



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 01:35 pm GMT

PDB ID : 1GOS
Title : HUMAN MONOAMINE OXIDASE B
Authors : Binda, C.; Newton-Vinson, P.; Hubalek, F.; Edmondson, D.E.; Mattevi, A.
Deposited on : 2001-10-26
Resolution : 3.00 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

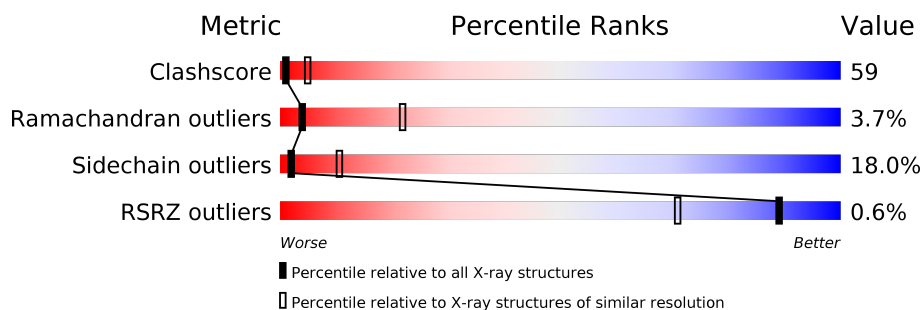
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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. 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	520	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 25%, orange 25%, yellow 55%, green 14%, grey 14%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 25% 55% 14% • • </div> </div>
1	B	520	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 31%, yellow 49%, orange 13%, red 5%, grey 3%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 31% 49% 13% • 5% </div> </div>

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
3	NYP	A	601	X	-	X	X
3	NYP	B	601	X	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8020 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 MONOAMINE OXIDASE.

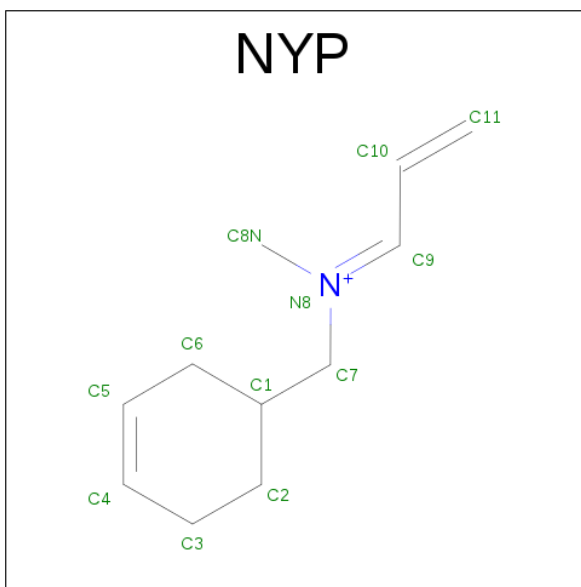
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	0	0	0
			3958	2531	678	725	24			
1	B	493	Total	C	N	O	S	0	0	0
			3932	2515	674	719	24			

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



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

- Molecule 3 is N-[(E)-METHYL](PHENYL)-N-[(E)-2-PROPENYLIDENE]METHANAMINIUM (three-letter code: NYP) (formula: $C_{11}H_{18}N$).

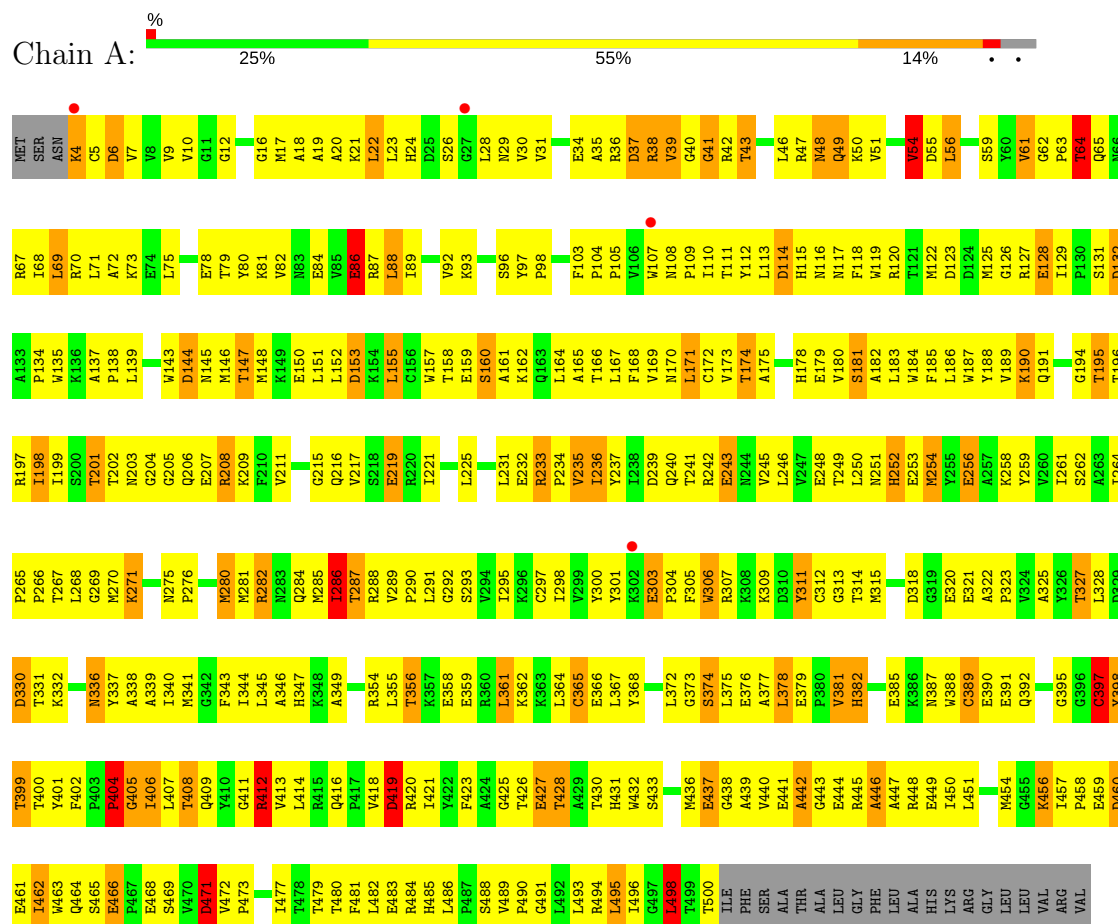


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			12	11	1		
3	B	1	Total	C	N	0	0
			12	11	1		

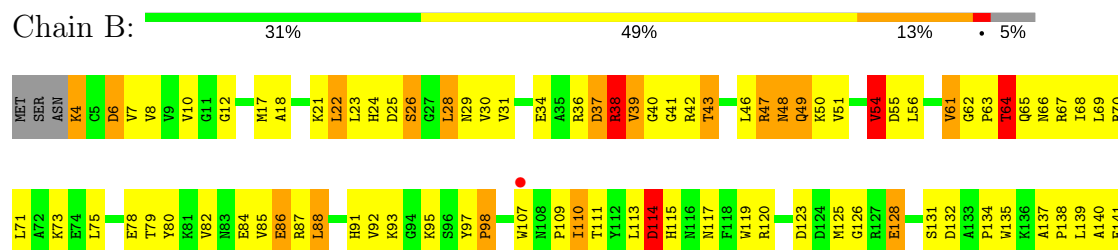
3 Residue-property plots

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: MONOAMINE OXIDASE



• Molecule 1: MONOAMINE OXIDASE



T479	E142	R208	L345	R415	G156	L158	L496	GLY	H178	G194	T195	G405	P473	T477
T480	W143	K209	A346	Q416	Q215	W157	T496	LEU	E179	G194	T195	P467	T478	
F481	D144	F210	H347	P417	Q216	E159	H431	THR	W180	T196	R197	E468		
L482	N145	V211	K348	V418	Q217	S160	W432	THR	S181	I198	I199	S469		
E483	T146	Q212	A349	D419	E218	A161	S433	THR	A182	S200	S201	V470		
R484	T147	G212	R350	R420	R220	K162	G434	ALA	L183	T202	T203	D471		
H485	M148		K351	I421	I221			ALA	W184	N203	G204	V472		
L486	K149			Y422	I222			THR	F185	G205		P473		
P487	E150		R354	F423	D223			LEU	L186			E467		
S488	L151		L355	A424	D227			THR	W187			S469		
V489	L152		T356	G425				THR	Y188			V470		
P490			K357	T426				ALA	W189			D471		
G491			E358	E427				ALA	K190			V472		
			R359	T428				ALA	Q191			E466		
			L361	A429				ALA				P467		
			L364	T430				ALA				E467		
			G365	H431				LEU				E468		
			E366	W432				THR				S469		
			L367	S433				THR				V470		
			E368	G434				THR				D471		
			Y368					THR				V472		
			A369					ALA				P473		
			K370					ALA				E477		
			V371					ALA				T478		
			L372					ALA						
			G373					LEU						
			S374					LEU						
			L375					LEU						
			E376					LEU						
			A377					ALA						
			L378					ALA						
								HIS						
								LYS						
								ARG						
								GLY						
								LEU						
								LEU						
								VAL						
								ARG						
								VAL						
								VAL						

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	138.80Å 224.30Å 87.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.00 14.90 – 3.08	Depositor EDS
% Data completeness (in resolution range)	95.3 (40.00-3.00) 94.5 (14.90-3.08)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 3.06Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.229 , 0.271 0.228 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	64.2	Xtriage
Anisotropy	0.746	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	8020	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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: NYP, 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	0.71	0/4055	1.17	20/5504 (0.4%)
1	B	0.79	1/4029 (0.0%)	1.21	27/5468 (0.5%)
All	All	0.75	1/8084 (0.0%)	1.19	47/10972 (0.4%)

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	1	2
1	B	0	2
All	All	1	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	306	TRP	CB-CG	-5.13	1.41	1.50

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	123	ASP	CB-CG-OD2	10.68	127.92	118.30
1	B	310	ASP	CB-CG-OD2	8.16	125.64	118.30
1	A	54	VAL	CB-CA-C	-7.89	96.41	111.40
1	A	419	ASP	CB-CG-OD2	7.88	125.39	118.30
1	A	471	ASP	CB-CG-OD2	7.64	125.18	118.30
1	A	330	ASP	CB-CG-OD2	7.32	124.89	118.30
1	B	471	ASP	CB-CG-OD2	7.22	124.80	118.30
1	B	144	ASP	CB-CG-OD2	7.02	124.61	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	ASP	CB-CG-OD2	6.93	124.54	118.30
1	B	375	LEU	CA-CB-CG	-6.79	99.69	115.30
1	B	37	ASP	CB-CG-OD2	6.72	124.35	118.30
1	B	223	ASP	CB-CG-OD2	6.70	124.33	118.30
1	B	471	ASP	CB-CG-OD1	-6.53	112.42	118.30
1	A	132	ASP	CB-CG-OD2	6.53	124.17	118.30
1	A	144	ASP	CB-CG-OD2	6.46	124.12	118.30
1	A	64	THR	N-CA-C	6.35	128.13	111.00
1	B	54	VAL	CB-CA-C	-6.31	99.41	111.40
1	A	397	CYS	N-CA-C	6.14	127.58	111.00
1	A	114	ASP	CB-CG-OD2	6.02	123.72	118.30
1	B	398	TYR	CB-CG-CD2	-6.01	117.39	121.00
1	A	404	PRO	C-N-CA	-5.99	109.71	122.30
1	A	235	VAL	CB-CA-C	-5.95	100.09	111.40
1	B	114	ASP	CB-CG-OD2	5.90	123.61	118.30
1	A	123	ASP	CB-CG-OD2	5.82	123.54	118.30
1	B	173	VAL	CB-CA-C	-5.77	100.44	111.40
1	B	398	TYR	CB-CG-CD1	5.64	124.38	121.00
1	B	227	ASP	CB-CG-OD2	5.63	123.37	118.30
1	B	98	PRO	N-CD-CG	-5.62	94.77	103.20
1	A	56	LEU	CB-CG-CD2	-5.61	101.46	111.00
1	A	406	ILE	N-CA-C	5.58	126.06	111.00
1	B	330	ASP	CB-CG-OD2	5.56	123.31	118.30
1	B	28	LEU	CA-CB-CG	-5.56	102.51	115.30
1	B	329	ASP	CB-CG-OD2	5.56	123.30	118.30
1	B	55	ASP	CB-CG-OD2	5.44	123.20	118.30
1	B	397	CYS	N-CA-C	5.34	125.43	111.00
1	A	286	ILE	CB-CA-C	-5.29	101.03	111.60
1	A	460	ASP	CB-CG-OD2	5.27	123.04	118.30
1	B	295	ILE	CB-CA-C	-5.25	101.10	111.60
1	B	407	LEU	CA-CB-CG	-5.23	103.27	115.30
1	B	38	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	B	25	ASP	CB-CG-OD2	5.18	122.96	118.30
1	B	37	ASP	CB-CG-OD1	-5.16	113.66	118.30
1	A	498	LEU	CA-CB-CG	5.11	127.06	115.30
1	B	254	MET	CG-SD-CE	5.11	108.38	100.20
1	A	153	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	311	TYR	CB-CA-C	-5.07	100.26	110.40
1	B	64	THR	N-CA-C	5.03	124.59	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	64	THR	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	397	CYS	Peptide
1	A	405	GLY	Peptide
1	B	397	CYS	Peptide
1	B	405	GLY	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3958	0	3959	533	0
1	B	3932	0	3931	435	0
2	A	53	0	29	7	0
2	B	53	0	29	3	0
3	A	12	0	16	12	0
3	B	12	0	16	8	0
All	All	8020	0	7980	945	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 59.

All (945) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:THR:CG2	1:B:208:ARG:HD3	1.66	1.25
1:A:79:THR:CG2	1:A:208:ARG:HD3	1.70	1.20
1:B:175:ALA:HB1	1:B:179:GLU:OE1	1.40	1.19
1:A:82:VAL:HG23	1:A:207:GLU:O	1.43	1.19
1:A:22:LEU:O	1:A:22:LEU:HD12	1.37	1.18
1:A:65:GLN:HB3	1:A:437:GLU:HG3	1.24	1.15
1:B:22:LEU:O	1:B:22:LEU:HD12	1.42	1.15
1:B:82:VAL:HG23	1:B:207:GLU:O	1.45	1.15
1:B:480:THR:HB	1:B:483:GLU:HB2	1.30	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:VAL:HG12	1:B:174:THR:N	1.57	1.12
1:B:88:LEU:N	1:B:88:LEU:HD23	1.49	1.12
1:A:304:PRO:HB2	1:A:307:ARG:HD2	1.28	1.12
1:A:51:VAL:HG11	1:A:54:VAL:HG22	1.32	1.12
1:B:64:THR:HG22	1:B:432:TRP:HE1	1.03	1.10
1:A:480:THR:HB	1:A:483:GLU:HB2	1.33	1.10
1:A:79:THR:HG21	1:A:208:ARG:HD3	1.31	1.09
1:A:236:ILE:HD11	1:A:250:LEU:HD12	1.32	1.09
1:B:79:THR:HG21	1:B:208:ARG:HD3	1.29	1.08
1:A:171:LEU:HD13	3:A:601:NYP:H3	1.35	1.08
1:B:125:MET:HE2	1:B:186:LEU:HD11	1.10	1.06
1:A:175:ALA:HB1	1:A:179:GLU:OE1	1.56	1.05
1:A:236:ILE:HD13	1:B:236:ILE:HD13	1.33	1.05
1:A:88:LEU:N	1:A:88:LEU:HD23	1.67	1.04
1:B:323:PRO:HD2	1:B:367:LEU:HD22	1.40	1.04
1:B:264:ILE:CG2	1:B:268:LEU:HB2	1.89	1.03
1:A:456:LYS:O	1:A:457:ILE:HG13	1.56	1.02
1:B:125:MET:HE2	1:B:186:LEU:CD1	1.87	1.02
1:A:304:PRO:HB2	1:A:307:ARG:CD	1.90	1.00
1:B:236:ILE:HD11	1:B:250:LEU:HD12	1.40	1.00
1:A:174:THR:CG2	1:A:293:SER:H	1.75	0.99
1:A:233:ARG:NH1	1:A:253:GLU:OE2	1.96	0.99
1:A:327:THR:O	1:A:328:LEU:HD23	1.63	0.99
1:B:249:THR:HG22	1:B:251:ASN:H	1.22	0.99
1:B:65:GLN:HB3	1:B:437:GLU:HG3	1.41	0.98
1:A:64:THR:HG22	1:A:432:TRP:HE1	1.25	0.98
1:B:249:THR:CG2	1:B:251:ASN:HB2	1.92	0.98
1:A:117:ASN:ND2	1:A:488:SER:HB3	1.80	0.97
1:B:10:VAL:HG22	1:B:235:VAL:HG21	1.45	0.96
1:A:174:THR:CG2	1:A:174:THR:O	2.13	0.96
1:A:67:ARG:N	1:A:437:GLU:OE2	1.98	0.96
1:B:173:VAL:CG1	1:B:174:THR:N	2.29	0.96
1:B:264:ILE:HG23	1:B:268:LEU:HB2	1.45	0.96
1:B:456:LYS:O	1:B:457:ILE:HG13	1.65	0.95
1:B:22:LEU:HD12	1:B:22:LEU:C	1.79	0.95
1:A:117:ASN:HD22	1:A:488:SER:HB3	1.29	0.95
1:B:79:THR:HG21	1:B:208:ARG:CD	1.97	0.95
1:A:264:ILE:HG23	1:A:268:LEU:HB2	1.48	0.94
1:A:201:THR:HG22	1:A:202:THR:N	1.80	0.94
1:A:87:ARG:C	1:A:88:LEU:HD23	1.88	0.93
1:B:264:ILE:HG22	1:B:265:PRO:O	1.67	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:GLU:O	1:B:420:ARG:NH1	2.01	0.93
1:A:270:MET:HG2	1:A:286:ILE:CG2	1.98	0.92
1:B:125:MET:CE	1:B:186:LEU:HD11	1.99	0.92
1:B:64:THR:HG22	1:B:432:TRP:NE1	1.85	0.92
1:B:171:LEU:HD13	3:B:601:NYP:H3	1.50	0.92
1:B:79:THR:CG2	1:B:208:ARG:CD	2.49	0.91
1:A:174:THR:CG2	1:A:293:SER:N	2.34	0.91
1:B:67:ARG:N	1:B:437:GLU:OE2	2.03	0.91
1:A:125:MET:CE	1:A:186:LEU:HD11	2.01	0.91
1:B:304:PRO:HB2	1:B:307:ARG:HD2	1.52	0.91
1:A:22:LEU:C	1:A:22:LEU:HD12	1.81	0.91
1:A:258:LYS:O	1:A:259:TYR:CG	2.23	0.91
1:B:88:LEU:N	1:B:88:LEU:CD2	2.27	0.90
1:A:125:MET:HE2	1:A:186:LEU:HD11	1.50	0.90
1:B:173:VAL:HG12	1:B:174:THR:H	1.32	0.90
1:B:448:ARG:NH1	1:B:464:GLN:HB2	1.87	0.90
1:B:171:LEU:O	1:B:171:LEU:HD22	1.72	0.89
1:A:71:LEU:O	1:A:75:LEU:HD12	1.71	0.89
1:A:448:ARG:NH1	1:A:464:GLN:HB2	1.88	0.89
1:B:49:GLN:HG3	1:B:50:LYS:N	1.87	0.88
1:B:174:THR:CG2	1:B:293:SER:H	1.87	0.88
1:B:51:VAL:HG11	1:B:54:VAL:HG22	1.53	0.88
1:B:249:THR:HG22	1:B:251:ASN:HB2	1.52	0.87
1:A:65:GLN:CB	1:A:437:GLU:HG3	2.04	0.87
1:B:70:ARG:NH2	1:B:444:GLU:OE2	2.07	0.87
1:A:323:PRO:HD2	1:A:367:LEU:HD22	1.56	0.87
1:A:315:MET:H	1:A:327:THR:HG22	1.40	0.87
1:A:174:THR:HG21	1:A:293:SER:N	1.90	0.87
1:B:201:THR:HG22	1:B:202:THR:N	1.87	0.87
1:A:171:LEU:HD13	3:A:601:NYP:C3	2.04	0.87
1:A:171:LEU:CD1	3:A:601:NYP:H3	2.04	0.86
1:A:249:THR:HG22	1:A:251:ASN:H	1.40	0.86
1:A:49:GLN:HG3	1:A:50:LYS:N	1.89	0.86
1:A:286:ILE:HG22	1:A:286:ILE:O	1.74	0.86
1:B:71:LEU:O	1:B:75:LEU:HD12	1.76	0.85
1:B:87:ARG:C	1:B:88:LEU:HD23	1.96	0.85
1:A:79:THR:HG21	1:A:208:ARG:CD	2.06	0.85
1:A:79:THR:HG23	1:A:208:ARG:HD3	1.57	0.85
1:B:216:GLN:HA	1:B:219:GLU:HG3	1.56	0.85
1:A:191:GLN:HE22	1:A:433:SER:N	1.75	0.85
1:B:270:MET:HG2	1:B:286:ILE:CG2	2.07	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:LYS:O	1:B:259:TYR:CG	2.30	0.84
1:B:471:ASP:OD1	1:B:471:ASP:N	2.01	0.84
1:A:174:THR:O	1:A:174:THR:HG22	1.78	0.84
1:B:268:LEU:O	1:B:271:LYS:HB2	1.78	0.84
1:B:79:THR:HG23	1:B:208:ARG:HD3	1.60	0.84
1:A:471:ASP:N	1:A:471:ASP:OD1	2.06	0.83
1:A:268:LEU:O	1:A:271:LYS:HB2	1.79	0.83
1:B:425:GLY:O	1:B:428:THR:HB	1.79	0.83
1:B:408:THR:HG22	1:B:409:GLN:HG2	1.61	0.82
1:A:147:THR:HG22	1:A:150:GLU:H	1.45	0.82
1:A:304:PRO:CB	1:A:307:ARG:HD2	2.10	0.82
1:B:270:MET:HG2	1:B:286:ILE:HG22	1.62	0.82
1:A:480:THR:O	1:A:481:PHE:C	2.16	0.82
1:A:488:SER:HB2	1:A:490:PRO:HD2	1.61	0.82
1:A:327:THR:C	1:A:328:LEU:HD23	2.00	0.82
1:A:243:GLU:O	1:A:420:ARG:NH1	2.13	0.81
1:B:240:GLN:OE1	1:B:419:ASP:HB3	1.79	0.81
1:B:315:MET:CE	1:B:327:THR:HG21	2.09	0.81
1:B:144:ASP:OD2	1:B:408:THR:HB	1.80	0.81
1:A:41:GLY:C	1:A:43:THR:H	1.85	0.80
1:A:88:LEU:CD2	1:A:88:LEU:N	2.45	0.80
1:B:174:THR:O	1:B:174:THR:CG2	2.29	0.80
1:B:173:VAL:CG1	1:B:174:THR:H	1.92	0.79
1:A:264:ILE:CG2	1:A:268:LEU:HB2	2.12	0.79
1:B:327:THR:O	1:B:328:LEU:HD23	1.82	0.79
1:B:289:VAL:O	1:B:289:VAL:HG23	1.79	0.79
1:A:64:THR:HG22	1:A:432:TRP:NE1	1.98	0.79
1:B:65:GLN:CB	1:B:437:GLU:HG3	2.12	0.79
1:A:41:GLY:N	1:A:43:THR:HG22	1.98	0.78
1:A:448:ARG:HD2	1:A:461:GLU:O	1.83	0.78
1:A:258:LYS:O	1:A:259:TYR:CD1	2.36	0.78
1:B:86:GLU:N	1:B:86:GLU:OE2	2.16	0.78
1:A:251:ASN:O	1:A:252:HIS:HB2	1.83	0.78
1:A:79:THR:CG2	1:A:208:ARG:CD	2.60	0.78
1:A:129:ILE:O	1:A:190:LYS:HE2	1.83	0.77
1:B:249:THR:HG21	1:B:251:ASN:HB2	1.66	0.77
1:B:251:ASN:O	1:B:252:HIS:HB2	1.84	0.77
1:A:173:VAL:HG12	1:A:174:THR:H	1.48	0.77
1:A:174:THR:HG22	1:A:293:SER:H	1.48	0.77
1:A:209:LYS:NZ	1:A:330:ASP:OD1	2.17	0.77
1:A:30:VAL:CG1	1:A:31:VAL:N	2.47	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:LEU:CD2	1:B:171:LEU:O	2.33	0.76
1:B:47:ARG:NH2	1:B:219:GLU:OE1	2.17	0.76
1:A:265:PRO:HD2	1:A:268:LEU:HD12	1.68	0.76
1:B:174:THR:O	1:B:174:THR:HG23	1.84	0.76
1:B:125:MET:CE	1:B:186:LEU:CD1	2.62	0.76
1:A:79:THR:HG21	1:A:208:ARG:HH11	1.50	0.76
1:A:64:THR:CG2	1:A:432:TRP:HE1	1.98	0.76
1:B:92:VAL:HG22	1:B:318:ASP:CB	2.15	0.76
1:A:86:GLU:N	1:A:86:GLU:OE2	2.18	0.75
1:A:65:GLN:HB3	1:A:437:GLU:CG	2.13	0.75
1:B:174:THR:CG2	1:B:293:SER:N	2.49	0.75
1:B:171:LEU:CD1	3:B:601:NYP:H3	2.15	0.75
1:A:10:VAL:HG22	1:A:235:VAL:HG21	1.69	0.75
1:B:117:ASN:ND2	1:B:488:SER:HB3	2.01	0.74
1:B:174:THR:HG21	1:B:293:SER:N	2.02	0.74
1:A:236:ILE:CD1	1:A:250:LEU:HD12	2.13	0.74
1:B:174:THR:HG22	1:B:293:SER:H	1.51	0.74
1:B:171:LEU:HD13	3:B:601:NYP:C3	2.17	0.74
1:B:315:MET:H	1:B:327:THR:HG22	1.52	0.74
1:A:293:SER:HB3	1:A:389:CYS:SG	2.28	0.74
1:A:288:ARG:NH2	1:B:291:LEU:O	2.20	0.74
1:A:286:ILE:O	1:A:286:ILE:CG2	2.36	0.74
1:B:253:GLU:OE1	1:B:255:TYR:OH	2.02	0.74
1:B:117:ASN:HD22	1:B:488:SER:CB	2.00	0.73
1:B:64:THR:CG2	1:B:432:TRP:HE1	1.93	0.73
1:A:428:THR:HG23	1:A:445:ARG:HH12	1.53	0.73
1:A:120:ARG:NH2	1:A:486:LEU:O	2.22	0.73
1:B:7:VAL:HG22	1:B:259:TYR:HB2	1.69	0.73
1:A:171:LEU:CD1	3:A:601:NYP:H2	2.18	0.73
1:A:173:VAL:HG12	1:A:174:THR:N	2.02	0.72
1:A:356:THR:OG1	1:A:359:GLU:HG3	1.87	0.72
1:A:282:ARG:NH2	1:A:423:PHE:CE2	2.57	0.72
1:B:480:THR:O	1:B:481:PHE:C	2.28	0.72
1:B:54:VAL:CG1	1:B:300:TYR:OH	2.35	0.72
1:A:287:THR:HG23	1:A:287:THR:O	1.88	0.72
1:B:209:LYS:NZ	1:B:330:ASP:OD1	2.22	0.72
1:A:71:LEU:O	1:A:75:LEU:CD1	2.37	0.72
1:B:188:TYR:O	1:B:191:GLN:HG3	1.89	0.72
1:B:22:LEU:CD1	1:B:22:LEU:C	2.56	0.72
1:A:249:THR:CG2	1:A:251:ASN:HB2	2.19	0.71
1:B:78:GLU:O	1:B:211:VAL:HG23	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:THR:HG22	1:A:251:ASN:HB2	1.72	0.71
1:A:264:ILE:HG23	1:A:268:LEU:CB	2.19	0.71
1:A:300:TYR:CD2	1:A:339:ALA:HB2	2.25	0.71
1:A:37:ASP:O	1:A:231:LEU:HD13	1.90	0.71
1:A:285:MET:C	1:A:287:THR:H	1.92	0.71
1:B:111:THR:HG23	1:B:158:THR:HG21	1.72	0.71
1:B:41:GLY:C	1:B:43:THR:H	1.94	0.71
1:A:408:THR:HG22	1:A:409:GLN:HG2	1.71	0.71
1:A:43:THR:O	1:A:43:THR:HG22	1.90	0.71
2:A:600:FAD:O2A	2:A:600:FAD:O5'	2.07	0.70
2:B:600:FAD:O5'	2:B:600:FAD:O2A	2.07	0.70
1:A:240:GLN:OE1	1:A:419:ASP:HB3	1.90	0.70
1:A:43:THR:CG2	1:A:43:THR:O	2.39	0.70
1:A:174:THR:HG23	1:A:174:THR:O	1.92	0.70
1:A:425:GLY:O	1:A:428:THR:HB	1.91	0.70
1:A:428:THR:CG2	1:A:445:ARG:HH12	2.05	0.70
1:A:28:LEU:HD13	1:A:454:MET:HE1	1.73	0.70
1:B:10:VAL:CG2	1:B:235:VAL:HG21	2.22	0.70
1:B:88:LEU:H	1:B:88:LEU:HD23	1.54	0.70
1:A:117:ASN:HD22	1:A:488:SER:CB	2.03	0.70
1:B:239:ASP:OD1	1:B:241:THR:HB	1.92	0.70
1:B:249:THR:HG22	1:B:251:ASN:N	2.02	0.69
1:B:28:LEU:HD13	1:B:454:MET:HE1	1.74	0.69
1:B:117:ASN:HD22	1:B:488:SER:HB3	1.56	0.69
1:A:291:LEU:HD23	1:A:400:THR:HA	1.74	0.69
1:A:314:THR:HA	1:A:327:THR:O	1.92	0.69
1:B:198:ILE:HG22	1:B:199:ILE:HG13	1.73	0.69
1:B:445:ARG:HD2	1:B:463:TRP:CZ2	2.27	0.69
1:A:275:ASN:HA	1:A:276:PRO:C	2.13	0.69
1:B:63:PRO:HG2	1:B:204:GLY:HA2	1.73	0.69
1:B:265:PRO:HD2	1:B:268:LEU:HD12	1.74	0.69
1:B:275:ASN:HA	1:B:276:PRO:C	2.13	0.69
1:B:293:SER:HB3	1:B:389:CYS:SG	2.32	0.69
1:B:12:GLY:HA3	1:B:34:GLU:OE1	1.93	0.68
1:B:315:MET:HE2	1:B:327:THR:HG21	1.74	0.68
1:B:79:THR:HG21	1:B:208:ARG:HH11	1.58	0.68
1:B:387:ASN:O	1:B:390:GLU:HG2	1.93	0.68
1:B:300:TYR:CD2	1:B:339:ALA:HB2	2.29	0.68
1:A:143:TRP:HA	1:A:146:MET:CE	2.24	0.68
1:B:37:ASP:OD1	1:B:37:ASP:N	2.16	0.68
1:A:488:SER:CB	1:A:490:PRO:HD2	2.25	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:THR:HG22	1:A:400:THR:H	1.60	0.67
1:A:22:LEU:C	1:A:22:LEU:CD1	2.59	0.67
1:A:54:VAL:HG13	1:A:300:TYR:OH	1.95	0.67
1:B:240:GLN:NE2	1:B:421:ILE:HG13	2.10	0.67
1:A:280:MET:HG3	1:B:389:CYS:HB3	1.76	0.67
1:A:364:LEU:O	1:A:367:LEU:HB3	1.94	0.67
1:B:236:ILE:HG22	1:B:237:TYR:HB2	1.77	0.67
1:A:34:GLU:OE1	2:A:600:FAD:O3B	2.12	0.67
1:A:451:LEU:HB3	1:A:457:ILE:HD12	1.77	0.67
1:B:320:GLU:OE2	1:B:347:HIS:CE1	2.46	0.67
1:B:431:HIS:O	1:B:432:TRP:C	2.29	0.67
1:A:82:VAL:CG2	1:A:207:GLU:O	2.33	0.67
1:A:119:TRP:CE3	1:A:195:THR:HG21	2.29	0.67
1:A:37:ASP:OD1	1:A:37:ASP:N	2.28	0.67
1:B:92:VAL:HG22	1:B:318:ASP:HB2	1.77	0.67
1:A:315:MET:CE	1:A:327:THR:HG21	2.24	0.67
1:B:428:THR:CG2	1:B:445:ARG:HH12	2.06	0.67
1:A:448:ARG:NH1	1:A:462:ILE:O	2.28	0.66
1:B:220:ARG:HA	1:B:223:ASP:OD2	1.95	0.66
1:A:86:GLU:HG2	1:A:312:CYS:HB3	1.77	0.66
1:A:431:HIS:CD2	1:A:432:TRP:CD1	2.84	0.66
1:B:54:VAL:HG13	1:B:300:TYR:OH	1.95	0.66
1:B:456:LYS:O	1:B:457:ILE:CG1	2.40	0.66
1:A:445:ARG:HD2	1:A:463:TRP:CZ2	2.31	0.66
1:B:315:MET:HE3	1:B:327:THR:HG21	1.76	0.66
1:B:291:LEU:HD23	1:B:400:THR:HA	1.77	0.66
1:A:51:VAL:HG11	1:A:54:VAL:CG2	2.19	0.66
1:A:24:HIS:C	1:A:26:SER:H	1.99	0.65
1:A:264:ILE:HG22	1:A:265:PRO:O	1.96	0.65
1:B:264:ILE:HG23	1:B:268:LEU:CB	2.23	0.65
1:A:304:PRO:CB	1:A:307:ARG:CD	2.71	0.65
1:A:343:PHE:HB3	1:A:345:LEU:HD21	1.78	0.65
1:A:275:ASN:OD1	1:A:276:PRO:HA	1.97	0.65
1:A:51:VAL:CG1	1:A:54:VAL:HG22	2.19	0.65
1:A:399:THR:CG2	1:A:400:THR:H	2.08	0.65
1:A:270:MET:HG2	1:A:286:ILE:HG22	1.78	0.65
1:B:30:VAL:CG1	1:B:31:VAL:N	2.59	0.65
1:A:4:LYS:HB2	1:A:256:GLU:HG3	1.78	0.65
1:B:286:ILE:HG22	1:B:286:ILE:O	1.96	0.65
1:B:43:THR:HG22	1:B:43:THR:O	1.97	0.65
1:B:428:THR:HG23	1:B:445:ARG:HH12	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:ILE:HG22	1:A:237:TYR:HB2	1.79	0.65
1:A:174:THR:HG22	1:A:292:GLY:CA	2.27	0.65
1:A:168:PHE:CG	1:A:168:PHE:O	2.50	0.64
1:A:191:GLN:HE22	1:A:433:SER:CA	2.09	0.64
1:A:491:GLY:O	1:A:494:ARG:HG2	1.96	0.64
1:B:134:PRO:HG2	1:B:407:LEU:HD21	1.78	0.64
1:B:65:GLN:HB3	1:B:437:GLU:CG	2.22	0.64
1:A:47:ARG:NH2	1:A:219:GLU:OE1	2.28	0.64
1:B:264:ILE:CG2	1:B:268:LEU:CB	2.73	0.64
1:B:304:PRO:CB	1:B:307:ARG:HD2	2.27	0.64
1:A:456:LYS:O	1:A:457:ILE:CG1	2.39	0.64
1:B:387:ASN:OD1	1:B:389:CYS:HB2	1.97	0.64
1:B:448:ARG:NH1	1:B:462:ILE:O	2.30	0.64
1:A:216:GLN:HA	1:A:219:GLU:HG3	1.80	0.64
1:A:174:THR:CG2	1:A:292:GLY:HA3	2.28	0.64
1:A:144:ASP:OD2	1:A:408:THR:HB	1.96	0.64
1:B:323:PRO:HD2	1:B:367:LEU:CD2	2.25	0.64
1:B:233:ARG:NH1	1:B:253:GLU:OE2	2.30	0.64
1:A:287:THR:HG22	1:A:288:ARG:HG3	1.79	0.64
1:A:236:ILE:HG22	1:A:237:TYR:CB	2.28	0.64
1:A:86:GLU:HB2	1:A:312:CYS:N	2.13	0.64
1:A:456:LYS:C	1:A:457:ILE:HG13	2.18	0.64
1:A:248:GLU:OE2	1:B:252:HIS:NE2	2.30	0.64
1:A:28:LEU:CD1	1:A:454:MET:CE	2.76	0.63
1:A:267:THR:HG22	1:B:270:MET:CE	2.29	0.63
1:A:426:THR:C	1:A:428:THR:H	2.01	0.63
1:B:406:ILE:O	1:B:407:LEU:C	2.35	0.63
1:A:89:ILE:CG2	1:A:96:SER:HB3	2.29	0.63
1:A:125:MET:CE	1:A:186:LEU:CD1	2.76	0.63
1:A:315:MET:N	1:A:327:THR:HG22	2.12	0.63
1:A:381:VAL:O	1:A:381:VAL:HG13	1.99	0.63
1:B:216:GLN:CA	1:B:219:GLU:HG3	2.27	0.63
1:A:171:LEU:HD13	3:A:601:NYP:C2	2.29	0.63
1:B:448:ARG:HD2	1:B:461:GLU:O	1.98	0.63
1:A:109:PRO:C	1:A:111:THR:H	2.02	0.63
1:B:147:THR:HG22	1:B:150:GLU:H	1.64	0.63
1:A:446:ALA:O	1:A:449:GLU:HB2	1.99	0.62
1:B:36:ARG:NH1	1:B:391:GLU:OE1	2.32	0.62
1:A:270:MET:HG2	1:A:286:ILE:HG21	1.81	0.62
1:A:12:GLY:HA3	1:A:34:GLU:OE1	1.99	0.62
1:A:236:ILE:CD1	1:B:236:ILE:HD13	2.20	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:VAL:HG23	1:A:289:VAL:O	1.99	0.62
1:A:30:VAL:HG12	1:A:31:VAL:N	2.14	0.62
1:A:41:GLY:H	1:A:43:THR:HG22	1.63	0.62
1:A:258:LYS:O	1:A:259:TYR:CD2	2.52	0.62
1:A:171:LEU:HD13	3:A:601:NYP:H2	1.82	0.62
1:A:489:VAL:N	1:A:490:PRO:CD	2.62	0.62
1:B:191:GLN:HE22	1:B:433:SER:N	1.96	0.62
1:B:428:THR:O	1:B:428:THR:HG23	2.00	0.62
1:B:41:GLY:C	1:B:43:THR:N	2.51	0.62
1:B:249:THR:HG22	1:B:251:ASN:CB	2.28	0.62
1:A:126:GLY:C	1:A:128:GLU:H	2.02	0.62
1:A:240:GLN:NE2	1:A:418:VAL:O	2.23	0.62
1:A:252:HIS:CE1	1:B:248:GLU:OE2	2.52	0.61
1:A:285:MET:C	1:A:287:THR:N	2.53	0.61
1:B:92:VAL:HG22	1:B:318:ASP:HB3	1.82	0.61
1:B:343:PHE:HB3	1:B:345:LEU:HD21	1.82	0.61
1:A:178:HIS:CE1	1:B:145:ASN:OD1	2.53	0.61
1:A:287:THR:HG23	1:B:290:PRO:HB3	1.83	0.61
1:B:400:THR:OG1	1:B:427:GLU:OE1	2.10	0.61
1:A:233:ARG:NH1	1:A:253:GLU:CD	2.53	0.61
1:B:182:ALA:O	1:B:183:LEU:C	2.38	0.61
1:B:320:GLU:OE2	1:B:347:HIS:NE2	2.33	0.61
1:A:46:LEU:HB3	1:A:54:VAL:HG23	1.82	0.61
1:B:337:TYR:O	1:B:338:ALA:C	2.35	0.61
1:A:191:GLN:NE2	1:A:433:SER:N	2.48	0.61
1:B:54:VAL:HG11	1:B:300:TYR:OH	2.00	0.61
1:B:34:GLU:OE1	2:B:600:FAD:O3B	2.19	0.61
1:A:151:LEU:O	1:A:155:LEU:HB2	2.01	0.60
1:B:70:ARG:HH22	1:B:444:GLU:CD	2.04	0.60
1:A:168:PHE:CE1	1:A:199:ILE:HD11	2.36	0.60
1:A:28:LEU:HD11	1:A:454:MET:CE	2.32	0.60
1:A:55:ASP:OD2	1:A:59:SER:OG	2.18	0.60
1:B:258:LYS:O	1:B:259:TYR:CD2	2.54	0.60
1:B:446:ALA:O	1:B:449:GLU:N	2.33	0.60
1:A:41:GLY:C	1:A:43:THR:N	2.51	0.60
1:A:79:THR:HG22	1:A:80:TYR:N	2.15	0.60
1:A:426:THR:HG23	1:A:427:GLU:N	2.16	0.60
1:B:126:GLY:C	1:B:128:GLU:H	2.05	0.60
1:A:236:ILE:O	1:A:236:ILE:CG2	2.48	0.60
1:A:209:LYS:CE	1:A:330:ASP:OD1	2.50	0.59
1:A:173:VAL:CG1	1:A:174:THR:H	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:LEU:HD12	1:A:395:GLY:C	2.23	0.59
1:A:5:CYS:SG	1:A:6:ASP:N	2.75	0.59
1:A:171:LEU:HD11	3:A:601:NYP:H2	1.84	0.59
1:A:75:LEU:N	1:A:75:LEU:HD12	2.17	0.59
1:A:28:LEU:HD11	1:A:454:MET:HE3	1.83	0.59
1:B:426:THR:C	1:B:428:THR:H	2.05	0.59
1:B:71:LEU:O	1:B:75:LEU:CD1	2.49	0.59
1:B:6:ASP:HB2	1:B:29:ASN:HB2	1.83	0.59
1:A:68:ILE:HD12	1:A:436:MET:HB3	1.85	0.59
1:B:313:GLY:O	1:B:327:THR:CG2	2.50	0.59
1:B:63:PRO:HG2	1:B:204:GLY:CA	2.32	0.59
1:A:267:THR:HG22	1:B:270:MET:HE1	1.84	0.59
1:B:67:ARG:NH2	1:B:466:GLU:HG2	2.17	0.59
1:A:378:LEU:HD23	1:A:378:LEU:N	2.16	0.59
1:A:79:THR:CG2	1:A:80:TYR:N	2.66	0.58
1:B:307:ARG:O	1:B:310:ASP:N	2.32	0.58
1:A:28:LEU:CD1	1:A:454:MET:HE1	2.33	0.58
1:B:68:ILE:HG22	1:B:437:GLU:HG2	1.85	0.58
1:B:456:LYS:C	1:B:457:ILE:HG13	2.22	0.58
1:A:172:CYS:SG	3:A:601:NYP:H5	2.44	0.58
1:A:252:HIS:ND1	1:B:252:HIS:CE1	2.72	0.58
1:A:6:ASP:HB2	1:A:29:ASN:O	2.03	0.58
1:A:41:GLY:H	1:A:43:THR:CG2	2.14	0.58
1:B:21:LYS:O	1:B:22:LEU:C	2.39	0.58
1:A:7:VAL:HG22	1:A:259:TYR:HB2	1.84	0.58
1:B:79:THR:HG23	1:B:208:ARG:CD	2.25	0.58
1:B:206:GLN:NE2	3:B:601:NYP:H8N1	2.19	0.58
1:A:30:VAL:HG13	1:A:31:VAL:N	2.18	0.58
1:B:233:ARG:CD	1:B:251:ASN:HD22	2.17	0.58
1:A:30:VAL:O	1:A:31:VAL:HG23	2.04	0.57
1:A:413:VAL:HG12	1:A:413:VAL:O	2.04	0.57
1:B:489:VAL:N	1:B:490:PRO:CD	2.67	0.57
1:A:285:MET:O	1:A:287:THR:N	2.38	0.57
1:B:346:ALA:O	1:B:349:ALA:N	2.36	0.57
1:B:285:MET:C	1:B:287:THR:H	2.08	0.57
1:A:119:TRP:HE3	1:A:195:THR:HG21	1.67	0.57
1:A:482:LEU:O	1:A:486:LEU:HG	2.04	0.57
1:B:291:LEU:HD22	1:B:399:THR:C	2.24	0.57
1:A:134:PRO:HD2	1:A:135:TRP:CE3	2.40	0.57
1:A:215:GLY:O	1:A:219:GLU:HG2	2.04	0.57
1:B:157:TRP:CZ2	1:B:490:PRO:HG3	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:LEU:C	1:B:171:LEU:HD22	2.25	0.57
1:B:85:VAL:HB	1:B:86:GLU:OE2	2.04	0.57
1:A:236:ILE:HD13	1:B:236:ILE:CD1	2.23	0.56
1:A:24:HIS:C	1:A:26:SER:N	2.54	0.56
1:A:315:MET:HE3	1:A:327:THR:HG21	1.86	0.56
1:A:438:GLY:O	1:A:439:ALA:C	2.39	0.56
1:A:126:GLY:O	1:A:190:LYS:HD3	2.06	0.56
1:A:23:LEU:O	1:A:26:SER:HB3	2.05	0.56
1:A:92:VAL:O	1:A:93:LYS:HB2	2.05	0.56
1:B:249:THR:CG2	1:B:251:ASN:CB	2.78	0.56
1:B:285:MET:CE	1:B:414:LEU:HD23	2.35	0.56
1:A:126:GLY:C	1:A:128:GLU:N	2.58	0.56
1:A:10:VAL:CG2	1:A:235:VAL:HG21	2.33	0.56
1:A:291:LEU:HD22	1:A:399:THR:O	2.05	0.56
1:B:290:PRO:O	1:B:400:THR:HA	2.06	0.56
1:A:38:ARG:NH2	1:A:41:GLY:O	2.37	0.56
1:B:48:ASN:OD1	1:B:48:ASN:C	2.44	0.56
1:B:236:ILE:HG22	1:B:237:TYR:CB	2.36	0.56
1:B:287:THR:HG23	1:B:287:THR:O	2.05	0.56
1:B:54:VAL:HG13	1:B:300:TYR:HH	1.70	0.56
1:B:38:ARG:NH2	1:B:41:GLY:O	2.39	0.56
1:B:428:THR:O	1:B:428:THR:CG2	2.52	0.56
1:A:291:LEU:HD22	1:A:399:THR:C	2.26	0.56
1:A:285:MET:HE1	1:A:414:LEU:HD23	1.88	0.56
1:A:40:GLY:CA	1:A:43:THR:HG22	2.36	0.55
1:A:48:ASN:OD1	1:A:48:ASN:C	2.43	0.55
1:B:430:THR:HB	1:B:441:GLU:OE2	2.06	0.55
1:B:24:HIS:C	1:B:26:SER:H	2.09	0.55
1:B:426:THR:HB	1:B:439:ALA:HB2	1.88	0.55
1:A:119:TRP:CE3	1:A:195:THR:CG2	2.88	0.55
1:A:147:THR:HG22	1:A:147:THR:O	2.05	0.55
1:A:80:TYR:CE2	1:A:209:LYS:HB2	2.41	0.55
1:A:481:PHE:O	1:A:485:HIS:HD2	1.89	0.55
1:A:86:GLU:H	1:A:86:GLU:CD	2.08	0.55
1:B:82:VAL:CG2	1:B:207:GLU:O	2.36	0.55
1:B:24:HIS:C	1:B:26:SER:N	2.59	0.55
1:A:290:PRO:HB3	1:B:287:THR:HG23	1.87	0.55
1:B:65:GLN:CA	1:B:437:GLU:HG3	2.37	0.55
1:A:174:THR:CG2	1:A:292:GLY:CA	2.84	0.55
1:B:171:LEU:CD2	1:B:171:LEU:C	2.70	0.55
1:A:252:HIS:CE1	1:B:252:HIS:ND1	2.75	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:GLU:CB	1:B:304:PRO:CD	2.84	0.55
1:A:188:TYR:O	1:A:191:GLN:HG3	2.06	0.55
1:A:309:LYS:NZ	1:A:373:GLY:O	2.40	0.55
1:A:291:LEU:HD12	1:A:395:GLY:CA	2.37	0.55
1:B:126:GLY:C	1:B:128:GLU:N	2.60	0.55
1:A:114:ASP:O	1:A:115:HIS:C	2.43	0.55
1:A:125:MET:HE2	1:A:186:LEU:CD1	2.30	0.55
1:A:239:ASP:OD1	1:A:241:THR:HB	2.07	0.55
1:A:458:PRO:O	1:A:459:GLU:C	2.46	0.55
1:A:78:GLU:O	1:A:211:VAL:HG23	2.07	0.55
1:B:110:ILE:O	1:B:110:ILE:HG22	2.07	0.55
1:B:444:GLU:HB3	1:B:448:ARG:HH21	1.71	0.55
1:A:320:GLU:C	1:A:322:ALA:H	2.10	0.54
1:A:387:ASN:O	1:A:390:GLU:HG2	2.06	0.54
1:B:92:VAL:CG2	1:B:318:ASP:HB2	2.36	0.54
1:B:41:GLY:N	1:B:43:THR:HG22	2.22	0.54
1:A:173:VAL:CG1	1:A:174:THR:N	2.68	0.54
1:A:291:LEU:HD12	1:A:395:GLY:HA3	1.89	0.54
1:A:295:ILE:HG12	1:A:387:ASN:HB2	1.88	0.54
1:A:301:TYR:O	1:A:338:ALA:HB3	2.07	0.54
1:A:303:GLU:CB	1:A:304:PRO:CD	2.85	0.54
1:A:406:ILE:O	1:A:407:LEU:C	2.45	0.54
1:B:171:LEU:CD1	3:B:601:NYP:H2	2.37	0.54
1:B:392:GLN:HG2	1:B:393:TYR:CE1	2.43	0.54
1:A:431:HIS:O	1:A:432:TRP:C	2.45	0.54
1:B:287:THR:HG22	1:B:288:ARG:HG3	1.89	0.54
1:A:171:LEU:HA	1:A:345:LEU:HD13	1.88	0.54
1:B:332:LYS:HB3	1:B:333:PRO:CD	2.36	0.54
1:A:365:CYS:O	1:A:366:GLU:C	2.45	0.54
1:A:430:THR:HB	1:A:441:GLU:OE2	2.06	0.54
1:B:198:ILE:CG2	1:B:199:ILE:N	2.69	0.54
1:A:16:GLY:O	1:A:19:ALA:N	2.40	0.54
1:B:258:LYS:O	1:B:259:TYR:CD1	2.61	0.54
1:B:315:MET:N	1:B:327:THR:HG22	2.22	0.54
1:A:271:LYS:HD3	1:B:270:MET:O	2.07	0.54
1:B:346:ALA:O	1:B:347:HIS:C	2.45	0.54
1:A:480:THR:O	1:A:482:LEU:N	2.41	0.53
1:B:159:GLU:O	1:B:160:SER:C	2.45	0.53
1:B:232:GLU:C	1:B:234:PRO:HD3	2.29	0.53
1:A:92:VAL:HG22	1:A:318:ASP:HB2	1.91	0.53
1:A:315:MET:HE2	1:A:327:THR:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:LEU:HA	1:A:345:LEU:CD1	2.39	0.53
1:B:198:ILE:HG22	1:B:199:ILE:N	2.23	0.53
1:B:120:ARG:NH2	1:B:486:LEU:O	2.38	0.53
1:A:305:PHE:CE1	1:A:306:TRP:HZ3	2.26	0.53
1:A:405:GLY:C	1:A:406:ILE:HG13	2.29	0.53
1:B:285:MET:O	1:B:287:THR:N	2.42	0.53
1:B:304:PRO:HB2	1:B:307:ARG:CD	2.32	0.53
1:B:87:ARG:C	1:B:88:LEU:CD2	2.71	0.53
1:A:269:GLY:C	1:A:271:LYS:H	2.11	0.53
1:B:331:THR:OG1	1:B:338:ALA:HA	2.09	0.53
1:B:388:TRP:O	1:B:389:CYS:C	2.46	0.53
1:A:236:ILE:O	1:A:236:ILE:HG23	2.08	0.53
1:A:269:GLY:C	1:A:271:LYS:N	2.62	0.53
1:A:62:GLY:O	1:A:63:PRO:C	2.47	0.53
1:B:413:VAL:O	1:B:413:VAL:HG12	2.07	0.53
1:A:251:ASN:O	1:A:252:HIS:CB	2.51	0.53
1:A:168:PHE:CD1	1:A:168:PHE:O	2.62	0.52
1:B:365:CYS:O	1:B:368:TYR:N	2.43	0.52
1:B:64:THR:O	1:B:64:THR:HG23	2.08	0.52
1:A:174:THR:HG22	1:A:293:SER:N	2.14	0.52
1:A:167:LEU:HD11	1:A:325:ALA:HB1	1.91	0.52
1:B:40:GLY:CA	1:B:43:THR:HG22	2.39	0.52
1:A:198:ILE:HG22	1:A:199:ILE:HG13	1.90	0.52
1:A:21:LYS:O	1:A:22:LEU:C	2.46	0.52
1:A:297:CYS:C	1:A:298:ILE:HD12	2.30	0.52
1:A:36:ARG:NH1	1:A:391:GLU:OE1	2.43	0.52
1:B:368:TYR:O	1:B:372:LEU:HB2	2.09	0.52
1:B:41:GLY:H	1:B:43:THR:CG2	2.23	0.52
1:B:431:HIS:O	1:B:433:SER:N	2.42	0.52
1:B:51:VAL:HG12	1:B:51:VAL:O	2.10	0.52
1:A:240:GLN:CD	1:A:419:ASP:HB3	2.29	0.52
1:B:49:GLN:CG	1:B:50:LYS:N	2.67	0.52
1:A:426:THR:C	1:A:428:THR:N	2.61	0.52
1:A:64:THR:O	1:A:64:THR:HG23	2.10	0.52
1:A:337:TYR:O	1:A:338:ALA:C	2.47	0.52
1:B:481:PHE:O	1:B:485:HIS:HD2	1.93	0.52
1:B:336:ASN:HB3	1:B:337:TYR:HD1	1.74	0.52
1:A:110:ILE:HG22	1:A:110:ILE:O	2.10	0.52
1:A:275:ASN:OD1	1:A:276:PRO:CA	2.58	0.52
1:A:285:MET:CE	1:A:414:LEU:HA	2.40	0.52
1:A:480:THR:O	1:A:483:GLU:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:THR:O	1:B:207:GLU:OE1	2.27	0.52
1:B:30:VAL:HG12	1:B:31:VAL:N	2.25	0.52
1:A:249:THR:HG21	1:A:251:ASN:HB2	1.92	0.51
1:A:264:ILE:CG2	1:A:268:LEU:CB	2.84	0.51
1:B:458:PRO:O	1:B:459:GLU:C	2.47	0.51
1:A:388:TRP:O	1:A:390:GLU:N	2.43	0.51
1:A:236:ILE:HD11	1:A:250:LEU:CD1	2.23	0.51
1:A:337:TYR:N	1:A:337:TYR:CD1	2.77	0.51
1:B:209:LYS:HZ3	1:B:330:ASP:CG	2.13	0.51
1:B:249:THR:C	1:B:251:ASN:N	2.63	0.51
1:B:40:GLY:HA3	1:B:43:THR:HG22	1.92	0.51
1:B:91:HIS:HA	1:B:95:LYS:O	2.11	0.51
1:B:446:ALA:O	1:B:447:ALA:C	2.47	0.51
1:A:320:GLU:OE2	1:A:347:HIS:CE1	2.64	0.51
1:A:269:GLY:O	1:A:271:LYS:N	2.43	0.51
1:A:285:MET:CE	1:A:414:LEU:HD23	2.41	0.51
1:A:293:SER:CB	1:A:389:CYS:SG	2.98	0.51
1:A:40:GLY:C	1:A:43:THR:HG22	2.31	0.51
1:B:167:LEU:O	1:B:168:PHE:C	2.46	0.51
1:B:51:VAL:CG1	1:B:51:VAL:O	2.59	0.51
1:A:313:GLY:O	1:A:327:THR:CG2	2.59	0.51
1:A:134:PRO:HG2	1:A:407:LEU:HD21	1.92	0.51
1:B:285:MET:CE	1:B:414:LEU:HA	2.41	0.51
1:A:246:LEU:HD23	1:A:256:GLU:HB3	1.91	0.51
1:B:17:MET:O	1:B:18:ALA:C	2.48	0.51
1:B:189:VAL:HG12	1:B:194:GLY:HA2	1.92	0.51
1:A:291:LEU:O	1:B:288:ARG:NH2	2.44	0.51
1:A:54:VAL:CG1	1:A:300:TYR:OH	2.58	0.51
1:B:171:LEU:HD13	3:B:601:NYP:C2	2.41	0.51
1:B:6:ASP:HB2	1:B:29:ASN:O	2.11	0.51
1:A:426:THR:HG23	1:A:427:GLU:HG2	1.92	0.51
1:A:459:GLU:O	1:A:462:ILE:HG13	2.10	0.51
1:B:270:MET:CG	1:B:286:ILE:HG22	2.37	0.51
1:B:309:LYS:NZ	1:B:373:GLY:O	2.44	0.51
1:B:241:THR:HG22	1:B:242:ARG:HG3	1.93	0.50
1:B:285:MET:HE1	1:B:414:LEU:HD23	1.92	0.50
1:A:327:THR:HA	1:A:341:MET:O	2.10	0.50
1:A:389:CYS:HB3	1:B:280:MET:HG3	1.94	0.50
1:B:240:GLN:CD	1:B:419:ASP:HB3	2.32	0.50
1:B:313:GLY:O	1:B:327:THR:HG22	2.11	0.50
1:A:109:PRO:C	1:A:111:THR:N	2.65	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:ARG:NH2	1:B:423:PHE:CE2	2.80	0.50
1:A:111:THR:HG23	1:A:158:THR:HG21	1.93	0.50
1:B:117:ASN:ND2	1:B:488:SER:CB	2.67	0.50
1:B:151:LEU:O	1:B:155:LEU:HB2	2.12	0.50
1:A:365:CYS:O	1:A:368:TYR:N	2.45	0.50
1:B:442:ALA:O	1:B:443:GLY:C	2.50	0.50
1:A:216:GLN:O	1:A:217:VAL:C	2.47	0.50
1:B:168:PHE:CE1	1:B:172:CYS:SG	3.05	0.50
1:A:290:PRO:O	1:A:400:THR:HA	2.11	0.50
1:B:381:VAL:O	1:B:382:HIS:HB2	2.12	0.50
1:A:364:LEU:HB3	1:A:368:TYR:CE1	2.46	0.50
1:A:144:ASP:OD2	1:A:408:THR:CB	2.60	0.50
1:A:6:ASP:OD2	1:A:28:LEU:HD22	2.12	0.50
1:A:88:LEU:O	1:A:98:PRO:HA	2.12	0.50
1:A:134:PRO:HG3	1:A:187:TRP:CD1	2.47	0.49
1:A:266:PRO:O	1:A:267:THR:C	2.51	0.49
1:A:336:ASN:HB3	1:A:337:TYR:HD1	1.77	0.49
1:A:448:ARG:NH1	1:A:464:GLN:CB	2.69	0.49
1:A:446:ALA:O	1:A:447:ALA:C	2.50	0.49
1:A:79:THR:HG23	1:A:208:ARG:CD	2.35	0.49
1:B:282:ARG:O	1:B:285:MET:N	2.45	0.49
1:A:196:THR:O	1:A:197:ARG:C	2.49	0.49
1:A:198:ILE:HG22	1:A:199:ILE:N	2.28	0.49
1:A:291:LEU:HD23	1:A:400:THR:CA	2.43	0.49
1:A:411:GLY:O	1:A:413:VAL:N	2.45	0.49
1:B:167:LEU:HD11	1:B:325:ALA:HB1	1.93	0.49
1:B:327:THR:HA	1:B:341:MET:O	2.12	0.49
1:B:75:LEU:N	1:B:75:LEU:HD12	2.26	0.49
1:A:209:LYS:HZ1	1:A:330:ASP:CG	2.15	0.49
1:B:236:ILE:CD1	1:B:250:LEU:HD12	2.28	0.49
1:A:446:ALA:O	1:A:449:GLU:N	2.43	0.49
1:A:89:ILE:HG23	1:A:96:SER:HB3	1.94	0.49
1:A:306:TRP:CZ3	1:A:340:ILE:HD11	2.48	0.49
1:B:171:LEU:HD13	3:B:601:NYP:H2	1.94	0.49
1:A:148:MET:O	1:A:152:LEU:HG	2.13	0.49
1:A:68:ILE:HG22	1:A:437:GLU:HG2	1.95	0.49
1:B:134:PRO:HD2	1:B:135:TRP:CZ3	2.48	0.49
1:A:204:GLY:O	1:A:205:GLY:C	2.51	0.49
1:A:92:VAL:HG22	1:A:318:ASP:CB	2.43	0.49
1:B:405:GLY:C	1:B:406:ILE:HG13	2.33	0.49
1:B:426:THR:OG1	1:B:434:GLY:N	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ARG:NH2	1:A:466:GLU:HG2	2.28	0.49
1:B:167:LEU:C	1:B:169:VAL:N	2.66	0.49
1:B:280:MET:O	1:B:281:MET:C	2.48	0.49
1:B:337:TYR:N	1:B:337:TYR:CD1	2.80	0.49
1:B:62:GLY:O	1:B:63:PRO:C	2.50	0.49
1:A:443:GLY:O	1:A:446:ALA:HB3	2.13	0.48
1:A:448:ARG:HH12	1:A:464:GLN:HB2	1.76	0.48
1:A:55:ASP:OD2	1:A:59:SER:CB	2.61	0.48
1:B:8:VAL:O	1:B:260:VAL:HA	2.12	0.48
1:B:28:LEU:HD13	1:B:454:MET:CE	2.42	0.48
1:B:392:GLN:HG2	1:B:393:TYR:CD1	2.48	0.48
1:A:346:ALA:O	1:A:347:HIS:C	2.50	0.48
1:A:171:LEU:HD22	1:A:171:LEU:O	2.14	0.48
1:A:426:THR:O	1:A:428:THR:N	2.46	0.48
1:B:215:GLY:O	1:B:219:GLU:HG2	2.13	0.48
1:B:437:GLU:O	1:B:438:GLY:C	2.52	0.48
1:B:79:THR:HG23	1:B:208:ARG:CB	2.44	0.48
1:A:42:ARG:CZ	2:A:600:FAD:H5'1	2.43	0.48
1:A:445:ARG:NE	1:A:449:GLU:OE2	2.45	0.48
1:A:270:MET:CG	1:A:286:ILE:CG2	2.84	0.48
1:A:240:GLN:NE2	1:A:421:ILE:HG13	2.28	0.48
1:B:75:LEU:HD21	1:B:221:ILE:HG12	1.94	0.48
1:A:413:VAL:O	1:A:413:VAL:CG1	2.61	0.48
1:A:438:GLY:O	1:A:440:VAL:N	2.46	0.48
2:A:600:FAD:O2'	2:A:600:FAD:H9	2.13	0.48
1:A:153:ASP:HA	1:A:162:LYS:HE2	1.95	0.48
1:A:97:TYR:N	1:A:97:TYR:CD1	2.82	0.48
1:B:157:TRP:CE2	1:B:490:PRO:HG3	2.49	0.48
1:B:43:THR:CG2	1:B:43:THR:O	2.56	0.48
1:A:215:GLY:O	1:A:216:GLN:C	2.51	0.48
1:A:246:LEU:CD2	1:A:256:GLU:HB3	2.44	0.48
1:A:320:GLU:OE2	1:A:347:HIS:NE2	2.47	0.48
1:A:385:GLU:O	1:A:385:GLU:HG3	2.13	0.48
1:B:138:PRO:O	1:B:139:LEU:HD23	2.13	0.48
1:B:280:MET:HG2	1:B:281:MET:N	2.27	0.48
1:A:42:ARG:NH2	2:A:600:FAD:O3P	2.42	0.48
1:A:6:ASP:CB	1:A:29:ASN:O	2.62	0.48
1:A:362:LYS:O	1:A:366:GLU:HG3	2.12	0.47
1:A:184:TRP:CZ2	1:A:401:TYR:HA	2.49	0.47
1:B:426:THR:C	1:B:428:THR:N	2.63	0.47
1:B:448:ARG:NH1	1:B:464:GLN:CB	2.70	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:448:ARG:HH12	1:B:464:GLN:HB2	1.75	0.47
1:B:4:LYS:HB2	1:B:256:GLU:HG3	1.96	0.47
1:A:258:LYS:C	1:A:259:TYR:CG	2.87	0.47
1:A:300:TYR:CE2	1:A:339:ALA:HB2	2.49	0.47
1:A:65:GLN:CA	1:A:437:GLU:HG3	2.43	0.47
1:A:206:GLN:NE2	3:A:601:NYP:H8N1	2.29	0.47
1:A:250:LEU:HD21	1:B:237:TYR:CE1	2.49	0.47
1:B:6:ASP:O	1:B:257:ALA:HB1	2.14	0.47
1:A:182:ALA:O	1:A:183:LEU:C	2.50	0.47
1:A:267:THR:HG22	1:B:270:MET:HE2	1.96	0.47
1:A:134:PRO:HG3	1:A:187:TRP:NE1	2.30	0.47
1:A:30:VAL:HG13	1:A:31:VAL:H	1.80	0.47
1:B:119:TRP:CE3	1:B:195:THR:HG21	2.50	0.47
1:A:28:LEU:CD1	1:A:454:MET:HE3	2.41	0.47
1:A:70:ARG:HG2	1:A:70:ARG:O	2.07	0.47
1:B:114:ASP:O	1:B:115:HIS:C	2.52	0.47
1:B:184:TRP:CZ2	1:B:401:TYR:HA	2.48	0.47
1:A:135:TRP:CH2	1:A:412:ARG:HA	2.50	0.47
1:A:284:GLN:O	1:A:287:THR:HG22	2.15	0.47
1:A:361:LEU:O	1:A:362:LYS:C	2.53	0.47
1:B:489:VAL:HB	1:B:490:PRO:HD3	1.96	0.47
1:A:137:ALA:O	1:A:138:PRO:C	2.51	0.47
1:A:413:VAL:O	1:A:414:LEU:C	2.54	0.47
1:A:485:HIS:O	1:A:486:LEU:C	2.50	0.47
1:B:270:MET:HG2	1:B:286:ILE:HG21	1.94	0.47
1:B:450:ILE:CG2	1:B:454:MET:HE2	2.45	0.47
1:B:413:VAL:O	1:B:413:VAL:CG1	2.63	0.47
1:A:249:THR:HG22	1:A:251:ASN:CB	2.43	0.47
1:A:355:LEU:HB3	1:A:359:GLU:HB2	1.97	0.47
1:A:444:GLU:HB3	1:A:448:ARG:HH21	1.80	0.47
1:A:495:LEU:HD12	1:A:495:LEU:HA	1.62	0.47
1:A:69:LEU:O	1:A:72:ALA:HB3	2.15	0.47
1:A:270:MET:CG	1:A:286:ILE:HG22	2.46	0.46
1:B:194:GLY:O	1:B:195:THR:C	2.53	0.46
1:B:358:GLU:H	1:B:358:GLU:HG2	1.33	0.46
1:A:171:LEU:CD2	1:A:171:LEU:O	2.63	0.46
1:A:291:LEU:CD2	1:A:399:THR:O	2.64	0.46
1:B:282:ARG:CZ	1:B:423:PHE:CZ	2.99	0.46
1:B:407:LEU:HA	1:B:407:LEU:HD12	1.32	0.46
1:B:446:ALA:O	1:B:449:GLU:HB2	2.15	0.46
1:B:381:VAL:O	1:B:381:VAL:HG13	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:MET:HB2	1:A:280:MET:HE2	1.60	0.46
1:A:298:ILE:N	1:A:298:ILE:HD12	2.30	0.46
1:B:171:LEU:HA	1:B:171:LEU:HD23	1.64	0.46
1:B:171:LEU:HA	1:B:345:LEU:CD1	2.45	0.46
1:B:495:LEU:HD12	1:B:495:LEU:HA	1.62	0.46
1:B:233:ARG:HD2	1:B:251:ASN:HD22	1.80	0.46
1:B:285:MET:C	1:B:287:THR:N	2.68	0.46
1:B:387:ASN:OD1	1:B:387:ASN:C	2.53	0.46
1:A:191:GLN:NE2	1:A:433:SER:HB3	2.31	0.46
1:B:196:THR:O	1:B:197:ARG:C	2.53	0.46
1:B:275:ASN:OD1	1:B:276:PRO:HA	2.16	0.46
1:B:375:LEU:O	1:B:376:GLU:C	2.52	0.46
1:B:113:LEU:HA	1:B:113:LEU:HD23	1.79	0.46
1:B:168:PHE:CD1	1:B:168:PHE:O	2.69	0.46
1:B:97:TYR:CD1	1:B:97:TYR:N	2.84	0.46
1:A:17:MET:O	1:A:18:ALA:C	2.53	0.46
1:A:440:VAL:O	1:A:441:GLU:C	2.53	0.46
1:A:56:LEU:HA	1:A:56:LEU:HD23	1.22	0.46
1:B:184:TRP:O	1:B:187:TRP:HB3	2.16	0.46
1:A:320:GLU:C	1:A:322:ALA:N	2.69	0.46
3:A:601:NYP:H6	3:A:601:NYP:H8N1	1.97	0.46
1:A:61:VAL:O	1:A:61:VAL:HG12	2.14	0.46
1:A:9:VAL:HG22	1:A:261:ILE:HB	1.98	0.46
1:A:320:GLU:O	1:A:322:ALA:N	2.49	0.46
1:A:445:ARG:HD2	1:A:463:TRP:CH2	2.51	0.46
1:B:233:ARG:HD3	1:B:233:ARG:HA	1.66	0.46
1:B:236:ILE:HD11	1:B:250:LEU:CD1	2.28	0.46
1:A:167:LEU:C	1:A:169:VAL:N	2.69	0.45
1:A:451:LEU:CB	1:A:457:ILE:HD12	2.44	0.45
1:A:113:LEU:CD2	1:A:486:LEU:HB3	2.46	0.45
1:B:174:THR:HG22	1:B:293:SER:N	2.20	0.45
1:B:174:THR:HG22	1:B:292:GLY:CA	2.46	0.45
1:A:198:ILE:CG2	1:A:199:ILE:N	2.79	0.45
1:B:275:ASN:CA	1:B:276:PRO:C	2.84	0.45
1:B:480:THR:O	1:B:484:ARG:HG2	2.16	0.45
1:A:104:PRO:HA	1:A:105:PRO:HD3	1.86	0.45
1:A:178:HIS:CG	1:B:145:ASN:HB3	2.51	0.45
1:A:189:VAL:HG12	1:A:194:GLY:HA2	1.99	0.45
1:A:358:GLU:H	1:A:358:GLU:HG2	1.21	0.45
1:A:80:TYR:CG	1:A:80:TYR:O	2.70	0.45
1:B:167:LEU:O	1:B:169:VAL:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:THR:CG2	1:B:292:GLY:HA3	2.46	0.45
1:B:75:LEU:H	1:B:75:LEU:HD12	1.81	0.45
1:A:143:TRP:HA	1:A:146:MET:HE3	1.96	0.45
1:A:23:LEU:O	1:A:26:SER:CB	2.64	0.45
1:A:280:MET:HB3	1:A:280:MET:HE3	1.68	0.45
1:A:343:PHE:HB3	1:A:345:LEU:CD2	2.46	0.45
1:B:375:LEU:HA	1:B:375:LEU:HD23	1.65	0.45
1:B:86:GLU:CD	1:B:86:GLU:H	2.19	0.45
1:A:173:VAL:HG21	1:A:184:TRP:CZ3	2.51	0.45
1:A:188:TYR:O	1:A:189:VAL:C	2.55	0.45
1:A:457:ILE:HA	1:A:458:PRO:HD3	1.81	0.45
1:A:86:GLU:N	1:A:86:GLU:CD	2.66	0.45
1:B:137:ALA:O	1:B:138:PRO:C	2.55	0.45
1:B:30:VAL:HG13	1:B:31:VAL:N	2.31	0.45
1:B:456:LYS:HB3	1:B:456:LYS:HE2	1.85	0.45
1:A:489:VAL:O	1:A:493:LEU:HG	2.16	0.45
1:B:207:GLU:HG2	1:B:208:ARG:HG2	1.98	0.45
1:A:164:LEU:HD12	1:A:164:LEU:O	2.17	0.45
1:A:216:GLN:CA	1:A:219:GLU:HG3	2.46	0.45
1:A:498:LEU:O	1:A:498:LEU:HD12	2.17	0.45
1:B:134:PRO:HD2	1:B:135:TRP:CE3	2.51	0.45
1:B:291:LEU:HD22	1:B:399:THR:O	2.17	0.45
1:B:41:GLY:H	1:B:43:THR:HG22	1.82	0.45
1:A:169:VAL:O	1:A:170:ASN:C	2.54	0.45
1:A:42:ARG:HB3	2:A:600:FAD:C8M	2.47	0.45
1:A:480:THR:CB	1:A:483:GLU:HB2	2.24	0.45
1:B:109:PRO:C	1:B:111:THR:H	2.19	0.45
1:B:168:PHE:CE1	1:B:199:ILE:HD11	2.52	0.45
1:B:79:THR:CG2	1:B:208:ARG:HH11	2.27	0.45
1:B:442:ALA:O	1:B:445:ARG:N	2.50	0.45
1:A:134:PRO:HD2	1:A:135:TRP:CZ3	2.52	0.44
1:B:457:ILE:HG23	1:B:458:PRO:HD2	1.99	0.44
1:B:86:GLU:HG2	1:B:312:CYS:HB3	1.99	0.44
1:A:387:ASN:OD1	1:A:389:CYS:HB2	2.17	0.44
1:A:407:LEU:HA	1:A:407:LEU:HD12	1.63	0.44
1:A:191:GLN:NE2	1:A:433:SER:H	2.14	0.44
1:B:144:ASP:OD2	1:B:408:THR:CB	2.59	0.44
1:B:291:LEU:HD23	1:B:400:THR:CA	2.45	0.44
1:A:159:GLU:O	1:A:160:SER:C	2.55	0.44
1:A:168:PHE:CD1	1:A:199:ILE:HD11	2.52	0.44
1:A:298:ILE:HG21	1:A:300:TYR:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:ILE:CG2	1:A:454:MET:HE2	2.48	0.44
1:B:119:TRP:O	1:B:120:ARG:C	2.54	0.44
1:B:457:ILE:HG23	1:B:461:GLU:HB2	1.99	0.44
1:B:86:GLU:HG2	1:B:312:CYS:CA	2.47	0.44
1:A:280:MET:HG2	1:A:281:MET:N	2.32	0.44
1:B:139:LEU:HA	1:B:139:LEU:HD23	1.42	0.44
1:B:151:LEU:O	1:B:152:LEU:C	2.54	0.44
1:B:202:THR:HG22	1:B:203:ASN:N	2.31	0.44
1:B:445:ARG:CD	1:B:463:TRP:CZ2	2.99	0.44
1:A:191:GLN:NE2	1:A:433:SER:O	2.51	0.44
1:B:216:GLN:O	1:B:217:VAL:C	2.55	0.44
1:B:236:ILE:CG2	1:B:236:ILE:O	2.63	0.44
1:B:79:THR:HG22	1:B:80:TYR:N	2.32	0.44
1:B:119:TRP:CE3	1:B:195:THR:CG2	3.00	0.44
1:A:303:GLU:CB	1:A:304:PRO:HD2	2.48	0.44
1:A:300:TYR:HD2	1:A:339:ALA:HB2	1.79	0.44
1:A:157:TRP:CE2	1:A:490:PRO:HG3	2.52	0.44
1:B:285:MET:HE2	1:B:414:LEU:HD23	2.00	0.44
1:A:239:ASP:OD1	1:A:239:ASP:C	2.56	0.44
1:A:249:THR:CG2	1:A:251:ASN:CB	2.93	0.44
1:A:270:MET:HE1	1:B:267:THR:HG22	2.00	0.44
1:A:282:ARG:CZ	1:A:423:PHE:CZ	3.01	0.44
1:A:285:MET:HE1	1:A:414:LEU:HA	2.00	0.44
1:A:86:GLU:HB2	1:A:311:TYR:C	2.38	0.44
1:A:388:TRP:O	1:A:389:CYS:C	2.55	0.44
1:A:468:GLU:OE2	1:A:473:PRO:HA	2.17	0.44
1:A:54:VAL:HG13	1:A:300:TYR:HH	1.82	0.44
1:A:6:ASP:HB2	1:A:29:ASN:HB2	1.99	0.44
1:A:480:THR:HG22	1:A:482:LEU:H	1.83	0.44
1:A:145:ASN:OD1	1:B:178:HIS:CE1	2.71	0.44
1:B:249:THR:O	1:B:252:HIS:N	2.42	0.44
1:B:378:LEU:HD22	1:B:378:LEU:HA	1.83	0.44
1:A:202:THR:HG22	1:A:203:ASN:N	2.33	0.43
1:A:287:THR:CG2	1:A:288:ARG:HG3	2.46	0.43
1:A:304:PRO:O	1:A:307:ARG:HD2	2.17	0.43
1:A:381:VAL:O	1:A:382:HIS:HB2	2.18	0.43
1:A:445:ARG:CD	1:A:463:TRP:CH2	3.00	0.43
1:B:471:ASP:C	1:B:473:PRO:HD3	2.37	0.43
1:A:75:LEU:HD21	1:A:221:ILE:HG12	1.99	0.43
3:A:601:NYP:H6	3:A:601:NYP:C8N	2.49	0.43
1:B:184:TRP:O	1:B:185:PHE:C	2.55	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:GLN:NE2	1:B:433:SER:HB3	2.32	0.43
1:B:260:VAL:O	1:B:421:ILE:HA	2.18	0.43
1:B:66:ASN:ND2	1:B:468:GLU:HA	2.33	0.43
1:A:139:LEU:HA	1:A:139:LEU:HD23	1.67	0.43
1:A:207:GLU:HG2	1:A:208:ARG:HG2	1.99	0.43
1:A:233:ARG:HA	1:A:233:ARG:HD3	1.77	0.43
1:A:295:ILE:HG22	1:A:297:CYS:SG	2.58	0.43
1:A:146:MET:HB2	1:A:146:MET:HE2	1.85	0.43
1:A:184:TRP:O	1:A:187:TRP:HB3	2.17	0.43
1:A:443:GLY:O	1:A:444:GLU:C	2.55	0.43
1:A:471:ASP:C	1:A:473:PRO:HD3	2.39	0.43
1:A:79:THR:CG2	1:A:208:ARG:HH11	2.24	0.43
1:A:23:LEU:HA	1:A:23:LEU:HD23	1.84	0.43
1:A:23:LEU:O	1:A:26:SER:N	2.49	0.43
1:A:35:ALA:HB1	1:A:234:PRO:HG3	2.00	0.43
1:A:362:LYS:HG2	1:A:366:GLU:OE2	2.19	0.43
1:A:42:ARG:HA	1:A:388:TRP:CZ3	2.54	0.43
1:B:241:THR:HG22	1:B:242:ARG:N	2.32	0.43
1:A:161:ALA:O	1:A:162:LYS:C	2.56	0.43
1:A:171:LEU:CD1	3:A:601:NYP:C2	2.90	0.43
1:A:264:ILE:HG21	1:A:268:LEU:C	2.39	0.43
1:A:372:LEU:HD23	1:A:372:LEU:HA	1.59	0.43
1:A:70:ARG:NH2	1:A:444:GLU:OE2	2.51	0.43
1:B:79:THR:CG2	1:B:80:TYR:N	2.81	0.43
1:B:344:ILE:HG22	1:B:349:ALA:HA	2.01	0.43
1:B:79:THR:HG23	1:B:208:ARG:HB3	1.99	0.43
1:A:438:GLY:O	1:A:441:GLU:N	2.52	0.43
1:A:157:TRP:CZ2	1:A:490:PRO:HG3	2.54	0.43
1:A:49:GLN:CG	1:A:50:LYS:N	2.74	0.43
1:B:61:VAL:HG12	1:B:61:VAL:O	2.17	0.43
1:B:86:GLU:N	1:B:86:GLU:CD	2.69	0.43
1:A:331:THR:OG1	1:A:338:ALA:HA	2.19	0.43
1:B:258:LYS:C	1:B:259:TYR:CG	2.90	0.43
1:A:267:THR:O	1:A:267:THR:HG22	2.18	0.42
1:A:332:LYS:HD3	1:A:332:LYS:HA	1.78	0.42
1:A:442:ALA:O	1:A:443:GLY:C	2.56	0.42
1:B:430:THR:HG22	1:B:430:THR:O	2.19	0.42
1:B:480:THR:HG22	1:B:482:LEU:H	1.83	0.42
1:A:346:ALA:O	1:A:349:ALA:N	2.52	0.42
1:A:480:THR:O	1:A:484:ARG:HG2	2.19	0.42
1:A:117:ASN:O	1:A:118:PHE:C	2.56	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:VAL:CG1	1:A:236:ILE:N	2.78	0.42
1:A:374:SER:O	1:A:375:LEU:C	2.56	0.42
1:A:377:ALA:C	1:A:379:GLU:H	2.23	0.42
1:A:459:GLU:O	1:A:460:ASP:C	2.57	0.42
1:A:252:HIS:HE1	1:B:248:GLU:OE2	2.00	0.42
1:B:236:ILE:HD12	1:B:250:LEU:HA	2.01	0.42
1:B:28:LEU:CD1	1:B:454:MET:CE	2.98	0.42
1:B:38:ARG:HH11	1:B:38:ARG:HD3	1.65	0.42
1:B:171:LEU:HD11	3:B:601:NYP:H2	2.02	0.42
1:A:264:ILE:O	1:A:265:PRO:C	2.57	0.42
1:A:270:MET:CE	1:B:267:THR:HG22	2.49	0.42
1:B:286:ILE:CG2	1:B:286:ILE:O	2.65	0.42
1:B:445:ARG:HD3	1:B:463:TRP:CH2	2.54	0.42
1:B:56:LEU:HD23	1:B:56:LEU:HA	1.47	0.42
1:B:314:THR:HA	1:B:327:THR:O	2.20	0.42
1:B:317:ILE:HD13	1:B:371:VAL:HG21	2.01	0.42
1:B:23:LEU:O	1:B:26:SER:CB	2.68	0.42
1:B:427:GLU:H	1:B:427:GLU:HG2	1.10	0.42
1:B:46:LEU:HB3	1:B:54:VAL:HG23	2.02	0.42
1:B:51:VAL:HG22	1:B:300:TYR:CE1	2.55	0.42
1:A:457:ILE:HG23	1:A:461:GLU:HB2	2.02	0.42
1:A:70:ARG:HH22	1:A:444:GLU:CD	2.22	0.42
1:B:236:ILE:HG21	1:B:236:ILE:HD13	1.65	0.42
1:B:286:ILE:HG21	1:B:286:ILE:HD13	1.50	0.42
1:A:55:ASP:OD2	1:A:59:SER:HB2	2.20	0.42
1:B:139:LEU:O	1:B:140:ALA:C	2.58	0.42
1:B:219:GLU:H	1:B:219:GLU:HG2	1.56	0.42
1:B:332:LYS:HB3	1:B:333:PRO:HD2	2.02	0.42
1:B:426:THR:O	1:B:428:THR:N	2.53	0.42
1:B:88:LEU:O	1:B:98:PRO:HA	2.20	0.42
1:A:143:TRP:O	1:A:182:ALA:HB3	2.19	0.42
1:A:79:THR:HG23	1:A:208:ARG:CB	2.49	0.42
1:A:313:GLY:O	1:A:327:THR:HG23	2.20	0.42
1:B:457:ILE:HA	1:B:458:PRO:HD3	1.83	0.42
1:A:115:HIS:O	1:A:116:ASN:C	2.57	0.41
1:A:171:LEU:CD2	1:A:171:LEU:C	2.88	0.41
1:A:411:GLY:C	1:A:413:VAL:H	2.24	0.41
1:B:119:TRP:HE3	1:B:195:THR:HG21	1.86	0.41
1:B:341:MET:HE2	1:B:341:MET:HB3	1.83	0.41
1:A:181:SER:O	1:A:182:ALA:C	2.57	0.41
1:A:445:ARG:HH11	1:A:445:ARG:HD3	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ASN:CA	1:A:276:PRO:C	2.87	0.41
1:A:67:ARG:HG3	1:A:437:GLU:OE2	2.21	0.41
1:B:147:THR:O	1:B:148:MET:C	2.56	0.41
1:A:237:TYR:CE1	1:B:250:LEU:HD21	2.56	0.41
1:A:267:THR:HG21	1:B:287:THR:OG1	2.21	0.41
1:B:355:LEU:HB3	1:B:359:GLU:HB2	2.02	0.41
1:B:195:THR:O	1:B:196:THR:C	2.58	0.41
1:B:303:GLU:HB3	1:B:304:PRO:CD	2.48	0.41
1:B:416:GLN:HA	1:B:417:PRO:HD3	1.81	0.41
1:B:490:PRO:O	1:B:491:GLY:C	2.58	0.41
1:A:151:LEU:HD12	1:A:151:LEU:O	2.21	0.41
1:A:402:PHE:HZ	1:A:414:LEU:HD11	1.84	0.41
1:A:414:LEU:HD23	1:A:414:LEU:HA	1.94	0.41
1:A:84:GLU:OE2	1:A:201:THR:HB	2.20	0.41
1:B:141:GLU:O	1:B:142:GLU:C	2.56	0.41
1:B:266:PRO:O	1:B:267:THR:C	2.57	0.41
1:B:303:GLU:HB3	1:B:304:PRO:HD3	2.03	0.41
1:B:365:CYS:O	1:B:366:GLU:C	2.59	0.41
1:A:165:ALA:O	1:A:168:PHE:HB3	2.20	0.41
1:A:250:LEU:HD21	1:B:237:TYR:CD1	2.55	0.41
1:A:41:GLY:HA3	2:A:600:FAD:O2A	2.21	0.41
1:A:79:THR:HG23	1:A:208:ARG:HB3	2.03	0.41
1:B:388:TRP:O	1:B:390:GLU:N	2.53	0.41
1:A:103:PHE:HA	1:A:104:PRO:HD3	1.75	0.41
1:A:165:ALA:O	1:A:166:THR:C	2.58	0.41
1:A:167:LEU:O	1:A:169:VAL:N	2.54	0.41
1:A:184:TRP:O	1:A:185:PHE:C	2.55	0.41
1:A:388:TRP:C	1:A:390:GLU:N	2.74	0.41
1:B:191:GLN:HE22	1:B:433:SER:CA	2.33	0.41
1:B:42:ARG:NH2	2:B:600:FAD:O3P	2.53	0.41
1:A:174:THR:HG22	1:A:292:GLY:HA3	1.91	0.41
1:A:304:PRO:HB2	1:A:307:ARG:HD3	1.93	0.41
1:A:373:GLY:C	1:A:374:SER:OG	2.59	0.41
1:A:89:ILE:HG21	1:A:96:SER:HB3	2.01	0.41
1:B:451:LEU:HB3	1:B:457:ILE:HD12	2.02	0.41
1:B:92:VAL:CG1	1:B:93:LYS:N	2.84	0.41
1:B:97:TYR:HA	1:B:98:PRO:HD3	1.70	0.41
1:A:286:ILE:HD13	1:A:286:ILE:HG21	1.64	0.41
1:A:392:GLN:O	1:A:392:GLN:HG3	2.20	0.41
1:A:418:VAL:O	1:A:418:VAL:HG12	2.20	0.41
1:B:161:ALA:O	1:B:162:LYS:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:VAL:HG23	1:B:257:ALA:O	2.21	0.41
1:B:282:ARG:O	1:B:283:ASN:C	2.59	0.41
1:B:413:VAL:O	1:B:414:LEU:C	2.58	0.41
1:B:46:LEU:HA	1:B:46:LEU:HD12	1.75	0.41
1:A:108:ASN:O	1:A:112:TYR:N	2.54	0.41
1:A:148:MET:HB3	1:A:148:MET:HE2	1.95	0.41
1:A:16:GLY:O	1:A:20:ALA:N	2.40	0.41
1:A:169:VAL:C	1:A:171:LEU:N	2.72	0.41
1:A:225:LEU:HA	1:A:225:LEU:HD23	1.62	0.41
1:A:245:VAL:O	1:A:256:GLU:HA	2.21	0.41
1:A:437:GLU:O	1:A:438:GLY:C	2.58	0.41
1:A:71:LEU:O	1:A:72:ALA:C	2.58	0.41
1:B:233:ARG:NH1	1:B:253:GLU:CD	2.74	0.41
1:B:480:THR:CB	1:B:483:GLU:HB2	2.23	0.41
1:A:242:ARG:HB3	1:A:243:GLU:H	1.67	0.41
1:A:92:VAL:HG12	1:A:93:LYS:HG3	2.03	0.41
1:A:271:LYS:HA	1:A:271:LYS:HD3	1.95	0.40
1:A:375:LEU:O	1:A:376:GLU:C	2.57	0.40
1:B:174:THR:HG22	1:B:174:THR:O	2.17	0.40
1:B:39:VAL:HG13	1:B:39:VAL:O	2.21	0.40
1:A:75:LEU:CD2	1:A:221:ILE:HG12	2.51	0.40
1:A:254:MET:HB3	1:A:254:MET:HE3	1.72	0.40
1:A:344:ILE:HG22	1:A:349:ALA:HA	2.04	0.40
1:B:304:PRO:O	1:B:305:PHE:C	2.59	0.40
1:A:436:MET:O	1:A:437:GLU:C	2.59	0.40
1:B:411:GLY:C	1:B:413:VAL:H	2.23	0.40
1:A:108:ASN:O	1:A:111:THR:HB	2.22	0.40
1:A:235:VAL:HG12	1:A:236:ILE:N	2.30	0.40
1:A:252:HIS:ND1	1:B:252:HIS:ND1	2.69	0.40
1:A:450:ILE:O	1:A:451:LEU:C	2.60	0.40
1:A:175:ALA:CB	1:A:179:GLU:OE1	2.47	0.40
1:A:28:LEU:HA	1:A:28:LEU:HD23	1.51	0.40
1:A:407:LEU:O	1:A:411:GLY:HA3	2.20	0.40
1:B:126:GLY:O	1:B:128:GLU:N	2.55	0.40

There are no symmetry-related clashes.

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	495/520 (95%)	391 (79%)	83 (17%)	21 (4%)	3	18
1	B	491/520 (94%)	400 (82%)	76 (16%)	15 (3%)	5	26
All	All	986/1040 (95%)	791 (80%)	159 (16%)	36 (4%)	4	22

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	389	CYS
1	B	286	ILE
1	B	442	ALA
1	B	446	ALA
1	A	252	HIS
1	A	286	ILE
1	A	398	TYR
1	A	446	ALA
1	A	496	ILE
1	B	132	ASP
1	B	195	THR
1	B	252	HIS
1	A	122	MET
1	A	132	ASP
1	A	321	GLU
1	A	365	CYS
1	A	408	THR
1	B	398	TYR
1	A	419	ASP
1	A	442	ALA
1	B	212	GLY
1	B	365	CYS
1	B	408	THR
1	B	412	ARG
1	A	86	GLU

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Mol	Chain	Res	Type
1	A	127	ARG
1	A	382	HIS
1	A	404	PRO
1	A	412	ARG
1	B	110	ILE
1	B	419	ASP
1	A	336	ASN
1	B	114	ASP
1	B	389	CYS
1	A	41	GLY
1	A	39	VAL

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	426/444 (96%)	353 (83%)	73 (17%)	2	12
1	B	423/444 (95%)	343 (81%)	80 (19%)	2	9
All	All	849/888 (96%)	696 (82%)	153 (18%)	2	10

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	6	ASP
1	A	22	LEU
1	A	38	ARG
1	A	39	VAL
1	A	43	THR
1	A	48	ASN
1	A	49	GLN
1	A	54	VAL
1	A	61	VAL
1	A	64	THR
1	A	69	LEU

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Mol	Chain	Res	Type
1	A	73	LYS
1	A	81	LYS
1	A	86	GLU
1	A	88	LEU
1	A	107	TRP
1	A	128	GLU
1	A	131	SER
1	A	147	THR
1	A	155	LEU
1	A	160	SER
1	A	171	LEU
1	A	174	THR
1	A	180	VAL
1	A	181	SER
1	A	190	LYS
1	A	195	THR
1	A	198	ILE
1	A	201	THR
1	A	208	ARG
1	A	219	GLU
1	A	232	GLU
1	A	233	ARG
1	A	236	ILE
1	A	243	GLU
1	A	254	MET
1	A	256	GLU
1	A	262	SER
1	A	271	LYS
1	A	280	MET
1	A	282	ARG
1	A	287	THR
1	A	303	GLU
1	A	306	TRP
1	A	327	THR
1	A	354	ARG
1	A	356	THR
1	A	361	LEU
1	A	374	SER
1	A	378	LEU
1	A	381	VAL
1	A	397	CYS
1	A	398	TYR

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Mol	Chain	Res	Type
1	A	399	THR
1	A	404	PRO
1	A	412	ARG
1	A	416	GLN
1	A	427	GLU
1	A	428	THR
1	A	437	GLU
1	A	456	LYS
1	A	462	ILE
1	A	465	SER
1	A	466	GLU
1	A	469	SER
1	A	471	ASP
1	A	472	VAL
1	A	477	ILE
1	A	479	THR
1	A	495	LEU
1	A	498	LEU
1	A	500	THR
1	B	4	LYS
1	B	6	ASP
1	B	22	LEU
1	B	26	SER
1	B	38	ARG
1	B	39	VAL
1	B	43	THR
1	B	47	ARG
1	B	48	ASN
1	B	49	GLN
1	B	54	VAL
1	B	61	VAL
1	B	64	THR
1	B	69	LEU
1	B	73	LYS
1	B	84	GLU
1	B	86	GLU
1	B	88	LEU
1	B	107	TRP
1	B	128	GLU
1	B	131	SER
1	B	147	THR
1	B	155	LEU

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Mol	Chain	Res	Type
1	B	160	SER
1	B	171	LEU
1	B	174	THR
1	B	180	VAL
1	B	181	SER
1	B	190	LYS
1	B	195	THR
1	B	198	ILE
1	B	201	THR
1	B	202	THR
1	B	219	GLU
1	B	232	GLU
1	B	233	ARG
1	B	236	ILE
1	B	241	THR
1	B	243	GLU
1	B	254	MET
1	B	256	GLU
1	B	262	SER
1	B	271	LYS
1	B	280	MET
1	B	282	ARG
1	B	287	THR
1	B	303	GLU
1	B	306	TRP
1	B	327	THR
1	B	337	TYR
1	B	341	MET
1	B	351	LYS
1	B	354	ARG
1	B	356	THR
1	B	361	LEU
1	B	364	LEU
1	B	370	LYS
1	B	374	SER
1	B	378	LEU
1	B	381	VAL
1	B	397	CYS
1	B	398	TYR
1	B	399	THR
1	B	408	THR
1	B	412	ARG

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Mol	Chain	Res	Type
1	B	416	GLN
1	B	427	GLU
1	B	428	THR
1	B	437	GLU
1	B	441	GLU
1	B	456	LYS
1	B	462	ILE
1	B	465	SER
1	B	466	GLU
1	B	469	SER
1	B	471	ASP
1	B	477	ILE
1	B	478	THR
1	B	479	THR
1	B	495	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	HIS
1	A	83	ASN
1	A	90	HIS
1	A	116	ASN
1	A	178	HIS
1	A	191	GLN
1	A	206	GLN
1	A	216	GLN
1	A	251	ASN
1	A	431	HIS
1	A	485	HIS
1	B	24	HIS
1	B	116	ASN
1	B	178	HIS
1	B	206	GLN
1	B	251	ASN
1	B	431	HIS
1	B	485	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	FAD	A	600	1,3	51,58,58	1.40	7 (13%)	54,89,89	2.12	12 (22%)
3	NYP	A	601	2	9,12,12	3.53	8 (88%)	8,14,14	3.58	5 (62%)
2	FAD	B	600	1,3	51,58,58	1.43	6 (11%)	54,89,89	2.21	17 (31%)
3	NYP	B	601	2	9,12,12	3.68	8 (88%)	8,14,14	3.57	5 (62%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	600	1,3	-	0/28/50/50	0/6/6/6
3	NYP	A	601	2	1/1/2/6	0/4/15/15	0/1/1/1
2	FAD	B	600	1,3	-	0/28/50/50	0/6/6/6
3	NYP	B	601	2	1/1/2/6	0/4/15/15	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	NYP	C2-C3	-5.54	1.40	1.52
3	B	601	NYP	C2-C3	-5.32	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	NYP	C2-C1	-4.69	1.39	1.52
3	B	601	NYP	C2-C1	-4.16	1.40	1.52
3	A	601	NYP	C6-C5	-4.11	1.40	1.49
3	B	601	NYP	C6-C5	-4.00	1.40	1.49
3	A	601	NYP	C7-C1	-2.96	1.50	1.53
3	B	601	NYP	C7-C1	-2.95	1.50	1.53
2	B	600	FAD	C2B-C1B	-2.40	1.49	1.53
3	A	601	NYP	C3-C4	-2.36	1.40	1.48
3	B	601	NYP	C3-C4	-2.25	1.41	1.48
2	A	600	FAD	C6-C5X	-2.23	1.38	1.41
2	A	600	FAD	C9A-C5X	-2.04	1.38	1.42
2	B	600	FAD	C2A-N1A	2.38	1.38	1.33
3	B	601	NYP	C9-C10	2.68	1.50	1.42
3	A	601	NYP	C9-C10	2.69	1.50	1.42
2	A	600	FAD	C4-N3	2.74	1.38	1.33
3	A	601	NYP	C5-C4	2.74	1.39	1.32
2	A	600	FAD	C2A-N1A	2.75	1.39	1.33
2	B	600	FAD	C4-N3	2.98	1.38	1.33
3	B	601	NYP	C5-C4	3.11	1.40	1.32
2	A	600	FAD	C10-N1	3.23	1.37	1.33
2	A	600	FAD	C4X-N5	3.27	1.38	1.33
2	B	600	FAD	C4X-N5	3.35	1.38	1.33
2	B	600	FAD	C10-N1	3.55	1.38	1.33
3	A	601	NYP	C9-N8	3.64	1.32	1.30
2	A	600	FAD	C2A-N3A	4.01	1.38	1.32
2	B	600	FAD	C2A-N3A	4.34	1.39	1.32
3	B	601	NYP	C9-N8	5.44	1.33	1.30

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	FAD	N3A-C2A-N1A	-8.84	121.16	128.86
2	B	600	FAD	N3A-C2A-N1A	-7.21	122.58	128.86
2	A	600	FAD	C4X-C10-N10	-3.59	118.03	120.52
2	A	600	FAD	O3'-C3'-C2'	-3.54	100.04	108.82
2	A	600	FAD	C9A-C5X-N5	-3.45	117.10	122.24
2	B	600	FAD	C5A-C6A-N6A	-3.36	113.63	120.47
2	B	600	FAD	C9A-C5X-N5	-3.21	117.46	122.24
2	B	600	FAD	C4X-C10-N10	-3.20	118.30	120.52
2	B	600	FAD	O3'-C3'-C2'	-3.03	101.31	108.82
2	B	600	FAD	C7M-C7-C8	-3.00	114.43	120.72
3	A	601	NYP	C11-C10-C9	-2.90	116.85	122.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	FAD	C4X-C4-N3	-2.87	119.40	123.48
2	A	600	FAD	C4X-C4-N3	-2.38	120.09	123.48
3	B	601	NYP	C11-C10-C9	-2.36	117.82	122.05
2	A	600	FAD	C5B-C4B-C3B	-2.33	106.42	115.29
2	B	600	FAD	C10-C4X-N5	-2.25	118.00	120.59
2	A	600	FAD	C7-C6-C5X	-2.24	117.61	121.08
2	B	600	FAD	C7-C6-C5X	-2.04	117.92	121.08
2	B	600	FAD	C5B-C4B-C3B	-2.04	107.51	115.29
2	A	600	FAD	C5A-C6A-N6A	-2.03	116.33	120.47
2	A	600	FAD	N6A-C6A-N1A	2.08	122.88	118.77
2	B	600	FAD	C1B-N9A-C4A	2.24	130.50	126.64
2	B	600	FAD	C4X-N5-C5X	2.45	119.35	116.76
2	B	600	FAD	C4-C4X-N5	2.82	121.77	118.68
3	B	601	NYP	C2-C3-C4	2.84	118.40	112.29
2	B	600	FAD	C5X-C9A-N10	3.04	119.91	117.66
2	A	600	FAD	O5'-P-O1P	3.04	121.51	109.25
2	B	600	FAD	N6A-C6A-N1A	3.29	125.28	118.77
3	B	601	NYP	C2-C1-C7	3.35	118.18	111.34
2	B	600	FAD	C4B-O4B-C1B	3.40	113.39	109.77
3	A	601	NYP	C2-C1-C7	3.62	118.72	111.34
3	A	601	NYP	C2-C3-C4	3.72	120.28	112.29
3	A	601	NYP	C3-C2-C1	4.34	119.56	112.32
3	B	601	NYP	C3-C2-C1	4.63	120.06	112.32
2	A	600	FAD	C4-N3-C2	5.05	119.58	115.16
2	A	600	FAD	C5X-C9A-N10	5.65	121.86	117.66
3	A	601	NYP	C2-C1-C6	6.52	120.67	109.38
2	B	600	FAD	C4-N3-C2	6.79	121.10	115.16
3	B	601	NYP	C2-C1-C6	7.02	121.52	109.38

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	601	NYP	C1
3	A	601	NYP	C1

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	FAD	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	NYP	12	0
2	B	600	FAD	3	0
3	B	601	NYP	8	0

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	497/520 (95%)	-0.15	4 (0%) 86 64	27, 44, 74, 100	0
1	B	493/520 (94%)	-0.40	2 (0%) 92 77	27, 44, 73, 91	0
All	All	990/1040 (95%)	-0.27	6 (0%) 89 71	27, 44, 74, 100	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	107	TRP	2.9
1	B	243	GLU	2.8
1	A	27	GLY	2.7
1	B	107	TRP	2.1
1	A	4	LYS	2.1
1	A	302	LYS	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	NYP	A	601	12/12	0.87	0.27	3.88	46,53,58,59	0
3	NYP	B	601	12/12	0.91	0.21	1.23	46,53,58,58	0
2	FAD	A	600	53/53	0.90	0.21	-0.11	24,35,45,49	0
2	FAD	B	600	53/53	0.96	0.14	-1.05	23,35,45,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.