



Full wwPDB X-ray Structure Validation Report ⓘ

May 12, 2020 – 11:12 pm BST

PDB ID : 4DJI
Title : Structure of glutamate-GABA antiporter GadC
Authors : Ma, D.; Lu, P.L.; Yan, C.Y.; Fan, C.; Yin, P.; Wang, J.W.; Shi, Y.G.
Deposited on : 2012-02-02
Resolution : 3.19 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

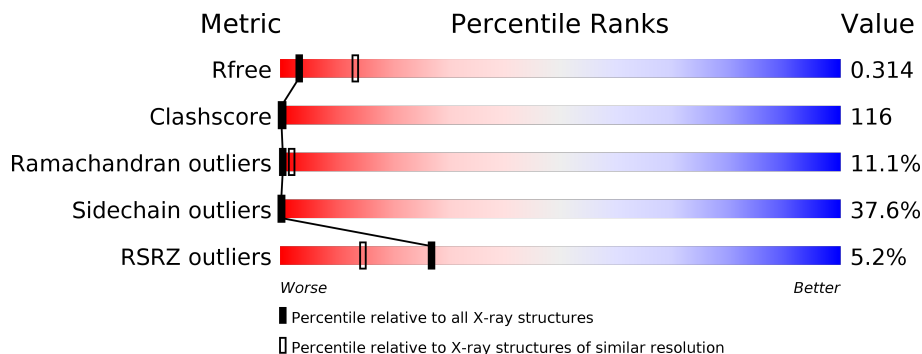
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1467 (3.20-3.16)
Clashscore	141614	1599 (3.20-3.16)
Ramachandran outliers	138981	1574 (3.20-3.16)
Sidechain outliers	138945	1573 (3.20-3.16)
RSRZ outliers	127900	1423 (3.20-3.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	511	
1	B	511	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7342 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.

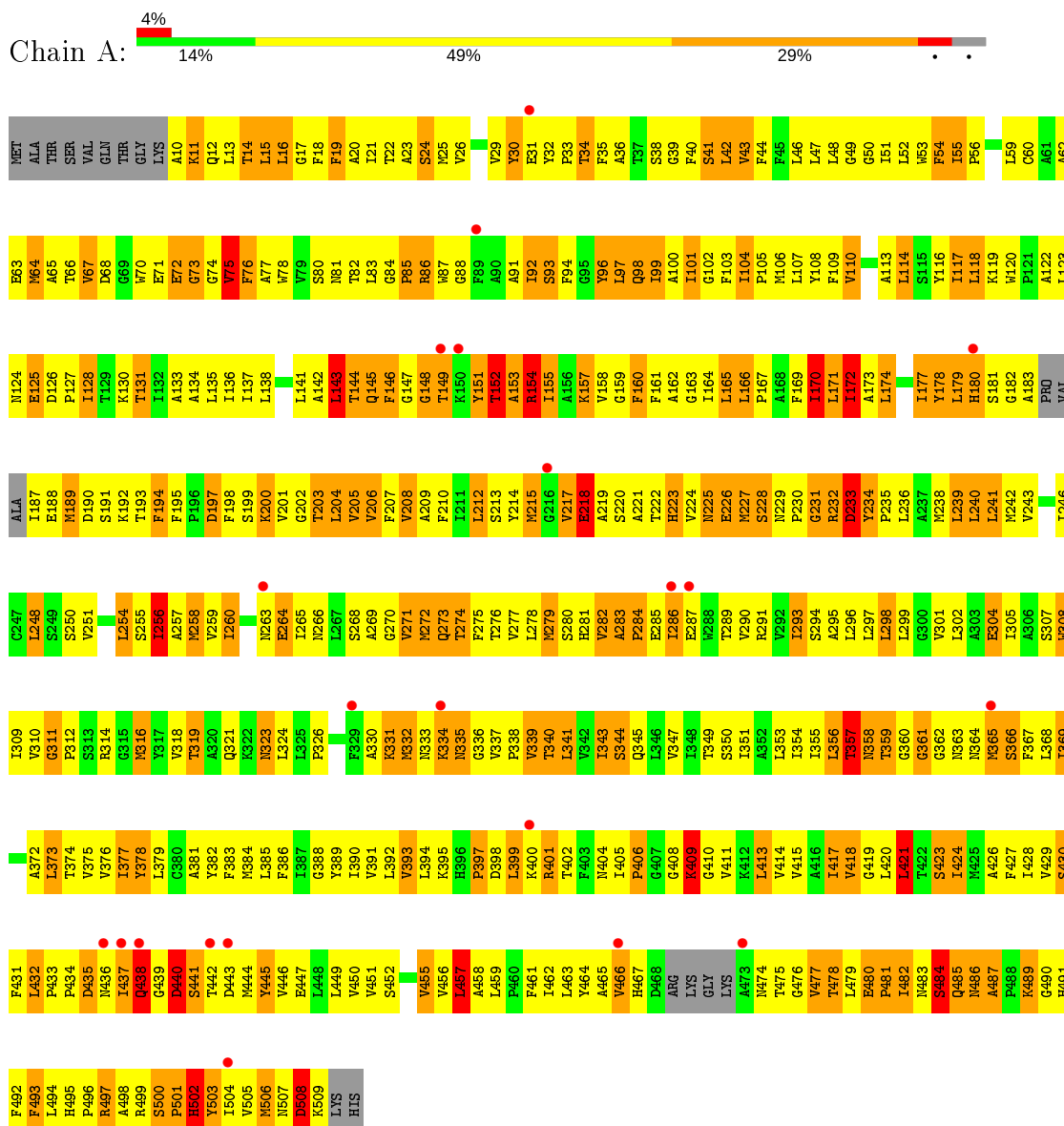
- Molecule 1 is a protein called Probable glutamate/gamma-aminobutyrate antiporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	493	Total 3732	C 2493	N 581	O 636	S 22	0	0	0
1	B	480	Total 3610	C 2417	N 556	O 616	S 21	0	0	0

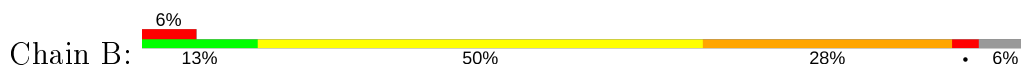
3 Residue-property plots

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

- Molecule 1: Probable glutamate/gamma-aminobutyrate antiporter



- Molecule 1: Probable glutamate/gamma-aminobutyrate antiporter



H491	F492	F493	L494	H495	P496	R497	A498	R499	S500	P501	H502	Y503	I504	VAL	MET	ASN	ASP	LYS	LYS	HIS																																										
F431	L432	P433	P434	M436	L437	Q438	G439	D440	S441	T442	D443	M444	Y445	V446	E447	L448	L449	V450	V451	F452	L453	L454	V455	V456	L457	A458	L459	P460	F461	L462	L463	Y464	A465	V466	H467	ASP	ARG	LYS	GLY	LYS	ALA	ASN	T475	G476	V477	T478	L479	E480	P481	L482	M483	S484	Q485	M486	A487	P488	K489	G490				
A370	L371	A372	L373	T374	V375	V376	I377	Y378	L379	C380	A381	Y382	F383	M384	L385	F386	I387	G388	Y389	I390	V391	L392	V393	L394	K395	H396	P397	ASP	LEU	LYS	ARG	T402	F403	M404	I405	G408	K409	G410	V411	K412	L413	V414	V415	A416	I417	V418	G419	L420	L421	T422	G362	M363	N364	M365	S366	F367	L428	V429	S430			
M308	I309	V310	G311	S312	S313	G314	G315	M316	V317	V318	T319	A320	Q321	K322	N323	L324	L325	P326	F329	A330	K331	M332	N333	K334	M335	G336	V337	P338	V339	T340	L341	V342	I343	S344	Q345	L346	V347	T348	T349	S350	I351	A352	L353	I354	L355	A356	T357	N358	T359	G360	N361	L362	A363	S364	S365	F366	L367	I368	I369			
L246	C247	L248	S249	S250	V251	G252	G253	L256	A257	M258	V259	L260	P261	G262	M263	E264	L265	M266	S268	A269	G270	V271	M272	Q273	T274	F275	T276	V277	L278	M279	S280	H281	V282	A283	F284	E285	L286	T289	V290	V292	I293	S294	A295	L296	L297	L298	L299	G300	V301	L302	A303	E304	A306	S307								
M246	E125	P126	P127	M128	T129	K130	T131	I132	A133	I136	I137	L138	M139	L140	L141	A142	I143	T144	Q145	F146	G147	G148	T149	K150	Y151	T152	A153	R154	I155	A156	K157	V158	G159	Q98	F160	F161	A162	G163	I164	I165	L166	I167	A168	F169	I170	L171	I172	A173	L174	A175	A176	I177	Y178	L179	I180	S181	G182	A183	PRO			
VAL	A186	I187	E188	M189	D190	S191	K192	T193	F194	F195	P196	D197	F198	S199	K200	V201	G202	T203	L204	V205	F206	F207	A208	A209	F210	I211	L212	S213	Y214	I215	G216	V217	A218	A219	S220	A221	T222	R223	V224	M225	E226	M227	S228	N229	P230	G231	R232	D233	Y234	F235	L236	A237	M238	L239	L240	L241	M242	V243				
A81	A82	E83	M84	A85	T86	V87	D88	G89	E71	E72	G73	G74	F75	F76	A77	A78	V79	S80	M81	T82	T83	L83	S84	M85	V86	M87	A88	V89	Y90	I92	S93	F94	G95	L96	L97	S98	Q98	I99	A100	I101	G102	F103	I104	P105	M106	F109	V110	L111	G112	A113	L114	S115	Y116	I117	I118	I119	M120	A121	A122	L123		
MET	ALA	THR	SER	VAL	GLN	THR	GLY	LYS	ALA	LYS	O12	L13	T14	L15	L16	G17	F18	F19	A20	I21	T22	A23	S24	M25	V26	M27	A28	V29	Y30	I92	S93	E31	Y32	P33	T34	F35	A36	T37	S38	G39	F40	S41	L42	V43	F44	F45	L46	L47	L48	G49	G50	I51	L52	W53	F54	I55	L118	P56	V57	G58	L59	C60

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.62Å 105.42Å 188.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.52 – 3.19 35.52 – 3.19	Depositor EDS
% Data completeness (in resolution range)	84.2 (35.52-3.19) 84.6 (35.52-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 3.18Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.310 , 0.328 0.300 , 0.314	Depositor DCC
R_{free} test set	1138 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	107.4	Xtrriage
Anisotropy	0.971	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 87.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7342	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

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	0.77	0/3826	0.81	9/5222 (0.2%)
1	B	0.70	0/3700	0.79	5/5054 (0.1%)
All	All	0.74	0/7526	0.80	14/10276 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	234	TYR	CB-CA-C	-8.67	93.07	110.40
1	B	215	MET	CG-SD-CE	8.39	113.62	100.20
1	B	41	SER	CB-CA-C	8.19	125.65	110.10
1	A	234	TYR	N-CA-C	7.97	132.52	111.00
1	A	482	ILE	CB-CA-C	-7.76	96.09	111.60
1	B	42	LEU	CB-CA-C	-6.50	97.84	110.20
1	A	215	MET	CG-SD-CE	5.92	109.67	100.20
1	A	170	ILE	O-C-N	-5.91	113.24	122.70
1	B	371	LEU	CB-CG-CD2	-5.87	101.03	111.00
1	A	421	LEU	CA-CB-CG	-5.54	102.57	115.30
1	A	443	ASP	CB-CG-OD2	5.46	123.21	118.30
1	B	443	ASP	CB-CG-OD2	5.35	123.11	118.30
1	A	256	ILE	CB-CA-C	-5.23	101.14	111.60
1	A	508	ASP	CB-CG-OD2	5.18	122.97	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	170	ILE	Mainchain
1	A	75	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	3732	0	3867	887	0
1	B	3610	0	3738	860	0
All	All	7342	0	7605	1738	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 116.

All (1738) 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:157:LYS:HG2	1:A:493:PHE:CD2	1.38	1.57
1:A:117:ILE:HG22	1:A:118:LEU:CD1	1.33	1.55
1:B:395:LYS:CE	1:B:396:HIS:HE1	1.18	1.53
1:A:160:PHE:CE1	1:A:165:LEU:HD23	1.46	1.51
1:A:202:GLY:CA	1:A:434:PRO:HG3	1.05	1.49
1:B:55:ILE:CG2	1:B:56:PRO:HD3	1.00	1.46
1:A:202:GLY:HA3	1:A:434:PRO:CG	1.00	1.45
1:B:395:LYS:HE2	1:B:396:HIS:CE1	1.49	1.44
1:B:55:ILE:HG22	1:B:56:PRO:CD	0.97	1.43
1:B:15:LEU:HD23	1:B:16:LEU:N	1.35	1.37
1:B:53:TRP:CH2	1:B:382:TYR:CE1	2.10	1.37
1:B:395:LYS:CE	1:B:396:HIS:CE1	2.06	1.35
1:B:447:GLU:O	1:B:451:VAL:HG23	1.29	1.33
1:B:160:PHE:CE1	1:B:165:LEU:HD21	1.64	1.31
1:B:15:LEU:CD2	1:B:16:LEU:N	1.95	1.30
1:A:457:LEU:HD12	1:A:457:LEU:O	1.34	1.25
1:A:154:ARG:NH2	1:A:489:LYS:HE3	1.47	1.24
1:A:117:ILE:CG2	1:A:118:LEU:CD1	2.16	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:432:LEU:O	1:B:432:LEU:HD12	1.36	1.21
1:A:347:VAL:CG1	1:A:351:ILE:HD11	1.70	1.20
1:B:15:LEU:HD23	1:B:15:LEU:C	1.55	1.20
1:A:15:LEU:C	1:A:15:LEU:HD23	1.58	1.20
1:A:215:MET:CE	1:A:378:TYR:HB3	1.72	1.20
1:A:386:PHE:O	1:A:390:ILE:HD12	1.42	1.19
1:A:339:VAL:O	1:A:343:ILE:HG23	1.42	1.19
1:A:154:ARG:HH21	1:A:489:LYS:CG	1.53	1.19
1:A:491:HIS:O	1:A:494:LEU:HB2	1.40	1.18
1:B:286:ILE:HG22	1:B:289:THR:CG2	1.73	1.18
1:B:53:TRP:CZ2	1:B:382:TYR:CD1	2.32	1.18
1:A:154:ARG:NH2	1:A:489:LYS:CE	2.07	1.17
1:B:124:ASN:O	1:B:130:LYS:HE2	1.41	1.17
1:A:224:VAL:O	1:A:227:MET:HB2	1.45	1.17
1:A:117:ILE:CG2	1:A:118:LEU:HD12	1.74	1.16
1:A:76:PHE:HB2	1:A:92:ILE:HG13	1.23	1.15
1:A:143:LEU:C	1:A:143:LEU:HD12	1.55	1.15
1:A:15:LEU:HD22	1:A:16:LEU:HD23	1.22	1.15
1:A:134:ALA:CB	1:A:353:LEU:HD21	1.77	1.15
1:A:160:PHE:CE1	1:A:165:LEU:CD2	2.30	1.15
1:A:172:ILE:CD1	1:A:251:VAL:HG11	1.77	1.15
1:A:485:GLN:HA	1:A:485:GLN:NE2	1.47	1.15
1:A:347:VAL:O	1:A:351:ILE:HG13	1.44	1.14
1:A:477:VAL:HG11	1:A:506:MET:HB3	1.26	1.14
1:B:41:SER:HB3	1:B:196:PRO:HG3	1.25	1.14
1:A:449:LEU:HD12	1:A:449:LEU:O	1.41	1.14
1:A:145:GLN:NE2	1:A:145:GLN:HA	1.61	1.13
1:B:215:MET:HE3	1:B:378:TYR:HB3	1.16	1.13
1:A:157:LYS:CG	1:A:493:PHE:HD2	1.62	1.13
1:A:397:PRO:HD2	1:A:398:ASP:H	1.11	1.13
1:B:262:GLY:HA2	1:B:265:ILE:HG13	1.31	1.13
1:A:75:VAL:HG12	1:A:78:TRP:CE3	1.83	1.12
1:A:125:GLU:O	1:A:127:PRO:HD3	1.45	1.12
1:A:128:ILE:O	1:A:128:ILE:HD12	1.48	1.12
1:A:259:VAL:HG21	1:A:278:LEU:HD21	1.13	1.12
1:B:489:LYS:H	1:B:489:LYS:CD	1.62	1.12
1:B:170:ILE:HG22	1:B:275:PHE:CZ	1.85	1.12
1:B:99:ILE:CD1	1:B:312:PRO:HG3	1.80	1.11
1:B:485:GLN:NE2	1:B:485:GLN:HA	1.47	1.11
1:B:166:LEU:HB3	1:B:167:PRO:HD3	1.18	1.11
1:A:432:LEU:O	1:A:432:LEU:HD12	1.52	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:LEU:HD23	1:B:204:LEU:N	1.60	1.10
1:A:286:ILE:HG22	1:A:289:THR:HB	1.29	1.09
1:B:53:TRP:CZ2	1:B:382:TYR:CE1	2.38	1.09
1:A:157:LYS:CG	1:A:493:PHE:CD2	2.33	1.09
1:B:47:LEU:HD23	1:B:246:ILE:HD11	1.12	1.09
1:A:154:ARG:HH21	1:A:489:LYS:HG3	1.13	1.09
1:B:323:ASN:O	1:B:324:LEU:HD13	1.52	1.08
1:A:44:PHE:HB2	1:A:194:PHE:CE2	1.89	1.07
1:A:203:THR:HG22	1:A:204:LEU:HD23	1.30	1.07
1:B:99:ILE:HD13	1:B:312:PRO:HG3	1.18	1.07
1:B:34:THR:O	1:B:37:THR:HG22	1.53	1.07
1:A:364:ASN:ND2	1:A:438:GLN:HG3	1.70	1.07
1:A:495:HIS:HD2	1:A:497:ARG:HB2	1.18	1.07
1:A:149:THR:CG2	1:A:314:ARG:HH22	1.66	1.06
1:B:229:ASN:O	1:B:233:ASP:HB2	1.51	1.06
1:A:337:VAL:HG22	1:A:337:VAL:O	1.56	1.06
1:B:215:MET:CE	1:B:378:TYR:HB3	1.85	1.06
1:B:489:LYS:HD2	1:B:489:LYS:N	1.54	1.06
1:A:154:ARG:HH21	1:A:489:LYS:CD	1.67	1.06
1:B:286:ILE:CG2	1:B:289:THR:CG2	2.33	1.05
1:A:330:ALA:O	1:A:331:LYS:HG2	1.55	1.05
1:B:57:VAL:O	1:B:61:ALA:HB2	1.57	1.05
1:B:160:PHE:HE1	1:B:165:LEU:HD21	0.89	1.05
1:B:337:VAL:O	1:B:337:VAL:HG22	1.55	1.04
1:A:75:VAL:HG12	1:A:78:TRP:CZ3	1.91	1.04
1:B:161:PHE:CD1	1:B:165:LEU:CD1	2.40	1.04
1:A:15:LEU:CD2	1:A:16:LEU:HD23	1.87	1.04
1:B:36:ALA:HB1	1:B:257:ALA:HB2	1.37	1.03
1:A:234:TYR:HB3	1:A:235:PRO:HD3	1.40	1.03
1:A:421:LEU:HD11	1:B:424:ILE:HD12	1.40	1.03
1:A:117:ILE:O	1:A:291:ARG:NH2	1.92	1.03
1:B:286:ILE:HG22	1:B:289:THR:HG22	1.35	1.03
1:B:501:PRO:O	1:B:502:HIS:HD2	1.42	1.02
1:A:98:GLN:HB2	1:A:377:ILE:HG22	1.41	1.02
1:B:395:LYS:HE3	1:B:396:HIS:CE1	1.91	1.02
1:A:353:LEU:O	1:A:357:THR:HG23	1.60	1.01
1:A:157:LYS:O	1:A:161:PHE:HD1	1.42	1.01
1:A:272:MET:CE	1:A:297:LEU:HD12	1.91	1.00
1:B:99:ILE:HD13	1:B:312:PRO:CG	1.90	1.00
1:A:202:GLY:HA3	1:A:434:PRO:CD	1.89	1.00
1:A:215:MET:HE2	1:A:378:TYR:HB3	1.42	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ILE:HB	1:A:56:PRO:HD3	1.42	1.00
1:A:74:GLY:O	1:A:75:VAL:HG13	1.61	1.00
1:A:74:GLY:O	1:A:75:VAL:HG22	1.61	1.00
1:B:53:TRP:CH2	1:B:382:TYR:HE1	1.73	1.00
1:B:36:ALA:HB2	1:B:253:GLY:O	1.59	1.00
1:B:35:PHE:O	1:B:42:LEU:HD21	1.61	1.00
1:A:21:ILE:HB	1:A:492:PHE:CE2	1.95	1.00
1:B:194:PHE:CE1	1:B:195:PHE:CE2	2.49	1.00
1:B:67:VAL:HG21	1:B:70:TRP:CE3	1.96	1.00
1:B:308:TRP:NE1	1:B:498:ALA:HB2	1.75	1.00
1:B:98:GLN:OE1	1:B:99:ILE:HG13	1.62	1.00
1:B:160:PHE:HE1	1:B:165:LEU:CD2	1.74	0.99
1:B:47:LEU:HD23	1:B:246:ILE:CD1	1.91	0.99
1:A:124:ASN:HA	1:A:130:LYS:HE2	1.42	0.99
1:B:31:GLU:C	1:B:33:PRO:HD2	1.82	0.99
1:B:53:TRP:HH2	1:B:382:TYR:CE1	1.76	0.99
1:A:347:VAL:HG13	1:A:351:ILE:HD11	1.43	0.99
1:B:166:LEU:HB3	1:B:167:PRO:CD	1.92	0.99
1:A:397:PRO:CD	1:A:398:ASP:H	1.74	0.99
1:B:41:SER:O	1:B:44:PHE:HB3	1.62	0.99
1:B:187:ILE:HG22	1:B:187:ILE:O	1.59	0.99
1:B:321:GLN:HE22	1:B:479:LEU:CD2	1.76	0.99
1:A:21:ILE:HB	1:A:492:PHE:CD2	1.97	0.99
1:B:141:LEU:CD1	1:B:306:ALA:HB2	1.91	0.99
1:B:310:VAL:O	1:B:310:VAL:HG22	1.62	0.99
1:B:42:LEU:O	1:B:46:LEU:HB2	1.60	0.99
1:B:109:PHE:HD2	1:B:301:VAL:HG21	1.28	0.98
1:B:145:GLN:HE21	1:B:145:GLN:HA	1.20	0.98
1:B:161:PHE:CD1	1:B:165:LEU:HD11	1.99	0.98
1:A:26:VAL:CG1	1:A:248:LEU:HD23	1.93	0.98
1:B:359:THR:HG22	1:B:359:THR:O	1.64	0.98
1:A:172:ILE:HD12	1:A:251:VAL:HG11	1.41	0.98
1:A:250:SER:O	1:A:254:LEU:HD12	1.63	0.98
1:B:30:TYR:CE1	1:B:301:VAL:HG22	1.98	0.98
1:A:506:MET:O	1:A:509:LYS:HD3	1.63	0.98
1:A:264:GLU:OE2	1:A:264:GLU:HA	1.61	0.98
1:A:134:ALA:HB1	1:A:353:LEU:HD21	1.42	0.98
1:B:489:LYS:HD2	1:B:489:LYS:H	1.08	0.98
1:B:25:MET:HB2	1:B:495:HIS:CE1	1.99	0.98
1:A:15:LEU:C	1:A:15:LEU:CD2	2.32	0.97
1:B:63:GLU:OE1	1:B:405:ILE:HG13	1.64	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:ALA:O	1:A:376:VAL:HG22	1.63	0.97
1:A:483:ASN:O	1:A:485:GLN:N	1.95	0.97
1:B:161:PHE:HD1	1:B:165:LEU:HD12	1.28	0.97
1:A:272:MET:HE2	1:A:297:LEU:HD12	1.43	0.97
1:B:196:PRO:HB2	1:B:198:PHE:CE1	1.98	0.97
1:B:25:MET:CB	1:B:495:HIS:HE1	1.76	0.97
1:A:116:TYR:CD1	1:A:272:MET:HB2	2.00	0.96
1:A:364:ASN:HD22	1:A:438:GLN:HG3	1.28	0.96
1:B:151:TYR:CD1	1:B:151:TYR:N	2.30	0.96
1:B:96:TYR:CD2	1:B:97:LEU:HD23	2.00	0.96
1:A:486:ASN:HB3	1:A:503:TYR:OH	1.64	0.96
1:B:194:PHE:HD1	1:B:195:PHE:CD2	1.83	0.96
1:B:70:TRP:CH2	1:B:392:LEU:HD11	1.99	0.96
1:B:362:GLY:H	1:B:440:ASP:HB3	1.28	0.96
1:A:485:GLN:HA	1:A:485:GLN:HE21	1.26	0.96
1:A:67:VAL:HG12	1:A:70:TRP:HB2	1.46	0.96
1:B:166:LEU:CD1	1:B:166:LEU:C	2.30	0.96
1:A:135:LEU:CD2	1:A:350:SER:OG	2.14	0.95
1:A:154:ARG:HH22	1:A:489:LYS:CE	1.75	0.95
1:B:82:THR:HG21	1:B:388:GLY:O	1.65	0.95
1:A:431:PHE:O	1:A:446:VAL:HG22	1.65	0.95
1:B:194:PHE:CD1	1:B:195:PHE:CD2	2.54	0.95
1:A:118:LEU:CD1	1:A:118:LEU:N	2.30	0.95
1:B:194:PHE:HD1	1:B:195:PHE:HD2	1.03	0.95
1:A:143:LEU:HG	1:A:144:THR:N	1.77	0.95
1:A:215:MET:HE1	1:A:378:TYR:HB3	1.48	0.95
1:A:478:THR:OG1	1:A:505:VAL:CG2	2.15	0.95
1:B:266:ASN:C	1:B:266:ASN:HD22	1.70	0.95
1:B:166:LEU:C	1:B:166:LEU:HD12	1.86	0.95
1:A:485:GLN:CA	1:A:485:GLN:NE2	2.30	0.95
1:B:194:PHE:HE1	1:B:195:PHE:CE2	1.83	0.95
1:A:421:LEU:CD1	1:B:424:ILE:HD12	1.96	0.95
1:A:134:ALA:HB3	1:A:353:LEU:HD21	1.49	0.94
1:A:73:GLY:HA3	1:A:77:ALA:CB	1.97	0.94
1:A:73:GLY:HA3	1:A:77:ALA:HB2	1.49	0.94
1:B:283:ALA:HB1	1:B:286:ILE:HD12	1.46	0.94
1:B:215:MET:HE3	1:B:378:TYR:CB	1.97	0.94
1:A:160:PHE:HE1	1:A:165:LEU:HD23	1.29	0.94
1:B:372:ALA:HB1	1:B:449:LEU:HD11	1.49	0.94
1:B:109:PHE:CD2	1:B:301:VAL:HG21	2.02	0.94
1:B:99:ILE:CD1	1:B:312:PRO:CG	2.46	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:485:GLN:NE2	1:B:485:GLN:CA	2.30	0.94
1:B:53:TRP:HZ2	1:B:382:TYR:CD1	1.83	0.94
1:B:160:PHE:CE1	1:B:165:LEU:CD2	2.49	0.94
1:B:13:LEU:HD22	1:B:17:GLY:HA3	1.50	0.93
1:B:194:PHE:CD1	1:B:195:PHE:HD2	1.86	0.93
1:B:286:ILE:HG23	1:B:289:THR:HB	1.46	0.93
1:A:154:ARG:NH2	1:A:489:LYS:HG3	1.83	0.93
1:A:149:THR:HG23	1:A:314:ARG:HH22	1.31	0.93
1:B:15:LEU:HD21	1:B:16:LEU:HD13	1.49	0.93
1:B:485:GLN:HE21	1:B:485:GLN:HA	1.26	0.93
1:B:145:GLN:NE2	1:B:145:GLN:HA	1.84	0.93
1:B:362:GLY:HA3	1:B:440:ASP:OD2	1.65	0.93
1:B:321:GLN:NE2	1:B:479:LEU:HD21	1.82	0.93
1:B:204:LEU:CD2	1:B:204:LEU:N	2.30	0.92
1:A:483:ASN:C	1:A:485:GLN:H	1.72	0.92
1:A:172:ILE:HD11	1:A:251:VAL:HG11	1.49	0.92
1:A:67:VAL:HG23	1:A:401:ARG:HG3	1.51	0.92
1:B:15:LEU:HD23	1:B:16:LEU:CA	2.00	0.92
1:B:503:TYR:O	1:B:504:ILE:CB	2.17	0.92
1:A:94:PHE:HB2	1:A:381:ALA:HB2	1.50	0.92
1:B:170:ILE:O	1:B:174:LEU:HB2	1.70	0.92
1:B:76:PHE:C	1:B:76:PHE:CD2	2.43	0.92
1:B:141:LEU:HD12	1:B:306:ALA:HB2	1.50	0.91
1:B:32:TYR:N	1:B:33:PRO:HD2	1.83	0.91
1:A:194:PHE:HD2	1:A:194:PHE:O	1.51	0.91
1:B:170:ILE:HG22	1:B:275:PHE:CE1	2.04	0.91
1:B:141:LEU:HD12	1:B:306:ALA:CB	2.01	0.91
1:A:154:ARG:HH22	1:A:489:LYS:HE3	1.11	0.91
1:A:212:LEU:HD12	1:A:375:VAL:HG23	1.50	0.91
1:B:25:MET:CB	1:B:495:HIS:CE1	2.53	0.91
1:A:143:LEU:C	1:A:143:LEU:CD1	2.30	0.91
1:A:435:ASP:HA	1:A:442:THR:OG1	1.71	0.91
1:A:154:ARG:NH2	1:A:489:LYS:CD	2.32	0.91
1:A:76:PHE:HD1	1:A:76:PHE:O	1.54	0.91
1:A:120:TRP:NE1	1:A:122:ALA:HB3	1.85	0.90
1:A:310:VAL:HG13	1:A:311:GLY:H	1.36	0.90
1:B:447:GLU:O	1:B:451:VAL:CG2	2.16	0.90
1:B:151:TYR:H	1:B:151:TYR:HD1	0.96	0.90
1:B:96:TYR:HD2	1:B:97:LEU:HD23	1.35	0.90
1:B:145:GLN:CA	1:B:145:GLN:HE21	1.83	0.90
1:B:286:ILE:CG2	1:B:289:THR:HG21	2.00	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:LYS:HG2	1:A:493:PHE:CE2	2.06	0.90
1:B:30:TYR:HE1	1:B:301:VAL:HG22	1.31	0.90
1:B:151:TYR:HD1	1:B:151:TYR:N	1.69	0.90
1:A:364:ASN:HD22	1:A:438:GLN:CG	1.84	0.90
1:B:25:MET:HB2	1:B:495:HIS:HE1	1.30	0.90
1:B:427:PHE:HZ	1:B:453:PHE:CE2	1.88	0.90
1:B:117:ILE:HG13	1:B:294:SER:HB2	1.53	0.90
1:B:51:ILE:HG22	1:B:52:LEU:HD23	1.53	0.89
1:A:117:ILE:HG22	1:A:118:LEU:HD11	1.53	0.89
1:A:101:ILE:HG13	1:A:373:LEU:HD13	1.52	0.89
1:B:269:ALA:HB1	1:B:272:MET:CE	2.01	0.89
1:B:15:LEU:HD22	1:B:16:LEU:N	1.86	0.89
1:B:321:GLN:NE2	1:B:479:LEU:CD2	2.35	0.89
1:A:109:PHE:HE1	1:A:271:VAL:HG21	1.37	0.89
1:B:76:PHE:C	1:B:76:PHE:HD2	1.75	0.89
1:A:117:ILE:CG2	1:A:118:LEU:HD11	2.03	0.88
1:B:395:LYS:HG3	1:B:396:HIS:ND1	1.88	0.88
1:B:383:PHE:O	1:B:387:ILE:HD12	1.72	0.88
1:B:48:LEU:HD23	1:B:48:LEU:N	1.87	0.88
1:A:29:VAL:HG23	1:A:30:TYR:N	1.89	0.88
1:A:504:ILE:O	1:A:504:ILE:HG22	1.72	0.88
1:B:194:PHE:CE1	1:B:195:PHE:HE2	1.90	0.88
1:B:22:THR:O	1:B:241:LEU:HD21	1.72	0.88
1:A:347:VAL:CG1	1:A:351:ILE:CD1	2.51	0.88
1:A:98:GLN:CB	1:A:377:ILE:HG22	2.03	0.88
1:B:283:ALA:CB	1:B:286:ILE:HD12	2.04	0.88
1:B:313:SER:O	1:B:316:MET:N	2.07	0.88
1:B:146:PHE:HE1	1:B:342:VAL:HG11	1.38	0.88
1:B:161:PHE:HD1	1:B:165:LEU:CD1	1.80	0.88
1:B:395:LYS:O	1:B:396:HIS:ND1	2.05	0.88
1:B:25:MET:HA	1:B:495:HIS:CE1	2.09	0.88
1:B:321:GLN:HE22	1:B:479:LEU:HD22	1.38	0.87
1:A:485:GLN:CA	1:A:485:GLN:HE21	1.87	0.87
1:A:172:ILE:CG2	1:A:173:ALA:N	2.37	0.87
1:A:505:VAL:O	1:A:505:VAL:HG23	1.71	0.87
1:B:124:ASN:HD21	1:B:268:SER:CB	1.87	0.87
1:A:63:GLU:OE1	1:A:405:ILE:HG13	1.74	0.87
1:A:82:THR:HB	1:A:391:VAL:CG1	2.03	0.87
1:B:157:LYS:HG3	1:B:493:PHE:HE2	1.38	0.87
1:B:308:TRP:CD1	1:B:498:ALA:HB1	2.09	0.87
1:A:98:GLN:HG3	1:A:378:TYR:CD2	2.10	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:VAL:HG11	1:A:413:LEU:HD21	1.54	0.87
1:B:347:VAL:O	1:B:351:ILE:HB	1.75	0.87
1:A:145:GLN:CA	1:A:145:GLN:NE2	2.30	0.87
1:A:304:GLU:O	1:A:308:TRP:CE3	2.28	0.86
1:A:42:LEU:O	1:A:46:LEU:HG	1.74	0.86
1:B:69:GLY:C	1:B:70:TRP:HD1	1.78	0.86
1:B:165:LEU:O	1:B:168:ALA:HB3	1.75	0.86
1:B:286:ILE:HG22	1:B:286:ILE:O	1.75	0.86
1:B:55:ILE:CB	1:B:56:PRO:HD3	2.04	0.86
1:A:356:LEU:HD22	1:A:369:ILE:CG2	2.05	0.86
1:B:166:LEU:CB	1:B:167:PRO:HD3	2.05	0.86
1:A:145:GLN:CA	1:A:145:GLN:HE21	1.85	0.86
1:A:332:MET:HG3	1:A:338:PRO:CA	2.04	0.86
1:B:485:GLN:HE21	1:B:485:GLN:CA	1.87	0.86
1:A:143:LEU:CG	1:A:144:THR:N	2.35	0.86
1:A:172:ILE:HG22	1:A:173:ALA:H	1.41	0.86
1:A:172:ILE:HD12	1:A:251:VAL:CG1	2.05	0.86
1:B:77:ALA:O	1:B:81:ASN:HB2	1.74	0.86
1:A:283:ALA:HB1	1:A:285:GLU:OE2	1.75	0.86
1:A:154:ARG:NH2	1:A:489:LYS:CG	2.39	0.86
1:B:25:MET:CA	1:B:495:HIS:HE1	1.87	0.86
1:A:163:GLY:O	1:A:167:PRO:HD2	1.75	0.86
1:A:19:PHE:C	1:A:19:PHE:HD2	1.78	0.86
1:A:202:GLY:C	1:A:434:PRO:HG3	1.96	0.86
1:B:434:PRO:O	1:B:435:ASP:HB2	1.74	0.86
1:A:109:PHE:HD2	1:A:301:VAL:HG21	1.40	0.85
1:A:347:VAL:HG12	1:A:351:ILE:HD11	1.57	0.85
1:A:15:LEU:HD23	1:A:15:LEU:O	1.76	0.85
1:B:27:MET:HE1	1:B:248:LEU:HG	1.57	0.85
1:A:26:VAL:HG12	1:A:248:LEU:HD23	1.59	0.85
1:A:330:ALA:C	1:A:331:LYS:HG2	1.95	0.85
1:A:286:ILE:O	1:A:289:THR:HG22	1.77	0.85
1:A:19:PHE:C	1:A:19:PHE:CD2	2.48	0.85
1:A:178:TYR:CD2	1:A:178:TYR:C	2.50	0.85
1:B:317:TYR:HD2	1:B:479:LEU:HD11	1.41	0.85
1:B:37:THR:OG1	1:B:438:GLN:NE2	2.08	0.85
1:B:70:TRP:CZ3	1:B:392:LEU:HD11	2.11	0.85
1:A:215:MET:CE	1:A:378:TYR:CB	2.55	0.85
1:A:229:ASN:O	1:A:233:ASP:HB2	1.77	0.84
1:B:55:ILE:HG22	1:B:56:PRO:CG	2.05	0.84
1:B:308:TRP:NE1	1:B:498:ALA:CB	2.39	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:PRO:O	1:A:502:HIS:CG	2.30	0.84
1:A:13:LEU:HD12	1:A:226:GLU:HB2	1.58	0.84
1:A:204:LEU:O	1:A:206:VAL:N	2.11	0.84
1:A:495:HIS:CD2	1:A:497:ARG:HB2	2.08	0.84
1:B:194:PHE:O	1:B:194:PHE:CD1	2.30	0.84
1:A:160:PHE:CZ	1:A:165:LEU:CD2	2.60	0.84
1:A:353:LEU:O	1:A:357:THR:CG2	2.25	0.84
1:A:143:LEU:HD12	1:A:143:LEU:O	1.78	0.84
1:A:135:LEU:HD21	1:A:350:SER:OG	1.76	0.84
1:A:135:LEU:HD23	1:A:350:SER:OG	1.78	0.84
1:A:67:VAL:HG11	1:A:70:TRP:CE3	2.13	0.84
1:B:286:ILE:CG2	1:B:289:THR:HB	2.07	0.84
1:B:51:ILE:CG2	1:B:52:LEU:HD23	2.07	0.84
1:A:399:LEU:CD2	1:A:400:LYS:H	1.90	0.84
1:A:449:LEU:HD12	1:A:449:LEU:C	1.91	0.84
1:A:418:VAL:HG12	1:A:419:GLY:N	1.91	0.83
1:A:15:LEU:HD23	1:A:16:LEU:N	1.92	0.83
1:A:212:LEU:HD12	1:A:375:VAL:CG2	2.08	0.83
1:B:298:LEU:HG	1:B:302:LEU:CD1	2.08	0.83
1:B:276:THR:HG22	1:B:277:VAL:N	1.92	0.83
1:B:501:PRO:O	1:B:502:HIS:CD2	2.29	0.83
1:A:149:THR:CG2	1:A:314:ARG:NH2	2.41	0.83
1:B:189:MET:O	1:B:190:ASP:O	1.96	0.83
1:A:347:VAL:HG12	1:A:351:ILE:CD1	2.08	0.83
1:A:44:PHE:HB2	1:A:194:PHE:HE2	1.40	0.83
1:A:85:PRO:O	1:A:87:TRP:N	2.11	0.83
1:B:34:THR:O	1:B:37:THR:CG2	2.25	0.83
1:A:74:GLY:C	1:A:75:VAL:HG13	1.99	0.83
1:B:96:TYR:CD2	1:B:97:LEU:CD2	2.62	0.83
1:A:119:LYS:HG2	1:A:291:ARG:HH12	1.42	0.83
1:B:221:ALA:O	1:B:224:VAL:HG23	1.79	0.83
1:B:47:LEU:CD2	1:B:246:ILE:HD11	2.04	0.83
1:B:234:TYR:C	1:B:234:TYR:HD2	1.81	0.82
1:B:42:LEU:O	1:B:46:LEU:N	2.12	0.82
1:B:395:LYS:HE2	1:B:396:HIS:HE1	0.66	0.82
1:A:234:TYR:HB3	1:A:235:PRO:CD	2.10	0.82
1:B:173:ALA:O	1:B:176:ALA:HB3	1.79	0.82
1:A:202:GLY:HA3	1:A:434:PRO:CB	2.06	0.82
1:A:73:GLY:CA	1:A:77:ALA:HB2	2.09	0.82
1:B:170:ILE:HD13	1:B:293:ILE:HD12	1.60	0.82
1:A:221:ALA:O	1:A:224:VAL:HG23	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:VAL:CG2	1:A:278:LEU:HD21	2.05	0.82
1:A:477:VAL:CG1	1:A:506:MET:HB3	2.10	0.82
1:B:395:LYS:C	1:B:396:HIS:HD1	1.83	0.82
1:A:161:PHE:CE1	1:A:493:PHE:CE2	2.67	0.82
1:B:308:TRP:CD1	1:B:498:ALA:CB	2.62	0.81
1:A:433:PRO:HG3	1:A:445:TYR:CD2	2.15	0.81
1:B:62:ALA:O	1:B:66:THR:HG23	1.79	0.81
1:A:259:VAL:HG21	1:A:278:LEU:CD2	2.05	0.81
1:A:279:MET:SD	1:A:289:THR:CG2	2.68	0.81
1:A:66:THR:HB	1:A:402:THR:HB	1.59	0.81
1:A:160:PHE:C	1:A:160:PHE:CD1	2.54	0.81
1:B:35:PHE:C	1:B:42:LEU:HD21	2.01	0.81
1:B:97:LEU:HD23	1:B:97:LEU:H	1.45	0.81
1:B:246:ILE:HG22	1:B:247:CYS:N	1.95	0.81
1:B:51:ILE:HG22	1:B:52:LEU:CD2	2.09	0.81
1:A:46:LEU:HD23	1:A:210:PHE:HD1	1.45	0.81
1:A:17:GLY:O	1:A:21:ILE:HG23	1.81	0.81
1:A:478:THR:OG1	1:A:505:VAL:HG21	1.79	0.81
1:A:504:ILE:HG22	1:A:506:MET:HG2	1.61	0.81
1:B:27:MET:CE	1:B:248:LEU:HG	2.10	0.81
1:B:30:TYR:HE1	1:B:301:VAL:CG2	1.94	0.81
1:A:272:MET:N	1:A:272:MET:HE3	1.96	0.81
1:A:177:ILE:O	1:A:180:HIS:HB2	1.81	0.80
1:A:26:VAL:CG1	1:A:248:LEU:CD2	2.59	0.80
1:B:99:ILE:HD12	1:B:312:PRO:HB3	1.62	0.80
1:B:45:PHE:O	1:B:47:LEU:N	2.14	0.80
1:A:166:LEU:O	1:A:166:LEU:CD2	2.30	0.80
1:B:141:LEU:HD11	1:B:306:ALA:HB2	1.63	0.80
1:B:393:VAL:HG12	1:B:393:VAL:O	1.80	0.80
1:A:15:LEU:CD2	1:A:16:LEU:CD2	2.59	0.80
1:B:128:ILE:HG13	1:B:129:THR:N	1.94	0.80
1:B:59:LEU:N	1:B:59:LEU:HD23	1.95	0.80
1:A:109:PHE:CE1	1:A:271:VAL:HG21	2.16	0.80
1:A:120:TRP:CD1	1:A:122:ALA:HB3	2.17	0.80
1:A:173:ALA:O	1:A:177:ILE:HG13	1.82	0.80
1:A:109:PHE:CD2	1:A:301:VAL:HG21	2.16	0.80
1:A:432:LEU:O	1:A:432:LEU:CD1	2.30	0.80
1:A:74:GLY:O	1:A:75:VAL:CG1	2.30	0.80
1:A:98:GLN:HE21	1:A:98:GLN:CA	1.94	0.80
1:B:371:LEU:HD23	1:B:371:LEU:N	1.94	0.80
1:B:25:MET:HA	1:B:495:HIS:HE1	1.45	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:GLY:HA2	1:B:54:PHE:HB3	1.64	0.80
1:A:25:MET:CE	1:A:496:PRO:HG2	2.12	0.80
1:B:163:GLY:O	1:B:167:PRO:HG2	1.82	0.80
1:B:60:CYS:HB2	1:B:389:TYR:CD1	2.17	0.80
1:B:210:PHE:O	1:B:213:SER:HB2	1.80	0.80
1:B:103:PHE:CZ	1:B:308:TRP:HB2	2.16	0.80
1:B:103:PHE:O	1:B:106:MET:HB2	1.82	0.79
1:A:397:PRO:CD	1:A:398:ASP:N	2.42	0.79
1:A:166:LEU:O	1:A:166:LEU:HD23	1.83	0.79
1:B:337:VAL:O	1:B:337:VAL:CG2	2.30	0.79
1:B:353:LEU:CD1	1:B:353:LEU:O	2.30	0.79
1:B:57:VAL:O	1:B:61:ALA:CB	2.30	0.79
1:A:362:GLY:H	1:A:440:ASP:HB3	1.45	0.79
1:A:74:GLY:O	1:A:75:VAL:CG2	2.30	0.79
1:A:98:GLN:NE2	1:A:99:ILE:N	2.30	0.79
1:B:49:GLY:HA3	1:B:214:TYR:CE2	2.18	0.79
1:B:439:GLY:O	1:B:440:ASP:O	2.01	0.79
1:A:386:PHE:O	1:A:390:ILE:CD1	2.30	0.79
1:B:362:GLY:HA3	1:B:440:ASP:CG	2.02	0.79
1:A:221:ALA:O	1:A:224:VAL:N	2.16	0.79
1:B:187:ILE:CG2	1:B:187:ILE:O	2.31	0.79
1:B:353:LEU:HD12	1:B:353:LEU:C	2.02	0.79
1:A:15:LEU:CD2	1:A:16:LEU:N	2.46	0.79
1:A:340:THR:O	1:A:344:SER:HB3	1.82	0.79
1:A:52:LEU:O	1:A:56:PRO:HG2	1.83	0.78
1:B:161:PHE:CE1	1:B:165:LEU:HD11	2.18	0.78
1:B:234:TYR:C	1:B:234:TYR:CD2	2.53	0.78
1:A:50:GLY:HA2	1:A:54:PHE:HB3	1.64	0.78
1:B:67:VAL:CG2	1:B:70:TRP:CE3	2.66	0.78
1:A:172:ILE:HG22	1:A:173:ALA:N	1.97	0.78
1:B:76:PHE:O	1:B:76:PHE:CD2	2.36	0.78
1:A:484:SER:O	1:A:485:GLN:NE2	2.17	0.78
1:B:286:ILE:CG2	1:B:289:THR:CB	2.60	0.78
1:A:25:MET:HE2	1:A:496:PRO:HG2	1.65	0.78
1:B:129:THR:O	1:B:130:LYS:C	2.22	0.78
1:B:434:PRO:O	1:B:435:ASP:CB	2.31	0.78
1:A:364:ASN:ND2	1:A:438:GLN:CG	2.44	0.78
1:B:152:THR:O	1:B:155:ILE:N	2.17	0.78
1:B:215:MET:CE	1:B:378:TYR:CB	2.60	0.78
1:B:234:TYR:HE2	1:B:238:MET:CG	1.97	0.77
1:A:157:LYS:O	1:A:161:PHE:CD1	2.33	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:PRO:O	1:A:406:PRO:HG2	1.85	0.77
1:B:221:ALA:O	1:B:224:VAL:CG2	2.32	0.77
1:B:96:TYR:HD2	1:B:97:LEU:CD2	1.96	0.77
1:A:194:PHE:CD2	1:A:194:PHE:O	2.35	0.77
1:A:202:GLY:N	1:A:434:PRO:HG3	1.98	0.77
1:B:70:TRP:CH2	1:B:392:LEU:CD1	2.67	0.77
1:A:118:LEU:HD13	1:A:118:LEU:N	1.96	0.77
1:A:98:GLN:CB	1:A:377:ILE:CG2	2.63	0.77
1:B:246:ILE:CG2	1:B:247:CYS:N	2.47	0.77
1:B:70:TRP:O	1:B:72:GLU:N	2.18	0.77
1:A:178:TYR:HD2	1:A:178:TYR:C	1.85	0.77
1:A:275:PHE:HB3	1:A:290:VAL:HG22	1.67	0.77
1:B:98:GLN:HE22	1:B:497:ARG:HB3	1.50	0.77
1:A:337:VAL:CG2	1:A:337:VAL:O	2.30	0.77
1:B:166:LEU:HD12	1:B:167:PRO:N	1.99	0.77
1:B:259:VAL:HG21	1:B:278:LEU:HD11	1.66	0.77
1:B:353:LEU:CD1	1:B:353:LEU:C	2.53	0.77
1:A:44:PHE:CB	1:A:194:PHE:CE2	2.68	0.77
1:A:19:PHE:CD2	1:A:23:ALA:HB2	2.19	0.77
1:A:44:PHE:CB	1:A:194:PHE:HE2	1.97	0.77
1:A:98:GLN:HB2	1:A:377:ILE:CG2	2.14	0.77
1:A:106:MET:HB3	1:A:305:ILE:HD11	1.64	0.77
1:A:501:PRO:O	1:A:502:HIS:CB	2.30	0.76
1:B:202:GLY:O	1:B:205:VAL:HG12	1.85	0.76
1:B:395:LYS:HG3	1:B:396:HIS:HD1	1.48	0.76
1:A:161:PHE:HE1	1:A:493:PHE:HE2	1.31	0.76
1:B:286:ILE:HG21	1:B:289:THR:HG21	1.64	0.76
1:B:427:PHE:CZ	1:B:453:PHE:CE2	2.72	0.76
1:A:109:PHE:HE1	1:A:271:VAL:CG2	1.99	0.76
1:A:215:MET:HE1	1:A:378:TYR:CB	2.13	0.76
1:A:393:VAL:HG11	1:A:413:LEU:CD2	2.15	0.76
1:B:353:LEU:HD12	1:B:353:LEU:O	1.84	0.76
1:B:197:ASP:O	1:B:199:SER:N	2.16	0.76
1:A:125:GLU:O	1:A:127:PRO:CD	2.30	0.76
1:A:203:THR:HG22	1:A:204:LEU:CD2	2.13	0.76
1:A:55:ILE:HB	1:A:56:PRO:CD	2.15	0.76
1:A:119:LYS:HG2	1:A:291:ARG:NH1	2.00	0.76
1:A:375:VAL:O	1:A:379:LEU:HD23	1.86	0.75
1:B:36:ALA:O	1:B:39:GLY:N	2.16	0.75
1:B:494:LEU:O	1:B:499:ARG:HD3	1.87	0.75
1:A:437:ILE:HD11	1:A:442:THR:CG2	2.15	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:LEU:HD22	1:B:16:LEU:H	1.50	0.75
1:A:118:LEU:N	1:A:118:LEU:HD12	2.00	0.75
1:A:336:GLY:O	1:A:337:VAL:CG1	2.34	0.75
1:A:117:ILE:HG22	1:A:118:LEU:HD12	0.77	0.75
1:B:129:THR:O	1:B:131:THR:N	2.19	0.75
1:B:59:LEU:H	1:B:59:LEU:HD23	1.48	0.75
1:A:166:LEU:C	1:A:166:LEU:CD2	2.55	0.75
1:A:334:LYS:O	1:A:335:ASN:CB	2.34	0.75
1:B:393:VAL:O	1:B:393:VAL:CG1	2.35	0.75
1:A:166:LEU:HB3	1:A:167:PRO:HD3	1.69	0.75
1:A:449:LEU:O	1:A:449:LEU:CD1	2.30	0.75
1:A:457:LEU:HD12	1:A:457:LEU:C	1.92	0.75
1:A:19:PHE:CE2	1:A:23:ALA:HB2	2.22	0.75
1:A:116:TYR:OH	1:A:273:GLN:HG3	1.87	0.75
1:A:339:VAL:HG23	1:A:343:ILE:CG2	2.17	0.75
1:A:456:VAL:C	1:A:458:ALA:H	1.90	0.75
1:B:334:LYS:O	1:B:335:ASN:CB	2.34	0.75
1:A:21:ILE:HD12	1:A:223:HIS:ND1	2.00	0.74
1:A:117:ILE:O	1:A:291:ARG:CZ	2.35	0.74
1:B:269:ALA:HB1	1:B:272:MET:HE2	1.69	0.74
1:B:126:ASP:O	1:B:130:LYS:HB2	1.87	0.74
1:B:145:GLN:OE1	1:B:152:THR:CG2	2.34	0.74
1:B:266:ASN:C	1:B:266:ASN:ND2	2.36	0.74
1:A:29:VAL:CG2	1:A:30:TYR:N	2.51	0.74
1:B:233:ASP:O	1:B:236:LEU:HB2	1.87	0.74
1:B:113:ALA:HA	1:B:272:MET:SD	2.28	0.74
1:B:46:LEU:O	1:B:46:LEU:HD12	1.88	0.74
1:B:172:ILE:HG12	1:B:251:VAL:HG11	1.67	0.74
1:A:149:THR:HG21	1:A:314:ARG:NH1	2.02	0.74
1:B:204:LEU:HD23	1:B:204:LEU:H	1.50	0.74
1:B:310:VAL:O	1:B:310:VAL:CG2	2.36	0.74
1:B:267:LEU:HB2	1:B:364:ASN:OD1	1.86	0.74
1:A:332:MET:HG3	1:A:338:PRO:HA	1.67	0.74
1:A:70:TRP:HZ2	1:A:81:ASN:CB	2.01	0.74
1:B:29:VAL:HA	1:B:32:TYR:CD1	2.23	0.74
1:A:272:MET:CE	1:A:297:LEU:CD1	2.66	0.74
1:A:98:GLN:HE21	1:A:98:GLN:N	1.84	0.74
1:A:53:TRP:O	1:A:56:PRO:HD2	1.87	0.74
1:B:355:ILE:HG12	1:B:356:LEU:N	2.03	0.74
1:A:96:TYR:C	1:A:96:TYR:CD2	2.61	0.74
1:B:71:GLU:HB3	1:B:225:ASN:HD21	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:ALA:CB	1:B:272:MET:CE	2.66	0.74
1:A:143:LEU:HG	1:A:144:THR:H	1.50	0.73
1:B:124:ASN:HD21	1:B:268:SER:HB3	1.50	0.73
1:A:178:TYR:CD1	1:A:278:LEU:HD22	2.23	0.73
1:A:397:PRO:HD2	1:A:398:ASP:N	1.95	0.73
1:B:234:TYR:O	1:B:236:LEU:N	2.21	0.73
1:A:351:ILE:O	1:A:355:ILE:HG13	1.87	0.73
1:A:98:GLN:CA	1:A:377:ILE:HG21	2.18	0.73
1:A:282:VAL:O	1:A:283:ALA:HB2	1.86	0.73
1:A:332:MET:HG2	1:A:338:PRO:N	2.02	0.73
1:A:70:TRP:CZ2	1:A:81:ASN:CB	2.71	0.73
1:B:24:SER:CB	1:B:493:PHE:O	2.36	0.73
1:B:137:ILE:O	1:B:140:ALA:HB3	1.88	0.73
1:B:298:LEU:O	1:B:302:LEU:HD12	1.89	0.73
1:B:315:GLY:CA	1:B:500:SER:HB2	2.18	0.73
1:B:374:THR:CG2	1:B:375:VAL:N	2.51	0.73
1:B:432:LEU:CD1	1:B:432:LEU:O	2.29	0.73
1:B:67:VAL:HG23	1:B:70:TRP:HB2	1.70	0.73
1:A:194:PHE:HD2	1:A:194:PHE:C	1.91	0.73
1:A:205:VAL:O	1:A:208:VAL:HG22	1.88	0.73
1:B:80:SER:OG	1:B:85:PRO:HA	1.88	0.73
1:A:23:ALA:HA	1:A:241:LEU:HD21	1.71	0.72
1:B:161:PHE:CD1	1:B:165:LEU:HD12	2.12	0.72
1:B:66:THR:OG1	1:B:403:PHE:N	2.22	0.72
1:A:46:LEU:HD23	1:A:210:PHE:CD1	2.24	0.72
1:A:41:SER:O	1:A:44:PHE:HB3	1.88	0.72
1:A:246:ILE:O	1:A:250:SER:OG	2.06	0.72
1:A:442:THR:HB	1:A:445:TYR:CB	2.19	0.72
1:B:53:TRP:HH2	1:B:382:TYR:CZ	2.06	0.72
1:A:506:MET:O	1:A:509:LYS:CD	2.36	0.72
1:B:98:GLN:NE2	1:B:497:ARG:HB3	2.04	0.72
1:B:32:TYR:N	1:B:33:PRO:CD	2.53	0.72
1:B:311:GLY:H	1:B:312:PRO:CD	2.01	0.72
1:B:323:ASN:O	1:B:324:LEU:CD1	2.35	0.72
1:B:170:ILE:CD1	1:B:293:ILE:HD12	2.19	0.72
1:B:172:ILE:CG1	1:B:251:VAL:HG11	2.19	0.72
1:B:265:ILE:O	1:B:438:GLN:HG2	1.90	0.72
1:A:149:THR:HG21	1:A:314:ARG:HH12	1.53	0.71
1:B:145:GLN:OE1	1:B:152:THR:HG22	1.89	0.71
1:B:226:GLU:O	1:B:227:MET:O	2.07	0.71
1:B:365:MET:HG3	1:B:437:ILE:HD12	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:477:VAL:HG13	1:B:478:THR:N	2.04	0.71
1:B:55:ILE:CG2	1:B:56:PRO:CD	1.89	0.71
1:A:272:MET:HE1	1:A:297:LEU:CD1	2.21	0.71
1:A:298:LEU:O	1:A:302:LEU:HG	1.91	0.71
1:A:149:THR:HG21	1:A:314:ARG:NH2	2.04	0.71
1:A:442:THR:HB	1:A:445:TYR:HB2	1.71	0.71
1:A:82:THR:HB	1:A:391:VAL:HG12	1.70	0.71
1:B:126:ASP:OD1	1:B:127:PRO:HD2	1.90	0.71
1:A:101:ILE:N	1:A:101:ILE:HD13	2.06	0.71
1:A:149:THR:O	1:A:149:THR:OG1	2.09	0.71
1:A:215:MET:HE2	1:A:378:TYR:CB	2.16	0.71
1:A:67:VAL:HG11	1:A:70:TRP:CD2	2.26	0.71
1:B:110:VAL:HG23	1:B:301:VAL:HG11	1.72	0.71
1:B:332:MET:HE2	1:B:336:GLY:HA2	1.71	0.71
1:B:129:THR:O	1:B:132:ILE:N	2.24	0.71
1:B:170:ILE:CG2	1:B:275:PHE:CZ	2.71	0.71
1:A:224:VAL:O	1:A:227:MET:CB	2.34	0.71
1:B:35:PHE:O	1:B:42:LEU:CD2	2.39	0.71
1:B:362:GLY:N	1:B:440:ASP:HB3	2.05	0.71
1:B:203:THR:C	1:B:204:LEU:HD23	2.10	0.70
1:A:99:ILE:HG23	1:A:99:ILE:O	1.89	0.70
1:B:82:THR:CG2	1:B:391:VAL:CG1	2.69	0.70
1:A:431:PHE:O	1:A:446:VAL:CG2	2.39	0.70
1:A:67:VAL:HG12	1:A:70:TRP:CB	2.21	0.70
1:B:24:SER:HB2	1:B:493:PHE:O	1.90	0.70
1:A:22:THR:HG22	1:A:22:THR:O	1.90	0.70
1:A:399:LEU:HD22	1:A:400:LYS:H	1.55	0.70
1:A:153:ALA:HB1	1:A:489:LYS:O	1.91	0.70
1:A:506:MET:O	1:A:507:ASN:HB2	1.91	0.70
1:B:482:ILE:C	1:B:483:ASN:OD1	2.30	0.70
1:A:66:THR:HG21	1:A:224:VAL:HG11	1.73	0.70
1:B:70:TRP:CZ3	1:B:392:LEU:CD1	2.74	0.70
1:B:377:ILE:CD1	1:B:456:VAL:HG11	2.22	0.70
1:B:70:TRP:O	1:B:71:GLU:C	2.29	0.70
1:A:456:VAL:C	1:A:458:ALA:N	2.42	0.70
1:B:200:LYS:O	1:B:201:VAL:C	2.30	0.70
1:A:285:GLU:HG3	1:A:286:ILE:HG12	1.73	0.70
1:A:347:VAL:O	1:A:351:ILE:CG1	2.33	0.70
1:A:96:TYR:C	1:A:96:TYR:HD2	1.94	0.70
1:A:106:MET:CB	1:A:305:ILE:HD11	2.22	0.70
1:B:269:ALA:HB1	1:B:272:MET:HE1	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:LEU:HB3	1:A:167:PRO:CD	2.22	0.69
1:A:476:GLY:O	1:A:477:VAL:CG1	2.40	0.69
1:B:15:LEU:CD2	1:B:16:LEU:HD13	2.22	0.69
1:B:146:PHE:HE1	1:B:342:VAL:CG1	2.03	0.69
1:A:104:ILE:HB	1:A:105:PRO:HD3	1.75	0.69
1:A:71:GLU:HB2	1:A:72:GLU:OE1	1.92	0.69
1:B:258:MET:HE2	1:B:259:VAL:HG23	1.74	0.69
1:B:70:TRP:C	1:B:72:GLU:N	2.42	0.69
1:A:336:GLY:O	1:A:337:VAL:HG13	1.93	0.69
1:B:124:ASN:ND2	1:B:268:SER:OG	2.25	0.69
1:A:437:ILE:C	1:A:438:GLN:HG2	2.11	0.69
1:B:194:PHE:CD1	1:B:195:PHE:CE2	2.79	0.69
1:A:143:LEU:CD1	1:A:144:THR:N	2.55	0.69
1:A:279:MET:C	1:A:281:HIS:H	1.95	0.69
1:A:272:MET:HE1	1:A:297:LEU:HD12	1.74	0.69
1:A:124:ASN:ND2	1:A:269:ALA:HB2	2.07	0.69
1:B:427:PHE:HZ	1:B:453:PHE:HE2	1.35	0.69
1:B:97:LEU:HD23	1:B:97:LEU:N	2.06	0.69
1:A:174:LEU:HD22	1:A:278:LEU:HB3	1.73	0.69
1:A:160:PHE:CZ	1:A:165:LEU:HD23	2.13	0.69
1:A:283:ALA:O	1:A:285:GLU:HG2	1.93	0.69
1:A:435:ASP:OD2	1:A:435:ASP:C	2.30	0.69
1:A:279:MET:HG2	1:A:287:GLU:HA	1.75	0.68
1:B:414:VAL:O	1:B:418:VAL:HG23	1.93	0.68
1:B:24:SER:HB3	1:B:493:PHE:HA	1.75	0.68
1:B:234:TYR:CE2	1:B:238:MET:CG	2.76	0.68
1:A:200:LYS:HG3	1:A:201:VAL:N	2.07	0.68
1:A:50:GLY:HA2	1:A:54:PHE:CB	2.24	0.68
1:B:166:LEU:C	1:B:166:LEU:HD13	2.11	0.68
1:B:117:ILE:HD11	1:B:295:ALA:N	2.07	0.68
1:B:82:THR:HG22	1:B:391:VAL:HG11	1.74	0.68
1:A:19:PHE:CE2	1:A:23:ALA:CB	2.76	0.68
1:A:445:TYR:C	1:A:445:TYR:HD1	1.96	0.68
1:B:329:PHE:O	1:B:330:ALA:HB2	1.93	0.68
1:B:69:GLY:C	1:B:70:TRP:CD1	2.66	0.68
1:A:279:MET:SD	1:A:289:THR:HG21	2.34	0.68
1:A:98:GLN:HA	1:A:377:ILE:HG21	1.76	0.68
1:A:478:THR:OG1	1:A:505:VAL:HG22	1.92	0.68
1:B:166:LEU:C	1:B:168:ALA:H	1.95	0.68
1:B:34:THR:C	1:B:37:THR:HG22	2.14	0.68
1:A:173:ALA:O	1:A:177:ILE:CG1	2.42	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:LEU:HD22	1:B:278:LEU:HB3	1.76	0.68
1:A:321:GLN:HE22	1:A:476:GLY:HA3	1.59	0.68
1:A:70:TRP:HZ2	1:A:81:ASN:HB3	1.59	0.68
1:B:174:LEU:CD2	1:B:278:LEU:HB3	2.23	0.68
1:B:332:MET:HE2	1:B:336:GLY:CA	2.24	0.68
1:A:13:LEU:HB2	1:A:227:MET:HA	1.76	0.67
1:A:74:GLY:O	1:A:75:VAL:CB	2.43	0.67
1:A:101:ILE:HG13	1:A:373:LEU:CD1	2.25	0.67
1:A:197:ASP:O	1:A:203:THR:OG1	2.06	0.67
1:B:29:VAL:HB	1:B:32:TYR:CD1	2.30	0.67
1:B:479:LEU:O	1:B:481:PRO:HD3	1.95	0.67
1:A:118:LEU:O	1:A:119:LYS:C	2.29	0.67
1:A:194:PHE:CD2	1:A:194:PHE:C	2.64	0.67
1:B:191:SER:C	1:B:193:THR:H	1.98	0.67
1:B:194:PHE:C	1:B:194:PHE:CD1	2.67	0.67
1:B:194:PHE:CE1	1:B:195:PHE:CD2	2.82	0.67
1:B:377:ILE:HG12	1:B:456:VAL:HG11	1.76	0.67
1:A:55:ILE:CB	1:A:56:PRO:HD3	2.21	0.67
1:B:364:ASN:HB2	1:B:440:ASP:OD1	1.95	0.67
1:A:282:VAL:O	1:A:283:ALA:CB	2.43	0.67
1:A:202:GLY:CA	1:A:434:PRO:CG	1.96	0.67
1:A:503:TYR:CD2	1:A:503:TYR:N	2.62	0.67
1:B:146:PHE:O	1:B:148:GLY:N	2.28	0.67
1:A:339:VAL:HG23	1:A:343:ILE:HG21	1.76	0.67
1:B:45:PHE:C	1:B:47:LEU:H	1.98	0.67
1:B:311:GLY:O	1:B:500:SER:HB3	1.94	0.67
1:A:434:PRO:O	1:A:435:ASP:CB	2.43	0.66
1:A:439:GLY:O	1:A:440:ASP:C	2.30	0.66
1:A:501:PRO:O	1:A:502:HIS:HB3	1.95	0.66
1:A:75:VAL:CG1	1:A:78:TRP:CZ3	2.73	0.66
1:B:339:VAL:HG23	1:B:343:ILE:HD12	1.76	0.66
1:A:100:ALA:O	1:A:349:THR:HG23	1.94	0.66
1:B:15:LEU:HD22	1:B:16:LEU:HD22	1.76	0.66
1:B:71:GLU:HB3	1:B:225:ASN:ND2	2.10	0.66
1:A:143:LEU:HD12	1:A:144:THR:N	2.10	0.66
1:B:104:ILE:N	1:B:105:PRO:HD2	2.11	0.66
1:B:161:PHE:CE1	1:B:165:LEU:CD1	2.78	0.66
1:B:351:ILE:O	1:B:355:ILE:CG2	2.43	0.66
1:A:26:VAL:HG11	1:A:248:LEU:CD2	2.25	0.66
1:B:351:ILE:HG22	1:B:352:ALA:N	2.11	0.66
1:B:78:TRP:N	1:B:78:TRP:CD1	2.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:GLY:N	1:B:312:PRO:CD	2.55	0.66
1:B:99:ILE:HD12	1:B:312:PRO:CB	2.24	0.66
1:B:365:MET:CG	1:B:437:ILE:HD12	2.26	0.66
1:A:134:ALA:HB1	1:A:353:LEU:CD2	2.21	0.66
1:A:161:PHE:CE1	1:A:493:PHE:HE2	2.10	0.66
1:B:29:VAL:HB	1:B:32:TYR:CE1	2.30	0.66
1:B:380:CYS:O	1:B:383:PHE:HB2	1.96	0.66
1:B:47:LEU:CD2	1:B:246:ILE:CD1	2.69	0.66
1:B:307:SER:HB2	1:B:494:LEU:HD11	1.77	0.66
1:A:203:THR:CG2	1:A:204:LEU:HD23	2.18	0.66
1:B:298:LEU:CD1	1:B:302:LEU:HD11	2.25	0.66
1:A:30:TYR:O	1:A:33:PRO:HD2	1.96	0.66
1:B:65:ALA:O	1:B:71:GLU:HA	1.95	0.66
1:A:151:TYR:HB2	1:A:155:ILE:HD11	1.78	0.65
1:A:353:LEU:HD12	1:A:357:THR:HG21	1.76	0.65
1:B:127:PRO:O	1:B:131:THR:CG2	2.44	0.65
1:A:347:VAL:HG13	1:A:351:ILE:CD1	2.24	0.65
1:A:462:ILE:O	1:A:466:VAL:HG23	1.96	0.65
1:A:70:TRP:CZ2	1:A:81:ASN:HB2	2.31	0.65
1:B:103:PHE:HZ	1:B:308:TRP:HB2	1.60	0.65
1:B:351:ILE:CG2	1:B:352:ALA:N	2.60	0.65
1:B:420:LEU:O	1:B:420:LEU:HD12	1.95	0.65
1:A:242:MET:O	1:A:246:ILE:HG13	1.96	0.65
1:A:72:GLU:N	1:A:72:GLU:OE1	2.30	0.65
1:B:359:THR:CG2	1:B:359:THR:O	2.38	0.65
1:A:151:TYR:O	1:A:152:THR:C	2.33	0.65
1:B:222:THR:C	1:B:224:VAL:N	2.48	0.65
1:A:373:LEU:O	1:A:376:VAL:HG23	1.96	0.65
1:B:22:THR:O	1:B:241:LEU:CD2	2.44	0.65
1:A:171:LEU:HD22	1:A:171:LEU:C	2.17	0.65
1:A:364:ASN:ND2	1:A:438:GLN:HB2	2.12	0.65
1:B:166:LEU:O	1:B:168:ALA:N	2.30	0.65
1:A:125:GLU:OE1	1:A:125:GLU:N	2.30	0.65
1:B:367:PHE:O	1:B:370:ALA:N	2.27	0.65
1:A:149:THR:HG21	1:A:314:ARG:CZ	2.27	0.65
1:B:395:LYS:HG3	1:B:396:HIS:CE1	2.31	0.65
1:B:396:HIS:N	1:B:397:PRO:HD3	2.12	0.65
1:A:205:VAL:O	1:A:205:VAL:HG22	1.94	0.64
1:A:98:GLN:C	1:A:98:GLN:NE2	2.50	0.64
1:B:124:ASN:ND2	1:B:268:SER:CB	2.59	0.64
1:B:70:TRP:HH2	1:B:392:LEU:CD1	2.10	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:TRP:HE1	1:A:122:ALA:HB3	1.61	0.64
1:A:445:TYR:CD1	1:A:445:TYR:C	2.70	0.64
1:A:157:LYS:HD3	1:A:493:PHE:CE2	2.33	0.64
1:B:286:ILE:O	1:B:289:THR:HG22	1.98	0.64
1:A:283:ALA:O	1:A:285:GLU:N	2.30	0.64
1:A:32:TYR:N	1:A:33:PRO:CD	2.60	0.64
1:A:465:ALA:O	1:A:466:VAL:C	2.35	0.64
1:B:234:TYR:CE2	1:B:238:MET:SD	2.90	0.64
1:A:202:GLY:CA	1:A:434:PRO:CD	2.60	0.64
1:A:435:ASP:OD2	1:A:436:ASN:N	2.30	0.64
1:B:67:VAL:O	1:B:68:ASP:C	2.34	0.64
1:A:212:LEU:CD1	1:A:375:VAL:HG23	2.26	0.64
1:B:259:VAL:HG21	1:B:278:LEU:CD1	2.27	0.64
1:B:229:ASN:O	1:B:233:ASP:CB	2.38	0.64
1:B:276:THR:CG2	1:B:277:VAL:N	2.60	0.64
1:B:374:THR:HG22	1:B:375:VAL:H	1.63	0.64
1:B:82:THR:CG2	1:B:391:VAL:HG11	2.27	0.64
1:B:95:GLY:O	1:B:98:GLN:HB3	1.97	0.64
1:B:336:GLY:O	1:B:337:VAL:CG1	2.46	0.64
1:A:332:MET:CG	1:A:338:PRO:N	2.60	0.64
1:A:399:LEU:HD23	1:A:400:LYS:H	1.62	0.64
1:B:101:ILE:HG12	1:B:373:LEU:HD13	1.79	0.64
1:B:128:ILE:CG1	1:B:129:THR:N	2.61	0.64
1:A:456:VAL:O	1:A:458:ALA:N	2.30	0.64
1:B:390:ILE:HG22	1:B:394:LEU:HG	1.80	0.64
1:B:25:MET:CA	1:B:495:HIS:CE1	2.69	0.64
1:A:124:ASN:ND2	1:A:269:ALA:CB	2.61	0.63
1:A:266:ASN:O	1:A:270:GLY:HA3	1.98	0.63
1:A:279:MET:O	1:A:281:HIS:N	2.31	0.63
1:B:395:LYS:O	1:B:395:LYS:HG3	1.98	0.63
1:B:51:ILE:CG2	1:B:52:LEU:CD2	2.72	0.63
1:A:225:ASN:O	1:A:227:MET:N	2.32	0.63
1:A:85:PRO:O	1:A:86:ARG:C	2.36	0.63
1:A:117:ILE:C	1:A:118:LEU:HD12	2.18	0.63
1:A:171:LEU:CD2	1:A:171:LEU:C	2.66	0.63
1:A:98:GLN:CA	1:A:98:GLN:NE2	2.56	0.63
1:A:222:THR:C	1:A:224:VAL:H	2.00	0.63
1:A:483:ASN:C	1:A:485:GLN:N	2.39	0.63
1:B:376:VAL:HG11	1:B:453:PHE:CG	2.33	0.63
1:B:98:GLN:OE1	1:B:99:ILE:CG1	2.42	0.63
1:A:76:PHE:CD1	1:A:76:PHE:O	2.45	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:THR:O	1:B:224:VAL:N	2.30	0.63
1:B:311:GLY:H	1:B:312:PRO:HD2	1.64	0.63
1:A:154:ARG:HH21	1:A:489:LYS:CE	1.86	0.63
1:A:452:SER:O	1:A:456:VAL:HG23	1.98	0.63
1:B:166:LEU:C	1:B:168:ALA:N	2.51	0.63
1:B:36:ALA:CB	1:B:253:GLY:O	2.42	0.63
1:B:357:THR:CG2	1:B:358:ASN:N	2.62	0.63
1:A:321:GLN:HE22	1:A:477:VAL:H	1.44	0.63
1:A:76:PHE:HD1	1:A:76:PHE:C	2.01	0.63
1:B:99:ILE:HD12	1:B:312:PRO:CG	2.28	0.63
1:B:409:LYS:O	1:B:413:LEU:HB2	1.99	0.63
1:A:166:LEU:HD22	1:A:166:LEU:C	2.19	0.63
1:A:160:PHE:C	1:A:160:PHE:HD1	2.02	0.63
1:A:335:ASN:H	1:A:506:MET:CE	2.11	0.63
1:B:308:TRP:CD1	1:B:498:ALA:HB2	2.33	0.63
1:A:124:ASN:O	1:A:130:LYS:HE3	1.98	0.62
1:B:146:PHE:CE1	1:B:342:VAL:HG11	2.29	0.62
1:B:377:ILE:HD11	1:B:456:VAL:HG11	1.81	0.62
1:A:152:THR:CG2	1:A:307:SER:HA	2.29	0.62
1:A:222:THR:C	1:A:224:VAL:N	2.50	0.62
1:A:31:GLU:HB3	1:A:35:PHE:CE2	2.34	0.62
1:A:336:GLY:H	1:A:506:MET:CE	2.12	0.62
1:B:160:PHE:CD1	1:B:165:LEU:HD21	2.27	0.62
1:B:234:TYR:HB3	1:B:235:PRO:CD	2.29	0.62
1:B:262:GLY:HA2	1:B:265:ILE:CG1	2.19	0.62
1:A:232:ARG:O	1:A:236:LEU:HD23	2.00	0.62
1:B:234:TYR:HB3	1:B:235:PRO:HD3	1.81	0.62
1:A:70:TRP:HZ3	1:A:392:LEU:HD13	1.65	0.62
1:A:85:PRO:O	1:A:88:GLY:N	2.32	0.62
1:B:269:ALA:CB	1:B:272:MET:HE1	2.29	0.62
1:A:163:GLY:O	1:A:167:PRO:CD	2.47	0.62
1:A:208:VAL:HG23	1:A:209:ALA:H	1.65	0.62
1:A:279:MET:HE2	1:A:279:MET:HA	1.82	0.62
1:B:172:ILE:HG22	1:B:173:ALA:N	2.14	0.62
1:A:11:LYS:CG	1:A:226:GLU:HA	2.29	0.62
1:A:279:MET:SD	1:A:289:THR:HG22	2.39	0.62
1:A:505:VAL:CG2	1:A:505:VAL:O	2.43	0.62
1:B:117:ILE:HD11	1:B:295:ALA:CA	2.30	0.62
1:A:336:GLY:C	1:A:337:VAL:HG12	2.20	0.62
1:A:406:PRO:O	1:A:406:PRO:CG	2.46	0.62
1:B:126:ASP:CG	1:B:127:PRO:HD2	2.20	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:ARG:O	1:A:233:ASP:C	2.36	0.61
1:A:117:ILE:HD12	1:A:294:SER:HB3	1.82	0.61
1:A:332:MET:CG	1:A:338:PRO:CA	2.78	0.61
1:A:399:LEU:HB3	1:A:401:ARG:HH21	1.65	0.61
1:B:374:THR:HG22	1:B:375:VAL:N	2.15	0.61
1:A:163:GLY:O	1:A:167:PRO:HG2	1.99	0.61
1:B:60:CYS:HB2	1:B:389:TYR:CE1	2.35	0.61
1:B:279:MET:O	1:B:283:ALA:N	2.27	0.61
1:B:483:ASN:N	1:B:483:ASN:OD1	2.30	0.61
1:A:166:LEU:HD22	1:A:166:LEU:O	1.99	0.61
1:A:197:ASP:OD1	1:A:199:SER:HB2	2.00	0.61
1:A:433:PRO:HB3	1:A:442:THR:HG21	1.82	0.61
1:A:68:ASP:HB2	1:A:400:LYS:HB2	1.83	0.61
1:A:75:VAL:O	1:A:75:VAL:HG23	2.00	0.61
1:B:353:LEU:O	1:B:353:LEU:HD13	1.98	0.61
1:B:317:TYR:CD2	1:B:479:LEU:HD11	2.30	0.61
1:B:489:LYS:O	1:B:490:GLY:C	2.37	0.61
1:A:359:THR:HG22	1:A:360:GLY:N	2.16	0.61
1:A:433:PRO:HG3	1:A:445:TYR:CG	2.36	0.61
1:A:223:HIS:HE1	1:A:492:PHE:CE2	2.19	0.61
1:B:222:THR:O	1:B:225:ASN:N	2.28	0.61
1:A:356:LEU:HD22	1:A:369:ILE:HG21	1.83	0.61
1:B:15:LEU:CD2	1:B:16:LEU:CA	2.70	0.61
1:B:341:LEU:HA	1:B:344:SER:HB3	1.83	0.61
1:B:29:VAL:C	1:B:31:GLU:H	2.04	0.61
1:A:379:LEU:HD12	1:A:383:PHE:CZ	2.36	0.61
1:A:76:PHE:CD1	1:A:76:PHE:C	2.70	0.61
1:B:133:ALA:O	1:B:137:ILE:HG13	2.01	0.60
1:A:101:ILE:HG22	1:A:374:THR:OG1	2.01	0.60
1:B:377:ILE:CG1	1:B:456:VAL:HG11	2.30	0.60
1:A:18:PHE:O	1:A:21:ILE:HG12	2.00	0.60
1:B:19:PHE:O	1:B:23:ALA:HB2	2.01	0.60
1:B:67:VAL:HG23	1:B:70:TRP:CB	2.30	0.60
1:A:330:ALA:C	1:A:331:LYS:CG	2.69	0.60
1:A:476:GLY:O	1:A:477:VAL:HG13	2.02	0.60
1:A:309:ILE:O	1:A:309:ILE:HG22	2.01	0.60
1:B:390:ILE:O	1:B:394:LEU:HB2	2.01	0.60
1:A:122:ALA:O	1:A:126:ASP:HB2	2.01	0.60
1:A:279:MET:HA	1:A:282:VAL:HG23	1.82	0.60
1:A:78:TRP:CD1	1:A:78:TRP:N	2.64	0.60
1:B:123:LEU:O	1:B:130:LYS:HG2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:PHE:CE2	1:B:238:MET:HE3	2.37	0.60
1:B:265:ILE:O	1:B:438:GLN:CG	2.50	0.60
1:B:181:SER:O	1:B:182:GLY:C	2.40	0.60
1:B:50:GLY:HA3	1:B:242:MET:CG	2.32	0.60
1:A:202:GLY:O	1:A:205:VAL:HG12	2.02	0.60
1:A:457:LEU:O	1:A:461:PHE:HD2	1.84	0.60
1:B:336:GLY:O	1:B:337:VAL:HG13	2.02	0.60
1:B:392:LEU:HA	1:B:396:HIS:HB2	1.84	0.60
1:B:60:CYS:HA	1:B:405:ILE:HD11	1.83	0.60
1:A:67:VAL:CG1	1:A:70:TRP:HB2	2.29	0.60
1:B:234:TYR:HD2	1:B:235:PRO:N	1.99	0.60
1:B:326:PRO:HB2	1:B:329:PHE:CD2	2.37	0.60
1:B:157:LYS:CG	1:B:493:PHE:HE2	2.13	0.60
1:B:56:PRO:O	1:B:60:CYS:SG	2.54	0.60
1:A:293:ILE:HA	1:A:296:LEU:HD12	1.84	0.59
1:A:433:PRO:CG	1:A:445:TYR:CD2	2.84	0.59
1:B:42:LEU:O	1:B:46:LEU:CB	2.43	0.59
1:A:272:MET:H	1:A:272:MET:HE3	1.64	0.59
1:A:40:PHE:O	1:A:43:VAL:HG23	2.01	0.59
1:A:172:ILE:HG23	1:A:173:ALA:N	2.17	0.59
1:A:152:THR:HG21	1:A:307:SER:HA	1.84	0.59
1:A:501:PRO:C	1:A:502:HIS:CG	2.72	0.59
1:B:131:THR:CG2	1:B:357:THR:HG21	2.33	0.59
1:B:194:PHE:CG	1:B:194:PHE:O	2.54	0.59
1:B:103:PHE:CE1	1:B:308:TRP:CE3	2.90	0.59
1:B:234:TYR:C	1:B:236:LEU:N	2.53	0.59
1:A:152:THR:O	1:A:153:ALA:C	2.39	0.59
1:A:94:PHE:CB	1:A:381:ALA:HB2	2.27	0.59
1:A:503:TYR:H	1:A:503:TYR:HD2	1.45	0.59
1:A:68:ASP:HB2	1:A:400:LYS:CB	2.32	0.59
1:B:103:PHE:CE1	1:B:308:TRP:HE3	2.20	0.59
1:A:113:ALA:HA	1:A:272:MET:SD	2.41	0.59
1:B:157:LYS:HG3	1:B:493:PHE:CE2	2.30	0.59
1:B:44:PHE:CD2	1:B:196:PRO:CD	2.86	0.59
1:A:339:VAL:O	1:A:339:VAL:HG23	2.03	0.59
1:A:38:SER:HG	1:A:41:SER:HB2	1.67	0.59
1:B:351:ILE:HG22	1:B:352:ALA:H	1.66	0.59
1:B:376:VAL:CG1	1:B:453:PHE:CD1	2.85	0.59
1:B:43:VAL:O	1:B:47:LEU:HB2	2.03	0.59
1:B:21:ILE:HD11	1:B:484:SER:HB2	1.85	0.59
1:B:339:VAL:HG23	1:B:339:VAL:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:PRO:O	1:A:231:GLY:C	2.39	0.59
1:A:373:LEU:HD22	1:A:377:ILE:HD12	1.85	0.59
1:B:170:ILE:HD13	1:B:293:ILE:CD1	2.32	0.59
1:B:59:LEU:CD2	1:B:59:LEU:N	2.63	0.59
1:B:106:MET:HB3	1:B:305:ILE:HD11	1.85	0.58
1:B:127:PRO:O	1:B:131:THR:HG22	2.03	0.58
1:B:362:GLY:CA	1:B:440:ASP:CG	2.70	0.58
1:A:283:ALA:HB1	1:A:285:GLU:CD	2.23	0.58
1:B:15:LEU:HD23	1:B:16:LEU:HA	1.83	0.58
1:B:171:LEU:HG	1:B:172:ILE:N	2.17	0.58
1:A:128:ILE:HD12	1:A:128:ILE:C	2.17	0.58
1:A:128:ILE:O	1:A:128:ILE:CD1	2.38	0.58
1:A:157:LYS:HD3	1:A:493:PHE:HE2	1.67	0.58
1:B:234:TYR:HE2	1:B:238:MET:HG3	1.69	0.58
1:A:203:THR:HG22	1:A:204:LEU:N	2.19	0.58
1:A:319:THR:HA	1:A:324:LEU:HD12	1.84	0.58
1:A:476:GLY:C	1:A:477:VAL:HG13	2.23	0.58
1:B:120:TRP:HD1	1:B:121:PRO:HD2	1.68	0.58
1:A:421:LEU:HD12	1:B:424:ILE:HD12	1.85	0.58
1:A:343:ILE:HG13	1:A:344:SER:N	2.18	0.58
1:A:417:ILE:HD11	1:B:424:ILE:HG22	1.85	0.58
1:A:434:PRO:O	1:A:435:ASP:CG	2.41	0.58
1:B:234:TYR:HE2	1:B:238:MET:SD	2.23	0.58
1:A:101:ILE:CG1	1:A:373:LEU:HD13	2.31	0.58
1:A:385:LEU:HD23	1:A:385:LEU:C	2.23	0.58
1:A:73:GLY:HA3	1:A:77:ALA:HB3	1.82	0.58
1:A:172:ILE:CD1	1:A:251:VAL:CG1	2.65	0.58
1:A:482:ILE:HG22	1:A:483:ASN:N	2.19	0.58
1:A:64:MET:HE3	1:A:78:TRP:CE3	2.38	0.58
1:B:286:ILE:CG2	1:B:286:ILE:O	2.48	0.58
1:B:191:SER:O	1:B:193:THR:N	2.37	0.58
1:B:30:TYR:OH	1:B:164:ILE:HD11	2.04	0.58
1:B:170:ILE:CG2	1:B:275:PHE:CE1	2.82	0.58
1:B:44:PHE:CE2	1:B:196:PRO:HD2	2.39	0.58
1:B:234:TYR:O	1:B:237:ALA:N	2.36	0.58
1:A:198:PHE:O	1:B:395:LYS:HD3	2.03	0.57
1:B:26:VAL:HG23	1:B:27:MET:CE	2.34	0.57
1:A:101:ILE:CD1	1:A:101:ILE:N	2.68	0.57
1:B:246:ILE:HG22	1:B:247:CYS:H	1.69	0.57
1:B:46:LEU:O	1:B:46:LEU:CD1	2.52	0.57
1:A:445:TYR:HE1	1:A:449:LEU:HD23	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:462:ILE:O	1:B:466:VAL:HB	2.04	0.57
1:B:495:HIS:O	1:B:498:ALA:N	2.37	0.57
1:A:98:GLN:HG3	1:A:378:TYR:HD2	1.67	0.57
1:B:82:THR:CG2	1:B:391:VAL:HB	2.33	0.57
1:B:439:GLY:C	1:B:440:ASP:O	2.41	0.57
1:A:465:ALA:O	1:A:467:HIS:N	2.37	0.57
1:A:80:SER:HA	1:A:84:GLY:O	2.04	0.57
1:A:19:PHE:HE2	1:A:23:ALA:CB	2.17	0.57
1:A:242:MET:CE	1:A:246:ILE:HD11	2.34	0.57
1:B:152:THR:O	1:B:156:ALA:N	2.36	0.57
1:B:204:LEU:O	1:B:207:PHE:N	2.30	0.57
1:B:47:LEU:O	1:B:51:ILE:HB	2.05	0.57
1:A:146:PHE:O	1:A:148:GLY:N	2.30	0.57
1:B:279:MET:HE3	1:B:286:ILE:CG2	2.35	0.57
1:A:365:MET:O	1:A:369:ILE:HB	2.05	0.57
1:A:67:VAL:CG2	1:A:401:ARG:HG3	2.30	0.57
1:A:421:LEU:HD11	1:B:424:ILE:CD1	2.25	0.57
1:A:154:ARG:CZ	1:A:489:LYS:HG3	2.35	0.57
1:A:504:ILE:O	1:A:504:ILE:CG2	2.45	0.57
1:B:234:TYR:C	1:B:236:LEU:H	2.06	0.57
1:A:200:LYS:NZ	1:A:200:LYS:CB	2.67	0.57
1:A:333:ASN:O	1:A:334:LYS:C	2.42	0.57
1:A:67:VAL:HA	1:A:400:LYS:O	2.05	0.57
1:A:44:PHE:CG	1:A:194:PHE:HE2	2.23	0.57
1:B:124:ASN:C	1:B:124:ASN:OD1	2.43	0.57
1:A:256:ILE:HA	1:A:274:THR:OG1	2.04	0.56
1:A:286:ILE:O	1:A:289:THR:CG2	2.51	0.56
1:A:353:LEU:HD12	1:A:357:THR:CG2	2.35	0.56
1:A:399:LEU:HD23	1:A:400:LYS:N	2.19	0.56
1:B:126:ASP:OD2	1:B:128:ILE:HG23	2.05	0.56
1:B:390:ILE:HD11	1:B:416:ALA:HB3	1.86	0.56
1:A:491:HIS:O	1:A:494:LEU:CB	2.34	0.56
1:B:53:TRP:O	1:B:54:PHE:C	2.44	0.56
1:B:163:GLY:HA2	1:B:167:PRO:HG2	1.88	0.56
1:B:377:ILE:HG12	1:B:456:VAL:CG1	2.35	0.56
1:B:60:CYS:CA	1:B:405:ILE:HD11	2.35	0.56
1:B:92:ILE:CG2	1:B:93:SER:N	2.69	0.56
1:A:389:TYR:O	1:A:392:LEU:HB3	2.06	0.56
1:A:435:ASP:O	1:A:441:SER:HA	2.05	0.56
1:B:298:LEU:C	1:B:302:LEU:HD12	2.26	0.56
1:B:342:VAL:O	1:B:346:LEU:HG	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:GLY:C	1:A:337:VAL:CG1	2.74	0.56
1:A:427:PHE:O	1:A:430:SER:HB2	2.05	0.56
1:B:396:HIS:N	1:B:397:PRO:CD	2.68	0.56
1:A:12:GLN:HG3	1:A:228:SER:HB2	1.86	0.56
1:A:53:TRP:O	1:A:54:PHE:C	2.43	0.56
1:B:178:TYR:OH	1:B:183:ALA:C	2.44	0.56
1:B:336:GLY:C	1:B:337:VAL:HG12	2.26	0.56
1:A:373:LEU:HA	1:A:376:VAL:CG2	2.35	0.56
1:A:178:TYR:CD2	1:A:178:TYR:O	2.59	0.56
1:A:357:THR:OG1	1:A:358:ASN:N	2.38	0.56
1:A:392:LEU:O	1:A:393:VAL:C	2.44	0.56
1:A:484:SER:C	1:A:485:GLN:HE21	2.10	0.56
1:B:120:TRP:CE3	1:B:123:LEU:HD22	2.40	0.56
1:B:226:GLU:OE2	1:B:483:ASN:HB3	2.06	0.56
1:A:477:VAL:HG21	1:A:504:ILE:HG23	1.88	0.55
1:B:41:SER:CB	1:B:196:PRO:HG3	2.18	0.55
1:B:103:PHE:CZ	1:B:308:TRP:CB	2.89	0.55
1:A:263:ASN:O	1:A:438:GLN:HB3	2.05	0.55
1:B:289:THR:CG2	1:B:290:VAL:N	2.70	0.55
1:B:44:PHE:O	1:B:47:LEU:HB2	2.06	0.55
1:B:45:PHE:C	1:B:47:LEU:N	2.58	0.55
1:A:266:ASN:O	1:A:270:GLY:CA	2.54	0.55
1:B:279:MET:HE3	1:B:286:ILE:HG21	1.87	0.55
1:B:92:ILE:HG23	1:B:93:SER:N	2.21	0.55
1:A:170:ILE:O	1:A:174:LEU:HB2	2.06	0.55
1:A:364:ASN:ND2	1:A:438:GLN:CB	2.69	0.55
1:A:378:TYR:CD1	1:A:382:TYR:CE2	2.94	0.55
1:B:48:LEU:CD2	1:B:48:LEU:N	2.60	0.55
1:A:11:LYS:HG3	1:A:226:GLU:HB3	1.88	0.55
1:A:337:VAL:O	1:A:338:PRO:C	2.43	0.55
1:B:277:VAL:O	1:B:281:HIS:HB2	2.06	0.55
1:B:65:ALA:O	1:B:71:GLU:CA	2.55	0.55
1:A:11:LYS:HA	1:A:11:LYS:CE	2.36	0.55
1:A:373:LEU:O	1:A:376:VAL:CG2	2.55	0.55
1:A:399:LEU:CD2	1:A:400:LYS:N	2.67	0.55
1:B:131:THR:HB	1:B:357:THR:HG21	1.88	0.55
1:B:47:LEU:HA	1:B:246:ILE:HD11	1.87	0.55
1:B:298:LEU:HG	1:B:302:LEU:HD12	1.88	0.55
1:B:32:TYR:HB3	1:B:256:ILE:HD11	1.88	0.55
1:B:408:GLY:O	1:B:412:LYS:HB2	2.06	0.55
1:A:225:ASN:C	1:A:227:MET:H	2.10	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ILE:HD11	1:A:295:ALA:N	2.21	0.55
1:B:337:VAL:O	1:B:338:PRO:C	2.43	0.55
1:A:117:ILE:CB	1:A:118:LEU:CD1	2.84	0.55
1:A:179:LEU:HD22	1:A:179:LEU:O	2.07	0.55
1:A:182:GLY:O	1:A:183:ALA:HB2	2.07	0.55
1:B:171:LEU:HA	1:B:275:PHE:CE1	2.42	0.55
1:B:215:MET:HE1	1:B:375:VAL:HA	1.88	0.55
1:B:340:THR:O	1:B:344:SER:HB2	2.07	0.55
1:B:82:THR:HG23	1:B:391:VAL:CG1	2.37	0.55
1:B:403:PHE:C	1:B:404:ASN:HD22	2.09	0.55
1:A:286:ILE:HG22	1:A:289:THR:CB	2.20	0.54
1:A:501:PRO:O	1:A:502:HIS:CD2	2.59	0.54
1:B:323:ASN:O	1:B:324:LEU:HD22	2.06	0.54
1:B:352:ALA:HA	1:B:355:ILE:HG23	1.88	0.54
1:A:11:LYS:HE3	1:A:11:LYS:HA	1.89	0.54
1:A:331:LYS:O	1:A:338:PRO:HA	2.07	0.54
1:A:394:LEU:HD11	1:A:413:LEU:HD11	1.89	0.54
1:A:154:ARG:HE	1:A:489:LYS:HG3	1.71	0.54
1:A:93:SER:O	1:A:97:LEU:HB2	2.07	0.54
1:B:308:TRP:HE1	1:B:498:ALA:CB	2.20	0.54
1:A:336:GLY:O	1:A:337:VAL:HG12	2.06	0.54
1:B:89:PHE:O	1:B:92:ILE:HG22	2.07	0.54
1:A:116:TYR:OH	1:A:273:GLN:CG	2.56	0.54
1:A:434:PRO:O	1:A:435:ASP:HB3	2.08	0.54
1:B:227:MET:HA	1:B:227:MET:HE2	1.90	0.54
1:B:230:PRO:O	1:B:231:GLY:C	2.46	0.54
1:B:237:ALA:O	1:B:241:LEU:N	2.29	0.54
1:B:116:TYR:OH	1:B:273:GLN:HG3	2.08	0.54
1:B:298:LEU:HG	1:B:302:LEU:HD11	1.87	0.54
1:B:325:LEU:HB3	1:B:326:PRO:HD2	1.89	0.54
1:B:36:ALA:HB1	1:B:257:ALA:CB	2.25	0.54
1:B:63:GLU:OE1	1:B:389:TYR:OH	2.16	0.54
1:A:223:HIS:CE1	1:A:492:PHE:CE2	2.96	0.54
1:A:19:PHE:O	1:A:23:ALA:HB2	2.07	0.54
1:A:339:VAL:HG23	1:A:343:ILE:HG23	1.89	0.54
1:A:423:SER:O	1:A:424:ILE:C	2.46	0.54
1:B:117:ILE:HD11	1:B:295:ALA:HA	1.89	0.54
1:B:321:GLN:C	1:B:323:ASN:H	2.10	0.54
1:B:395:LYS:CG	1:B:395:LYS:O	2.54	0.54
1:A:207:PHE:O	1:A:210:PHE:N	2.40	0.54
1:A:232:ARG:O	1:A:234:TYR:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:ILE:HD12	1:A:273:GLN:HE21	1.72	0.54
1:A:25:MET:HB2	1:A:495:HIS:CE1	2.42	0.54
1:B:162:ALA:O	1:B:296:LEU:HD22	2.08	0.54
1:A:15:LEU:HD22	1:A:16:LEU:N	2.22	0.54
1:A:225:ASN:C	1:A:227:MET:N	2.58	0.54
1:A:22:THR:CG2	1:A:25:MET:HE2	2.38	0.54
1:A:19:PHE:HE2	1:A:23:ALA:HB1	1.71	0.54
1:B:58:GLY:O	1:B:61:ALA:HB3	2.08	0.54
1:B:70:TRP:CD1	1:B:70:TRP:N	2.71	0.54
1:A:363:ASN:N	1:A:440:ASP:OD2	2.41	0.54
1:B:222:THR:C	1:B:224:VAL:H	2.09	0.54
1:B:356:LEU:CD2	1:B:369:ILE:HG21	2.38	0.54
1:B:411:VAL:HA	1:B:414:VAL:HG12	1.89	0.54
1:B:93:SER:CB	1:B:460:PRO:HB3	2.39	0.54
1:B:82:THR:HG22	1:B:391:VAL:CG1	2.36	0.54
1:A:275:PHE:HB3	1:A:290:VAL:CG2	2.34	0.53
1:A:360:GLY:O	1:A:361:GLY:O	2.26	0.53
1:B:332:MET:HE3	1:B:338:PRO:N	2.23	0.53
1:B:350:SER:O	1:B:354:ILE:HG13	2.08	0.53
1:B:64:MET:HE3	1:B:78:TRP:HB3	1.90	0.53
1:A:265:ILE:HG22	1:A:265:ILE:O	2.08	0.53
1:B:437:ILE:O	1:B:438:GLN:C	2.45	0.53
1:A:217:VAL:O	1:A:219:ALA:N	2.41	0.53
1:A:279:MET:C	1:A:281:HIS:N	2.61	0.53
1:B:55:ILE:CB	1:B:56:PRO:CD	2.68	0.53
1:A:222:THR:O	1:A:224:VAL:N	2.41	0.53
1:B:491:HIS:C	1:B:491:HIS:CD2	2.81	0.53
1:A:138:LEU:C	1:A:138:LEU:CD2	2.77	0.53
1:A:160:PHE:CZ	1:A:165:LEU:HD21	2.43	0.53
1:A:215:MET:HE2	1:A:378:TYR:CG	2.43	0.53
1:A:405:ILE:CG2	1:A:406:PRO:HD2	2.38	0.53
1:A:75:VAL:HG12	1:A:78:TRP:CD2	2.41	0.53
1:B:351:ILE:O	1:B:355:ILE:HG22	2.07	0.53
1:A:117:ILE:HG21	1:A:118:LEU:HD11	1.89	0.53
1:B:40:PHE:O	1:B:40:PHE:HD2	1.92	0.53
1:B:444:MET:O	1:B:445:TYR:C	2.45	0.53
1:B:308:TRP:HE1	1:B:498:ALA:HB2	1.69	0.53
1:A:161:PHE:HE1	1:A:493:PHE:CE2	2.07	0.53
1:A:96:TYR:HB2	1:A:316:MET:HG3	1.89	0.53
1:B:23:ALA:C	1:B:25:MET:H	2.11	0.53
1:A:321:GLN:NE2	1:A:476:GLY:HA3	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:ARG:HD2	1:A:87:TRP:CZ2	2.43	0.53
1:B:142:ALA:HA	1:B:309:ILE:HG21	1.90	0.53
1:A:123:LEU:O	1:A:130:LYS:HG2	2.08	0.53
1:A:204:LEU:C	1:A:206:VAL:N	2.62	0.53
1:A:146:PHE:C	1:A:148:GLY:H	2.12	0.53
1:A:242:MET:HE3	1:A:246:ILE:HD11	1.89	0.53
1:A:44:PHE:HB2	1:A:194:PHE:CD2	2.42	0.53
1:B:166:LEU:O	1:B:166:LEU:HD13	2.08	0.52
1:B:50:GLY:HA3	1:B:242:MET:SD	2.49	0.52
1:B:53:TRP:CZ2	1:B:382:TYR:HD1	2.17	0.52
1:B:60:CYS:N	1:B:405:ILE:HD11	2.24	0.52
1:B:70:TRP:C	1:B:72:GLU:H	2.13	0.52
1:A:124:ASN:HD21	1:A:269:ALA:HB2	1.71	0.52
1:B:433:PRO:HB2	1:B:434:PRO:CD	2.39	0.52
1:B:82:THR:O	1:B:83:LEU:HD23	2.09	0.52
1:B:29:VAL:HA	1:B:32:TYR:CE1	2.43	0.52
1:B:32:TYR:O	1:B:35:PHE:HB2	2.09	0.52
1:B:40:PHE:C	1:B:42:LEU:H	2.13	0.52
1:A:15:LEU:HD22	1:A:16:LEU:CD2	2.13	0.52
1:A:239:LEU:O	1:A:243:VAL:HG23	2.10	0.52
1:B:103:PHE:O	1:B:106:MET:CB	2.56	0.52
1:B:131:THR:HG22	1:B:357:THR:HG21	1.92	0.52
1:B:160:PHE:O	1:B:164:ILE:HB	2.09	0.52
1:B:175:ALA:O	1:B:178:TYR:HB3	2.09	0.52
1:A:224:VAL:O	1:A:227:MET:N	2.36	0.52
1:A:332:MET:HG3	1:A:338:PRO:CB	2.40	0.52
1:A:408:GLY:O	1:A:410:GLY:N	2.41	0.52
1:B:208:VAL:CG1	1:B:371:LEU:HB3	2.40	0.52
1:B:212:LEU:O	1:B:213:SER:C	2.45	0.52
1:A:160:PHE:HE1	1:A:165:LEU:CD2	1.97	0.52
1:B:392:LEU:C	1:B:394:LEU:H	2.12	0.52
1:A:428:ILE:O	1:A:430:SER:N	2.43	0.52
1:A:476:GLY:O	1:A:477:VAL:HG12	2.09	0.52
1:B:166:LEU:CD1	1:B:166:LEU:O	2.57	0.52
1:A:15:LEU:HD21	1:A:16:LEU:CD2	2.37	0.52
1:A:205:VAL:O	1:A:205:VAL:CG2	2.56	0.52
1:A:335:ASN:H	1:A:506:MET:HE1	1.74	0.52
1:B:376:VAL:HG11	1:B:453:PHE:CD1	2.45	0.52
1:A:399:LEU:CB	1:A:401:ARG:HH21	2.23	0.52
1:A:65:ALA:O	1:A:71:GLU:HA	2.10	0.52
1:B:109:PHE:CD2	1:B:301:VAL:CG2	2.87	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:ASN:HD21	1:B:268:SER:HB3	1.75	0.52
1:B:82:THR:HG21	1:B:391:VAL:HB	1.90	0.52
1:A:310:VAL:CG1	1:A:311:GLY:H	2.18	0.51
1:B:332:MET:HE1	1:B:338:PRO:HD3	1.91	0.51
1:B:336:GLY:C	1:B:337:VAL:CG1	2.79	0.51
1:B:349:THR:O	1:B:353:LEU:N	2.43	0.51
1:A:250:SER:O	1:A:254:LEU:CD1	2.50	0.51
1:A:13:LEU:CB	1:A:227:MET:HA	2.41	0.51
1:A:55:ILE:CB	1:A:56:PRO:CD	2.77	0.51
1:B:76:PHE:HD2	1:B:76:PHE:O	1.81	0.51
1:A:143:LEU:O	1:A:144:THR:C	2.45	0.51
1:A:504:ILE:CG2	1:A:506:MET:HG2	2.35	0.51
1:A:42:LEU:HD21	1:A:254:LEU:HG	1.93	0.51
1:B:111:LEU:HD12	1:B:130:LYS:HD3	1.92	0.51
1:B:484:SER:O	1:B:485:GLN:NE2	2.40	0.51
1:B:75:VAL:HG23	1:B:76:PHE:N	2.26	0.51
1:B:146:PHE:C	1:B:148:GLY:H	2.14	0.51
1:B:395:LYS:CG	1:B:396:HIS:CE1	2.94	0.51
1:A:10:ALA:O	1:A:11:LYS:HD2	2.11	0.51
1:A:124:ASN:CA	1:A:130:LYS:HE2	2.29	0.51
1:A:200:LYS:HB2	1:A:200:LYS:HZ2	1.76	0.51
1:A:124:ASN:HD21	1:A:269:ALA:CB	2.22	0.51
1:A:226:GLU:OE2	1:A:484:SER:HB3	2.10	0.51
1:A:64:MET:CE	1:A:78:TRP:CE3	2.94	0.51
1:B:338:PRO:HB2	1:B:341:LEU:CD1	2.41	0.51
1:B:393:VAL:HG11	1:B:413:LEU:CD2	2.41	0.51
1:A:67:VAL:O	1:A:68:ASP:C	2.46	0.51
1:B:59:LEU:O	1:B:61:ALA:N	2.44	0.51
1:A:38:SER:O	1:A:39:GLY:C	2.46	0.51
1:A:433:PRO:HG2	1:A:445:TYR:HB3	1.93	0.51
1:A:98:GLN:CA	1:A:377:ILE:CG2	2.89	0.51
1:B:24:SER:HB3	1:B:493:PHE:O	2.10	0.51
1:A:29:VAL:HA	1:A:32:TYR:CD2	2.46	0.50
1:B:175:ALA:O	1:B:178:TYR:CB	2.59	0.50
1:B:29:VAL:HA	1:B:32:TYR:CG	2.46	0.50
1:A:154:ARG:NE	1:A:489:LYS:HG3	2.26	0.50
1:A:310:VAL:HG13	1:A:311:GLY:N	2.16	0.50
1:A:434:PRO:O	1:A:435:ASP:OD2	2.30	0.50
1:A:442:THR:HG21	1:A:445:TYR:HD2	1.75	0.50
1:A:25:MET:HE1	1:A:496:PRO:HG2	1.89	0.50
1:A:96:TYR:CD1	1:A:316:MET:HG3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:MET:HE3	1:B:378:TYR:CG	2.46	0.50
1:B:374:THR:HG23	1:B:375:VAL:N	2.27	0.50
1:B:437:ILE:O	1:B:439:GLY:N	2.44	0.50
1:A:272:MET:HE3	1:A:272:MET:CA	2.41	0.50
1:B:138:LEU:O	1:B:138:LEU:HD22	2.10	0.50
1:B:159:GLY:HA2	1:B:162:ALA:HB3	1.93	0.50
1:B:307:SER:CB	1:B:494:LEU:HD11	2.39	0.50
1:A:131:THR:O	1:A:135:LEU:HD12	2.12	0.50
1:A:217:VAL:C	1:A:219:ALA:N	2.62	0.50
1:A:338:PRO:HG2	1:A:338:PRO:O	2.12	0.50
1:A:347:VAL:HG12	1:A:351:ILE:HD12	1.91	0.50
1:A:442:THR:HB	1:A:445:TYR:HB3	1.90	0.50
1:B:186:ALA:C	1:B:188:GLU:H	2.13	0.50
1:B:209:ALA:HB2	1:B:371:LEU:HD12	1.93	0.50
1:B:436:ASN:OD1	1:B:436:ASN:O	2.30	0.50
1:B:489:LYS:H	1:B:489:LYS:HD3	1.66	0.50
1:B:51:ILE:HG22	1:B:52:LEU:CG	2.40	0.50
1:A:19:PHE:HD2	1:A:20:ALA:N	2.10	0.50
1:A:22:THR:CG2	1:A:25:MET:CE	2.90	0.50
1:A:101:ILE:HG22	1:A:374:THR:HG1	1.76	0.50
1:A:263:ASN:O	1:A:263:ASN:OD1	2.30	0.50
1:A:67:VAL:HG12	1:A:70:TRP:CG	2.46	0.50
1:B:124:ASN:OD1	1:B:124:ASN:O	2.30	0.50
1:B:76:PHE:O	1:B:80:SER:HB2	2.12	0.50
1:A:204:LEU:C	1:A:206:VAL:H	2.14	0.50
1:A:217:VAL:C	1:A:219:ALA:H	2.15	0.50
1:A:31:GLU:O	1:A:35:PHE:CD2	2.65	0.50
1:A:355:ILE:O	1:A:359:THR:HB	2.11	0.50
1:A:356:LEU:HD22	1:A:369:ILE:HG22	1.91	0.50
1:A:423:SER:O	1:A:426:ALA:N	2.45	0.50
1:B:170:ILE:HG22	1:B:275:PHE:HZ	1.63	0.50
1:B:67:VAL:O	1:B:69:GLY:N	2.45	0.50
1:A:170:ILE:HG22	1:A:275:PHE:CZ	2.47	0.50
1:A:187:ILE:CB	1:A:258:MET:O	2.60	0.50
1:A:208:VAL:HG23	1:A:209:ALA:N	2.26	0.50
1:B:234:TYR:CD2	1:B:235:PRO:N	2.77	0.50
1:A:163:GLY:O	1:A:167:PRO:CG	2.59	0.50
1:A:254:LEU:O	1:A:258:MET:HG2	2.12	0.50
1:A:433:PRO:HB2	1:A:442:THR:OG1	2.12	0.50
1:A:486:ASN:O	1:A:487:ALA:O	2.30	0.50
1:A:55:ILE:HG22	1:A:56:PRO:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:LYS:O	1:B:201:VAL:O	2.30	0.50
1:B:279:MET:CE	1:B:286:ILE:HG21	2.41	0.50
1:B:486:ASN:O	1:B:487:ALA:O	2.30	0.50
1:A:29:VAL:CG2	1:A:30:TYR:H	2.25	0.49
1:A:98:GLN:HG2	1:A:374:THR:HG23	1.92	0.49
1:A:85:PRO:HB2	1:A:464:TYR:OH	2.12	0.49
1:B:31:GLU:O	1:B:34:THR:HG23	2.11	0.49
1:A:117:ILE:HD11	1:A:294:SER:C	2.32	0.49
1:A:71:GLU:HB3	1:A:225:ASN:HD21	1.76	0.49
1:A:22:THR:OG1	1:A:220:SER:OG	2.12	0.49
1:A:308:TRP:N	1:A:308:TRP:HE3	2.10	0.49
1:A:312:PRO:HG3	1:A:498:ALA:HA	1.93	0.49
1:B:129:THR:C	1:B:131:THR:N	2.65	0.49
1:B:146:PHE:C	1:B:148:GLY:N	2.65	0.49
1:B:386:PHE:CE1	1:B:419:GLY:HA3	2.47	0.49
1:B:444:MET:O	1:B:445:TYR:O	2.30	0.49
1:A:34:THR:O	1:A:34:THR:OG1	2.30	0.49
1:A:38:SER:OG	1:A:41:SER:HB2	2.13	0.49
1:B:128:ILE:O	1:B:131:THR:HG23	2.12	0.49
1:B:338:PRO:O	1:B:338:PRO:HG2	2.12	0.49
1:A:118:LEU:HD13	1:A:118:LEU:H	1.71	0.49
1:A:480:GLU:O	1:A:481:PRO:C	2.51	0.49
1:B:437:ILE:HD11	1:B:442:THR:HG22	1.95	0.49
1:B:442:THR:OG1	1:B:442:THR:O	2.30	0.49
1:A:200:LYS:HG3	1:A:201:VAL:H	1.76	0.49
1:A:357:THR:O	1:A:359:THR:N	2.44	0.49
1:A:379:LEU:CD1	1:A:423:SER:HB3	2.42	0.49
1:B:266:ASN:ND2	1:B:268:SER:N	2.61	0.49
1:B:117:ILE:CG1	1:B:294:SER:HB2	2.35	0.49
1:A:197:ASP:CG	1:A:199:SER:HB2	2.33	0.49
1:A:428:ILE:C	1:A:430:SER:N	2.66	0.49
1:A:439:GLY:O	1:A:440:ASP:O	2.30	0.49
1:A:82:THR:HB	1:A:391:VAL:HG11	1.89	0.49
1:A:98:GLN:C	1:A:98:GLN:CD	2.69	0.49
1:B:141:LEU:HD12	1:B:306:ALA:CA	2.42	0.49
1:B:191:SER:C	1:B:193:THR:N	2.64	0.49
1:B:267:LEU:O	1:B:268:SER:C	2.49	0.49
1:B:362:GLY:H	1:B:440:ASP:CB	2.11	0.49
1:B:428:ILE:O	1:B:430:SER:N	2.45	0.49
1:B:432:LEU:HD12	1:B:432:LEU:C	2.23	0.49
1:A:492:PHE:C	1:A:494:LEU:H	2.15	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:LEU:O	1:B:300:GLY:C	2.49	0.49
1:B:426:ALA:O	1:B:430:SER:OG	2.25	0.49
1:B:197:ASP:C	1:B:199:SER:N	2.65	0.49
1:B:50:GLY:O	1:B:55:ILE:HB	2.13	0.49
1:A:170:ILE:HG21	1:A:293:ILE:HD12	1.95	0.49
1:A:198:PHE:O	1:B:395:LYS:CD	2.61	0.49
1:A:274:THR:CG2	1:A:275:PHE:N	2.75	0.49
1:B:189:MET:O	1:B:190:ASP:C	2.49	0.49
1:A:160:PHE:HD1	1:A:161:PHE:N	2.11	0.49
1:A:223:HIS:CE1	1:A:492:PHE:HE2	2.31	0.49
1:A:229:ASN:O	1:A:229:ASN:OD1	2.30	0.49
1:A:256:ILE:HG22	1:A:257:ALA:N	2.20	0.49
1:B:150:LYS:HB3	1:B:150:LYS:HE3	1.47	0.49
1:B:266:ASN:HD22	1:B:267:LEU:N	2.09	0.49
1:B:266:ASN:ND2	1:B:267:LEU:N	2.61	0.49
1:B:480:GLU:HA	1:B:481:PRO:HD2	1.67	0.49
1:A:204:LEU:O	1:A:205:VAL:C	2.51	0.48
1:A:264:GLU:OE2	1:A:264:GLU:CA	2.45	0.48
1:A:410:GLY:O	1:A:411:VAL:C	2.52	0.48
1:A:466:VAL:HG12	1:A:467:HIS:HB2	1.94	0.48
1:A:71:GLU:CD	1:A:71:GLU:H	2.16	0.48
1:A:96:TYR:O	1:A:96:TYR:CD2	2.66	0.48
1:B:276:THR:HG22	1:B:277:VAL:H	1.74	0.48
1:A:120:TRP:C	1:A:122:ALA:H	2.16	0.48
1:B:120:TRP:NE1	1:B:122:ALA:HB3	2.28	0.48
1:B:138:LEU:HD22	1:B:138:LEU:C	2.33	0.48
1:B:333:ASN:O	1:B:334:LYS:C	2.49	0.48
1:B:365:MET:HE1	1:B:442:THR:HA	1.93	0.48
1:B:64:MET:HE3	1:B:78:TRP:CB	2.44	0.48
1:A:101:ILE:HG21	1:A:373:LEU:HB3	1.95	0.48
1:A:229:ASN:C	1:A:229:ASN:OD1	2.51	0.48
1:A:74:GLY:C	1:A:75:VAL:CG1	2.69	0.48
1:A:91:ALA:HB2	1:A:384:MET:SD	2.53	0.48
1:B:181:SER:O	1:B:182:GLY:O	2.30	0.48
1:B:496:PRO:O	1:B:497:ARG:C	2.45	0.48
1:A:157:LYS:CD	1:A:493:PHE:CE2	2.96	0.48
1:A:433:PRO:HD3	1:A:446:VAL:CG2	2.44	0.48
1:B:234:TYR:CB	1:B:235:PRO:CD	2.90	0.48
1:B:294:SER:O	1:B:295:ALA:C	2.49	0.48
1:B:63:GLU:OE2	1:B:404:ASN:HA	2.13	0.48
1:B:66:THR:OG1	1:B:402:THR:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:TYR:O	1:B:97:LEU:C	2.51	0.48
1:A:456:VAL:O	1:A:459:LEU:N	2.44	0.48
1:B:44:PHE:CD2	1:B:196:PRO:HD2	2.48	0.48
1:B:263:ASN:O	1:B:263:ASN:OD1	2.30	0.48
1:B:31:GLU:HB2	1:B:35:PHE:CE2	2.49	0.48
1:B:484:SER:C	1:B:485:GLN:HE21	2.17	0.48
1:A:157:LYS:CG	1:A:493:PHE:CE2	2.84	0.48
1:A:63:GLU:OE1	1:A:405:ILE:CG1	2.57	0.48
1:B:389:TYR:CE2	1:B:393:VAL:HG21	2.49	0.48
1:B:459:LEU:CB	1:B:460:PRO:CD	2.92	0.48
1:B:51:ILE:HG23	1:B:52:LEU:HD23	1.92	0.48
1:A:200:LYS:NZ	1:A:200:LYS:HB2	2.27	0.48
1:B:13:LEU:O	1:B:227:MET:HE2	2.14	0.48
1:B:21:ILE:CD1	1:B:484:SER:HB2	2.42	0.48
1:A:104:ILE:HB	1:A:105:PRO:CD	2.43	0.48
1:A:54:PHE:CD1	1:A:214:TYR:CD1	3.02	0.48
1:A:22:THR:HG23	1:A:25:MET:HE2	1.95	0.48
1:A:117:ILE:CD1	1:A:294:SER:HB3	2.44	0.48
1:A:32:TYR:N	1:A:33:PRO:HD2	2.27	0.48
1:A:401:ARG:HB2	1:A:404:ASN:OD1	2.13	0.48
1:A:455:VAL:HG13	1:A:455:VAL:O	2.14	0.48
1:B:141:LEU:CD1	1:B:306:ALA:CB	2.69	0.48
1:B:221:ALA:O	1:B:224:VAL:CB	2.62	0.48
1:B:260:ILE:HD11	1:B:274:THR:HA	1.95	0.48
1:B:40:PHE:O	1:B:40:PHE:CD2	2.66	0.48
1:A:155:ILE:HG12	1:A:155:ILE:H	1.43	0.48
1:A:275:PHE:CE2	1:A:293:ILE:HG21	2.49	0.48
1:A:393:VAL:CG1	1:A:413:LEU:HD21	2.36	0.48
1:B:22:THR:HG21	1:B:220:SER:OG	2.14	0.48
1:A:272:MET:HE1	1:A:297:LEU:HD13	1.96	0.48
1:A:433:PRO:CG	1:A:445:TYR:CG	2.97	0.48
1:A:476:GLY:C	1:A:477:VAL:CG1	2.82	0.48
1:A:417:ILE:HG23	1:B:421:LEU:HD23	1.95	0.48
1:B:69:GLY:O	1:B:70:TRP:HD1	1.94	0.48
1:A:124:ASN:HA	1:A:130:LYS:CE	2.29	0.47
1:A:304:GLU:O	1:A:308:TRP:CZ3	2.67	0.47
1:B:356:LEU:HD22	1:B:369:ILE:HG21	1.96	0.47
1:B:357:THR:HG22	1:B:358:ASN:N	2.29	0.47
1:A:162:ALA:O	1:A:166:LEU:HB2	2.14	0.47
1:A:66:THR:O	1:A:401:ARG:HA	2.14	0.47
1:A:141:LEU:HA	1:A:144:THR:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:MET:SD	1:A:504:ILE:HG21	2.54	0.47
1:B:386:PHE:HD2	1:B:386:PHE:H	1.63	0.47
1:B:59:LEU:HB3	1:B:405:ILE:HD13	1.95	0.47
1:A:19:PHE:HE1	1:A:240:LEU:HD22	1.80	0.47
1:B:163:GLY:O	1:B:167:PRO:CG	2.59	0.47
1:B:226:GLU:O	1:B:227:MET:C	2.53	0.47
1:B:495:HIS:O	1:B:499:ARG:HG2	2.14	0.47
1:B:67:VAL:CG2	1:B:70:TRP:CD2	2.97	0.47
1:B:222:THR:HG23	1:B:223:HIS:N	2.29	0.47
1:A:142:ALA:O	1:A:143:LEU:C	2.52	0.47
1:A:323:ASN:O	1:A:324:LEU:C	2.53	0.47
1:A:386:PHE:HB2	1:A:420:LEU:HD13	1.97	0.47
1:A:70:TRP:CZ3	1:A:392:LEU:HD13	2.48	0.47
1:A:83:LEU:O	1:A:87:TRP:HD1	1.96	0.47
1:B:261:PRO:HD2	1:B:264:GLU:CB	2.44	0.47
1:A:155:ILE:O	1:A:159:GLY:N	2.35	0.47
1:A:206:VAL:O	1:A:207:PHE:C	2.53	0.47
1:A:356:LEU:CD2	1:A:369:ILE:CG2	2.87	0.47
1:A:435:ASP:OD2	1:A:436:ASN:ND2	2.48	0.47
1:A:21:ILE:CD1	1:A:223:HIS:ND1	2.74	0.47
1:A:22:THR:O	1:A:22:THR:CG2	2.61	0.47
1:B:163:GLY:C	1:B:167:PRO:HG2	2.34	0.47
1:A:46:LEU:CD2	1:A:210:PHE:CD1	2.95	0.47
1:B:395:LYS:C	1:B:396:HIS:ND1	2.61	0.47
1:B:82:THR:CG2	1:B:391:VAL:CB	2.93	0.47
1:A:437:ILE:HD11	1:A:442:THR:HG21	1.95	0.47
1:B:221:ALA:O	1:B:224:VAL:HB	2.14	0.47
1:B:260:ILE:O	1:B:262:GLY:N	2.47	0.47
1:B:44:PHE:CE2	1:B:198:PHE:HZ	2.33	0.47
1:B:479:LEU:O	1:B:481:PRO:CD	2.62	0.47
1:A:486:ASN:HB3	1:A:503:TYR:HH	1.71	0.47
1:A:52:LEU:N	1:A:52:LEU:HD23	2.30	0.47
1:B:78:TRP:N	1:B:78:TRP:HD1	2.12	0.47
1:A:283:ALA:O	1:A:284:PRO:C	2.53	0.46
1:B:351:ILE:O	1:B:355:ILE:HG23	2.14	0.46
1:B:380:CYS:O	1:B:383:PHE:N	2.48	0.46
1:B:40:PHE:C	1:B:42:LEU:N	2.68	0.46
1:A:411:VAL:HA	1:A:414:VAL:HG12	1.97	0.46
1:A:83:LEU:O	1:A:87:TRP:CD1	2.69	0.46
1:B:22:THR:CG2	1:B:220:SER:OG	2.64	0.46
1:B:109:PHE:CE2	1:B:301:VAL:HG21	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:ILE:CD1	1:B:312:PRO:CB	2.89	0.46
1:A:67:VAL:CG1	1:A:70:TRP:CD2	2.98	0.46
1:B:127:PRO:HG2	1:B:128:ILE:H	1.80	0.46
1:B:417:ILE:O	1:B:421:LEU:HD12	2.15	0.46
1:B:49:GLY:HA3	1:B:214:TYR:HE2	1.75	0.46
1:A:11:LYS:HG3	1:A:226:GLU:HA	1.95	0.46
1:A:143:LEU:O	1:A:146:PHE:HB2	2.14	0.46
1:A:259:VAL:HG12	1:A:259:VAL:O	2.15	0.46
1:A:364:ASN:N	1:A:440:ASP:OD2	2.49	0.46
1:A:397:PRO:CG	1:A:398:ASP:N	2.78	0.46
1:A:489:LYS:HG2	1:A:489:LYS:H	1.26	0.46
1:B:131:THR:CB	1:B:357:THR:HG21	2.45	0.46
1:B:127:PRO:O	1:B:131:THR:HG23	2.15	0.46
1:B:312:PRO:O	1:B:313:SER:C	2.54	0.46
1:B:373:LEU:HD22	1:B:377:ILE:HD12	1.97	0.46
1:A:178:TYR:HD2	1:A:179:LEU:N	2.13	0.46
1:A:290:VAL:HG12	1:A:291:ARG:N	2.31	0.46
1:A:336:GLY:H	1:A:506:MET:HE2	1.81	0.46
1:A:15:LEU:HD23	1:A:16:LEU:CA	2.46	0.46
1:A:160:PHE:HA	1:A:164:ILE:HD12	1.97	0.46
1:A:202:GLY:CA	1:A:434:PRO:HD3	2.43	0.46
1:A:29:VAL:HA	1:A:32:TYR:CE2	2.50	0.46
1:A:408:GLY:O	1:A:409:LYS:C	2.54	0.46
1:B:392:LEU:C	1:B:394:LEU:N	2.69	0.46
1:B:372:ALA:CB	1:B:449:LEU:HD11	2.33	0.46
1:A:118:LEU:O	1:A:119:LYS:O	2.33	0.46
1:A:507:ASN:O	1:A:508:ASP:O	2.34	0.46
1:A:60:CYS:HB3	1:A:389:TYR:CD1	2.51	0.46
1:B:246:ILE:O	1:B:250:SER:HB3	2.16	0.46
1:B:131:THR:CG2	1:B:357:THR:CG2	2.93	0.46
1:B:437:ILE:CD1	1:B:442:THR:HG22	2.46	0.46
1:B:110:VAL:HG23	1:B:301:VAL:CG1	2.42	0.46
1:B:211:ILE:HG22	1:B:215:MET:SD	2.55	0.46
1:B:289:THR:HG23	1:B:290:VAL:N	2.30	0.46
1:B:29:VAL:O	1:B:31:GLU:N	2.48	0.46
1:A:220:SER:O	1:A:220:SER:OG	2.31	0.46
1:A:340:THR:O	1:A:344:SER:CB	2.60	0.46
1:A:157:LYS:HA	1:A:493:PHE:HD2	1.80	0.46
1:B:493:PHE:O	1:B:494:LEU:C	2.51	0.46
1:B:98:GLN:NE2	1:B:497:ARG:HD2	2.31	0.46
1:B:66:THR:HG1	1:B:402:THR:HA	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:LEU:HA	1:A:123:LEU:HD23	1.80	0.46
1:B:151:TYR:HB2	1:B:152:THR:H	1.55	0.46
1:B:166:LEU:CB	1:B:167:PRO:CD	2.66	0.46
1:B:222:THR:O	1:B:223:HIS:C	2.54	0.46
1:B:112:GLY:HA3	1:B:269:ALA:HB3	1.97	0.46
1:B:28:ALA:O	1:B:31:GLU:HG3	2.16	0.46
1:B:146:PHE:CE1	1:B:342:VAL:CG1	2.93	0.46
1:B:376:VAL:HG13	1:B:427:PHE:HE1	1.81	0.46
1:B:71:GLU:HG3	1:B:71:GLU:H	1.38	0.46
1:A:221:ALA:C	1:A:223:HIS:N	2.68	0.45
1:A:350:SER:O	1:A:354:ILE:HG13	2.16	0.45
1:A:198:PHE:O	1:B:395:LYS:HB2	2.15	0.45
1:B:47:LEU:HD23	1:B:47:LEU:HA	1.52	0.45
1:A:96:TYR:HD1	1:A:316:MET:HG3	1.79	0.45
1:A:55:ILE:O	1:A:56:PRO:C	2.53	0.45
1:B:137:ILE:O	1:B:140:ALA:N	2.49	0.45
1:B:45:PHE:O	1:B:46:LEU:C	2.54	0.45
1:A:212:LEU:O	1:A:213:SER:C	2.54	0.45
1:A:457:LEU:HD11	1:A:461:PHE:CE2	2.51	0.45
1:B:114:LEU:HA	1:B:114:LEU:HD23	1.47	0.45
1:B:444:MET:O	1:B:448:LEU:HB2	2.16	0.45
1:A:401:ARG:CB	1:A:404:ASN:OD1	2.64	0.45
1:B:262:GLY:CA	1:B:265:ILE:HG13	2.22	0.45
1:A:231:GLY:O	1:A:235:PRO:HD2	2.16	0.45
1:B:115:SER:O	1:B:116:TYR:C	2.54	0.45
1:B:206:VAL:C	1:B:208:VAL:H	2.19	0.45
1:B:308:TRP:CE2	1:B:498:ALA:HB2	2.48	0.45
1:A:116:TYR:CE1	1:A:272:MET:HB2	2.49	0.45
1:A:157:LYS:HG3	1:A:490:GLY:HA3	1.98	0.45
1:B:23:ALA:C	1:B:25:MET:N	2.70	0.45
1:B:298:LEU:CG	1:B:302:LEU:HD11	2.45	0.45
1:B:329:PHE:O	1:B:330:ALA:CB	2.58	0.45
1:B:484:SER:O	1:B:484:SER:OG	2.30	0.45
1:A:157:LYS:HA	1:A:493:PHE:CD2	2.52	0.45
1:A:495:HIS:CD2	1:A:497:ARG:H	2.34	0.45
1:B:208:VAL:O	1:B:375:VAL:HG21	2.17	0.45
1:B:433:PRO:CB	1:B:434:PRO:CD	2.95	0.45
1:B:65:ALA:O	1:B:71:GLU:N	2.50	0.45
1:B:72:GLU:HA	1:B:73:GLY:HA3	1.64	0.45
1:A:32:TYR:HB2	1:A:33:PRO:HD3	1.99	0.45
1:A:85:PRO:C	1:A:87:TRP:N	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:LEU:O	1:B:205:VAL:C	2.56	0.45
1:B:299:LEU:HD22	1:B:299:LEU:HA	1.78	0.45
1:B:394:LEU:HD22	1:B:394:LEU:HA	1.80	0.45
1:A:204:LEU:HD23	1:A:204:LEU:N	2.32	0.45
1:B:117:ILE:HG22	1:B:118:LEU:N	2.29	0.45
1:B:127:PRO:HB2	1:B:358:ASN:OD1	2.16	0.45
1:A:226:GLU:C	1:A:227:MET:O	2.51	0.45
1:A:232:ARG:HG3	1:A:236:LEU:HD23	1.98	0.45
1:B:376:VAL:HG13	1:B:427:PHE:CE1	2.52	0.45
1:B:441:SER:O	1:B:441:SER:OG	2.31	0.45
1:A:152:THR:O	1:A:154:ARG:N	2.49	0.44
1:B:289:THR:O	1:B:293:ILE:HG12	2.17	0.44
1:B:379:LEU:HD23	1:B:379:LEU:HA	1.65	0.44
1:A:26:VAL:CG1	1:A:26:VAL:O	2.62	0.44
1:B:278:LEU:O	1:B:282:VAL:N	2.48	0.44
1:B:386:PHE:HE1	1:B:419:GLY:HA3	1.83	0.44
1:B:74:GLY:O	1:B:77:ALA:N	2.41	0.44
1:A:83:LEU:HD21	1:A:388:GLY:HA2	1.99	0.44
1:A:88:GLY:O	1:A:92:ILE:HB	2.18	0.44
1:B:145:GLN:HG3	1:B:310:VAL:CG1	2.47	0.44
1:B:234:TYR:O	1:B:235:PRO:C	2.54	0.44
1:B:177:ILE:HD11	1:B:282:VAL:HG21	1.99	0.44
1:B:309:ILE:HG22	1:B:309:ILE:O	2.18	0.44
1:B:356:LEU:CD2	1:B:369:ILE:CG2	2.95	0.44
1:B:157:LYS:CG	1:B:493:PHE:CE2	2.94	0.44
1:B:315:GLY:N	1:B:500:SER:HB2	2.31	0.44
1:B:60:CYS:CB	1:B:389:TYR:CE1	3.00	0.44
1:A:224:VAL:O	1:A:225:ASN:C	2.55	0.44
1:A:171:LEU:HD21	1:A:255:SER:HB3	1.99	0.44
1:A:82:THR:CB	1:A:391:VAL:HG12	2.46	0.44
1:B:345:GLN:HG2	1:B:346:LEU:N	2.32	0.44
1:A:19:PHE:CE1	1:A:240:LEU:HD22	2.53	0.44
1:A:338:PRO:CG	1:A:338:PRO:O	2.65	0.44
1:B:307:SER:OG	1:B:308:TRP:HD1	2.01	0.44
1:B:405:ILE:HB	1:B:412:LYS:HG2	1.99	0.44
1:A:19:PHE:CE2	1:A:23:ALA:HB1	2.47	0.44
1:A:66:THR:CG2	1:A:224:VAL:HG11	2.45	0.44
1:A:279:MET:HE2	1:A:282:VAL:HG21	1.99	0.44
1:A:373:LEU:O	1:A:373:LEU:HD22	2.17	0.44
1:A:399:LEU:CB	1:A:401:ARG:NH2	2.80	0.44
1:A:368:LEU:HD22	1:A:437:ILE:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:ASN:O	1:A:475:THR:OG1	2.31	0.44
1:A:321:GLN:NE2	1:A:477:VAL:H	2.14	0.44
1:A:494:LEU:HD12	1:A:494:LEU:HA	1.72	0.44
1:B:137:ILE:O	1:B:140:ALA:CB	2.62	0.44
1:A:14:THR:O	1:A:17:GLY:N	2.49	0.44
1:A:154:ARG:HH22	1:A:489:LYS:NZ	2.13	0.44
1:A:154:ARG:O	1:A:158:VAL:HG23	2.18	0.44
1:A:167:PRO:HG2	1:A:297:LEU:HD23	1.98	0.44
1:A:435:ASP:CA	1:A:442:THR:OG1	2.53	0.44
1:A:49:GLY:O	1:A:54:PHE:N	2.51	0.44
1:B:199:SER:OG	1:B:199:SER:O	2.30	0.44
1:B:206:VAL:C	1:B:208:VAL:N	2.71	0.44
1:B:224:VAL:O	1:B:227:MET:HB2	2.18	0.44
1:B:29:VAL:C	1:B:31:GLU:N	2.69	0.44
1:B:365:MET:CG	1:B:437:ILE:CD1	2.95	0.44
1:B:315:GLY:HA2	1:B:500:SER:HB2	1.98	0.44
1:B:98:GLN:OE1	1:B:99:ILE:N	2.50	0.44
1:A:442:THR:CG2	1:A:445:TYR:HD2	2.31	0.44
1:B:158:VAL:O	1:B:162:ALA:CB	2.65	0.44
1:B:196:PRO:HB2	1:B:198:PHE:CD1	2.48	0.44
1:B:36:ALA:CB	1:B:257:ALA:HB2	2.27	0.44
1:B:298:LEU:HD11	1:B:302:LEU:HD11	2.00	0.44
1:B:332:MET:HE3	1:B:332:MET:HB3	1.71	0.44
1:B:417:ILE:HD12	1:B:417:ILE:HA	1.88	0.44
1:A:178:TYR:OH	1:A:183:ALA:HA	2.18	0.44
1:A:332:MET:HG3	1:A:338:PRO:HB3	1.99	0.44
1:A:98:GLN:N	1:A:377:ILE:HG21	2.32	0.44
1:B:117:ILE:HG22	1:B:118:LEU:CD1	2.48	0.44
1:B:29:VAL:CB	1:B:32:TYR:CE1	2.98	0.44
1:B:98:GLN:CD	1:B:497:ARG:HH11	2.22	0.44
1:A:207:PHE:O	1:A:208:VAL:C	2.55	0.43
1:A:50:GLY:CA	1:A:54:PHE:HB3	2.44	0.43
1:A:62:ALA:O	1:A:63:GLU:C	2.56	0.43
1:B:30:TYR:HD1	1:B:109:PHE:CD2	2.36	0.43
1:B:203:THR:C	1:B:204:LEU:CD2	2.81	0.43
1:B:236:LEU:O	1:B:237:ALA:C	2.57	0.43
1:B:31:GLU:C	1:B:33:PRO:CD	2.71	0.43
1:B:332:MET:CE	1:B:338:PRO:HD3	2.48	0.43
1:B:51:ILE:HG22	1:B:52:LEU:HG	2.00	0.43
1:A:283:ALA:HB1	1:A:285:GLU:HG2	2.00	0.43
1:A:449:LEU:C	1:A:449:LEU:CD1	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:THR:O	1:A:505:VAL:HG22	2.17	0.43
1:B:177:ILE:HD11	1:B:282:VAL:CG2	2.48	0.43
1:B:212:LEU:HD12	1:B:212:LEU:O	2.17	0.43
1:B:338:PRO:O	1:B:338:PRO:CG	2.66	0.43
1:B:90:ALA:O	1:B:91:ALA:C	2.56	0.43
1:A:104:ILE:HG22	1:A:108:TYR:CZ	2.53	0.43
1:A:145:GLN:N	1:A:145:GLN:HE21	2.14	0.43
1:A:231:GLY:O	1:A:235:PRO:CD	2.66	0.43
1:A:242:MET:HE2	1:A:246:ILE:CD1	2.49	0.43
1:A:283:ALA:C	1:A:285:GLU:N	2.70	0.43
1:B:196:PRO:HB2	1:B:198:PHE:HE1	1.67	0.43
1:B:369:ILE:HG13	1:B:445:TYR:CE1	2.53	0.43
1:A:102:GLY:O	1:A:105:PRO:HD2	2.18	0.43
1:A:151:TYR:O	1:A:154:ARG:N	2.52	0.43
1:A:161:PHE:O	1:A:162:ALA:C	2.57	0.43
1:A:355:ILE:O	1:A:359:THR:CB	2.67	0.43
1:B:313:SER:O	1:B:316:MET:CA	2.67	0.43
1:B:340:THR:O	1:B:344:SER:CB	2.65	0.43
1:A:170:ILE:HD13	1:A:293:ILE:CD1	2.48	0.43
1:A:218:GLU:HG3	1:A:218:GLU:H	1.40	0.43
1:A:377:ILE:HG22	1:A:378:TYR:N	2.33	0.43
1:A:405:ILE:HG23	1:A:406:PRO:HD2	2.00	0.43
1:B:350:SER:O	1:B:354:ILE:CG1	2.66	0.43
1:B:325:LEU:HD23	1:B:463:LEU:HD23	1.99	0.43
1:A:266:ASN:HB2	1:A:273:GLN:OE1	2.19	0.43
1:A:417:ILE:HD13	1:A:417:ILE:HA	1.67	0.43
1:B:106:MET:HG2	1:B:305:ILE:HG12	2.00	0.43
1:B:454:LEU:HD12	1:B:454:LEU:HA	1.80	0.43
1:B:494:LEU:HA	1:B:494:LEU:HD12	1.77	0.43
1:A:125:GLU:C	1:A:127:PRO:HD3	2.29	0.43
1:A:248:LEU:HD12	1:A:248:LEU:HA	1.81	0.43
1:A:411:VAL:O	1:A:415:VAL:HB	2.18	0.43
1:A:73:GLY:HA2	1:A:77:ALA:HB2	1.98	0.43
1:B:261:PRO:HD2	1:B:264:GLU:HB2	2.01	0.43
1:B:341:LEU:O	1:B:342:VAL:C	2.56	0.43
1:B:70:TRP:HZ3	1:B:392:LEU:CD1	2.25	0.43
1:A:31:GLU:HB3	1:A:35:PHE:HE2	1.79	0.43
1:A:34:THR:HG21	1:A:367:PHE:HE2	1.84	0.43
1:A:38:SER:OG	1:A:38:SER:O	2.30	0.43
1:A:447:GLU:O	1:A:450:VAL:N	2.50	0.43
1:B:259:VAL:CG2	1:B:278:LEU:HD11	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:501:PRO:C	1:B:502:HIS:CD2	2.91	0.43
1:B:51:ILE:HD13	1:B:51:ILE:HA	1.74	0.43
1:B:90:ALA:O	1:B:93:SER:HB2	2.19	0.43
1:B:96:TYR:O	1:B:98:GLN:N	2.52	0.43
1:A:124:ASN:O	1:A:363:ASN:OD1	2.37	0.43
1:A:445:TYR:O	1:A:445:TYR:HD1	2.00	0.43
1:A:76:PHE:HB2	1:A:92:ILE:CG1	2.18	0.43
1:B:279:MET:HE3	1:B:286:ILE:HB	2.00	0.43
1:B:312:PRO:O	1:B:315:GLY:N	2.51	0.43
1:B:466:VAL:HG13	1:B:466:VAL:O	2.18	0.43
1:B:50:GLY:HA2	1:B:54:PHE:CB	2.41	0.43
1:A:500:SER:OG	1:A:501:PRO:N	2.49	0.42
1:B:243:VAL:O	1:B:246:ILE:HG22	2.19	0.42
1:B:303:ALA:O	1:B:304:GLU:C	2.53	0.42
1:A:130:LYS:O	1:A:134:ALA:N	2.50	0.42
1:A:206:VAL:CG1	1:A:207:PHE:N	2.82	0.42
1:A:456:VAL:O	1:A:457:LEU:C	2.57	0.42
1:A:44:PHE:O	1:A:47:LEU:HB2	2.18	0.42
1:B:145:GLN:HG3	1:B:310:VAL:HG12	2.00	0.42
1:B:49:GLY:CA	1:B:214:TYR:CE2	2.98	0.42
1:B:349:THR:O	1:B:353:LEU:HB2	2.19	0.42
1:B:427:PHE:CZ	1:B:453:PHE:CZ	3.07	0.42
1:A:256:ILE:HD11	1:A:270:GLY:O	2.20	0.42
1:A:413:LEU:N	1:A:413:LEU:HD23	2.33	0.42
1:A:495:HIS:HD2	1:A:497:ARG:CB	2.08	0.42
1:A:67:VAL:CG1	1:A:70:TRP:CG	3.03	0.42
1:B:170:ILE:CD1	1:B:293:ILE:CD1	2.94	0.42
1:B:172:ILE:CG1	1:B:251:VAL:CG1	2.96	0.42
1:B:177:ILE:HG13	1:B:178:TYR:N	2.34	0.42
1:B:54:PHE:O	1:B:55:ILE:C	2.57	0.42
1:B:55:ILE:CG2	1:B:56:PRO:N	2.50	0.42
1:B:69:GLY:O	1:B:70:TRP:CD1	2.73	0.42
1:B:93:SER:OG	1:B:460:PRO:HB3	2.19	0.42
1:A:117:ILE:C	1:A:118:LEU:CD1	2.81	0.42
1:A:24:SER:O	1:A:24:SER:OG	2.38	0.42
1:A:29:VAL:O	1:A:32:TYR:HB2	2.19	0.42
1:A:408:GLY:C	1:A:410:GLY:N	2.73	0.42
1:B:345:GLN:O	1:B:349:THR:CG2	2.67	0.42
1:B:101:ILE:HG22	1:B:374:THR:CB	2.50	0.42
1:A:107:LEU:O	1:A:110:VAL:HB	2.20	0.42
1:A:146:PHE:C	1:A:148:GLY:N	2.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ARG:O	1:A:155:ILE:C	2.57	0.42
1:A:165:LEU:HA	1:A:165:LEU:HD13	1.86	0.42
1:A:259:VAL:HG12	1:A:277:VAL:HG11	2.00	0.42
1:A:338:PRO:HB2	1:A:341:LEU:CD1	2.49	0.42
1:A:96:TYR:HD2	1:A:96:TYR:O	2.02	0.42
1:B:390:ILE:O	1:B:394:LEU:CB	2.67	0.42
1:B:495:HIS:ND1	1:B:496:PRO:HD2	2.34	0.42
1:B:208:VAL:HG12	1:B:371:LEU:HB3	2.02	0.42
1:A:33:PRO:O	1:A:36:ALA:HB3	2.19	0.42
1:A:373:LEU:CA	1:A:376:VAL:HG22	2.49	0.42
1:A:457:LEU:CD1	1:A:461:PHE:HE2	2.33	0.42
1:A:97:LEU:HD13	1:A:97:LEU:HA	1.53	0.42
1:B:356:LEU:HD21	1:B:369:ILE:CG2	2.49	0.42
1:B:436:ASN:CG	1:B:436:ASN:O	2.57	0.42
1:B:64:MET:O	1:B:67:VAL:CG2	2.68	0.42
1:B:95:GLY:HA2	1:B:378:TYR:CE1	2.55	0.42
1:A:457:LEU:CD1	1:A:461:PHE:CE2	3.03	0.42
1:B:233:ASP:O	1:B:236:LEU:CB	2.65	0.42
1:B:29:VAL:CB	1:B:32:TYR:CD1	3.02	0.42
1:B:339:VAL:CG2	1:B:343:ILE:HD12	2.47	0.42
1:B:55:ILE:HA	1:B:55:ILE:HD12	1.91	0.42
1:B:124:ASN:O	1:B:130:LYS:CE	2.35	0.42
1:B:112:GLY:HA3	1:B:269:ALA:CB	2.50	0.42
1:B:311:GLY:N	1:B:312:PRO:HD2	2.29	0.42
1:B:393:VAL:HG11	1:B:413:LEU:HD23	2.01	0.42
1:B:447:GLU:N	1:B:447:GLU:OE2	2.45	0.42
1:A:104:ILE:N	1:A:105:PRO:CD	2.82	0.42
1:A:124:ASN:O	1:A:130:LYS:CE	2.66	0.42
1:A:19:PHE:O	1:A:19:PHE:CD2	2.70	0.42
1:A:506:MET:O	1:A:507:ASN:CB	2.63	0.42
1:B:145:GLN:CA	1:B:145:GLN:NE2	2.55	0.42
1:A:170:ILE:HG22	1:A:275:PHE:CE1	2.55	0.41
1:A:309:ILE:O	1:A:309:ILE:CG2	2.67	0.41
1:B:234:TYR:CE2	1:B:238:MET:HG2	2.53	0.41
1:B:60:CYS:HA	1:B:389:TYR:CE1	2.55	0.41
1:A:102:GLY:C	1:A:105:PRO:HD2	2.40	0.41
1:A:120:TRP:O	1:A:122:ALA:N	2.49	0.41
1:A:188:GLU:O	1:A:189:MET:O	2.37	0.41
1:A:362:GLY:N	1:A:440:ASP:HB3	2.24	0.41
1:B:207:PHE:HA	1:B:210:PHE:CD2	2.55	0.41
1:A:138:LEU:C	1:A:138:LEU:HD23	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:ARG:C	1:A:234:TYR:N	2.73	0.41
1:A:332:MET:HG2	1:A:336:GLY:C	2.40	0.41
1:A:83:LEU:CD2	1:A:388:GLY:HA2	2.51	0.41
1:B:29:VAL:CA	1:B:32:TYR:CD1	2.97	0.41
1:B:433:PRO:HA	1:B:434:PRO:HD3	1.89	0.41
1:A:135:LEU:CD2	1:A:350:SER:HG	2.30	0.41
1:A:336:GLY:H	1:A:506:MET:HE1	1.82	0.41
1:A:405:ILE:HG22	1:A:406:PRO:HD2	2.01	0.41
1:B:32:TYR:CE2	1:B:249:SER:HA	2.56	0.41
1:B:103:PHE:CE1	1:B:308:TRP:HB2	2.52	0.41
1:B:320:ALA:HB1	1:B:330:ALA:HB2	2.02	0.41
1:B:70:TRP:HH2	1:B:392:LEU:HD11	1.64	0.41
1:A:114:LEU:O	1:A:118:LEU:HD13	2.20	0.41
1:A:161:PHE:CE1	1:A:493:PHE:CZ	3.07	0.41
1:A:221:ALA:O	1:A:222:THR:C	2.59	0.41
1:A:276:THR:OG1	1:A:290:VAL:HG11	2.21	0.41
1:B:131:THR:HG22	1:B:357:THR:CG2	2.50	0.41
1:B:158:VAL:O	1:B:162:ALA:N	2.35	0.41
1:B:66:THR:CB	1:B:402:THR:HA	2.50	0.41
1:A:114:LEU:HD23	1:A:114:LEU:HA	1.52	0.41
1:A:48:LEU:HD12	1:A:207:PHE:HE2	1.86	0.41
1:A:83:LEU:HD12	1:A:384:MET:HB3	2.02	0.41
1:B:44:PHE:HE2	1:B:198:PHE:HZ	1.68	0.41
1:B:218:GLU:HG3	1:B:218:GLU:H	1.41	0.41
1:B:380:CYS:O	1:B:381:ALA:C	2.59	0.41
1:A:191:SER:OG	1:A:192:LYS:N	2.54	0.41
1:A:232:ARG:CG	1:A:233:ASP:N	2.84	0.41
1:A:260:ILE:HD12	1:A:273:GLN:NE2	2.35	0.41
1:A:404:ASN:O	1:A:405:ILE:C	2.56	0.41
1:A:96:TYR:CB	1:A:316:MET:HG3	2.50	0.41
1:B:110:VAL:O	1:B:114:LEU:HB2	2.20	0.41
1:B:205:VAL:HG13	1:B:206:VAL:N	2.36	0.41
1:A:495:HIS:HA	1:A:496:PRO:HD3	1.91	0.41
1:B:67:VAL:HG23	1:B:70:TRP:CG	2.56	0.41
1:A:133:ALA:O	1:A:137:ILE:HG13	2.21	0.41
1:A:225:ASN:O	1:A:226:GLU:C	2.60	0.41
1:A:333:ASN:OD1	1:A:339:VAL:HG11	2.21	0.41
1:A:373:LEU:HA	1:A:373:LEU:HD23	1.90	0.41
1:A:433:PRO:HD3	1:A:446:VAL:HG23	2.02	0.41
1:B:13:LEU:O	1:B:227:MET:CE	2.68	0.41
1:B:148:GLY:C	1:B:150:LYS:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:LEU:O	1:B:168:ALA:CB	2.58	0.41
1:B:13:LEU:CD2	1:B:17:GLY:HA3	2.36	0.41
1:B:371:LEU:O	1:B:374:THR:HG22	2.21	0.41
1:B:82:THR:HG23	1:B:391:VAL:HG12	2.02	0.41
1:B:435:ASP:HA	1:B:442:THR:OG1	2.20	0.41
1:A:104:ILE:HG12	1:A:104:ILE:H	1.54	0.41
1:A:104:ILE:N	1:A:105:PRO:HD2	2.36	0.41
1:A:194:PHE:CD2	1:A:195:PHE:CD1	3.08	0.41
1:A:357:THR:HA	1:A:366:SER:HB3	2.02	0.41
1:A:379:LEU:HD12	1:A:383:PHE:CE1	2.54	0.41
1:B:200:LYS:HB2	1:B:203:THR:HG21	2.03	0.41
1:B:24:SER:HB3	1:B:493:PHE:CA	2.48	0.41
1:B:439:GLY:O	1:B:440:ASP:C	2.58	0.41
1:B:376:VAL:HG12	1:B:453:PHE:CD1	2.56	0.41
1:B:485:GLN:O	1:B:486:ASN:O	2.39	0.41
1:B:495:HIS:O	1:B:496:PRO:C	2.57	0.41
1:A:230:PRO:O	1:A:231:GLY:O	2.38	0.41
1:B:106:MET:O	1:B:109:PHE:N	2.54	0.41
1:B:51:ILE:HG22	1:B:52:LEU:N	2.35	0.41
1:A:200:LYS:HZ3	1:A:200:LYS:HB3	1.87	0.40
1:A:455:VAL:HG12	1:A:456:VAL:HG22	2.04	0.40
1:B:163:GLY:CA	1:B:167:PRO:HG2	2.51	0.40
1:A:124:ASN:ND2	1:A:269:ALA:HB3	2.36	0.40
1:A:53:TRP:O	1:A:56:PRO:CD	2.63	0.40
1:B:390:ILE:CD1	1:B:416:ALA:HB3	2.50	0.40
1:B:58:GLY:HA3	1:B:238:MET:CE	2.51	0.40
1:A:250:SER:O	1:A:254:LEU:HB2	2.20	0.40
1:A:178:TYR:HD1	1:A:278:LEU:HD22	1.83	0.40
1:B:46:LEU:HD12	1:B:246:ILE:HG13	2.04	0.40
1:B:293:ILE:O	1:B:296:LEU:HB2	2.21	0.40
1:B:300:GLY:O	1:B:303:ALA:HB3	2.22	0.40
1:B:103:PHE:CD1	1:B:308:TRP:HE3	2.39	0.40
1:B:325:LEU:O	1:B:326:PRO:C	2.58	0.40
1:B:436:ASN:OD1	1:B:436:ASN:C	2.60	0.40
1:A:234:TYR:CB	1:A:235:PRO:CD	2.85	0.40
1:A:238:MET:HE3	1:A:238:MET:HB3	1.89	0.40
1:A:59:LEU:HB3	1:A:405:ILE:HD13	2.04	0.40
1:A:485:GLN:O	1:A:486:ASN:O	2.39	0.40
1:B:36:ALA:O	1:B:37:THR:C	2.59	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	487/511 (95%)	374 (77%)	59 (12%)	54 (11%)	0 2
1	B	472/511 (92%)	336 (71%)	84 (18%)	52 (11%)	0 2
All	All	959/1022 (94%)	710 (74%)	143 (15%)	106 (11%)	0 2

All (106) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	VAL
1	A	86	ARG
1	A	152	THR
1	A	231	GLY
1	A	280	SER
1	A	283	ALA
1	A	335	ASN
1	A	466	VAL
1	A	484	SER
1	A	486	ASN
1	A	501	PRO
1	A	502	HIS
1	B	46	LEU
1	B	59	LEU
1	B	71	GLU
1	B	96	TYR
1	B	151	TYR
1	B	182	GLY
1	B	190	ASP
1	B	227	MET
1	B	330	ALA
1	B	335	ASN
1	B	440	ASP
1	B	442	THR
1	B	486	ASN

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Mol	Chain	Res	Type
1	A	54	PHE
1	A	85	PRO
1	A	153	ALA
1	A	205	VAL
1	A	226	GLU
1	A	311	GLY
1	A	356	LEU
1	A	361	GLY
1	A	393	VAL
1	A	409	LYS
1	A	429	VAL
1	A	457	LEU
1	A	477	VAL
1	B	30	TYR
1	B	68	ASP
1	B	130	LYS
1	B	147	GLY
1	B	201	VAL
1	B	223	HIS
1	B	231	GLY
1	B	324	LEU
1	B	367	PHE
1	B	429	VAL
1	B	433	PRO
1	B	438	GLN
1	B	445	TYR
1	A	55	ILE
1	A	143	LEU
1	A	154	ARG
1	A	218	GLU
1	A	223	HIS
1	A	284	PRO
1	A	334	LYS
1	A	357	THR
1	A	358	ASN
1	A	359	THR
1	A	508	ASP
1	B	54	PHE
1	B	115	SER
1	B	192	LYS
1	B	198	PHE
1	B	235	PRO

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Mol	Chain	Res	Type
1	B	312	PRO
1	B	322	LYS
1	A	110	VAL
1	A	147	GLY
1	A	189	MET
1	A	225	ASN
1	A	233	ASP
1	A	326	PRO
1	A	423	SER
1	A	424	ILE
1	A	440	ASP
1	A	487	ALA
1	B	41	SER
1	B	60	CYS
1	B	97	LEU
1	B	166	LEU
1	B	167	PRO
1	B	268	SER
1	B	487	ALA
1	A	481	PRO
1	B	164	ILE
1	B	298	LEU
1	B	323	ASN
1	B	334	LYS
1	B	396	HIS
1	A	406	PRO
1	A	438	GLN
1	B	121	PRO
1	B	490	GLY
1	A	73	GLY
1	A	172	ILE
1	B	251	VAL
1	B	261	PRO
1	A	148	GLY
1	B	310	VAL
1	B	459	LEU
1	A	397	PRO
1	B	326	PRO
1	A	208	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	394/414 (95%)	249 (63%)	145 (37%)	0	0
1	B	380/414 (92%)	234 (62%)	146 (38%)	0	0
All	All	774/828 (94%)	483 (62%)	291 (38%)	0	0

All (291) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	14	THR
1	A	15	LEU
1	A	16	LEU
1	A	19	PHE
1	A	24	SER
1	A	30	TYR
1	A	34	THR
1	A	41	SER
1	A	42	LEU
1	A	43	VAL
1	A	51	ILE
1	A	64	MET
1	A	67	VAL
1	A	72	GLU
1	A	76	PHE
1	A	92	ILE
1	A	93	SER
1	A	96	TYR
1	A	97	LEU
1	A	98	GLN
1	A	99	ILE
1	A	101	ILE
1	A	103	PHE
1	A	104	ILE
1	A	114	LEU
1	A	117	ILE

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Mol	Chain	Res	Type
1	A	118	LEU
1	A	125	GLU
1	A	128	ILE
1	A	131	THR
1	A	136	ILE
1	A	143	LEU
1	A	144	THR
1	A	145	GLN
1	A	146	PHE
1	A	149	THR
1	A	151	TYR
1	A	152	THR
1	A	154	ARG
1	A	155	ILE
1	A	157	LYS
1	A	160	PHE
1	A	165	LEU
1	A	166	LEU
1	A	169	PHE
1	A	170	ILE
1	A	171	LEU
1	A	172	ILE
1	A	174	LEU
1	A	177	ILE
1	A	178	TYR
1	A	179	LEU
1	A	180	HIS
1	A	181	SER
1	A	190	ASP
1	A	193	THR
1	A	194	PHE
1	A	197	ASP
1	A	200	LYS
1	A	203	THR
1	A	204	LEU
1	A	206	VAL
1	A	212	LEU
1	A	217	VAL
1	A	218	GLU
1	A	227	MET
1	A	228	SER
1	A	232	ARG

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Mol	Chain	Res	Type
1	A	233	ASP
1	A	239	LEU
1	A	240	LEU
1	A	241	LEU
1	A	248	LEU
1	A	254	LEU
1	A	256	ILE
1	A	258	MET
1	A	260	ILE
1	A	264	GLU
1	A	268	SER
1	A	271	VAL
1	A	272	MET
1	A	273	GLN
1	A	274	THR
1	A	279	MET
1	A	282	VAL
1	A	286	ILE
1	A	293	ILE
1	A	298	LEU
1	A	299	LEU
1	A	304	GLU
1	A	308	TRP
1	A	316	MET
1	A	318	VAL
1	A	319	THR
1	A	323	ASN
1	A	331	LYS
1	A	332	MET
1	A	339	VAL
1	A	340	THR
1	A	341	LEU
1	A	343	ILE
1	A	344	SER
1	A	345	GLN
1	A	357	THR
1	A	365	MET
1	A	366	SER
1	A	369	ILE
1	A	373	LEU
1	A	377	ILE
1	A	378	TYR

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Mol	Chain	Res	Type
1	A	395	LYS
1	A	399	LEU
1	A	401	ARG
1	A	409	LYS
1	A	413	LEU
1	A	417	ILE
1	A	418	VAL
1	A	421	LEU
1	A	430	SER
1	A	432	LEU
1	A	435	ASP
1	A	437	ILE
1	A	438	GLN
1	A	440	ASP
1	A	441	SER
1	A	444	MET
1	A	445	TYR
1	A	451	VAL
1	A	455	VAL
1	A	457	LEU
1	A	463	LEU
1	A	478	THR
1	A	479	LEU
1	A	480	GLU
1	A	484	SER
1	A	485	GLN
1	A	489	LYS
1	A	493	PHE
1	A	497	ARG
1	A	499	ARG
1	A	500	SER
1	A	502	HIS
1	A	503	TYR
1	A	506	MET
1	B	13	LEU
1	B	14	THR
1	B	15	LEU
1	B	24	SER
1	B	26	VAL
1	B	27	MET
1	B	31	GLU
1	B	34	THR

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Mol	Chain	Res	Type
1	B	38	SER
1	B	41	SER
1	B	43	VAL
1	B	46	LEU
1	B	47	LEU
1	B	48	LEU
1	B	51	ILE
1	B	55	ILE
1	B	59	LEU
1	B	67	VAL
1	B	68	ASP
1	B	71	GLU
1	B	76	PHE
1	B	78	TRP
1	B	80	SER
1	B	97	LEU
1	B	98	GLN
1	B	103	PHE
1	B	104	ILE
1	B	106	MET
1	B	111	LEU
1	B	114	LEU
1	B	117	ILE
1	B	123	LEU
1	B	128	ILE
1	B	130	LYS
1	B	131	THR
1	B	132	ILE
1	B	136	ILE
1	B	138	LEU
1	B	144	THR
1	B	145	GLN
1	B	149	THR
1	B	151	TYR
1	B	154	ARG
1	B	164	ILE
1	B	165	LEU
1	B	166	LEU
1	B	169	PHE
1	B	171	LEU
1	B	172	ILE
1	B	174	LEU

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Mol	Chain	Res	Type
1	B	179	LEU
1	B	181	SER
1	B	187	ILE
1	B	188	GLU
1	B	189	MET
1	B	192	LYS
1	B	194	PHE
1	B	199	SER
1	B	203	THR
1	B	204	LEU
1	B	208	VAL
1	B	211	ILE
1	B	213	SER
1	B	215	MET
1	B	217	VAL
1	B	218	GLU
1	B	228	SER
1	B	232	ARG
1	B	233	ASP
1	B	234	TYR
1	B	239	LEU
1	B	240	LEU
1	B	246	ILE
1	B	248	LEU
1	B	250	SER
1	B	256	ILE
1	B	260	ILE
1	B	263	ASN
1	B	266	ASN
1	B	267	LEU
1	B	271	VAL
1	B	272	MET
1	B	275	PHE
1	B	276	THR
1	B	278	LEU
1	B	279	MET
1	B	281	HIS
1	B	282	VAL
1	B	291	ARG
1	B	294	SER
1	B	299	LEU
1	B	304	GLU

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Mol	Chain	Res	Type
1	B	307	SER
1	B	316	MET
1	B	318	VAL
1	B	323	ASN
1	B	324	LEU
1	B	331	LYS
1	B	332	MET
1	B	334	LYS
1	B	339	VAL
1	B	340	THR
1	B	341	LEU
1	B	345	GLN
1	B	349	THR
1	B	351	ILE
1	B	353	LEU
1	B	354	ILE
1	B	355	ILE
1	B	356	LEU
1	B	357	THR
1	B	369	ILE
1	B	373	LEU
1	B	374	THR
1	B	377	ILE
1	B	378	TYR
1	B	384	MET
1	B	385	LEU
1	B	392	LEU
1	B	394	LEU
1	B	395	LYS
1	B	396	HIS
1	B	402	THR
1	B	404	ASN
1	B	423	SER
1	B	424	ILE
1	B	435	ASP
1	B	438	GLN
1	B	441	SER
1	B	444	MET
1	B	448	LEU
1	B	449	LEU
1	B	454	LEU
1	B	457	LEU

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Mol	Chain	Res	Type
1	B	462	ILE
1	B	464	TYR
1	B	477	VAL
1	B	478	THR
1	B	479	LEU
1	B	480	GLU
1	B	483	ASN
1	B	485	GLN
1	B	489	LYS
1	B	491	HIS
1	B	499	ARG
1	B	500	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	GLN
1	A	145	GLN
1	A	225	ASN
1	A	321	GLN
1	A	364	ASN
1	A	436	ASN
1	A	485	GLN
1	A	495	HIS
1	B	124	ASN
1	B	145	GLN
1	B	225	ASN
1	B	266	ASN
1	B	321	GLN
1	B	323	ASN
1	B	345	GLN
1	B	404	ASN
1	B	438	GLN
1	B	485	GLN
1	B	491	HIS
1	B	495	HIS
1	B	502	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	493/511 (96%)	0.04	21 (4%) 35 21	47, 95, 150, 198	0
1	B	480/511 (93%)	0.16	30 (6%) 20 11	51, 115, 177, 251	0
All	All	973/1022 (95%)	0.10	51 (5%) 27 15	47, 105, 168, 251	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	150	LYS	5.2
1	B	480	GLU	4.8
1	B	435	ASP	4.5
1	B	504	ILE	3.9
1	B	196	PRO	3.9
1	A	443	ASP	3.7
1	B	197	ASP	3.5
1	A	287	GLU	3.5
1	B	466	VAL	3.4
1	B	119	LYS	3.2
1	B	14	THR	3.2
1	A	504	ILE	3.1
1	B	228	SER	3.1
1	B	213	SER	2.9
1	B	154	ARG	2.9
1	A	473	ALA	2.8
1	B	436	ASN	2.8
1	B	478	THR	2.7
1	B	27	MET	2.7
1	A	89	PHE	2.6
1	B	195	PHE	2.6
1	B	334	LYS	2.5
1	B	30	TYR	2.5
1	A	329	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	332	MET	2.5
1	A	438	GLN	2.5
1	A	442	THR	2.5
1	A	334	LYS	2.5
1	B	12	GLN	2.4
1	A	436	ASN	2.4
1	A	180	HIS	2.4
1	A	149	THR	2.4
1	B	28	ALA	2.3
1	B	479	LEU	2.3
1	A	365	MET	2.3
1	B	502	HIS	2.3
1	B	264	GLU	2.3
1	A	216	GLY	2.2
1	A	263	ASN	2.2
1	B	215	MET	2.2
1	A	286	ILE	2.1
1	B	285	GLU	2.1
1	B	219	ALA	2.1
1	A	31	GLU	2.1
1	A	437	ILE	2.1
1	A	466	VAL	2.1
1	A	400	LYS	2.0
1	B	304	GLU	2.0
1	B	336	GLY	2.0
1	B	105	PRO	2.0
1	B	326	PRO	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](#)

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.