



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:37 PM GMT

PDB ID : 1PV7  
Title : Crystal structure of lactose permease with TDG  
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Deposited on : 2003-06-26  
Resolution : 3.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

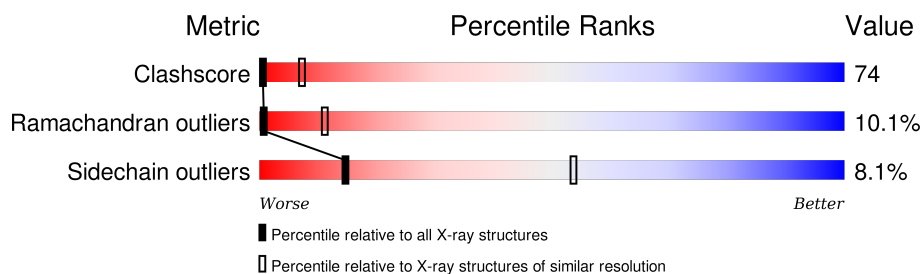
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	417	 23% 63% 14%
1	B	417	 24% 62% 13% .

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6626 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.

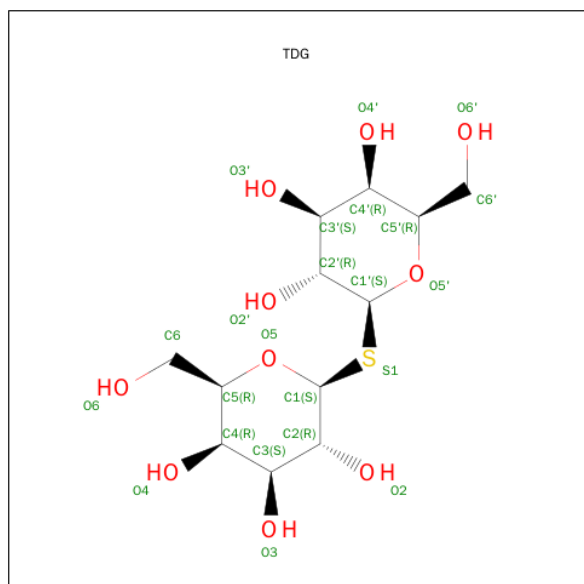
- Molecule 1 is a protein called Lactose permease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	0	0	0
			3290	2222	506	541	21			
1	B	417	Total	C	N	O	S	0	0	0
			3290	2222	506	541	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	154	GLY	CYS	ENGINEERED	UNP P02920
B	154	GLY	CYS	ENGINEERED	UNP P02920

- Molecule 2 is THIODIGALACTOSIDE (three-letter code: TDG) (formula:  $C_{12}H_{22}O_{10}S$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			23	12	10	1		

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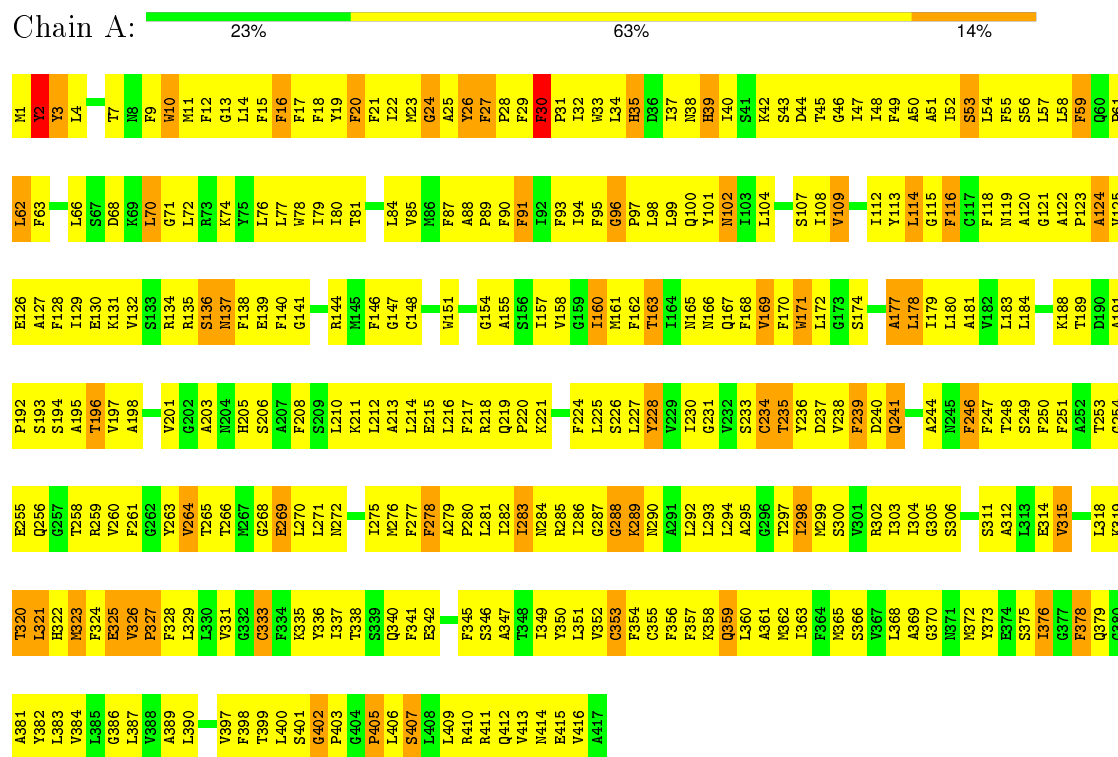
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	O	S	0	0
			23	12	10	1		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

#### • Molecule 1: Lactose permease



#### • Molecule 1: Lactose permease



A195	R289	V326	L390
I196	V260	F327	
V197	F261	F328	V397
A198	G262	L329	F398
	Y263	L330	T399
V201	V264	V331	L400
R202		G332	S401
A203	G268	C333	G402
I204	E269	F334	
H205	L270	K335	P405
S206	L271	Y336	L406
A207	L272	I337	S407
F208	I273	T338	L408
S209		S339	L409
I210	I275	Q340	R410
L211	M276	F341	R411
L212	F277		Q412
A213	F278	A347	V413
L214	A279	T348	N414
E215	P280	L349	E415
F217	L281	Y350	V416
R218	I282	L351	
Q219	I283	V352	A417
P220		C353	
K221	I286	F354	
	G287	C355	
	G288	F356	
F224	K289	F357	
L225	N290	K358	
S226	A291	Q359	
L227	L292	L360	
Y228	L293	A361	
V229	L294	K362	
I230	A295	T363	
G231	G296	F364	
V232	T297	K365	
S233	I298	S366	
G234	N299	V367	
T235	S300	L368	
Y236	V301	A369	
D237	R302	G370	
V238	I303	N371	
F239	I304	K372	
D240	G305	Y373	
Q241	S306	E374	
Q242		S375	
F243	S311	I376	
A244	A312	G377	
I245	L313	F378	
F246	E314	Q379	
F247	V315	G380	
T248		A381	
S249	L318	Y382	
F250	K319	L383	
F251	T320	V384	
A252	L321	L385	
T253	K322	G386	
G254	M323	L387	
E255	F324	V388	
Q256	E325	A389	

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.35Å 125.84Å 188.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	4.00 – 3.60	Depositor
% Data completeness (in resolution range)	(Not available) (4.00-3.60)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.271 , 0.296	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6626	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

## 5 Model quality [i](#)

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

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

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	0.69	1/3387 (0.0%)	0.84	2/4588 (0.0%)
1	B	0.67	1/3387 (0.0%)	0.84	2/4588 (0.0%)
All	All	0.68	2/6774 (0.0%)	0.84	4/9176 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	315	VAL	CB-CG1	-5.82	1.40	1.52
1	B	315	VAL	CB-CG1	-5.50	1.41	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	LEU	CA-CB-CG	5.74	128.50	115.30
1	B	70	LEU	CA-CB-CG	5.67	128.34	115.30
1	B	114	LEU	N-CA-C	-5.12	97.18	111.00
1	A	114	LEU	N-CA-C	-5.00	97.49	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3290	0	3333	504	0
1	B	3290	0	3333	490	0
2	A	23	0	22	0	0
2	B	23	0	22	0	0
All	All	6626	0	6710	990	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 74.

All (990) 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:30:PHE:HB3	1:A:31:PRO:HD3	1.29	1.10
1:B:87:PHE:HB3	1:B:174:SER:HB2	1.36	1.08
1:B:256:GLN:OE1	1:B:259:ARG:HD2	1.54	1.07
1:B:30:PHE:HB3	1:B:31:PRO:HD3	1.31	1.07
1:A:293:LEU:HD13	1:A:397:VAL:HG22	1.36	1.06
1:A:77:LEU:HD12	1:A:80:ILE:HD12	1.38	1.05
1:A:256:GLN:OE1	1:A:259:ARG:HD2	1.54	1.05
1:B:293:LEU:HD13	1:B:397:VAL:HG22	1.40	1.04
1:A:74:LYS:HD2	1:A:74:LYS:H	1.25	1.01
1:A:87:PHE:HB3	1:A:174:SER:HB2	1.39	1.00
1:A:34:LEU:HB3	1:A:40:ILE:HG21	1.47	0.96
1:A:279:ALA:O	1:A:283:ILE:HG12	1.66	0.96
1:B:104:LEU:HG	1:B:108:ILE:HD11	1.44	0.95
1:B:74:LYS:H	1:B:74:LYS:HD2	1.29	0.95
1:B:34:LEU:HB3	1:B:40:ILE:HG21	1.49	0.95
1:B:16:PHE:HB3	1:B:147:GLY:HA3	1.49	0.94
1:B:50:ALA:HB2	1:B:366:SER:HB2	1.49	0.94
1:B:90:PHE:CG	1:B:114:LEU:HD13	2.03	0.93
1:A:30:PHE:HB3	1:A:31:PRO:CD	1.97	0.93
1:A:90:PHE:CG	1:A:114:LEU:HD13	2.04	0.93
1:B:52:ILE:HA	1:B:112:ILE:HG21	1.49	0.92
1:B:30:PHE:HB3	1:B:31:PRO:CD	2.01	0.91
1:B:264:VAL:HG11	1:B:319:LYS:HG2	1.52	0.90
1:B:279:ALA:O	1:B:283:ILE:HG12	1.71	0.90
1:A:104:LEU:HG	1:A:108:ILE:HD11	1.50	0.90
1:A:52:ILE:HA	1:A:112:ILE:HG21	1.50	0.89
1:A:234:CYS:SG	1:A:365:MET:SD	2.70	0.89
1:B:234:CYS:SG	1:B:365:MET:SD	2.71	0.89
1:B:88:ALA:HB3	1:B:89:PRO:HD3	1.53	0.88
1:A:283:ILE:HG13	1:A:331:VAL:CG1	2.04	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:VAL:HG11	1:A:319:LYS:HG2	1.55	0.88
1:A:16:PHE:HB3	1:A:147:GLY:HA3	1.56	0.88
1:A:50:ALA:HB2	1:A:366:SER:HB2	1.54	0.87
1:A:88:ALA:HB3	1:A:89:PRO:HD3	1.55	0.87
1:A:108:ILE:HG22	1:A:112:ILE:HD11	1.55	0.87
1:B:27:PHE:HB3	1:B:28:PRO:CD	2.05	0.86
1:B:77:LEU:HD12	1:B:80:ILE:HD12	1.54	0.86
1:B:283:ILE:HG13	1:B:331:VAL:CG1	2.05	0.85
1:A:27:PHE:HB3	1:A:28:PRO:CD	2.07	0.85
1:A:37:ILE:HD13	1:A:166:ASN:HD22	1.40	0.85
1:B:22:ILE:HD11	1:B:177:ALA:HB1	1.59	0.85
1:A:276:MET:HA	1:A:279:ALA:HB2	1.59	0.84
1:A:121:GLY:O	1:A:124:ALA:HB3	1.78	0.84
1:A:196:THR:HG21	1:A:201:VAL:HB	1.58	0.84
1:B:74:LYS:N	1:B:74:LYS:HD2	1.92	0.84
1:B:415:GLU:OE1	1:B:415:GLU:HA	1.76	0.84
1:B:251:PHE:CE2	1:B:260:VAL:HG21	2.13	0.84
1:B:180:LEU:O	1:B:184:LEU:HG	1.78	0.84
1:B:276:MET:HA	1:B:279:ALA:HB2	1.57	0.84
1:B:90:PHE:CD1	1:B:94:ILE:HD12	2.13	0.83
1:A:22:ILE:HD11	1:A:177:ALA:HB1	1.59	0.83
1:A:74:LYS:N	1:A:74:LYS:HD2	1.92	0.83
1:B:279:ALA:HB3	1:B:280:PRO:HD3	1.62	0.82
1:A:279:ALA:HB3	1:A:280:PRO:HD3	1.61	0.82
1:B:44:ASP:OD1	1:B:104:LEU:HD22	1.80	0.82
1:B:283:ILE:HG13	1:B:331:VAL:HG11	1.62	0.81
1:B:195:ALA:O	1:B:196:THR:HG22	1.80	0.81
1:B:108:ILE:HG22	1:B:112:ILE:HD11	1.62	0.81
1:A:283:ILE:HG13	1:A:331:VAL:HG11	1.60	0.81
1:B:85:VAL:HG22	1:B:178:LEU:HB2	1.63	0.80
1:A:27:PHE:HB3	1:A:28:PRO:HD2	1.63	0.80
1:A:180:LEU:O	1:A:184:LEU:HG	1.82	0.80
1:A:415:GLU:HA	1:A:415:GLU:OE1	1.82	0.80
1:B:121:GLY:O	1:B:124:ALA:HB3	1.81	0.80
1:A:268:GLY:HA3	1:A:323:MET:CE	2.13	0.79
1:B:27:PHE:HB3	1:B:28:PRO:HD2	1.64	0.79
1:A:85:VAL:HG22	1:A:178:LEU:HB2	1.65	0.79
1:A:251:PHE:CE2	1:A:260:VAL:HG21	2.17	0.78
1:B:368:LEU:O	1:B:372:MET:HG3	1.83	0.78
1:A:37:ILE:HD13	1:A:166:ASN:ND2	1.98	0.78
1:B:104:LEU:O	1:B:108:ILE:HG13	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:LEU:HD13	1:B:40:ILE:CD1	2.14	0.78
1:B:37:ILE:HD13	1:B:166:ASN:HD22	1.46	0.78
1:A:90:PHE:CE2	1:A:95:PHE:HE1	2.02	0.78
1:A:293:LEU:HD11	1:A:397:VAL:HA	1.65	0.78
1:B:208:PHE:HA	1:B:212:LEU:HD12	1.65	0.77
1:B:268:GLY:HA3	1:B:323:MET:CE	2.15	0.77
1:A:172:LEU:HD13	1:B:183:LEU:HD12	1.66	0.77
1:B:196:THR:HG21	1:B:201:VAL:HB	1.66	0.77
1:B:34:LEU:HB3	1:B:40:ILE:CG2	2.15	0.77
1:A:34:LEU:HB3	1:A:40:ILE:CG2	2.15	0.77
1:A:90:PHE:CD1	1:A:94:ILE:HD12	2.20	0.76
1:A:42:LYS:NZ	1:A:373:TYR:HB3	2.01	0.76
1:A:208:PHE:HA	1:A:212:LEU:HD12	1.67	0.76
1:B:20:PHE:H	1:B:20:PHE:HD1	1.34	0.75
1:B:293:LEU:HD11	1:B:397:VAL:HA	1.66	0.75
1:A:20:PHE:HD1	1:A:20:PHE:H	1.34	0.75
1:A:93:PHE:O	1:A:97:PRO:HG2	1.85	0.75
1:A:122:ALA:HB3	1:A:123:PRO:CD	2.17	0.75
1:A:44:ASP:OD1	1:A:104:LEU:HD22	1.86	0.75
1:B:42:LYS:NZ	1:B:373:TYR:HB3	2.02	0.74
1:A:195:ALA:O	1:A:196:THR:HG22	1.88	0.74
1:B:409:LEU:O	1:B:413:VAL:HG23	1.87	0.74
1:A:151:TRP:HD1	1:A:269:GLU:HG3	1.52	0.74
1:A:99:LEU:HG	1:A:107:SER:OG	1.88	0.74
1:A:275:ILE:HG21	1:A:327:PRO:HG3	1.70	0.73
1:A:246:PHE:HB2	1:A:378:PHE:CD2	2.23	0.73
1:B:93:PHE:O	1:B:97:PRO:HG2	1.89	0.73
1:A:333:CYS:O	1:A:337:ILE:HG13	1.88	0.73
1:B:4:LEU:HD22	1:B:10:TRP:CZ3	2.23	0.73
1:A:74:LYS:H	1:A:74:LYS:CD	1.99	0.73
1:A:48:ILE:HA	1:A:108:ILE:HG23	1.71	0.73
1:B:333:CYS:O	1:B:337:ILE:HG13	1.88	0.73
1:B:66:LEU:O	1:B:70:LEU:HG	1.89	0.73
1:A:259:ARG:O	1:A:263:TYR:HD1	1.71	0.72
1:A:34:LEU:HD13	1:A:40:ILE:CD1	2.19	0.72
1:B:90:PHE:CZ	1:B:95:PHE:HE1	2.07	0.72
1:A:278:PHE:N	1:A:278:PHE:HD1	1.88	0.72
1:A:119:ASN:O	1:A:123:PRO:HD2	1.89	0.72
1:A:22:ILE:HB	1:A:118:PHE:HZ	1.52	0.72
1:B:48:ILE:HA	1:B:108:ILE:HG23	1.72	0.72
1:B:268:GLY:HA3	1:B:323:MET:HE2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:PHE:HD1	1:B:278:PHE:N	1.87	0.72
1:A:90:PHE:CZ	1:A:95:PHE:HE1	2.08	0.72
1:B:289:LYS:HE3	1:B:400:LEU:HB3	1.72	0.72
1:A:409:LEU:O	1:A:413:VAL:HG23	1.89	0.72
1:A:66:LEU:O	1:A:70:LEU:HG	1.90	0.71
1:B:74:LYS:H	1:B:74:LYS:CD	2.01	0.71
1:A:20:PHE:HD2	1:A:151:TRP:HB2	1.55	0.71
1:B:246:PHE:HB2	1:B:378:PHE:CD2	2.25	0.71
1:A:337:ILE:CD1	1:A:350:TYR:HE1	2.03	0.71
1:B:122:ALA:HB3	1:B:123:PRO:CD	2.19	0.71
1:A:34:LEU:HD13	1:A:40:ILE:HD13	1.73	0.71
1:B:411:ARG:O	1:B:414:ASN:HB3	1.90	0.71
1:A:225:LEU:HD13	1:A:336:TYR:CE2	2.26	0.71
1:B:90:PHE:CD2	1:B:114:LEU:HD13	2.25	0.71
1:A:282:ILE:O	1:A:286:ILE:HG13	1.92	0.70
1:B:122:ALA:HB3	1:B:123:PRO:HD2	1.73	0.70
1:A:4:LEU:HD22	1:A:10:TRP:CZ3	2.26	0.70
1:B:289:LYS:HD2	1:B:401:SER:O	1.91	0.70
1:B:22:ILE:HB	1:B:118:PHE:HZ	1.55	0.70
1:B:215:GLU:O	1:B:218:ARG:HB3	1.91	0.70
1:B:275:ILE:HG21	1:B:327:PRO:HG3	1.72	0.70
1:B:250:PHE:O	1:B:312:ALA:HB2	1.91	0.70
1:A:55:PHE:CZ	1:A:113:TYR:HE1	2.10	0.70
1:B:278:PHE:CD1	1:B:278:PHE:N	2.59	0.70
1:A:326:VAL:HB	1:A:327:PRO:CD	2.22	0.70
1:A:338:THR:HG21	1:A:415:GLU:OE2	1.92	0.70
1:A:250:PHE:O	1:A:312:ALA:HB2	1.92	0.70
1:B:208:PHE:HA	1:B:212:LEU:CD1	2.22	0.70
1:B:198:ALA:HB3	1:B:201:VAL:CG2	2.21	0.69
1:B:246:PHE:CD1	1:B:246:PHE:C	2.65	0.69
1:A:55:PHE:O	1:A:59:PHE:HB2	1.92	0.69
1:A:130:GLU:HG3	1:A:140:PHE:CD2	2.28	0.69
1:A:208:PHE:HA	1:A:212:LEU:CD1	2.23	0.69
1:A:10:TRP:HE1	1:B:168:PHE:HD1	1.38	0.69
1:A:268:GLY:HA3	1:A:323:MET:HE3	1.74	0.69
1:B:151:TRP:HD1	1:B:269:GLU:HG3	1.56	0.69
1:B:119:ASN:O	1:B:123:PRO:HD2	1.93	0.69
1:B:282:ILE:O	1:B:286:ILE:HG13	1.93	0.69
1:B:259:ARG:O	1:B:263:TYR:HD1	1.76	0.68
1:B:20:PHE:HD2	1:B:151:TRP:HB2	1.58	0.68
1:B:337:ILE:CD1	1:B:350:TYR:HE1	2.07	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:PHE:O	1:B:96:GLY:C	2.31	0.68
1:A:215:GLU:O	1:A:218:ARG:HB3	1.93	0.68
1:A:278:PHE:N	1:A:278:PHE:CD1	2.60	0.68
1:B:277:PHE:HD2	1:B:278:PHE:CE1	2.12	0.68
1:B:165:ASN:O	1:B:168:PHE:HB3	1.93	0.68
1:B:283:ILE:HG13	1:B:331:VAL:HG12	1.76	0.68
1:B:329:LEU:O	1:B:333:CYS:HB2	1.94	0.68
1:A:368:LEU:O	1:A:372:MET:HG3	1.94	0.68
1:B:326:VAL:HB	1:B:327:PRO:CD	2.22	0.67
1:A:90:PHE:CD2	1:A:114:LEU:HD13	2.28	0.67
1:A:168:PHE:CZ	1:A:172:LEU:HD12	2.29	0.67
1:A:246:PHE:CD1	1:A:246:PHE:C	2.68	0.67
1:B:34:LEU:CB	1:B:40:ILE:HG21	2.23	0.67
1:B:17:PHE:HD2	1:B:18:PHE:CD1	2.12	0.67
1:B:44:ASP:HA	1:B:104:LEU:HD21	1.75	0.67
1:B:55:PHE:CZ	1:B:113:TYR:HE1	2.11	0.67
1:B:90:PHE:HD1	1:B:94:ILE:HD12	1.57	0.67
1:B:99:LEU:HG	1:B:107:SER:OG	1.95	0.67
1:A:172:LEU:HD13	1:B:183:LEU:CD1	2.24	0.67
1:B:198:ALA:HB3	1:B:201:VAL:HG23	1.75	0.67
1:B:37:ILE:HD13	1:B:166:ASN:ND2	2.09	0.67
1:A:34:LEU:O	1:A:38:ASN:N	2.26	0.67
1:B:50:ALA:HB2	1:B:366:SER:CB	2.25	0.66
1:A:151:TRP:CD1	1:A:269:GLU:HG3	2.30	0.66
1:B:90:PHE:CE2	1:B:95:PHE:HE1	2.13	0.66
1:B:22:ILE:HD11	1:B:177:ALA:CB	2.24	0.66
1:A:283:ILE:HG13	1:A:331:VAL:HG12	1.76	0.66
1:B:104:LEU:CG	1:B:108:ILE:HD11	2.24	0.66
1:B:20:PHE:O	1:B:24:GLY:N	2.22	0.66
1:B:34:LEU:HD13	1:B:40:ILE:HD13	1.76	0.66
1:A:412:GLN:O	1:A:416:VAL:HG23	1.95	0.66
1:A:196:THR:OG1	1:A:201:VAL:HG11	1.95	0.66
1:A:268:GLY:HA3	1:A:323:MET:HE2	1.77	0.66
1:A:91:PHE:HB3	1:A:170:PHE:CE2	2.31	0.65
1:A:289:LYS:HD2	1:A:401:SER:O	1.96	0.65
1:B:412:GLN:O	1:B:416:VAL:HG23	1.95	0.65
1:A:77:LEU:O	1:A:80:ILE:HB	1.95	0.65
1:A:411:ARG:O	1:A:414:ASN:HB3	1.95	0.65
1:B:81:THR:O	1:B:85:VAL:HG23	1.96	0.65
1:A:104:LEU:O	1:A:108:ILE:HG13	1.96	0.65
1:A:22:ILE:HD11	1:A:177:ALA:CB	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:ILE:O	1:B:234:CYS:HB2	1.96	0.65
1:A:44:ASP:HA	1:A:104:LEU:HD21	1.78	0.65
1:A:49:PHE:HB3	1:A:241:GLN:OE1	1.97	0.65
1:A:22:ILE:HB	1:A:118:PHE:CZ	2.31	0.65
1:A:1:MET:H2	1:A:4:LEU:HB2	1.61	0.65
1:B:49:PHE:HB3	1:B:241:GLN:OE1	1.97	0.65
1:A:55:PHE:CZ	1:A:113:TYR:CE1	2.84	0.65
1:A:95:PHE:O	1:A:96:GLY:C	2.35	0.64
1:B:225:LEU:HD13	1:B:336:TYR:CE2	2.32	0.64
1:A:303:ILE:HG21	1:A:386:GLY:CA	2.26	0.64
1:A:90:PHE:CE2	1:A:95:PHE:CE1	2.85	0.64
1:B:1:MET:H2	1:B:4:LEU:HB2	1.62	0.64
1:A:289:LYS:HE3	1:A:400:LEU:HB3	1.79	0.64
1:B:48:ILE:HA	1:B:108:ILE:CG2	2.28	0.64
1:B:268:GLY:O	1:B:271:LEU:N	2.22	0.64
1:A:55:PHE:CE2	1:A:113:TYR:HE1	2.15	0.64
1:B:136:SER:O	1:B:137:ASN:CB	2.46	0.64
1:A:34:LEU:CB	1:A:40:ILE:HG21	2.24	0.64
1:B:338:THR:HG21	1:B:415:GLU:OE2	1.97	0.64
1:B:246:PHE:HD1	1:B:246:PHE:C	2.00	0.64
1:B:55:PHE:O	1:B:59:PHE:HB2	1.97	0.64
1:A:165:ASN:O	1:A:168:PHE:HB3	1.97	0.64
1:B:168:PHE:O	1:B:171:TRP:HB2	1.97	0.63
1:B:22:ILE:HB	1:B:118:PHE:CZ	2.33	0.63
1:A:122:ALA:HB3	1:A:123:PRO:HD2	1.80	0.63
1:A:63:PHE:CE1	1:A:76:LEU:HD21	2.33	0.63
1:A:1:MET:N	1:A:4:LEU:HB2	2.13	0.63
1:B:271:LEU:O	1:B:275:ILE:HG13	1.98	0.63
1:B:196:THR:OG1	1:B:201:VAL:HG11	1.97	0.63
1:B:130:GLU:HG3	1:B:140:PHE:CD2	2.34	0.63
1:B:303:ILE:HG21	1:B:386:GLY:CA	2.28	0.63
1:A:76:LEU:HD12	1:A:79:ILE:HD12	1.81	0.63
1:B:1:MET:HB2	1:B:3:TYR:CZ	2.34	0.62
1:A:48:ILE:HA	1:A:108:ILE:CG2	2.29	0.62
1:B:63:PHE:CE2	1:B:124:ALA:HB2	2.34	0.62
1:A:230:ILE:O	1:A:234:CYS:HB2	2.00	0.62
1:A:303:ILE:O	1:A:306:SER:N	2.33	0.62
1:A:13:GLY:O	1:A:146:PHE:HD2	1.82	0.62
1:B:52:ILE:HA	1:B:112:ILE:CG2	2.24	0.62
1:B:236:TYR:CE1	1:B:299:MET:HG2	2.34	0.62
1:A:246:PHE:HD1	1:A:246:PHE:C	2.03	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:THR:HG22	1:B:254:GLY:N	2.15	0.62
1:B:12:PHE:CD2	1:B:129:ILE:HG12	2.35	0.62
1:B:91:PHE:HB3	1:B:170:PHE:CE2	2.34	0.62
1:A:399:THR:HG22	1:A:399:THR:O	2.00	0.61
1:A:168:PHE:O	1:A:171:TRP:HB2	1.99	0.61
1:B:55:PHE:CZ	1:B:113:TYR:CE1	2.87	0.61
1:B:33:TRP:HA	1:B:37:ILE:HD12	1.82	0.61
1:B:90:PHE:CE2	1:B:114:LEU:HB3	2.35	0.61
1:A:85:VAL:HG13	1:A:178:LEU:HD22	1.83	0.61
1:B:44:ASP:O	1:B:48:ILE:HG13	2.00	0.61
1:A:12:PHE:CD2	1:A:129:ILE:HG12	2.34	0.61
1:A:196:THR:CG2	1:A:201:VAL:HB	2.29	0.61
1:B:216:LEU:HD23	1:B:219:GLN:OE1	2.00	0.61
1:B:100:GLN:HA	1:B:100:GLN:OE1	2.01	0.61
1:A:373:TYR:HE1	1:A:382:TYR:HE1	1.48	0.61
1:A:98:LEU:HB2	1:A:107:SER:OG	2.00	0.61
1:A:90:PHE:CB	1:A:114:LEU:HD13	2.31	0.61
1:A:85:VAL:CG1	1:A:178:LEU:HD22	2.30	0.61
1:B:373:TYR:HE1	1:B:382:TYR:HE1	1.47	0.61
1:A:277:PHE:HD2	1:A:278:PHE:CE1	2.19	0.61
1:A:376:ILE:HG22	1:A:376:ILE:O	2.01	0.61
1:A:139:GLU:C	1:A:141:GLY:H	2.03	0.61
1:A:139:GLU:C	1:A:141:GLY:N	2.54	0.61
1:A:81:THR:O	1:A:85:VAL:HG23	2.01	0.60
1:B:77:LEU:HD11	1:B:125:VAL:HG22	1.83	0.60
1:A:390:LEU:HD23	1:A:390:LEU:C	2.21	0.60
1:A:340:GLN:NE2	1:A:401:SER:OG	2.35	0.60
1:B:151:TRP:CD1	1:B:269:GLU:HG3	2.36	0.60
1:A:17:PHE:HD2	1:A:18:PHE:CD2	2.19	0.60
1:A:61:PRO:HG3	1:A:355:CYS:SG	2.41	0.60
1:B:407:SER:HG	1:B:410:ARG:HB2	1.66	0.60
1:B:356:PHE:CG	1:B:356:PHE:O	2.55	0.60
1:A:52:ILE:HA	1:A:112:ILE:CG2	2.26	0.60
1:B:215:GLU:OE1	1:B:215:GLU:C	2.39	0.60
1:B:40:ILE:CG1	1:B:44:ASP:HB2	2.31	0.60
1:A:40:ILE:CG1	1:A:44:ASP:HB2	2.31	0.60
1:A:29:PHE:CE1	1:A:33:TRP:CD1	2.89	0.60
1:B:34:LEU:HD13	1:B:40:ILE:HD12	1.84	0.60
1:A:226:SER:O	1:A:227:LEU:C	2.40	0.60
1:A:63:PHE:CE2	1:A:124:ALA:HB2	2.37	0.60
1:B:390:LEU:C	1:B:390:LEU:HD23	2.22	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:PRO:O	1:A:331:VAL:HG23	2.01	0.60
1:B:29:PHE:CE1	1:B:33:TRP:CD1	2.90	0.60
1:B:179:ILE:O	1:B:183:LEU:HB2	2.02	0.60
1:B:85:VAL:CG1	1:B:178:LEU:HD22	2.31	0.59
1:A:329:LEU:O	1:A:333:CYS:HB2	2.02	0.59
1:A:33:TRP:HH2	1:A:95:PHE:HB2	1.67	0.59
1:A:63:PHE:CD1	1:A:76:LEU:HD21	2.37	0.59
1:A:198:ALA:HB3	1:A:201:VAL:CG2	2.32	0.59
1:A:163:THR:HG21	1:A:255:GLU:HA	1.84	0.59
1:B:85:VAL:HG13	1:B:178:LEU:HD22	1.84	0.59
1:B:292:LEU:O	1:B:295:ALA:HB3	2.01	0.59
1:A:77:LEU:HD11	1:A:125:VAL:HG22	1.83	0.59
1:A:1:MET:HB2	1:A:3:TYR:CZ	2.37	0.59
1:B:4:LEU:HD22	1:B:10:TRP:HZ3	1.66	0.59
1:A:172:LEU:CD1	1:B:183:LEU:HD12	2.32	0.59
1:A:239:PHE:HD1	1:A:240:ASP:N	2.00	0.59
1:A:136:SER:O	1:A:137:ASN:CB	2.50	0.59
1:A:20:PHE:O	1:A:24:GLY:N	2.27	0.59
1:B:268:GLY:HA3	1:B:323:MET:HE3	1.84	0.59
1:A:4:LEU:HD22	1:A:10:TRP:CH2	2.38	0.59
1:A:42:LYS:HZ3	1:A:373:TYR:HB3	1.68	0.59
1:B:76:LEU:HD12	1:B:79:ILE:HD12	1.84	0.59
1:B:13:GLY:O	1:B:146:PHE:HD2	1.85	0.59
1:B:226:SER:O	1:B:227:LEU:C	2.41	0.58
1:B:277:PHE:CD2	1:B:278:PHE:HE1	2.21	0.58
1:B:90:PHE:CB	1:B:114:LEU:HD13	2.33	0.58
1:B:42:LYS:HZ2	1:B:373:TYR:HB3	1.66	0.58
1:B:1:MET:N	1:B:4:LEU:HB2	2.17	0.58
1:A:104:LEU:CG	1:A:108:ILE:HD11	2.28	0.58
1:B:286:ILE:HG22	1:B:290:ASN:HB2	1.85	0.58
1:A:90:PHE:HD1	1:A:94:ILE:HD12	1.65	0.58
1:A:216:LEU:HD23	1:A:219:GLN:OE1	2.03	0.58
1:A:286:ILE:HG22	1:A:290:ASN:HB2	1.85	0.58
1:B:37:ILE:HD11	1:B:162:PHE:CZ	2.39	0.58
1:A:98:LEU:HB3	1:A:107:SER:HB2	1.84	0.58
1:B:319:LYS:O	1:B:320:THR:C	2.41	0.58
1:B:4:LEU:HD22	1:B:10:TRP:CH2	2.39	0.58
1:B:239:PHE:HD1	1:B:240:ASP:N	2.00	0.58
1:B:127:ALA:O	1:B:130:GLU:HB3	2.02	0.58
1:A:253:THR:HG22	1:A:254:GLY:N	2.19	0.58
1:A:292:LEU:O	1:A:295:ALA:HB3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:TRP:CE3	1:B:171:TRP:HA	2.38	0.58
1:A:390:LEU:HD23	1:A:390:LEU:O	2.03	0.58
1:A:165:ASN:OD1	1:A:167:GLN:HB3	2.04	0.58
1:A:25:ALA:O	1:A:29:PHE:HB3	2.04	0.58
1:A:42:LYS:HZ2	1:A:373:TYR:HB3	1.68	0.58
1:B:163:THR:HG21	1:B:255:GLU:HG3	1.84	0.58
1:B:17:PHE:CD2	1:B:18:PHE:CE1	2.92	0.58
1:A:234:CYS:SG	1:A:361:ALA:HB1	2.42	0.58
1:A:271:LEU:O	1:A:275:ILE:HG13	2.04	0.58
1:B:55:PHE:CD2	1:B:112:ILE:HB	2.39	0.58
1:A:215:GLU:C	1:A:215:GLU:OE1	2.43	0.57
1:A:9:PHE:HD2	1:A:10:TRP:HE3	1.51	0.57
1:B:55:PHE:CE2	1:B:113:TYR:HE1	2.22	0.57
1:B:319:LYS:O	1:B:322:HIS:N	2.28	0.57
1:A:38:ASN:O	1:A:39:HIS:C	2.42	0.57
1:B:28:PRO:O	1:B:31:PRO:HD2	2.03	0.57
1:A:4:LEU:HD22	1:A:10:TRP:HZ3	1.69	0.57
1:B:20:PHE:N	1:B:20:PHE:CD1	2.71	0.57
1:B:34:LEU:O	1:B:38:ASN:N	2.36	0.57
1:A:369:ALA:O	1:A:370:GLY:C	2.42	0.57
1:A:49:PHE:O	1:A:52:ILE:HB	2.03	0.57
1:B:399:THR:HG22	1:B:399:THR:O	2.04	0.57
1:A:248:THR:HG22	1:A:248:THR:O	2.02	0.57
1:B:40:ILE:HG12	1:B:44:ASP:HB2	1.86	0.57
1:A:100:GLN:HA	1:A:100:GLN:OE1	2.03	0.57
1:B:55:PHE:HD2	1:B:112:ILE:HB	1.69	0.57
1:B:163:THR:HG21	1:B:255:GLU:HA	1.85	0.57
1:B:17:PHE:HD2	1:B:18:PHE:CE1	2.22	0.57
1:A:90:PHE:CE2	1:A:114:LEU:HB3	2.39	0.57
1:A:20:PHE:N	1:A:20:PHE:CD1	2.71	0.57
1:A:326:VAL:N	1:A:327:PRO:HD2	2.20	0.57
1:B:139:GLU:C	1:B:141:GLY:N	2.58	0.57
1:B:303:ILE:O	1:B:306:SER:N	2.38	0.56
1:B:369:ALA:O	1:B:370:GLY:C	2.43	0.56
1:B:54:LEU:HG	1:B:58:LEU:HD12	1.87	0.56
1:A:2:TYR:CE1	1:A:137:ASN:ND2	2.73	0.56
1:A:134:ARG:NH1	1:A:203:ALA:HA	2.18	0.56
1:B:134:ARG:NH1	1:B:203:ALA:HA	2.20	0.56
1:A:179:ILE:O	1:A:183:LEU:HB2	2.05	0.56
1:B:305:GLY:O	1:B:318:LEU:HD11	2.04	0.56
1:A:9:PHE:CD2	1:A:10:TRP:HE3	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:ARG:O	1:A:263:TYR:CD1	2.58	0.56
1:A:239:PHE:HE2	1:A:303:ILE:HA	1.70	0.56
1:B:347:ALA:O	1:B:351:LEU:HD12	2.04	0.56
1:A:305:GLY:O	1:A:318:LEU:HD11	2.05	0.56
1:A:85:VAL:HG13	1:A:178:LEU:HB2	1.87	0.56
1:A:14:LEU:HD23	1:A:146:PHE:HE2	1.69	0.56
1:A:335:LYS:HA	1:A:338:THR:HG22	1.87	0.56
1:B:139:GLU:C	1:B:141:GLY:H	2.07	0.56
1:A:356:PHE:CG	1:A:356:PHE:O	2.58	0.56
1:B:155:ALA:O	1:B:158:VAL:HB	2.05	0.56
1:A:99:LEU:CD2	1:A:107:SER:HB3	2.36	0.55
1:A:198:ALA:HB3	1:A:201:VAL:HG23	1.87	0.55
1:B:340:GLN:NE2	1:B:401:SER:OG	2.39	0.55
1:B:63:PHE:HE2	1:B:124:ALA:HB2	1.71	0.55
1:B:299:MET:O	1:B:300:SER:C	2.45	0.55
1:B:407:SER:OG	1:B:410:ARG:HB2	2.06	0.55
1:B:33:TRP:O	1:B:37:ILE:HB	2.06	0.55
1:A:155:ALA:O	1:A:158:VAL:HB	2.06	0.55
1:A:171:TRP:CE3	1:A:171:TRP:HA	2.41	0.55
1:A:277:PHE:C	1:A:278:PHE:HD1	2.09	0.55
1:B:305:GLY:O	1:B:318:LEU:CD1	2.54	0.55
1:B:327:PRO:O	1:B:331:VAL:HG23	2.07	0.55
1:B:362:MET:O	1:B:363:ILE:C	2.45	0.55
1:B:4:LEU:CD2	1:B:10:TRP:HZ3	2.20	0.55
1:A:54:LEU:HG	1:A:58:LEU:HD12	1.88	0.55
1:B:246:PHE:HD1	1:B:247:PHE:N	2.04	0.55
1:A:1:MET:HB2	1:A:3:TYR:CE1	2.41	0.55
1:A:25:ALA:O	1:A:29:PHE:CB	2.54	0.55
1:B:16:PHE:HB3	1:B:147:GLY:CA	2.32	0.55
1:A:319:LYS:O	1:A:320:THR:C	2.45	0.55
1:B:85:VAL:HG22	1:B:178:LEU:CB	2.36	0.55
1:B:239:PHE:HE2	1:B:303:ILE:HA	1.72	0.55
1:B:277:PHE:C	1:B:278:PHE:HD1	2.10	0.55
1:A:178:LEU:HG	1:A:179:ILE:N	2.22	0.55
1:B:27:PHE:CB	1:B:28:PRO:CD	2.84	0.55
1:B:365:MET:O	1:B:366:SER:C	2.46	0.55
1:A:13:GLY:O	1:A:146:PHE:CD2	2.60	0.55
1:B:120:ALA:O	1:B:123:PRO:HG2	2.07	0.55
1:B:10:TRP:O	1:B:14:LEU:HG	2.06	0.55
1:A:113:TYR:C	1:A:115:GLY:N	2.58	0.55
1:A:63:PHE:HE2	1:A:124:ALA:HB2	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:TYR:O	1:B:102:ASN:HB2	2.06	0.55
1:A:341:PHE:CD2	1:A:349:ILE:HD11	2.42	0.54
1:A:98:LEU:HD13	1:A:107:SER:HA	1.88	0.54
1:A:228:TYR:CZ	1:A:292:LEU:HB3	2.42	0.54
1:B:9:PHE:HD2	1:B:10:TRP:HE3	1.53	0.54
1:A:33:TRP:O	1:A:37:ILE:HB	2.06	0.54
1:A:211:LYS:O	1:A:212:LEU:C	2.46	0.54
1:A:294:LEU:HD23	1:A:328:PHE:CE2	2.43	0.54
1:B:13:GLY:O	1:B:146:PHE:CD2	2.60	0.54
1:B:11:MET:O	1:B:14:LEU:HB2	2.08	0.54
1:B:9:PHE:CD2	1:B:10:TRP:HE3	2.25	0.54
1:A:29:PHE:O	1:A:33:TRP:N	2.32	0.54
1:B:165:ASN:OD1	1:B:167:GLN:HB3	2.07	0.54
1:A:20:PHE:CD2	1:A:151:TRP:HB2	2.40	0.54
1:A:99:LEU:HD21	1:A:107:SER:HB3	1.90	0.54
1:A:239:PHE:C	1:A:239:PHE:CD1	2.80	0.54
1:A:85:VAL:HG22	1:A:178:LEU:CB	2.37	0.54
1:B:98:LEU:HB3	1:B:107:SER:HB2	1.90	0.54
1:B:239:PHE:CE2	1:B:303:ILE:HG12	2.43	0.54
1:B:85:VAL:HG13	1:B:178:LEU:HB2	1.90	0.54
1:A:327:PRO:HG2	1:A:328:PHE:H	1.72	0.54
1:A:40:ILE:HG12	1:A:44:ASP:HB2	1.89	0.54
1:B:90:PHE:CE2	1:B:95:PHE:CE1	2.94	0.53
1:B:196:THR:CG2	1:B:201:VAL:HB	2.34	0.53
1:A:168:PHE:HZ	1:A:172:LEU:HD12	1.72	0.53
1:A:4:LEU:CD2	1:A:10:TRP:HZ3	2.22	0.53
1:A:12:PHE:C	1:A:14:LEU:N	2.61	0.53
1:A:90:PHE:CZ	1:A:95:PHE:CE1	2.95	0.53
1:B:29:PHE:O	1:B:33:TRP:N	2.33	0.53
1:B:340:GLN:HE22	1:B:405:PRO:HB3	1.73	0.53
1:B:77:LEU:O	1:B:80:ILE:HB	2.08	0.53
1:B:228:TYR:CZ	1:B:292:LEU:HB3	2.43	0.53
1:B:62:LEU:HD11	1:B:66:LEU:HD11	1.88	0.53
1:A:101:TYR:O	1:A:102:ASN:HB2	2.08	0.53
1:B:2:TYR:CE1	1:B:137:ASN:ND2	2.77	0.53
1:A:55:PHE:HD2	1:A:112:ILE:HB	1.73	0.53
1:B:335:LYS:HA	1:B:338:THR:HG22	1.90	0.53
1:B:38:ASN:O	1:B:39:HIS:C	2.47	0.53
1:A:365:MET:O	1:A:366:SER:C	2.45	0.53
1:A:78:TRP:C	1:A:80:ILE:N	2.61	0.53
1:B:12:PHE:C	1:B:14:LEU:N	2.61	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:MET:HA	1:B:279:ALA:CB	2.34	0.53
1:B:294:LEU:HD23	1:B:328:PHE:CE2	2.44	0.53
1:B:85:VAL:CG2	1:B:178:LEU:HB2	2.34	0.53
1:A:277:PHE:CD2	1:A:278:PHE:HE1	2.27	0.53
1:A:311:SER:OG	1:A:314:GLU:CB	2.57	0.53
1:A:63:PHE:CD2	1:A:120:ALA:HB1	2.43	0.53
1:B:113:TYR:O	1:B:116:PHE:CD2	2.62	0.53
1:B:1:MET:HB2	1:B:3:TYR:CE1	2.44	0.53
1:B:277:PHE:CD2	1:B:278:PHE:CE1	2.94	0.53
1:A:53:SER:O	1:A:56:SER:N	2.40	0.53
1:B:277:PHE:HB3	1:B:278:PHE:CD1	2.44	0.53
1:A:44:ASP:O	1:A:48:ILE:HG13	2.09	0.52
1:B:14:LEU:HD23	1:B:146:PHE:HE2	1.74	0.52
1:B:376:ILE:O	1:B:376:ILE:HG22	2.09	0.52
1:B:264:VAL:HG11	1:B:319:LYS:CG	2.33	0.52
1:A:383:LEU:O	1:A:387:LEU:HB2	2.09	0.52
1:B:20:PHE:CD2	1:B:151:TRP:HB2	2.41	0.52
1:B:383:LEU:O	1:B:387:LEU:HB2	2.09	0.52
1:B:325:GLU:O	1:B:325:GLU:HG2	2.08	0.52
1:B:178:LEU:HG	1:B:179:ILE:N	2.25	0.52
1:A:210:LEU:O	1:A:214:LEU:N	2.22	0.52
1:B:297:THR:O	1:B:298:ILE:C	2.48	0.52
1:B:98:LEU:HB2	1:B:107:SER:OG	2.10	0.52
1:A:246:PHE:HD1	1:A:247:PHE:N	2.06	0.52
1:A:358:LYS:O	1:A:360:LEU:N	2.43	0.52
1:A:340:GLN:HE22	1:A:405:PRO:HB3	1.73	0.52
1:B:336:TYR:OH	1:B:401:SER:HB3	2.10	0.52
1:A:121:GLY:HA2	1:A:124:ALA:HB3	1.90	0.52
1:B:61:PRO:HG3	1:B:355:CYS:SG	2.49	0.52
1:A:108:ILE:O	1:A:109:VAL:C	2.47	0.52
1:A:116:PHE:C	1:A:116:PHE:CD1	2.83	0.52
1:A:14:LEU:O	1:A:17:PHE:N	2.42	0.52
1:B:25:ALA:O	1:B:29:PHE:HB3	2.09	0.52
1:B:379:GLN:O	1:B:382:TYR:HB2	2.08	0.52
1:A:55:PHE:CD2	1:A:112:ILE:HB	2.45	0.52
1:A:32:ILE:CD1	1:A:258:THR:HG23	2.40	0.52
1:B:205:HIS:CG	1:B:206:SER:H	2.27	0.52
1:A:85:VAL:CG2	1:A:178:LEU:HB2	2.37	0.52
1:B:278:PHE:HB2	1:B:282:ILE:HD11	1.91	0.52
1:A:205:HIS:CG	1:A:206:SER:H	2.28	0.52
1:A:22:ILE:CB	1:A:118:PHE:HZ	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:CYS:SG	1:A:361:ALA:CB	2.98	0.51
1:B:248:THR:O	1:B:248:THR:HG22	2.10	0.51
1:B:341:PHE:CD2	1:B:349:ILE:HD11	2.46	0.51
1:A:236:TYR:CE1	1:A:299:MET:HG2	2.45	0.51
1:A:121:GLY:C	1:A:124:ALA:HB3	2.30	0.51
1:A:37:ILE:HD11	1:A:162:PHE:CZ	2.44	0.51
1:A:277:PHE:HD2	1:A:278:PHE:HE1	1.58	0.51
1:B:33:TRP:HH2	1:B:95:PHE:HB2	1.75	0.51
1:A:55:PHE:CE2	1:A:113:TYR:CE1	2.98	0.51
1:A:311:SER:OG	1:A:314:GLU:HB2	2.10	0.51
1:A:7:THR:O	1:A:11:MET:HG2	2.11	0.51
1:A:163:THR:HG21	1:A:255:GLU:HG3	1.92	0.51
1:A:407:SER:OG	1:A:410:ARG:HB2	2.10	0.51
1:A:276:MET:HA	1:A:279:ALA:CB	2.36	0.51
1:B:14:LEU:O	1:B:17:PHE:N	2.43	0.51
1:B:236:TYR:O	1:B:239:PHE:HB3	2.10	0.51
1:A:236:TYR:O	1:A:239:PHE:HB3	2.09	0.51
1:B:210:LEU:O	1:B:214:LEU:N	2.19	0.51
1:B:239:PHE:C	1:B:239:PHE:CD1	2.83	0.51
1:A:239:PHE:CE2	1:A:303:ILE:HG12	2.45	0.51
1:A:305:GLY:O	1:A:318:LEU:CD1	2.59	0.51
1:A:376:ILE:O	1:A:376:ILE:CG2	2.59	0.51
1:B:192:PRO:HG2	1:B:197:VAL:HA	1.93	0.51
1:B:24:GLY:O	1:B:25:ALA:C	2.49	0.51
1:B:25:ALA:O	1:B:29:PHE:CB	2.59	0.51
1:B:42:LYS:HZ3	1:B:373:TYR:HB3	1.73	0.51
1:B:88:ALA:HB3	1:B:89:PRO:CD	2.36	0.51
1:A:29:PHE:CE1	1:A:170:PHE:CZ	2.99	0.51
1:B:320:THR:O	1:B:322:HIS:N	2.43	0.51
1:A:62:LEU:HD11	1:A:66:LEU:HD11	1.92	0.51
1:A:347:ALA:O	1:A:351:LEU:HD12	2.10	0.51
1:B:29:PHE:CE1	1:B:170:PHE:CZ	2.99	0.51
1:B:23:MET:O	1:B:24:GLY:C	2.49	0.51
1:B:33:TRP:CZ3	1:B:38:ASN:ND2	2.79	0.51
1:B:293:LEU:CD1	1:B:397:VAL:HA	2.37	0.51
1:A:239:PHE:CE2	1:A:303:ILE:HA	2.46	0.51
1:A:362:MET:O	1:A:363:ILE:C	2.47	0.51
1:A:18:PHE:CE1	1:A:180:LEU:HD12	2.46	0.51
1:B:124:ALA:O	1:B:127:ALA:N	2.44	0.51
1:B:49:PHE:O	1:B:52:ILE:HB	2.11	0.50
1:A:104:LEU:HG	1:A:108:ILE:CD1	2.34	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:PHE:CD2	1:A:144:ARG:HA	2.47	0.50
1:B:113:TYR:C	1:B:115:GLY:N	2.62	0.50
1:B:116:PHE:CD1	1:B:116:PHE:C	2.83	0.50
1:B:268:GLY:O	1:B:270:LEU:N	2.45	0.50
1:A:50:ALA:HB2	1:A:366:SER:CB	2.34	0.50
1:B:246:PHE:HB2	1:B:378:PHE:CE2	2.46	0.50
1:B:163:THR:CG2	1:B:255:GLU:HG3	2.41	0.50
1:A:325:GLU:O	1:A:325:GLU:HG2	2.09	0.50
1:A:168:PHE:CZ	1:A:172:LEU:CD1	2.93	0.50
1:A:168:PHE:O	1:A:171:TRP:N	2.45	0.50
1:A:221:LYS:HD2	1:A:341:PHE:CZ	2.46	0.50
1:A:373:TYR:CE1	1:A:382:TYR:HE1	2.28	0.50
1:B:358:LYS:O	1:B:359:GLN:C	2.50	0.50
1:A:3:TYR:O	1:A:9:PHE:CG	2.64	0.50
1:B:211:LYS:O	1:B:212:LEU:C	2.48	0.50
1:A:38:ASN:O	1:A:40:ILE:N	2.45	0.50
1:A:16:PHE:CE1	1:A:129:ILE:HG21	2.46	0.50
1:B:108:ILE:O	1:B:109:VAL:C	2.50	0.50
1:A:299:MET:O	1:A:300:SER:C	2.50	0.50
1:A:372:MET:HE3	1:A:384:VAL:HG11	1.94	0.50
1:A:85:VAL:HG11	1:A:178:LEU:HD13	1.93	0.50
1:B:26:TYR:CD1	1:B:27:PHE:N	2.80	0.50
1:B:239:PHE:CE2	1:B:303:ILE:HA	2.47	0.50
1:B:63:PHE:CD2	1:B:120:ALA:HB1	2.46	0.50
1:A:135:ARG:NH1	1:A:193:SER:OG	2.44	0.50
1:A:268:GLY:O	1:A:271:LEU:N	2.25	0.50
1:B:230:ILE:O	1:B:234:CYS:CB	2.59	0.50
1:A:45:THR:O	1:A:48:ILE:N	2.44	0.50
1:B:84:LEU:O	1:B:87:PHE:HB2	2.12	0.49
1:A:225:LEU:HD13	1:A:336:TYR:HE2	1.75	0.49
1:A:293:LEU:CD1	1:A:397:VAL:HA	2.38	0.49
1:B:99:LEU:CD2	1:B:107:SER:HB3	2.42	0.49
1:A:127:ALA:O	1:A:130:GLU:HB3	2.12	0.49
1:A:224:PHE:CD1	1:A:224:PHE:N	2.78	0.49
1:A:24:GLY:O	1:A:25:ALA:C	2.49	0.49
1:B:168:PHE:O	1:B:171:TRP:N	2.45	0.49
1:B:234:CYS:SG	1:B:361:ALA:HB1	2.52	0.49
1:A:122:ALA:CB	1:A:123:PRO:CD	2.90	0.49
1:A:30:PHE:CB	1:A:31:PRO:CD	2.78	0.49
1:A:225:LEU:O	1:A:228:TYR:HB3	2.12	0.49
1:B:98:LEU:HD13	1:B:107:SER:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:PHE:CD2	1:A:303:ILE:HG12	2.47	0.49
1:B:12:PHE:O	1:B:15:PHE:N	2.45	0.49
1:B:90:PHE:CZ	1:B:114:LEU:HB3	2.48	0.49
1:B:1:MET:O	1:B:3:TYR:N	2.46	0.49
1:B:236:TYR:CG	1:B:299:MET:SD	3.06	0.49
1:B:23:MET:HG2	1:B:151:TRP:HZ3	1.76	0.49
1:B:48:ILE:O	1:B:52:ILE:HG13	2.12	0.49
1:A:226:SER:O	1:A:230:ILE:N	2.46	0.49
1:A:278:PHE:HB2	1:A:282:ILE:HD11	1.94	0.49
1:B:166:ASN:OD1	1:B:167:GLN:N	2.45	0.49
1:B:293:LEU:HD13	1:B:397:VAL:CG2	2.27	0.49
1:B:45:THR:O	1:B:48:ILE:N	2.45	0.49
1:A:279:ALA:HB1	1:A:331:VAL:HG21	1.94	0.49
1:A:9:PHE:HD2	1:A:10:TRP:CE3	2.31	0.49
1:B:99:LEU:CD2	1:B:104:LEU:HD12	2.43	0.49
1:A:399:THR:O	1:A:399:THR:CG2	2.59	0.49
1:B:219:GLN:NE2	1:B:221:LYS:HE3	2.28	0.49
1:B:37:ILE:O	1:B:37:ILE:HG22	2.11	0.49
1:A:372:MET:O	1:A:376:ILE:HB	2.11	0.49
1:A:235:THR:HG21	1:A:389:ALA:HB2	1.95	0.49
1:B:293:LEU:O	1:B:294:LEU:C	2.51	0.49
1:B:326:VAL:N	1:B:327:PRO:HD2	2.28	0.49
1:A:121:GLY:HA2	1:A:124:ALA:CB	2.42	0.49
1:A:17:PHE:HD2	1:A:18:PHE:CE2	2.31	0.49
1:A:4:LEU:CD2	1:A:10:TRP:CZ3	2.96	0.49
1:A:17:PHE:CD2	1:A:18:PHE:CE2	3.01	0.49
1:A:246:PHE:HB2	1:A:378:PHE:CE2	2.47	0.49
1:B:154:GLY:O	1:B:158:VAL:HG23	2.13	0.49
1:A:98:LEU:CD1	1:A:107:SER:HA	2.42	0.48
1:A:34:LEU:HA	1:A:38:ASN:HB2	1.94	0.48
1:B:224:PHE:N	1:B:224:PHE:CD1	2.79	0.48
1:A:148:CYS:O	1:A:151:TRP:HB3	2.13	0.48
1:A:28:PRO:O	1:A:31:PRO:HD2	2.12	0.48
1:A:3:TYR:O	1:A:9:PHE:CD2	2.66	0.48
1:B:271:LEU:HD23	1:B:323:MET:HB2	1.95	0.48
1:B:121:GLY:C	1:B:124:ALA:HB3	2.32	0.48
1:A:9:PHE:CD2	1:A:10:TRP:CE3	3.01	0.48
1:B:239:PHE:CD2	1:B:303:ILE:HG12	2.47	0.48
1:A:113:TYR:O	1:A:116:PHE:CD2	2.67	0.48
1:A:33:TRP:HA	1:A:37:ILE:HD12	1.95	0.48
1:A:78:TRP:C	1:A:80:ILE:H	2.16	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:PHE:O	1:A:94:ILE:HB	2.13	0.48
1:A:289:LYS:HG3	1:A:400:LEU:HD23	1.96	0.48
1:A:293:LEU:HD13	1:A:397:VAL:CG2	2.24	0.48
1:B:279:ALA:HB1	1:B:331:VAL:HG21	1.94	0.48
1:A:50:ALA:O	1:A:51:ALA:C	2.51	0.48
1:A:381:ALA:O	1:A:384:VAL:N	2.40	0.48
1:A:11:MET:O	1:A:14:LEU:HB2	2.12	0.48
1:B:121:GLY:HA2	1:B:124:ALA:HB3	1.94	0.48
1:B:61:PRO:O	1:B:65:LEU:HG	2.13	0.48
1:B:358:LYS:O	1:B:360:LEU:N	2.46	0.48
1:A:34:LEU:HD13	1:A:40:ILE:HD12	1.96	0.48
1:A:40:ILE:CD1	1:A:48:ILE:HD12	2.42	0.48
1:A:122:ALA:O	1:A:126:GLU:HG3	2.12	0.48
1:A:124:ALA:O	1:A:127:ALA:N	2.46	0.48
1:A:14:LEU:O	1:A:15:PHE:C	2.51	0.48
1:B:399:THR:CG2	1:B:399:THR:O	2.61	0.48
1:A:135:ARG:HD3	1:A:135:ARG:O	2.14	0.48
1:B:311:SER:OG	1:B:314:GLU:CB	2.62	0.48
1:B:40:ILE:HD13	1:B:45:THR:HG22	1.96	0.48
1:A:264:VAL:HG11	1:A:319:LYS:CG	2.38	0.48
1:B:122:ALA:O	1:B:126:GLU:HG3	2.13	0.48
1:B:62:LEU:CD1	1:B:66:LEU:HD11	2.44	0.48
1:B:160:ILE:HG22	1:B:161:MET:N	2.29	0.48
1:B:226:SER:O	1:B:230:ILE:N	2.47	0.48
1:B:269:GLU:HA	1:B:272:ASN:HB2	1.95	0.48
1:B:29:PHE:HE1	1:B:33:TRP:CD1	2.31	0.48
1:A:192:PRO:HG2	1:A:197:VAL:HA	1.94	0.48
1:A:26:TYR:CD1	1:A:27:PHE:N	2.81	0.48
1:A:297:THR:O	1:A:298:ILE:C	2.52	0.47
1:A:281:LEU:O	1:A:285:ARG:HG3	2.14	0.47
1:A:91:PHE:HB3	1:A:170:PHE:HE2	1.79	0.47
1:B:161:MET:HB3	1:B:168:PHE:CE2	2.50	0.47
1:B:171:TRP:HE3	1:B:171:TRP:HA	1.78	0.47
1:B:18:PHE:CE2	1:B:180:LEU:HD12	2.49	0.47
1:A:244:ALA:O	1:A:247:PHE:N	2.47	0.47
1:A:224:PHE:HD1	1:A:224:PHE:N	2.12	0.47
1:A:358:LYS:O	1:A:359:GLN:C	2.50	0.47
1:A:48:ILE:O	1:A:52:ILE:HG13	2.15	0.47
1:A:303:ILE:O	1:A:304:ILE:C	2.52	0.47
1:A:51:ALA:O	1:A:52:ILE:C	2.52	0.47
1:A:166:ASN:OD1	1:A:167:GLN:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:VAL:HG21	1:B:178:LEU:HD13	1.97	0.47
1:A:328:PHE:HD1	1:A:328:PHE:H	1.63	0.47
1:A:366:SER:O	1:A:369:ALA:HB3	2.15	0.47
1:A:84:LEU:O	1:A:87:PHE:HB2	2.15	0.47
1:A:283:ILE:O	1:A:286:ILE:N	2.48	0.47
1:A:211:LYS:O	1:A:215:GLU:N	2.47	0.47
1:B:12:PHE:HE2	1:B:132:VAL:HG21	1.78	0.47
1:B:299:MET:O	1:B:302:ARG:N	2.47	0.47
1:B:327:PRO:HG2	1:B:328:PHE:H	1.79	0.47
1:B:49:PHE:O	1:B:50:ALA:C	2.52	0.47
1:B:372:MET:HE3	1:B:384:VAL:HG11	1.96	0.47
1:A:42:LYS:HG3	1:A:373:TYR:HB2	1.95	0.47
1:A:42:LYS:O	1:A:46:GLY:N	2.47	0.47
1:A:45:THR:O	1:A:46:GLY:C	2.53	0.47
1:A:47:ILE:O	1:A:48:ILE:C	2.52	0.47
1:B:14:LEU:O	1:B:17:PHE:HB3	2.15	0.47
1:B:349:ILE:O	1:B:353:CYS:N	2.34	0.47
1:B:78:TRP:C	1:B:80:ILE:N	2.68	0.47
1:B:148:CYS:O	1:B:151:TRP:HB3	2.14	0.47
1:B:90:PHE:CZ	1:B:95:PHE:CE1	2.96	0.47
1:A:320:THR:O	1:A:322:HIS:N	2.48	0.47
1:A:90:PHE:CZ	1:A:114:LEU:HB3	2.50	0.47
1:B:333:CYS:HG	1:B:354:PHE:HZ	1.63	0.47
1:A:369:ALA:O	1:A:372:MET:N	2.48	0.47
1:A:49:PHE:O	1:A:50:ALA:C	2.53	0.47
1:A:289:LYS:HD3	1:A:403:PRO:HG3	1.98	0.46
1:A:293:LEU:O	1:A:294:LEU:C	2.53	0.46
1:B:136:SER:O	1:B:137:ASN:HB2	2.15	0.46
1:B:122:ALA:CB	1:B:123:PRO:CD	2.92	0.46
1:B:154:GLY:O	1:B:155:ALA:C	2.53	0.46
1:A:29:PHE:HE1	1:A:33:TRP:CD1	2.31	0.46
1:B:14:LEU:O	1:B:15:PHE:C	2.53	0.46
1:B:328:PHE:HD1	1:B:328:PHE:H	1.61	0.46
1:A:239:PHE:C	1:A:239:PHE:HD1	2.17	0.46
1:A:40:ILE:HD12	1:A:48:ILE:HD12	1.95	0.46
1:B:319:LYS:O	1:B:321:LEU:N	2.48	0.46
1:B:4:LEU:CD2	1:B:10:TRP:CZ3	2.94	0.46
1:B:112:ILE:O	1:B:112:ILE:HG22	2.15	0.46
1:B:236:TYR:CD1	1:B:299:MET:SD	3.08	0.46
1:B:337:ILE:O	1:B:341:PHE:HB2	2.14	0.46
1:A:84:LEU:O	1:A:87:PHE:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:PHE:CD2	1:B:10:TRP:CE3	3.04	0.46
1:B:366:SER:O	1:B:369:ALA:HB3	2.16	0.46
1:B:372:MET:O	1:B:376:ILE:HB	2.15	0.46
1:B:51:ALA:O	1:B:52:ILE:C	2.54	0.46
1:A:151:TRP:CD1	1:A:269:GLU:CG	2.99	0.46
1:B:85:VAL:HG11	1:B:178:LEU:HD13	1.97	0.46
1:A:219:GLN:NE2	1:A:221:LYS:HE3	2.31	0.46
1:B:108:ILE:O	1:B:112:ILE:HG13	2.15	0.46
1:B:33:TRP:CE3	1:B:38:ASN:ND2	2.84	0.46
1:A:337:ILE:HG23	1:A:349:ILE:CD1	2.46	0.46
1:B:289:LYS:O	1:B:293:LEU:HG	2.16	0.46
1:A:42:LYS:HA	1:A:45:THR:OG1	2.16	0.46
1:B:237:ASP:O	1:B:238:VAL:C	2.53	0.46
1:A:20:PHE:HD1	1:A:20:PHE:N	2.07	0.46
1:B:225:LEU:O	1:B:228:TYR:HB3	2.15	0.46
1:A:12:PHE:O	1:A:14:LEU:N	2.48	0.46
1:A:326:VAL:HB	1:A:327:PRO:HD3	1.96	0.46
1:B:1:MET:O	1:B:4:LEU:N	2.27	0.46
1:B:47:ILE:O	1:B:48:ILE:C	2.55	0.46
1:A:98:LEU:HB3	1:A:107:SER:CB	2.46	0.46
1:A:44:ASP:HB3	1:A:104:LEU:CD1	2.46	0.46
1:A:247:PHE:HD1	1:A:315:VAL:CG1	2.29	0.46
1:B:230:ILE:HD11	1:B:357:PHE:HB3	1.98	0.46
1:B:29:PHE:CE1	1:B:170:PHE:CE1	3.04	0.46
1:B:228:TYR:OH	1:B:292:LEU:O	2.34	0.46
1:B:34:LEU:HA	1:B:38:ASN:HB2	1.98	0.46
1:B:99:LEU:HD22	1:B:104:LEU:HD12	1.97	0.45
1:B:211:LYS:O	1:B:215:GLU:N	2.49	0.45
1:B:50:ALA:O	1:B:51:ALA:C	2.53	0.45
1:A:239:PHE:CD1	1:A:240:ASP:N	2.83	0.45
1:A:303:ILE:C	1:A:305:GLY:N	2.69	0.45
1:A:237:ASP:O	1:A:238:VAL:C	2.53	0.45
1:B:350:TYR:O	1:B:351:LEU:C	2.54	0.45
1:A:303:ILE:CG2	1:A:386:GLY:HA3	2.47	0.45
1:B:22:ILE:CB	1:B:118:PHE:HZ	2.25	0.45
1:B:247:PHE:HD1	1:B:315:VAL:CG1	2.29	0.45
1:B:253:THR:CG2	1:B:254:GLY:N	2.80	0.45
1:B:80:ILE:O	1:B:81:THR:C	2.55	0.45
1:B:98:LEU:CB	1:B:107:SER:HB2	2.46	0.45
1:A:234:CYS:O	1:A:235:THR:C	2.55	0.45
1:A:337:ILE:O	1:A:341:PHE:HB2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:PHE:CD2	1:B:114:LEU:HD22	2.51	0.45
1:B:38:ASN:O	1:B:40:ILE:N	2.49	0.45
1:A:98:LEU:CB	1:A:107:SER:CB	2.94	0.45
1:A:57:LEU:HD13	1:A:355:CYS:O	2.16	0.45
1:B:390:LEU:O	1:B:390:LEU:HD23	2.16	0.45
1:B:20:PHE:CE2	1:B:144:ARG:NH1	2.85	0.45
1:B:292:LEU:HD21	1:B:333:CYS:N	2.32	0.45
1:A:264:VAL:O	1:A:265:THR:C	2.55	0.45
1:B:224:PHE:N	1:B:224:PHE:HD1	2.14	0.45
1:A:23:MET:HG2	1:A:151:TRP:HZ3	1.81	0.45
1:B:326:VAL:O	1:B:327:PRO:C	2.55	0.45
1:B:369:ALA:O	1:B:372:MET:N	2.50	0.45
1:A:233:SER:O	1:A:234:CYS:C	2.55	0.45
1:B:239:PHE:C	1:B:239:PHE:HD1	2.20	0.45
1:B:239:PHE:CD1	1:B:240:ASP:N	2.84	0.45
1:B:42:LYS:HG3	1:B:373:TYR:HB2	1.98	0.45
1:A:161:MET:HB3	1:A:168:PHE:CE2	2.51	0.45
1:A:37:ILE:O	1:A:37:ILE:HG22	2.16	0.45
1:A:333:CYS:HG	1:A:354:PHE:HZ	1.63	0.45
1:B:45:THR:O	1:B:46:GLY:C	2.55	0.45
1:A:372:MET:CE	1:A:384:VAL:HG21	2.47	0.45
1:B:121:GLY:HA2	1:B:124:ALA:CB	2.47	0.45
1:A:85:VAL:HG21	1:A:178:LEU:HD13	1.99	0.45
1:A:350:TYR:N	1:A:350:TYR:CD1	2.85	0.45
1:B:51:ALA:HB1	1:B:112:ILE:CD1	2.47	0.45
1:B:42:LYS:O	1:B:46:GLY:N	2.47	0.45
1:B:53:SER:O	1:B:56:SER:N	2.46	0.45
1:A:42:LYS:HD3	1:A:42:LYS:N	2.32	0.45
1:B:320:THR:C	1:B:322:HIS:N	2.70	0.45
1:B:195:ALA:O	1:B:196:THR:CG2	2.61	0.45
1:A:154:GLY:O	1:A:155:ALA:C	2.53	0.45
1:A:269:GLU:HA	1:A:272:ASN:HB2	1.99	0.44
1:B:16:PHE:CE1	1:B:129:ILE:HG21	2.52	0.44
1:A:98:LEU:CB	1:A:107:SER:HB2	2.46	0.44
1:A:78:TRP:O	1:A:80:ILE:N	2.51	0.44
1:A:208:PHE:CD2	1:A:351:LEU:HD13	2.52	0.44
1:A:349:ILE:O	1:A:353:CYS:N	2.36	0.44
1:B:3:TYR:O	1:B:9:PHE:CG	2.70	0.44
1:B:42:LYS:HA	1:B:45:THR:OG1	2.17	0.44
1:A:40:ILE:HD13	1:A:45:THR:HG22	2.00	0.44
1:B:19:TYR:HE2	1:B:122:ALA:HA	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:ARG:O	1:B:263:TYR:CD1	2.62	0.44
1:B:157:ILE:HG23	1:B:161:MET:HG3	1.99	0.44
1:B:372:MET:CE	1:B:384:VAL:HG21	2.48	0.44
1:B:99:LEU:HD21	1:B:107:SER:HB3	1.98	0.44
1:B:12:PHE:O	1:B:14:LEU:N	2.50	0.44
1:A:121:GLY:CA	1:A:124:ALA:HB3	2.48	0.44
1:A:250:PHE:CD1	1:A:250:PHE:N	2.86	0.44
1:A:288:GLY:O	1:A:290:ASN:N	2.51	0.44
1:A:289:LYS:O	1:A:293:LEU:HG	2.16	0.44
1:A:336:TYR:OH	1:A:401:SER:HB3	2.18	0.44
1:B:98:LEU:CD1	1:B:107:SER:HA	2.47	0.44
1:A:303:ILE:HG21	1:A:386:GLY:N	2.32	0.44
1:B:72:LEU:O	1:B:72:LEU:HG	2.17	0.44
1:A:160:ILE:HG22	1:A:161:MET:N	2.33	0.44
1:B:225:LEU:HD13	1:B:336:TYR:HE2	1.82	0.44
1:B:297:THR:O	1:B:300:SER:HB2	2.18	0.44
1:B:376:ILE:CG2	1:B:376:ILE:O	2.65	0.44
1:B:91:PHE:HB3	1:B:170:PHE:HE2	1.81	0.44
1:B:3:TYR:O	1:B:9:PHE:CD2	2.70	0.44
1:A:51:ALA:O	1:A:54:LEU:N	2.51	0.44
1:A:407:SER:HG	1:A:410:ARG:HB2	1.82	0.44
1:B:128:PHE:CD1	1:B:128:PHE:C	2.91	0.44
1:B:302:ARG:O	1:B:302:ARG:HG2	2.17	0.44
1:B:42:LYS:HD3	1:B:42:LYS:N	2.33	0.44
1:A:236:TYR:CG	1:A:299:MET:SD	3.11	0.44
1:A:299:MET:O	1:A:302:ARG:N	2.51	0.44
1:A:12:PHE:O	1:A:15:PHE:N	2.51	0.44
1:A:26:TYR:HD1	1:A:27:PHE:N	2.15	0.43
1:A:228:TYR:OH	1:A:292:LEU:O	2.35	0.43
1:B:381:ALA:O	1:B:384:VAL:N	2.43	0.43
1:B:95:PHE:HD1	1:B:95:PHE:H	1.66	0.43
1:B:97:PRO:O	1:B:98:LEU:C	2.53	0.43
1:A:32:ILE:HD12	1:A:258:THR:HG23	1.99	0.43
1:A:268:GLY:O	1:A:270:LEU:N	2.51	0.43
1:B:16:PHE:CD2	1:B:144:ARG:HA	2.54	0.43
1:B:303:ILE:C	1:B:305:GLY:N	2.70	0.43
1:B:329:LEU:HD12	1:B:329:LEU:HA	1.84	0.43
1:B:337:ILE:HG23	1:B:349:ILE:HD13	1.99	0.43
1:A:112:ILE:C	1:A:113:TYR:HD1	2.21	0.43
1:A:320:THR:C	1:A:322:HIS:N	2.71	0.43
1:A:62:LEU:CD1	1:A:66:LEU:HD11	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:LYS:HG2	1:A:203:ALA:HB2	2.00	0.43
1:A:95:PHE:HD1	1:A:95:PHE:H	1.65	0.43
1:A:319:LYS:O	1:A:321:LEU:N	2.51	0.43
1:A:23:MET:O	1:A:24:GLY:C	2.57	0.43
1:B:90:PHE:O	1:B:94:ILE:HG13	2.18	0.43
1:A:303:ILE:HG21	1:A:386:GLY:HA3	2.00	0.43
1:B:256:GLN:O	1:B:260:VAL:HG23	2.19	0.43
1:B:44:ASP:HB3	1:B:104:LEU:CD1	2.49	0.43
1:A:386:GLY:O	1:A:389:ALA:HB3	2.18	0.43
1:A:29:PHE:CE1	1:A:170:PHE:CE1	3.06	0.43
1:B:104:LEU:HG	1:B:108:ILE:CD1	2.31	0.43
1:B:37:ILE:HD11	1:B:162:PHE:CE1	2.53	0.43
1:B:51:ALA:O	1:B:54:LEU:N	2.50	0.43
1:A:297:THR:O	1:A:300:SER:HB2	2.19	0.43
1:A:93:PHE:O	1:A:97:PRO:CG	2.61	0.43
1:B:76:LEU:CD1	1:B:79:ILE:HD12	2.48	0.43
1:B:103:ILE:O	1:B:103:ILE:HG22	2.19	0.43
1:A:29:PHE:CD1	1:A:33:TRP:HB2	2.54	0.43
1:B:40:ILE:HG23	1:B:40:ILE:O	2.17	0.43
1:A:128:PHE:C	1:A:128:PHE:CD1	2.92	0.43
1:A:283:ILE:O	1:A:287:GLY:N	2.51	0.43
1:B:234:CYS:O	1:B:235:THR:C	2.57	0.43
1:B:352:VAL:O	1:B:357:PHE:HD2	2.02	0.43
1:A:134:ARG:NH1	1:A:203:ALA:CA	2.82	0.43
1:A:171:TRP:HA	1:A:171:TRP:HE3	1.80	0.43
1:B:337:ILE:HG23	1:B:349:ILE:CD1	2.48	0.43
1:B:352:VAL:O	1:B:357:PHE:HB2	2.19	0.43
1:A:230:ILE:O	1:A:234:CYS:CB	2.66	0.43
1:A:88:ALA:CB	1:A:89:PRO:HD3	2.37	0.43
1:A:225:LEU:HA	1:A:225:LEU:HD12	1.82	0.43
1:A:256:GLN:O	1:A:260:VAL:HG23	2.19	0.43
1:B:1:MET:O	1:B:2:TYR:C	2.58	0.43
1:B:303:ILE:CG2	1:B:386:GLY:HA3	2.49	0.43
1:A:12:PHE:O	1:A:13:GLY:C	2.55	0.43
1:A:68:ASP:O	1:A:71:GLY:N	2.52	0.43
1:A:80:ILE:HG22	1:A:84:LEU:CD1	2.49	0.42
1:B:85:VAL:HG22	1:B:178:LEU:CA	2.49	0.42
1:B:78:TRP:C	1:B:80:ILE:H	2.22	0.42
1:B:314:GLU:O	1:B:318:LEU:HG	2.19	0.42
1:A:352:VAL:O	1:A:357:PHE:HD2	2.02	0.42
1:A:72:LEU:O	1:A:72:LEU:HG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ALA:HB3	1:A:266:THR:OG1	2.18	0.42
1:B:228:TYR:O	1:B:229:VAL:C	2.58	0.42
1:B:381:ALA:O	1:B:384:VAL:HB	2.19	0.42
1:B:74:LYS:O	1:B:75:TYR:C	2.57	0.42
1:B:233:SER:O	1:B:234:CYS:C	2.57	0.42
1:B:340:GLN:OE1	1:B:405:PRO:HB3	2.20	0.42
1:B:9:PHE:HD2	1:B:10:TRP:CE3	2.34	0.42
1:B:215:GLU:OE1	1:B:216:LEU:N	2.52	0.42
1:A:154:GLY:O	1:A:158:VAL:HG23	2.20	0.42
1:A:1:MET:O	1:A:4:LEU:N	2.31	0.42
1:A:375:SER:C	1:A:376:ILE:HG13	2.40	0.42
1:A:122:ALA:C	1:A:124:ALA:N	2.73	0.42
1:B:213:ALA:O	1:B:217:PHE:HD1	2.02	0.42
1:B:227:LEU:O	1:B:231:GLY:N	2.44	0.42
1:B:350:TYR:CD1	1:B:350:TYR:N	2.87	0.42
1:A:34:LEU:O	1:A:35:HIS:O	2.37	0.42
1:A:12:PHE:HE2	1:A:132:VAL:HG21	1.84	0.42
1:B:246:PHE:CE1	1:B:250:PHE:CE1	3.07	0.42
1:A:61:PRO:CG	1:A:355:CYS:SG	3.08	0.42
1:A:213:ALA:O	1:A:217:PHE:HD1	2.03	0.42
1:B:136:SER:O	1:B:137:ASN:HB3	2.20	0.42
1:B:20:PHE:HB3	1:B:151:TRP:HB2	2.01	0.42
1:B:40:ILE:CD1	1:B:48:ILE:HD12	2.49	0.42
1:A:97:PRO:O	1:A:98:LEU:C	2.58	0.42
1:A:248:THR:CG2	1:A:248:THR:O	2.67	0.42
1:A:101:TYR:O	1:A:102:ASN:CB	2.68	0.42
1:B:287:GLY:O	1:B:288:GLY:C	2.57	0.42
1:B:326:VAL:HB	1:B:327:PRO:HD3	1.99	0.42
1:B:250:PHE:CD1	1:B:250:PHE:N	2.88	0.42
1:A:2:TYR:CZ	1:A:137:ASN:ND2	2.87	0.42
1:A:25:ALA:O	1:A:26:TYR:C	2.57	0.42
1:B:84:LEU:O	1:B:87:PHE:N	2.53	0.42
1:B:235:THR:HG21	1:B:389:ALA:HB2	2.01	0.42
1:B:386:GLY:O	1:B:389:ALA:HB3	2.20	0.42
1:A:88:ALA:HB3	1:A:89:PRO:CD	2.37	0.42
1:B:63:PHE:CZ	1:B:124:ALA:HB2	2.55	0.42
1:B:26:TYR:HD1	1:B:27:PHE:N	2.18	0.42
1:B:279:ALA:HB3	1:B:280:PRO:CD	2.41	0.42
1:B:40:ILE:HD12	1:B:48:ILE:HD12	2.00	0.42
1:A:375:SER:O	1:A:376:ILE:HG13	2.19	0.42
1:A:40:ILE:HG23	1:A:40:ILE:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:VAL:HG22	1:A:178:LEU:CA	2.50	0.41
1:A:85:VAL:HG22	1:A:178:LEU:HA	2.01	0.41
1:A:87:PHE:HD1	1:A:114:LEU:HD21	1.85	0.41
1:B:35:HIS:HB3	1:B:36:ASP:H	1.63	0.41
1:A:42:LYS:O	1:A:43:SER:C	2.58	0.41
1:A:127:ALA:O	1:A:128:PHE:C	2.57	0.41
1:B:243:PHE:O	1:B:246:PHE:HB3	2.20	0.41
1:B:244:ALA:O	1:B:247:PHE:N	2.53	0.41
1:B:188:LYS:HB2	1:B:189:THR:H	1.67	0.41
1:A:168:PHE:CD2	1:A:169:VAL:N	2.89	0.41
1:A:326:VAL:CB	1:A:327:PRO:CD	2.92	0.41
1:A:350:TYR:O	1:A:351:LEU:C	2.56	0.41
1:B:168:PHE:CD2	1:B:169:VAL:N	2.88	0.41
1:B:283:ILE:CG1	1:B:331:VAL:HG11	2.44	0.41
1:B:375:SER:O	1:B:376:ILE:HG13	2.20	0.41
1:A:112:ILE:O	1:A:112:ILE:HG22	2.20	0.41
1:B:85:VAL:HG22	1:B:178:LEU:HA	2.02	0.41
1:A:292:LEU:HD21	1:A:333:CYS:N	2.36	0.41
1:A:340:GLN:NE2	1:A:405:PRO:HB3	2.35	0.41
1:B:231:GLY:O	1:B:235:THR:OG1	2.24	0.41
1:B:303:ILE:HG21	1:B:386:GLY:N	2.35	0.41
1:B:244:ALA:O	1:B:245:ASN:C	2.56	0.41
1:B:134:ARG:HH11	1:B:203:ALA:CB	2.33	0.41
1:A:345:PHE:O	1:A:346:SER:C	2.59	0.41
1:A:27:PHE:CB	1:A:28:PRO:CD	2.85	0.41
1:A:80:ILE:O	1:A:81:THR:C	2.58	0.41
1:A:287:GLY:O	1:A:288:GLY:C	2.58	0.41
1:A:326:VAL:O	1:A:327:PRO:C	2.58	0.41
1:A:328:PHE:N	1:A:328:PHE:CD1	2.88	0.41
1:B:113:TYR:O	1:B:116:PHE:HD2	2.00	0.41
1:A:14:LEU:O	1:A:16:PHE:N	2.54	0.41
1:B:225:LEU:HD12	1:B:225:LEU:HA	1.80	0.41
1:B:303:ILE:O	1:B:304:ILE:C	2.56	0.41
1:B:340:GLN:NE2	1:B:405:PRO:HB3	2.35	0.41
1:B:57:LEU:HD13	1:B:355:CYS:O	2.21	0.41
1:A:1:MET:O	1:A:3:TYR:N	2.54	0.41
1:B:302:ARG:HG3	1:B:318:LEU:O	2.20	0.41
1:B:347:ALA:O	1:B:351:LEU:CD1	2.68	0.41
1:A:314:GLU:O	1:A:318:LEU:HG	2.21	0.41
1:A:135:ARG:NH2	1:A:191:ALA:O	2.46	0.41
1:B:29:PHE:CD1	1:B:33:TRP:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:PHE:CD2	1:B:351:LEU:HD13	2.56	0.41
1:B:7:THR:O	1:B:11:MET:HG2	2.21	0.41
1:A:379:GLN:O	1:A:382:TYR:HB2	2.21	0.41
1:A:12:PHE:HE2	1:A:128:PHE:CE1	2.39	0.41
1:A:19:TYR:HE2	1:A:122:ALA:HA	1.84	0.41
1:B:101:TYR:O	1:B:102:ASN:CB	2.68	0.41
1:A:283:ILE:O	1:A:284:ASN:C	2.59	0.41
1:B:294:LEU:O	1:B:298:ILE:HG13	2.21	0.41
1:B:367:VAL:O	1:B:368:LEU:C	2.58	0.41
1:B:98:LEU:CB	1:B:107:SER:CB	2.99	0.41
1:A:44:ASP:HB3	1:A:104:LEU:HD11	2.02	0.41
1:A:99:LEU:HD22	1:A:104:LEU:HD12	2.03	0.41
1:A:303:ILE:O	1:A:305:GLY:N	2.54	0.41
1:B:85:VAL:C	1:B:87:PHE:H	2.24	0.41
1:A:178:LEU:O	1:A:179:ILE:C	2.59	0.41
1:A:85:VAL:C	1:A:87:PHE:H	2.24	0.41
1:A:336:TYR:CZ	1:A:400:LEU:HD11	2.56	0.41
1:A:277:PHE:HB3	1:A:278:PHE:CD1	2.56	0.41
1:A:9:PHE:HE2	1:A:10:TRP:HZ3	1.69	0.41
1:B:379:GLN:HE21	1:B:379:GLN:HB3	1.67	0.41
1:B:328:PHE:N	1:B:328:PHE:CD1	2.89	0.41
1:B:50:ALA:HB1	1:B:363:ILE:HA	2.02	0.41
1:A:379:GLN:HB3	1:A:379:GLN:HE21	1.65	0.41
1:B:320:THR:C	1:B:322:HIS:H	2.24	0.41
1:A:16:PHE:HB3	1:A:147:GLY:CA	2.39	0.41
1:B:127:ALA:O	1:B:130:GLU:N	2.54	0.41
1:B:131:LYS:HG2	1:B:203:ALA:HB2	2.01	0.41
1:A:352:VAL:O	1:A:357:PHE:HB2	2.21	0.41
1:A:337:ILE:HG23	1:A:349:ILE:HD13	2.02	0.41
1:A:402:GLY:HA2	1:A:403:PRO:HD3	1.95	0.41
1:B:34:LEU:O	1:B:35:HIS:O	2.39	0.41
1:B:375:SER:C	1:B:376:ILE:HG13	2.42	0.41
1:A:108:ILE:O	1:A:112:ILE:HG13	2.21	0.41
1:B:247:PHE:CD1	1:B:315:VAL:CG1	3.04	0.41
1:B:27:PHE:HB3	1:B:28:PRO:HD3	1.97	0.40
1:A:53:SER:OG	1:A:363:ILE:HG13	2.20	0.40
1:A:79:ILE:HG22	1:A:79:ILE:O	2.20	0.40
1:B:127:ALA:O	1:B:130:GLU:CB	2.69	0.40
1:A:134:ARG:HH11	1:A:203:ALA:CB	2.34	0.40
1:B:154:GLY:O	1:B:158:VAL:N	2.44	0.40
1:A:342:GLU:HG3	1:A:342:GLU:H	1.67	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:VAL:O	1:A:162:PHE:N	2.47	0.40
1:A:260:VAL:O	1:A:263:TYR:HB2	2.21	0.40
1:A:302:ARG:HG2	1:A:302:ARG:O	2.21	0.40
1:A:361:ALA:O	1:A:362:MET:C	2.60	0.40
1:A:253:THR:CG2	1:A:254:GLY:N	2.83	0.40
1:A:337:ILE:HD12	1:A:350:TYR:HE1	1.83	0.40
1:B:290:ASN:O	1:B:291:ALA:C	2.59	0.40
1:A:211:LYS:HA	1:A:214:LEU:HB2	2.03	0.40
1:A:340:GLN:C	1:A:341:PHE:CD1	2.94	0.40
1:A:227:LEU:O	1:A:231:GLY:N	2.45	0.40
1:A:14:LEU:O	1:A:17:PHE:HB3	2.21	0.40
1:B:121:GLY:CA	1:B:124:ALA:HB3	2.51	0.40
1:B:79:ILE:O	1:B:79:ILE:HG22	2.20	0.40
1:A:157:ILE:HG23	1:A:161:MET:HG3	2.03	0.40
1:B:50:ALA:O	1:B:53:SER:HB3	2.21	0.40
1:A:99:LEU:CD2	1:A:104:LEU:HD12	2.52	0.40
1:A:188:LYS:HB2	1:A:189:THR:H	1.70	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	415/417 (100%)	261 (63%)	114 (28%)	40 (10%)	1	12
1	B	415/417 (100%)	261 (63%)	110 (26%)	44 (11%)	0	10
All	All	830/834 (100%)	522 (63%)	224 (27%)	84 (10%)	1	11

All (84) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	HIS

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Mol	Chain	Res	Type
1	A	102	ASN
1	A	160	ILE
1	A	196	THR
1	A	407	SER
1	B	35	HIS
1	B	102	ASN
1	B	160	ILE
1	B	320	THR
1	B	407	SER
1	A	39	HIS
1	A	96	GLY
1	A	137	ASN
1	A	269	GLU
1	A	289	LYS
1	A	320	THR
1	A	321	LEU
1	A	402	GLY
1	A	406	LEU
1	B	2	TYR
1	B	39	HIS
1	B	96	GLY
1	B	137	ASN
1	B	196	THR
1	B	235	THR
1	B	269	GLU
1	B	298	ILE
1	B	321	LEU
1	B	402	GLY
1	B	405	PRO
1	B	406	LEU
1	A	177	ALA
1	A	181	ALA
1	A	234	CYS
1	A	235	THR
1	A	359	GLN
1	A	378	PHE
1	B	26	TYR
1	B	124	ALA
1	B	177	ALA
1	B	234	CYS
1	B	289	LYS
1	B	378	PHE

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Mol	Chain	Res	Type
1	A	26	TYR
1	A	124	ALA
1	A	178	LEU
1	A	228	TYR
1	A	298	ILE
1	A	405	PRO
1	B	27	PHE
1	B	181	ALA
1	B	204	ASN
1	B	228	TYR
1	B	359	GLN
1	A	2	TYR
1	A	27	PHE
1	A	109	VAL
1	A	194	SER
1	B	75	TYR
1	B	117	CYS
1	B	239	PHE
1	B	416	VAL
1	A	376	ILE
1	B	24	GLY
1	B	194	SER
1	A	24	GLY
1	A	283	ILE
1	B	326	VAL
1	B	376	ILE
1	A	326	VAL
1	B	220	PRO
1	B	264	VAL
1	A	220	PRO
1	A	288	GLY
1	A	327	PRO
1	B	30	PHE
1	B	112	ILE
1	B	229	VAL
1	B	327	PRO
1	A	30	PHE
1	A	169	VAL
1	A	264	VAL
1	B	46	GLY
1	B	288	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	345/345 (100%)	317 (92%)	28 (8%)	15	54
1	B	345/345 (100%)	317 (92%)	28 (8%)	15	54
All	All	690/690 (100%)	634 (92%)	56 (8%)	15	54

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	TYR
1	A	3	TYR
1	A	10	TRP
1	A	16	PHE
1	A	20	PHE
1	A	21	PHE
1	A	30	PHE
1	A	53	SER
1	A	59	PHE
1	A	62	LEU
1	A	91	PHE
1	A	116	PHE
1	A	136	SER
1	A	138	PHE
1	A	163	THR
1	A	171	TRP
1	A	239	PHE
1	A	241	GLN
1	A	246	PHE
1	A	249	SER
1	A	261	PHE
1	A	278	PHE
1	A	323	MET
1	A	324	PHE
1	A	325	GLU
1	A	333	CYS
1	A	353	CYS

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Mol	Chain	Res	Type
1	A	398	PHE
1	B	2	TYR
1	B	3	TYR
1	B	10	TRP
1	B	20	PHE
1	B	21	PHE
1	B	30	PHE
1	B	53	SER
1	B	59	PHE
1	B	62	LEU
1	B	91	PHE
1	B	116	PHE
1	B	136	SER
1	B	138	PHE
1	B	171	TRP
1	B	239	PHE
1	B	241	GLN
1	B	246	PHE
1	B	249	SER
1	B	261	PHE
1	B	278	PHE
1	B	323	MET
1	B	324	PHE
1	B	325	GLU
1	B	333	CYS
1	B	366	SER
1	B	379	GLN
1	B	398	PHE
1	B	415	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	102	ASN
1	A	137	ASN
1	A	204	ASN
1	A	290	ASN
1	A	340	GLN
1	A	371	ASN
1	A	379	GLN
1	B	8	ASN

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Mol	Chain	Res	Type
1	B	60	GLN
1	B	102	ASN
1	B	137	ASN
1	B	204	ASN
1	B	290	ASN
1	B	340	GLN
1	B	371	ASN
1	B	379	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

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

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	TDG	A	500	-	24,24,24	2.05	7 (29%)	32,35,35	0.82	0
2	TDG	B	1500	-	24,24,24	1.84	7 (29%)	32,35,35	0.81	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TDG	A	500	-	-	0/8/48/48	0/2/2/2
2	TDG	B	1500	-	-	0/8/48/48	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1500	TDG	C4-C5	2.29	1.57	1.53
2	A	500	TDG	C1'-C2'	2.32	1.57	1.53
2	A	500	TDG	C3-C2	2.37	1.58	1.52
2	B	1500	TDG	O5'-C1'	2.56	1.46	1.42
2	B	1500	TDG	C3-C2	2.62	1.59	1.52
2	A	500	TDG	O5-C1	2.79	1.47	1.42
2	B	1500	TDG	C4'-C5'	3.09	1.59	1.53
2	B	1500	TDG	O5-C1	3.14	1.47	1.42
2	B	1500	TDG	C4'-C3'	3.34	1.61	1.52
2	A	500	TDG	O5'-C1'	3.64	1.48	1.42
2	A	500	TDG	C4'-C3'	3.83	1.62	1.52
2	B	1500	TDG	C1-S1	3.88	1.87	1.80
2	A	500	TDG	C4'-C5'	3.99	1.61	1.53
2	A	500	TDG	C1-S1	4.23	1.88	1.80

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.