2	B	501	FAD	O4B-C4B-C3B	2.60	110.31	105.15
2	B	501	FAD	O4B-C1B-N9A	2.56	113.01	108.09
2	A	501	FAD	C7M-C7-C6	-2.54	115.10	119.57
2	B	501	FAD	C4X-C10-N1	-2.51	118.44	124.59
2	A	501	FAD	C10-C4X-N5	-2.49	119.72	124.81
2	B	501	FAD	C4X-C10-N10	2.36	119.86	116.48
2	A	501	FAD	O2-C2-N1	-2.29	118.00	121.80
2	A	501	FAD	O4-C4-C4X	-2.19	120.75	126.53
2	A	501	FAD	O4B-C4B-C5B	2.16	116.25	109.33
2	B	501	FAD	C4A-N9A-C8A	2.14	107.98	105.74
2	A	501	FAD	O4'-C4'-C5'	-2.13	105.29	109.99
2	B	501	FAD	C4A-C5A-N7A	-2.10	108.18	110.58
2	A	501	FAD	N3A-C4A-N9A	2.02	130.61	127.17

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	FAD	C5B-O5B-PA-O2A
2	A	501	FAD	C5B-O5B-PA-O3P
2	A	501	FAD	C2B-C1B-N9A-C4A
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'

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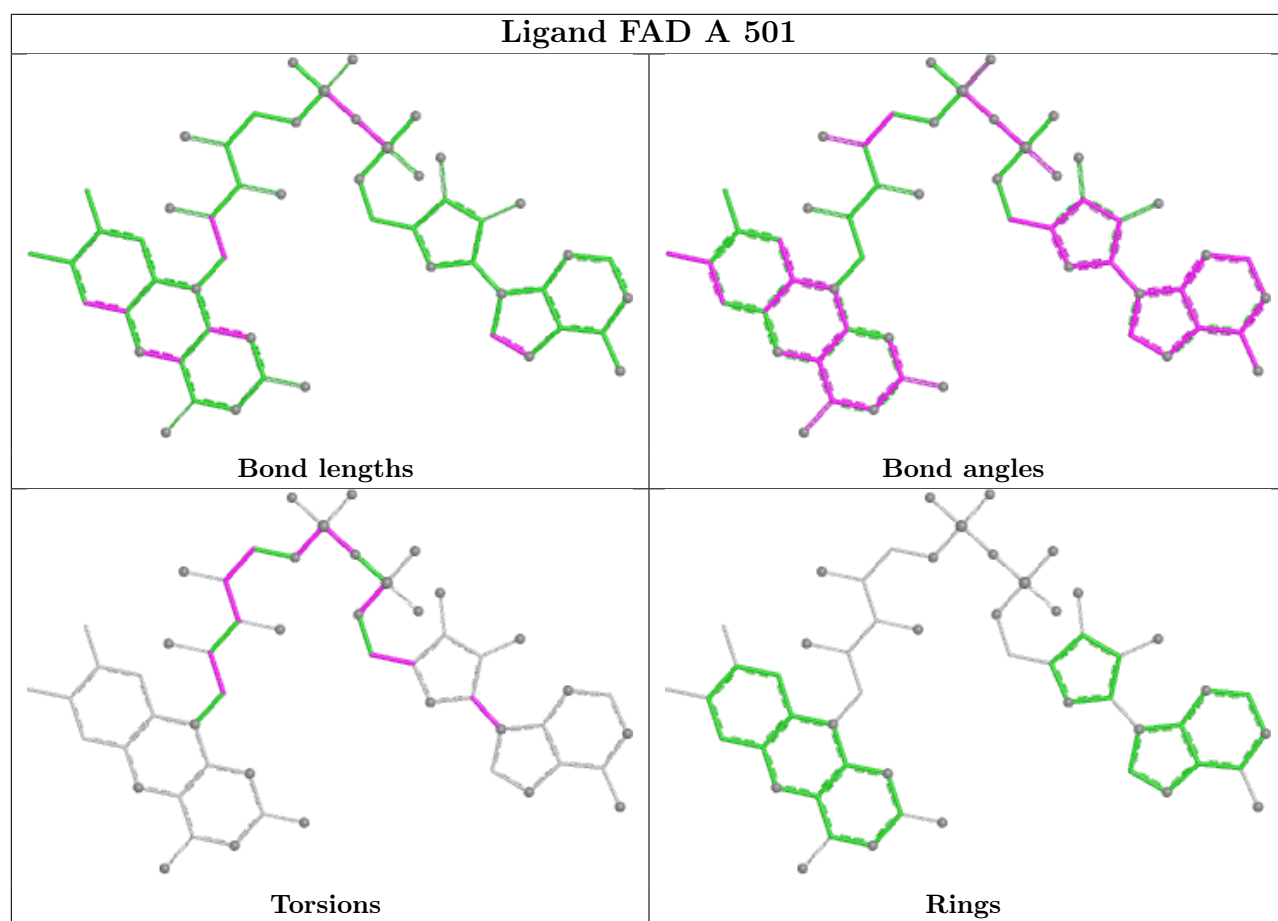
Mol	Chain	Res	Type	Atoms
2	A	501	FAD	O4'-C4'-C5'-O5'
2	A	501	FAD	C5'-O5'-P-O1P
2	A	501	FAD	C5'-O5'-P-O2P
2	A	501	FAD	C5'-O5'-P-O3P
2	B	501	FAD	C2'-C3'-C4'-O4'
2	B	501	FAD	C2'-C3'-C4'-C5'
2	B	501	FAD	O3'-C3'-C4'-O4'
2	B	501	FAD	O3'-C3'-C4'-C5'
2	B	501	FAD	C5'-O5'-P-O1P
2	B	501	FAD	C5'-O5'-P-O2P
2	B	501	FAD	C5'-O5'-P-O3P
2	A	501	FAD	C2B-C1B-N9A-C8A
2	B	501	FAD	O4B-C4B-C5B-O5B
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	A	501	FAD	C3B-C4B-C5B-O5B
2	B	501	FAD	O2'-C2'-C3'-O3'
2	A	501	FAD	C3'-C4'-C5'-O5'
2	B	501	FAD	P-O3P-PA-O1A
2	B	501	FAD	P-O3P-PA-O2A
2	B	501	FAD	PA-O3P-P-O2P

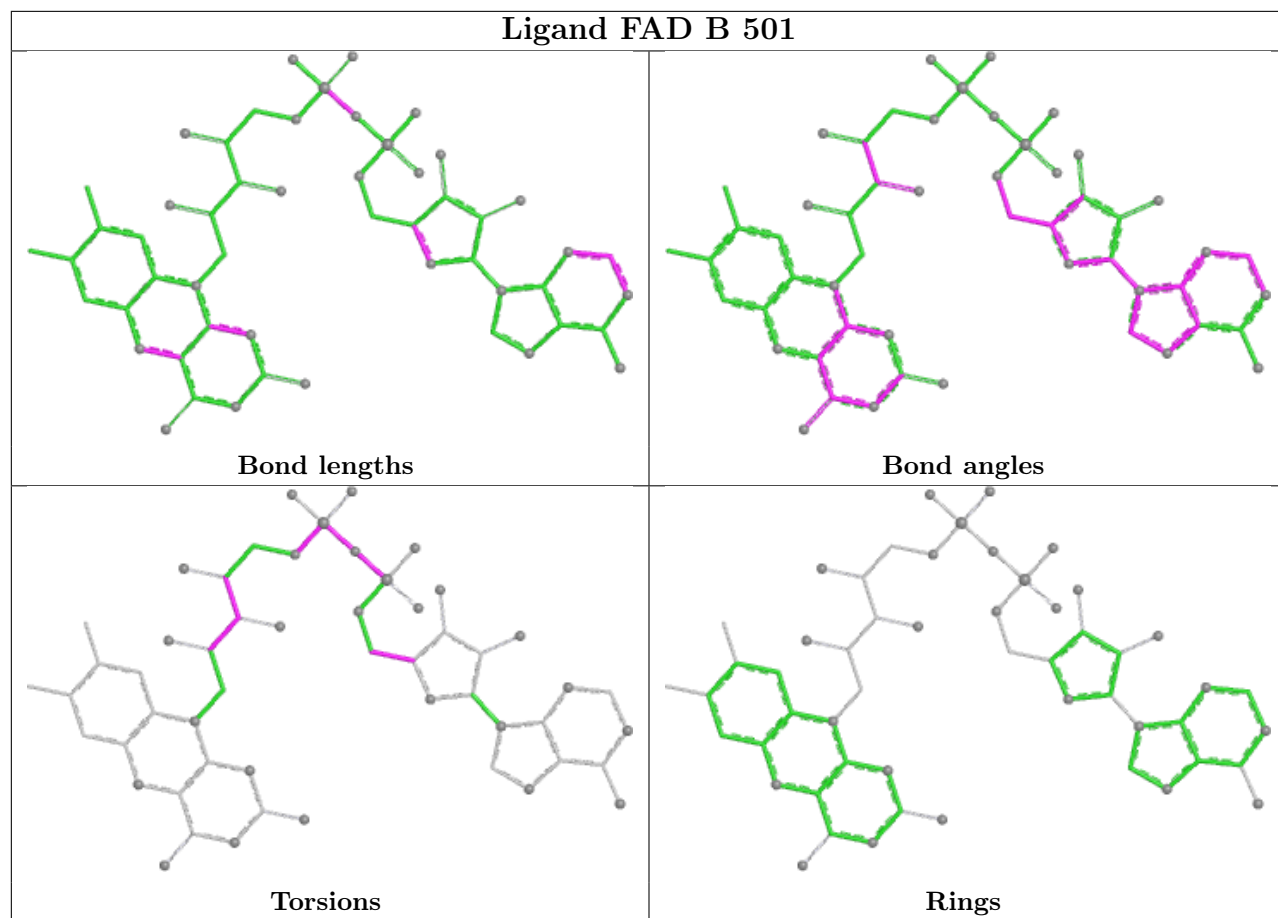
There are no ring outliers.

2 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	FAD	28	0
2	B	501	FAD	17	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%)	-0.35	7 (1%)	72 52	15, 29, 44, 53	11 (2%)
1	B	480/497 (96%)	-0.31	9 (1%)	66 45	14, 30, 46, 63	16 (3%)
All	All	954/994 (95%)	-0.33	16 (1%)	69 48	14, 30, 45, 63	27 (2%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	436	TYR	4.0
1	A	333	LYS	3.8
1	A	113	SER	3.5
1	A	12	ARG	3.4
1	B	12	ARG	3.3
1	B	13	GLU	3.0
1	B	91	LEU	3.0
1	A	163	LYS	3.0
1	A	7	LEU	2.8
1	B	478	ASP	2.7
1	A	162	GLN	2.7
1	B	481	ARG	2.6
1	B	11	PHE	2.6
1	B	386	PHE	2.4
1	A	475	GLU	2.4
1	B	108	GLN	2.1

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](#)

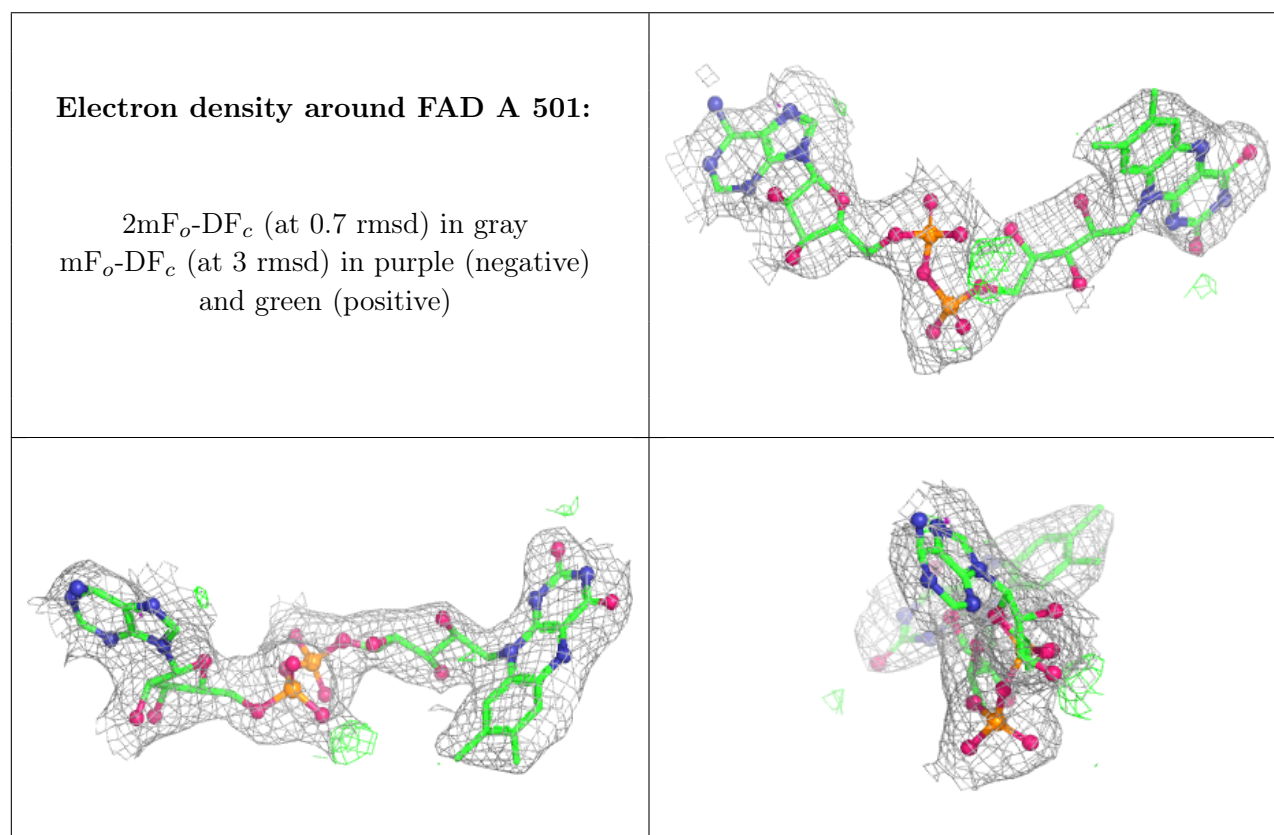
There are no oligosaccharides in this entry.

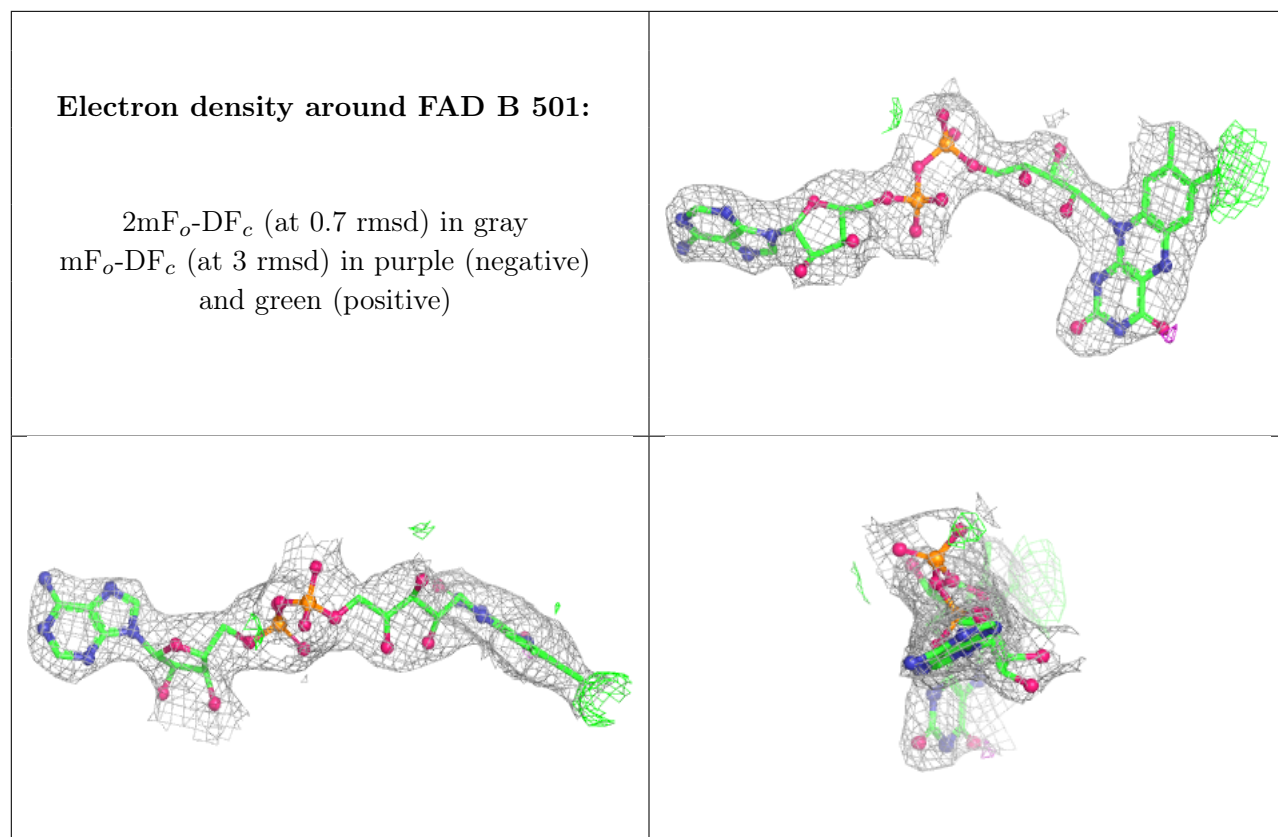
6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
2	FAD	A	501	53/53	0.95	0.08	8,19,39,40	0
2	FAD	B	501	53/53	0.95	0.08	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.