Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 04:44 PM EDT

PDB ID	:	1R1I
Title	:	STRUCTURAL ANALYSIS OF NEPRILYSIN WITH VARIOUS SPECIFIC AND POTENT INHIBITORS
Authors	:	Oefner, C.; Roques, B.P.; Fournie-Zaluski, M.C.; Dale, G.E.
Deposited on	:	2003-09-24
Resolution	:	2.60 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

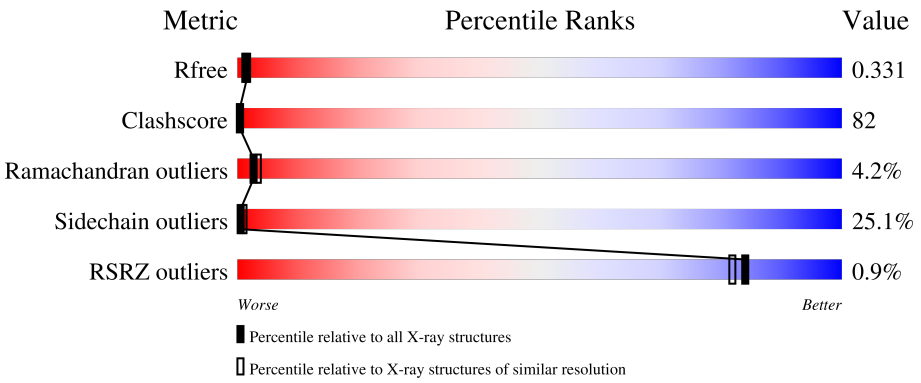
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	696	% 26% 53% 20% •

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	TI1	A	2001	X	-	-	-

2 Entry composition (i)

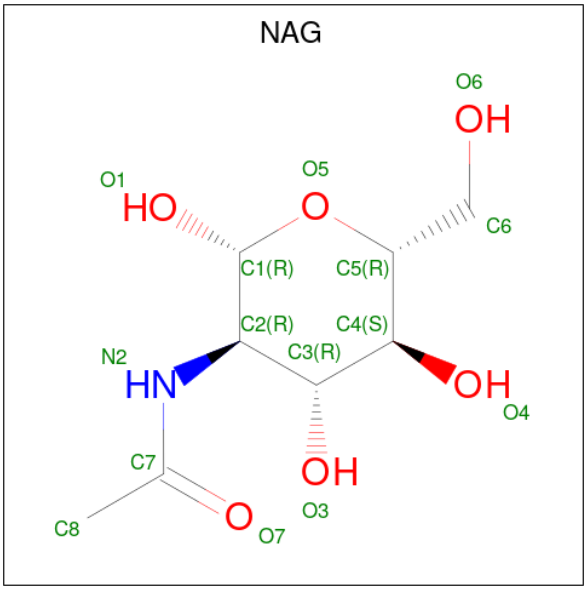
There are 5 unique types of molecules in this entry. The entry contains 5683 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Neprilysin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	696	5595	3538	957	1074	26	0	0	0

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

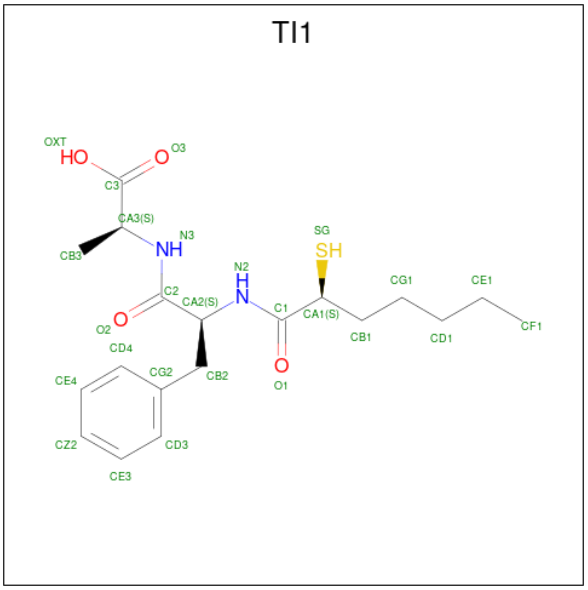


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	14	8	1	5	0	0
2	A	1	14	8	1	5	0	0
2	A	1	14	8	1	5	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	1	1	1	0	0

- Molecule 4 is [2(R,S)-2-SULFANYLHEPTANOYL]-PHE-ALA (three-letter code: TI1) (formula: $C_{19}H_{28}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	A	1	26	19	2	4	1	0	0

- Molecule 5 is water.

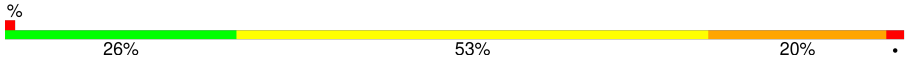
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	19	19	19	0	0

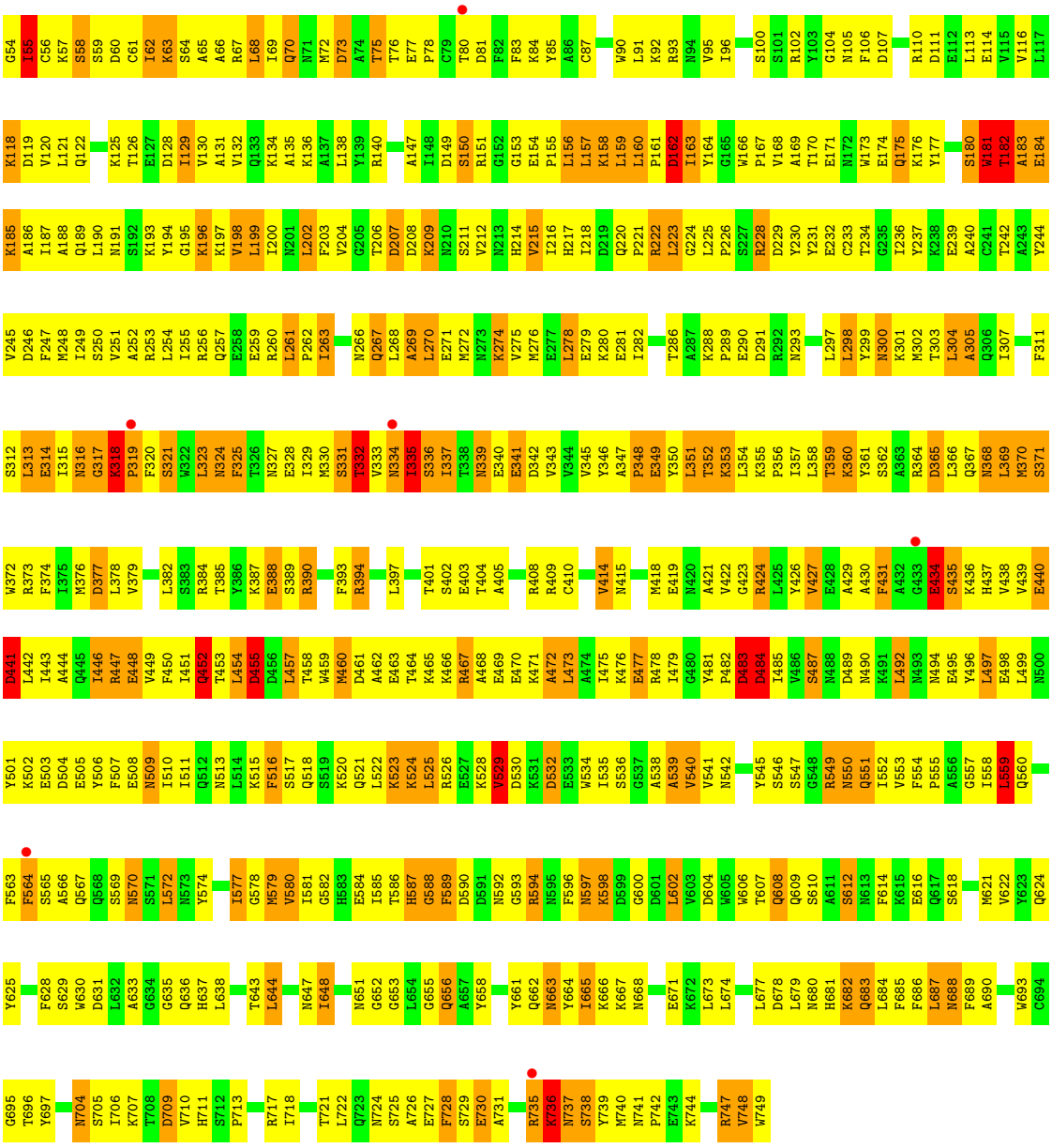
3 Residue-property plots (i)

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

- Molecule 1: Neprilysin

Chain A:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	108.84Å 108.84Å 113.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.60 19.98 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.2 (20.00-2.60) 97.2 (19.98-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.45 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.276 , 0.358 0.262 , 0.331	Depositor DCC
R_{free} test set	1186 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	61.9	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 54.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5683	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, ZN, TI1

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	0.65	0/5713	0.85	21/7727 (0.3%)

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	23

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	504	ASP	CB-CG-OD2	7.07	124.66	118.30
1	A	631	ASP	CB-CG-OD2	6.99	124.59	118.30
1	A	365	ASP	CB-CG-OD2	6.95	124.55	118.30
1	A	489	ASP	CB-CG-OD2	6.83	124.45	118.30
1	A	111	ASP	CB-CG-OD2	6.77	124.39	118.30
1	A	604	ASP	CB-CG-OD2	6.25	123.93	118.30
1	A	540	VAL	CB-CA-C	-6.16	99.69	111.40
1	A	207	ASP	CB-CG-OD2	6.10	123.79	118.30
1	A	162	ASP	CB-CG-OD2	5.94	123.65	118.30
1	A	709	ASP	CB-CG-OD2	5.82	123.54	118.30
1	A	110	ARG	NE-CZ-NH1	-5.72	117.44	120.30
1	A	484	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	455	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	291	ASP	CB-CG-OD2	5.45	123.20	118.30
1	A	532	ASP	CB-CG-OD2	5.44	123.20	118.30
1	A	377	ASP	CB-CG-OD2	5.43	123.19	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	483	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	73	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	60	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	441	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	119	ASP	CB-CG-OD2	5.07	122.86	118.30

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	170	THR	Peptide
1	A	181	TRP	Peptide
1	A	182	THR	Peptide
1	A	316	ASN	Peptide
1	A	317	GLY	Peptide
1	A	318	LYS	Peptide
1	A	332	THR	Peptide
1	A	335	ILE	Peptide
1	A	352	THR	Peptide
1	A	389	SER	Peptide
1	A	429	ALA	Peptide
1	A	431	PHE	Peptide
1	A	434	GLU	Peptide
1	A	452	GLN	Peptide
1	A	484	ASP	Peptide
1	A	487	SER	Peptide
1	A	523	LYS	Peptide
1	A	538	ALA	Peptide
1	A	539	ALA	Peptide
1	A	54	GLY	Peptide
1	A	587	HIS	Peptide
1	A	711	HIS	Peptide
1	A	737	ASN	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5595	0	5444	914	4
2	A	42	0	39	1	0
3	A	1	0	0	0	0
4	A	26	0	26	6	0
5	A	19	0	0	2	1
All	All	5683	0	5509	916	5

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 82.

All (916) 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:68:LEU:HD22	1:A:687:LEU:CD1	1.29	1.59
1:A:68:LEU:CD2	1:A:687:LEU:CD1	1.88	1.45
1:A:68:LEU:CD2	1:A:687:LEU:HD13	1.45	1.44
1:A:502:LYS:HD2	1:A:505:GLU:OE2	1.22	1.38
1:A:62:ILE:CD1	1:A:63:LYS:N	1.88	1.35
1:A:303:THR:OG1	1:A:305:ALA:HB3	1.22	1.35
1:A:182:THR:CG2	1:A:185:LYS:HD3	1.55	1.35
1:A:473:LEU:H	1:A:473:LEU:CD1	1.32	1.34
1:A:62:ILE:HD12	1:A:63:LYS:N	1.02	1.34
1:A:460:MET:HB3	1:A:465:LYS:CD	1.58	1.34
1:A:62:ILE:CD1	1:A:62:ILE:C	1.98	1.28
1:A:157:LEU:HD23	1:A:157:LEU:N	1.39	1.26
1:A:272:MET:O	1:A:275:VAL:CG1	1.85	1.24
1:A:314:GLU:OE1	1:A:319:PRO:HA	1.37	1.23
1:A:157:LEU:H	1:A:157:LEU:CD2	1.44	1.23
1:A:467:ARG:O	1:A:470:GLU:N	1.72	1.23
1:A:718:ILE:O	1:A:722:LEU:HD12	1.05	1.20
1:A:471:LYS:NZ	1:A:596:PHE:O	1.75	1.19
1:A:473:LEU:N	1:A:473:LEU:HD12	1.40	1.19
1:A:735:ARG:O	1:A:738:SER:OG	1.58	1.18
1:A:549:ARG:HH11	1:A:549:ARG:CG	1.52	1.18
1:A:549:ARG:HH11	1:A:549:ARG:HG2	1.05	1.17
1:A:469:GLU:O	1:A:472:ALA:HB3	1.41	1.17
1:A:202:LEU:HB2	1:A:218:ILE:CD1	1.75	1.16
1:A:207:ASP:HB2	1:A:215:VAL:CG2	1.76	1.15
1:A:460:MET:CB	1:A:465:LYS:HD3	1.77	1.15
1:A:345:VAL:CG1	1:A:348:PRO:HD3	1.76	1.13
1:A:718:ILE:O	1:A:722:LEU:CD1	1.94	1.13
1:A:153:GLY:O	1:A:156:LEU:HD21	1.45	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:THR:HG22	1:A:185:LYS:CD	1.80	1.12
1:A:336:SER:O	1:A:337:ILE:HD13	1.48	1.11
1:A:403:GLU:OE2	1:A:404:THR:HG22	1.51	1.11
1:A:193:LYS:NZ	1:A:515:LYS:HE2	1.67	1.09
1:A:214:HIS:NE2	1:A:524:LYS:HD2	1.68	1.09
1:A:209:LYS:N	1:A:209:LYS:HD2	1.48	1.09
1:A:472:ALA:HB3	1:A:473:LEU:CD1	1.83	1.09
1:A:506:TYR:CZ	1:A:510:ILE:HD11	1.87	1.08
1:A:272:MET:O	1:A:275:VAL:HG12	1.47	1.08
1:A:261:LEU:HD23	1:A:262:PRO:HD2	1.24	1.08
1:A:68:LEU:HD23	1:A:687:LEU:HD13	1.34	1.07
1:A:318:LYS:HB3	1:A:319:PRO:C	1.76	1.06
1:A:209:LYS:HD3	1:A:299:TYR:CE2	1.91	1.06
1:A:345:VAL:HG12	1:A:348:PRO:HD3	1.10	1.06
1:A:426:TYR:O	1:A:430:ALA:HB3	1.56	1.06
1:A:68:LEU:CD2	1:A:687:LEU:HD12	1.70	1.05
1:A:62:ILE:HD12	1:A:63:LYS:CA	1.87	1.05
1:A:315:ILE:CD1	1:A:320:PHE:HB2	1.85	1.05
1:A:472:ALA:HB3	1:A:473:LEU:HD12	1.36	1.05
1:A:214:HIS:CD2	1:A:524:LYS:HD2	1.93	1.04
1:A:315:ILE:HD12	1:A:320:PHE:HB2	1.35	1.04
1:A:303:THR:OG1	1:A:305:ALA:CB	2.04	1.04
1:A:116:VAL:O	1:A:120:VAL:HG13	1.56	1.03
1:A:202:LEU:HD12	1:A:202:LEU:O	1.58	1.03
1:A:739:TYR:CD1	1:A:740:MET:HE3	1.92	1.03
1:A:439:VAL:CG1	1:A:443:ILE:HD11	1.88	1.03
1:A:202:LEU:CD1	1:A:202:LEU:C	2.25	1.02
1:A:261:LEU:HD23	1:A:262:PRO:CD	1.89	1.02
1:A:439:VAL:HG13	1:A:443:ILE:HD11	1.35	1.02
1:A:62:ILE:C	1:A:62:ILE:HD13	1.77	1.02
1:A:157:LEU:N	1:A:157:LEU:CD2	2.05	1.01
1:A:198:VAL:HG21	1:A:370:MET:HB3	1.42	1.01
1:A:662:GLN:O	1:A:665:ILE:HB	1.60	1.01
1:A:62:ILE:HD12	1:A:62:ILE:C	1.63	1.01
1:A:314:GLU:OE1	1:A:319:PRO:CA	2.08	1.00
1:A:418:MET:O	1:A:422:VAL:HG23	1.61	1.00
1:A:55:ILE:HD13	1:A:55:ILE:H	1.26	1.00
1:A:469:GLU:O	1:A:472:ALA:CB	2.10	1.00
1:A:222:ARG:C	1:A:223:LEU:HD23	1.81	0.99
1:A:193:LYS:CE	1:A:515:LYS:HE2	1.91	0.99
1:A:366:LEU:O	1:A:370:MET:HG3	1.61	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:GLN:OE1	5:A:15:HOH:O	1.79	0.98
1:A:461:ASP:OD1	1:A:607:THR:HG21	1.63	0.98
1:A:209:LYS:HG2	1:A:299:TYR:OH	1.62	0.98
1:A:434:GLU:HA	1:A:437:HIS:CE1	1.97	0.98
1:A:311:PHE:HE1	1:A:352:THR:OG1	1.45	0.98
1:A:160:LEU:N	1:A:161:PRO:HD3	1.76	0.97
1:A:261:LEU:CD2	1:A:262:PRO:HD2	1.94	0.97
1:A:244:TYR:HE2	1:A:376:MET:CE	1.76	0.97
1:A:739:TYR:CE1	1:A:740:MET:HE1	1.99	0.96
1:A:58:SER:O	1:A:62:ILE:HG23	1.64	0.96
1:A:549:ARG:HG2	1:A:549:ARG:NH1	1.76	0.96
1:A:90:TRP:CZ3	1:A:695:GLY:HA2	2.01	0.95
1:A:333:VAL:HG22	1:A:333:VAL:O	1.64	0.95
1:A:209:LYS:HG2	1:A:299:TYR:CZ	2.01	0.95
1:A:502:LYS:CD	1:A:505:GLU:OE2	2.14	0.95
1:A:671:GLU:HG3	1:A:681:HIS:CD2	2.01	0.95
1:A:62:ILE:CD1	1:A:63:LYS:CA	2.43	0.95
1:A:354:LEU:HG	1:A:358:LEU:HD11	1.48	0.94
1:A:159:LEU:C	1:A:161:PRO:CD	2.36	0.94
1:A:462:ALA:HA	1:A:465:LYS:HG2	1.49	0.94
1:A:607:THR:OG1	1:A:610:SER:HB2	1.65	0.94
1:A:318:LYS:HB3	1:A:319:PRO:O	1.66	0.94
1:A:454:LEU:HA	1:A:457:LEU:HD12	1.50	0.94
1:A:156:LEU:O	1:A:159:LEU:N	2.01	0.94
1:A:153:GLY:O	1:A:156:LEU:CD2	2.16	0.93
1:A:184:GLU:O	1:A:188:ALA:CB	2.16	0.93
1:A:323:LEU:CD1	1:A:327:ASN:HD22	1.80	0.93
1:A:62:ILE:HD12	1:A:63:LYS:H	1.30	0.93
1:A:353:LYS:O	1:A:356:PRO:HG2	1.69	0.93
1:A:658:TYR:CE2	1:A:727:GLU:HG3	2.04	0.93
1:A:439:VAL:CG1	1:A:443:ILE:CD1	2.46	0.92
1:A:156:LEU:O	1:A:160:LEU:CD2	2.16	0.91
1:A:244:TYR:HE2	1:A:376:MET:HE2	1.33	0.91
1:A:135:ALA:O	1:A:138:LEU:HB3	1.70	0.91
1:A:121:LEU:O	1:A:136:LYS:HD3	1.71	0.91
1:A:160:LEU:N	1:A:161:PRO:CD	2.34	0.91
1:A:415:ASN:HA	1:A:422:VAL:HG21	1.53	0.91
1:A:274:LYS:HA	1:A:274:LYS:HE3	1.50	0.90
1:A:303:THR:HA	1:A:341:GLU:O	1.71	0.90
1:A:658:TYR:CD2	1:A:727:GLU:HG2	2.06	0.89
1:A:202:LEU:HB2	1:A:218:ILE:HD12	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:ALA:CB	1:A:473:LEU:HD12	2.02	0.89
1:A:298:LEU:O	1:A:300:ASN:ND2	2.06	0.89
1:A:722:LEU:HD23	1:A:728:PHE:CE2	2.08	0.89
1:A:202:LEU:HD12	1:A:202:LEU:C	1.90	0.88
1:A:204:VAL:O	1:A:521:GLN:NE2	2.06	0.88
1:A:718:ILE:HG23	1:A:722:LEU:HD11	1.56	0.88
1:A:439:VAL:HG13	1:A:443:ILE:CD1	2.02	0.88
1:A:451:ILE:HD11	1:A:472:ALA:HB1	1.56	0.88
1:A:68:LEU:HD21	1:A:687:LEU:HD13	1.56	0.87
1:A:739:TYR:CE1	1:A:740:MET:CE	2.57	0.87
1:A:658:TYR:CD2	1:A:727:GLU:CG	2.57	0.87
1:A:354:LEU:HG	1:A:358:LEU:CD1	2.05	0.87
1:A:312:SER:O	1:A:313:LEU:HD23	1.73	0.86
1:A:118:LYS:CE	1:A:122:GLN:HE22	1.88	0.86
1:A:184:GLU:O	1:A:188:ALA:HB2	1.73	0.86
1:A:193:LYS:HE3	1:A:515:LYS:HE2	1.57	0.86
1:A:722:LEU:HD23	1:A:728:PHE:CD2	2.11	0.86
1:A:158:LYS:HA	1:A:158:LYS:HZ2	1.40	0.86
1:A:658:TYR:CE2	1:A:727:GLU:CG	2.59	0.86
1:A:462:ALA:HA	1:A:465:LYS:CG	2.05	0.86
1:A:272:MET:C	1:A:275:VAL:HG12	1.96	0.86
1:A:263:ILE:N	1:A:263:ILE:HD13	1.91	0.85
1:A:327:ASN:ND2	1:A:337:ILE:O	2.08	0.85
1:A:718:ILE:C	1:A:722:LEU:HD12	1.95	0.85
1:A:160:LEU:CD2	1:A:160:LEU:H	1.90	0.85
1:A:182:THR:CG2	1:A:185:LYS:CD	2.48	0.85
1:A:739:TYR:CD1	1:A:740:MET:CE	2.58	0.85
1:A:300:ASN:N	1:A:300:ASN:HD22	1.74	0.85
1:A:118:LYS:CE	1:A:122:GLN:NE2	2.40	0.85
1:A:199:LEU:HB3	1:A:200:ILE:HD12	1.58	0.85
1:A:272:MET:O	1:A:275:VAL:HG13	1.75	0.85
1:A:314:GLU:OE1	1:A:314:GLU:HA	1.73	0.85
1:A:323:LEU:HD11	1:A:337:ILE:O	1.75	0.85
1:A:318:LYS:HB3	1:A:319:PRO:CA	2.04	0.85
1:A:182:THR:HG22	1:A:185:LYS:HD3	0.87	0.84
1:A:214:HIS:NE2	1:A:524:LYS:CD	2.39	0.84
1:A:454:LEU:HD12	1:A:455:ASP:H	1.41	0.84
1:A:209:LYS:HE3	1:A:602:LEU:HB3	1.59	0.84
1:A:207:ASP:HB2	1:A:215:VAL:HG22	1.59	0.84
1:A:529:VAL:HG12	1:A:529:VAL:O	1.75	0.84
1:A:68:LEU:HD22	1:A:687:LEU:HD12	0.84	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:622:VAL:HG23	1:A:644:LEU:HD22	1.60	0.83
1:A:738:SER:O	1:A:741:ASN:N	2.09	0.83
1:A:208:ASP:C	1:A:209:LYS:HD2	1.98	0.83
1:A:313:LEU:CD1	1:A:358:LEU:HD22	2.08	0.83
1:A:180:SER:O	1:A:181:TRP:O	1.96	0.83
1:A:378:LEU:HD22	1:A:507:PHE:CZ	2.14	0.82
1:A:300:ASN:ND2	1:A:300:ASN:N	2.28	0.82
1:A:461:ASP:O	1:A:465:LYS:HG2	1.78	0.81
1:A:118:LYS:HE2	1:A:122:GLN:NE2	1.94	0.81
1:A:209:LYS:CE	1:A:602:LEU:HB3	2.11	0.81
1:A:558:ILE:O	1:A:560:GLN:N	2.11	0.81
1:A:202:LEU:HB2	1:A:218:ILE:HD11	1.63	0.81
1:A:193:LYS:HZ1	1:A:515:LYS:HE2	1.43	0.81
1:A:156:LEU:O	1:A:160:LEU:HD22	1.81	0.81
1:A:56:CYS:SG	1:A:58:SER:HB3	2.20	0.81
1:A:323:LEU:HD12	1:A:327:ASN:HD22	1.45	0.80
1:A:355:LYS:N	1:A:356:PRO:HD2	1.96	0.80
1:A:530:ASP:OD1	1:A:532:ASP:N	2.14	0.80
1:A:739:TYR:HE1	1:A:740:MET:HE1	1.44	0.80
1:A:158:LYS:HA	1:A:158:LYS:NZ	1.97	0.80
1:A:182:THR:OG1	1:A:184:GLU:HG2	1.81	0.80
1:A:156:LEU:C	1:A:160:LEU:CD2	2.50	0.80
1:A:159:LEU:C	1:A:161:PRO:HD2	2.01	0.80
1:A:472:ALA:CB	1:A:473:LEU:CD1	2.57	0.80
1:A:58:SER:O	1:A:62:ILE:N	2.15	0.80
1:A:209:LYS:HE3	1:A:602:LEU:CB	2.12	0.80
1:A:202:LEU:C	1:A:202:LEU:HD13	1.99	0.80
1:A:281:GLU:OE1	1:A:361:TYR:OH	2.00	0.80
1:A:366:LEU:C	1:A:370:MET:HE2	2.02	0.80
1:A:590:ASP:OD1	1:A:592:ASN:N	2.15	0.80
1:A:438:VAL:O	1:A:441:ASP:OD2	2.00	0.79
1:A:505:GLU:OE1	1:A:508:GLU:HG2	1.81	0.79
1:A:424:ARG:O	1:A:427:VAL:HG23	1.82	0.79
1:A:182:THR:N	1:A:185:LYS:HE2	1.97	0.79
1:A:498:GLU:O	1:A:498:GLU:HG3	1.82	0.79
1:A:303:THR:HG1	1:A:305:ALA:HB3	1.45	0.79
1:A:439:VAL:HG12	1:A:443:ILE:CD1	2.13	0.79
1:A:718:ILE:HG23	1:A:722:LEU:CD1	2.13	0.79
1:A:622:VAL:HG23	1:A:644:LEU:CD2	2.12	0.79
1:A:643:THR:HB	1:A:647:ASN:ND2	1.98	0.78
1:A:160:LEU:N	1:A:160:LEU:HD22	1.98	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:TRP:O	1:A:372:TRP:CD2	2.36	0.78
1:A:621:MET:HE1	1:A:651:ASN:HB2	1.66	0.78
1:A:341:GLU:OE2	1:A:341:GLU:HA	1.83	0.77
1:A:643:THR:HB	1:A:647:ASN:HD21	1.49	0.77
1:A:461:ASP:OD1	1:A:607:THR:CG2	2.31	0.77
1:A:164:TYR:CE2	1:A:185:LYS:HE3	2.20	0.77
1:A:354:LEU:HA	1:A:357:ILE:HD12	1.65	0.77
1:A:472:ALA:HB3	1:A:473:LEU:HD11	1.64	0.77
1:A:460:MET:HB3	1:A:465:LYS:HD3	0.81	0.77
1:A:118:LYS:HE3	1:A:122:GLN:HE22	1.48	0.76
1:A:202:LEU:CD2	1:A:218:ILE:HD11	2.16	0.76
1:A:62:ILE:CD1	1:A:63:LYS:HA	2.15	0.76
1:A:303:THR:C	1:A:305:ALA:N	2.38	0.76
1:A:470:GLU:HG2	1:A:598:LYS:NZ	1.99	0.76
1:A:62:ILE:HD13	1:A:62:ILE:O	1.83	0.76
1:A:244:TYR:CE2	1:A:376:MET:CE	2.67	0.76
1:A:372:TRP:O	1:A:372:TRP:CG	2.38	0.76
1:A:501:TYR:OH	1:A:513:ASN:OD1	2.03	0.76
1:A:256:ARG:O	1:A:259:GLU:N	2.19	0.75
1:A:434:GLU:HA	1:A:437:HIS:ND1	2.00	0.75
1:A:300:ASN:HD22	1:A:300:ASN:H	1.34	0.75
1:A:245:VAL:O	1:A:249:ILE:HG13	1.85	0.75
1:A:451:ILE:O	1:A:454:LEU:HD11	1.86	0.75
1:A:483:ASP:O	1:A:484:ASP:C	2.25	0.75
1:A:140:ARG:NH2	1:A:503:GLU:OE1	2.17	0.75
1:A:184:GLU:HB3	1:A:325:PHE:HB2	1.67	0.75
1:A:202:LEU:HD13	1:A:203:PHE:N	2.02	0.74
1:A:594:ARG:HG3	1:A:594:ARG:HH11	1.52	0.74
1:A:72:MET:SD	1:A:677:LEU:HD21	2.28	0.74
1:A:515:LYS:O	1:A:516:PHE:O	2.04	0.74
1:A:207:ASP:HB2	1:A:215:VAL:HG23	1.68	0.74
1:A:68:LEU:HD21	1:A:687:LEU:CD1	2.14	0.74
1:A:160:LEU:H	1:A:160:LEU:HD22	1.50	0.74
1:A:196:LYS:NZ	1:A:377:ASP:OD1	2.19	0.74
1:A:454:LEU:HA	1:A:457:LEU:CD1	2.16	0.74
1:A:588:GLY:HA3	1:A:589:PHE:CD2	2.22	0.74
1:A:549:ARG:CG	1:A:549:ARG:NH1	2.26	0.74
1:A:467:ARG:O	1:A:470:GLU:HB2	1.87	0.74
1:A:58:SER:C	1:A:62:ILE:HG23	2.08	0.74
1:A:426:TYR:O	1:A:430:ALA:CB	2.35	0.74
1:A:372:TRP:CE2	1:A:376:MET:HE3	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:ARG:HH11	1:A:549:ARG:HG3	1.46	0.73
1:A:558:ILE:HG23	1:A:559:LEU:HD23	1.70	0.73
1:A:228:ARG:NH2	1:A:286:THR:O	2.22	0.73
1:A:718:ILE:CG2	1:A:722:LEU:CD1	2.66	0.73
1:A:134:LYS:HE2	1:A:499:LEU:O	1.87	0.73
1:A:263:ILE:N	1:A:263:ILE:CD1	2.52	0.73
1:A:318:LYS:CB	1:A:319:PRO:CA	2.66	0.73
1:A:154:GLU:HG3	1:A:155:PRO:HD3	1.70	0.73
1:A:255:ILE:O	1:A:259:GLU:HG2	1.89	0.73
1:A:303:THR:O	1:A:305:ALA:N	2.22	0.73
1:A:138:LEU:HD23	1:A:414:VAL:HB	1.68	0.73
1:A:302:MET:O	1:A:343:VAL:N	2.21	0.73
1:A:168:VAL:H	1:A:368:ASN:HD21	1.34	0.73
1:A:278:LEU:HB3	1:A:369:LEU:HD23	1.71	0.72
1:A:244:TYR:CE2	1:A:376:MET:HE2	2.22	0.72
1:A:570:ASN:N	1:A:570:ASN:HD22	1.87	0.72
1:A:180:SER:O	1:A:181:TRP:C	2.28	0.72
1:A:274:LYS:HA	1:A:274:LYS:CE	2.18	0.72
1:A:167:PRO:HD2	1:A:368:ASN:ND2	2.04	0.72
1:A:156:LEU:CD1	1:A:382:LEU:HD11	2.20	0.72
1:A:722:LEU:CD2	1:A:728:PHE:CE2	2.73	0.72
1:A:473:LEU:H	1:A:473:LEU:HD12	0.58	0.71
1:A:323:LEU:CD1	1:A:327:ASN:ND2	2.51	0.71
1:A:160:LEU:HA	1:A:163:ILE:HD11	1.72	0.71
1:A:394:ARG:HH21	1:A:402:SER:N	1.89	0.71
1:A:441:ASP:O	1:A:444:ALA:HB3	1.90	0.71
1:A:191:ASN:O	1:A:195:GLY:HA2	1.91	0.71
1:A:271:GLU:HB3	1:A:272:MET:HE3	1.73	0.71
1:A:372:TRP:CZ2	1:A:376:MET:HE3	2.26	0.71
1:A:118:LYS:HE2	1:A:122:GLN:CD	2.11	0.71
1:A:160:LEU:O	1:A:163:ILE:HG12	1.91	0.71
1:A:382:LEU:O	1:A:387:LYS:HE2	1.90	0.70
1:A:588:GLY:HA3	1:A:589:PHE:CE2	2.26	0.70
1:A:662:GLN:O	1:A:665:ILE:CB	2.37	0.70
1:A:460:MET:CB	1:A:465:LYS:CD	2.49	0.70
1:A:559:LEU:HD23	1:A:559:LEU:N	2.06	0.70
1:A:311:PHE:HE1	1:A:352:THR:HG1	0.75	0.70
1:A:671:GLU:HG3	1:A:681:HIS:HD2	1.56	0.70
1:A:166:TRP:CE3	1:A:255:ILE:HD12	2.27	0.70
1:A:275:VAL:HG23	1:A:369:LEU:HD22	1.74	0.70
1:A:193:LYS:HE3	1:A:515:LYS:CE	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:LEU:HD12	1:A:323:LEU:O	1.91	0.69
1:A:453:THR:HG22	1:A:457:LEU:HD11	1.73	0.69
1:A:461:ASP:OD1	1:A:607:THR:CB	2.40	0.69
1:A:447:ARG:NH2	1:A:475:ILE:O	2.24	0.69
1:A:140:ARG:HH21	1:A:503:GLU:CD	1.94	0.69
1:A:244:TYR:HE2	1:A:376:MET:HE1	1.57	0.69
1:A:156:LEU:O	1:A:160:LEU:HD23	1.93	0.69
1:A:366:LEU:HB3	1:A:370:MET:HE2	1.75	0.69
1:A:59:SER:HA	1:A:62:ILE:HG13	1.73	0.69
1:A:272:MET:HA	1:A:272:MET:CE	2.22	0.69
1:A:403:GLU:CD	1:A:404:THR:HG22	2.13	0.69
1:A:149:ASP:O	1:A:150:SER:C	2.30	0.69
1:A:202:LEU:CB	1:A:218:ILE:CD1	2.65	0.69
1:A:69:ILE:HD11	1:A:677:LEU:HG	1.74	0.69
1:A:182:THR:HG23	1:A:185:LYS:HD3	1.69	0.69
1:A:461:ASP:CG	1:A:607:THR:HG21	2.14	0.68
1:A:125:LYS:HB2	1:A:128:ASP:OD1	1.92	0.68
1:A:157:LEU:HD23	1:A:157:LEU:H	0.60	0.68
1:A:274:LYS:HD2	1:A:274:LYS:N	2.09	0.68
1:A:441:ASP:OD2	1:A:442:LEU:N	2.25	0.68
1:A:156:LEU:HD11	1:A:382:LEU:HD11	1.75	0.68
1:A:184:GLU:O	1:A:188:ALA:HB3	1.93	0.68
1:A:184:GLU:CB	1:A:325:PHE:HB2	2.22	0.68
1:A:353:LYS:O	1:A:356:PRO:CG	2.42	0.68
1:A:496:TYR:O	1:A:499:LEU:HB2	1.94	0.68
1:A:622:VAL:CG2	1:A:644:LEU:HD22	2.22	0.68
1:A:134:LYS:NZ	1:A:499:LEU:O	2.27	0.68
1:A:424:ARG:HD2	1:A:485:ILE:O	1.94	0.68
1:A:156:LEU:HD11	1:A:382:LEU:CD1	2.25	0.67
1:A:437:HIS:HA	1:A:440:GLU:CD	2.14	0.67
1:A:439:VAL:C	1:A:443:ILE:HD12	2.15	0.67
1:A:590:ASP:O	1:A:594:ARG:HB3	1.94	0.67
1:A:160:LEU:N	1:A:160:LEU:CD2	2.54	0.67
1:A:282:ILE:O	1:A:286:THR:HG23	1.94	0.67
1:A:193:LYS:HG2	1:A:515:LYS:HE3	1.77	0.67
1:A:454:LEU:HD12	1:A:455:ASP:N	2.10	0.66
1:A:321:SER:OG	1:A:324:ASN:HB2	1.95	0.66
1:A:554:PHE:CZ	1:A:581:ILE:HA	2.30	0.66
1:A:268:LEU:O	1:A:270:LEU:N	2.28	0.66
1:A:55:ILE:HA	1:A:673:LEU:O	1.94	0.66
1:A:156:LEU:C	1:A:159:LEU:H	1.99	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:LEU:CD1	1:A:455:ASP:OD1	2.43	0.66
1:A:65:ALA:O	1:A:69:ILE:HD12	1.94	0.66
1:A:663:ASN:HA	1:A:666:LYS:HG3	1.76	0.66
1:A:154:GLU:N	1:A:155:PRO:CD	2.59	0.66
1:A:181:TRP:C	1:A:185:LYS:HE2	2.15	0.66
1:A:209:LYS:CD	1:A:299:TYR:CE2	2.75	0.66
1:A:216:ILE:HG13	1:A:525:LEU:HD21	1.77	0.66
1:A:347:ALA:HB1	1:A:350:TYR:HB3	1.78	0.66
1:A:209:LYS:CG	1:A:299:TYR:CZ	2.78	0.66
1:A:134:LYS:CE	1:A:499:LEU:O	2.44	0.66
1:A:209:LYS:N	1:A:209:LYS:CD	2.37	0.66
1:A:209:LYS:HD3	1:A:299:TYR:CZ	2.31	0.66
1:A:607:THR:OG1	1:A:610:SER:CB	2.40	0.66
1:A:166:TRP:CZ3	1:A:255:ILE:HD12	2.31	0.65
1:A:209:LYS:CE	1:A:602:LEU:CB	2.72	0.65
1:A:658:TYR:CE2	1:A:727:GLU:HB3	2.31	0.65
1:A:318:LYS:CB	1:A:319:PRO:C	2.61	0.65
1:A:55:ILE:H	1:A:55:ILE:CD1	1.96	0.65
1:A:272:MET:HA	1:A:272:MET:HE2	1.77	0.65
1:A:502:LYS:O	1:A:505:GLU:HB2	1.96	0.65
1:A:67:ARG:HH22	1:A:688:ASN:HD21	1.43	0.65
1:A:350:TYR:CZ	1:A:354:LEU:HD13	2.32	0.65
1:A:506:TYR:CE2	1:A:510:ILE:HD11	2.31	0.65
1:A:184:GLU:HB3	1:A:325:PHE:CB	2.26	0.65
1:A:372:TRP:CZ2	1:A:376:MET:CE	2.79	0.65
1:A:454:LEU:CA	1:A:457:LEU:HD12	2.25	0.65
1:A:509:ASN:N	1:A:509:ASN:HD22	1.94	0.65
1:A:440:GLU:O	1:A:443:ILE:HB	1.97	0.65
1:A:549:ARG:HB3	1:A:551:GLN:HB2	1.77	0.65
1:A:597:ASN:C	1:A:597:ASN:OD1	2.35	0.65
1:A:268:LEU:C	1:A:270:LEU:H	1.98	0.65
1:A:467:ARG:O	1:A:470:GLU:CA	2.45	0.65
1:A:525:LEU:HD12	1:A:525:LEU:C	2.17	0.65
1:A:354:LEU:HD23	1:A:358:LEU:HD21	1.79	0.64
1:A:467:ARG:O	1:A:470:GLU:CB	2.45	0.64
1:A:469:GLU:O	1:A:473:LEU:HD11	1.97	0.64
1:A:244:TYR:CE2	1:A:376:MET:HE1	2.32	0.64
1:A:303:THR:C	1:A:305:ALA:H	2.00	0.64
1:A:159:LEU:O	1:A:161:PRO:CD	2.44	0.64
1:A:525:LEU:HD12	1:A:525:LEU:O	1.98	0.64
1:A:580:VAL:HG22	4:A:2001:TI1:CE4	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:LEU:HA	1:A:160:LEU:HD23	1.79	0.64
1:A:739:TYR:HD1	1:A:740:MET:HE3	1.57	0.64
1:A:271:GLU:HB3	1:A:272:MET:CE	2.27	0.64
1:A:347:ALA:N	1:A:348:PRO:CD	2.60	0.64
1:A:207:ASP:CB	1:A:215:VAL:CG2	2.68	0.64
1:A:251:VAL:O	1:A:255:ILE:HG13	1.98	0.64
1:A:625:TYR:HA	1:A:628:PHE:CD2	2.33	0.64
1:A:441:ASP:CG	1:A:442:LEU:N	2.51	0.64
1:A:686:PHE:CE1	1:A:728:PHE:HA	2.33	0.64
1:A:164:TYR:CZ	1:A:185:LYS:HG3	2.32	0.64
1:A:586:THR:HG1	1:A:656:GLN:HE22	1.46	0.64
1:A:589:PHE:CD2	1:A:589:PHE:N	2.65	0.63
1:A:275:VAL:HG13	1:A:276:MET:N	2.12	0.63
1:A:314:GLU:OE1	1:A:314:GLU:CA	2.44	0.63
1:A:439:VAL:O	1:A:443:ILE:HD12	1.99	0.63
1:A:482:PRO:HB3	1:A:484:ASP:HB2	1.80	0.63
1:A:540:VAL:HG12	1:A:541:VAL:N	2.12	0.63
1:A:547:SER:O	1:A:600:GLY:HA2	1.96	0.63
1:A:347:ALA:N	1:A:348:PRO:HD2	2.13	0.63
1:A:470:GLU:HG2	1:A:598:LYS:HZ2	1.63	0.63
1:A:718:ILE:HG22	1:A:722:LEU:HD13	1.81	0.63
1:A:471:LYS:HZ1	1:A:596:PHE:HB2	1.63	0.63
1:A:545:TYR:OH	1:A:550:ASN:ND2	2.31	0.63
1:A:658:TYR:HE2	1:A:727:GLU:HG3	1.60	0.63
1:A:730:GLU:C	1:A:730:GLU:CD	2.57	0.62
1:A:748:VAL:CG2	1:A:749:TRP:CD1	2.82	0.62
1:A:225:LEU:HB3	1:A:226:PRO:CD	2.30	0.62
1:A:436:LYS:O	1:A:440:GLU:HG2	1.99	0.62
1:A:540:VAL:O	1:A:557:GLY:HA3	2.00	0.62
1:A:621:MET:HE1	1:A:651:ASN:HD22	1.64	0.62
1:A:333:VAL:O	1:A:333:VAL:CG2	2.38	0.62
1:A:570:ASN:HD22	1:A:570:ASN:H	1.44	0.62
1:A:678:ASP:O	1:A:679:LEU:HD23	1.99	0.62
1:A:225:LEU:HD13	1:A:230:TYR:HB3	1.82	0.62
1:A:323:LEU:HD11	1:A:327:ASN:ND2	2.14	0.62
1:A:102:ARG:HG2	1:A:107:ASP:OD2	2.00	0.61
1:A:268:LEU:C	1:A:270:LEU:N	2.49	0.61
1:A:315:ILE:CD1	1:A:320:PHE:CB	2.73	0.61
1:A:262:PRO:C	1:A:263:ILE:HD13	2.21	0.61
1:A:275:VAL:HG13	1:A:276:MET:H	1.63	0.61
1:A:621:MET:SD	1:A:648:ILE:HA	2.40	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:TRP:CZ2	1:A:104:GLY:HA2	2.35	0.61
1:A:621:MET:CE	1:A:651:ASN:ND2	2.63	0.61
1:A:368:ASN:O	1:A:372:TRP:HB3	2.01	0.61
1:A:655:GLY:O	1:A:656:GLN:C	2.36	0.61
1:A:358:LEU:CD1	1:A:358:LEU:N	2.63	0.61
1:A:509:ASN:N	1:A:509:ASN:ND2	2.48	0.61
1:A:76:THR:O	1:A:78:PRO:HD3	2.01	0.61
1:A:223:LEU:HD23	1:A:223:LEU:N	2.15	0.61
1:A:125:LYS:CB	1:A:128:ASP:OD1	2.49	0.60
1:A:469:GLU:O	1:A:473:LEU:CD1	2.49	0.60
1:A:471:LYS:NZ	1:A:593:GLY:O	2.34	0.60
1:A:434:GLU:O	1:A:435:SER:C	2.40	0.60
1:A:482:PRO:HD3	1:A:534:TRP:CE2	2.36	0.60
1:A:513:ASN:O	1:A:516:PHE:HB3	2.00	0.60
1:A:565:SER:C	1:A:567:GLN:H	2.03	0.60
1:A:157:LEU:CA	1:A:160:LEU:HD23	2.32	0.60
1:A:367:GLN:O	1:A:371:SER:HB2	2.00	0.60
1:A:58:SER:O	1:A:61:CYS:HB2	2.02	0.60
1:A:81:ASP:C	1:A:81:ASP:OD1	2.40	0.60
1:A:453:THR:HG22	1:A:457:LEU:CD1	2.32	0.60
1:A:680:ASN:O	1:A:683:GLN:HG3	2.01	0.60
1:A:159:LEU:O	1:A:161:PRO:HD2	2.01	0.60
1:A:366:LEU:HB3	1:A:370:MET:CE	2.32	0.60
1:A:461:ASP:OD1	1:A:607:THR:OG1	2.19	0.60
1:A:278:LEU:HD13	1:A:369:LEU:HD23	1.83	0.60
1:A:390:ARG:O	1:A:390:ARG:HG2	2.01	0.60
1:A:345:VAL:CG1	1:A:348:PRO:CD	2.68	0.59
1:A:272:MET:CE	1:A:272:MET:CA	2.80	0.59
1:A:336:SER:C	1:A:337:ILE:HD13	2.20	0.59
1:A:193:LYS:CE	1:A:515:LYS:CE	2.74	0.59
1:A:202:LEU:HD23	1:A:218:ILE:HD11	1.83	0.59
1:A:216:ILE:HG13	1:A:525:LEU:CD2	2.31	0.59
1:A:168:VAL:HG22	1:A:168:VAL:O	2.02	0.59
1:A:182:THR:H	1:A:185:LYS:HE2	1.65	0.59
1:A:358:LEU:N	1:A:358:LEU:HD12	2.17	0.59
1:A:686:PHE:CZ	1:A:728:PHE:HA	2.38	0.59
1:A:135:ALA:O	1:A:138:LEU:CB	2.50	0.59
1:A:506:TYR:OH	1:A:510:ILE:HD11	2.03	0.59
1:A:706:ILE:HG22	1:A:707:LYS:HD3	1.84	0.59
1:A:725:SER:HB3	1:A:728:PHE:HB2	1.83	0.59
1:A:222:ARG:O	1:A:223:LEU:HD23	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:GLU:OE2	1:A:318:LYS:C	2.41	0.59
1:A:315:ILE:HD11	1:A:320:PHE:HB2	1.79	0.59
1:A:354:LEU:O	1:A:358:LEU:HD13	2.02	0.59
1:A:577:ILE:HD12	1:A:577:ILE:O	2.02	0.59
1:A:460:MET:HB3	1:A:465:LYS:CE	2.30	0.58
1:A:584:GLU:O	1:A:587:HIS:HB2	2.04	0.58
1:A:185:LYS:O	1:A:189:GLN:N	2.33	0.58
1:A:303:THR:O	1:A:304:LEU:C	2.41	0.58
1:A:424:ARG:HG3	1:A:485:ILE:O	2.03	0.58
1:A:231:TYR:O	1:A:280:LYS:HE2	2.04	0.58
1:A:249:ILE:O	1:A:250:SER:C	2.42	0.58
1:A:579:MET:HE2	1:A:689:PHE:HE2	1.68	0.58
1:A:329:ILE:O	1:A:332:THR:HB	2.03	0.58
1:A:388:GLU:O	1:A:390:ARG:N	2.36	0.58
1:A:684:LEU:HA	1:A:687:LEU:HB2	1.86	0.58
1:A:690:ALA:HA	1:A:718:ILE:CD1	2.33	0.58
1:A:278:LEU:HB3	1:A:369:LEU:CD2	2.34	0.58
1:A:621:MET:HE1	1:A:651:ASN:ND2	2.19	0.58
1:A:704:ASN:HD22	1:A:704:ASN:C	2.08	0.58
1:A:713:PRO:O	1:A:717:ARG:HG3	2.03	0.58
1:A:451:ILE:O	1:A:454:LEU:CD1	2.52	0.57
1:A:471:LYS:NZ	1:A:596:PHE:C	2.57	0.57
1:A:159:LEU:O	1:A:161:PRO:N	2.36	0.57
1:A:451:ILE:O	1:A:452:GLN:C	2.43	0.57
1:A:114:GLU:OE1	1:A:408:ARG:HG2	2.04	0.57
1:A:466:LYS:O	1:A:469:GLU:HB3	2.04	0.57
1:A:470:GLU:HG2	1:A:598:LYS:HZ1	1.67	0.57
1:A:629:SER:OG	1:A:635:GLY:O	2.20	0.57
1:A:357:ILE:O	1:A:360:LYS:HG2	2.04	0.57
1:A:690:ALA:HA	1:A:718:ILE:HD13	1.86	0.57
1:A:149:ASP:O	1:A:151:ARG:N	2.38	0.57
1:A:267:GLN:HE21	1:A:267:GLN:HA	1.69	0.57
1:A:540:VAL:CG1	1:A:541:VAL:N	2.67	0.57
1:A:132:VAL:CG1	1:A:136:LYS:HE3	2.35	0.56
1:A:202:LEU:HD22	1:A:218:ILE:HD11	1.86	0.56
1:A:289:PRO:HD2	1:A:290:GLU:OE2	2.05	0.56
1:A:435:SER:O	1:A:437:HIS:N	2.39	0.56
1:A:570:ASN:N	1:A:570:ASN:ND2	2.52	0.56
1:A:725:SER:O	1:A:728:PHE:HB3	2.05	0.56
1:A:354:LEU:CD2	1:A:358:LEU:HD21	2.36	0.56
1:A:559:LEU:HB3	1:A:564:PHE:CZ	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:VAL:HG22	4:A:2001:TI1:CD4	2.36	0.56
1:A:673:LEU:N	1:A:673:LEU:HD12	2.20	0.56
1:A:718:ILE:CG2	1:A:722:LEU:HD13	2.35	0.56
1:A:153:GLY:C	1:A:155:PRO:HD2	2.25	0.56
1:A:366:LEU:CB	1:A:370:MET:HE2	2.35	0.56
1:A:69:ILE:CD1	1:A:677:LEU:HG	2.35	0.56
1:A:221:PRO:O	1:A:223:LEU:CD2	2.53	0.56
1:A:482:PRO:O	1:A:485:ILE:HG12	2.06	0.56
1:A:250:SER:HA	1:A:253:ARG:NH1	2.20	0.56
1:A:630:TRP:CE3	1:A:706:ILE:HG13	2.41	0.56
1:A:478:ARG:CZ	1:A:551:GLN:OE1	2.53	0.56
1:A:439:VAL:HG12	1:A:479:ILE:HD13	1.87	0.56
1:A:490:ASN:O	1:A:494:ASN:HB2	2.06	0.56
1:A:618:SER:HB2	1:A:648:ILE:HD11	1.88	0.56
1:A:160:LEU:H	1:A:160:LEU:HD23	1.70	0.55
1:A:181:TRP:HZ3	1:A:316:ASN:HB2	1.72	0.55
1:A:355:LYS:N	1:A:356:PRO:CD	2.69	0.55
1:A:461:ASP:OD2	1:A:461:ASP:C	2.43	0.55
1:A:680:ASN:OD1	1:A:683:GLN:CG	2.54	0.55
1:A:468:ALA:O	1:A:469:GLU:C	2.45	0.55
1:A:157:LEU:N	1:A:157:LEU:HD22	2.16	0.55
1:A:530:ASP:OD1	1:A:532:ASP:HB2	2.06	0.55
1:A:330:MET:C	1:A:332:THR:H	2.10	0.55
1:A:658:TYR:CE2	1:A:727:GLU:CB	2.88	0.55
1:A:261:LEU:CB	1:A:262:PRO:HD2	2.37	0.55
1:A:362:SER:OG	1:A:365:ASP:N	2.23	0.55
1:A:680:ASN:OD1	1:A:683:GLN:HG2	2.06	0.55
1:A:214:HIS:CD2	1:A:524:LYS:CD	2.81	0.55
1:A:459:TRP:CH2	1:A:614:PHE:HD2	2.25	0.55
1:A:478:ARG:NE	1:A:551:GLN:OE1	2.39	0.55
1:A:569:SER:O	1:A:572:LEU:HD12	2.07	0.55
1:A:232:GLU:O	1:A:233:CYS:HB2	2.06	0.55
1:A:653:GLY:HA2	1:A:656:GLN:NE2	2.22	0.55
1:A:199:LEU:C	1:A:200:ILE:HD12	2.28	0.55
1:A:216:ILE:CD1	1:A:525:LEU:HD21	2.37	0.55
1:A:403:GLU:HG3	1:A:404:THR:N	2.22	0.55
1:A:70:GLN:HG2	1:A:93:ARG:NH1	2.22	0.55
1:A:209:LYS:HD3	1:A:299:TYR:CD2	2.37	0.55
1:A:323:LEU:CD1	1:A:337:ILE:O	2.54	0.55
1:A:477:GLU:HA	1:A:552:ILE:HG13	1.87	0.55
1:A:524:LYS:O	1:A:525:LEU:C	2.45	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:597:ASN:ND2	5:A:6:HOH:O	2.33	0.55
1:A:159:LEU:O	1:A:160:LEU:C	2.44	0.54
1:A:199:LEU:HB3	1:A:200:ILE:CD1	2.34	0.54
1:A:454:LEU:HD12	1:A:455:ASP:OD1	2.06	0.54
1:A:565:SER:C	1:A:567:GLN:N	2.59	0.54
1:A:709:ASP:OD1	1:A:710:VAL:N	2.41	0.54
1:A:354:LEU:HD23	1:A:358:LEU:CD2	2.36	0.54
1:A:394:ARG:HH21	1:A:401:THR:C	2.10	0.54
1:A:478:ARG:NH2	1:A:551:GLN:OE1	2.40	0.54
1:A:96:ILE:HD11	1:A:696:THR:HG23	1.90	0.54
1:A:256:ARG:O	1:A:257:GLN:C	2.45	0.54
1:A:84:LYS:O	1:A:85:TYR:C	2.46	0.54
1:A:193:LYS:O	1:A:515:LYS:HA	2.08	0.54
1:A:315:ILE:HD13	1:A:320:PHE:CD2	2.42	0.54
1:A:333:VAL:O	1:A:334:ASN:C	2.46	0.54
1:A:522:LEU:C	1:A:524:LYS:H	2.11	0.54
1:A:612:SER:O	1:A:616:GLU:HB2	2.07	0.54
1:A:169:ALA:HA	1:A:256:ARG:HE	1.73	0.54
1:A:132:VAL:HG13	1:A:136:LYS:HE3	1.89	0.53
1:A:594:ARG:HH11	1:A:594:ARG:CG	2.20	0.53
1:A:464:THR:O	1:A:465:LYS:C	2.44	0.53
1:A:621:MET:CE	1:A:651:ASN:HD22	2.22	0.53
1:A:354:LEU:HG	1:A:358:LEU:HD13	1.90	0.53
1:A:337:ILE:CD1	1:A:526:ARG:NH2	2.72	0.53
1:A:730:GLU:CD	1:A:730:GLU:O	2.46	0.53
1:A:554:PHE:HZ	1:A:581:ILE:HA	1.73	0.53
1:A:191:ASN:OD1	1:A:518:GLN:NE2	2.42	0.53
1:A:622:VAL:HG23	1:A:644:LEU:HD21	1.91	0.53
1:A:129:ILE:O	1:A:131:ALA:N	2.42	0.53
1:A:247:PHE:O	1:A:248:MET:C	2.46	0.53
1:A:267:GLN:HG3	1:A:267:GLN:O	2.06	0.53
1:A:293:ASN:C	1:A:293:ASN:OD1	2.45	0.53
1:A:198:VAL:HG21	1:A:370:MET:CB	2.26	0.53
1:A:535:ILE:HD11	1:A:553:VAL:HG21	1.90	0.53
1:A:350:TYR:CE2	1:A:354:LEU:HD13	2.43	0.53
1:A:621:MET:HE1	1:A:651:ASN:CB	2.38	0.53
1:A:156:LEU:O	1:A:160:LEU:N	2.41	0.53
1:A:736:LYS:O	1:A:738:SER:N	2.42	0.53
1:A:69:ILE:CG1	1:A:677:LEU:HG	2.39	0.52
1:A:358:LEU:CD1	1:A:358:LEU:H	2.21	0.52
1:A:382:LEU:O	1:A:387:LYS:CE	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:LYS:NZ	1:A:158:LYS:CA	2.72	0.52
1:A:314:GLU:OE2	1:A:318:LYS:O	2.27	0.52
1:A:471:LYS:O	1:A:472:ALA:C	2.47	0.52
1:A:718:ILE:HG22	1:A:722:LEU:CD1	2.39	0.52
1:A:318:LYS:CB	1:A:319:PRO:HA	2.39	0.52
1:A:643:THR:CB	1:A:647:ASN:HD21	2.22	0.52
1:A:741:ASN:N	1:A:742:PRO:HD3	2.24	0.52
1:A:167:PRO:HD2	1:A:368:ASN:HD22	1.74	0.52
1:A:366:LEU:O	1:A:370:MET:CG	2.47	0.52
1:A:482:PRO:HD3	1:A:534:TRP:CD2	2.44	0.52
1:A:580:VAL:CG2	4:A:2001:TI1:CE4	2.87	0.52
1:A:472:ALA:CB	1:A:473:LEU:HD11	2.36	0.52
1:A:230:TYR:HE2	1:A:240:ALA:CB	2.22	0.52
1:A:439:VAL:CG1	1:A:443:ILE:HD12	2.35	0.52
1:A:515:LYS:O	1:A:516:PHE:C	2.48	0.52
1:A:346:TYR:C	1:A:348:PRO:HD2	2.29	0.52
1:A:621:MET:O	1:A:622:VAL:C	2.48	0.52
1:A:680:ASN:OD1	1:A:680:ASN:C	2.48	0.52
1:A:225:LEU:HB3	1:A:226:PRO:HD2	1.91	0.52
1:A:471:LYS:CE	1:A:596:PHE:O	2.57	0.52
1:A:541:VAL:HG12	1:A:541:VAL:O	2.09	0.52
1:A:388:GLU:C	1:A:390:ARG:H	2.13	0.51
1:A:662:GLN:HA	1:A:665:ILE:CG1	2.40	0.51
1:A:156:LEU:O	1:A:159:LEU:CA	2.58	0.51
2:A:754:NAG:O6	2:A:754:NAG:O4	2.16	0.51
1:A:203:PHE:CE2	1:A:217:HIS:HB2	2.44	0.51
1:A:437:HIS:HA	1:A:440:GLU:CG	2.41	0.51
1:A:636:GLN:OE1	1:A:707:LYS:NZ	2.44	0.51
1:A:748:VAL:HG22	1:A:749:TRP:N	2.24	0.51
1:A:355:LYS:O	1:A:359:THR:OG1	2.11	0.51
1:A:467:ARG:O	1:A:468:ALA:C	2.47	0.51
1:A:505:GLU:HB3	1:A:508:GLU:HB2	1.92	0.51
1:A:565:SER:O	1:A:567:GLN:N	2.43	0.51
1:A:164:TYR:OH	1:A:185:LYS:HG3	2.11	0.51
1:A:159:LEU:O	1:A:162:ASP:N	2.34	0.51
1:A:182:THR:H	1:A:185:LYS:CE	2.23	0.51
1:A:315:ILE:O	1:A:316:ASN:HB3	2.11	0.51
1:A:337:ILE:HD11	1:A:526:ARG:NH2	2.26	0.51
1:A:156:LEU:HD13	1:A:382:LEU:HD11	1.92	0.51
1:A:199:LEU:HD23	1:A:199:LEU:N	2.26	0.51
1:A:209:LYS:HE3	1:A:602:LEU:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:VAL:HG13	1:A:248:MET:SD	2.51	0.51
1:A:665:ILE:O	1:A:666:LYS:C	2.49	0.51
1:A:65:ALA:O	1:A:69:ILE:CD1	2.59	0.51
1:A:421:ALA:HB2	1:A:496:TYR:CE2	2.46	0.51
1:A:439:VAL:HG11	1:A:479:ILE:HG23	1.93	0.51
1:A:446:ILE:HG21	1:A:581:ILE:HG22	1.93	0.51
1:A:588:GLY:CA	1:A:589:PHE:CD2	2.93	0.51
1:A:83:PHE:O	1:A:87:CYS:HB2	2.11	0.51
1:A:390:ARG:O	1:A:390:ARG:CG	2.57	0.51
1:A:193:LYS:HG3	1:A:515:LYS:HG2	1.93	0.51
1:A:405:ALA:O	1:A:408:ARG:HB2	2.11	0.51
1:A:633:ALA:CB	1:A:706:ILE:HD12	2.41	0.51
1:A:209:LYS:CD	1:A:299:TYR:CZ	2.94	0.50
1:A:546:SER:HB3	1:A:549:ARG:HB2	1.93	0.50
1:A:693:TRP:CH2	1:A:717:ARG:NH1	2.79	0.50
1:A:216:ILE:CG1	1:A:525:LEU:HD21	2.42	0.50
1:A:625:TYR:O	1:A:628:PHE:HB2	2.10	0.50
1:A:590:ASP:OD1	1:A:590:ASP:C	2.49	0.50
1:A:69:ILE:HD11	1:A:677:LEU:CG	2.42	0.50
1:A:658:TYR:O	1:A:661:TYR:N	2.42	0.50
1:A:69:ILE:HA	1:A:72:MET:HG2	1.93	0.50
1:A:182:THR:O	1:A:185:LYS:HG2	2.11	0.50
1:A:200:ILE:HD12	1:A:200:ILE:N	2.27	0.50
1:A:597:ASN:CG	1:A:598:LYS:N	2.63	0.50
1:A:168:VAL:HA	1:A:271:GLU:OE1	2.11	0.50
1:A:460:MET:O	1:A:465:LYS:HE2	2.12	0.50
1:A:747:ARG:HG3	1:A:748:VAL:N	2.26	0.50
1:A:164:TYR:HE2	1:A:185:LYS:HE3	1.73	0.49
1:A:298:LEU:HD13	1:A:346:TYR:CD1	2.47	0.49
1:A:718:ILE:C	1:A:722:LEU:CD1	2.70	0.49
1:A:261:LEU:HB3	1:A:262:PRO:HD2	1.93	0.49
1:A:408:ARG:C	1:A:410:CYS:H	2.15	0.49
1:A:696:THR:OG1	1:A:697:TYR:N	2.36	0.49
1:A:436:LYS:O	1:A:440:GLU:CG	2.60	0.49
1:A:225:LEU:HD12	1:A:231:TYR:CZ	2.48	0.49
1:A:408:ARG:C	1:A:410:CYS:N	2.64	0.49
1:A:423:GLY:O	1:A:427:VAL:HG22	2.13	0.49
1:A:427:VAL:HG11	1:A:481:TYR:CD2	2.47	0.49
1:A:579:MET:HE2	1:A:689:PHE:CE2	2.47	0.49
1:A:166:TRP:O	1:A:167:PRO:C	2.51	0.49
1:A:167:PRO:CD	1:A:368:ASN:ND2	2.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:LEU:O	1:A:269:ALA:C	2.50	0.49
1:A:382:LEU:HD21	1:A:507:PHE:CE2	2.48	0.49
1:A:437:HIS:O	1:A:440:GLU:OE2	2.30	0.49
1:A:313:LEU:HD22	1:A:355:LYS:HB2	1.95	0.49
1:A:183:ALA:O	1:A:187:ILE:HB	2.12	0.49
1:A:288:LYS:HB3	1:A:290:GLU:OE2	2.13	0.49
1:A:378:LEU:HD22	1:A:507:PHE:CE2	2.48	0.49
1:A:182:THR:O	1:A:183:ALA:C	2.51	0.49
1:A:490:ASN:O	1:A:494:ASN:N	2.46	0.49
1:A:78:PRO:HG3	1:A:85:TYR:CE1	2.48	0.48
1:A:173:TRP:O	1:A:174:GLU:C	2.51	0.48
1:A:394:ARG:NH2	1:A:402:SER:N	2.56	0.48
1:A:528:LYS:O	1:A:529:VAL:C	2.51	0.48
1:A:72:MET:SD	1:A:677:LEU:CD2	3.01	0.48
1:A:387:LYS:O	1:A:388:GLU:C	2.50	0.48
1:A:69:ILE:HD11	1:A:677:LEU:CD1	2.44	0.48
1:A:403:GLU:CG	1:A:404:THR:N	2.76	0.48
1:A:621:MET:HE2	1:A:651:ASN:ND2	2.26	0.48
1:A:225:LEU:HD12	1:A:231:TYR:CE2	2.49	0.48
1:A:193:LYS:CG	1:A:515:LYS:HE3	2.43	0.48
1:A:461:ASP:OD2	1:A:463:GLU:HG2	2.13	0.48
1:A:545:TYR:CZ	1:A:546:SER:O	2.66	0.48
1:A:658:TYR:CZ	1:A:727:GLU:HB3	2.48	0.48
1:A:427:VAL:HG12	1:A:431:PHE:HD1	1.79	0.48
1:A:725:SER:HB3	1:A:728:PHE:CB	2.43	0.48
1:A:549:ARG:NH1	1:A:549:ARG:HG3	2.13	0.48
1:A:356:PRO:C	1:A:359:THR:OG1	2.52	0.48
1:A:350:TYR:CZ	1:A:354:LEU:CD1	2.97	0.48
1:A:250:SER:HA	1:A:253:ARG:HH12	1.78	0.48
1:A:535:ILE:CG1	1:A:553:VAL:HG21	2.44	0.48
1:A:73:ASP:OD1	1:A:75:THR:HG23	2.13	0.47
1:A:131:ALA:CB	1:A:492:LEU:HD13	2.44	0.47
1:A:196:LYS:NZ	1:A:373:ARG:O	2.38	0.47
1:A:247:PHE:CZ	1:A:390:ARG:HB2	2.49	0.47
1:A:121:LEU:O	1:A:136:LYS:CD	2.55	0.47
1:A:160:LEU:HA	1:A:163:ILE:CD1	2.42	0.47
1:A:252:ALA:O	1:A:256:ARG:HG3	2.13	0.47
1:A:404:THR:HG23	1:A:409:ARG:HD3	1.96	0.47
1:A:469:GLU:O	1:A:472:ALA:HB2	2.08	0.47
1:A:552:ILE:HG21	1:A:585:ILE:HG13	1.96	0.47
1:A:173:TRP:O	1:A:175:GLN:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:LEU:HB3	1:A:526:ARG:HG2	1.97	0.47
1:A:58:SER:O	1:A:61:CYS:N	2.47	0.47
1:A:156:LEU:HB2	1:A:160:LEU:HD21	1.95	0.47
1:A:217:HIS:O	1:A:218:ILE:HD13	2.13	0.47
1:A:439:VAL:O	1:A:442:LEU:HB2	2.14	0.47
1:A:505:GLU:OE1	1:A:508:GLU:CG	2.59	0.47
1:A:290:GLU:OE2	1:A:290:GLU:N	2.46	0.47
1:A:58:SER:O	1:A:62:ILE:CG2	2.52	0.47
1:A:168:VAL:O	1:A:168:VAL:CG2	2.63	0.47
1:A:372:TRP:CZ2	1:A:376:MET:HE2	2.49	0.47
1:A:622:VAL:CG2	1:A:644:LEU:CD2	2.88	0.47
1:A:690:ALA:O	1:A:718:ILE:HD11	2.14	0.47
1:A:185:LYS:HG2	1:A:186:ALA:H	1.80	0.47
1:A:199:LEU:N	1:A:199:LEU:CD2	2.76	0.47
1:A:313:LEU:HD11	1:A:358:LEU:HD22	1.93	0.47
1:A:577:ILE:O	1:A:581:ILE:HD12	2.15	0.47
1:A:76:THR:CG2	1:A:77:GLU:N	2.77	0.47
1:A:461:ASP:C	1:A:465:LYS:HG2	2.36	0.47
1:A:542:ASN:OD1	4:A:2001:TI1:HB21	2.14	0.47
1:A:96:ILE:HG22	1:A:100:SER:HB2	1.98	0.46
1:A:460:MET:O	1:A:465:LYS:CE	2.63	0.46
1:A:588:GLY:C	1:A:589:PHE:CD2	2.89	0.46
1:A:76:THR:HG22	1:A:77:GLU:N	2.30	0.46
1:A:154:GLU:N	1:A:155:PRO:HD3	2.29	0.46
1:A:331:SER:HA	1:A:334:ASN:HA	1.98	0.46
1:A:496:TYR:O	1:A:499:LEU:N	2.40	0.46
1:A:191:ASN:O	1:A:195:GLY:CA	2.61	0.46
1:A:451:ILE:HD11	1:A:472:ALA:CB	2.36	0.46
1:A:506:TYR:O	1:A:510:ILE:HG12	2.16	0.46
1:A:66:ALA:O	1:A:70:GLN:HB2	2.16	0.46
1:A:278:LEU:HD22	1:A:282:ILE:HD12	1.98	0.46
1:A:190:LEU:O	1:A:195:GLY:N	2.48	0.46
1:A:199:LEU:CB	1:A:200:ILE:HD12	2.40	0.46
1:A:394:ARG:NH2	1:A:402:SER:CA	2.79	0.46
1:A:129:ILE:O	1:A:130:VAL:C	2.55	0.46
1:A:207:ASP:OD1	1:A:301:LYS:NZ	2.49	0.46
1:A:209:LYS:HE2	1:A:602:LEU:HB3	1.92	0.46
1:A:262:PRO:C	1:A:263:ILE:CD1	2.84	0.46
1:A:630:TRP:CZ3	1:A:706:ILE:HG13	2.51	0.46
1:A:408:ARG:O	1:A:409:ARG:C	2.54	0.46
1:A:449:VAL:HA	1:A:452:GLN:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:651:ASN:OD1	1:A:721:THR:HA	2.16	0.46
1:A:153:GLY:C	1:A:155:PRO:CD	2.84	0.45
1:A:156:LEU:C	1:A:160:LEU:HD23	2.31	0.45
1:A:278:LEU:HD22	1:A:282:ILE:CD1	2.46	0.45
1:A:297:LEU:HD23	1:A:297:LEU:N	2.30	0.45
1:A:435:SER:O	1:A:436:LYS:C	2.55	0.45
1:A:577:ILE:CG2	1:A:578:GLY:N	2.80	0.45
1:A:664:TYR:CE2	1:A:668:ASN:ND2	2.84	0.45
1:A:331:SER:O	1:A:331:SER:OG	2.26	0.45
1:A:545:TYR:CE2	1:A:546:SER:O	2.70	0.45
1:A:579:MET:HE1	4:A:2001:TI1:HE4	1.99	0.45
1:A:680:ASN:OD1	1:A:682:LYS:N	2.50	0.45
1:A:239:GLU:O	1:A:240:ALA:C	2.55	0.45
1:A:261:LEU:CB	1:A:262:PRO:CD	2.95	0.45
1:A:522:LEU:O	1:A:524:LYS:N	2.49	0.45
1:A:313:LEU:CD2	1:A:355:LYS:HB2	2.46	0.45
1:A:566:ALA:HB3	1:A:567:GLN:OE1	2.16	0.45
1:A:156:LEU:C	1:A:160:LEU:HD21	2.33	0.45
1:A:236:ILE:HD13	1:A:636:GLN:HE22	1.82	0.45
1:A:680:ASN:OD1	1:A:683:GLN:HG3	2.17	0.45
1:A:442:LEU:HD23	1:A:442:LEU:HA	1.84	0.45
1:A:482:PRO:HG3	1:A:534:TRP:NE1	2.32	0.45
4:A:2001:TI1:HN2	4:A:2001:TI1:HB12	1.44	0.45
1:A:190:LEU:HD23	1:A:190:LEU:HA	1.68	0.44
1:A:323:LEU:O	1:A:327:ASN:HB2	2.17	0.44
1:A:662:GLN:HA	1:A:665:ILE:HG13	1.99	0.44
1:A:207:ASP:HB2	1:A:215:VAL:HG21	1.84	0.44
1:A:454:LEU:HD12	1:A:454:LEU:N	2.31	0.44
1:A:574:TYR:CB	1:A:685:PHE:HE2	2.31	0.44
1:A:147:ALA:O	1:A:150:SER:HB2	2.17	0.44
1:A:315:ILE:CD1	1:A:320:PHE:CD2	3.00	0.44
1:A:507:PHE:O	1:A:510:ILE:HB	2.17	0.44
1:A:727:GLU:H	1:A:727:GLU:CD	2.20	0.44
1:A:448:GLU:O	1:A:452:GLN:N	2.41	0.44
1:A:597:ASN:OD1	1:A:598:LYS:N	2.50	0.44
1:A:643:THR:O	1:A:644:LEU:C	2.55	0.44
1:A:736:LYS:C	1:A:738:SER:H	2.19	0.44
1:A:166:TRP:HE3	1:A:255:ILE:HD12	1.78	0.44
1:A:272:MET:CE	1:A:272:MET:N	2.80	0.44
1:A:298:LEU:HD23	1:A:298:LEU:HA	1.77	0.44
1:A:157:LEU:N	1:A:160:LEU:CD2	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:PRO:O	1:A:223:LEU:HD23	2.17	0.44
1:A:735:ARG:O	1:A:736:LYS:C	2.55	0.44
1:A:68:LEU:HD23	1:A:687:LEU:CD1	2.02	0.44
1:A:96:ILE:CG2	1:A:100:SER:HB2	2.48	0.44
1:A:382:LEU:O	1:A:387:LYS:NZ	2.51	0.44
1:A:509:ASN:O	1:A:510:ILE:C	2.55	0.44
1:A:577:ILE:HD13	1:A:577:ILE:HA	1.72	0.44
1:A:156:LEU:HA	1:A:159:LEU:HB2	1.99	0.44
1:A:175:GLN:O	1:A:175:GLN:HG3	2.17	0.44
1:A:254:LEU:O	1:A:255:ILE:C	2.56	0.44
1:A:69:ILE:HG13	1:A:677:LEU:HG	2.00	0.44
1:A:209:LYS:CE	1:A:602:LEU:HB2	2.48	0.44
1:A:315:ILE:O	1:A:316:ASN:CB	2.66	0.44
1:A:366:LEU:O	1:A:370:MET:HE2	2.18	0.44
1:A:374:PHE:CE2	1:A:378:LEU:HD11	2.53	0.44
1:A:415:ASN:HD21	1:A:539:ALA:HB1	1.82	0.44
1:A:525:LEU:HD13	1:A:525:LEU:HA	1.42	0.44
1:A:182:THR:HG23	1:A:185:LYS:CG	2.48	0.43
1:A:214:HIS:CE1	1:A:524:LYS:NZ	2.86	0.43
1:A:378:LEU:HD21	1:A:511:ILE:HD11	1.99	0.43
1:A:450:PHE:CD1	1:A:450:PHE:C	2.90	0.43
1:A:209:LYS:HE2	1:A:602:LEU:CB	2.46	0.43
1:A:247:PHE:O	1:A:251:VAL:HG23	2.18	0.43
1:A:275:VAL:O	1:A:369:LEU:HD22	2.19	0.43
1:A:570:ASN:O	1:A:574:TYR:HD2	2.00	0.43
1:A:239:GLU:O	1:A:242:THR:N	2.52	0.43
1:A:490:ASN:O	1:A:494:ASN:CB	2.66	0.43
1:A:159:LEU:HD12	1:A:159:LEU:HA	1.82	0.43
1:A:384:ARG:HD3	1:A:384:ARG:HA	1.68	0.43
1:A:459:TRP:CZ3	1:A:606:TRP:HZ3	2.37	0.43
1:A:494:ASN:HA	1:A:497:LEU:HD12	2.01	0.43
1:A:230:TYR:O	1:A:233:CYS:N	2.52	0.43
1:A:726:ALA:C	1:A:728:PHE:N	2.69	0.43
1:A:134:LYS:O	1:A:135:ALA:C	2.55	0.43
1:A:199:LEU:HA	1:A:199:LEU:HD22	1.63	0.43
1:A:220:GLN:HB2	1:A:221:PRO:HD2	1.99	0.43
1:A:272:MET:HE3	1:A:272:MET:N	2.33	0.43
1:A:499:LEU:HD23	1:A:499:LEU:HA	1.78	0.43
1:A:682:LYS:O	1:A:685:PHE:HB3	2.18	0.43
1:A:95:VAL:HG12	1:A:96:ILE:O	2.19	0.43
1:A:256:ARG:NH1	1:A:262:PRO:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:VAL:CG2	1:A:369:LEU:HD22	2.46	0.43
1:A:522:LEU:C	1:A:524:LYS:N	2.72	0.43
1:A:662:GLN:O	1:A:663:ASN:C	2.57	0.43
1:A:149:ASP:C	1:A:151:ARG:N	2.71	0.43
1:A:193:LYS:HB3	1:A:194:TYR:CD2	2.54	0.43
1:A:231:TYR:OH	1:A:279:GLU:OE1	2.25	0.43
1:A:345:VAL:HG12	1:A:345:VAL:O	2.19	0.43
1:A:403:GLU:HG2	1:A:409:ARG:HD2	2.01	0.43
1:A:728:PHE:O	1:A:731:ALA:HB3	2.18	0.43
1:A:209:LYS:HE3	1:A:602:LEU:HB2	1.99	0.43
1:A:311:PHE:CE1	1:A:352:THR:OG1	2.36	0.43
1:A:403:GLU:OE2	1:A:404:THR:CG2	2.44	0.43
1:A:521:GLN:O	1:A:524:LYS:HB2	2.19	0.43
1:A:726:ALA:O	1:A:727:GLU:C	2.56	0.43
1:A:216:ILE:HD11	1:A:525:LEU:CD2	2.49	0.42
1:A:662:GLN:O	1:A:665:ILE:N	2.52	0.42
1:A:722:LEU:C	1:A:724:ASN:H	2.21	0.42
1:A:193:LYS:NZ	1:A:515:LYS:CE	2.59	0.42
1:A:247:PHE:C	1:A:249:ILE:N	2.71	0.42
1:A:313:LEU:O	1:A:320:PHE:N	2.45	0.42
1:A:424:ARG:CD	1:A:485:ILE:O	2.64	0.42
1:A:579:MET:SD	1:A:689:PHE:HE2	2.42	0.42
1:A:652:GLY:O	1:A:656:GLN:HB2	2.20	0.42
1:A:164:TYR:OH	1:A:185:LYS:HB2	2.19	0.42
1:A:229:ASP:O	1:A:232:GLU:HB2	2.19	0.42
1:A:184:GLU:CA	1:A:325:PHE:HB2	2.49	0.42
1:A:335:ILE:HG23	1:A:336:SER:N	2.35	0.42
1:A:706:ILE:O	1:A:706:ILE:CG2	2.66	0.42
1:A:447:ARG:O	1:A:450:PHE:HB3	2.18	0.42
1:A:356:PRO:O	1:A:359:THR:OG1	2.38	0.42
1:A:394:ARG:NH2	1:A:401:THR:C	2.73	0.42
1:A:451:ILE:O	1:A:453:THR:N	2.53	0.42
1:A:564:PHE:O	1:A:564:PHE:CD2	2.72	0.42
1:A:589:PHE:C	1:A:590:ASP:O	2.56	0.42
1:A:722:LEU:C	1:A:724:ASN:N	2.73	0.42
1:A:131:ALA:HB1	1:A:492:LEU:HD13	2.01	0.42
1:A:202:LEU:HA	1:A:218:ILE:HD13	2.02	0.42
1:A:256:ARG:HH11	1:A:256:ARG:HD3	1.73	0.42
1:A:354:LEU:O	1:A:357:ILE:N	2.53	0.42
1:A:621:MET:SD	1:A:648:ILE:HG13	2.60	0.42
1:A:621:MET:CE	1:A:651:ASN:HB2	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:SER:O	1:A:62:ILE:HD12	2.20	0.42
1:A:358:LEU:HD13	1:A:358:LEU:H	1.84	0.42
1:A:464:THR:OG1	1:A:607:THR:HG23	2.19	0.42
1:A:471:LYS:HZ1	1:A:596:PHE:CB	2.30	0.42
1:A:471:LYS:O	1:A:472:ALA:O	2.38	0.42
1:A:478:ARG:HE	1:A:551:GLN:CD	2.23	0.42
1:A:439:VAL:HG12	1:A:443:ILE:HD12	1.95	0.42
1:A:440:GLU:HA	1:A:443:ILE:CD1	2.50	0.42
1:A:535:ILE:CD1	1:A:553:VAL:HG21	2.50	0.42
1:A:275:VAL:CG1	1:A:276:MET:N	2.82	0.41
1:A:278:LEU:CD1	1:A:369:LEU:HD23	2.49	0.41
1:A:393:PHE:O	1:A:397:LEU:HG	2.20	0.41
1:A:181:TRP:CZ3	1:A:316:ASN:HB2	2.52	0.41
1:A:184:GLU:HG2	1:A:184:GLU:H	1.24	0.41
1:A:193:LYS:HZ2	1:A:515:LYS:HE2	1.75	0.41
1:A:728:PHE:O	1:A:731:ALA:N	2.53	0.41
1:A:55:ILE:HD13	1:A:55:ILE:N	2.10	0.41
1:A:246:ASP:O	1:A:249:ILE:HB	2.20	0.41
1:A:340:GLU:OE2	1:A:340:GLU:O	2.39	0.41
1:A:447:ARG:NH1	1:A:475:ILE:O	2.53	0.41
1:A:335:ILE:HG23	1:A:336:SER:H	1.85	0.41
1:A:313:LEU:HD13	1:A:358:LEU:HD22	1.98	0.41
1:A:342:ASP:C	1:A:343:VAL:HG23	2.40	0.41
1:A:499:LEU:HD13	1:A:501:TYR:OH	2.19	0.41
1:A:563:PHE:HB3	1:A:577:ILE:N	2.35	0.41
1:A:579:MET:CE	1:A:689:PHE:HE2	2.33	0.41
1:A:690:ALA:HA	1:A:718:ILE:HD11	2.03	0.41
1:A:748:VAL:HG22	1:A:749:TRP:CD1	2.54	0.41
1:A:185:LYS:CG	1:A:186:ALA:N	2.83	0.41
1:A:454:LEU:H	1:A:454:LEU:HG	1.41	0.41
1:A:155:PRO:HB3	1:A:507:PHE:CD1	2.56	0.41
1:A:312:SER:O	1:A:313:LEU:CD2	2.58	0.41
1:A:565:SER:O	1:A:566:ALA:C	2.57	0.41
1:A:462:ALA:HA	1:A:465:LYS:HG3	1.94	0.41
1:A:135:ALA:O	1:A:138:LEU:N	2.53	0.41
1:A:198:VAL:CG2	1:A:370:MET:HB3	2.31	0.41
1:A:216:ILE:CD1	1:A:525:LEU:CD2	2.99	0.41
1:A:347:ALA:O	1:A:348:PRO:C	2.59	0.41
1:A:355:LYS:CB	1:A:356:PRO:CD	2.98	0.41
1:A:414:VAL:CG2	1:A:415:ASN:N	2.82	0.41
1:A:574:TYR:C	1:A:685:PHE:CE2	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:633:ALA:HB1	1:A:706:ILE:HD12	2.02	0.41
1:A:305:ALA:C	1:A:307:ILE:N	2.74	0.41
1:A:408:ARG:O	1:A:410:CYS:N	2.54	0.41
1:A:435:SER:C	1:A:437:HIS:N	2.74	0.41
1:A:481:TYR:HD1	1:A:482:PRO:O	2.03	0.41
1:A:105:ASN:O	1:A:106:PHE:C	2.59	0.40
1:A:164:TYR:HA	1:A:177:TYR:CD1	2.56	0.40
1:A:349:GLU:O	1:A:353:LYS:HB2	2.21	0.40
1:A:351:LEU:O	1:A:352:THR:C	2.57	0.40
1:A:693:TRP:CZ2	1:A:717:ARG:CZ	3.04	0.40
1:A:69:ILE:HD12	1:A:69:ILE:H	1.86	0.40
1:A:182:THR:HG23	1:A:185:LYS:CD	2.39	0.40
1:A:224:GLY:HA3	1:A:244:TYR:OH	2.20	0.40
1:A:261:LEU:HD23	1:A:262:PRO:HD3	1.91	0.40
1:A:449:VAL:O	1:A:452:GLN:HB2	2.22	0.40
1:A:535:ILE:HD11	1:A:553:VAL:CG2	2.51	0.40
1:A:535:ILE:HG12	1:A:553:VAL:HG21	2.02	0.40
1:A:536:SER:HB3	1:A:555:PRO:HG3	2.02	0.40
1:A:463:GLU:HG3	1:A:607:THR:CG2	2.51	0.40
1:A:582:GLY:O	1:A:586:THR:OG1	2.35	0.40
1:A:69:ILE:CD1	1:A:677:LEU:CD1	3.00	0.40
1:A:135:ALA:HA	1:A:418:MET:SD	2.61	0.40
1:A:465:LYS:HG2	1:A:465:LYS:H	1.67	0.40
1:A:517:SER:O	1:A:520:LYS:HB3	2.22	0.40
1:A:217:HIS:ND1	1:A:217:HIS:N	2.70	0.40
1:A:249:ILE:O	1:A:251:VAL:N	2.55	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:16:HOH:O	5:A:16:HOH:O[4_556]	1.18	1.02
1:A:175:GLN:NE2	1:A:261:LEU:C[6_765]	1.74	0.46
1:A:175:GLN:NE2	1:A:261:LEU:O[6_765]	1.91	0.29
1:A:490:ASN:ND2	1:A:609:GLN:OE1[5_665]	2.02	0.18
1:A:175:GLN:NE2	1:A:261:LEU:CA[6_765]	2.08	0.12

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	694/696 (100%)	584 (84%)	81 (12%)	29 (4%)	3 3

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	181	TRP
1	A	183	ALA
1	A	269	ALA
1	A	304	LEU
1	A	318	LYS
1	A	435	SER
1	A	472	ALA
1	A	516	PHE
1	A	529	VAL
1	A	638	LEU
1	A	665	ILE
1	A	736	LYS
1	A	55	ILE
1	A	150	SER
1	A	305	ALA
1	A	452	GLN
1	A	588	GLY
1	A	737	ASN
1	A	388	GLU
1	A	559	LEU
1	A	608	GLN
1	A	663	ASN
1	A	339	ASN
1	A	624	GLN
1	A	728	PHE
1	A	334	ASN
1	A	348	PRO
1	A	317	GLY

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Mol	Chain	Res	Type
1	A	319	PRO

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	605/605 (100%)	453 (75%)	152 (25%)	0 1

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	ILE
1	A	57	LYS
1	A	58	SER
1	A	62	ILE
1	A	63	LYS
1	A	64	SER
1	A	68	LEU
1	A	70	GLN
1	A	75	THR
1	A	80	THR
1	A	91	LEU
1	A	92	LYS
1	A	113	LEU
1	A	118	LYS
1	A	126	THR
1	A	129	ILE
1	A	156	LEU
1	A	157	LEU
1	A	158	LYS
1	A	159	LEU
1	A	160	LEU
1	A	162	ASP
1	A	163	ILE
1	A	171	GLU
1	A	175	GLN

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Mol	Chain	Res	Type
1	A	176	LYS
1	A	180	SER
1	A	182	THR
1	A	184	GLU
1	A	185	LYS
1	A	196	LYS
1	A	197	LYS
1	A	198	VAL
1	A	199	LEU
1	A	202	LEU
1	A	206	THR
1	A	209	LYS
1	A	211	SER
1	A	212	VAL
1	A	215	VAL
1	A	222	ARG
1	A	223	LEU
1	A	228	ARG
1	A	234	THR
1	A	237	TYR
1	A	260	ARG
1	A	261	LEU
1	A	263	ILE
1	A	266	ASN
1	A	267	GLN
1	A	270	LEU
1	A	274	LYS
1	A	278	LEU
1	A	298	LEU
1	A	300	ASN
1	A	313	LEU
1	A	314	GLU
1	A	318	LYS
1	A	321	SER
1	A	323	LEU
1	A	324	ASN
1	A	325	PHE
1	A	328	GLU
1	A	331	SER
1	A	332	THR
1	A	335	ILE
1	A	336	SER

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Mol	Chain	Res	Type
1	A	337	ILE
1	A	339	ASN
1	A	341	GLU
1	A	349	GLU
1	A	351	LEU
1	A	353	LYS
1	A	359	THR
1	A	360	LYS
1	A	364	ARG
1	A	368	ASN
1	A	369	LEU
1	A	370	MET
1	A	371	SER
1	A	379	VAL
1	A	385	THR
1	A	390	ARG
1	A	394	ARG
1	A	414	VAL
1	A	419	GLU
1	A	424	ARG
1	A	427	VAL
1	A	434	GLU
1	A	440	GLU
1	A	441	ASP
1	A	446	ILE
1	A	447	ARG
1	A	448	GLU
1	A	452	GLN
1	A	454	LEU
1	A	455	ASP
1	A	457	LEU
1	A	458	THR
1	A	460	MET
1	A	467	ARG
1	A	473	LEU
1	A	476	LYS
1	A	477	GLU
1	A	483	ASP
1	A	484	ASP
1	A	487	SER
1	A	492	LEU
1	A	495	GLU

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Mol	Chain	Res	Type
1	A	497	LEU
1	A	509	ASN
1	A	523	LYS
1	A	524	LYS
1	A	525	LEU
1	A	529	VAL
1	A	549	ARG
1	A	550	ASN
1	A	551	GLN
1	A	559	LEU
1	A	564	PHE
1	A	570	ASN
1	A	572	LEU
1	A	577	ILE
1	A	579	MET
1	A	580	VAL
1	A	589	PHE
1	A	594	ARG
1	A	597	ASN
1	A	598	LYS
1	A	602	LEU
1	A	608	GLN
1	A	612	SER
1	A	637	HIS
1	A	644	LEU
1	A	648	ILE
1	A	656	GLN
1	A	667	LYS
1	A	674	LEU
1	A	682	LYS
1	A	683	GLN
1	A	687	LEU
1	A	688	ASN
1	A	704	ASN
1	A	705	SER
1	A	729	SER
1	A	730	GLU
1	A	735	ARG
1	A	736	LYS
1	A	738	SER
1	A	744	LYS
1	A	747	ARG

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Mol	Chain	Res	Type
1	A	748	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	ASN
1	A	122	GLN
1	A	257	GLN
1	A	267	GLN
1	A	284	ASN
1	A	300	ASN
1	A	316	ASN
1	A	327	ASN
1	A	339	ASN
1	A	368	ASN
1	A	509	ASN
1	A	518	GLN
1	A	550	ASN
1	A	570	ASN
1	A	609	GLN
1	A	619	GLN
1	A	647	ASN
1	A	651	ASN
1	A	656	GLN
1	A	668	ASN
1	A	688	ASN
1	A	704	ASN
1	A	741	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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	$\#\|Z\| > 2$
4	TI1	A	2001	3	24,26,26	1.07	2 (8%)	28,33,33	1.29	3 (10%)
2	NAG	A	753	1	14,14,15	0.73	0	17,19,21	1.74	5 (29%)
2	NAG	A	752	1	14,14,15	0.71	0	17,19,21	1.80	3 (17%)
2	NAG	A	754	1	14,14,15	0.68	0	17,19,21	2.14	5 (29%)

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	NAG	A	753	1	-	2/6/23/26	0/1/1/1
2	NAG	A	752	1	-	4/6/23/26	0/1/1/1
4	TI1	A	2001	3	1/1/6/8	4/27/29/29	0/1/1/1
2	NAG	A	754	1	-	4/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2001	TI1	CA3-C3	-3.47	1.47	1.52
4	A	2001	TI1	CA1-C1	-2.22	1.49	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	752	NAG	C1-O5-C5	-5.73	104.51	112.19
2	A	754	NAG	C1-O5-C5	-5.65	104.62	112.19
2	A	754	NAG	C2-N2-C7	-3.54	118.16	122.90
2	A	754	NAG	O5-C5-C6	3.48	114.44	107.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	2001	TI1	CA2-N2-C1	-3.39	114.36	121.65
2	A	753	NAG	O5-C1-C2	-3.30	106.18	111.29
4	A	2001	TI1	CG2-CB2-CA2	-3.20	104.84	113.36
2	A	752	NAG	O5-C1-C2	-3.08	106.53	111.29
2	A	753	NAG	C1-O5-C5	-2.80	108.43	112.19
4	A	2001	TI1	OXT-C3-CA3	2.80	123.07	113.84
2	A	753	NAG	C2-N2-C7	-2.65	119.34	122.90
2	A	752	NAG	O5-C5-C6	2.53	112.59	107.66
2	A	753	NAG	C6-C5-C4	2.38	118.86	113.02
2	A	754	NAG	C4-C3-C2	-2.31	107.63	111.02
2	A	754	NAG	O5-C1-C2	-2.30	107.74	111.29
2	A	753	NAG	C3-C4-C5	-2.09	106.44	110.23

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	2001	TI1	CA1

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2001	TI1	SG-CA1-CB1-CG1
2	A	754	NAG	C4-C5-C6-O6
2	A	752	NAG	C8-C7-N2-C2
2	A	752	NAG	O7-C7-N2-C2
4	A	2001	TI1	C1-CA1-CB1-CG1
2	A	754	NAG	O5-C5-C6-O6
4	A	2001	TI1	O1-C1-CA1-CB1
2	A	754	NAG	C8-C7-N2-C2
4	A	2001	TI1	N2-C1-CA1-CB1
2	A	754	NAG	O7-C7-N2-C2
2	A	753	NAG	O5-C5-C6-O6
2	A	752	NAG	C4-C5-C6-O6
2	A	753	NAG	C4-C5-C6-O6
2	A	752	NAG	O5-C5-C6-O6

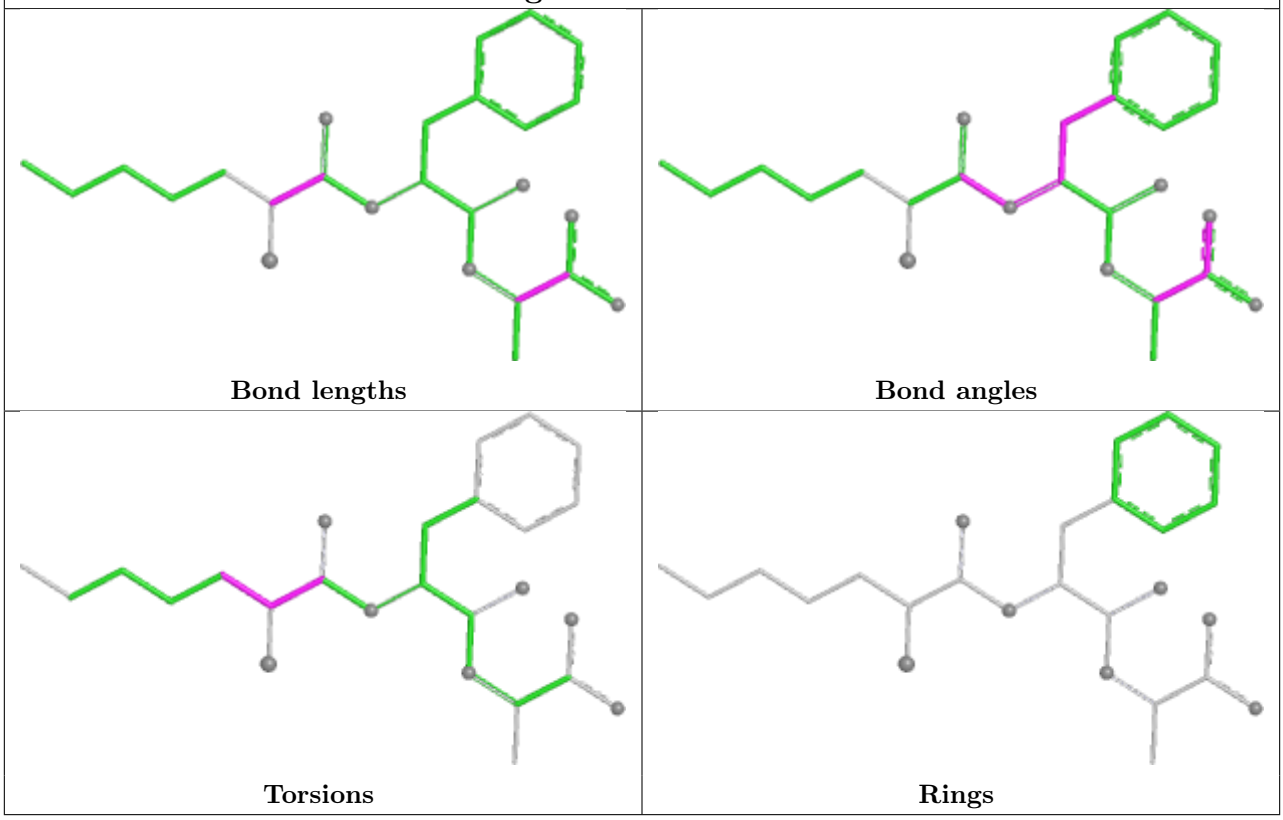
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2001	TI1	6	0
2	A	754	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand TI1 A 2001



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	696/696 (100%)	-0.19	6 (0%)	84	82	25, 52, 78, 93	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	319	PRO	3.1
1	A	735	ARG	2.7
1	A	334	ASN	2.6
1	A	564	PHE	2.6
1	A	433	GLY	2.2
1	A	80	THR	2.2

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 monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	A	753	14/15	0.83	0.29	72,83,86,87	0

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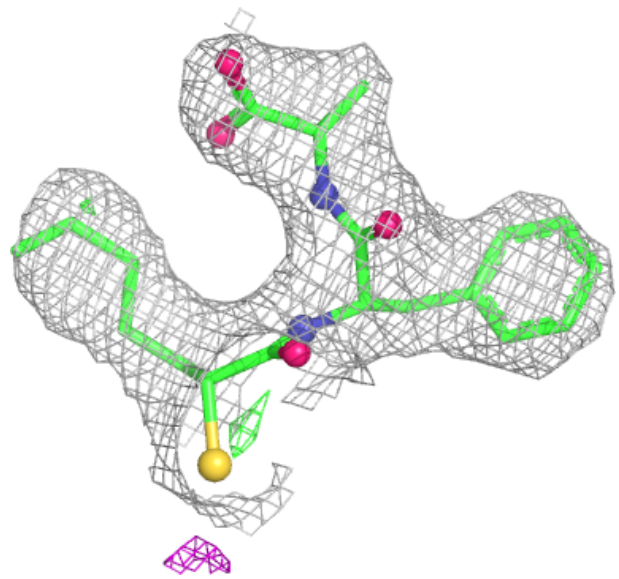
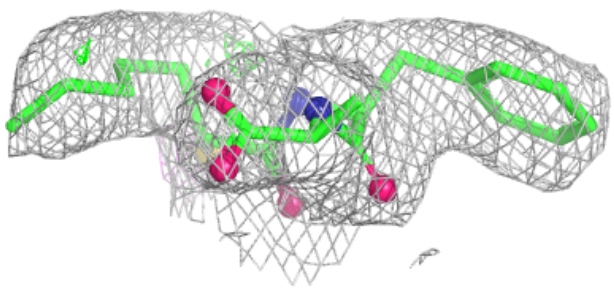
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	A	754	14/15	0.89	0.24	56,59,69,71	0
2	NAG	A	752	14/15	0.93	0.15	56,62,67,69	0
4	TI1	A	2001	26/26	0.95	0.14	35,46,55,56	0
3	ZN	A	1001	1/1	0.99	0.02	35,35,35,35	0

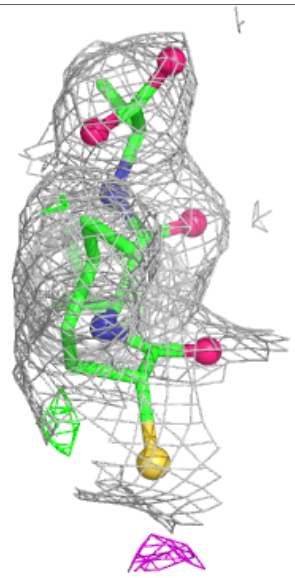
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TI1 A 2001:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.