



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 05:34 pm BST

PDB ID : 1GPD
Title : STUDIES OF ASYMMETRY IN THE THREE-DIMENSIONAL STRUCTURE OF LOBSTER D-GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE
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Deposited on : 1975-07-01
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

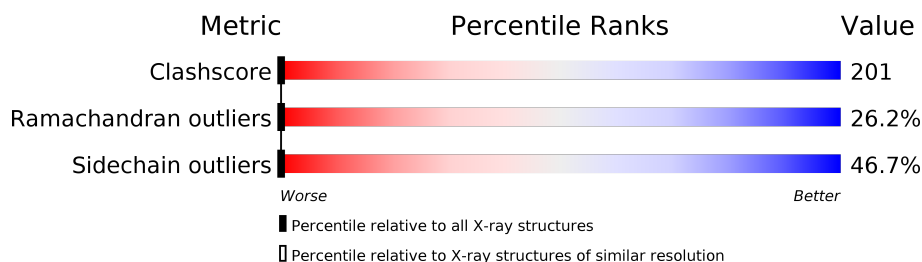
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	G	334	
1	R	334	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	R	338	-	-	X	-

2 Entry composition [i](#)

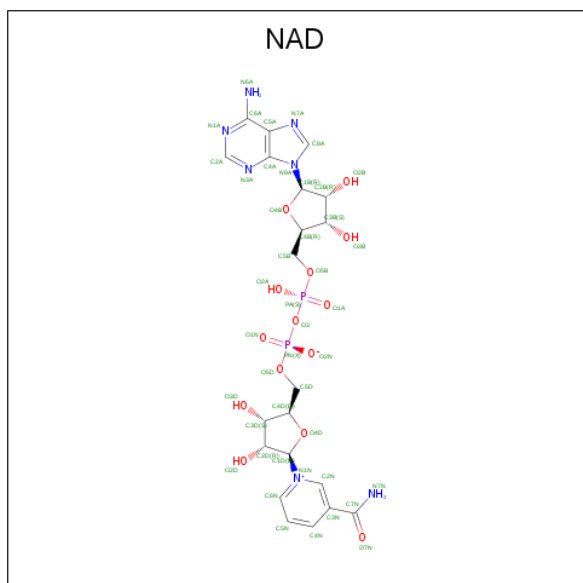
There are 3 unique types of molecules in this entry. The entry contains 5112 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 D-GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	334	Total	C	N	O	S	0	0	0
			2510	1593	419	483	15			
1	R	334	Total	C	N	O	S	0	0	0
			2510	1593	419	483	15			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	R	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



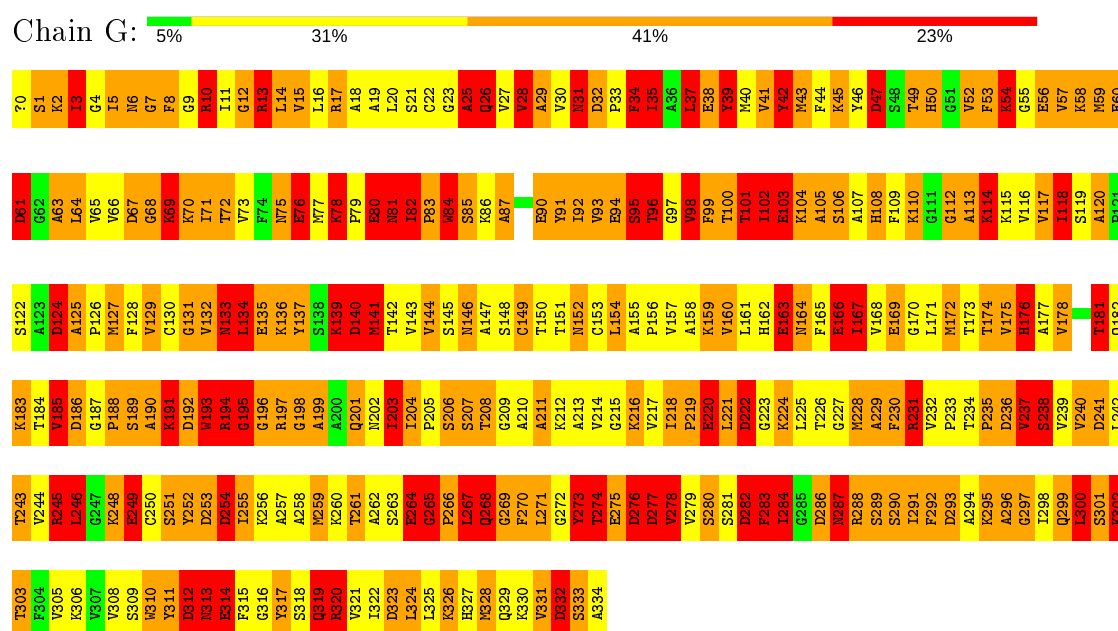
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	R	1	Total	P	0	0
			1	1		
3	R	1	Total	P	0	0
			1	1		
3	R	1	Total	P	0	0
			1	1		
3	R	1	Total	P	0	0
			1	1		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: D-GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE



K302	T303	F304	V305	K306	V307	V308	S309	V310	Y311	D312	N313	E314	F315	G316	Y317	S318	Q319	R320	V321	I322	D323	I324	L325	K326	H327	M328	Q329	K330	V331	D332	S333	A334
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4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	149.00Å 139.10Å 80.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5112	wwPDB-VP
Average B, all atoms (Å ²)	0.0	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: PO4, NAD, ACE

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	G	1.18	30/2554 (1.2%)	2.05	168/3453 (4.9%)
1	R	1.18	30/2554 (1.2%)	1.88	130/3453 (3.8%)
All	All	1.18	60/5108 (1.2%)	1.97	298/6906 (4.3%)

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	G	0	5
1	R	0	7
All	All	0	12

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	84	TRP	NE1-CE2	-7.38	1.27	1.37
1	R	84	TRP	NE1-CE2	-7.35	1.27	1.37
1	R	310	TRP	NE1-CE2	-7.34	1.28	1.37
1	R	193	TRP	NE1-CE2	-7.33	1.28	1.37
1	G	310	TRP	NE1-CE2	-7.31	1.28	1.37
1	G	193	TRP	NE1-CE2	-7.28	1.28	1.37
1	G	164	ASN	CG-OD1	7.05	1.39	1.24
1	R	164	ASN	CG-OD1	7.04	1.39	1.24
1	R	287	ASN	CG-OD1	7.04	1.39	1.24
1	G	152	ASN	CG-OD1	7.04	1.39	1.24
1	R	133	ASN	CG-OD1	7.04	1.39	1.24
1	R	81	ASN	CG-OD1	7.03	1.39	1.24
1	R	75	ASN	CG-OD1	7.03	1.39	1.24
1	G	133	ASN	CG-OD1	7.03	1.39	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	146	ASN	CG-OD1	7.03	1.39	1.24
1	R	202	ASN	CG-OD1	7.02	1.39	1.24
1	R	313	ASN	CG-OD1	7.02	1.39	1.24
1	G	202	ASN	CG-OD1	7.02	1.39	1.24
1	G	75	ASN	CG-OD1	7.01	1.39	1.24
1	R	152	ASN	CG-OD1	7.01	1.39	1.24
1	G	287	ASN	CG-OD1	7.01	1.39	1.24
1	R	31	ASN	CG-OD1	7.01	1.39	1.24
1	G	31	ASN	CG-OD1	7.00	1.39	1.24
1	R	146	ASN	CG-OD1	7.00	1.39	1.24
1	G	313	ASN	CG-OD1	6.99	1.39	1.24
1	G	81	ASN	CG-OD1	6.99	1.39	1.24
1	G	166	GLU	CD-OE1	-5.30	1.19	1.25
1	G	135	GLU	CD-OE1	-5.30	1.19	1.25
1	R	135	GLU	CD-OE1	-5.30	1.19	1.25
1	G	275	GLU	CD-OE1	-5.27	1.19	1.25
1	R	103	GLU	CD-OE1	-5.27	1.19	1.25
1	G	38	GLU	CD-OE1	-5.26	1.19	1.25
1	R	60	GLU	CD-OE1	-5.25	1.19	1.25
1	G	264	GLU	CD-OE1	-5.24	1.19	1.25
1	R	169	GLU	CD-OE1	-5.24	1.19	1.25
1	G	103	GLU	CD-OE1	-5.24	1.19	1.25
1	G	220	GLU	CD-OE1	-5.24	1.19	1.25
1	G	169	GLU	CD-OE1	-5.23	1.19	1.25
1	R	264	GLU	CD-OE1	-5.23	1.19	1.25
1	G	90	GLU	CD-OE1	-5.23	1.20	1.25
1	R	38	GLU	CD-OE1	-5.22	1.20	1.25
1	R	166	GLU	CD-OE1	-5.22	1.20	1.25
1	R	314	GLU	CD-OE1	-5.22	1.20	1.25
1	G	60	GLU	CD-OE1	-5.22	1.20	1.25
1	G	76	GLU	CD-OE1	-5.22	1.20	1.25
1	G	314	GLU	CD-OE1	-5.22	1.20	1.25
1	G	94	GLU	CD-OE1	-5.21	1.20	1.25
1	R	163	GLU	CD-OE1	-5.21	1.20	1.25
1	R	56	GLU	CD-OE1	-5.21	1.20	1.25
1	R	220	GLU	CD-OE1	-5.21	1.20	1.25
1	R	94	GLU	CD-OE1	-5.21	1.20	1.25
1	R	275	GLU	CD-OE1	-5.20	1.20	1.25
1	G	249	GLU	CD-OE1	-5.20	1.20	1.25
1	G	163	GLU	CD-OE1	-5.20	1.20	1.25
1	R	249	GLU	CD-OE1	-5.20	1.20	1.25
1	R	90	GLU	CD-OE1	-5.18	1.20	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	56	GLU	CD-OE1	-5.17	1.20	1.25
1	R	76	GLU	CD-OE1	-5.17	1.20	1.25
1	R	80	GLU	CD-OE1	-5.15	1.20	1.25
1	G	80	GLU	CD-OE1	-5.12	1.20	1.25

All (298) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	277	ASP	N-CA-C	13.71	148.02	111.00
1	G	300	LEU	N-CA-C	13.61	147.75	111.00
1	R	198	GLY	N-CA-C	12.19	143.56	113.10
1	R	195	GLY	N-CA-C	12.14	143.44	113.10
1	G	198	GLY	N-CA-C	12.06	143.25	113.10
1	G	221	LEU	N-CA-C	-11.91	78.83	111.00
1	G	96	THR	N-CA-C	11.89	143.11	111.00
1	G	300	LEU	CB-CA-C	-11.52	88.31	110.20
1	G	28	VAL	N-CA-C	11.45	141.92	111.00
1	G	32	ASP	N-CA-C	11.28	141.44	111.00
1	G	277	ASP	CB-CA-C	-10.79	88.82	110.40
1	G	141	MET	N-CA-C	10.71	139.91	111.00
1	R	238	SER	N-CA-C	10.69	139.87	111.00
1	G	311	TYR	N-CA-C	10.63	139.71	111.00
1	G	275	GLU	N-CA-C	-10.38	82.97	111.00
1	R	248	LYS	N-CA-C	10.02	138.05	111.00
1	R	250	CYS	N-CA-C	10.02	138.04	111.00
1	G	28	VAL	CB-CA-C	-9.98	92.44	111.40
1	G	286	ASP	N-CA-C	-9.90	84.28	111.00
1	R	181	THR	N-CA-C	-9.35	85.76	111.00
1	G	246	LEU	N-CA-C	9.24	135.95	111.00
1	R	238	SER	CB-CA-C	-9.19	92.63	110.10
1	G	10	ARG	N-CA-C	9.15	135.70	111.00
1	G	25	ALA	N-CA-CB	-9.11	97.35	110.10
1	G	8	PHE	N-CA-C	-9.04	86.58	111.00
1	R	46	TYR	N-CA-C	9.04	135.42	111.00
1	G	118	ILE	N-CA-C	8.95	135.15	111.00
1	G	172	MET	N-CA-C	8.94	135.13	111.00
1	G	118	ILE	CB-CA-C	-8.90	93.79	111.60
1	R	5	ILE	N-CA-C	8.90	135.02	111.00
1	R	5	ILE	CB-CA-C	-8.89	93.82	111.60
1	G	32	ASP	CB-CA-C	-8.81	92.78	110.40
1	G	5	ILE	CB-CA-C	-8.78	94.05	111.60
1	G	5	ILE	N-CA-C	8.77	134.68	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	25	ALA	N-CA-C	8.76	134.64	111.00
1	G	141	MET	CB-CA-C	-8.72	92.97	110.40
1	R	248	LYS	CB-CA-C	-8.71	92.97	110.40
1	G	191	LYS	N-CA-C	8.60	134.22	111.00
1	R	25	ALA	N-CA-CB	-8.44	98.29	110.10
1	R	272	GLY	N-CA-C	8.40	134.09	113.10
1	G	321	VAL	N-CA-C	-8.37	88.41	111.00
1	R	250	CYS	CB-CA-C	-8.35	93.70	110.40
1	R	237	VAL	N-CA-C	8.34	133.51	111.00
1	R	172	MET	N-CA-C	8.22	133.20	111.00
1	G	183	LYS	N-CA-C	8.16	133.03	111.00
1	R	191	LYS	N-CA-C	8.16	133.02	111.00
1	G	202	ASN	N-CA-C	8.15	133.02	111.00
1	G	61	ASP	N-CA-C	8.15	133.01	111.00
1	R	25	ALA	N-CA-C	8.11	132.90	111.00
1	G	176	HIS	N-CA-C	8.08	132.83	111.00
1	R	28	VAL	N-CA-C	8.08	132.81	111.00
1	G	10	ARG	CB-CA-C	-8.07	94.26	110.40
1	R	239	VAL	N-CA-C	7.96	132.49	111.00
1	R	302	LYS	N-CA-C	7.88	132.28	111.00
1	G	311	TYR	CB-CA-C	-7.86	94.69	110.40
1	G	246	LEU	CB-CA-C	-7.80	95.38	110.20
1	G	9	GLY	N-CA-C	-7.72	93.80	113.10
1	R	300	LEU	N-CA-C	7.71	131.81	111.00
1	G	76	GLU	N-CA-C	7.70	131.79	111.00
1	R	286	ASP	N-CA-C	-7.69	90.23	111.00
1	G	238	SER	N-CA-C	7.66	131.68	111.00
1	G	195	GLY	N-CA-C	7.64	132.19	113.10
1	G	229	ALA	N-CA-CB	-7.64	99.41	110.10
1	G	181	THR	N-CA-C	7.59	131.51	111.00
1	G	191	LYS	CB-CA-C	-7.55	95.30	110.40
1	G	63	ALA	N-CA-CB	-7.50	99.61	110.10
1	G	203	ILE	N-CA-C	-7.48	90.81	111.00
1	R	227	GLY	N-CA-C	7.43	131.68	113.10
1	G	67	ASP	N-CA-C	-7.42	90.96	111.00
1	R	186	ASP	CB-CG-OD1	7.38	124.94	118.30
1	G	95	SER	N-CA-C	-7.37	91.09	111.00
1	G	286	ASP	CB-CG-OD1	7.35	124.92	118.30
1	R	236	ASP	CB-CG-OD1	7.35	124.92	118.30
1	R	293	ASP	CB-CG-OD1	7.35	124.92	118.30
1	G	236	ASP	CB-CG-OD1	7.35	124.91	118.30
1	R	237	VAL	CB-CA-C	-7.34	97.45	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	192	ASP	CB-CG-OD1	7.34	124.91	118.30
1	R	67	ASP	CB-CG-OD1	7.34	124.90	118.30
1	R	100	THR	N-CA-C	-7.34	91.19	111.00
1	R	140	ASP	CB-CG-OD1	7.34	124.90	118.30
1	R	253	ASP	CB-CG-OD1	7.33	124.90	118.30
1	G	61	ASP	CB-CG-OD1	7.33	124.90	118.30
1	G	229	ALA	N-CA-C	7.33	130.80	111.00
1	R	61	ASP	CB-CG-OD1	7.33	124.90	118.30
1	R	241	ASP	CB-CG-OD1	7.33	124.90	118.30
1	R	286	ASP	CB-CG-OD1	7.32	124.89	118.30
1	G	140	ASP	CB-CG-OD1	7.32	124.89	118.30
1	G	222	ASP	CB-CG-OD1	7.32	124.89	118.30
1	G	254	ASP	CB-CG-OD1	7.32	124.89	118.30
1	G	227	GLY	N-CA-C	7.32	131.39	113.10
1	G	282	ASP	CB-CG-OD1	7.32	124.88	118.30
1	G	47	ASP	CB-CG-OD1	7.31	124.88	118.30
1	G	124	ASP	CB-CG-OD1	7.31	124.88	118.30
1	G	293	ASP	CB-CG-OD1	7.31	124.88	118.30
1	G	323	ASP	CB-CG-OD1	7.31	124.88	118.30
1	G	277	ASP	CB-CG-OD1	7.31	124.88	118.30
1	R	32	ASP	CB-CG-OD1	7.31	124.88	118.30
1	G	186	ASP	CB-CG-OD1	7.31	124.88	118.30
1	G	312	ASP	CB-CG-OD1	7.31	124.88	118.30
1	R	277	ASP	CB-CG-OD1	7.31	124.88	118.30
1	G	67	ASP	CB-CG-OD1	7.31	124.88	118.30
1	R	332	ASP	CB-CG-OD1	7.31	124.88	118.30
1	G	276	ASP	CB-CG-OD1	7.31	124.88	118.30
1	G	167	ILE	CB-CA-C	-7.30	96.99	111.60
1	R	222	ASP	CB-CG-OD1	7.30	124.87	118.30
1	G	192	ASP	CB-CG-OD1	7.30	124.87	118.30
1	R	323	ASP	CB-CG-OD1	7.29	124.86	118.30
1	G	32	ASP	CB-CG-OD1	7.29	124.86	118.30
1	G	172	MET	CB-CA-C	-7.29	95.82	110.40
1	G	241	ASP	CB-CG-OD1	7.29	124.86	118.30
1	G	253	ASP	CB-CG-OD1	7.29	124.86	118.30
1	G	332	ASP	CB-CG-OD1	7.29	124.86	118.30
1	R	312	ASP	CB-CG-OD1	7.28	124.85	118.30
1	R	276	ASP	CB-CG-OD1	7.28	124.85	118.30
1	R	282	ASP	CB-CG-OD1	7.28	124.85	118.30
1	R	47	ASP	CB-CG-OD1	7.28	124.85	118.30
1	R	124	ASP	CB-CG-OD1	7.25	124.82	118.30
1	G	251	SER	N-CA-C	-7.24	91.45	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	236	ASP	N-CA-C	7.24	130.55	111.00
1	R	254	ASP	CB-CG-OD1	7.23	124.81	118.30
1	R	191	LYS	CB-CA-C	-7.21	95.98	110.40
1	G	183	LYS	CB-CA-C	-7.20	96.00	110.40
1	G	76	GLU	CB-CA-C	-7.19	96.02	110.40
1	G	63	ALA	N-CA-C	7.16	130.34	111.00
1	G	268	GLN	N-CA-C	7.16	130.34	111.00
1	R	334	ALA	N-CA-CB	-7.15	100.10	110.10
1	R	128	PHE	N-CA-C	7.13	130.25	111.00
1	R	9	GLY	N-CA-C	-7.10	95.35	113.10
1	R	28	VAL	CB-CA-C	-7.08	97.94	111.40
1	R	302	LYS	CB-CA-C	-6.97	96.47	110.40
1	R	268	GLN	N-CA-C	6.96	129.78	111.00
1	G	221	LEU	CB-CA-C	6.92	123.35	110.20
1	R	118	ILE	CB-CA-C	-6.92	97.77	111.60
1	G	167	ILE	N-CA-C	6.90	129.64	111.00
1	G	310	TRP	N-CA-C	6.89	129.61	111.00
1	G	56	GLU	N-CA-C	-6.88	92.44	111.00
1	R	267	LEU	N-CA-C	6.84	129.46	111.00
1	R	334	ALA	N-CA-C	6.82	129.41	111.00
1	R	175	VAL	N-CA-C	-6.77	92.73	111.00
1	R	3	ILE	CB-CA-C	-6.73	98.14	111.60
1	R	172	MET	CB-CA-C	-6.71	96.98	110.40
1	R	229	ALA	N-CA-CB	-6.68	100.75	110.10
1	G	238	SER	CB-CA-C	-6.64	97.48	110.10
1	R	204	ILE	CB-CA-C	-6.64	98.32	111.60
1	G	31	ASN	N-CA-C	6.60	128.83	111.00
1	R	46	TYR	CB-CA-C	-6.60	97.21	110.40
1	G	265	GLY	N-CA-C	6.50	129.36	113.10
1	R	300	LEU	CB-CA-C	-6.49	97.86	110.20
1	G	290	SER	N-CA-C	-6.49	93.49	111.00
1	G	96	THR	CB-CA-C	-6.46	94.17	111.60
1	R	71	ILE	CB-CA-C	-6.43	98.75	111.60
1	R	118	ILE	N-CA-C	6.43	128.35	111.00
1	G	220	GLU	N-CA-C	-6.41	93.70	111.00
1	R	29	ALA	N-CA-C	-6.41	93.71	111.00
1	R	229	ALA	N-CA-C	6.35	128.15	111.00
1	G	267	LEU	N-CA-C	6.29	127.99	111.00
1	G	61	ASP	CB-CA-C	-6.28	97.84	110.40
1	G	202	ASN	CB-CA-C	-6.28	97.85	110.40
1	R	3	ILE	N-CA-C	6.21	127.78	111.00
1	G	78	LYS	N-CA-C	-6.20	94.27	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	319	GLN	N-CA-C	6.17	127.67	111.00
1	G	175	VAL	N-CA-C	-6.13	94.45	111.00
1	R	77	MET	N-CA-C	-6.12	94.46	111.00
1	R	204	ILE	N-CA-C	6.07	127.37	111.00
1	G	60	GLU	N-CA-C	-6.06	94.63	111.00
1	G	178	VAL	N-CA-C	6.04	127.31	111.00
1	G	50	HIS	N-CA-C	6.01	127.24	111.00
1	G	176	HIS	CB-CA-C	-5.92	98.56	110.40
1	G	192	ASP	N-CA-C	-5.91	95.05	111.00
1	G	286	ASP	CB-CA-C	5.90	122.20	110.40
1	R	58	LYS	N-CA-C	5.89	126.91	111.00
1	G	237	VAL	N-CA-C	5.85	126.78	111.00
1	G	314	GLU	OE1-CD-OE2	5.83	130.29	123.30
1	G	56	GLU	OE1-CD-OE2	5.82	130.29	123.30
1	G	135	GLU	OE1-CD-OE2	5.82	130.28	123.30
1	G	166	GLU	OE1-CD-OE2	5.82	130.28	123.30
1	G	248	LYS	N-CA-C	5.82	126.70	111.00
1	R	94	GLU	OE1-CD-OE2	5.82	130.28	123.30
1	R	56	GLU	OE1-CD-OE2	5.81	130.28	123.30
1	G	60	GLU	OE1-CD-OE2	5.81	130.28	123.30
1	R	169	GLU	OE1-CD-OE2	5.80	130.26	123.30
1	R	71	ILE	N-CA-C	5.79	126.64	111.00
1	R	267	LEU	CB-CA-C	-5.79	99.19	110.20
1	G	222	ASP	N-CA-C	-5.79	95.36	111.00
1	R	60	GLU	OE1-CD-OE2	5.79	130.25	123.30
1	R	103	GLU	OE1-CD-OE2	5.79	130.25	123.30
1	R	38	GLU	OE1-CD-OE2	5.79	130.24	123.30
1	G	264	GLU	OE1-CD-OE2	5.79	130.24	123.30
1	R	135	GLU	OE1-CD-OE2	5.79	130.24	123.30
1	R	275	GLU	OE1-CD-OE2	5.79	130.24	123.30
1	G	249	GLU	OE1-CD-OE2	5.78	130.24	123.30
1	G	103	GLU	OE1-CD-OE2	5.78	130.23	123.30
1	R	166	GLU	OE1-CD-OE2	5.78	130.23	123.30
1	R	264	GLU	OE1-CD-OE2	5.78	130.23	123.30
1	G	38	GLU	OE1-CD-OE2	5.78	130.23	123.30
1	G	275	GLU	OE1-CD-OE2	5.78	130.23	123.30
1	R	90	GLU	OE1-CD-OE2	5.77	130.22	123.30
1	R	80	GLU	OE1-CD-OE2	5.77	130.22	123.30
1	G	90	GLU	OE1-CD-OE2	5.76	130.22	123.30
1	G	76	GLU	OE1-CD-OE2	5.76	130.21	123.30
1	G	94	GLU	OE1-CD-OE2	5.76	130.21	123.30
1	G	297	GLY	N-CA-C	-5.76	98.71	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	76	GLU	OE1-CD-OE2	5.76	130.21	123.30
1	G	80	GLU	OE1-CD-OE2	5.75	130.21	123.30
1	G	169	GLU	OE1-CD-OE2	5.75	130.21	123.30
1	R	249	GLU	OE1-CD-OE2	5.75	130.20	123.30
1	G	220	GLU	OE1-CD-OE2	5.75	130.20	123.30
1	G	163	GLU	OE1-CD-OE2	5.74	130.19	123.30
1	R	314	GLU	OE1-CD-OE2	5.74	130.19	123.30
1	R	163	GLU	OE1-CD-OE2	5.74	130.19	123.30
1	R	220	GLU	OE1-CD-OE2	5.73	130.18	123.30
1	G	204	ILE	CB-CA-C	-5.70	100.19	111.60
1	R	245	ARG	N-CA-C	-5.64	95.76	111.00
1	G	185	VAL	N-CA-C	-5.64	95.77	111.00
1	R	137	TYR	N-CA-C	5.64	126.22	111.00
1	G	274	THR	N-CA-C	-5.63	95.80	111.00
1	G	82	ILE	CB-CA-C	-5.62	100.36	111.60
1	G	35	ILE	N-CA-C	-5.58	95.94	111.00
1	G	8	PHE	CB-CA-C	5.57	121.53	110.40
1	R	236	ASP	CB-CA-C	-5.56	99.28	110.40
1	G	269	GLY	N-CA-C	-5.56	99.20	113.10
1	G	55	GLY	N-CA-C	-5.49	99.38	113.10
1	G	178	VAL	CB-CA-C	-5.41	101.12	111.40
1	R	179	THR	N-CA-C	5.40	125.59	111.00
1	R	58	LYS	CB-CA-C	-5.38	99.63	110.40
1	R	251	SER	N-CA-C	-5.36	96.54	111.00
1	G	267	LEU	CB-CA-C	-5.32	100.10	110.20
1	G	248	LYS	CB-CA-C	-5.32	99.77	110.40
1	R	295	LYS	N-CA-C	5.29	125.28	111.00
1	G	275	GLU	CB-CA-C	5.26	120.93	110.40
1	G	237	VAL	CB-CA-C	-5.26	101.41	111.40
1	R	128	PHE	CB-CA-C	-5.25	99.90	110.40
1	R	82	ILE	CB-CA-C	-5.24	101.12	111.60
1	R	85	SER	N-CA-C	-5.23	96.87	111.00
1	R	301	SER	N-CA-C	-5.23	96.88	111.00
1	G	301	SER	N-CA-C	5.22	125.10	111.00
1	R	84	TRP	N-CA-C	-5.19	96.99	111.00
1	G	278	VAL	N-CA-C	-5.18	97.03	111.00
1	G	135	GLU	CG-CD-OE2	-5.17	107.95	118.30
1	G	166	GLU	CG-CD-OE2	-5.17	107.95	118.30
1	G	264	GLU	CG-CD-OE2	-5.17	107.96	118.30
1	R	56	GLU	CG-CD-OE2	-5.17	107.97	118.30
1	R	103	GLU	CG-CD-OE2	-5.17	107.97	118.30
1	R	135	GLU	CG-CD-OE2	-5.17	107.97	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	264	GLU	CG-CD-OE2	-5.17	107.97	118.30
1	G	103	GLU	CG-CD-OE2	-5.17	107.97	118.30
1	G	76	GLU	CG-CD-OE2	-5.16	107.97	118.30
1	R	94	GLU	CG-CD-OE2	-5.16	107.97	118.30
1	R	169	GLU	CG-CD-OE2	-5.16	107.97	118.30
1	G	314	GLU	CG-CD-OE2	-5.16	107.97	118.30
1	R	60	GLU	CG-CD-OE2	-5.16	107.98	118.30
1	G	163	GLU	CG-CD-OE2	-5.16	107.98	118.30
1	G	38	GLU	CG-CD-OE2	-5.16	107.98	118.30
1	R	38	GLU	CG-CD-OE2	-5.16	107.99	118.30
1	R	166	GLU	CG-CD-OE2	-5.16	107.99	118.30
1	G	249	GLU	CG-CD-OE2	-5.15	108.00	118.30
1	R	249	GLU	CG-CD-OE2	-5.15	107.99	118.30
1	G	56	GLU	CG-CD-OE2	-5.15	108.01	118.30
1	G	169	GLU	CG-CD-OE2	-5.15	108.00	118.30
1	G	220	GLU	CG-CD-OE2	-5.15	108.00	118.30
1	R	80	GLU	CG-CD-OE2	-5.15	108.00	118.30
1	G	60	GLU	CG-CD-OE2	-5.15	108.01	118.30
1	G	312	ASP	N-CA-C	-5.15	97.11	111.00
1	G	90	GLU	CG-CD-OE2	-5.14	108.01	118.30
1	G	114	LYS	N-CA-C	-5.14	97.11	111.00
1	R	275	GLU	CG-CD-OE2	-5.14	108.01	118.30
1	R	273	TYR	CB-CG-CD1	-5.14	117.91	121.00
1	G	275	GLU	CG-CD-OE2	-5.14	108.02	118.30
1	R	90	GLU	CG-CD-OE2	-5.14	108.02	118.30
1	R	220	GLU	CG-CD-OE2	-5.13	108.03	118.30
1	R	76	GLU	CG-CD-OE2	-5.13	108.03	118.30
1	G	94	GLU	CG-CD-OE2	-5.13	108.04	118.30
1	R	314	GLU	CG-CD-OE2	-5.13	108.04	118.30
1	R	163	GLU	CG-CD-OE2	-5.13	108.05	118.30
1	G	80	GLU	CG-CD-OE2	-5.12	108.05	118.30
1	G	317	TYR	CB-CG-CD1	-5.11	117.93	121.00
1	R	42	TYR	CB-CG-CD1	-5.11	117.94	121.00
1	G	3	ILE	CB-CA-C	-5.10	101.39	111.60
1	R	317	TYR	CB-CG-CD1	-5.10	117.94	121.00
1	G	311	TYR	CB-CG-CD1	-5.09	117.94	121.00
1	G	207	SER	N-CA-C	5.09	124.74	111.00
1	G	7	GLY	N-CA-C	5.08	125.81	113.10
1	G	39	TYR	CB-CG-CD1	-5.07	117.96	121.00
1	R	91	TYR	CB-CG-CD1	-5.07	117.96	121.00
1	G	273	TYR	CB-CG-CD1	-5.06	117.97	121.00
1	R	252	TYR	CB-CG-CD1	-5.06	117.97	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	252	TYR	CB-CG-CD1	-5.05	117.97	121.00
1	G	31	ASN	CB-CA-C	-5.05	100.30	110.40
1	G	46	TYR	CB-CG-CD1	-5.05	117.97	121.00
1	G	91	TYR	CB-CG-CD1	-5.05	117.97	121.00
1	R	137	TYR	CB-CG-CD1	-5.05	117.97	121.00
1	G	102	ILE	CB-CA-C	-5.04	101.51	111.60
1	G	137	TYR	CB-CG-CD1	-5.04	117.97	121.00
1	R	8	PHE	N-CA-C	-5.04	97.39	111.00
1	G	42	TYR	CB-CG-CD1	-5.04	117.98	121.00
1	R	80	GLU	N-CA-C	-5.01	97.47	111.00
1	R	39	TYR	CB-CG-CD1	-5.01	118.00	121.00
1	G	54	LYS	N-CA-C	-5.01	97.48	111.00

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	13	ARG	Sidechain
1	G	194	ARG	Sidechain
1	G	231	ARG	Sidechain
1	G	245	ARG	Sidechain
1	G	320	ARG	Sidechain
1	R	13	ARG	Sidechain
1	R	194	ARG	Sidechain
1	R	197	ARG	Sidechain
1	R	231	ARG	Sidechain
1	R	245	ARG	Sidechain
1	R	288	ARG	Sidechain
1	R	320	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	2510	0	2519	1064	7
1	R	2510	0	2522	1004	7
2	G	44	0	26	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R	44	0	26	8	0
3	R	4	0	0	8	0
All	All	5112	0	5093	2047	7

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 201.

All (2047) 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:G:117:VAL:HG21	1:G:328:MET:SD	1.23	1.70
1:R:324:LEU:HD11	1:R:328:MET:SD	1.24	1.66
1:G:173:THR:HG22	1:G:228:MET:SD	1.39	1.60
1:R:137:TYR:CD1	1:R:331:VAL:HG11	1.47	1.47
1:R:5:ILE:CG1	1:R:30:VAL:HG13	1.02	1.47
1:R:154:LEU:C	1:R:156:PRO:HD2	1.25	1.46
1:R:149:CYS:SG	2:R:339:NAD:C4N	2.06	1.43
1:R:5:ILE:CG1	1:R:30:VAL:CG1	1.97	1.41
1:G:117:VAL:CG2	1:G:328:MET:SD	2.08	1.40
1:R:8:PHE:CZ	1:R:44:PHE:HB2	1.56	1.39
1:R:126:PRO:HB3	1:R:141:MET:SD	1.64	1.38
1:G:0:ACE:CH3	1:G:26:GLN:HB2	1.54	1.37
1:G:237:VAL:CG2	1:G:284:ILE:HG13	1.51	1.36
1:G:26:GLN:C	1:G:26:GLN:HE21	1.28	1.36
1:R:324:LEU:CD1	1:R:328:MET:SD	2.14	1.35
1:G:237:VAL:HG21	1:G:284:ILE:CG1	1.54	1.35
1:R:92:ILE:HD11	1:R:113:ALA:CB	1.55	1.34
1:R:5:ILE:CD1	1:R:30:VAL:HG13	1.56	1.34
1:R:170:GLY:O	1:R:225:LEU:HD23	1.25	1.33
1:G:0:ACE:C	1:G:26:GLN:HB2	1.47	1.32
1:R:167:ILE:HG13	1:R:246:LEU:CD2	1.58	1.32
1:R:14:LEU:CD1	1:R:18:ALA:HB2	1.59	1.32
1:G:0:ACE:H1	1:G:26:GLN:CA	1.60	1.32
1:G:3:ILE:CD1	1:G:93:VAL:HG12	1.57	1.31
1:R:26:GLN:O	1:R:27:VAL:CG2	1.77	1.31
1:G:3:ILE:HD11	1:G:93:VAL:CG1	1.59	1.30
1:G:269:GLY:O	1:G:289:SER:HB2	1.28	1.30
1:G:3:ILE:O	1:G:28:VAL:HB	1.24	1.30
1:G:0:ACE:O	1:G:26:GLN:HG2	1.26	1.29
1:G:237:VAL:CG2	1:G:284:ILE:CG1	2.08	1.29
1:G:298:ILE:O	1:G:299:GLN:NE2	1.63	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:84:TRP:NE1	1:R:92:ILE:HG21	1.45	1.28
1:G:267:LEU:O	1:G:270:PHE:CD1	1.87	1.28
1:R:92:ILE:CD1	1:R:113:ALA:HB1	1.63	1.28
1:G:324:LEU:HD11	1:G:328:MET:SD	1.72	1.28
1:G:251:SER:OG	1:G:254:ASP:HB2	1.15	1.28
1:G:126:PRO:HG3	1:G:143:VAL:O	1.20	1.28
1:R:207:SER:O	1:R:208:THR:CG2	1.82	1.27
1:G:218:ILE:CG2	1:G:221:LEU:HD13	1.65	1.27
1:G:32:ASP:OD1	2:G:335:NAD:H1B	1.24	1.27
1:G:0:ACE:H1	1:G:26:GLN:CB	1.63	1.26
1:G:126:PRO:CG	1:G:143:VAL:O	1.83	1.26
1:G:252:TYR:CB	1:G:300:LEU:HD22	1.64	1.26
1:G:42:TYR:OH	1:R:197:ARG:CD	1.84	1.26
1:G:330:LYS:O	1:G:334:ALA:CA	1.84	1.26
1:R:64:LEU:O	1:R:71:ILE:HG23	1.34	1.25
1:G:176:HIS:ND1	1:G:238:SER:OG	1.69	1.25
1:R:45:LYS:HE3	1:R:57:VAL:CG2	1.67	1.25
1:G:312:ASP:O	1:G:312:ASP:OD1	1.54	1.24
1:G:13:ARG:HH22	1:G:43:MET:CE	1.48	1.24
1:G:0:ACE:H1	1:G:26:GLN:N	1.51	1.24
1:G:132:VAL:O	1:G:134:LEU:HD22	1.37	1.23
1:R:31:ASN:O	1:R:32:ASP:OD1	1.55	1.23
1:G:224:LYS:O	1:G:225:LEU:HD23	1.33	1.23
1:R:5:ILE:HG13	1:R:30:VAL:CG1	1.64	1.23
1:G:26:GLN:NE2	1:G:27:VAL:N	1.87	1.22
1:G:10:ARG:HB2	2:G:335:NAD:O1N	1.31	1.22
1:G:137:TYR:CE2	1:G:331:VAL:HG11	1.73	1.22
1:R:17:ARG:HG2	1:R:53:PHE:CE1	1.73	1.22
1:G:319:GLN:HB3	1:G:320:ARG:NH1	1.54	1.22
1:G:330:LYS:O	1:G:334:ALA:HA	1.33	1.22
1:R:94:GLU:OE2	1:R:96:THR:N	1.72	1.22
1:G:0:ACE:CH3	1:G:26:GLN:CB	2.18	1.21
1:G:79:PRO:O	1:G:82:ILE:HG23	1.35	1.21
1:G:96:THR:HG22	1:G:97:GLY:N	1.39	1.21
1:G:173:THR:CG2	1:G:228:MET:SD	2.28	1.21
1:R:240:VAL:HG13	1:R:309:SER:OG	1.39	1.21
1:R:180:ALA:O	1:R:181:THR:OG1	1.58	1.21
1:R:35:ILE:CG2	1:R:40:MET:SD	2.29	1.21
1:G:0:ACE:C	1:G:26:GLN:HG2	1.61	1.21
1:G:33:PRO:CD	1:G:75:ASN:O	1.88	1.20
1:G:286:ASP:O	1:G:287:ASN:HB2	1.41	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:252:TYR:CZ	1:G:298:ILE:HG12	1.76	1.20
1:R:177:ALA:O	1:R:178:VAL:HG23	1.38	1.20
1:G:33:PRO:CG	1:G:76:GLU:O	1.90	1.20
1:R:282:ASP:O	1:R:284:ILE:N	1.74	1.20
1:G:159:LYS:O	1:G:163:GLU:CG	1.90	1.19
1:G:320:ARG:HA	1:G:323:ASP:HB2	1.24	1.19
1:R:177:ALA:HB1	1:R:234:THR:O	1.42	1.19
1:G:324:LEU:C	1:G:324:LEU:HD13	1.58	1.18
1:R:184:THR:O	1:R:185:VAL:HG23	1.02	1.18
1:G:96:THR:CG2	1:G:97:GLY:N	2.05	1.18
1:R:208:THR:OG1	3:R:338:PO4:P	2.02	1.18
1:R:92:ILE:CD1	1:R:113:ALA:CB	2.18	1.18
1:R:286:ASP:O	1:R:287:ASN:HB2	1.44	1.18
1:G:273:TYR:CE2	1:G:275:GLU:HG2	1.78	1.17
1:G:269:GLY:O	1:G:289:SER:CB	1.93	1.17
1:G:252:TYR:HB2	1:G:300:LEU:HD22	1.17	1.17
1:R:184:THR:O	1:R:185:VAL:CG2	1.93	1.17
1:R:76:GLU:CB	1:R:82:ILE:HG22	1.73	1.16
1:G:240:VAL:HG12	1:G:311:TYR:CE1	1.80	1.16
1:G:324:LEU:C	1:G:324:LEU:CD1	2.12	1.16
1:G:26:GLN:CA	1:G:26:GLN:HE21	1.58	1.16
1:R:126:PRO:CB	1:R:141:MET:SD	2.33	1.16
1:G:256:LYS:O	1:G:273:TYR:HE1	1.26	1.16
1:R:37:LEU:CD1	1:R:59:MET:HB2	1.75	1.16
1:R:9:GLY:C	1:R:13:ARG:HE	1.49	1.16
1:G:322:ILE:HG22	1:G:326:LYS:HE2	1.28	1.15
1:G:0:ACE:C	1:G:26:GLN:CB	2.13	1.15
1:R:154:LEU:C	1:R:156:PRO:CD	2.14	1.15
1:R:45:LYS:HE2	1:R:57:VAL:HG22	1.27	1.15
1:R:26:GLN:O	1:R:27:VAL:HG23	0.98	1.15
1:R:45:LYS:CE	1:R:57:VAL:CG2	2.23	1.15
1:R:167:ILE:CG1	1:R:246:LEU:CD2	2.24	1.14
1:G:219:PRO:HA	1:G:222:ASP:HB2	1.24	1.14
1:G:271:LEU:O	1:G:291:ILE:HA	1.43	1.14
1:G:23:GLY:O	1:G:25:ALA:HB2	1.42	1.14
1:R:76:GLU:HB2	1:R:82:ILE:CG2	1.78	1.14
1:G:159:LYS:O	1:G:163:GLU:HG2	1.45	1.14
1:G:299:GLN:HE21	1:G:299:GLN:HA	1.03	1.13
1:G:53:PHE:CE1	1:G:54:LYS:O	2.02	1.13
1:G:33:PRO:CB	1:G:75:ASN:O	1.95	1.13
1:R:146:ASN:OD1	1:R:317:TYR:HE1	1.29	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:319:GLN:CB	1:G:320:ARG:HH12	1.61	1.13
1:G:13:ARG:NH2	1:G:43:MET:HE1	1.63	1.13
1:R:274:THR:O	1:R:275:GLU:HG2	1.48	1.13
1:R:5:ILE:CD1	1:R:30:VAL:CG1	2.24	1.13
1:R:146:ASN:OD1	1:R:317:TYR:CE1	2.01	1.13
1:R:19:ALA:O	1:R:25:ALA:N	1.81	1.13
1:G:213:ALA:O	1:G:217:VAL:HG23	1.48	1.13
1:G:176:HIS:CE1	1:G:238:SER:OG	2.02	1.13
1:R:7:GLY:HA2	1:R:32:ASP:OD1	1.46	1.13
1:G:14:LEU:HD13	1:G:18:ALA:HB2	1.19	1.12
1:G:33:PRO:HG3	1:G:76:GLU:O	0.98	1.12
1:R:101:THR:OG1	1:R:124:ASP:OD2	1.67	1.12
1:R:5:ILE:HD11	1:R:30:VAL:CG1	1.79	1.12
1:R:45:LYS:CB	1:R:57:VAL:HG21	1.78	1.12
1:R:45:LYS:CE	1:R:57:VAL:HG22	1.79	1.12
1:G:322:ILE:CG2	1:G:326:LYS:HE2	1.79	1.12
1:R:286:ASP:OD2	1:R:288:ARG:NH1	1.82	1.12
1:R:327:HIS:O	1:R:331:VAL:HG23	1.49	1.11
1:R:45:LYS:HE3	1:R:57:VAL:HG23	1.29	1.11
1:R:29:ALA:HA	1:R:72:THR:O	1.49	1.11
1:G:17:ARG:NH2	1:G:53:PHE:HB2	1.63	1.11
1:G:252:TYR:OH	1:G:295:LYS:N	1.83	1.11
1:R:218:ILE:CD1	1:R:220:GLU:HB3	1.77	1.11
1:R:320:ARG:N	1:R:320:ARG:HD2	1.60	1.11
1:G:45:LYS:HE3	1:G:57:VAL:HG12	1.27	1.11
1:R:160:VAL:O	1:R:164:ASN:HB2	1.46	1.11
1:G:3:ILE:HG12	1:G:4:GLY:N	1.48	1.10
1:G:324:LEU:O	1:G:324:LEU:HD13	1.48	1.10
1:G:319:GLN:HB3	1:G:320:ARG:HH12	1.03	1.10
1:R:5:ILE:HG12	1:R:30:VAL:HG13	1.17	1.10
1:G:255:ILE:CG2	1:G:256:LYS:N	2.12	1.10
1:R:84:TRP:O	1:R:86:LYS:N	1.84	1.10
1:R:162:HIS:ND1	1:R:166:GLU:O	1.83	1.09
1:R:113:ALA:O	1:R:114:LYS:HG3	1.53	1.09
1:R:218:ILE:O	1:R:218:ILE:HG23	1.40	1.09
1:G:32:ASP:OD1	2:G:335:NAD:C1B	1.99	1.09
1:G:33:PRO:O	1:G:34:PHE:HB2	1.40	1.09
1:G:256:LYS:O	1:G:273:TYR:CE1	2.06	1.09
1:R:104:LYS:O	1:R:107:ALA:HB3	1.50	1.09
1:G:0:ACE:C	1:G:26:GLN:CG	2.21	1.09
1:G:255:ILE:HG22	1:G:256:LYS:N	1.35	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:184:THR:C	1:R:185:VAL:HG23	1.71	1.09
1:G:128:PHE:CZ	1:G:136:LYS:HB3	1.88	1.09
1:G:118:ILE:HG22	1:G:119:SER:H	1.17	1.08
1:R:17:ARG:HG2	1:R:53:PHE:HE1	0.93	1.08
1:G:218:ILE:CG2	1:G:221:LEU:CD1	2.31	1.08
1:G:45:LYS:CD	1:G:57:VAL:HG11	1.83	1.08
1:R:170:GLY:C	1:R:225:LEU:HD23	1.73	1.08
1:R:207:SER:O	1:R:208:THR:HG22	0.91	1.08
1:G:137:TYR:CD2	1:G:331:VAL:HG11	1.89	1.08
1:R:129:VAL:O	1:R:133:ASN:HB3	1.50	1.08
1:G:1:SER:N	1:G:26:GLN:HB2	1.67	1.07
1:G:320:ARG:NH2	1:G:323:ASP:OD1	1.86	1.07
1:R:91:TYR:CE1	1:R:329:GLN:NE2	2.21	1.07
1:G:284:ILE:O	1:G:284:ILE:HG22	1.47	1.07
1:R:26:GLN:HA	1:R:26:GLN:HE21	1.03	1.07
1:R:207:SER:C	1:R:208:THR:HG22	1.72	1.07
1:G:40:MET:SD	1:G:73:VAL:CG1	2.41	1.07
1:R:167:ILE:CG1	1:R:246:LEU:HD23	1.84	1.07
1:G:154:LEU:C	1:G:156:PRO:HD2	1.75	1.07
1:G:17:ARG:HH21	1:G:53:PHE:HB2	0.96	1.07
1:R:320:ARG:H	1:R:320:ARG:HD2	0.98	1.07
1:G:320:ARG:HA	1:G:323:ASP:CB	1.83	1.07
1:R:167:ILE:HG12	1:R:246:LEU:HD23	1.36	1.07
1:R:26:GLN:CA	1:R:26:GLN:HE21	1.67	1.07
1:R:23:GLY:O	1:R:25:ALA:CB	2.02	1.07
1:G:251:SER:OG	1:G:254:ASP:CB	2.03	1.06
1:G:38:GLU:O	1:G:41:VAL:HG13	1.56	1.06
1:R:209:GLY:N	3:R:338:PO4:P	2.28	1.06
1:G:191:LYS:O	1:G:191:LYS:CG	1.98	1.06
1:G:33:PRO:CG	1:G:75:ASN:O	2.03	1.06
1:G:83:PRO:O	1:G:84:TRP:HB2	1.56	1.06
1:G:82:ILE:HD11	1:G:84:TRP:CD2	1.91	1.06
1:R:107:ALA:O	1:R:110:LYS:HB2	1.56	1.06
1:G:218:ILE:HG21	1:G:221:LEU:CD1	1.85	1.06
1:R:5:ILE:HG13	1:R:30:VAL:HG13	1.08	1.06
1:R:35:ILE:HG22	1:R:40:MET:SD	1.95	1.06
1:G:37:LEU:CD2	1:G:38:GLU:H	1.68	1.05
1:G:191:LYS:O	1:G:191:LYS:HG2	1.53	1.05
1:G:14:LEU:HD12	1:G:318:SER:HB3	1.35	1.05
1:R:23:GLY:O	1:R:25:ALA:HB2	1.49	1.05
1:R:14:LEU:HD11	1:R:18:ALA:HB2	1.37	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:195:GLY:O	1:R:197:ARG:N	1.90	1.05
1:G:218:ILE:O	1:G:218:ILE:HG22	1.57	1.05
1:G:239:VAL:HB	1:G:310:TRP:CE3	1.92	1.05
1:G:176:HIS:ND1	1:G:238:SER:CB	2.20	1.04
1:G:150:THR:HA	1:G:311:TYR:CE2	1.92	1.04
1:G:117:VAL:CG2	1:G:328:MET:CE	2.35	1.04
1:R:35:ILE:HD12	1:R:43:MET:HE2	1.35	1.04
1:R:37:LEU:HD12	1:R:59:MET:HB2	1.08	1.04
1:R:161:LEU:HB3	1:R:167:ILE:HD12	1.38	1.04
1:G:176:HIS:CE1	1:G:238:SER:HG	1.75	1.04
1:G:33:PRO:HG3	1:G:76:GLU:C	1.77	1.04
1:G:45:LYS:CE	1:G:57:VAL:CG1	2.35	1.04
1:R:270:PHE:O	1:R:271:LEU:HB2	1.53	1.04
1:G:160:VAL:O	1:G:164:ASN:HB2	1.58	1.04
1:G:13:ARG:HH22	1:G:43:MET:HE1	0.87	1.04
1:G:14:LEU:CD1	1:G:18:ALA:HB2	1.88	1.04
1:G:153:CYS:O	1:G:156:PRO:CG	2.05	1.03
1:G:127:MET:O	1:G:128:PHE:CD1	2.11	1.03
1:G:26:GLN:C	1:G:26:GLN:NE2	2.07	1.03
1:R:167:ILE:HG22	1:R:167:ILE:O	1.53	1.03
1:R:284:ILE:O	1:R:284:ILE:HG22	1.55	1.03
1:R:84:TRP:O	1:R:85:SER:C	1.95	1.03
1:R:35:ILE:HG21	1:R:40:MET:SD	1.97	1.02
1:G:100:THR:O	1:G:101:THR:HB	1.52	1.02
1:G:249:GLU:OE2	1:G:302:LYS:CE	2.07	1.02
1:G:324:LEU:HD12	1:G:325:LEU:N	1.73	1.02
1:R:106:SER:O	1:R:109:PHE:HB2	1.58	1.02
1:R:279:VAL:O	1:R:280:SER:HB2	1.60	1.02
1:G:280:SER:O	1:G:310:TRP:CH2	2.13	1.02
1:G:41:VAL:HG22	1:G:42:TYR:H	1.22	1.02
1:R:107:ALA:HA	1:R:110:LYS:HD3	1.05	1.02
1:G:127:MET:O	1:G:128:PHE:HD1	1.40	1.02
1:G:41:VAL:HG22	1:G:42:TYR:N	1.74	1.02
1:G:53:PHE:CZ	1:G:54:LYS:O	2.11	1.02
1:R:117:VAL:C	1:R:118:ILE:HD13	1.77	1.02
1:R:137:TYR:CD1	1:R:331:VAL:CG1	2.41	1.02
1:R:289:SER:OG	1:R:320:ARG:CZ	2.07	1.02
1:G:331:VAL:HG12	1:G:332:ASP:H	1.23	1.02
1:R:116:VAL:HG12	1:R:118:ILE:HD11	1.40	1.01
1:R:8:PHE:HZ	1:R:44:PHE:CB	1.73	1.01
1:G:237:VAL:HG23	1:G:284:ILE:HG12	1.37	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:42:TYR:OH	1:R:197:ARG:HD2	1.60	1.01
1:G:40:MET:HE1	1:G:73:VAL:HB	1.42	1.01
1:G:40:MET:CE	1:G:73:VAL:HB	1.91	1.01
1:R:209:GLY:CA	3:R:338:PO4:P	2.49	1.01
1:G:113:ALA:O	1:G:114:LYS:HG2	1.60	1.01
1:G:49:THR:OG1	1:G:236:ASP:HB2	1.61	1.01
1:R:232:VAL:HG23	1:R:233:PRO:HD2	1.05	1.01
1:G:33:PRO:HD3	1:G:75:ASN:O	1.61	1.00
1:G:8:PHE:CE2	1:G:44:PHE:HB2	1.96	1.00
1:R:191:LYS:O	1:R:192:ASP:HB2	1.61	1.00
1:R:27:VAL:HG12	1:R:28:VAL:N	1.73	1.00
1:R:42:TYR:HD2	1:R:43:MET:N	1.59	1.00
1:R:167:ILE:HG13	1:R:246:LEU:HD22	1.03	1.00
1:G:273:TYR:HE2	1:G:275:GLU:CG	1.74	1.00
1:G:273:TYR:HE2	1:G:275:GLU:HG2	0.86	1.00
1:G:249:GLU:OE2	1:G:302:LYS:HD2	1.61	1.00
1:R:146:ASN:HB3	1:R:317:TYR:OH	1.58	1.00
1:R:107:ALA:HA	1:R:110:LYS:CD	1.91	1.00
1:R:207:SER:C	1:R:208:THR:CG2	2.24	1.00
1:R:27:VAL:CG1	1:R:28:VAL:H	1.73	1.00
1:R:322:ILE:HG22	1:R:326:LYS:CE	1.91	1.00
1:R:240:VAL:CG1	1:R:309:SER:OG	2.10	1.00
1:R:232:VAL:CG2	1:R:233:PRO:HD2	1.92	1.00
1:G:96:THR:HG22	1:G:97:GLY:H	1.22	1.00
1:R:194:ARG:HH11	1:R:194:ARG:HG3	1.19	1.00
1:R:264:GLU:HG2	1:R:265:GLY:N	1.69	1.00
1:R:27:VAL:HG12	1:R:28:VAL:H	1.23	1.00
1:G:237:VAL:HG23	1:G:284:ILE:CG1	1.91	1.00
1:G:276:ASP:O	1:G:277:ASP:HB2	1.61	0.99
1:R:17:ARG:NH2	1:R:22:CYS:SG	2.34	0.99
1:G:45:LYS:HE3	1:G:57:VAL:CG1	1.92	0.99
1:R:199:ALA:O	1:R:233:PRO:HB3	1.62	0.99
1:G:289:SER:OG	1:G:320:ARG:HD2	1.62	0.99
1:G:238:SER:O	1:G:311:TYR:HB2	1.62	0.99
1:R:176:HIS:CD2	1:R:177:ALA:O	2.13	0.99
1:G:150:THR:HA	1:G:311:TYR:CZ	1.97	0.99
1:G:33:PRO:HB3	1:G:75:ASN:O	1.63	0.99
1:G:218:ILE:HG21	1:G:221:LEU:HD13	1.01	0.99
1:R:185:VAL:O	1:R:186:ASP:OD1	1.81	0.99
1:G:193:TRP:CD1	1:G:195:GLY:HA2	1.98	0.99
1:G:53:PHE:CD1	1:G:54:LYS:O	2.14	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:26:GLN:C	1:R:27:VAL:HG23	1.83	0.99
1:G:118:ILE:HG22	1:G:119:SER:N	1.69	0.99
1:R:11:ILE:CG2	1:R:12:GLY:N	2.26	0.99
1:G:42:TYR:OH	1:R:197:ARG:HD3	1.61	0.99
1:R:79:PRO:O	1:R:80:GLU:C	2.00	0.98
1:G:232:VAL:HB	1:G:233:PRO:HD2	1.42	0.98
1:R:104:LYS:O	1:R:107:ALA:CB	2.11	0.98
1:G:235:PRO:CB	1:R:201:GLN:NE2	2.25	0.98
1:R:155:ALA:N	1:R:156:PRO:HD2	1.78	0.98
1:R:107:ALA:CA	1:R:110:LYS:HD3	1.93	0.98
1:R:9:GLY:O	1:R:13:ARG:NE	1.97	0.98
1:R:232:VAL:HG23	1:R:233:PRO:CD	1.92	0.98
1:R:322:ILE:HG22	1:R:326:LYS:HE3	1.45	0.98
1:R:76:GLU:HB2	1:R:82:ILE:HG22	1.01	0.98
1:G:299:GLN:HE21	1:G:299:GLN:CA	1.75	0.98
1:R:162:HIS:CD2	1:R:221:LEU:HD12	1.99	0.98
1:R:26:GLN:HA	1:R:26:GLN:NE2	1.71	0.98
1:R:8:PHE:CE2	1:R:44:PHE:HB2	1.98	0.98
1:G:150:THR:HA	1:G:311:TYR:OH	1.63	0.98
1:R:109:PHE:HE1	1:R:142:THR:HG21	1.29	0.98
1:R:194:ARG:NH1	1:R:194:ARG:HG3	1.70	0.98
1:G:153:CYS:O	1:G:156:PRO:HG2	1.61	0.97
1:G:0:ACE:H1	1:G:26:GLN:HB2	1.23	0.97
1:G:14:LEU:CD2	1:G:315:PHE:CE2	2.47	0.97
1:G:177:ALA:HB2	1:G:237:VAL:O	1.63	0.97
1:R:18:ALA:HA	1:R:22:CYS:SG	2.04	0.97
1:R:45:LYS:HB3	1:R:57:VAL:HG21	1.43	0.97
1:G:106:SER:HB3	1:G:109:PHE:CE1	1.99	0.97
1:G:162:HIS:O	1:G:166:GLU:N	1.97	0.97
1:R:84:TRP:HB3	1:R:112:GLY:O	1.64	0.97
1:G:215:GLY:O	1:G:219:PRO:N	1.97	0.97
1:G:267:LEU:HA	1:G:270:PHE:CE1	1.99	0.97
1:R:167:ILE:O	1:R:167:ILE:CG2	2.10	0.97
1:R:217:VAL:O	1:R:218:ILE:HG22	1.63	0.97
1:G:249:GLU:OE2	1:G:302:LYS:CD	2.12	0.97
1:R:209:GLY:HA3	3:R:338:PO4:P	2.03	0.97
1:G:1:SER:O	1:G:2:LYS:HB3	1.65	0.97
1:G:0:ACE:CH3	1:G:26:GLN:CA	2.43	0.97
1:G:14:LEU:CD2	1:G:315:PHE:HE2	1.77	0.96
1:R:3:ILE:CG1	1:R:4:GLY:N	2.27	0.96
1:G:255:ILE:HG22	1:G:256:LYS:H	1.24	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:137:TYR:HE2	1:G:331:VAL:CG1	1.79	0.96
1:G:331:VAL:HG12	1:G:332:ASP:N	1.81	0.96
1:G:37:LEU:HD23	1:G:38:GLU:H	1.29	0.96
1:R:211:ALA:CB	1:R:226:THR:HA	1.95	0.96
1:R:255:ILE:HG23	1:R:256:LYS:H	1.25	0.96
1:G:235:PRO:HB3	1:R:201:GLN:NE2	1.79	0.96
1:G:14:LEU:HG	1:G:315:PHE:CE2	1.99	0.96
1:R:109:PHE:CZ	1:R:142:THR:HG23	1.99	0.96
1:R:253:ASP:HA	1:R:256:LYS:HE2	1.46	0.96
1:G:191:LYS:O	1:G:192:ASP:HB3	1.65	0.96
1:G:40:MET:SD	1:G:73:VAL:HB	2.05	0.96
1:R:149:CYS:SG	2:R:339:NAD:H4N	2.02	0.96
1:G:159:LYS:O	1:G:163:GLU:HG3	1.62	0.96
1:G:3:ILE:CG1	1:G:4:GLY:N	2.29	0.96
1:R:177:ALA:C	1:R:178:VAL:HG23	1.81	0.96
1:R:82:ILE:HG13	1:R:82:ILE:O	1.63	0.96
1:G:137:TYR:CE2	1:G:331:VAL:CG1	2.49	0.95
1:G:117:VAL:HG21	1:G:328:MET:CE	1.92	0.95
1:G:319:GLN:HB3	1:G:320:ARG:CZ	1.96	0.95
1:G:37:LEU:CG	1:G:38:GLU:H	1.78	0.95
1:G:23:GLY:O	1:G:25:ALA:CB	2.13	0.95
1:R:127:MET:O	1:R:128:PHE:CD1	2.18	0.95
1:R:45:LYS:HB2	1:R:57:VAL:HG21	1.44	0.95
1:G:13:ARG:NH2	1:G:43:MET:CE	2.20	0.95
1:G:237:VAL:CG2	1:G:284:ILE:HG12	1.88	0.95
1:G:26:GLN:HE21	1:G:27:VAL:N	1.56	0.95
1:R:11:ILE:HG22	1:R:12:GLY:N	1.80	0.95
1:R:129:VAL:HG13	1:R:217:VAL:CG1	1.96	0.95
1:G:50:HIS:NE2	1:G:315:PHE:CD2	2.34	0.95
1:G:292:PHE:C	1:G:292:PHE:CD2	2.39	0.95
1:R:137:TYR:HD1	1:R:331:VAL:CG1	1.79	0.95
1:G:313:ASN:O	1:G:314:GLU:C	2.06	0.95
1:R:255:ILE:HG23	1:R:256:LYS:N	1.80	0.95
1:G:267:LEU:HA	1:G:270:PHE:HE1	1.31	0.94
1:R:126:PRO:CG	1:R:143:VAL:O	2.16	0.94
1:R:14:LEU:CD1	1:R:18:ALA:CB	2.46	0.94
1:G:41:VAL:O	1:G:57:VAL:HG21	1.67	0.94
1:R:295:LYS:O	1:R:296:ALA:C	2.06	0.94
1:G:41:VAL:CG2	1:G:42:TYR:N	2.30	0.94
1:R:17:ARG:CZ	1:R:18:ALA:HA	1.97	0.94
1:R:10:ARG:NH1	1:R:314:GLU:OE1	2.00	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:280:SER:HB3	1:R:282:ASP:OD1	1.66	0.94
1:R:17:ARG:CG	1:R:53:PHE:HE1	1.79	0.94
1:G:10:ARG:HG3	2:G:335:NAD:O2N	1.68	0.94
1:G:270:PHE:O	1:G:271:LEU:HB2	1.67	0.94
1:R:184:THR:C	1:R:185:VAL:CG2	2.33	0.94
1:G:95:SER:O	1:G:96:THR:HB	1.64	0.94
1:G:161:LEU:O	1:G:165:PHE:HB2	1.68	0.94
1:R:37:LEU:HD12	1:R:59:MET:CB	1.98	0.94
1:G:274:THR:OG1	1:G:276:ASP:HB2	1.68	0.93
1:R:157:VAL:HG21	1:R:242:LEU:HD13	1.50	0.93
1:R:219:PRO:O	1:R:220:GLU:C	2.03	0.93
1:R:245:ARG:HA	1:R:303:THR:O	1.67	0.93
1:R:85:SER:O	1:R:88:GLY:N	2.01	0.93
1:G:330:LYS:O	1:G:334:ALA:N	1.99	0.93
1:R:127:MET:HE2	1:R:216:LYS:HD2	1.49	0.93
1:R:154:LEU:HD21	1:R:172:MET:HE3	1.47	0.93
1:R:9:GLY:C	1:R:13:ARG:NE	2.22	0.93
1:G:14:LEU:HD21	1:G:315:PHE:CE2	2.04	0.93
1:G:241:ASP:OD1	1:G:306:LYS:NZ	2.01	0.93
1:R:170:GLY:C	1:R:225:LEU:CD2	2.37	0.93
1:R:170:GLY:O	1:R:225:LEU:CD2	2.17	0.93
1:G:240:VAL:HG12	1:G:311:TYR:HE1	1.26	0.93
1:R:129:VAL:HG13	1:R:217:VAL:HG11	1.50	0.92
1:G:235:PRO:CB	1:R:201:GLN:HE21	1.83	0.92
1:G:178:VAL:HG22	1:G:235:PRO:HA	1.49	0.92
1:R:214:VAL:O	1:R:217:VAL:HG23	1.68	0.92
1:R:45:LYS:HB2	1:R:57:VAL:CG2	1.99	0.92
1:R:84:TRP:HE1	1:R:92:ILE:HG21	1.24	0.92
1:G:298:ILE:O	1:G:298:ILE:HD12	1.67	0.92
1:G:105:ALA:O	1:G:108:HIS:HB2	1.69	0.92
1:G:128:PHE:CE2	1:G:137:TYR:HB2	2.04	0.92
1:G:162:HIS:ND1	1:G:166:GLU:O	2.01	0.92
1:R:176:HIS:NE2	1:R:177:ALA:O	2.03	0.92
1:R:92:ILE:CD1	1:R:113:ALA:HB2	2.00	0.91
1:G:263:SER:CB	1:G:271:LEU:HD12	2.00	0.91
1:G:283:PHE:HA	1:G:286:ASP:HB2	1.49	0.91
1:G:10:ARG:HB2	2:G:335:NAD:PN	2.09	0.91
1:G:268:GLN:HE21	1:G:268:GLN:HA	1.35	0.91
1:G:299:GLN:NE2	1:G:299:GLN:HA	1.85	0.91
1:G:37:LEU:HD23	1:G:38:GLU:N	1.86	0.91
1:R:154:LEU:HD21	1:R:172:MET:CE	1.99	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:132:VAL:HG11	1:G:218:ILE:HG13	1.49	0.91
1:G:328:MET:O	1:G:332:ASP:OD2	1.88	0.91
1:G:58:LYS:O	1:G:65:VAL:HG13	1.70	0.91
1:R:180:ALA:C	1:R:181:THR:OG1	2.00	0.91
1:R:237:VAL:HG22	1:R:284:ILE:CD1	2.00	0.91
1:G:45:LYS:CE	1:G:57:VAL:HG11	1.99	0.91
1:R:237:VAL:HG22	1:R:284:ILE:HD11	1.50	0.91
1:G:128:PHE:O	1:G:129:VAL:HG12	1.70	0.91
1:G:10:ARG:CB	2:G:335:NAD:O1N	2.18	0.91
1:G:102:ILE:HG12	1:G:103:GLU:N	1.86	0.90
1:R:3:ILE:HG12	1:R:4:GLY:N	1.84	0.90
1:R:165:PHE:CB	1:R:246:LEU:HD13	2.02	0.90
1:R:93:VAL:HA	1:R:117:VAL:O	1.70	0.90
1:R:252:TYR:HE1	1:R:294:ALA:HB1	1.35	0.90
1:R:274:THR:O	1:R:275:GLU:CG	2.19	0.90
1:G:249:GLU:CD	1:G:302:LYS:NZ	2.25	0.90
1:R:137:TYR:CE1	1:R:331:VAL:HG11	2.06	0.90
1:R:42:TYR:CD2	1:R:43:MET:N	2.39	0.90
1:R:64:LEU:O	1:R:71:ILE:CG2	2.18	0.90
1:G:45:LYS:HG2	1:G:53:PHE:HB3	1.51	0.90
1:G:218:ILE:O	1:G:218:ILE:CG2	2.20	0.90
1:G:2:LYS:CE	1:G:90:GLU:CG	2.49	0.90
1:R:176:HIS:CD2	1:R:177:ALA:N	2.40	0.90
1:G:129:VAL:CG1	1:G:147:ALA:HB2	2.02	0.90
1:G:3:ILE:HG12	1:G:4:GLY:H	1.33	0.90
1:G:40:MET:CE	1:G:73:VAL:CB	2.50	0.90
1:R:222:ASP:OD2	1:R:222:ASP:O	1.89	0.90
1:G:302:LYS:HG3	1:G:303:THR:N	1.83	0.89
1:R:17:ARG:NE	1:R:18:ALA:N	2.19	0.89
1:R:149:CYS:SG	2:R:339:NAD:C5N	2.61	0.89
1:G:153:CYS:SG	1:G:310:TRP:O	2.30	0.89
1:G:2:LYS:HE3	1:G:90:GLU:CG	2.01	0.89
1:G:41:VAL:HG23	1:G:57:VAL:HG22	1.52	0.89
1:R:218:ILE:O	1:R:218:ILE:CG2	2.20	0.89
1:R:161:LEU:HB3	1:R:167:ILE:CD1	2.03	0.89
1:G:252:TYR:HB3	1:G:300:LEU:HD22	1.52	0.89
1:R:92:ILE:HD11	1:R:113:ALA:HB1	0.90	0.89
1:G:322:ILE:HG22	1:G:326:LYS:CE	2.03	0.88
1:G:6:ASN:HB2	1:G:94:GLU:HG2	1.55	0.88
1:R:124:ASP:O	1:R:125:ALA:HB3	1.72	0.88
1:G:320:ARG:CA	1:G:323:ASP:HB2	2.03	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:45:LYS:HB2	1:G:57:VAL:HG21	1.51	0.88
1:R:292:PHE:CD1	1:R:292:PHE:C	2.46	0.88
1:G:14:LEU:O	1:G:18:ALA:N	2.05	0.88
1:G:216:LYS:NZ	1:G:222:ASP:OD2	2.07	0.88
1:R:126:PRO:HG2	1:R:143:VAL:O	1.74	0.88
1:R:162:HIS:O	1:R:166:GLU:N	2.06	0.88
1:G:77:MET:O	1:G:78:LYS:HB2	1.71	0.88
1:G:119:SER:O	1:G:120:ALA:HB2	1.74	0.88
1:G:162:HIS:O	1:G:166:GLU:CA	2.22	0.88
1:R:109:PHE:CZ	1:R:114:LYS:O	2.27	0.88
1:G:19:ALA:O	1:G:25:ALA:N	2.07	0.88
1:R:137:TYR:HE2	1:R:144:VAL:HG11	1.39	0.88
1:R:232:VAL:HG22	1:R:234:THR:H	1.38	0.88
1:R:14:LEU:HD13	1:R:18:ALA:HB2	1.53	0.87
1:R:84:TRP:NE1	1:R:92:ILE:CG2	2.34	0.87
1:R:118:ILE:HG22	1:R:119:SER:N	1.89	0.87
1:G:14:LEU:CG	1:G:315:PHE:CE2	2.57	0.87
1:G:206:SER:O	1:G:229:ALA:N	2.07	0.87
1:R:8:PHE:CZ	1:R:44:PHE:CB	2.50	0.87
1:G:40:MET:HE1	1:G:73:VAL:CB	2.05	0.87
1:R:195:GLY:O	1:R:197:ARG:HG3	1.73	0.87
1:G:82:ILE:HD11	1:G:84:TRP:CG	2.10	0.87
1:R:219:PRO:O	1:R:222:ASP:N	2.08	0.87
1:G:117:VAL:HG23	1:G:328:MET:HE3	1.57	0.87
1:G:219:PRO:CA	1:G:222:ASP:HB2	2.05	0.87
1:G:292:PHE:CD2	1:G:293:ASP:N	2.42	0.87
1:G:129:VAL:O	1:G:133:ASN:HB3	1.73	0.87
1:R:267:LEU:HD22	1:R:267:LEU:H	1.39	0.87
1:R:5:ILE:HD11	1:R:30:VAL:HG11	1.52	0.87
1:G:251:SER:HG	1:G:254:ASP:HB2	1.39	0.87
1:R:119:SER:O	1:R:120:ALA:CB	2.22	0.87
1:R:180:ALA:C	1:R:181:THR:HG1	1.74	0.87
1:R:137:TYR:HE1	1:R:332:ASP:OD2	1.56	0.87
1:G:124:ASP:O	1:G:125:ALA:CB	2.23	0.86
1:R:289:SER:OG	1:R:320:ARG:NE	2.07	0.86
1:R:154:LEU:O	1:R:156:PRO:HD2	1.74	0.86
1:G:162:HIS:O	1:G:166:GLU:HA	1.74	0.86
1:R:6:ASN:O	1:R:95:SER:HB3	1.76	0.86
1:G:129:VAL:HG11	1:G:147:ALA:HB2	1.57	0.86
1:G:14:LEU:HD12	1:G:318:SER:CB	2.03	0.86
1:R:217:VAL:O	1:R:218:ILE:CG2	2.23	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:185:VAL:O	1:G:186:ASP:OD2	1.92	0.86
1:G:3:ILE:O	1:G:28:VAL:CB	2.18	0.86
1:G:53:PHE:CE2	1:G:54:LYS:O	2.28	0.86
1:R:198:GLY:O	1:R:199:ALA:CB	2.22	0.86
1:R:211:ALA:HB3	1:R:226:THR:HA	1.55	0.86
1:R:279:VAL:HG11	1:R:283:PHE:CE2	2.09	0.86
1:G:189:SER:O	1:G:190:ALA:HB2	1.75	0.86
1:G:267:LEU:O	1:G:270:PHE:CE1	2.29	0.86
1:R:137:TYR:CE2	1:R:144:VAL:HG11	2.10	0.86
1:R:74:PHE:CE1	1:R:83:PRO:HG2	2.10	0.86
1:R:109:PHE:CE1	1:R:142:THR:HG21	2.11	0.86
1:R:322:ILE:CG2	1:R:326:LYS:HE2	2.04	0.86
1:G:32:ASP:CG	2:G:335:NAD:H1B	1.95	0.86
1:R:154:LEU:CA	1:R:156:PRO:HD2	2.03	0.86
1:G:49:THR:OG1	1:G:236:ASP:CB	2.24	0.85
1:R:211:ALA:HB2	1:R:226:THR:CA	2.06	0.85
1:G:101:THR:OG1	1:G:124:ASP:OD2	1.94	0.85
1:R:177:ALA:O	1:R:178:VAL:CG2	2.23	0.85
1:R:94:GLU:C	1:R:94:GLU:CD	2.33	0.85
1:R:189:SER:O	1:R:190:ALA:CB	2.24	0.85
1:R:58:LYS:O	1:R:65:VAL:HG13	1.73	0.85
1:G:142:THR:HG23	1:G:143:VAL:HG13	1.56	0.85
1:G:215:GLY:O	1:G:219:PRO:CA	2.24	0.85
1:G:235:PRO:CG	1:R:201:GLN:HE21	1.88	0.85
1:G:320:ARG:HA	1:G:323:ASP:CG	1.95	0.85
1:R:264:GLU:HG2	1:R:265:GLY:H	1.41	0.85
1:G:289:SER:OG	1:G:320:ARG:CD	2.24	0.85
1:R:59:MET:O	1:R:59:MET:HG3	1.77	0.85
1:R:7:GLY:CA	1:R:32:ASP:OD1	2.25	0.85
1:R:11:ILE:HG22	1:R:12:GLY:H	1.42	0.84
1:R:109:PHE:HZ	1:R:142:THR:HG23	1.40	0.84
1:R:166:GLU:HG2	1:R:167:ILE:H	1.40	0.84
1:R:74:PHE:CD1	1:R:83:PRO:HG2	2.13	0.84
1:R:84:TRP:CE3	1:R:84:TRP:HA	2.12	0.84
1:G:106:SER:HB3	1:G:109:PHE:HE1	1.43	0.84
1:G:147:ALA:HB1	1:G:151:THR:HG22	1.58	0.84
1:G:215:GLY:HA3	1:G:222:ASP:HA	1.57	0.84
1:G:26:GLN:CD	1:G:27:VAL:H	1.81	0.84
1:R:94:GLU:OE1	1:R:96:THR:OG1	1.94	0.84
1:G:26:GLN:HA	1:G:26:GLN:HE21	1.42	0.84
1:G:115:LYS:NZ	1:G:332:ASP:OD1	2.10	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:124:ASP:O	1:R:125:ALA:CB	2.25	0.84
1:G:240:VAL:CG1	1:G:311:TYR:CE1	2.61	0.84
1:R:218:ILE:HD11	1:R:220:GLU:HB3	1.59	0.84
1:G:155:ALA:N	1:G:156:PRO:HD2	1.92	0.84
1:R:100:THR:O	1:R:101:THR:HB	1.77	0.84
1:R:29:ALA:CA	1:R:72:THR:O	2.24	0.84
1:G:292:PHE:CG	1:G:293:ASP:N	2.45	0.84
1:G:284:ILE:O	1:G:284:ILE:CG2	2.25	0.84
1:G:324:LEU:CD1	1:G:328:MET:HB2	2.07	0.84
1:G:45:LYS:CE	1:G:57:VAL:HG12	2.00	0.84
1:R:92:ILE:HD13	1:R:113:ALA:CB	2.08	0.84
1:G:175:VAL:HG22	1:G:230:PHE:HD2	1.40	0.83
1:R:109:PHE:CE2	1:R:114:LYS:O	2.31	0.83
1:R:142:THR:HG22	1:R:143:VAL:HG13	1.60	0.83
1:G:26:GLN:CA	1:G:26:GLN:NE2	2.28	0.83
1:G:40:MET:SD	1:G:73:VAL:HG11	2.18	0.83
1:G:2:LYS:HE3	1:G:90:GLU:CD	1.97	0.83
1:R:283:PHE:HA	1:R:286:ASP:HB2	1.59	0.83
1:G:235:PRO:HG3	1:R:201:GLN:HE21	1.43	0.83
1:R:129:VAL:CG1	1:R:217:VAL:HG11	2.08	0.83
1:G:162:HIS:HA	1:G:167:ILE:HG13	1.60	0.83
1:G:102:ILE:O	1:G:106:SER:OG	1.96	0.83
1:G:10:ARG:NH1	1:R:185:VAL:HG12	1.92	0.83
1:G:236:ASP:O	1:G:237:VAL:HB	1.77	0.83
1:R:14:LEU:O	1:R:15:VAL:C	2.15	0.83
1:G:249:GLU:CD	1:G:302:LYS:HZ3	1.82	0.83
1:G:332:ASP:OD2	1:G:332:ASP:N	2.03	0.83
1:G:91:TYR:CZ	1:G:115:LYS:HG3	2.13	0.83
1:R:10:ARG:NH2	1:R:47:ASP:OD1	2.10	0.83
1:G:252:TYR:CZ	1:G:298:ILE:CG1	2.61	0.83
1:G:45:LYS:CG	1:G:57:VAL:HG11	2.09	0.83
1:R:18:ALA:CA	1:R:22:CYS:SG	2.67	0.83
1:G:134:LEU:HD13	1:G:134:LEU:H	1.43	0.83
1:G:156:PRO:HG3	1:G:290:SER:CB	2.09	0.83
1:G:324:LEU:CD1	1:G:328:MET:SD	2.63	0.83
1:R:324:LEU:HD21	1:R:328:MET:SD	2.19	0.83
1:R:55:GLY:O	1:R:56:GLU:HB3	1.79	0.83
1:R:149:CYS:SG	2:R:339:NAD:C3N	2.66	0.83
1:R:17:ARG:HE	1:R:18:ALA:N	1.76	0.83
1:R:188:PRO:O	1:R:189:SER:HB2	1.79	0.83
1:G:124:ASP:O	1:G:125:ALA:HB3	1.77	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:127:MET:CE	1:R:216:LYS:HD2	2.09	0.82
1:G:18:ALA:O	1:G:22:CYS:HB2	1.80	0.82
1:G:324:LEU:CD1	1:G:325:LEU:N	2.35	0.82
1:G:40:MET:SD	1:G:73:VAL:CB	2.68	0.82
1:R:100:THR:O	1:R:101:THR:CB	2.26	0.82
1:G:17:ARG:HH21	1:G:53:PHE:CB	1.88	0.82
1:R:137:TYR:CE1	1:R:331:VAL:CG1	2.63	0.82
1:G:0:ACE:CH3	1:G:26:GLN:N	2.39	0.82
1:R:109:PHE:HD2	1:R:113:ALA:HB3	1.45	0.82
1:R:274:THR:C	1:R:275:GLU:HG2	2.00	0.82
1:G:109:PHE:HA	1:G:113:ALA:HB3	1.62	0.82
1:G:302:LYS:CG	1:G:303:THR:N	2.39	0.82
1:G:198:GLY:O	1:G:199:ALA:CB	2.28	0.81
1:R:27:VAL:CG1	1:R:28:VAL:N	2.35	0.81
1:G:128:PHE:O	1:G:129:VAL:CG1	2.28	0.81
1:G:132:VAL:HG21	1:G:217:VAL:O	1.80	0.81
1:R:238:SER:HB3	1:R:311:TYR:CE2	2.15	0.81
1:R:137:TYR:CE1	1:R:332:ASP:OD2	2.33	0.81
1:G:40:MET:SD	1:G:73:VAL:HG12	2.20	0.81
1:R:109:PHE:CE2	1:R:114:LYS:C	2.54	0.81
1:G:289:SER:HB2	1:G:320:ARG:HE	1.43	0.81
1:G:40:MET:HE1	1:G:73:VAL:CG2	2.11	0.81
1:G:147:ALA:HB1	1:G:151:THR:CG2	2.11	0.81
1:G:26:GLN:HA	1:G:26:GLN:NE2	1.93	0.81
1:R:109:PHE:CE1	1:R:142:THR:CG2	2.62	0.81
1:R:177:ALA:C	1:R:178:VAL:CG2	2.48	0.81
1:G:14:LEU:HD13	1:G:18:ALA:CB	2.06	0.81
1:G:263:SER:HB2	1:G:271:LEU:HD12	1.60	0.81
1:R:26:GLN:O	1:R:27:VAL:CB	2.29	0.81
1:R:324:LEU:HD21	1:R:328:MET:HG3	1.63	0.81
1:G:26:GLN:NE2	1:G:27:VAL:H	1.79	0.80
1:G:221:LEU:O	1:G:222:ASP:CB	2.29	0.80
1:R:211:ALA:HB2	1:R:226:THR:N	1.96	0.80
1:G:0:ACE:O	1:G:26:GLN:CG	2.20	0.80
1:G:228:MET:HG2	1:G:229:ALA:N	1.95	0.80
1:G:268:GLN:HE21	1:G:268:GLN:CA	1.93	0.80
1:G:298:ILE:O	1:G:299:GLN:CD	2.19	0.80
1:G:37:LEU:CG	1:G:38:GLU:N	2.44	0.80
1:R:100:THR:O	1:R:101:THR:HG22	1.80	0.80
1:G:117:VAL:CG2	1:G:328:MET:HE3	2.09	0.80
1:R:137:TYR:CE2	1:R:328:MET:HG2	2.17	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:155:ALA:N	1:R:156:PRO:CD	2.40	0.80
1:R:286:ASP:O	1:R:287:ASN:CB	2.28	0.80
1:R:126:PRO:HG2	1:R:144:VAL:HA	1.64	0.80
1:G:126:PRO:HG2	1:G:143:VAL:O	1.81	0.79
1:G:266:PRO:O	1:G:268:GLN:HG2	1.81	0.79
1:R:280:SER:CB	1:R:282:ASP:OD1	2.29	0.79
1:G:41:VAL:C	1:G:57:VAL:CG2	2.51	0.79
1:G:263:SER:HA	1:G:271:LEU:CD1	2.12	0.79
1:R:126:PRO:HG3	1:R:143:VAL:O	1.83	0.79
1:R:211:ALA:CB	1:R:226:THR:CA	2.59	0.79
1:G:331:VAL:CG1	1:G:332:ASP:N	2.43	0.79
1:R:10:ARG:HH11	1:R:314:GLU:CD	1.85	0.79
1:R:169:GLU:OE1	1:R:245:ARG:NH1	2.15	0.79
1:G:256:LYS:HD2	1:G:294:ALA:HB1	1.63	0.79
1:G:41:VAL:O	1:G:57:VAL:CG2	2.31	0.79
1:R:154:LEU:O	1:R:156:PRO:CD	2.29	0.79
1:R:126:PRO:CG	1:R:141:MET:SD	2.71	0.79
1:G:14:LEU:HD22	1:G:17:ARG:HB3	1.63	0.79
1:R:252:TYR:O	1:R:255:ILE:CG2	2.31	0.79
1:R:252:TYR:CE1	1:R:294:ALA:HB1	2.18	0.79
1:R:45:LYS:CE	1:R:57:VAL:HG23	2.04	0.79
1:G:10:ARG:NH1	1:R:185:VAL:CG1	2.46	0.79
1:G:282:ASP:O	1:G:283:PHE:C	2.21	0.79
1:R:0:ACE:H1	1:R:26:GLN:HG2	1.64	0.79
1:R:167:ILE:HA	1:R:246:LEU:HB3	1.63	0.79
1:R:291:ILE:O	1:R:310:TRP:HB2	1.82	0.79
1:G:2:LYS:HE2	1:G:90:GLU:CG	2.13	0.79
1:G:8:PHE:HE2	1:G:44:PHE:HB2	1.44	0.79
1:R:100:THR:O	1:R:101:THR:CG2	2.31	0.79
1:G:50:HIS:HE2	1:G:315:PHE:HD2	1.28	0.78
1:G:331:VAL:HG12	1:G:332:ASP:OD2	1.82	0.78
1:R:169:GLU:CD	1:R:245:ARG:NH1	2.36	0.78
1:G:116:VAL:HB	1:G:143:VAL:HG12	1.65	0.78
1:R:152:ASN:O	1:R:156:PRO:HD3	1.83	0.78
1:R:270:PHE:O	1:R:271:LEU:CB	2.29	0.78
1:G:2:LYS:HE2	1:G:90:GLU:HG2	1.65	0.78
1:R:16:LEU:C	1:R:16:LEU:HD13	2.04	0.78
1:G:119:SER:HA	1:G:317:TYR:OH	1.83	0.78
1:R:1:SER:O	1:R:2:LYS:HB2	1.81	0.78
1:G:322:ILE:O	1:G:326:LYS:HG2	1.83	0.78
1:R:259:MET:O	1:R:263:SER:HB3	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:118:ILE:CG2	1:G:119:SER:N	2.47	0.78
1:R:129:VAL:O	1:R:133:ASN:CB	2.32	0.78
1:G:137:TYR:HE2	1:G:331:VAL:HG11	1.32	0.78
1:R:125:ALA:HB1	1:R:126:PRO:HD2	1.66	0.78
1:R:322:ILE:HG22	1:R:326:LYS:HE2	1.65	0.78
1:G:53:PHE:CG	1:G:54:LYS:N	2.50	0.78
1:R:168:VAL:O	1:R:169:GLU:HB2	1.82	0.78
1:G:319:GLN:HB3	1:G:320:ARG:NH2	1.97	0.77
1:G:3:ILE:HG13	1:G:91:TYR:O	1.84	0.77
1:R:41:VAL:O	1:R:45:LYS:HB3	1.84	0.77
1:G:168:VAL:HG12	1:G:245:ARG:HH12	1.49	0.77
1:G:252:TYR:CE1	1:G:298:ILE:HG12	2.19	0.77
1:G:260:LYS:HG2	1:G:261:THR:N	1.97	0.77
1:R:113:ALA:O	1:R:114:LYS:CG	2.31	0.77
1:R:165:PHE:HB2	1:R:246:LEU:HD13	1.65	0.77
1:G:197:ARG:HG2	1:G:197:ARG:HH11	1.50	0.77
1:G:6:ASN:O	1:G:95:SER:OG	2.02	0.77
1:R:92:ILE:HD13	1:R:113:ALA:HB2	1.66	0.77
1:R:37:LEU:HD22	1:R:73:VAL:HG21	1.66	0.77
1:R:154:LEU:CD2	1:R:172:MET:CE	2.62	0.77
1:R:284:ILE:O	1:R:284:ILE:CG2	2.31	0.77
1:G:76:GLU:HG3	1:G:82:ILE:HA	1.66	0.77
1:R:320:ARG:CD	1:R:320:ARG:N	2.44	0.77
1:R:45:LYS:CB	1:R:57:VAL:CG2	2.56	0.77
1:G:252:TYR:OH	1:G:298:ILE:HG12	1.84	0.77
1:G:295:LYS:O	1:G:298:ILE:HG23	1.84	0.77
1:G:91:TYR:OH	1:G:332:ASP:CG	2.23	0.77
1:G:96:THR:HG21	1:G:99:PHE:HB2	1.66	0.77
1:G:239:VAL:HG23	1:G:309:SER:O	1.82	0.77
1:R:8:PHE:HZ	1:R:44:PHE:HB2	0.96	0.77
1:R:79:PRO:O	1:R:82:ILE:N	2.18	0.77
1:G:117:VAL:HA	1:G:144:VAL:O	1.86	0.76
1:G:214:VAL:HG11	1:G:225:LEU:HD12	1.66	0.76
1:G:84:TRP:CE3	1:G:84:TRP:HA	2.21	0.76
1:G:84:TRP:NE1	1:G:108:HIS:NE2	2.33	0.76
1:R:109:PHE:HE2	1:R:114:LYS:C	1.87	0.76
1:G:270:PHE:O	1:G:271:LEU:CB	2.31	0.76
1:G:86:LYS:O	1:G:87:ALA:HB3	1.86	0.76
1:R:161:LEU:HD22	1:R:244:VAL:HG21	1.66	0.76
1:R:166:GLU:O	1:R:167:ILE:HB	1.85	0.76
1:R:189:SER:O	1:R:190:ALA:HB3	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:119:SER:O	1:G:120:ALA:CB	2.33	0.76
1:G:195:GLY:O	1:G:197:ARG:N	2.18	0.76
1:R:272:GLY:O	1:R:273:TYR:CB	2.33	0.76
1:G:218:ILE:HG23	1:G:221:LEU:HD12	1.67	0.76
1:G:26:GLN:CD	1:G:27:VAL:N	2.38	0.76
1:G:146:ASN:HB3	1:G:317:TYR:OH	1.85	0.76
1:R:11:ILE:HD13	1:R:15:VAL:HG23	1.67	0.76
1:R:260:LYS:HG2	1:R:261:THR:N	1.99	0.76
1:R:322:ILE:CG2	1:R:326:LYS:CE	2.63	0.76
1:G:3:ILE:CG1	1:G:4:GLY:H	1.94	0.76
1:G:267:LEU:C	1:G:270:PHE:CD1	2.59	0.76
1:R:176:HIS:CD2	1:R:177:ALA:H	2.02	0.76
1:G:154:LEU:HD21	1:G:240:VAL:HG21	1.68	0.76
1:G:6:ASN:OD1	1:G:94:GLU:OE2	2.04	0.76
1:G:134:LEU:N	1:G:134:LEU:HD13	2.01	0.75
1:G:191:LYS:HG3	1:G:191:LYS:O	1.86	0.75
1:R:166:GLU:HG2	1:R:167:ILE:N	2.01	0.75
1:R:17:ARG:NH1	1:R:21:SER:OG	2.18	0.75
1:R:84:TRP:HE3	1:R:84:TRP:HA	1.48	0.75
1:G:76:GLU:HG3	1:G:82:ILE:CA	2.15	0.75
1:R:126:PRO:HG3	1:R:141:MET:SD	2.26	0.75
1:G:188:PRO:O	1:G:189:SER:HB3	1.87	0.75
1:G:286:ASP:O	1:G:287:ASN:CB	2.29	0.75
1:G:295:LYS:O	1:G:298:ILE:N	2.18	0.75
1:G:218:ILE:HG23	1:G:221:LEU:CD1	2.16	0.75
1:R:5:ILE:HG13	1:R:30:VAL:HG12	1.64	0.75
1:G:167:ILE:O	1:G:167:ILE:HG22	1.82	0.75
1:G:189:SER:O	1:G:190:ALA:CB	2.34	0.75
1:G:37:LEU:HG	1:G:38:GLU:H	1.49	0.75
1:R:252:TYR:O	1:R:255:ILE:HG22	1.87	0.75
1:G:125:ALA:HB1	1:G:126:PRO:HD2	1.68	0.75
1:G:42:TYR:HD1	1:G:43:MET:N	1.84	0.75
1:G:94:GLU:O	1:G:118:ILE:CG2	2.35	0.75
1:R:256:LYS:HD3	1:R:294:ALA:HB1	1.68	0.75
1:G:119:SER:HB2	1:G:317:TYR:HE2	1.52	0.75
1:G:176:HIS:CE1	1:G:238:SER:CB	2.67	0.75
1:R:272:GLY:O	1:R:273:TYR:HB3	1.85	0.75
1:G:1:SER:N	1:G:26:GLN:CB	2.42	0.75
1:R:170:GLY:HA2	1:R:244:VAL:CG1	2.17	0.75
1:R:157:VAL:HG13	1:R:161:LEU:HD12	1.69	0.75
1:G:305:VAL:HG22	1:G:306:LYS:N	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:45:LYS:NZ	1:G:57:VAL:CG1	2.50	0.74
1:G:40:MET:CE	1:G:73:VAL:CG2	2.65	0.74
1:G:53:PHE:O	1:G:54:LYS:CB	2.35	0.74
1:G:45:LYS:HD2	1:G:57:VAL:HG11	1.67	0.74
1:G:228:MET:N	1:G:228:MET:HE3	2.02	0.74
1:G:182:GLN:OE1	1:G:231:ARG:HB3	1.86	0.74
1:G:127:MET:C	1:G:128:PHE:HD1	1.91	0.74
1:G:132:VAL:HG11	1:G:218:ILE:CG1	2.17	0.74
1:R:217:VAL:O	1:R:218:ILE:CB	2.36	0.74
1:G:267:LEU:HG	1:G:271:LEU:HD21	1.68	0.74
1:G:26:GLN:CG	1:G:27:VAL:H	1.97	0.74
1:R:1:SER:HB2	1:R:329:GLN:HG3	1.69	0.74
1:R:283:PHE:N	1:R:283:PHE:CD2	2.55	0.74
1:R:327:HIS:ND1	1:R:331:VAL:HG21	2.02	0.74
1:G:10:ARG:CG	2:G:335:NAD:O2N	2.36	0.74
1:G:10:ARG:HH11	1:R:185:VAL:CG1	2.01	0.74
1:G:183:LYS:O	1:G:198:GLY:O	2.06	0.74
1:R:324:LEU:HD21	1:R:328:MET:CG	2.18	0.74
1:G:37:LEU:HG	1:G:38:GLU:N	2.03	0.74
1:R:130:CYS:O	1:R:133:ASN:OD1	2.06	0.74
1:R:299:GLN:O	1:R:305:VAL:HG23	1.88	0.74
1:G:11:ILE:O	1:G:15:VAL:HG23	1.87	0.73
1:G:53:PHE:CG	1:G:54:LYS:O	2.41	0.73
1:R:142:THR:CG2	1:R:143:VAL:HG13	2.17	0.73
1:R:99:PHE:HE1	2:R:339:NAD:N1A	1.86	0.73
1:G:252:TYR:OH	1:G:295:LYS:CA	2.36	0.73
1:R:188:PRO:O	1:R:189:SER:CB	2.37	0.73
1:R:41:VAL:HG12	1:R:64:LEU:CD1	2.18	0.73
1:R:301:SER:O	1:R:304:PHE:O	2.05	0.73
1:G:269:GLY:O	1:G:289:SER:HB3	1.86	0.73
1:G:2:LYS:CE	1:G:90:GLU:HG3	2.17	0.73
1:R:166:GLU:CG	1:R:167:ILE:N	2.51	0.73
1:R:247:GLY:O	1:R:248:LYS:HB2	1.87	0.73
1:R:28:VAL:HG23	1:R:29:ALA:O	1.81	0.73
1:R:50:HIS:CE1	1:R:314:GLU:HB2	2.24	0.73
1:R:6:ASN:HB3	1:R:94:GLU:OE1	1.88	0.73
1:G:240:VAL:CG1	1:G:311:TYR:HE1	2.01	0.73
1:G:5:ILE:HG22	1:G:6:ASN:N	2.04	0.73
1:G:106:SER:HA	1:G:109:PHE:CE1	2.24	0.73
1:R:12:GLY:HA2	1:R:15:VAL:HB	1.71	0.73
1:R:279:VAL:HG11	1:R:283:PHE:CZ	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:172:MET:O	1:G:228:MET:CE	2.37	0.73
1:R:243:THR:HG22	1:R:304:PHE:CZ	2.23	0.73
1:G:198:GLY:O	1:G:199:ALA:HB2	1.89	0.73
1:R:218:ILE:HD13	1:R:220:GLU:HB3	1.71	0.73
1:R:324:LEU:HD13	1:R:324:LEU:C	2.08	0.73
1:G:14:LEU:HG	1:G:315:PHE:CD2	2.24	0.73
1:G:49:THR:HG1	1:G:236:ASP:CB	2.01	0.73
1:G:86:LYS:O	1:G:87:ALA:CB	2.36	0.73
1:R:327:HIS:CE1	1:R:331:VAL:HG21	2.23	0.73
1:G:6:ASN:CB	1:G:94:GLU:HG2	2.19	0.72
1:G:249:GLU:OE2	1:G:302:LYS:NZ	2.22	0.72
1:G:259:MET:O	1:G:263:SER:N	2.18	0.72
1:G:42:TYR:HH	1:R:197:ARG:HD3	1.54	0.72
1:G:154:LEU:C	1:G:156:PRO:CD	2.57	0.72
1:G:1:SER:O	1:G:2:LYS:CB	2.37	0.72
1:G:252:TYR:HB2	1:G:300:LEU:CD2	2.10	0.72
1:G:239:VAL:HB	1:G:310:TRP:CZ3	2.23	0.72
1:R:252:TYR:CD2	1:R:298:ILE:HG13	2.24	0.72
1:G:197:ARG:HD3	1:R:42:TYR:OH	1.88	0.72
1:G:40:MET:HE3	1:G:73:VAL:HG21	1.69	0.72
1:G:41:VAL:CG2	1:G:57:VAL:HG22	2.19	0.72
1:R:109:PHE:CZ	1:R:142:THR:CG2	2.72	0.72
1:G:128:PHE:HZ	1:G:136:LYS:HB3	1.50	0.72
1:G:215:GLY:O	1:G:218:ILE:C	2.27	0.72
1:G:264:GLU:HG2	1:G:265:GLY:N	2.05	0.72
1:G:91:TYR:OH	1:G:332:ASP:OD1	2.06	0.72
1:R:45:LYS:HE2	1:R:57:VAL:CG2	2.02	0.72
1:G:132:VAL:CG2	1:G:217:VAL:HG12	2.20	0.72
1:G:324:LEU:HD13	1:G:328:MET:HB2	1.71	0.72
1:R:238:SER:CB	1:R:311:TYR:CE2	2.72	0.72
1:R:91:TYR:HE1	1:R:329:GLN:NE2	1.88	0.72
1:G:165:PHE:O	1:G:166:GLU:HB2	1.90	0.72
1:G:33:PRO:N	1:G:75:ASN:O	2.21	0.72
1:R:26:GLN:CA	1:R:26:GLN:NE2	2.41	0.72
1:R:325:LEU:O	1:R:329:GLN:HB2	1.88	0.72
1:G:8:PHE:CD1	1:G:30:VAL:HG11	2.25	0.71
1:G:150:THR:CA	1:G:311:TYR:CE2	2.72	0.71
1:G:77:MET:O	1:G:78:LYS:CB	2.38	0.71
1:R:162:HIS:CG	1:R:221:LEU:HD12	2.26	0.71
1:G:184:THR:C	1:G:185:VAL:HG23	2.10	0.71
1:G:289:SER:CB	1:G:320:ARG:HE	2.02	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:37:LEU:CD2	1:G:38:GLU:N	2.47	0.71
1:G:79:PRO:C	1:G:82:ILE:HG23	2.09	0.71
1:G:238:SER:O	1:G:311:TYR:CB	2.37	0.71
1:G:40:MET:CE	1:G:73:VAL:HG21	2.20	0.71
1:R:137:TYR:HE2	1:R:144:VAL:CG1	2.02	0.71
1:R:198:GLY:O	1:R:199:ALA:HB2	1.90	0.71
1:R:35:ILE:HG21	1:R:40:MET:CE	2.21	0.71
1:G:128:PHE:CE2	1:G:136:LYS:HB3	2.25	0.71
1:G:246:LEU:HD11	1:G:250:CYS:HB3	1.72	0.71
1:G:92:ILE:CG1	1:G:116:VAL:HG22	2.20	0.71
1:R:50:HIS:HD2	1:R:315:PHE:HD2	1.36	0.71
1:G:159:LYS:HA	1:G:163:GLU:OE2	1.90	0.71
1:G:41:VAL:HG12	1:G:64:LEU:HD11	1.73	0.71
1:R:295:LYS:O	1:R:297:GLY:N	2.22	0.71
1:R:71:ILE:HG13	1:R:71:ILE:O	1.81	0.71
1:R:129:VAL:HB	1:R:152:ASN:OD1	1.89	0.71
1:R:12:GLY:O	1:R:13:ARG:C	2.29	0.71
1:G:154:LEU:O	1:G:157:VAL:HG12	1.91	0.71
1:G:313:ASN:ND2	1:G:313:ASN:H	1.89	0.71
1:R:157:VAL:CG1	1:R:158:ALA:N	2.53	0.71
1:G:118:ILE:CG2	1:G:119:SER:H	2.02	0.71
1:G:322:ILE:HG23	1:G:326:LYS:HE2	1.72	0.71
1:G:186:ASP:OD1	1:G:197:ARG:HG2	1.91	0.70
1:R:279:VAL:CG1	1:R:283:PHE:CE2	2.73	0.70
1:G:215:GLY:O	1:G:219:PRO:HA	1.90	0.70
1:G:12:GLY:O	1:G:15:VAL:N	2.23	0.70
1:R:213:ALA:O	1:R:215:GLY:N	2.24	0.70
1:G:186:ASP:OD1	1:G:197:ARG:NH1	2.24	0.70
1:R:165:PHE:CG	1:R:246:LEU:HD13	2.27	0.70
1:G:53:PHE:O	1:G:54:LYS:HG3	1.91	0.70
1:R:267:LEU:H	1:R:267:LEU:CD2	2.04	0.70
1:R:129:VAL:HG13	1:R:217:VAL:HG13	1.73	0.70
1:R:245:ARG:HG2	1:R:245:ARG:NH1	2.05	0.70
1:R:195:GLY:O	1:R:196:GLY:C	2.29	0.70
1:R:324:LEU:CD2	1:R:328:MET:SD	2.80	0.70
1:G:14:LEU:HD21	1:G:315:PHE:HE2	1.48	0.69
1:R:298:ILE:O	1:R:298:ILE:HD13	1.92	0.69
1:G:249:GLU:OE2	1:G:302:LYS:HE2	1.93	0.69
1:G:53:PHE:CD2	1:G:54:LYS:O	2.45	0.69
1:G:267:LEU:CA	1:G:270:PHE:CE1	2.75	0.69
1:R:137:TYR:HD1	1:R:137:TYR:O	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:305:VAL:HG22	1:R:306:LYS:N	2.08	0.69
1:R:41:VAL:HB	1:R:57:VAL:HB	1.74	0.69
1:R:94:GLU:CD	1:R:96:THR:OG1	2.29	0.69
1:G:58:LYS:HG3	1:G:59:MET:N	2.06	0.69
1:R:168:VAL:O	1:R:169:GLU:CB	2.39	0.69
1:G:79:PRO:O	1:G:80:GLU:C	2.31	0.69
1:R:267:LEU:O	1:R:270:PHE:CD1	2.46	0.69
1:G:10:ARG:HH12	1:R:185:VAL:HG12	1.53	0.69
1:R:84:TRP:CD1	1:R:92:ILE:HG21	2.27	0.69
1:G:330:LYS:C	1:G:334:ALA:HA	2.13	0.69
1:R:146:ASN:CB	1:R:317:TYR:OH	2.37	0.69
1:G:322:ILE:CG2	1:G:326:LYS:CE	2.64	0.69
1:G:59:MET:CB	1:G:64:LEU:HD13	2.23	0.69
1:G:14:LEU:HB3	1:G:318:SER:OG	1.93	0.69
1:G:206:SER:N	1:G:229:ALA:O	2.25	0.69
1:G:280:SER:O	1:G:310:TRP:HH2	1.71	0.69
1:G:270:PHE:HA	1:G:289:SER:HB3	1.75	0.69
1:G:129:VAL:HG12	1:G:147:ALA:H	1.58	0.68
1:G:184:THR:O	1:G:185:VAL:HG23	1.93	0.68
1:G:151:THR:CG2	1:G:213:ALA:HB1	2.23	0.68
1:G:53:PHE:O	1:G:54:LYS:CG	2.41	0.68
1:R:324:LEU:CG	1:R:328:MET:SD	2.81	0.68
1:G:14:LEU:O	1:G:15:VAL:C	2.29	0.68
1:R:178:VAL:HG12	1:R:179:THR:H	1.57	0.68
1:R:178:VAL:HG21	1:R:313:ASN:OD1	1.94	0.68
1:R:11:ILE:HG23	1:R:12:GLY:N	2.07	0.68
1:R:252:TYR:C	1:R:252:TYR:CD1	2.67	0.68
1:G:130:CYS:SG	1:G:320:ARG:HB3	2.33	0.68
1:G:289:SER:OG	1:G:320:ARG:NE	2.25	0.68
1:R:170:GLY:HA2	1:R:244:VAL:HG13	1.76	0.68
1:R:93:VAL:HG22	1:R:117:VAL:HG12	1.75	0.68
1:G:106:SER:CB	1:G:109:PHE:CE1	2.74	0.68
1:G:149:CYS:O	1:G:311:TYR:HE2	1.77	0.68
1:R:127:MET:HE2	1:R:216:LYS:CD	2.22	0.68
1:R:252:TYR:O	1:R:256:LYS:HG2	1.92	0.68
1:R:319:GLN:HB3	1:R:320:ARG:CZ	2.22	0.68
1:R:50:HIS:CE1	1:R:236:ASP:OD2	2.47	0.68
1:G:53:PHE:O	1:G:54:LYS:HB2	1.93	0.68
1:R:127:MET:HB2	1:R:216:LYS:HD3	1.75	0.68
1:G:129:VAL:HG12	1:G:147:ALA:HB2	1.76	0.68
1:G:324:LEU:HD11	1:G:328:MET:HB2	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:33:PRO:O	1:G:34:PHE:CB	2.29	0.68
1:R:65:VAL:O	1:R:65:VAL:HG22	1.93	0.68
1:R:76:GLU:HG3	1:R:82:ILE:HA	1.76	0.68
1:G:282:ASP:O	1:G:284:ILE:HB	1.94	0.68
1:R:328:MET:O	1:R:329:GLN:C	2.32	0.68
1:R:279:VAL:O	1:R:280:SER:CB	2.39	0.68
1:R:7:GLY:HA2	1:R:32:ASP:CG	2.13	0.68
1:G:10:ARG:HH11	1:R:185:VAL:HG11	1.59	0.68
1:G:298:ILE:HD12	1:G:298:ILE:C	2.13	0.68
1:R:259:MET:O	1:R:263:SER:N	2.26	0.68
1:G:252:TYR:CB	1:G:300:LEU:CD2	2.59	0.67
1:G:45:LYS:HB2	1:G:57:VAL:CG2	2.22	0.67
1:G:45:LYS:HG3	1:G:57:VAL:CG1	2.24	0.67
1:G:49:THR:CG2	1:G:50:HIS:N	2.56	0.67
1:R:278:VAL:HG12	1:R:278:VAL:O	1.94	0.67
1:G:39:TYR:CD1	1:G:43:MET:HG3	2.29	0.67
1:G:33:PRO:CA	1:G:75:ASN:O	2.40	0.67
1:G:79:PRO:O	1:G:82:ILE:N	2.27	0.67
1:R:10:ARG:HA	1:R:13:ARG:NE	2.09	0.67
1:R:118:ILE:N	1:R:118:ILE:HD13	2.07	0.67
1:G:132:VAL:CG2	1:G:217:VAL:O	2.42	0.67
1:G:30:VAL:N	1:G:72:THR:O	2.26	0.67
1:G:117:VAL:CG2	1:G:144:VAL:HG13	2.24	0.67
1:G:189:SER:OG	1:G:190:ALA:N	2.21	0.67
1:G:267:LEU:CA	1:G:270:PHE:CD1	2.78	0.67
1:G:83:PRO:O	1:G:84:TRP:CB	2.38	0.67
1:G:194:ARG:O	1:G:196:GLY:N	2.26	0.67
1:G:270:PHE:O	1:G:271:LEU:HD23	1.94	0.67
1:G:289:SER:O	1:G:291:ILE:HG22	1.93	0.67
1:R:255:ILE:CG2	1:R:256:LYS:N	2.58	0.67
1:R:266:PRO:HG2	1:R:267:LEU:HD22	1.75	0.67
1:G:267:LEU:HD22	1:G:267:LEU:H	1.60	0.67
1:G:27:VAL:HG22	1:G:28:VAL:H	1.58	0.67
1:R:119:SER:O	1:R:120:ALA:HB2	1.93	0.67
1:R:137:TYR:O	1:R:137:TYR:CD1	2.48	0.67
1:R:84:TRP:C	1:R:86:LYS:N	2.45	0.67
1:G:117:VAL:HG23	1:G:328:MET:CE	2.17	0.67
1:G:174:THR:HG23	1:G:229:ALA:HB2	1.76	0.67
1:G:295:LYS:HA	1:G:298:ILE:CG1	2.25	0.67
1:R:17:ARG:CZ	1:R:22:CYS:SG	2.83	0.67
1:R:255:ILE:CG2	1:R:256:LYS:H	2.06	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:261:THR:O	1:R:264:GLU:OE1	2.13	0.67
1:R:327:HIS:O	1:R:331:VAL:CG2	2.37	0.67
1:G:100:THR:O	1:G:101:THR:CB	2.34	0.67
1:G:150:THR:HA	1:G:311:TYR:HE2	1.58	0.67
1:G:177:ALA:HB1	1:G:235:PRO:O	1.94	0.67
1:R:274:THR:O	1:R:275:GLU:CB	2.43	0.67
1:R:3:ILE:HG13	1:R:4:GLY:N	2.09	0.67
1:G:263:SER:CA	1:G:271:LEU:HD12	2.25	0.67
1:G:277:ASP:CG	1:G:277:ASP:O	2.27	0.67
1:R:17:ARG:HD2	1:R:17:ARG:C	2.14	0.67
1:R:219:PRO:O	1:R:220:GLU:O	2.12	0.67
1:G:283:PHE:HE1	1:G:291:ILE:HG12	1.60	0.67
1:R:327:HIS:O	1:R:328:MET:O	2.12	0.67
1:R:84:TRP:CE2	1:R:92:ILE:HG21	2.28	0.67
1:G:319:GLN:HB2	1:G:320:ARG:HH12	1.56	0.66
1:R:180:ALA:O	1:R:181:THR:CB	2.41	0.66
1:R:74:PHE:HZ	1:R:86:LYS:O	1.78	0.66
1:G:166:GLU:O	1:G:167:ILE:HB	1.93	0.66
1:R:153:CYS:HA	1:R:290:SER:HB2	1.76	0.66
1:R:10:ARG:HE	1:R:13:ARG:HH11	1.42	0.66
1:R:119:SER:O	1:R:120:ALA:HB3	1.96	0.66
1:R:17:ARG:HB2	1:R:44:PHE:CZ	2.29	0.66
1:R:17:ARG:NH2	1:R:18:ALA:HA	2.09	0.66
1:R:35:ILE:HG21	1:R:40:MET:HE1	1.78	0.66
1:G:236:ASP:O	1:G:237:VAL:CB	2.43	0.66
1:G:177:ALA:H	1:G:238:SER:HG	1.43	0.66
1:R:126:PRO:HB3	1:R:141:MET:CE	2.24	0.66
1:R:138:SER:O	1:R:140:ASP:N	2.27	0.66
1:G:315:PHE:O	1:G:318:SER:HB2	1.95	0.66
1:G:324:LEU:O	1:G:328:MET:N	2.26	0.66
1:R:244:VAL:O	1:R:304:PHE:CD1	2.47	0.66
1:R:6:ASN:OD1	1:R:108:HIS:NE2	2.27	0.66
1:G:133:ASN:O	1:G:136:LYS:HB2	1.95	0.66
1:G:155:ALA:N	1:G:156:PRO:CD	2.58	0.66
1:G:302:LYS:HG2	1:G:303:THR:HG22	1.76	0.66
1:G:106:SER:O	1:G:109:PHE:N	2.28	0.66
1:G:14:LEU:HD21	1:G:315:PHE:CZ	2.30	0.66
1:G:67:ASP:O	1:G:69:LYS:N	2.29	0.66
1:R:252:TYR:O	1:R:252:TYR:CD1	2.49	0.66
1:G:313:ASN:O	1:G:315:PHE:N	2.28	0.66
1:G:64:LEU:O	1:G:71:ILE:HG22	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:328:MET:O	1:R:331:VAL:HB	1.96	0.66
1:G:238:SER:O	1:G:311:TYR:HD1	1.79	0.66
1:R:232:VAL:HG22	1:R:234:THR:N	2.10	0.66
1:R:84:TRP:O	1:R:86:LYS:CA	2.43	0.66
1:G:128:PHE:C	1:G:129:VAL:CG1	2.65	0.65
1:G:211:ALA:CB	1:G:225:LEU:O	2.44	0.65
1:G:175:VAL:HG22	1:G:230:PHE:CD2	2.28	0.65
1:G:238:SER:O	1:G:311:TYR:CD1	2.48	0.65
1:G:315:PHE:O	1:G:318:SER:N	2.29	0.65
1:R:161:LEU:CD2	1:R:244:VAL:HG21	2.26	0.65
1:R:35:ILE:HD12	1:R:43:MET:CE	2.18	0.65
1:G:102:ILE:O	1:G:106:SER:N	2.27	0.65
1:G:33:PRO:HB3	1:G:75:ASN:C	2.16	0.65
1:R:86:LYS:O	1:R:87:ALA:HB2	1.96	0.65
1:G:68:GLY:O	1:G:70:LYS:N	2.29	0.65
1:G:92:ILE:CD1	1:G:115:LYS:O	2.44	0.65
1:R:84:TRP:O	1:R:86:LYS:C	2.35	0.65
1:R:1:SER:O	1:R:2:LYS:CB	2.44	0.65
1:G:0:ACE:H1	1:G:25:ALA:C	2.16	0.65
1:G:249:GLU:CG	1:G:302:LYS:HZ2	2.10	0.65
1:R:299:GLN:NE2	1:R:299:GLN:HA	2.10	0.65
1:R:5:ILE:HG12	1:R:30:VAL:CG1	1.94	0.65
1:G:150:THR:CA	1:G:311:TYR:OH	2.42	0.65
1:G:27:VAL:O	1:G:28:VAL:HG12	1.96	0.65
1:R:17:ARG:O	1:R:20:LEU:HB3	1.96	0.65
1:R:283:PHE:CE1	1:R:291:ILE:HD11	2.31	0.65
1:R:64:LEU:CB	1:R:71:ILE:HG12	2.27	0.65
1:G:2:LYS:HG2	1:G:2:LYS:O	1.96	0.65
1:G:96:THR:HG22	1:G:97:GLY:CA	2.25	0.65
1:R:213:ALA:O	1:R:214:VAL:C	2.34	0.65
1:R:64:LEU:HB2	1:R:71:ILE:HG12	1.79	0.65
1:G:139:LYS:O	1:G:140:ASP:C	2.35	0.65
1:G:252:TYR:CE1	1:G:298:ILE:CG1	2.80	0.65
1:G:263:SER:HA	1:G:271:LEU:HD12	1.78	0.65
1:G:8:PHE:HD1	1:G:30:VAL:HG11	1.61	0.65
1:R:162:HIS:HA	1:R:166:GLU:O	1.97	0.65
1:R:261:THR:HG22	1:R:262:ALA:N	2.12	0.65
1:G:295:LYS:O	1:G:296:ALA:C	2.35	0.65
1:G:39:TYR:HD1	1:G:43:MET:HG3	1.62	0.65
1:G:178:VAL:CG2	1:G:235:PRO:HA	2.25	0.65
1:G:173:THR:HB	1:G:230:PHE:CZ	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:42:TYR:CD1	1:G:43:MET:N	2.65	0.64
1:G:162:HIS:CA	1:G:167:ILE:HG13	2.26	0.64
1:G:224:LYS:C	1:G:225:LEU:HD23	2.14	0.64
1:G:211:ALA:HB2	1:G:225:LEU:O	1.97	0.64
1:R:282:ASP:C	1:R:284:ILE:H	1.95	0.64
1:G:17:ARG:NH2	1:G:45:LYS:HA	2.12	0.64
1:R:102:ILE:HA	1:R:105:ALA:HB3	1.79	0.64
1:R:35:ILE:CG2	1:R:40:MET:CE	2.76	0.64
1:G:184:THR:O	1:G:185:VAL:CB	2.45	0.64
1:G:184:THR:O	1:G:185:VAL:HB	1.95	0.64
1:G:211:ALA:HB2	1:G:226:THR:HA	1.80	0.64
1:R:137:TYR:C	1:R:137:TYR:CD1	2.70	0.64
1:R:267:LEU:HD22	1:R:267:LEU:N	2.13	0.64
1:G:8:PHE:HE2	1:G:44:PHE:CB	2.11	0.64
1:R:106:SER:O	1:R:109:PHE:CB	2.43	0.64
1:R:263:SER:HB2	1:R:271:LEU:HD12	1.79	0.64
1:R:41:VAL:HG12	1:R:64:LEU:HD11	1.79	0.64
1:G:235:PRO:HB3	1:R:201:GLN:HE22	1.61	0.64
1:G:30:VAL:O	1:G:73:VAL:HA	1.97	0.64
1:G:31:ASN:HB3	1:G:84:TRP:CH2	2.32	0.64
1:R:116:VAL:HG12	1:R:118:ILE:CD1	2.22	0.64
1:R:50:HIS:HE1	1:R:236:ASP:OD2	1.81	0.64
1:R:60:GLU:O	1:R:62:GLY:N	2.30	0.64
1:R:9:GLY:C	1:R:13:ARG:CZ	2.65	0.64
1:R:198:GLY:O	1:R:199:ALA:HB3	1.98	0.64
1:G:113:ALA:O	1:G:114:LYS:CG	2.44	0.64
1:R:302:LYS:HG3	1:R:303:THR:HG22	1.79	0.64
1:R:31:ASN:O	1:R:32:ASP:CG	2.33	0.64
1:G:283:PHE:CD2	1:G:283:PHE:N	2.64	0.64
1:R:16:LEU:HD13	1:R:17:ARG:N	2.13	0.64
1:R:192:ASP:O	1:R:193:TRP:HB2	1.97	0.64
1:R:50:HIS:HD2	1:R:315:PHE:CD2	2.15	0.64
1:G:161:LEU:O	1:G:165:PHE:CB	2.44	0.63
1:G:324:LEU:HD12	1:G:325:LEU:CA	2.28	0.63
1:G:137:TYR:HE2	1:G:331:VAL:HG12	1.61	0.63
1:R:107:ALA:O	1:R:110:LYS:CB	2.41	0.63
1:R:17:ARG:CD	1:R:17:ARG:C	2.66	0.63
1:R:86:LYS:O	1:R:87:ALA:CB	2.46	0.63
1:G:126:PRO:HG2	1:G:144:VAL:HA	1.79	0.63
1:G:172:MET:O	1:G:228:MET:HE3	1.97	0.63
1:G:276:ASP:O	1:G:277:ASP:CB	2.42	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:137:TYR:HD2	1:G:331:VAL:HG11	1.60	0.63
1:R:223:GLY:C	1:R:225:LEU:H	2.01	0.63
1:R:313:ASN:H	1:R:313:ASN:ND2	1.94	0.63
1:G:153:CYS:O	1:G:156:PRO:CD	2.45	0.63
1:G:221:LEU:O	1:G:222:ASP:HB2	1.98	0.63
1:G:320:ARG:CZ	1:G:323:ASP:OD1	2.46	0.63
1:G:64:LEU:HD23	1:G:73:VAL:CG1	2.27	0.63
1:G:156:PRO:CG	1:G:290:SER:OG	2.47	0.63
1:G:45:LYS:CG	1:G:57:VAL:CG1	2.76	0.63
1:R:175:VAL:HG23	1:R:239:VAL:O	1.98	0.63
1:R:153:CYS:SG	1:R:240:VAL:HG11	2.38	0.63
1:R:60:GLU:O	1:R:63:ALA:N	2.31	0.63
1:R:67:ASP:O	1:R:69:LYS:HG3	1.97	0.63
1:G:319:GLN:CG	1:G:320:ARG:HH22	2.11	0.63
1:G:173:THR:HB	1:G:230:PHE:CE2	2.33	0.63
1:G:319:GLN:HB3	1:G:320:ARG:HH22	1.60	0.63
1:G:49:THR:HG22	1:G:50:HIS:H	1.64	0.63
1:G:84:TRP:HA	1:G:84:TRP:HE3	1.61	0.63
1:G:302:LYS:CG	1:G:303:THR:H	2.11	0.63
1:R:29:ALA:HB2	1:R:72:THR:HB	1.79	0.63
1:R:158:ALA:O	1:R:159:LYS:C	2.35	0.63
1:R:37:LEU:HD11	1:R:59:MET:HB2	1.79	0.63
1:R:79:PRO:O	1:R:80:GLU:O	2.16	0.63
1:G:232:VAL:HG23	1:G:234:THR:H	1.64	0.62
1:G:312:ASP:CG	1:G:312:ASP:O	2.36	0.62
1:G:96:THR:HG22	1:G:97:GLY:C	2.20	0.62
1:R:292:PHE:C	1:R:293:ASP:OD2	2.38	0.62
1:R:238:SER:CB	1:R:311:TYR:CZ	2.82	0.62
1:G:28:VAL:O	1:G:29:ALA:HB2	1.99	0.62
1:R:107:ALA:O	1:R:110:LYS:N	2.32	0.62
1:R:137:TYR:CZ	1:R:328:MET:HG2	2.34	0.62
1:R:239:VAL:HG22	1:R:239:VAL:O	1.98	0.62
1:R:41:VAL:CG2	1:R:42:TYR:N	2.62	0.62
1:G:102:ILE:CG1	1:G:103:GLU:N	2.62	0.62
1:G:210:ALA:O	1:G:214:VAL:HG23	1.99	0.62
1:R:157:VAL:HG12	1:R:158:ALA:N	2.15	0.62
1:R:279:VAL:CG1	1:R:283:PHE:HE2	2.11	0.62
1:G:268:GLN:C	1:G:270:PHE:N	2.52	0.62
1:G:146:ASN:HB3	1:G:317:TYR:CZ	2.33	0.62
1:G:53:PHE:O	1:G:54:LYS:HE2	1.99	0.62
1:R:127:MET:O	1:R:128:PHE:CG	2.53	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:157:VAL:HG12	1:R:158:ALA:H	1.62	0.62
1:R:329:GLN:OE1	1:R:329:GLN:HA	1.99	0.62
1:G:65:VAL:O	1:G:65:VAL:HG22	2.00	0.62
1:G:96:THR:OG1	1:G:99:PHE:HD2	1.82	0.62
1:R:94:GLU:HB3	1:R:118:ILE:HG23	1.82	0.62
1:R:259:MET:O	1:R:263:SER:CB	2.47	0.62
1:R:322:ILE:O	1:R:325:LEU:N	2.32	0.62
1:G:16:LEU:HD21	1:G:71:ILE:CD1	2.29	0.62
1:G:32:ASP:OD1	2:G:335:NAD:N9A	2.33	0.62
1:G:41:VAL:C	1:G:57:VAL:HG21	2.17	0.62
1:G:63:ALA:HB1	1:G:71:ILE:O	1.99	0.62
1:R:139:LYS:O	1:R:140:ASP:C	2.38	0.62
1:R:19:ALA:O	1:R:25:ALA:CA	2.48	0.62
1:R:211:ALA:CB	1:R:226:THR:N	2.62	0.62
1:R:169:GLU:O	1:R:244:VAL:HG12	2.00	0.62
1:G:139:LYS:O	1:G:141:MET:N	2.33	0.62
1:G:119:SER:HB2	1:G:317:TYR:CE2	2.34	0.62
1:R:324:LEU:O	1:R:324:LEU:HD22	2.00	0.62
1:R:13:ARG:HA	1:R:44:PHE:HD1	1.65	0.62
1:R:6:ASN:CB	1:R:94:GLU:OE1	2.48	0.62
1:G:106:SER:O	1:G:107:ALA:C	2.37	0.62
1:G:273:TYR:C	1:G:273:TYR:HD2	2.03	0.62
1:G:41:VAL:CB	1:G:57:VAL:HG22	2.29	0.62
1:R:176:HIS:CD2	1:R:231:ARG:HD2	2.34	0.62
1:R:222:ASP:C	1:R:222:ASP:OD2	2.38	0.62
1:R:41:VAL:HG12	1:R:64:LEU:HD12	1.82	0.62
1:G:191:LYS:O	1:G:192:ASP:CB	2.44	0.62
1:G:216:LYS:N	1:G:216:LYS:HD3	2.14	0.62
1:R:162:HIS:NE2	1:R:220:GLU:HG2	2.14	0.62
1:R:237:VAL:HG22	1:R:284:ILE:CG1	2.30	0.62
1:R:78:LYS:O	1:R:82:ILE:HG23	2.00	0.62
1:G:2:LYS:CE	1:G:90:GLU:HG2	2.24	0.61
1:R:50:HIS:CD2	1:R:315:PHE:HD2	2.17	0.61
1:G:159:LYS:C	1:G:163:GLU:HG3	2.21	0.61
1:G:237:VAL:HG21	1:G:284:ILE:HG13	0.69	0.61
1:R:117:VAL:O	1:R:118:ILE:HD13	1.99	0.61
1:R:283:PHE:HE1	1:R:291:ILE:HD11	1.63	0.61
1:R:28:VAL:CG2	1:R:29:ALA:O	2.48	0.61
1:R:191:LYS:O	1:R:192:ASP:CB	2.39	0.61
1:R:292:PHE:CD1	1:R:293:ASP:N	2.69	0.61
1:G:193:TRP:CD1	1:G:195:GLY:CA	2.79	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:264:GLU:HG2	1:G:265:GLY:H	1.65	0.61
2:G:335:NAD:N3A	2:G:335:NAD:H3B	2.16	0.61
1:R:160:VAL:O	1:R:164:ASN:CB	2.36	0.61
1:R:41:VAL:HG22	1:R:42:TYR:N	2.15	0.61
1:G:274:THR:OG1	1:G:276:ASP:CB	2.44	0.61
1:R:102:ILE:CG2	1:R:106:SER:OG	2.48	0.61
1:G:159:LYS:C	1:G:163:GLU:CG	2.67	0.61
1:R:117:VAL:HG21	1:R:324:LEU:HD11	1.81	0.61
1:R:8:PHE:CD2	1:R:43:MET:HE3	2.36	0.61
1:G:109:PHE:O	1:G:112:GLY:N	2.34	0.61
1:R:34:PHE:CD1	1:R:34:PHE:N	2.65	0.61
1:G:208:THR:HG23	1:G:209:GLY:N	2.15	0.61
1:G:41:VAL:CA	1:G:57:VAL:CG2	2.78	0.61
1:G:53:PHE:C	1:G:53:PHE:CD2	2.71	0.61
1:R:92:ILE:HD12	1:R:108:HIS:HB3	1.83	0.61
1:R:307:VAL:HG23	1:R:308:VAL:N	2.15	0.61
1:R:264:GLU:CG	1:R:265:GLY:H	2.11	0.60
1:R:65:VAL:O	1:R:65:VAL:CG2	2.49	0.60
1:G:273:TYR:C	1:G:273:TYR:CD2	2.74	0.60
1:G:42:TYR:C	1:G:42:TYR:CD1	2.74	0.60
1:R:153:CYS:HB2	1:R:311:TYR:HB3	1.82	0.60
1:G:177:ALA:HA	1:G:234:THR:O	2.00	0.60
1:G:305:VAL:HG22	1:G:306:LYS:H	1.64	0.60
1:R:154:LEU:O	1:R:156:PRO:N	2.33	0.60
1:R:166:GLU:O	1:R:167:ILE:CB	2.49	0.60
1:G:139:LYS:C	1:G:141:MET:N	2.49	0.60
1:G:232:VAL:HG23	1:G:234:THR:HB	1.83	0.60
1:R:232:VAL:C	1:R:234:THR:H	2.03	0.60
1:R:328:MET:O	1:R:331:VAL:N	2.34	0.60
1:R:92:ILE:HG13	1:R:115:LYS:O	2.02	0.60
1:G:94:GLU:O	1:G:118:ILE:HG22	2.00	0.60
1:G:12:GLY:O	1:G:13:ARG:C	2.40	0.60
1:R:14:LEU:O	1:R:16:LEU:N	2.33	0.60
1:R:176:HIS:CG	1:R:177:ALA:N	2.69	0.60
1:R:13:ARG:O	1:R:44:PHE:HE1	1.84	0.60
1:G:61:ASP:C	1:G:63:ALA:H	2.02	0.60
1:G:84:TRP:O	1:G:85:SER:C	2.39	0.60
1:R:118:ILE:CG2	1:R:119:SER:N	2.64	0.60
1:R:41:VAL:HB	1:R:57:VAL:C	2.22	0.60
1:G:289:SER:CB	1:G:320:ARG:NE	2.64	0.60
1:G:59:MET:HB2	1:G:64:LEU:HD13	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:218:ILE:CD1	1:R:220:GLU:CB	2.68	0.60
1:R:94:GLU:CD	1:R:95:SER:N	2.54	0.60
1:G:107:ALA:O	1:G:108:HIS:C	2.40	0.60
1:G:232:VAL:HB	1:G:233:PRO:CD	2.24	0.60
1:G:94:GLU:O	1:G:118:ILE:HG23	2.00	0.60
1:G:324:LEU:HD21	1:G:328:MET:SD	2.42	0.60
1:G:84:TRP:CD1	1:G:108:HIS:CD2	2.90	0.60
1:R:102:ILE:HG23	1:R:106:SER:OG	2.01	0.60
1:R:170:GLY:HA2	1:R:244:VAL:HG12	1.84	0.60
1:R:283:PHE:CA	1:R:286:ASP:HB2	2.30	0.60
1:R:324:LEU:HD13	1:R:325:LEU:N	2.17	0.60
1:R:35:ILE:CD1	1:R:43:MET:HE2	2.23	0.60
1:R:5:ILE:HG12	1:R:30:VAL:HA	1.84	0.60
1:G:156:PRO:HG3	1:G:290:SER:OG	2.01	0.59
1:R:109:PHE:O	1:R:110:LYS:O	2.20	0.59
1:R:10:ARG:N	1:R:13:ARG:HE	2.00	0.59
1:R:169:GLU:CD	1:R:245:ARG:HH11	2.05	0.59
1:R:45:LYS:HB2	1:R:57:VAL:HG22	1.83	0.59
1:R:23:GLY:O	1:R:25:ALA:HB3	1.95	0.59
1:R:266:PRO:HG2	1:R:267:LEU:CD2	2.32	0.59
1:G:13:ARG:HH22	1:G:43:MET:HE2	1.58	0.59
1:G:16:LEU:HD21	1:G:71:ILE:HD11	1.82	0.59
1:G:178:VAL:HG22	1:G:235:PRO:CA	2.30	0.59
1:G:311:TYR:O	1:G:312:ASP:C	2.40	0.59
1:G:92:ILE:HD13	1:G:115:LYS:O	2.01	0.59
1:R:17:ARG:NE	1:R:18:ALA:CA	2.65	0.59
1:R:217:VAL:C	1:R:218:ILE:HG22	2.22	0.59
1:R:327:HIS:C	1:R:331:VAL:HG23	2.22	0.59
1:G:150:THR:CA	1:G:311:TYR:HE2	2.12	0.59
1:G:259:MET:O	1:G:263:SER:CB	2.49	0.59
1:G:281:SER:O	1:G:282:ASP:O	2.19	0.59
1:R:137:TYR:HB3	1:R:327:HIS:HE1	1.67	0.59
1:R:161:LEU:HD22	1:R:167:ILE:HD11	1.85	0.59
1:R:253:ASP:O	1:R:256:LYS:HG3	2.01	0.59
1:R:41:VAL:O	1:R:57:VAL:HG21	2.01	0.59
1:G:157:VAL:O	1:G:161:LEU:HD12	2.02	0.59
1:R:170:GLY:CA	1:R:244:VAL:CG1	2.81	0.59
1:R:292:PHE:CG	1:R:293:ASP:N	2.69	0.59
1:R:47:ASP:O	1:R:51:GLY:N	2.33	0.59
1:G:137:TYR:CE1	1:G:144:VAL:HG11	2.37	0.59
1:G:295:LYS:HA	1:G:298:ILE:HG13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:45:LYS:CD	1:G:57:VAL:CG1	2.67	0.59
1:R:3:ILE:O	1:R:28:VAL:HB	2.02	0.59
1:R:91:TYR:HE1	1:R:329:GLN:HE22	1.43	0.59
1:R:77:MET:O	1:R:78:LYS:CB	2.50	0.59
1:G:190:ALA:O	1:G:193:TRP:HA	2.02	0.59
1:R:237:VAL:HG21	1:R:281:SER:HB2	1.84	0.59
1:G:267:LEU:HB3	1:G:271:LEU:HD23	1.84	0.59
1:G:79:PRO:O	1:G:82:ILE:CG2	2.30	0.59
1:R:10:ARG:NE	1:R:13:ARG:HH11	1.99	0.59
1:G:117:VAL:HG22	1:G:144:VAL:HG13	1.83	0.59
1:G:219:PRO:HA	1:G:222:ASP:CB	2.16	0.59
1:R:170:GLY:CA	1:R:244:VAL:HG12	2.33	0.59
1:R:154:LEU:O	1:R:157:VAL:N	2.36	0.58
1:G:130:CYS:O	1:G:131:GLY:O	2.21	0.58
1:G:26:GLN:CG	1:G:27:VAL:N	2.66	0.58
1:G:82:ILE:CD1	1:G:84:TRP:CD2	2.79	0.58
1:G:106:SER:CA	1:G:109:PHE:CE1	2.85	0.58
1:G:12:GLY:O	1:G:14:LEU:N	2.37	0.58
1:G:305:VAL:CG2	1:G:306:LYS:N	2.66	0.58
1:R:38:GLU:HG2	1:R:39:TYR:H	1.69	0.58
1:R:60:GLU:O	1:R:61:ASP:C	2.42	0.58
1:R:80:GLU:CG	1:R:107:ALA:HB1	2.33	0.58
1:G:119:SER:CB	1:G:317:TYR:HE2	2.15	0.58
1:G:146:ASN:HB3	1:G:317:TYR:CE1	2.39	0.58
1:G:53:PHE:CD2	1:G:54:LYS:N	2.71	0.58
1:R:13:ARG:HA	1:R:44:PHE:CD1	2.38	0.58
1:R:42:TYR:CD2	1:R:42:TYR:C	2.76	0.58
1:G:221:LEU:O	1:G:222:ASP:HB3	2.02	0.58
1:G:268:GLN:C	1:G:270:PHE:H	2.06	0.58
1:G:273:TYR:HA	1:G:292:PHE:O	2.02	0.58
1:R:109:PHE:HA	1:R:113:ALA:HB3	1.86	0.58
1:R:42:TYR:HD2	1:R:43:MET:H	1.46	0.58
1:G:184:THR:O	1:G:185:VAL:CG2	2.52	0.58
1:G:215:GLY:HA3	1:G:222:ASP:CA	2.31	0.58
1:G:8:PHE:CE2	1:G:44:PHE:CB	2.79	0.58
1:R:175:VAL:HB	1:R:239:VAL:HG13	1.86	0.58
1:R:279:VAL:HG12	1:R:280:SER:N	2.19	0.58
1:G:128:PHE:C	1:G:129:VAL:HG13	2.24	0.58
1:G:292:PHE:C	1:G:292:PHE:HD2	2.03	0.58
1:G:91:TYR:CE1	1:G:115:LYS:HG3	2.39	0.58
1:R:91:TYR:CE1	1:R:329:GLN:CD	2.75	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:129:VAL:CG1	1:G:147:ALA:CB	2.77	0.58
1:G:151:THR:HG21	1:G:213:ALA:HB1	1.84	0.58
1:G:42:TYR:OH	1:R:197:ARG:NE	2.36	0.58
1:G:52:VAL:CG2	1:G:53:PHE:N	2.66	0.58
1:R:176:HIS:CG	1:R:231:ARG:HD2	2.38	0.58
1:R:137:TYR:HD1	1:R:331:VAL:HG11	0.84	0.58
1:R:83:PRO:HB2	1:R:86:LYS:HB3	1.85	0.58
1:G:319:GLN:CB	1:G:320:ARG:HH22	2.16	0.58
1:R:329:GLN:OE1	1:R:329:GLN:CA	2.51	0.58
1:G:228:MET:H	1:G:228:MET:HE3	1.69	0.57
1:G:295:LYS:HA	1:G:298:ILE:HG12	1.85	0.57
1:G:103:GLU:O	1:G:107:ALA:N	2.24	0.57
1:R:327:HIS:O	1:R:328:MET:C	2.43	0.57
1:R:82:ILE:CD1	1:R:83:PRO:O	2.52	0.57
1:G:203:ILE:O	1:G:203:ILE:HG13	2.04	0.57
1:G:232:VAL:HG23	1:G:234:THR:CB	2.34	0.57
1:R:14:LEU:HG	1:R:318:SER:CB	2.34	0.57
1:R:232:VAL:CG2	1:R:233:PRO:CD	2.67	0.57
1:R:237:VAL:HG13	1:R:284:ILE:HG13	1.87	0.57
1:G:256:LYS:C	1:G:273:TYR:HE1	2.06	0.57
1:G:117:VAL:HG23	1:G:328:MET:SD	2.31	0.57
1:G:65:VAL:O	1:G:65:VAL:CG2	2.52	0.57
1:R:154:LEU:CD2	1:R:172:MET:HE1	2.34	0.57
1:G:182:GLN:OE1	1:G:231:ARG:CB	2.50	0.57
1:G:38:GLU:C	1:G:41:VAL:HG13	2.24	0.57
1:R:195:GLY:O	1:R:197:ARG:CG	2.50	0.57
1:G:59:MET:HG3	1:G:59:MET:O	1.98	0.57
1:G:76:GLU:OE2	1:G:76:GLU:CA	2.51	0.57
1:G:152:ASN:O	1:G:156:PRO:HD3	2.05	0.57
1:G:8:PHE:CZ	1:G:44:PHE:HB2	2.39	0.57
1:G:45:LYS:HA	1:G:53:PHE:HB2	1.86	0.57
1:R:12:GLY:CA	1:R:15:VAL:HB	2.34	0.57
1:R:176:HIS:O	1:R:231:ARG:HA	2.05	0.57
1:R:154:LEU:HD12	1:R:214:VAL:HG21	1.86	0.57
1:R:298:ILE:O	1:R:298:ILE:CD1	2.52	0.57
1:R:209:GLY:H	3:R:338:PO4:P	2.26	0.57
1:G:132:VAL:HG11	1:G:218:ILE:CD1	2.33	0.57
1:G:142:THR:CG2	1:G:143:VAL:N	2.68	0.57
1:G:79:PRO:HA	1:G:82:ILE:CG2	2.35	0.57
1:G:3:ILE:CD1	1:G:93:VAL:CG1	2.42	0.57
1:R:10:ARG:NH1	1:R:314:GLU:CD	2.55	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:240:VAL:O	1:R:308:VAL:HA	2.04	0.57
1:R:76:GLU:CG	1:R:82:ILE:HA	2.35	0.57
1:G:259:MET:O	1:G:263:SER:HB2	2.03	0.56
1:G:2:LYS:CG	1:G:2:LYS:O	2.53	0.56
1:G:106:SER:O	1:G:109:PHE:CG	2.58	0.56
1:R:21:SER:OG	1:R:22:CYS:N	2.39	0.56
1:R:252:TYR:CE1	1:R:256:LYS:HD3	2.40	0.56
1:R:322:ILE:O	1:R:323:ASP:C	2.43	0.56
1:G:267:LEU:HA	1:G:270:PHE:CD1	2.40	0.56
1:G:281:SER:O	1:G:282:ASP:C	2.43	0.56
1:R:10:ARG:CA	1:R:13:ARG:NE	2.68	0.56
1:R:115:LYS:HD3	1:R:115:LYS:N	2.20	0.56
1:R:215:GLY:O	1:R:219:PRO:N	2.39	0.56
1:G:82:ILE:HG13	1:G:82:ILE:O	1.96	0.56
1:R:120:ALA:HB1	1:R:121:PRO:HD2	1.86	0.56
1:R:211:ALA:HB1	1:R:225:LEU:C	2.26	0.56
1:R:298:ILE:O	1:R:298:ILE:CG1	2.53	0.56
1:G:298:ILE:C	1:G:299:GLN:NE2	2.53	0.56
1:R:261:THR:O	1:R:264:GLU:CD	2.44	0.56
1:R:79:PRO:O	1:R:81:ASN:N	2.38	0.56
1:G:84:TRP:CD1	1:G:108:HIS:NE2	2.74	0.56
1:R:256:LYS:HD3	1:R:294:ALA:CB	2.36	0.56
1:R:64:LEU:HD23	1:R:73:VAL:CG1	2.35	0.56
1:G:95:SER:HA	1:G:119:SER:OG	2.06	0.56
1:G:193:TRP:NE1	1:G:195:GLY:HA2	2.20	0.56
1:G:273:TYR:CE2	1:G:275:GLU:CG	2.63	0.56
1:R:84:TRP:NE1	1:R:108:HIS:CE1	2.74	0.56
1:R:179:THR:O	1:R:179:THR:CG2	2.53	0.56
1:G:275:GLU:O	1:G:276:ASP:C	2.43	0.56
1:G:52:VAL:HG23	1:G:53:PHE:N	2.21	0.56
1:R:10:ARG:N	1:R:13:ARG:NE	2.54	0.56
1:R:260:LYS:O	1:R:263:SER:HB3	2.06	0.56
1:R:305:VAL:CG2	1:R:306:LYS:N	2.68	0.56
1:G:133:ASN:C	1:G:133:ASN:ND2	2.59	0.56
1:G:172:MET:O	1:G:228:MET:HE1	2.05	0.56
1:G:39:TYR:O	1:G:40:MET:C	2.43	0.56
1:R:109:PHE:CE1	1:R:142:THR:HG23	2.31	0.56
1:R:210:ALA:O	1:R:214:VAL:HG23	2.06	0.56
1:G:204:ILE:HG22	1:G:205:PRO:O	2.05	0.56
1:G:264:GLU:CG	1:G:265:GLY:N	2.67	0.56
1:R:17:ARG:CZ	1:R:18:ALA:CA	2.77	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:25:ALA:O	1:R:26:GLN:HB2	2.06	0.56
1:G:18:ALA:C	1:G:22:CYS:HB2	2.26	0.56
1:G:283:PHE:HD2	1:G:283:PHE:N	2.03	0.56
1:G:252:TYR:OH	1:G:295:LYS:HA	2.05	0.56
1:G:96:THR:CG2	1:G:97:GLY:C	2.75	0.56
1:R:76:GLU:OE1	1:R:76:GLU:CA	2.54	0.56
1:G:50:HIS:NE2	1:G:315:PHE:HD2	1.91	0.55
1:R:283:PHE:CE1	1:R:291:ILE:CD1	2.89	0.55
1:G:218:ILE:CG2	1:G:221:LEU:HD12	2.21	0.55
1:G:174:THR:HG23	1:G:229:ALA:CB	2.37	0.55
1:G:14:LEU:HD23	1:G:315:PHE:HE2	1.67	0.55
1:R:170:GLY:C	1:R:225:LEU:HD21	2.25	0.55
1:G:14:LEU:HA	1:G:17:ARG:CB	2.37	0.55
1:G:239:VAL:HB	1:G:310:TRP:CD2	2.41	0.55
1:R:41:VAL:HB	1:R:57:VAL:O	2.06	0.55
1:R:17:ARG:NE	1:R:18:ALA:HA	2.21	0.55
1:R:94:GLU:C	1:R:94:GLU:OE2	2.44	0.55
1:G:133:ASN:ND2	1:G:134:LEU:N	2.54	0.55
1:G:305:VAL:CG2	1:G:306:LYS:H	2.20	0.55
1:R:150:THR:HG21	3:R:338:PO4:P	2.46	0.55
1:R:132:VAL:HG11	1:R:217:VAL:O	2.05	0.55
1:G:42:TYR:CZ	1:R:197:ARG:HD2	2.42	0.55
1:R:94:GLU:O	1:R:94:GLU:OE2	2.24	0.55
1:G:27:VAL:C	1:G:28:VAL:CG1	2.75	0.55
1:G:41:VAL:HA	1:G:57:VAL:HG23	1.87	0.55
1:R:59:MET:O	1:R:59:MET:CG	2.48	0.55
1:R:59:MET:C	1:R:59:MET:SD	2.85	0.55
1:G:13:ARG:NH2	1:G:43:MET:HE2	2.16	0.55
1:G:149:CYS:O	1:G:311:TYR:CE2	2.60	0.55
1:R:102:ILE:HG22	1:R:102:ILE:O	2.06	0.55
1:R:276:ASP:HB3	1:R:279:VAL:HG22	1.90	0.55
1:R:319:GLN:O	1:R:323:ASP:CG	2.45	0.55
1:G:173:THR:HA	1:G:228:MET:O	2.07	0.54
1:G:224:LYS:O	1:G:225:LEU:CD2	2.28	0.54
1:G:156:PRO:HG3	1:G:290:SER:HB2	1.85	0.54
1:R:161:LEU:CB	1:R:167:ILE:HD12	2.24	0.54
1:R:271:LEU:O	1:R:291:ILE:HA	2.06	0.54
1:R:35:ILE:CG2	1:R:40:MET:HE1	2.36	0.54
1:R:92:ILE:CG1	1:R:115:LYS:O	2.55	0.54
1:G:176:HIS:ND1	1:G:238:SER:HB3	2.20	0.54
1:G:277:ASP:OD1	1:G:278:VAL:HG22	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:45:LYS:HG3	1:G:57:VAL:HB	1.89	0.54
1:G:2:LYS:HE3	1:G:90:GLU:HG3	1.80	0.54
1:R:103:GLU:N	1:R:103:GLU:OE2	2.40	0.54
1:R:3:ILE:HG13	1:R:4:GLY:H	1.71	0.54
1:R:50:HIS:CE1	1:R:314:GLU:OE2	2.60	0.54
1:G:208:THR:HG23	1:G:210:ALA:N	2.22	0.54
1:G:252:TYR:HB3	1:G:300:LEU:CD2	2.29	0.54
1:R:215:GLY:O	1:R:218:ILE:C	2.46	0.54
1:R:74:PHE:HZ	1:R:87:ALA:HB2	1.70	0.54
1:G:255:ILE:HG22	1:G:256:LYS:CA	2.31	0.54
1:R:90:GLU:OE2	1:R:114:LYS:HD2	2.07	0.54
1:R:14:LEU:HD12	1:R:18:ALA:HB2	1.79	0.54
1:R:292:PHE:HD1	1:R:292:PHE:C	2.09	0.54
1:G:324:LEU:HD11	1:G:328:MET:CG	2.38	0.54
1:G:35:ILE:HG12	2:G:335:NAD:O2B	2.08	0.54
1:G:66:VAL:O	1:G:67:ASP:C	2.45	0.54
1:G:76:GLU:HB3	1:G:82:ILE:HG22	1.89	0.54
1:R:217:VAL:O	1:R:218:ILE:HB	2.06	0.54
1:G:129:VAL:HG12	1:G:147:ALA:CB	2.37	0.54
1:G:76:GLU:HA	1:G:76:GLU:OE2	2.07	0.54
1:G:82:ILE:HD11	1:G:84:TRP:CE3	2.41	0.54
1:R:17:ARG:HH21	1:R:18:ALA:HB2	1.72	0.54
1:R:237:VAL:CG2	1:R:284:ILE:HD11	2.33	0.54
1:R:289:SER:OG	1:R:320:ARG:NH2	2.40	0.54
1:G:14:LEU:O	1:G:17:ARG:N	2.41	0.54
1:R:243:THR:CG2	1:R:304:PHE:CZ	2.91	0.54
1:R:238:SER:HB2	1:R:311:TYR:CE2	2.42	0.54
1:R:91:TYR:CZ	1:R:329:GLN:CD	2.81	0.54
1:R:84:TRP:HE1	1:R:92:ILE:CG2	2.06	0.54
1:R:237:VAL:CG2	1:R:284:ILE:CD1	2.80	0.54
1:R:84:TRP:CE2	1:R:92:ILE:CG2	2.89	0.54
1:G:128:PHE:CE2	1:G:137:TYR:CB	2.84	0.54
1:G:129:VAL:HG11	1:G:147:ALA:CB	2.34	0.54
1:G:170:GLY:HA3	1:G:243:THR:O	2.07	0.54
1:G:147:ALA:CB	1:G:151:THR:HG22	2.33	0.54
1:G:271:LEU:N	1:G:290:SER:O	2.39	0.54
1:R:218:ILE:HD11	1:R:220:GLU:CB	2.35	0.54
1:R:238:SER:HB2	1:R:311:TYR:CZ	2.43	0.54
1:R:279:VAL:HG12	1:R:283:PHE:HE2	1.72	0.54
1:R:69:LYS:O	1:R:71:ILE:HG22	2.08	0.54
1:R:33:PRO:HG3	1:R:77:MET:HG2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:267:LEU:HG	1:G:271:LEU:CD2	2.37	0.53
1:R:16:LEU:O	1:R:17:ARG:C	2.46	0.53
1:R:186:ASP:OD2	1:R:197:ARG:NH2	2.41	0.53
1:R:0:ACE:CH3	1:R:26:GLN:HG2	2.35	0.53
1:G:27:VAL:C	1:G:28:VAL:HG12	2.28	0.53
1:R:211:ALA:CB	1:R:225:LEU:C	2.77	0.53
1:R:80:GLU:HG3	1:R:107:ALA:HB1	1.90	0.53
1:G:17:ARG:NH2	1:G:44:PHE:O	2.41	0.53
1:G:67:ASP:C	1:G:69:LYS:H	2.11	0.53
1:R:10:ARG:HH22	1:R:47:ASP:CG	2.10	0.53
1:R:16:LEU:CD1	1:R:16:LEU:C	2.77	0.53
1:R:194:ARG:CG	1:R:194:ARG:HH11	2.08	0.53
1:G:49:THR:CG2	1:G:50:HIS:H	2.21	0.53
1:G:309:SER:O	1:G:310:TRP:CD1	2.61	0.53
1:G:324:LEU:HD11	1:G:328:MET:CB	2.37	0.53
1:R:14:LEU:HD13	1:R:18:ALA:CB	2.25	0.53
1:R:176:HIS:CG	1:R:177:ALA:H	2.27	0.53
1:R:299:GLN:HE21	1:R:299:GLN:HA	1.74	0.53
1:G:272:GLY:O	1:G:273:TYR:HB3	2.09	0.53
1:R:102:ILE:CG2	1:R:106:SER:HG	2.22	0.53
1:G:161:LEU:O	1:G:165:PHE:N	2.42	0.53
1:G:166:GLU:O	1:G:167:ILE:CB	2.57	0.53
1:G:177:ALA:CB	1:G:234:THR:HG22	2.39	0.53
1:R:182:GLN:OE1	1:R:204:ILE:HG13	2.09	0.53
1:R:237:VAL:CG2	1:R:281:SER:HB2	2.39	0.53
1:R:76:GLU:HB3	1:R:82:ILE:HG22	1.80	0.53
1:G:173:THR:HG21	1:G:230:PHE:HZ	1.72	0.53
1:R:120:ALA:O	1:R:145:SER:OG	2.26	0.53
1:R:17:ARG:HE	1:R:18:ALA:H	1.54	0.53
1:R:237:VAL:HG22	1:R:284:ILE:HG13	1.90	0.53
1:G:168:VAL:HG13	1:G:224:LYS:HE2	1.90	0.53
1:G:252:TYR:CE1	1:G:298:ILE:HB	2.44	0.53
1:R:74:PHE:CZ	1:R:86:LYS:O	2.61	0.53
1:G:157:VAL:CG1	1:G:158:ALA:N	2.71	0.53
1:G:3:ILE:HG13	1:G:92:ILE:HA	1.90	0.53
1:R:85:SER:O	1:R:87:ALA:N	2.42	0.53
1:G:216:LYS:HZ3	1:G:222:ASP:CG	2.05	0.52
1:G:267:LEU:C	1:G:270:PHE:CE1	2.82	0.52
1:G:50:HIS:CE1	1:G:315:PHE:CD2	2.97	0.52
1:G:5:ILE:CG2	1:G:6:ASN:N	2.68	0.52
1:G:76:GLU:CB	1:G:82:ILE:HG22	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:14:LEU:HA	1:G:17:ARG:HB3	1.90	0.52
1:G:314:GLU:HG2	2:G:335:NAD:O7N	2.09	0.52
1:R:18:ALA:CB	1:R:22:CYS:SG	2.97	0.52
1:G:49:THR:HG1	1:G:236:ASP:HB2	1.62	0.52
1:G:282:ASP:O	1:G:284:ILE:N	2.42	0.52
1:G:41:VAL:HG12	1:G:64:LEU:CD1	2.37	0.52
1:R:282:ASP:N	1:R:282:ASP:OD1	2.33	0.52
1:R:50:HIS:HE1	1:R:314:GLU:HB2	1.71	0.52
1:G:158:ALA:O	1:G:159:LYS:C	2.46	0.52
1:R:16:LEU:HD12	1:R:44:PHE:CZ	2.45	0.52
1:R:305:VAL:HG22	1:R:306:LYS:H	1.74	0.52
1:R:322:ILE:O	1:R:324:LEU:N	2.42	0.52
1:R:90:GLU:OE2	1:R:90:GLU:HA	2.10	0.52
1:G:134:LEU:CD1	1:G:134:LEU:N	2.72	0.52
1:G:232:VAL:CG2	1:G:234:THR:HB	2.39	0.52
1:G:150:THR:HG23	1:G:311:TYR:OH	2.09	0.52
1:G:10:ARG:HD3	1:G:314:GLU:CD	2.30	0.52
1:G:172:MET:CE	1:G:210:ALA:HB2	2.38	0.52
1:R:153:CYS:SG	1:R:240:VAL:CG1	2.97	0.52
1:G:154:LEU:O	1:G:155:ALA:C	2.48	0.52
1:G:172:MET:HE1	1:G:210:ALA:HB2	1.91	0.52
1:G:235:PRO:CB	1:R:201:GLN:HE22	2.14	0.52
1:G:80:GLU:O	1:G:81:ASN:C	2.47	0.52
1:G:45:LYS:CB	1:G:57:VAL:HG21	2.32	0.52
1:G:95:SER:O	1:G:96:THR:CB	2.45	0.52
1:R:114:LYS:HB3	1:R:115:LYS:HD3	1.91	0.52
1:R:50:HIS:CE1	1:R:314:GLU:CB	2.92	0.52
1:R:27:VAL:HG21	1:R:69:LYS:HB3	1.90	0.52
1:G:187:GLY:O	1:G:188:PRO:O	2.27	0.52
1:G:249:GLU:HG3	1:G:302:LYS:HZ2	1.73	0.52
1:R:106:SER:O	1:R:109:PHE:N	2.42	0.52
1:G:176:HIS:CE1	1:G:238:SER:HB2	2.42	0.52
1:G:8:PHE:HD1	1:G:30:VAL:CG1	2.23	0.52
1:R:109:PHE:O	1:R:110:LYS:C	2.48	0.52
1:G:137:TYR:CE1	1:G:144:VAL:CG1	2.93	0.51
1:G:235:PRO:HB3	1:R:201:GLN:HE21	1.52	0.51
1:R:207:SER:C	1:R:208:THR:HG23	2.21	0.51
1:R:252:TYR:C	1:R:255:ILE:HG22	2.29	0.51
1:R:252:TYR:HD1	1:R:252:TYR:O	1.92	0.51
1:R:305:VAL:CG2	1:R:306:LYS:H	2.23	0.51
1:R:17:ARG:HB2	1:R:44:PHE:CE1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:153:CYS:O	1:G:156:PRO:HD2	2.10	0.51
1:R:127:MET:CE	1:R:216:LYS:CD	2.86	0.51
1:R:19:ALA:O	1:R:25:ALA:HA	2.10	0.51
1:R:312:ASP:OD1	1:R:315:PHE:CB	2.59	0.51
1:G:96:THR:HG1	1:G:99:PHE:HD2	1.45	0.51
1:R:192:ASP:O	1:R:193:TRP:CB	2.58	0.51
1:R:278:VAL:O	1:R:278:VAL:CG1	2.58	0.51
1:G:233:PRO:O	1:G:235:PRO:N	2.44	0.51
1:R:99:PHE:CE1	2:R:339:NAD:N1A	2.73	0.51
1:G:137:TYR:CE1	1:G:141:MET:CB	2.94	0.51
1:R:129:VAL:O	1:R:133:ASN:N	2.43	0.51
1:R:219:PRO:O	1:R:222:ASP:HB3	2.11	0.51
1:R:137:TYR:O	1:R:331:VAL:HG11	2.11	0.51
1:G:214:VAL:O	1:G:218:ILE:N	2.40	0.51
1:G:215:GLY:CA	1:G:222:ASP:HA	2.36	0.51
1:R:118:ILE:HG22	1:R:119:SER:H	1.74	0.51
1:G:263:SER:HA	1:G:271:LEU:HG	1.93	0.51
1:G:76:GLU:HG3	1:G:82:ILE:N	2.26	0.51
1:R:232:VAL:C	1:R:234:THR:N	2.63	0.51
1:G:101:THR:HG23	1:G:102:ILE:HD13	1.92	0.51
1:G:102:ILE:HG12	1:G:103:GLU:H	1.68	0.51
1:G:92:ILE:HG12	1:G:116:VAL:HG22	1.92	0.51
1:R:109:PHE:CE2	1:R:114:LYS:CA	2.94	0.51
1:R:94:GLU:HB3	1:R:118:ILE:HD12	1.91	0.51
1:G:249:GLU:CG	1:G:302:LYS:NZ	2.72	0.50
1:R:17:ARG:NH2	1:R:18:ALA:CA	2.74	0.50
1:R:264:GLU:O	1:R:265:GLY:O	2.29	0.50
1:R:312:ASP:OD1	1:R:315:PHE:HB3	2.11	0.50
1:G:105:ALA:O	1:G:108:HIS:CB	2.51	0.50
1:G:157:VAL:HG13	1:G:158:ALA:N	2.27	0.50
1:G:257:ALA:O	1:G:258:ALA:C	2.48	0.50
1:G:267:LEU:O	1:G:270:PHE:CG	2.55	0.50
1:R:108:HIS:O	1:R:109:PHE:C	2.49	0.50
1:R:162:HIS:O	1:R:166:GLU:CA	2.60	0.50
1:R:117:VAL:CG2	1:R:324:LEU:HD11	2.41	0.50
1:G:178:VAL:N	1:G:234:THR:O	2.40	0.50
1:G:31:ASN:HB3	1:G:84:TRP:CZ2	2.46	0.50
1:R:14:LEU:HA	1:R:17:ARG:HB3	1.94	0.50
1:G:18:ALA:O	1:G:22:CYS:N	2.44	0.50
1:R:132:VAL:C	1:R:134:LEU:HD22	2.31	0.50
1:R:138:SER:O	1:R:139:LYS:C	2.48	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:242:LEU:O	1:R:306:LYS:HA	2.11	0.50
1:R:60:GLU:HA	1:R:60:GLU:OE1	2.12	0.50
1:G:263:SER:HA	1:G:271:LEU:CG	2.41	0.50
1:G:266:PRO:HG2	1:G:267:LEU:HD22	1.94	0.50
1:G:45:LYS:CG	1:G:53:PHE:HB3	2.33	0.50
1:R:6:ASN:HB2	1:R:94:GLU:HA	1.94	0.50
1:G:98:VAL:O	1:G:100:THR:N	2.45	0.50
1:G:170:GLY:CA	1:G:243:THR:O	2.60	0.50
1:G:273:TYR:OH	1:G:275:GLU:OE1	2.30	0.50
1:G:149:CYS:C	1:G:311:TYR:HE2	2.14	0.50
1:G:91:TYR:OH	1:G:332:ASP:CB	2.59	0.50
1:R:113:ALA:O	1:R:114:LYS:CB	2.59	0.50
1:R:157:VAL:HG13	1:R:161:LEU:CD1	2.37	0.50
1:R:159:LYS:O	1:R:163:GLU:HG2	2.12	0.50
1:R:154:LEU:CD2	1:R:172:MET:HE3	2.28	0.50
1:R:176:HIS:CD2	1:R:231:ARG:CD	2.94	0.50
1:R:54:LYS:O	1:R:56:GLU:N	2.45	0.50
1:R:76:GLU:OE1	1:R:76:GLU:HA	2.12	0.50
1:R:128:PHE:HD2	1:R:144:VAL:CG2	2.24	0.50
1:R:154:LEU:O	1:R:155:ALA:C	2.50	0.50
1:R:50:HIS:CD2	1:R:315:PHE:CD2	2.95	0.50
1:R:8:PHE:HD2	1:R:43:MET:CE	2.24	0.50
1:R:80:GLU:O	1:R:81:ASN:C	2.49	0.50
1:R:84:TRP:CD1	1:R:92:ILE:HD13	2.47	0.50
1:G:84:TRP:HE1	1:G:108:HIS:CE1	2.30	0.50
1:R:1:SER:OG	1:R:2:LYS:N	2.44	0.50
1:G:215:GLY:CA	1:G:222:ASP:CA	2.90	0.50
1:G:193:TRP:HD1	1:G:195:GLY:HA2	1.71	0.49
1:R:162:HIS:NE2	1:R:221:LEU:HD12	2.26	0.49
1:R:277:ASP:O	1:R:295:LYS:HB3	2.12	0.49
1:G:155:ALA:HB2	1:G:217:VAL:HG11	1.94	0.49
1:R:137:TYR:CE2	1:R:328:MET:CG	2.94	0.49
1:R:169:GLU:O	1:R:244:VAL:HA	2.12	0.49
1:R:195:GLY:C	1:R:197:ARG:N	2.64	0.49
1:R:64:LEU:HD23	1:R:73:VAL:HG13	1.93	0.49
1:G:63:ALA:HB2	1:G:72:THR:HG23	1.93	0.49
1:R:110:LYS:O	1:R:112:GLY:N	2.45	0.49
1:R:8:PHE:HD2	1:R:43:MET:HE3	1.74	0.49
1:G:3:ILE:HD11	1:G:93:VAL:HG12	0.67	0.49
1:R:18:ALA:O	1:R:19:ALA:C	2.51	0.49
1:R:66:VAL:O	1:R:67:ASP:C	2.49	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:97:GLY:O	1:R:98:VAL:C	2.50	0.49
1:G:195:GLY:O	1:G:196:GLY:C	2.51	0.49
1:R:189:SER:O	1:R:190:ALA:HB2	2.09	0.49
1:R:194:ARG:HH22	1:R:204:ILE:HG22	1.78	0.49
1:G:3:ILE:CG1	1:G:91:TYR:O	2.59	0.49
1:R:240:VAL:HG11	1:R:309:SER:OG	2.10	0.49
1:R:104:LYS:CD	1:R:104:LYS:H	2.25	0.49
1:R:33:PRO:HB3	1:R:77:MET:HG2	1.94	0.49
1:G:182:GLN:OE1	1:G:231:ARG:HG2	2.12	0.49
1:G:49:THR:HG23	1:G:50:HIS:N	2.27	0.49
1:R:283:PHE:HD2	1:R:283:PHE:N	2.08	0.49
1:R:74:PHE:CZ	1:R:87:ALA:HB2	2.48	0.49
1:G:295:LYS:O	1:G:298:ILE:HG13	2.12	0.49
1:R:26:GLN:HE21	1:R:26:GLN:C	2.13	0.49
1:R:268:GLN:C	1:R:270:PHE:H	2.15	0.49
1:R:282:ASP:C	1:R:284:ILE:N	2.59	0.49
1:G:193:TRP:O	1:G:194:ARG:C	2.51	0.48
1:G:41:VAL:O	1:G:45:LYS:HB2	2.13	0.48
1:R:14:LEU:HD11	1:R:17:ARG:HH21	1.78	0.48
1:R:236:ASP:C	1:R:236:ASP:OD1	2.51	0.48
1:R:64:LEU:HB2	1:R:71:ILE:CG1	2.42	0.48
1:G:106:SER:O	1:G:109:PHE:CD1	2.66	0.48
1:G:18:ALA:O	1:G:22:CYS:CB	2.56	0.48
1:G:283:PHE:CE1	1:G:291:ILE:HG12	2.43	0.48
1:G:292:PHE:CZ	1:G:293:ASP:O	2.66	0.48
1:G:7:GLY:H	2:G:335:NAD:H8A	1.77	0.48
1:G:96:THR:CG2	1:G:99:PHE:HB2	2.38	0.48
1:R:10:ARG:O	1:R:11:ILE:C	2.50	0.48
1:R:302:LYS:HG3	1:R:303:THR:H	1.78	0.48
1:G:106:SER:HA	1:G:109:PHE:CZ	2.48	0.48
1:G:233:PRO:O	1:G:234:THR:C	2.51	0.48
1:G:236:ASP:O	1:G:284:ILE:HD11	2.14	0.48
1:R:104:LYS:O	1:R:107:ALA:N	2.47	0.48
1:G:61:ASP:C	1:G:63:ALA:N	2.67	0.48
1:G:71:ILE:O	1:G:71:ILE:CG2	2.52	0.48
1:G:15:VAL:HG11	1:G:93:VAL:HG11	1.95	0.48
1:R:219:PRO:O	1:R:221:LEU:N	2.47	0.48
1:G:283:PHE:CA	1:G:286:ASP:HB2	2.34	0.48
1:G:313:ASN:H	1:G:313:ASN:HD22	1.61	0.48
1:R:237:VAL:HG11	1:R:281:SER:O	2.14	0.48
1:R:50:HIS:NE2	1:R:315:PHE:HB2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:43:MET:CE	1:R:187:GLY:HA2	2.44	0.48
1:R:158:ALA:O	1:R:161:LEU:N	2.46	0.48
1:R:193:TRP:O	1:R:195:GLY:N	2.46	0.48
1:R:208:THR:O	1:R:209:GLY:C	2.52	0.48
1:R:223:GLY:O	1:R:225:LEU:N	2.46	0.48
1:R:29:ALA:CB	1:R:72:THR:HB	2.43	0.48
1:G:17:ARG:HH22	1:G:45:LYS:HA	1.78	0.48
1:G:38:GLU:O	1:G:41:VAL:CG1	2.46	0.48
1:G:79:PRO:HA	1:G:82:ILE:HG23	1.95	0.48
1:G:15:VAL:HG11	1:G:93:VAL:HG21	1.94	0.48
1:R:128:PHE:HD2	1:R:144:VAL:HG23	1.79	0.48
1:R:5:ILE:HG12	1:R:30:VAL:CB	2.44	0.48
1:R:72:THR:CG2	1:R:74:PHE:CE2	2.96	0.48
1:G:27:VAL:HG22	1:G:28:VAL:N	2.27	0.48
1:G:291:ILE:HG13	1:G:291:ILE:O	2.10	0.48
1:G:319:GLN:CB	1:G:320:ARG:NH1	2.35	0.48
1:R:150:THR:OG1	1:R:151:THR:N	2.45	0.48
1:G:189:SER:OG	1:R:39:TYR:OH	2.23	0.48
1:R:63:ALA:HB1	1:R:71:ILE:O	2.14	0.48
1:G:142:THR:HG23	1:G:143:VAL:N	2.29	0.48
1:G:251:SER:HG	1:G:254:ASP:CB	2.06	0.48
1:G:25:ALA:O	1:G:26:GLN:CB	2.61	0.48
1:G:292:PHE:CD2	1:G:293:ASP:CA	2.97	0.48
1:R:14:LEU:HD12	1:R:18:ALA:CB	2.39	0.48
1:R:193:TRP:O	1:R:194:ARG:C	2.51	0.48
1:R:18:ALA:HB1	1:R:22:CYS:SG	2.54	0.48
1:R:263:SER:HA	1:R:271:LEU:HG	1.96	0.48
1:R:2:LYS:HD2	1:R:90:GLU:HG2	1.95	0.48
1:R:137:TYR:O	1:R:331:VAL:CG1	2.62	0.48
1:R:327:HIS:CE1	1:R:331:VAL:CG2	2.96	0.48
1:R:331:VAL:O	1:R:334:ALA:HB2	2.14	0.48
1:R:80:GLU:HG2	1:R:107:ALA:HB1	1.94	0.47
1:R:147:ALA:HB1	1:R:151:THR:HB	1.96	0.47
1:R:20:LEU:HD22	1:R:20:LEU:C	2.34	0.47
1:R:72:THR:HG21	1:R:74:PHE:CE2	2.48	0.47
1:G:130:CYS:SG	1:G:323:ASP:HB2	2.54	0.47
1:G:236:ASP:OD1	1:G:237:VAL:N	2.47	0.47
1:R:211:ALA:O	1:R:214:VAL:HB	2.14	0.47
1:G:104:LYS:O	1:G:107:ALA:HB3	2.15	0.47
1:G:156:PRO:HG2	1:G:290:SER:OG	2.14	0.47
1:G:177:ALA:CA	1:G:234:THR:O	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:216:LYS:HD3	1:G:222:ASP:OD2	2.14	0.47
1:G:32:ASP:OD1	2:G:335:NAD:C8A	2.62	0.47
1:G:40:MET:CE	1:G:73:VAL:CG1	2.88	0.47
1:R:159:LYS:O	1:R:163:GLU:CG	2.62	0.47
1:G:263:SER:CA	1:G:271:LEU:CD1	2.85	0.47
1:R:10:ARG:HE	1:R:13:ARG:NH1	2.10	0.47
1:R:115:LYS:CD	1:R:115:LYS:N	2.77	0.47
1:G:256:LYS:HD2	1:G:294:ALA:CB	2.37	0.47
1:R:114:LYS:C	1:R:115:LYS:HD3	2.33	0.47
1:R:127:MET:C	1:R:128:PHE:CG	2.87	0.47
1:R:176:HIS:C	1:R:231:ARG:HG3	2.35	0.47
1:R:254:ASP:O	1:R:257:ALA:HB3	2.14	0.47
1:R:208:THR:HG1	3:R:338:PO4:P	2.30	0.47
1:R:41:VAL:CB	1:R:57:VAL:HB	2.43	0.47
1:G:324:LEU:HD12	1:G:325:LEU:HA	1.96	0.47
1:R:9:GLY:HA2	1:R:13:ARG:NH2	2.30	0.47
1:G:218:ILE:HG22	1:G:221:LEU:HB2	1.97	0.47
1:G:1:SER:C	1:G:26:GLN:HG3	2.35	0.47
1:G:252:TYR:CE1	1:G:298:ILE:CB	2.98	0.47
1:G:17:ARG:HH22	1:G:45:LYS:CA	2.27	0.47
1:G:49:THR:HG1	1:G:236:ASP:CG	2.18	0.47
1:R:256:LYS:CD	1:R:294:ALA:CB	2.93	0.47
1:R:5:ILE:HG21	1:R:15:VAL:HG11	1.97	0.47
1:G:322:ILE:O	1:G:326:LYS:CG	2.58	0.47
1:G:268:GLN:NE2	1:G:268:GLN:CA	2.66	0.47
1:G:252:TYR:HH	1:G:295:LYS:HG2	1.80	0.47
1:R:41:VAL:CG2	1:R:57:VAL:O	2.62	0.47
1:G:328:MET:O	1:G:329:GLN:C	2.53	0.47
1:R:135:GLU:O	1:R:136:LYS:C	2.52	0.47
1:R:208:THR:OG1	1:R:209:GLY:N	2.48	0.47
1:R:252:TYR:O	1:R:255:ILE:HG23	2.13	0.47
1:R:41:VAL:CA	1:R:57:VAL:HB	2.45	0.47
1:G:185:VAL:C	1:G:186:ASP:OD2	2.52	0.47
1:G:267:LEU:CA	1:G:270:PHE:HD1	2.27	0.47
1:G:34:PHE:O	1:G:35:ILE:HG12	2.15	0.47
1:R:110:LYS:O	1:R:111:GLY:C	2.53	0.47
1:R:122:SER:O	1:R:127:MET:HG3	2.15	0.47
1:G:177:ALA:HA	1:G:234:THR:HG22	1.97	0.46
1:G:71:ILE:HG22	1:G:71:ILE:O	2.15	0.46
1:R:280:SER:O	1:R:283:PHE:CE2	2.67	0.46
1:G:331:VAL:O	1:G:334:ALA:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:11:ILE:HD13	1:R:15:VAL:CG2	2.41	0.46
1:G:173:THR:CG2	1:G:230:PHE:CZ	2.98	0.46
1:G:256:LYS:HB2	1:G:294:ALA:HB2	1.98	0.46
1:G:7:GLY:HA2	2:G:335:NAD:O4B	2.14	0.46
1:G:327:HIS:CE1	1:G:331:VAL:HG21	2.51	0.46
1:G:32:ASP:OD2	2:G:335:NAD:H1B	2.16	0.46
1:R:54:LYS:O	1:R:55:GLY:C	2.53	0.46
1:G:142:THR:CG2	1:G:143:VAL:H	2.28	0.46
1:R:14:LEU:HD13	1:R:18:ALA:H	1.81	0.46
1:R:167:ILE:HD11	1:R:244:VAL:HG11	1.98	0.46
1:R:232:VAL:O	1:R:234:THR:N	2.49	0.46
1:R:312:ASP:O	1:R:316:GLY:N	2.45	0.46
1:R:327:HIS:ND1	1:R:331:VAL:CG2	2.74	0.46
1:G:324:LEU:HD12	1:G:325:LEU:HD23	1.97	0.46
1:R:41:VAL:CG1	1:R:64:LEU:HD11	2.44	0.46
1:G:198:GLY:O	1:G:199:ALA:HB3	2.13	0.46
1:G:1:SER:C	1:G:26:GLN:CG	2.84	0.46
1:G:252:TYR:CE2	1:G:298:ILE:CD1	2.98	0.46
1:G:319:GLN:HG3	1:G:320:ARG:HH22	1.80	0.46
1:G:79:PRO:CA	1:G:82:ILE:HG23	2.45	0.46
1:R:130:CYS:O	1:R:131:GLY:C	2.53	0.46
1:R:18:ALA:O	1:R:20:LEU:N	2.49	0.46
1:R:283:PHE:HE1	1:R:291:ILE:CD1	2.28	0.46
1:G:178:VAL:O	1:G:178:VAL:HG23	2.16	0.46
1:G:19:ALA:O	1:G:25:ALA:CA	2.63	0.46
1:R:138:SER:C	1:R:140:ASP:N	2.68	0.46
1:R:207:SER:O	1:R:208:THR:CB	2.55	0.46
1:R:260:LYS:O	1:R:263:SER:CB	2.63	0.46
1:R:245:ARG:CA	1:R:303:THR:O	2.54	0.46
1:R:332:ASP:OD2	1:R:332:ASP:N	2.48	0.46
1:R:150:THR:CG2	3:R:338:PO4:P	3.04	0.46
1:G:144:VAL:CG2	1:G:145:SER:N	2.79	0.46
1:G:197:ARG:CG	1:G:197:ARG:HH11	2.21	0.46
1:G:151:THR:HG23	1:G:213:ALA:HB1	1.94	0.46
1:R:176:HIS:HB3	1:R:231:ARG:HD2	1.98	0.46
1:R:221:LEU:CD2	1:R:225:LEU:HD12	2.46	0.46
1:R:245:ARG:C	1:R:246:LEU:HG	2.35	0.46
1:G:241:ASP:CG	1:G:306:LYS:NZ	2.67	0.46
1:G:298:ILE:CD1	1:G:298:ILE:C	2.82	0.45
1:G:45:LYS:HG3	1:G:57:VAL:CB	2.46	0.45
1:G:92:ILE:HG13	1:G:116:VAL:HG22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:261:THR:CG2	1:R:262:ALA:N	2.79	0.45
1:R:27:VAL:CG2	1:R:69:LYS:HB3	2.46	0.45
1:G:177:ALA:HB2	1:G:237:VAL:C	2.34	0.45
1:G:132:VAL:HG22	1:G:217:VAL:HG12	1.97	0.45
1:R:82:ILE:HD12	1:R:83:PRO:O	2.15	0.45
1:G:330:LYS:O	1:G:331:VAL:C	2.54	0.45
1:R:102:ILE:HG23	1:R:106:SER:HG	1.82	0.45
1:R:109:PHE:HZ	1:R:114:LYS:O	1.95	0.45
1:R:116:VAL:CG1	1:R:118:ILE:HD11	2.27	0.45
1:R:14:LEU:C	1:R:16:LEU:N	2.69	0.45
1:R:17:ARG:HB2	1:R:44:PHE:HZ	1.80	0.45
1:G:11:ILE:HG22	1:G:12:GLY:N	2.31	0.45
1:G:194:ARG:NE	1:G:207:SER:H	2.15	0.45
1:G:28:VAL:O	1:G:29:ALA:CB	2.64	0.45
1:G:37:LEU:O	1:G:38:GLU:C	2.54	0.45
1:G:52:VAL:HG23	1:G:53:PHE:H	1.81	0.45
1:R:17:ARG:O	1:R:20:LEU:CB	2.64	0.45
1:G:43:MET:HE1	1:R:187:GLY:HA2	1.98	0.45
1:R:176:HIS:CD2	1:R:177:ALA:C	2.89	0.45
1:R:31:ASN:OD1	1:R:32:ASP:N	2.50	0.45
1:R:313:ASN:HB2	2:R:339:NAD:O7N	2.17	0.45
1:R:26:GLN:C	1:R:27:VAL:CG2	2.56	0.45
1:R:324:LEU:CD1	1:R:324:LEU:C	2.81	0.45
1:G:40:MET:CE	1:G:73:VAL:HG11	2.46	0.45
1:R:107:ALA:O	1:R:108:HIS:C	2.53	0.45
1:G:163:GLU:H	1:G:163:GLU:HG2	1.57	0.45
1:G:324:LEU:CD1	1:G:325:LEU:CA	2.92	0.45
1:R:14:LEU:HG	1:R:318:SER:OG	2.16	0.45
1:R:54:LYS:HB3	1:R:55:GLY:H	1.49	0.45
1:G:10:ARG:HB2	2:G:335:NAD:O2N	2.17	0.45
1:G:208:THR:HG23	1:G:210:ALA:H	1.82	0.45
1:G:2:LYS:N	1:G:26:GLN:HG3	2.32	0.45
1:R:109:PHE:CE2	1:R:116:VAL:HG23	2.52	0.45
1:G:10:ARG:NE	1:G:314:GLU:OE1	2.50	0.45
1:G:267:LEU:CB	1:G:270:PHE:HD1	2.29	0.45
1:G:34:PHE:HD2	1:G:34:PHE:HA	1.70	0.45
1:R:187:GLY:O	1:R:188:PRO:O	2.35	0.45
1:R:224:LYS:O	1:R:225:LEU:HG	2.17	0.45
1:R:242:LEU:HG	1:R:243:THR:N	2.32	0.45
1:R:269:GLY:C	1:R:270:PHE:CD2	2.91	0.45
1:R:283:PHE:CD1	1:R:291:ILE:HD13	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:64:LEU:HA	1:R:64:LEU:HD13	1.76	0.45
1:G:260:LYS:O	1:G:263:SER:HB3	2.17	0.44
1:G:294:ALA:O	1:G:295:LYS:HB2	2.17	0.44
1:R:5:ILE:HG21	1:R:15:VAL:CG1	2.47	0.44
1:R:165:PHE:O	1:R:167:ILE:N	2.50	0.44
1:G:235:PRO:HB2	1:R:201:GLN:NE2	2.23	0.44
1:R:238:SER:HB3	1:R:311:TYR:CZ	2.50	0.44
1:R:5:ILE:HD11	1:R:30:VAL:CG2	2.47	0.44
1:G:201:GLN:H	1:G:201:GLN:HG2	1.30	0.44
1:R:137:TYR:HB3	1:R:327:HIS:CE1	2.49	0.44
1:G:104:LYS:H	1:G:104:LYS:HG3	1.55	0.44
1:G:132:VAL:O	1:G:134:LEU:CD2	2.32	0.44
1:G:17:ARG:NH1	1:G:44:PHE:O	2.51	0.44
1:G:17:ARG:NH2	1:G:53:PHE:CB	2.57	0.44
1:G:295:LYS:O	1:G:297:GLY:N	2.50	0.44
1:G:79:PRO:HA	1:G:82:ILE:HG21	1.98	0.44
1:R:163:GLU:H	1:R:163:GLU:HG2	1.67	0.44
1:G:270:PHE:O	1:G:271:LEU:CD2	2.63	0.44
1:R:17:ARG:NE	1:R:17:ARG:C	2.69	0.44
1:R:184:THR:O	1:R:185:VAL:CB	2.55	0.44
1:R:283:PHE:HD1	1:R:291:ILE:HD13	1.82	0.44
1:R:298:ILE:O	1:R:298:ILE:HG12	2.12	0.44
1:R:236:ASP:CG	1:R:314:GLU:HG3	2.38	0.44
1:R:324:LEU:CD2	1:R:328:MET:CG	2.94	0.44
1:G:193:TRP:CD1	1:G:195:GLY:N	2.85	0.44
1:R:193:TRP:CE3	1:R:193:TRP:HA	2.53	0.44
1:R:64:LEU:HD23	1:R:73:VAL:HG11	1.98	0.44
1:G:128:PHE:CE2	1:G:137:TYR:N	2.85	0.44
1:G:15:VAL:CG1	1:G:93:VAL:HG11	2.47	0.44
1:G:330:LYS:O	1:G:334:ALA:CB	2.59	0.44
1:R:178:VAL:HG22	1:R:235:PRO:O	2.17	0.44
1:R:215:GLY:O	1:R:218:ILE:N	2.51	0.44
1:R:170:GLY:CA	1:R:244:VAL:HG13	2.44	0.44
1:R:93:VAL:HG22	1:R:117:VAL:CG1	2.44	0.44
1:G:128:PHE:HE2	1:G:137:TYR:H	1.66	0.44
1:G:211:ALA:HB1	1:G:225:LEU:O	2.16	0.44
1:G:16:LEU:HD12	1:G:44:PHE:CZ	2.52	0.44
1:G:41:VAL:CA	1:G:57:VAL:HG22	2.48	0.44
1:G:256:LYS:O	1:G:273:TYR:CD1	2.67	0.44
2:G:335:NAD:C2B	2:G:335:NAD:N3A	2.81	0.44
1:R:146:ASN:C	1:R:317:TYR:HH	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:319:GLN:O	1:R:323:ASP:N	2.33	0.44
1:R:45:LYS:O	1:R:45:LYS:HG3	2.18	0.44
1:G:133:ASN:C	1:G:133:ASN:HD22	2.21	0.44
1:G:117:VAL:HG23	1:G:144:VAL:HG13	1.98	0.44
1:G:168:VAL:O	1:G:245:ARG:HB3	2.18	0.44
1:G:295:LYS:C	1:G:298:ILE:HG23	2.37	0.44
1:G:96:THR:HG21	1:G:99:PHE:CB	2.42	0.44
1:R:12:GLY:O	1:R:13:ARG:O	2.36	0.44
1:R:177:ALA:O	1:R:178:VAL:CB	2.65	0.44
1:R:320:ARG:HA	1:R:323:ASP:HB2	2.00	0.44
1:G:102:ILE:C	1:G:106:SER:HG	2.08	0.43
1:G:92:ILE:HD11	1:G:113:ALA:HB1	2.00	0.43
1:G:13:ARG:O	1:G:44:PHE:HE1	2.01	0.43
1:G:204:ILE:HG23	1:G:205:PRO:HD2	2.00	0.43
1:G:267:LEU:HB3	1:G:270:PHE:O	2.17	0.43
1:R:178:VAL:CG1	1:R:179:THR:H	2.19	0.43
1:R:94:GLU:CD	1:R:96:THR:N	2.63	0.43
1:G:283:PHE:O	1:G:284:ILE:C	2.54	0.43
1:G:291:ILE:O	1:G:291:ILE:CG1	2.64	0.43
1:G:142:THR:HG22	1:G:143:VAL:H	1.83	0.43
1:G:330:LYS:O	1:G:331:VAL:O	2.37	0.43
1:R:20:LEU:O	1:R:20:LEU:HD22	2.17	0.43
1:R:263:SER:O	1:R:264:GLU:C	2.56	0.43
1:R:16:LEU:HD23	1:R:28:VAL:CG1	2.48	0.43
1:R:37:LEU:O	1:R:38:GLU:C	2.55	0.43
1:G:119:SER:HA	1:G:317:TYR:CZ	2.53	0.43
1:G:174:THR:CG2	1:G:229:ALA:HB2	2.47	0.43
1:G:96:THR:OG1	1:G:99:PHE:CD2	2.62	0.43
1:R:193:TRP:C	1:R:195:GLY:N	2.69	0.43
1:R:283:PHE:CD1	1:R:291:ILE:CD1	3.01	0.43
1:R:291:ILE:O	1:R:310:TRP:CB	2.60	0.43
1:R:299:GLN:CA	1:R:299:GLN:NE2	2.79	0.43
1:G:127:MET:C	1:G:128:PHE:CD1	2.77	0.43
1:G:19:ALA:O	1:G:25:ALA:HA	2.18	0.43
1:G:267:LEU:HB3	1:G:270:PHE:HD1	1.83	0.43
1:G:325:LEU:O	1:G:329:GLN:HB2	2.19	0.43
1:G:91:TYR:OH	1:G:332:ASP:HB2	2.18	0.43
1:R:210:ALA:CB	1:R:227:GLY:HA3	2.48	0.43
1:R:223:GLY:C	1:R:225:LEU:N	2.68	0.43
1:R:326:LYS:H	1:R:326:LYS:HG2	1.61	0.43
1:G:17:ARG:HB2	1:G:44:PHE:HE1	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:293:ASP:OD2	1:G:296:ALA:HB2	2.19	0.43
1:G:117:VAL:CB	1:G:328:MET:CE	2.94	0.43
1:R:153:CYS:HB2	1:R:311:TYR:CB	2.46	0.43
1:R:175:VAL:HG23	1:R:239:VAL:HG22	2.00	0.43
1:R:211:ALA:HB1	1:R:225:LEU:O	2.19	0.43
1:R:278:VAL:HA	1:R:296:ALA:HA	1.99	0.43
1:G:161:LEU:O	1:G:165:PHE:CA	2.67	0.43
1:G:22:CYS:SG	1:G:319:GLN:OE1	2.76	0.43
1:R:105:ALA:O	1:R:106:SER:C	2.56	0.43
1:R:293:ASP:N	1:R:293:ASP:OD2	2.52	0.43
1:G:101:THR:OG1	1:G:124:ASP:CG	2.56	0.43
1:G:320:ARG:HG2	1:G:320:ARG:NH1	2.31	0.43
1:R:27:VAL:HG13	1:R:28:VAL:H	1.72	0.43
1:R:72:THR:CG2	1:R:73:VAL:N	2.81	0.43
1:G:109:PHE:HD2	1:G:113:ALA:HB3	1.83	0.43
1:G:309:SER:O	1:G:310:TRP:CG	2.71	0.43
1:G:40:MET:O	1:G:44:PHE:HB3	2.19	0.43
1:R:137:TYR:HE1	1:R:331:VAL:CG1	2.23	0.43
1:G:33:PRO:CD	1:G:76:GLU:O	2.63	0.43
1:R:94:GLU:OE2	1:R:95:SER:C	2.51	0.43
1:G:10:ARG:H	1:G:13:ARG:HH11	1.67	0.42
1:G:236:ASP:C	1:G:237:VAL:HG23	2.39	0.42
1:G:264:GLU:O	1:G:265:GLY:O	2.36	0.42
1:R:157:VAL:HG22	1:R:161:LEU:HD11	2.01	0.42
1:R:191:LYS:HG3	1:R:191:LYS:H	1.69	0.42
1:G:315:PHE:O	1:G:318:SER:CB	2.66	0.42
1:G:60:GLU:O	1:G:63:ALA:O	2.37	0.42
1:G:98:VAL:O	1:G:100:THR:HB	2.18	0.42
1:R:34:PHE:N	1:R:34:PHE:HD1	2.12	0.42
1:R:68:GLY:O	1:R:69:LYS:C	2.57	0.42
1:R:90:GLU:CA	1:R:90:GLU:OE2	2.67	0.42
1:G:243:THR:O	1:G:244:VAL:HG13	2.20	0.42
1:R:105:ALA:C	1:R:107:ALA:N	2.72	0.42
1:R:97:GLY:O	1:R:98:VAL:O	2.37	0.42
1:G:14:LEU:HD22	1:G:14:LEU:HA	1.85	0.42
1:G:13:ARG:O	1:G:17:ARG:HB2	2.18	0.42
1:G:242:LEU:HD21	1:G:244:VAL:HG13	2.01	0.42
1:G:286:ASP:OD1	1:G:288:ARG:NH1	2.42	0.42
1:G:10:ARG:CB	2:G:335:NAD:O2N	2.67	0.42
1:G:185:VAL:HG11	1:R:10:ARG:HD2	2.00	0.42
1:R:281:SER:O	1:R:282:ASP:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:107:ALA:O	1:G:109:PHE:N	2.52	0.42
1:G:10:ARG:HA	1:G:10:ARG:HE	1.83	0.42
1:G:137:TYR:HE1	1:G:144:VAL:HG12	1.83	0.42
1:G:58:LYS:HE3	1:G:58:LYS:HB2	1.67	0.42
1:G:64:LEU:HD23	1:G:73:VAL:HG12	1.98	0.42
1:R:129:VAL:C	1:R:133:ASN:HB3	2.33	0.42
1:R:137:TYR:CE1	1:R:331:VAL:HG12	2.52	0.42
1:G:133:ASN:CG	1:G:134:LEU:N	2.73	0.42
1:G:13:ARG:O	1:G:44:PHE:CE1	2.72	0.42
1:G:119:SER:HA	1:G:317:TYR:CE2	2.55	0.42
1:G:82:ILE:CD1	1:G:84:TRP:CE3	3.02	0.42
1:R:126:PRO:HB3	1:R:141:MET:HE1	2.01	0.42
1:G:129:VAL:HG23	1:G:131:GLY:H	1.85	0.42
1:G:313:ASN:O	1:G:314:GLU:O	2.37	0.42
1:G:319:GLN:CA	1:G:319:GLN:HE21	2.33	0.42
1:G:64:LEU:HA	1:G:64:LEU:HD13	1.87	0.42
1:G:2:LYS:HG3	1:G:90:GLU:OE2	2.20	0.42
1:G:99:PHE:HA	1:G:104:LYS:HD3	2.02	0.42
1:R:133:ASN:O	1:R:134:LEU:O	2.37	0.42
1:R:244:VAL:O	1:R:304:PHE:HA	2.20	0.42
1:R:2:LYS:O	1:R:91:TYR:HB2	2.20	0.42
1:G:289:SER:HB2	1:G:320:ARG:NE	2.20	0.42
1:G:10:ARG:CD	1:G:314:GLU:CD	2.88	0.42
1:G:98:VAL:O	1:G:99:PHE:C	2.58	0.42
1:R:275:GLU:O	1:R:276:ASP:HB3	2.19	0.42
1:R:311:TYR:O	1:R:311:TYR:CG	2.72	0.42
1:R:33:PRO:CB	1:R:77:MET:HG2	2.49	0.42
1:R:95:SER:C	1:R:96:THR:OG1	2.57	0.42
1:G:214:VAL:O	1:G:215:GLY:C	2.58	0.42
1:G:292:PHE:HB2	1:G:309:SER:CB	2.49	0.42
1:G:28:VAL:CG2	1:G:29:ALA:O	2.67	0.42
1:R:182:GLN:HE21	1:R:182:GLN:HB3	1.71	0.42
1:R:41:VAL:HA	1:R:57:VAL:HB	2.02	0.42
1:G:10:ARG:CA	1:G:10:ARG:HE	2.33	0.41
1:R:10:ARG:O	1:R:12:GLY:N	2.53	0.41
1:R:153:CYS:CB	1:R:311:TYR:HB3	2.48	0.41
1:G:0:ACE:CH3	1:G:26:GLN:CG	2.81	0.41
1:G:153:CYS:O	1:G:290:SER:OG	2.36	0.41
1:G:211:ALA:O	1:G:212:LYS:C	2.56	0.41
1:G:2:LYS:HE2	1:G:90:GLU:HG3	1.88	0.41
2:G:335:NAD:C3B	2:G:335:NAD:N3A	2.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:102:ILE:HG22	1:R:106:SER:HG	1.86	0.41
1:R:18:ALA:O	1:R:22:CYS:N	2.53	0.41
1:R:31:ASN:C	1:R:31:ASN:OD1	2.59	0.41
1:G:137:TYR:CD2	1:G:137:TYR:C	2.93	0.41
1:G:298:ILE:C	1:G:299:GLN:HE21	2.17	0.41
1:R:179:THR:O	1:R:179:THR:HG22	2.20	0.41
1:G:10:ARG:NH2	1:G:47:ASP:OD1	2.53	0.41
1:G:220:GLU:O	1:G:221:LEU:C	2.53	0.41
1:G:262:ALA:O	1:G:263:SER:C	2.58	0.41
1:G:310:TRP:HB3	1:G:311:TYR:H	1.33	0.41
1:R:92:ILE:O	1:R:116:VAL:HA	2.19	0.41
1:G:154:LEU:CD1	1:G:242:LEU:HD12	2.50	0.41
1:G:219:PRO:C	1:G:222:ASP:HB2	2.40	0.41
1:G:223:GLY:C	1:G:225:LEU:H	2.24	0.41
1:G:232:VAL:CB	1:G:233:PRO:HD2	2.29	0.41
1:G:251:SER:HG	1:G:254:ASP:CG	2.23	0.41
1:G:310:TRP:C	1:G:311:TYR:CD1	2.93	0.41
1:R:104:LYS:O	1:R:105:ALA:C	2.59	0.41
1:R:176:HIS:N	1:R:230:PHE:O	2.35	0.41
1:R:44:PHE:C	1:R:46:TYR:N	2.73	0.41
1:R:42:TYR:O	1:R:46:TYR:HB2	2.21	0.41
1:G:283:PHE:O	1:G:284:ILE:O	2.39	0.41
1:R:146:ASN:C	1:R:317:TYR:OH	2.59	0.41
1:R:148:SER:HB3	1:R:150:THR:HG23	2.02	0.41
1:R:133:ASN:O	1:R:134:LEU:C	2.58	0.41
1:R:221:LEU:HD22	1:R:225:LEU:HD12	2.03	0.41
1:R:77:MET:O	1:R:78:LYS:HB2	2.20	0.41
1:G:197:ARG:CG	1:G:197:ARG:NH1	2.83	0.41
1:G:206:SER:O	1:G:229:ALA:CA	2.68	0.41
1:G:177:ALA:HB2	1:G:234:THR:HG22	2.03	0.41
1:G:26:GLN:NE2	1:G:27:VAL:HB	2.35	0.41
1:G:82:ILE:O	1:G:82:ILE:CG1	2.63	0.41
1:R:116:VAL:HB	1:R:143:VAL:HG12	2.03	0.41
1:R:18:ALA:C	1:R:20:LEU:N	2.70	0.41
1:R:150:THR:OG1	1:R:209:GLY:O	2.25	0.41
1:R:129:VAL:CG1	1:R:217:VAL:CG1	2.77	0.41
1:R:26:GLN:O	1:R:27:VAL:HB	2.15	0.41
1:G:218:ILE:O	1:G:221:LEU:HB2	2.21	0.41
1:G:251:SER:OG	1:G:254:ASP:CG	2.59	0.41
1:G:34:PHE:O	1:G:35:ILE:CG1	2.68	0.41
1:R:102:ILE:CA	1:R:105:ALA:HB3	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:241:ASP:HA	1:R:307:VAL:O	2.21	0.41
1:R:237:VAL:HG21	1:R:281:SER:O	2.21	0.41
1:R:82:ILE:H	1:R:82:ILE:HG23	1.45	0.41
1:R:94:GLU:OE1	1:R:95:SER:N	2.53	0.41
1:G:35:ILE:HA	1:G:35:ILE:HD13	1.89	0.41
1:R:170:GLY:HA3	1:R:225:LEU:HD21	2.03	0.41
1:R:44:PHE:O	1:R:46:TYR:N	2.54	0.41
1:G:137:TYR:CD1	1:G:141:MET:SD	3.14	0.41
1:G:313:ASN:O	1:G:316:GLY:N	2.54	0.41
1:G:155:ALA:HB3	1:G:156:PRO:HD3	2.03	0.40
1:G:216:LYS:NZ	1:G:222:ASP:CG	2.68	0.40
1:G:252:TYR:CZ	1:G:298:ILE:CD1	3.04	0.40
1:R:135:GLU:O	1:R:137:TYR:N	2.54	0.40
1:R:10:ARG:CA	1:R:13:ARG:HE	2.29	0.40
1:R:147:ALA:HB1	1:R:151:THR:CG2	2.50	0.40
1:R:158:ALA:O	1:R:160:VAL:N	2.54	0.40
1:R:215:GLY:HA3	1:R:222:ASP:HB2	2.03	0.40
1:R:274:THR:HB	1:R:275:GLU:H	1.64	0.40
1:R:50:HIS:HE1	1:R:314:GLU:CB	2.34	0.40
1:G:213:ALA:O	1:G:217:VAL:CG2	2.41	0.40
1:G:265:GLY:HA3	1:G:266:PRO:HD2	1.91	0.40
1:G:1:SER:H	1:G:26:GLN:HB2	1.73	0.40
1:G:295:LYS:CA	1:G:298:ILE:CG1	2.97	0.40
1:G:326:LYS:H	1:G:326:LYS:HG2	1.57	0.40
1:R:1:SER:HB2	1:R:329:GLN:CG	2.45	0.40
1:R:218:ILE:HD12	1:R:220:GLU:HB3	1.85	0.40
1:R:176:HIS:HD2	1:R:231:ARG:CG	2.34	0.40
1:R:232:VAL:CG2	1:R:233:PRO:N	2.81	0.40
1:R:297:GLY:C	1:R:298:ILE:HG22	2.40	0.40
1:G:109:PHE:O	1:G:110:LYS:C	2.59	0.40
1:G:12:GLY:O	1:G:15:VAL:HG23	2.21	0.40
1:G:333:SER:C	1:G:334:ALA:OXT	2.60	0.40
1:G:61:ASP:O	1:G:63:ALA:N	2.55	0.40
1:R:104:LYS:HD3	1:R:104:LYS:H	1.86	0.40
1:R:10:ARG:N	1:R:13:ARG:CZ	2.84	0.40
1:R:318:SER:O	1:R:319:GLN:C	2.59	0.40
2:R:339:NAD:H2N	2:R:339:NAD:O5D	2.21	0.40
1:R:120:ALA:O	1:R:146:ASN:O	2.40	0.40
1:R:12:GLY:O	1:R:15:VAL:HB	2.22	0.40
1:R:15:VAL:HG12	1:R:16:LEU:N	2.36	0.40
1:R:267:LEU:O	1:R:270:PHE:CE1	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:153:CYS:SG	1:R:311:TYR:HB3	2.61	0.40
1:R:44:PHE:O	1:R:45:LYS:C	2.60	0.40
1:G:211:ALA:HB2	1:G:226:THR:CA	2.51	0.40
1:G:309:SER:C	1:G:310:TRP:CD1	2.94	0.40
1:G:310:TRP:O	1:G:311:TYR:CD1	2.75	0.40
1:R:172:MET:SD	1:R:210:ALA:HB1	2.62	0.40
1:R:181:THR:O	1:R:183:LYS:N	2.55	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.







Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:135:GLU:CB	1:R:220:GLU:OE2[4_555]	1.21	0.99
1:G:135:GLU:CG	1:R:220:GLU:OE2[4_555]	1.26	0.94
1:G:135:GLU:N	1:R:220:GLU:OE1[4_555]	1.32	0.88
1:G:135:GLU:CA	1:R:220:GLU:OE1[4_555]	1.53	0.67
1:G:135:GLU:CB	1:R:220:GLU:CD[4_555]	1.61	0.59
1:G:135:GLU:CB	1:R:220:GLU:OE1[4_555]	1.91	0.29
1:G:135:GLU:CA	1:R:220:GLU:CD[4_555]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	332/334 (99%)	178 (54%)	73 (22%)	81 (24%)		
1	R	332/334 (99%)	167 (50%)	72 (22%)	93 (28%)		
All	All	664/668 (99%)	345 (52%)	145 (22%)	174 (26%)		

All (174) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	2	LYS
1	G	10	ARG
1	G	13	ARG
1	G	25	ALA
1	G	28	VAL
1	G	34	PHE
1	G	54	LYS
1	G	61	ASP
1	G	68	GLY
1	G	69	LYS
1	G	76	GLU
1	G	83	PRO
1	G	99	PHE
1	G	113	ALA
1	G	120	ALA
1	G	125	ALA
1	G	159	LYS
1	G	185	VAL
1	G	188	PRO
1	G	189	SER
1	G	190	ALA
1	G	193	TRP
1	G	195	GLY
1	G	196	GLY
1	G	199	ALA
1	G	219	PRO
1	G	220	GLU
1	G	222	ASP
1	G	235	PRO
1	G	265	GLY
1	G	267	LEU
1	G	268	GLN
1	G	271	LEU
1	G	276	ASP
1	G	277	ASP
1	G	282	ASP
1	G	287	ASN
1	G	313	ASN
1	G	314	GLU
1	G	331	VAL
1	R	1	SER
1	R	2	LYS
1	R	10	ARG

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Mol	Chain	Res	Type
1	R	15	VAL
1	R	25	ALA
1	R	27	VAL
1	R	28	VAL
1	R	56	GLU
1	R	61	ASP
1	R	80	GLU
1	R	85	SER
1	R	86	LYS
1	R	87	ALA
1	R	101	THR
1	R	110	LYS
1	R	114	LYS
1	R	120	ALA
1	R	134	LEU
1	R	169	GLU
1	R	178	VAL
1	R	179	THR
1	R	181	THR
1	R	188	PRO
1	R	189	SER
1	R	190	ALA
1	R	195	GLY
1	R	196	GLY
1	R	199	ALA
1	R	214	VAL
1	R	218	ILE
1	R	220	GLU
1	R	265	GLY
1	R	268	GLN
1	R	271	LEU
1	R	273	TYR
1	R	275	GLU
1	R	280	SER
1	R	283	PHE
1	R	287	ASN
1	R	294	ALA
1	R	296	ALA
1	R	314	GLU
1	R	328	MET
1	R	329	GLN
1	G	1	SER

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Mol	Chain	Res	Type
1	G	29	ALA
1	G	37	LEU
1	G	78	LYS
1	G	84	TRP
1	G	87	ALA
1	G	96	THR
1	G	103	GLU
1	G	114	LYS
1	G	131	GLY
1	G	139	LYS
1	G	148	SER
1	G	169	GLU
1	G	237	VAL
1	G	278	VAL
1	G	302	LYS
1	R	11	ILE
1	R	29	ALA
1	R	55	GLY
1	R	98	VAL
1	R	111	GLY
1	R	125	ALA
1	R	136	LYS
1	R	139	LYS
1	R	159	LYS
1	R	167	ILE
1	R	185	VAL
1	R	209	GLY
1	R	235	PRO
1	R	248	LYS
1	R	279	VAL
1	R	282	ASP
1	R	302	LYS
1	G	12	GLY
1	G	53	PHE
1	G	80	GLU
1	G	101	THR
1	G	134	LEU
1	G	136	LYS
1	G	167	ILE
1	G	191	LYS
1	G	211	ALA
1	R	13	ARG

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Mol	Chain	Res	Type
1	R	54	LYS
1	R	79	PRO
1	R	84	TRP
1	R	105	ALA
1	R	122	SER
1	R	158	ALA
1	R	193	TRP
1	R	208	THR
1	R	224	LYS
1	R	277	ASP
1	R	289	SER
1	R	295	LYS
1	G	26	GLN
1	G	70	LYS
1	G	98	VAL
1	G	283	PHE
1	G	295	LYS
1	G	296	ALA
1	R	17	ARG
1	R	78	LYS
1	R	81	ASN
1	R	121	PRO
1	R	155	ALA
1	R	194	ARG
1	R	206	SER
1	R	212	LYS
1	R	222	ASP
1	R	323	ASP
1	G	105	ALA
1	G	181	THR
1	G	266	PRO
1	G	284	ILE
1	G	289	SER
1	G	332	ASP
1	R	103	GLU
1	R	166	GLU
1	R	182	GLN
1	R	202	ASN
1	G	41	VAL
1	G	166	GLU
1	R	112	GLY
1	R	192	ASP

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Mol	Chain	Res	Type
1	G	15	VAL
1	R	266	PRO
1	R	102	ILE
1	G	112	GLY
1	R	217	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	271/271 (100%)	149 (55%)	122 (45%)	0	0
1	R	271/271 (100%)	140 (52%)	131 (48%)	0	0
All	All	542/542 (100%)	289 (53%)	253 (47%)	0	0

All (253) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	3	ILE
1	G	6	ASN
1	G	10	ARG
1	G	13	ARG
1	G	14	LEU
1	G	17	ARG
1	G	20	LEU
1	G	21	SER
1	G	26	GLN
1	G	31	ASN
1	G	34	PHE
1	G	35	ILE
1	G	37	LEU
1	G	39	TYR
1	G	42	TYR
1	G	43	MET
1	G	45	LYS
1	G	47	ASP

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Mol	Chain	Res	Type
1	G	49	THR
1	G	52	VAL
1	G	56	GLU
1	G	57	VAL
1	G	58	LYS
1	G	59	MET
1	G	61	ASP
1	G	64	LEU
1	G	69	LYS
1	G	71	ILE
1	G	72	THR
1	G	80	GLU
1	G	81	ASN
1	G	82	ILE
1	G	84	TRP
1	G	85	SER
1	G	92	ILE
1	G	93	VAL
1	G	95	SER
1	G	96	THR
1	G	98	VAL
1	G	100	THR
1	G	101	THR
1	G	102	ILE
1	G	104	LYS
1	G	106	SER
1	G	108	HIS
1	G	110	LYS
1	G	117	VAL
1	G	118	ILE
1	G	122	SER
1	G	124	ASP
1	G	127	MET
1	G	129	VAL
1	G	132	VAL
1	G	133	ASN
1	G	134	LEU
1	G	139	LYS
1	G	140	ASP
1	G	141	MET
1	G	144	VAL
1	G	149	CYS

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Mol	Chain	Res	Type
1	G	154	LEU
1	G	160	VAL
1	G	163	GLU
1	G	171	LEU
1	G	174	THR
1	G	176	HIS
1	G	181	THR
1	G	191	LYS
1	G	194	ARG
1	G	197	ARG
1	G	201	GLN
1	G	203	ILE
1	G	206	SER
1	G	208	THR
1	G	216	LYS
1	G	218	ILE
1	G	220	GLU
1	G	224	LYS
1	G	228	MET
1	G	230	PHE
1	G	231	ARG
1	G	238	SER
1	G	240	VAL
1	G	243	THR
1	G	245	ARG
1	G	246	LEU
1	G	248	LYS
1	G	249	GLU
1	G	253	ASP
1	G	254	ASP
1	G	255	ILE
1	G	259	MET
1	G	261	THR
1	G	264	GLU
1	G	268	GLN
1	G	270	PHE
1	G	273	TYR
1	G	274	THR
1	G	278	VAL
1	G	279	VAL
1	G	280	SER
1	G	283	PHE

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Mol	Chain	Res	Type
1	G	284	ILE
1	G	287	ASN
1	G	288	ARG
1	G	291	ILE
1	G	292	PHE
1	G	299	GLN
1	G	300	LEU
1	G	301	SER
1	G	302	LYS
1	G	303	THR
1	G	308	VAL
1	G	312	ASP
1	G	313	ASN
1	G	319	GLN
1	G	320	ARG
1	G	324	LEU
1	G	326	LYS
1	G	328	MET
1	G	332	ASP
1	G	333	SER
1	R	2	LYS
1	R	3	ILE
1	R	5	ILE
1	R	11	ILE
1	R	13	ARG
1	R	14	LEU
1	R	15	VAL
1	R	17	ARG
1	R	20	LEU
1	R	22	CYS
1	R	26	GLN
1	R	28	VAL
1	R	32	ASP
1	R	37	LEU
1	R	39	TYR
1	R	40	MET
1	R	42	TYR
1	R	43	MET
1	R	45	LYS
1	R	47	ASP
1	R	52	VAL
1	R	54	LYS

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Mol	Chain	Res	Type
1	R	57	VAL
1	R	59	MET
1	R	60	GLU
1	R	64	LEU
1	R	67	ASP
1	R	71	ILE
1	R	73	VAL
1	R	75	ASN
1	R	76	GLU
1	R	77	MET
1	R	81	ASN
1	R	82	ILE
1	R	84	TRP
1	R	86	LYS
1	R	92	ILE
1	R	94	GLU
1	R	96	THR
1	R	100	THR
1	R	104	LYS
1	R	108	HIS
1	R	110	LYS
1	R	115	LYS
1	R	118	ILE
1	R	124	ASP
1	R	129	VAL
1	R	132	VAL
1	R	133	ASN
1	R	134	LEU
1	R	136	LYS
1	R	139	LYS
1	R	140	ASP
1	R	141	MET
1	R	142	THR
1	R	144	VAL
1	R	148	SER
1	R	150	THR
1	R	154	LEU
1	R	157	VAL
1	R	159	LYS
1	R	162	HIS
1	R	163	GLU
1	R	164	ASN

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Mol	Chain	Res	Type
1	R	165	PHE
1	R	166	GLU
1	R	167	ILE
1	R	171	LEU
1	R	172	MET
1	R	173	THR
1	R	178	VAL
1	R	179	THR
1	R	181	THR
1	R	184	THR
1	R	185	VAL
1	R	192	ASP
1	R	193	TRP
1	R	194	ARG
1	R	201	GLN
1	R	203	ILE
1	R	204	ILE
1	R	208	THR
1	R	217	VAL
1	R	218	ILE
1	R	221	LEU
1	R	222	ASP
1	R	224	LYS
1	R	228	MET
1	R	231	ARG
1	R	232	VAL
1	R	237	VAL
1	R	239	VAL
1	R	240	VAL
1	R	243	THR
1	R	244	VAL
1	R	245	ARG
1	R	246	LEU
1	R	252	TYR
1	R	253	ASP
1	R	254	ASP
1	R	255	ILE
1	R	261	THR
1	R	263	SER
1	R	264	GLU
1	R	270	PHE
1	R	271	LEU

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Mol	Chain	Res	Type
1	R	280	SER
1	R	282	ASP
1	R	283	PHE
1	R	284	ILE
1	R	287	ASN
1	R	291	ILE
1	R	292	PHE
1	R	293	ASP
1	R	298	ILE
1	R	300	LEU
1	R	301	SER
1	R	302	LYS
1	R	303	THR
1	R	306	LYS
1	R	310	TRP
1	R	313	ASN
1	R	315	PHE
1	R	318	SER
1	R	319	GLN
1	R	320	ARG
1	R	324	LEU
1	R	326	LYS
1	R	329	GLN
1	R	332	ASP
1	R	333	SER

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

Mol	Chain	Res	Type
1	G	6	ASN
1	G	26	GLN
1	G	75	ASN
1	G	133	ASN
1	G	268	GLN
1	G	299	GLN
1	G	313	ASN
1	G	319	GLN
1	G	327	HIS
1	R	26	GLN
1	R	50	HIS
1	R	75	ASN
1	R	133	ASN

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Mol	Chain	Res	Type
1	R	201	GLN
1	R	299	GLN
1	R	313	ASN
1	R	319	GLN
1	R	327	HIS

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](#)

Of 6 ligands modelled in this entry, 4 are modelled with single atom - leaving 2 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$
2	NAD	G	335	-	42,48,48	0.73	1 (2%)	50,73,73	0.88	3 (6%)
2	NAD	R	339	-	42,48,48	0.72	1 (2%)	50,73,73	1.70	4 (8%)

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	NAD	G	335	-	-	9/26/62/62	0/5/5/5
2	NAD	R	339	-	-	12/26/62/62	0/5/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	339	NAD	C8A-N7A	-2.55	1.30	1.34
2	G	335	NAD	C8A-N7A	-2.53	1.30	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	339	NAD	O2A-PA-O5B	7.85	144.21	107.75
2	R	339	NAD	O2A-PA-O1A	-7.30	76.17	112.24
2	G	335	NAD	O2A-PA-O5B	2.61	119.85	107.75
2	G	335	NAD	O4D-C1D-C2D	-2.41	103.41	106.93
2	R	339	NAD	O4D-C1D-C2D	-2.26	103.62	106.93
2	G	335	NAD	C5A-C6A-N6A	2.04	123.46	120.35
2	R	339	NAD	C5A-C6A-N6A	2.04	123.45	120.35

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	335	NAD	C5B-O5B-PA-O1A
2	G	335	NAD	C5B-O5B-PA-O2A
2	G	335	NAD	C5D-O5D-PN-O3
2	G	335	NAD	C5D-O5D-PN-O1N
2	G	335	NAD	O4D-C4D-C5D-O5D
2	R	339	NAD	C5B-O5B-PA-O1A
2	R	339	NAD	C5D-O5D-PN-O3
2	R	339	NAD	C5D-O5D-PN-O1N
2	R	339	NAD	C5D-O5D-PN-O2N
2	R	339	NAD	O4D-C4D-C5D-O5D
2	G	335	NAD	C3D-C4D-C5D-O5D
2	R	339	NAD	O4B-C4B-C5B-O5B
2	R	339	NAD	C3B-C4B-C5B-O5B
2	R	339	NAD	C3D-C4D-C5D-O5D
2	G	335	NAD	C5B-O5B-PA-O3
2	R	339	NAD	PN-O3-PA-O2A
2	G	335	NAD	C5D-O5D-PN-O2N
2	R	339	NAD	C4D-C5D-O5D-PN

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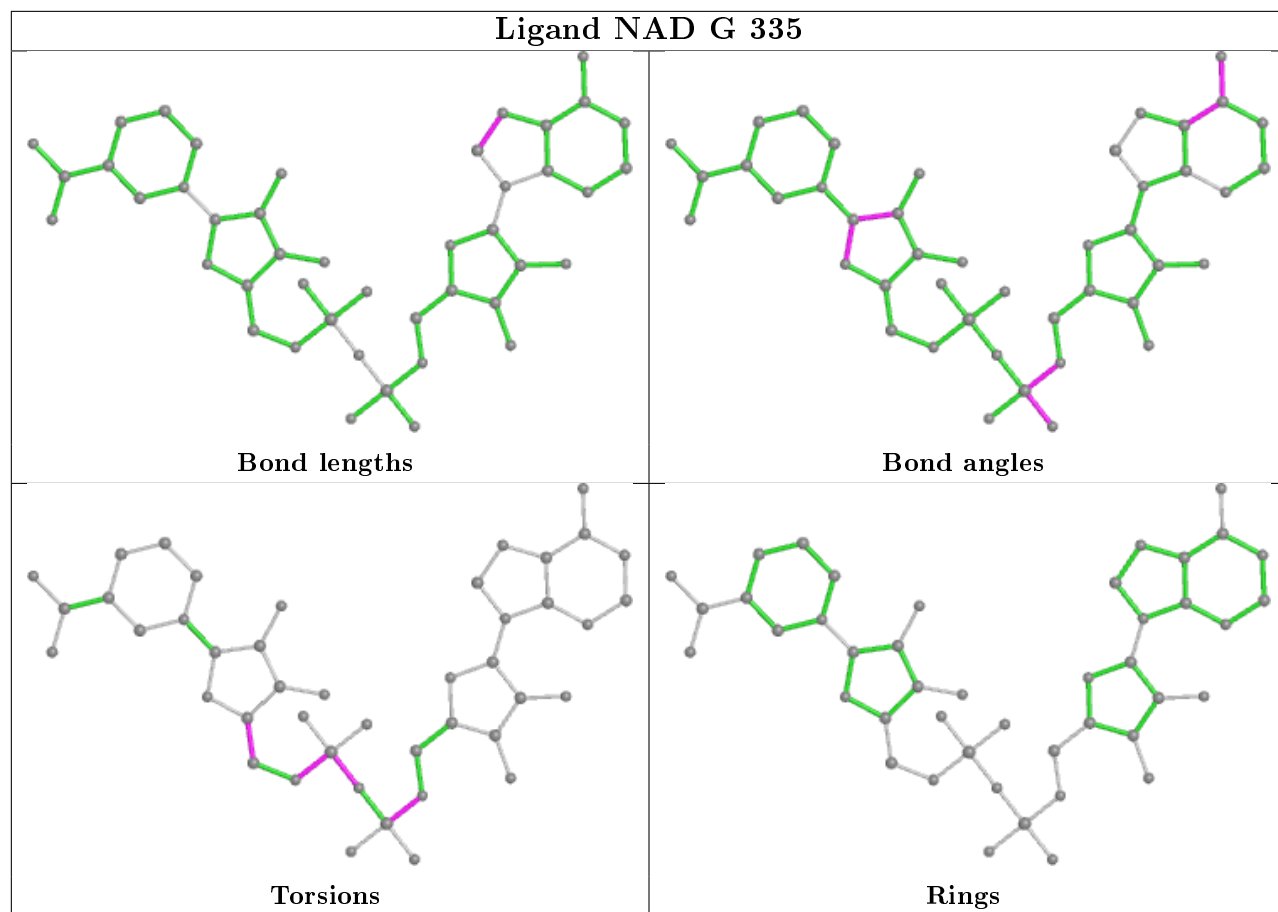
Mol	Chain	Res	Type	Atoms
2	R	339	NAD	PA-O3-PN-O2N
2	R	339	NAD	C5B-O5B-PA-O3
2	G	335	NAD	PA-O3-PN-O2N

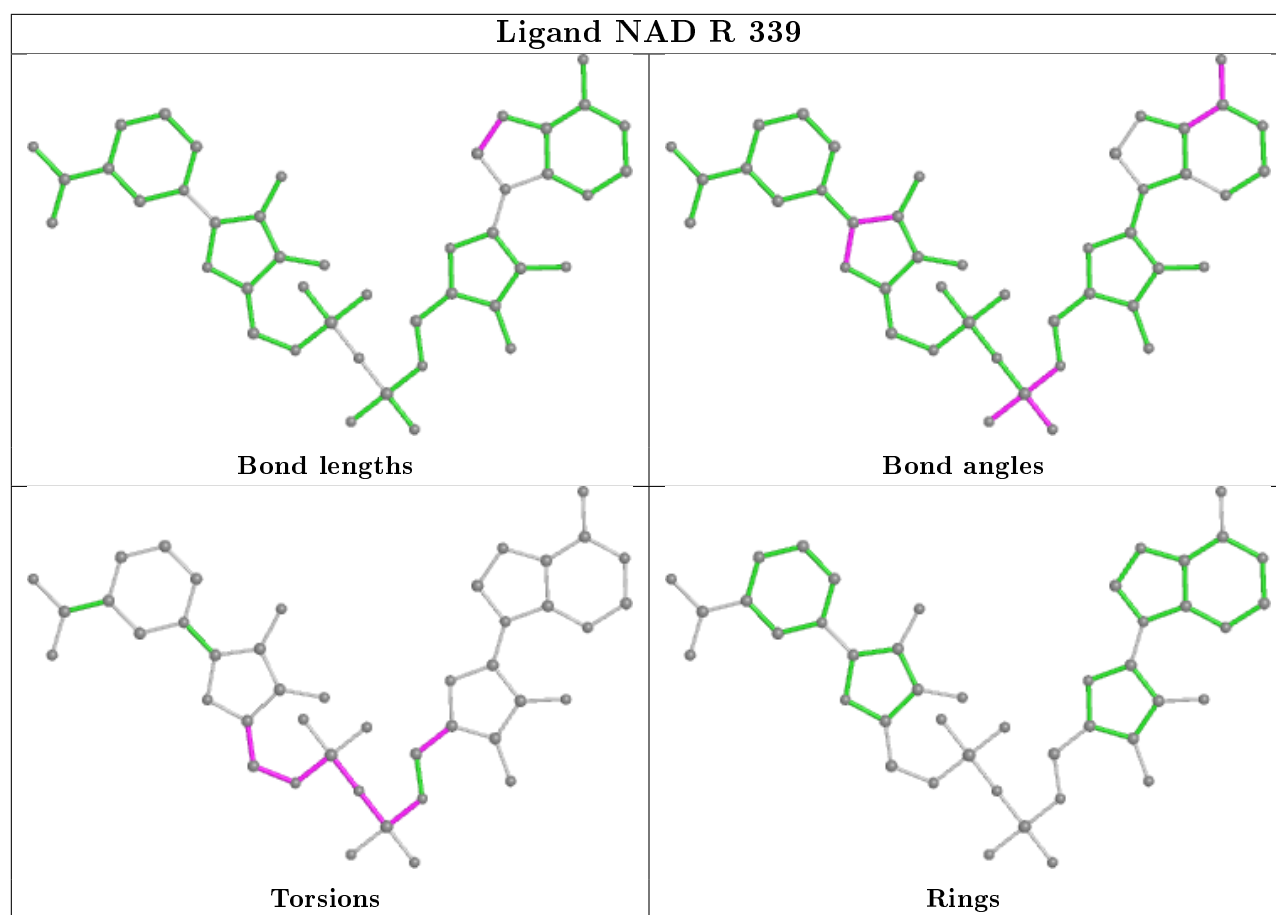
There are no ring outliers.

2 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	335	NAD	20	0
2	R	339	NAD	8	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.