



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:58 AM UTC

PDB ID : 3GPD / pdb_00003gpd
Title : TWINNING IN CRYSTALS OF HUMAN SKELETAL MUSCLE D-GLYCE
RALDEHYDE-3-PHOSPHATE DEHYDROGENASE
Authors : Watson, H.C.; Campbell, J.C.
Deposited on : 1983-06-20
Resolution : 3.50 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

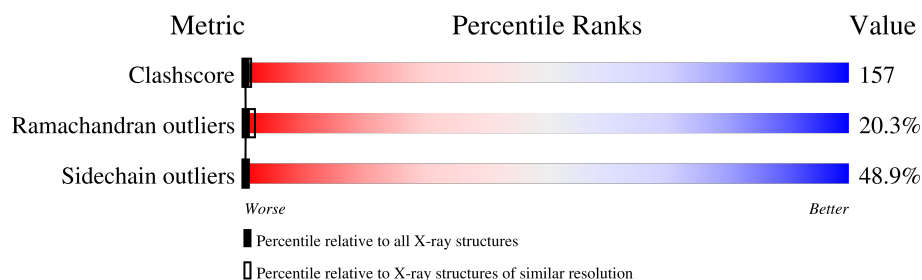
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	G	334	5% 31% 34% 29%
1	R	334	5% 38% 39% 18%

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
2	SO4	G	338	-	-	X	-
2	SO4	G	340	-	-	X	-
2	SO4	R	338	-	-	X	-
2	SO4	R	340	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAD	G	336	X	-	-	-

2 Entry composition [i](#)

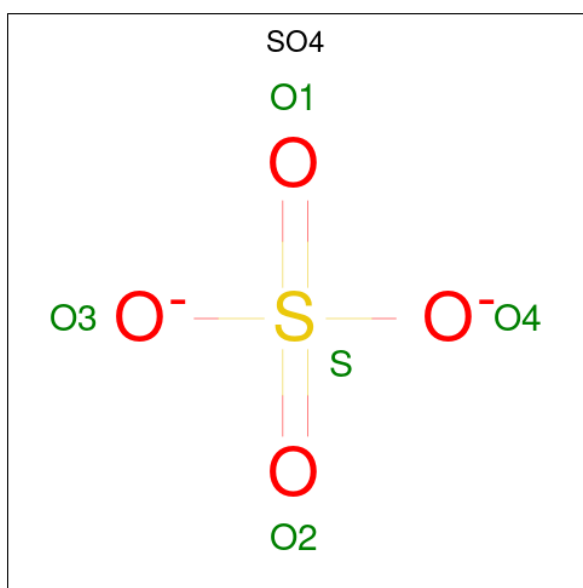
There are 3 unique types of molecules in this entry. The entry contains 5154 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

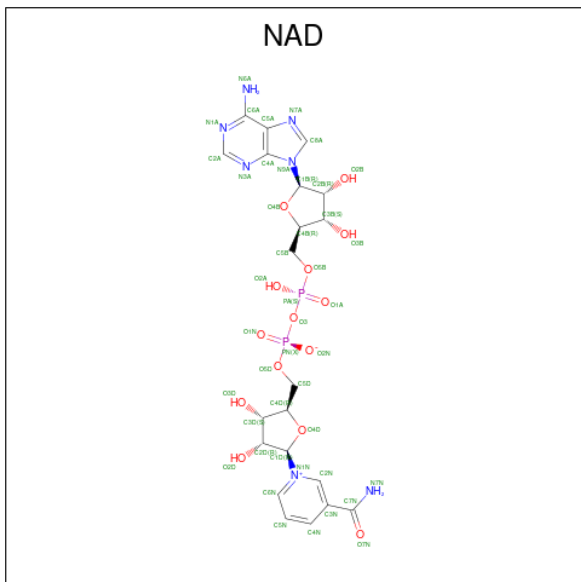
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	334	Total	C	N	O	S	0	0	0
			2523	1601	431	479	12			
1	G	334	Total	C	N	O	S	0	0	0
			2523	1601	431	479	12			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	R	1	Total	O	S	0	0
			5	4	1		
2	R	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $\text{C}_{21}\text{H}_{27}\text{N}_7\text{O}_{14}\text{P}_2$).



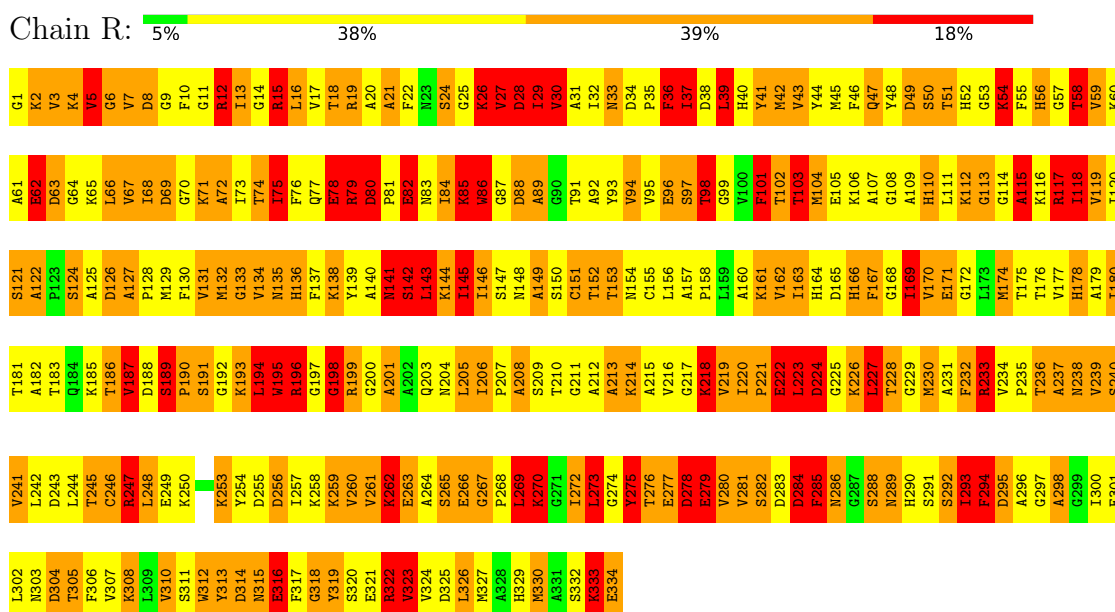
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	R	1	Total 44	C 21	N 7	O 14	P 2	0	0
3	G	1	Total 44	C 21	N 7	O 14	P 2	0	0

3 Residue-property plots

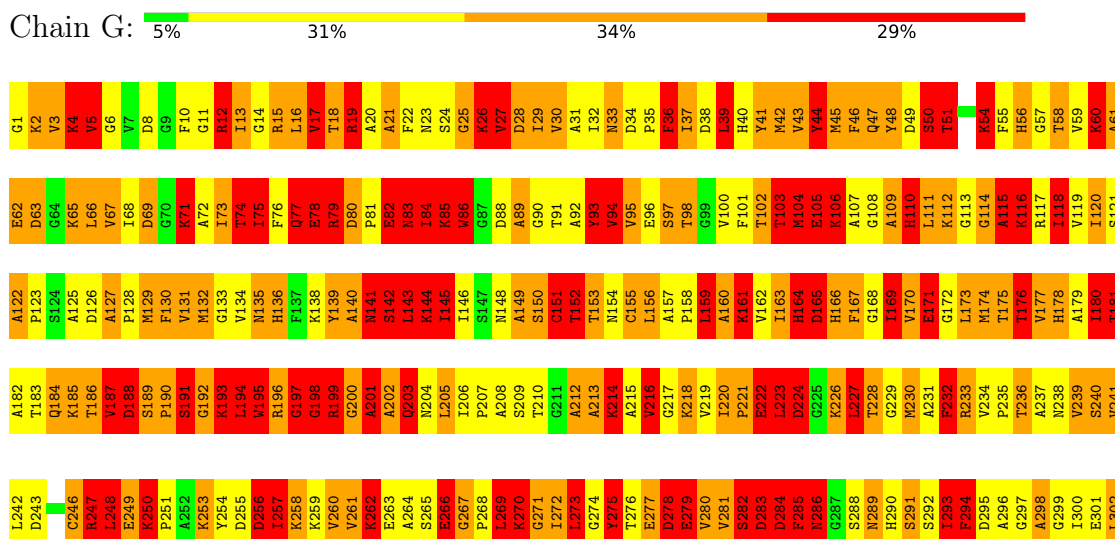
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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



• Molecule 1: D-GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE



K303	D304	T305	F306	V307	K308	L309	V310	S311	W312	Y313	D314	K315	E316	F317	G318	Y319	S320	E321	R322	V323	V324	D325	L326	M327	A328	H329	M330	A331	S332	K333	E334
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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	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	132.40Å 97.90Å 81.60Å 90.00° 114.30° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	0.330 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5154	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: SO4, NAD

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	1.89	69/2573 (2.7%)	2.47	195/3479 (5.6%)
1	R	1.46	17/2573 (0.7%)	1.97	99/3479 (2.8%)
All	All	1.69	86/5146 (1.7%)	2.23	294/6958 (4.2%)

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	279	GLU	N-CA	10.00	1.59	1.46
1	G	195	TRP	N-CA	9.56	1.58	1.46
1	G	198	GLY	N-CA	9.44	1.59	1.45
1	G	194	LEU	N-CA	8.97	1.57	1.46
1	G	278	ASP	CA-C	8.81	1.64	1.52
1	G	329	HIS	CB-CG	8.29	1.61	1.50
1	G	193	LYS	C-N	8.14	1.45	1.33
1	G	193	LYS	CA-C	8.11	1.63	1.52
1	G	94	VAL	N-CA	7.96	1.55	1.46
1	G	194	LEU	C-N	7.71	1.44	1.33
1	G	222	GLU	CA-C	7.39	1.62	1.52
1	R	279	GLU	N-CA	7.37	1.55	1.46
1	G	236	THR	N-CA	7.33	1.55	1.46
1	G	197	GLY	C-N	7.25	1.44	1.33
1	G	314	ASP	CA-CB	7.19	1.64	1.53
1	R	269	LEU	N-CA	7.16	1.54	1.46
1	G	78	GLU	CA-C	6.86	1.61	1.52
1	G	164	HIS	CB-CG	6.79	1.59	1.50
1	G	304	ASP	CA-CB	6.69	1.64	1.53
1	G	194	LEU	CA-C	6.61	1.61	1.52
1	G	271	GLY	N-CA	6.53	1.54	1.45
1	G	223	LEU	N-CA	6.47	1.54	1.46
1	G	86	TRP	NE1-CE2	-6.35	1.30	1.37
1	R	195	TRP	N-CA	6.34	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	86	TRP	NE1-CE2	-6.29	1.30	1.37
1	R	227	LEU	N-CA	6.28	1.53	1.45
1	R	195	TRP	NE1-CE2	-6.27	1.30	1.37
1	G	24	SER	N-CA	6.21	1.54	1.46
1	R	270	LYS	N-CA	6.20	1.54	1.46
1	R	278	ASP	CA-C	6.01	1.60	1.52
1	R	269	LEU	CA-C	5.94	1.60	1.52
1	G	291	SER	N-CA	5.92	1.53	1.46
1	R	333	LYS	CA-C	5.91	1.60	1.52
1	G	109	ALA	N-CA	5.91	1.53	1.46
1	G	195	TRP	CA-CB	5.90	1.63	1.53
1	G	169	ILE	C-N	-5.89	1.25	1.33
1	G	284	ASP	N-CA	5.87	1.53	1.46
1	G	278	ASP	N-CA	5.83	1.53	1.46
1	G	314	ASP	C-N	5.83	1.41	1.33
1	G	171	GLU	N-CA	5.81	1.53	1.46
1	G	74	THR	N-CA	5.81	1.52	1.45
1	G	181	THR	N-CA	-5.78	1.38	1.45
1	G	227	LEU	N-CA	5.64	1.52	1.46
1	G	103	THR	N-CA	5.63	1.53	1.46
1	G	195	TRP	NE1-CE2	-5.62	1.31	1.37
1	G	93	TYR	CA-C	5.61	1.59	1.52
1	R	96	GLU	N-CA	5.61	1.53	1.46
1	G	314	ASP	CA-C	5.58	1.60	1.53
1	G	282	SER	C-N	-5.53	1.25	1.33
1	R	312	TRP	NE1-CE2	-5.45	1.31	1.37
1	G	50	SER	C-N	-5.43	1.25	1.33
1	G	266	GLU	CA-CB	5.41	1.62	1.53
1	G	313	TYR	N-CA	5.41	1.53	1.46
1	R	208	ALA	N-CA	5.40	1.53	1.46
1	R	136	HIS	N-CA	5.40	1.53	1.46
1	G	69	ASP	N-CA	-5.39	1.38	1.46
1	G	224	ASP	N-CA	5.39	1.53	1.46
1	R	115	ALA	N-CA	5.39	1.53	1.46
1	G	312	TRP	NE1-CE2	-5.38	1.31	1.37
1	G	159	LEU	N-CA	5.38	1.52	1.46
1	G	78	GLU	N-CA	5.37	1.53	1.46
1	G	24	SER	CA-C	5.37	1.59	1.52
1	G	250	LYS	N-CA	5.36	1.53	1.45
1	R	145	ILE	N-CA	5.36	1.52	1.46
1	G	185	LYS	C-N	5.36	1.41	1.33
1	G	315	ASN	N-CA	5.33	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	144	LYS	N-CA	-5.32	1.39	1.46
1	G	36	PHE	CA-C	5.32	1.59	1.52
1	G	222	GLU	C-N	5.32	1.41	1.33
1	G	262	LYS	N-CA	5.30	1.53	1.46
1	G	204	ASN	CA-C	5.30	1.59	1.52
1	R	6	GLY	N-CA	5.27	1.50	1.45
1	G	290	HIS	N-CA	5.26	1.52	1.45
1	G	153	THR	CA-C	5.26	1.59	1.52
1	G	115	ALA	N-CA	5.25	1.52	1.46
1	G	224	ASP	CA-CB	5.22	1.62	1.53
1	G	135	ASN	N-CA	5.17	1.52	1.46
1	G	283	ASP	CA-CB	5.16	1.62	1.53
1	G	228	THR	N-CA	5.15	1.52	1.46
1	G	304	ASP	CA-C	5.13	1.59	1.52
1	G	106	LYS	N-CA	5.11	1.52	1.46
1	G	183	THR	N-CA	5.11	1.52	1.46
1	G	116	LYS	N-CA	5.07	1.52	1.46
1	G	270	LYS	CA-C	5.04	1.59	1.52
1	G	145	ILE	N-CA	5.02	1.51	1.46
1	G	262	LYS	CA-CB	5.01	1.61	1.53

All (294) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	85	LYS	O-C-N	14.05	135.56	121.79
1	G	279	GLU	O-C-N	12.91	139.77	122.59
1	R	27	VAL	O-C-N	12.75	138.50	122.57
1	G	293	ILE	O-C-N	12.64	136.05	123.03
1	G	278	ASP	O-C-N	-12.59	105.85	122.59
1	G	196	ARG	CB-CA-C	11.93	130.36	111.51
1	G	304	ASP	CA-CB-CG	11.83	124.43	112.60
1	G	314	ASP	CA-CB-CG	11.78	124.38	112.60
1	G	314	ASP	CB-CA-C	11.31	127.01	111.63
1	G	304	ASP	O-C-N	11.17	137.45	122.59
1	G	180	ILE	O-C-N	11.14	134.49	122.57
1	G	83	ASN	CA-C-N	-11.09	102.02	121.97
1	G	83	ASN	C-N-CA	-11.09	102.02	121.97
1	R	143	LEU	O-C-N	11.08	135.85	123.22
1	R	194	LEU	N-CA-CB	-10.77	103.33	114.10
1	G	223	LEU	O-C-N	-10.71	108.34	122.59
1	G	196	ARG	O-C-N	10.65	140.63	122.21
1	G	334	GLU	CA-C-O	10.57	138.76	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	28	ASP	O-C-N	10.46	136.51	122.59
1	G	201	ALA	O-C-N	10.29	136.28	122.59
1	R	36	PHE	CA-CB-CG	10.14	123.94	113.80
1	G	177	VAL	O-C-N	10.12	137.64	122.76
1	G	63	ASP	O-C-N	9.59	135.34	122.59
1	G	186	THR	O-C-N	9.53	134.08	123.22
1	G	94	VAL	O-C-N	-9.41	113.20	122.98
1	G	198	GLY	O-C-N	9.36	134.87	122.70
1	R	278	ASP	O-C-N	-9.29	110.23	122.59
1	R	180	ILE	O-C-N	9.24	132.68	122.61
1	G	280	VAL	O-C-N	9.19	134.05	122.57
1	G	36	PHE	CA-CB-CG	9.13	122.93	113.80
1	G	238	ASN	O-C-N	9.05	134.70	123.21
1	G	78	GLU	O-C-N	8.97	134.52	122.59
1	G	191	SER	O-C-N	8.93	134.47	122.59
1	R	36	PHE	CB-CA-C	-8.93	92.65	110.42
1	R	269	LEU	N-CA-C	8.76	120.52	110.97
1	G	303	ASN	N-CA-CB	-8.74	95.71	110.49
1	G	169	ILE	O-C-N	8.66	133.39	122.57
1	R	36	PHE	N-CA-CB	8.51	124.87	110.49
1	R	293	ILE	O-C-N	8.50	131.79	123.03
1	G	303	ASN	CA-CB-CG	8.48	121.08	112.60
1	G	313	TYR	CB-CA-C	-8.48	93.55	110.42
1	G	333	LYS	O-C-N	-8.47	111.33	122.59
1	G	290	HIS	CB-CA-C	-8.47	92.25	110.45
1	G	125	ALA	O-C-N	8.46	130.83	122.03
1	G	304	ASP	CA-C-N	8.45	137.69	121.54
1	G	304	ASP	C-N-CA	8.45	137.69	121.54
1	R	278	ASP	CB-CA-C	8.43	127.20	110.42
1	G	270	LYS	CA-C-N	8.42	129.46	120.03
1	G	270	LYS	C-N-CA	8.42	129.46	120.03
1	R	314	ASP	N-CA-C	-8.35	101.12	113.40
1	R	304	ASP	CA-CB-CG	8.35	120.95	112.60
1	G	229	GLY	O-C-N	8.21	132.95	123.51
1	R	218	LYS	O-C-N	8.17	130.82	122.08
1	G	27	VAL	O-C-N	8.16	132.77	122.57
1	G	209	SER	O-C-N	8.09	132.17	123.03
1	R	26	LYS	O-C-N	8.09	133.34	122.59
1	G	196	ARG	N-CA-C	-8.08	101.90	112.24
1	R	194	LEU	O-C-N	8.07	129.80	121.89
1	G	202	ALA	O-C-N	8.03	132.67	122.23
1	G	51	THR	CB-CA-C	8.03	125.28	110.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	290	HIS	CA-CB-CG	7.91	121.70	113.80
1	R	198	GLY	O-C-N	7.89	132.96	122.70
1	R	88	ASP	O-C-N	7.88	133.07	122.82
1	R	323	VAL	O-C-N	7.88	129.64	121.91
1	G	69	ASP	N-CA-CB	-7.79	100.36	112.13
1	G	118	ILE	O-C-N	-7.79	114.85	123.26
1	G	294	PHE	O-C-N	7.78	133.14	123.10
1	G	275	TYR	O-C-N	7.77	132.93	122.59
1	G	277	GLU	N-CA-C	-7.74	102.94	112.38
1	R	118	ILE	O-C-N	-7.72	114.16	123.03
1	R	50	SER	O-C-N	7.68	130.26	122.12
1	G	165	ASP	N-CA-CB	7.68	122.05	110.22
1	G	78	GLU	CA-C-N	7.63	133.93	122.95
1	G	78	GLU	C-N-CA	7.63	133.93	122.95
1	G	314	ASP	N-CA-C	-7.62	101.71	111.92
1	G	167	PHE	CB-CA-C	-7.55	98.47	110.85
1	R	136	HIS	CB-CA-C	-7.54	106.82	115.79
1	G	169	ILE	CB-CA-C	-7.53	98.95	111.29
1	G	222	GLU	CB-CA-C	7.51	125.37	110.42
1	G	60	LYS	O-C-N	7.49	132.88	123.15
1	R	94	VAL	O-C-N	-7.48	115.20	122.98
1	R	101	PHE	O-C-N	7.46	132.50	122.59
1	G	83	ASN	O-C-N	-7.43	114.24	122.12
1	G	197	GLY	CA-C-N	7.43	135.97	121.41
1	G	197	GLY	C-N-CA	7.43	135.97	121.41
1	R	27	VAL	CB-CA-C	7.40	123.42	111.29
1	G	219	VAL	N-CA-CB	-7.36	101.81	110.64
1	G	310	VAL	O-C-N	7.32	131.11	123.20
1	R	277	GLU	N-CA-C	-7.24	103.43	111.82
1	G	82	GLU	O-C-N	7.22	129.77	122.12
1	G	236	THR	CB-CA-C	-7.14	101.01	109.80
1	R	87	GLY	O-C-N	7.14	130.74	122.68
1	G	214	LYS	O-C-N	7.12	132.06	122.59
1	G	110	HIS	CA-CB-CG	-7.12	106.69	113.80
1	G	176	THR	O-C-N	7.06	131.57	123.31
1	R	79	ARG	O-C-N	7.04	131.28	122.84
1	G	219	VAL	CB-CA-C	7.03	121.22	111.94
1	R	269	LEU	CB-CA-C	-6.99	100.20	110.96
1	G	305	THR	N-CA-CB	-6.98	98.70	110.49
1	G	283	ASP	CA-CB-CG	6.97	119.57	112.60
1	R	87	GLY	N-CA-C	-6.96	105.74	114.16
1	R	151	CYS	O-C-N	6.91	129.28	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	232	PHE	CA-CB-CG	-6.89	106.91	113.80
1	R	142	SER	O-C-N	6.89	131.75	122.59
1	R	238	ASN	O-C-N	6.86	131.21	123.19
1	G	165	ASP	CB-CA-C	-6.85	97.96	110.63
1	G	289	ASN	CA-CB-CG	6.85	119.45	112.60
1	G	104	MET	N-CA-CB	6.84	119.92	110.01
1	R	177	VAL	O-C-N	6.81	131.08	122.57
1	G	204	ASN	CA-CB-CG	6.80	119.40	112.60
1	G	333	LYS	CB-CA-C	6.79	123.94	110.42
1	G	224	ASP	CA-CB-CG	6.79	119.39	112.60
1	G	247	ARG	O-C-N	-6.79	115.22	123.30
1	G	201	ALA	CA-C-N	6.75	132.13	120.58
1	G	201	ALA	C-N-CA	6.75	132.13	120.58
1	R	333	LYS	CA-C-N	6.74	133.83	121.70
1	R	333	LYS	C-N-CA	6.74	133.83	121.70
1	G	312	TRP	N-CA-C	6.72	116.85	108.19
1	G	285	PHE	O-C-N	-6.71	113.67	122.59
1	G	183	THR	N-CA-C	6.69	119.40	111.71
1	G	182	ALA	CA-C-N	6.68	129.90	120.28
1	G	182	ALA	C-N-CA	6.68	129.90	120.28
1	G	256	ASP	N-CA-C	6.62	118.29	111.14
1	R	232	PHE	CA-CB-CG	-6.60	107.20	113.80
1	R	29	ILE	N-CA-CB	-6.59	100.35	111.23
1	R	169	ILE	CB-CA-C	-6.59	100.47	111.29
1	R	277	GLU	O-C-N	6.58	130.36	122.27
1	G	140	ALA	O-C-N	6.55	130.87	123.27
1	G	141	ASN	O-C-N	6.55	131.30	122.59
1	G	79	ARG	O-C-N	6.54	132.93	122.99
1	G	186	THR	N-CA-CB	6.52	120.92	110.16
1	G	196	ARG	CA-C-N	6.46	134.07	121.41
1	G	196	ARG	C-N-CA	6.46	134.07	121.41
1	G	170	VAL	N-CA-C	-6.46	98.75	108.17
1	R	246	CYS	O-C-N	6.45	130.60	123.25
1	G	61	ALA	O-C-N	6.44	130.79	122.87
1	R	75	ILE	O-C-N	6.43	129.87	123.18
1	G	48	TYR	CB-CA-C	-6.43	100.50	110.78
1	G	304	ASP	N-CA-CB	-6.42	99.63	110.49
1	G	26	LYS	O-C-N	6.41	131.11	122.59
1	R	267	GLY	N-CA-C	6.40	125.40	112.34
1	G	185	LYS	CB-CA-C	-6.39	98.70	109.50
1	R	223	LEU	O-C-N	-6.38	114.10	122.59
1	G	23	ASN	CA-CB-CG	6.33	118.93	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	238	ASN	CA-C-N	6.32	133.34	121.97
1	G	238	ASN	C-N-CA	6.32	133.34	121.97
1	R	267	GLY	O-C-N	-6.31	115.46	121.77
1	G	33	ASN	CA-C-N	-6.31	114.34	122.98
1	G	33	ASN	C-N-CA	-6.31	114.34	122.98
1	R	133	GLY	CA-C-N	6.29	130.96	120.64
1	R	133	GLY	C-N-CA	6.29	130.96	120.64
1	G	289	ASN	O-C-N	6.26	130.92	122.59
1	G	110	HIS	O-C-N	6.26	129.31	122.11
1	G	216	VAL	CB-CA-C	6.26	120.59	112.14
1	G	267	GLY	N-CA-C	6.26	125.11	112.34
1	G	165	ASP	CA-CB-CG	6.24	118.84	112.60
1	G	21	ALA	N-CA-C	-6.19	103.84	111.33
1	G	253	LYS	CB-CA-C	-6.17	97.18	109.33
1	G	17	VAL	O-C-N	-6.16	115.87	121.91
1	G	5	VAL	O-C-N	6.15	129.55	122.97
1	R	96	GLU	CB-CA-C	-6.14	100.68	110.81
1	G	141	ASN	CA-CB-CG	6.13	118.73	112.60
1	G	102	THR	CB-CA-C	6.11	122.57	110.42
1	G	143	LEU	O-C-N	6.10	130.18	123.22
1	R	82	GLU	CB-CA-C	-6.09	100.64	110.74
1	R	5	VAL	CA-C-N	6.07	127.91	121.48
1	R	5	VAL	C-N-CA	6.07	127.91	121.48
1	G	82	GLU	N-CA-C	-6.05	104.00	111.33
1	G	203	GLN	N-CA-C	6.05	118.78	111.40
1	G	289	ASN	CA-C-N	6.05	132.21	121.75
1	G	289	ASN	C-N-CA	6.05	132.21	121.75
1	R	169	ILE	O-C-N	6.04	130.13	122.57
1	R	58	THR	O-C-N	6.04	130.63	122.59
1	G	313	TYR	CA-C-N	-6.02	113.56	122.35
1	G	313	TYR	C-N-CA	-6.02	113.56	122.35
1	G	218	LYS	O-C-N	6.00	128.48	122.12
1	G	75	ILE	O-C-N	6.00	129.74	123.26
1	G	212	ALA	O-C-N	5.96	128.44	122.12
1	G	277	GLU	O-C-N	5.96	130.13	122.39
1	G	197	GLY	O-C-N	5.94	130.43	122.70
1	G	280	VAL	CB-CA-C	5.93	121.01	111.29
1	R	310	VAL	O-C-N	5.92	129.62	123.05
1	G	110	HIS	CB-CA-C	-5.92	100.92	110.74
1	R	214	LYS	O-C-N	5.88	128.21	122.09
1	G	188	ASP	CA-CB-CG	-5.88	106.72	112.60
1	R	334	GLU	N-CA-C	5.84	127.35	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	313	TYR	N-CA-C	5.79	123.14	110.80
1	G	166	HIS	CA-CB-CG	-5.79	108.01	113.80
1	G	174	MET	CB-CA-C	-5.76	99.89	111.17
1	G	69	ASP	N-CA-C	-5.74	103.99	111.74
1	R	167	PHE	CB-CA-C	-5.73	101.77	109.16
1	G	185	LYS	N-CA-C	5.73	119.39	110.17
1	R	68	ILE	CB-CA-C	-5.71	106.17	112.68
1	G	326	LEU	CB-CA-C	5.67	121.94	110.38
1	G	169	ILE	N-CA-CB	5.66	120.57	111.23
1	G	248	LEU	CA-C-N	5.64	128.10	120.65
1	G	248	LEU	C-N-CA	5.64	128.10	120.65
1	R	294	PHE	O-C-N	5.63	129.37	122.84
1	G	46	PHE	O-C-N	5.63	127.89	122.03
1	G	192	GLY	CA-C-N	5.63	132.29	121.54
1	G	192	GLY	C-N-CA	5.63	132.29	121.54
1	G	200	GLY	O-C-N	5.61	129.99	122.70
1	R	82	GLU	O-C-N	5.60	128.56	122.11
1	G	5	VAL	CA-C-N	5.58	127.40	121.48
1	G	5	VAL	C-N-CA	5.58	127.40	121.48
1	G	260	VAL	N-CA-CB	5.58	116.70	110.62
1	G	65	LYS	O-C-N	5.55	129.62	122.68
1	G	195	TRP	O-C-N	5.53	129.94	122.59
1	G	193	LYS	CB-CA-C	5.50	121.37	110.42
1	G	120	ILE	O-C-N	5.48	128.68	122.98
1	R	194	LEU	CB-CA-C	5.48	115.25	109.83
1	G	130	PHE	O-C-N	5.47	131.21	122.61
1	G	199	ARG	N-CA-CB	-5.47	100.15	111.36
1	G	218	LYS	CA-C-N	5.47	127.55	120.88
1	G	218	LYS	C-N-CA	5.47	127.55	120.88
1	G	248	LEU	O-C-N	5.46	129.95	123.24
1	G	283	ASP	O-C-N	-5.45	114.93	121.64
1	R	285	PHE	O-C-N	-5.42	115.38	122.59
1	G	281	VAL	O-C-N	5.41	129.18	122.14
1	G	330	MET	N-CA-CB	5.40	118.66	110.28
1	G	139	TYR	N-CA-CB	5.38	118.01	109.51
1	G	296	ALA	N-CA-C	-5.37	103.60	110.53
1	G	222	GLU	N-CA-CB	-5.37	101.42	110.49
1	R	5	VAL	O-C-N	5.36	128.59	122.97
1	G	5	VAL	CB-CA-C	-5.36	103.19	110.90
1	G	192	GLY	O-C-N	5.35	132.44	123.93
1	G	247	ARG	N-CA-C	-5.34	100.19	108.90
1	R	322	ARG	NE-CZ-NH2	5.34	124.01	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	15	ARG	NE-CZ-NH2	5.34	124.01	119.20
1	G	54	LYS	O-C-N	-5.33	115.39	122.59
1	G	39	LEU	O-C-N	5.33	129.68	122.59
1	G	181	THR	O-C-N	5.33	130.38	122.97
1	G	282	SER	O-C-N	5.33	129.67	122.59
1	G	142	SER	CB-CA-C	5.32	122.10	110.18
1	R	12	ARG	NE-CZ-NH2	5.32	123.99	119.20
1	R	27	VAL	CA-C-N	5.32	131.70	121.54
1	R	27	VAL	C-N-CA	5.32	131.70	121.54
1	R	226	LYS	N-CA-C	-5.32	106.82	113.15
1	R	313	TYR	CA-C-N	-5.32	115.74	123.93
1	R	313	TYR	C-N-CA	-5.32	115.74	123.93
1	G	269	LEU	CB-CA-C	-5.32	102.53	110.88
1	R	19	ARG	NE-CZ-NH2	5.31	123.98	119.20
1	R	247	ARG	NE-CZ-NH2	5.31	123.98	119.20
1	R	208	ALA	N-CA-C	5.31	116.59	108.42
1	R	37	ILE	O-C-N	5.30	129.19	122.57
1	G	15	ARG	NE-CZ-NH2	5.30	123.97	119.20
1	R	233	ARG	NE-CZ-NH2	5.29	123.97	119.20
1	G	12	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	G	257	ILE	O-C-N	5.29	127.67	121.96
1	R	5	VAL	N-CA-C	5.29	116.47	108.96
1	G	151	CYS	O-C-N	5.28	129.62	122.59
1	G	214	LYS	CA-C-N	5.28	127.62	120.65
1	G	214	LYS	C-N-CA	5.28	127.62	120.65
1	R	224	ASP	CA-CB-CG	5.28	117.88	112.60
1	G	196	ARG	NE-CZ-NH2	5.27	123.95	119.20
1	R	79	ARG	NE-CZ-NH2	5.26	123.94	119.20
1	G	312	TRP	CB-CA-C	-5.26	102.99	114.10
1	G	69	ASP	CA-CB-CG	5.25	117.86	112.60
1	G	233	ARG	NE-CZ-NH2	5.25	123.92	119.20
1	G	213	ALA	O-C-N	5.24	128.29	122.11
1	R	62	GLU	CA-C-O	5.24	120.98	117.94
1	G	93	TYR	O-C-N	-5.24	117.09	123.27
1	R	196	ARG	NE-CZ-NH2	5.24	123.91	119.20
1	G	170	VAL	O-C-N	-5.22	117.43	123.07
1	R	219	VAL	N-CA-CB	-5.22	103.95	110.47
1	R	199	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	G	74	THR	CB-CA-C	-5.21	99.54	109.66
1	R	117	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	G	142	SER	O-C-N	5.20	129.09	122.33
1	G	286	ASN	O-C-N	5.20	129.68	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	25	GLY	O-C-N	5.20	129.46	122.70
1	R	7	VAL	N-CA-C	5.19	114.70	108.06
1	R	113	GLY	O-C-N	5.19	127.17	122.19
1	G	311	SER	O-C-N	-5.18	115.59	122.59
1	G	199	ARG	NE-CZ-NH2	5.18	123.86	119.20
1	R	6	GLY	O-C-N	-5.17	118.90	123.65
1	G	44	TYR	O-C-N	5.15	129.44	122.59
1	G	19	ARG	NE-CZ-NH2	5.13	123.82	119.20
1	R	194	LEU	N-CA-C	-5.12	105.73	113.51
1	R	182	ALA	O-C-N	5.11	127.97	122.15
1	G	79	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	R	21	ALA	O-C-N	5.09	127.52	122.12
1	R	319	TYR	O-C-N	5.09	127.32	122.03
1	R	314	ASP	N-CA-CB	-5.09	104.20	113.10
1	G	109	ALA	N-CA-C	5.08	116.89	111.36
1	G	247	ARG	NE-CZ-NH2	5.07	123.76	119.20
1	R	19	ARG	CA-C-N	5.06	127.48	120.29
1	R	19	ARG	C-N-CA	5.06	127.48	120.29
1	R	144	LYS	N-CA-C	-5.06	107.05	113.43
1	G	269	LEU	N-CA-CB	5.06	117.34	110.01
1	R	275	TYR	O-C-N	5.05	129.31	122.59
1	R	54	LYS	O-C-N	-5.05	116.00	122.72
1	G	16	LEU	N-CA-CB	5.05	117.33	110.01
1	R	103	THR	O-C-N	5.05	129.30	122.59

There are no chirality outliers.

There are no planarity outliers.

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	2523	0	2515	821	25
1	R	2523	0	2518	805	20
2	G	10	0	0	6	0
2	R	10	0	0	4	0
3	G	44	0	24	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	R	44	0	26	7	0
All	All	5154	0	5083	1612	25

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 157.

All (1612) 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:R:1:GLY:CA	1:R:28:ASP:HA	1.14	1.57
1:G:3:VAL:H	1:G:27:VAL:CG1	1.19	1.55
1:R:3:VAL:CB	1:R:27:VAL:HG13	1.32	1.55
1:R:1:GLY:C	1:R:28:ASP:HA	1.30	1.54
1:R:3:VAL:HG23	1:R:27:VAL:CG2	1.41	1.48
1:R:156:LEU:HD13	1:R:242:LEU:CD2	1.45	1.47
1:R:1:GLY:HA2	1:R:28:ASP:CA	1.45	1.46
1:R:16:LEU:HD12	1:R:320:SER:CB	1.46	1.45
1:G:156:LEU:HD13	1:G:242:LEU:CD2	1.50	1.42
1:G:26:LYS:HD2	1:G:27:VAL:N	1.33	1.42
1:R:3:VAL:HB	1:R:27:VAL:CG1	1.50	1.40
1:G:65:LYS:CG	1:G:73:ILE:O	1.68	1.39
1:G:156:LEU:CD1	1:G:242:LEU:HD21	1.52	1.37
1:R:16:LEU:CD1	1:R:320:SER:HB3	1.52	1.36
1:G:196:ARG:NH2	1:G:208:ALA:HB2	1.35	1.34
1:R:2:LYS:N	1:R:28:ASP:CA	1.91	1.33
1:R:1:GLY:CA	1:R:28:ASP:CA	2.02	1.33
1:G:16:LEU:HD12	1:G:320:SER:CB	1.58	1.33
1:R:196:ARG:NH1	1:R:196:ARG:HA	1.45	1.31
1:R:2:LYS:NZ	1:R:25:GLY:HA3	1.45	1.30
1:R:297:GLY:O	1:R:300:ILE:HG13	1.28	1.28
1:R:2:LYS:N	1:R:28:ASP:N	1.83	1.26
1:R:1:GLY:HA2	1:R:28:ASP:C	1.59	1.26
1:R:223:LEU:O	1:R:224:ASP:CB	1.78	1.26
1:G:2:LYS:HB2	1:G:26:LYS:CD	1.66	1.26
1:R:119:VAL:HG21	1:R:326:LEU:CD1	1.67	1.25
1:G:156:LEU:CD1	1:G:242:LEU:CD2	2.10	1.25
1:G:78:GLU:CG	1:G:84:ILE:HG22	1.68	1.24
1:G:257:ILE:O	1:G:260:VAL:HG12	1.36	1.24
1:R:186:THR:O	1:R:187:VAL:HG23	1.33	1.23
1:G:223:LEU:O	1:G:224:ASP:CB	1.86	1.23
1:G:3:VAL:N	1:G:27:VAL:HG13	1.16	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:40:HIS:O	1:R:43:VAL:HG13	1.35	1.22
1:R:257:ILE:O	1:R:260:VAL:HG12	1.36	1.22
1:R:259:LYS:O	1:R:262:LYS:HG3	1.31	1.22
1:R:26:LYS:HE2	1:R:28:ASP:N	1.55	1.21
1:G:117:ARG:HG3	1:G:334:GLU:OE1	1.40	1.21
1:R:196:ARG:HH11	1:R:196:ARG:CA	1.55	1.20
1:R:39:LEU:H	1:R:39:LEU:CD1	1.54	1.20
1:G:196:ARG:HH21	1:G:208:ALA:CB	1.55	1.19
1:G:291:SER:HB2	1:G:322:ARG:HD3	1.24	1.19
1:R:35:PRO:HG3	1:R:78:GLU:O	1.35	1.19
1:G:276:THR:OG1	1:G:278:ASP:HB2	1.39	1.19
1:G:254:TYR:OH	1:G:300:ILE:HG21	1.44	1.18
1:G:2:LYS:CB	1:G:26:LYS:HD2	1.74	1.18
1:R:1:GLY:C	1:R:28:ASP:CA	2.08	1.18
1:R:12:ARG:HB2	3:R:336:NAD:O2N	1.41	1.17
1:R:30:VAL:HG23	1:R:31:ALA:N	1.51	1.17
1:R:30:VAL:CG2	1:R:31:ALA:H	1.48	1.17
1:G:65:LYS:HG3	1:G:73:ILE:O	1.31	1.16
1:G:80:ASP:O	1:G:83:ASN:HB2	1.39	1.16
1:R:156:LEU:HD13	1:R:242:LEU:HD21	1.23	1.16
1:R:47:GLN:HG3	1:R:59:VAL:CG1	1.74	1.15
1:G:12:ARG:H	1:G:15:ARG:NH1	1.43	1.15
1:G:196:ARG:HA	1:G:196:ARG:HH11	1.07	1.15
1:G:254:TYR:CZ	1:G:300:ILE:HG21	1.81	1.15
1:R:149:ALA:HB1	1:R:153:THR:HG22	1.16	1.15
1:R:47:GLN:CG	1:R:59:VAL:HG11	1.76	1.15
1:R:196:ARG:HH21	1:R:208:ALA:HB2	1.00	1.14
1:G:276:THR:CG2	1:G:295:ASP:HB3	1.77	1.14
1:G:65:LYS:HB2	1:G:74:THR:HA	1.18	1.14
1:R:254:TYR:H	1:R:302:LEU:HD13	1.09	1.14
1:R:186:THR:O	1:R:187:VAL:CG2	1.96	1.13
1:R:176:THR:CG2	1:R:231:ALA:HB2	1.77	1.13
1:R:313:TYR:O	1:R:314:ASP:HB3	1.37	1.13
1:R:3:VAL:CB	1:R:27:VAL:CG1	2.17	1.13
1:R:37:ILE:O	1:R:42:MET:HE3	1.48	1.13
1:G:197:GLY:O	1:G:199:ARG:HB3	1.49	1.13
1:G:8:ASP:OD2	1:G:33:ASN:ND2	1.80	1.12
1:R:2:LYS:N	1:R:28:ASP:HA	1.57	1.12
1:R:156:LEU:HD22	1:R:174:MET:HE3	1.28	1.12
1:G:78:GLU:HG3	1:G:84:ILE:HG22	1.32	1.12
1:G:322:ARG:NH2	1:G:325:ASP:OD1	1.80	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:2:LYS:N	1:R:28:ASP:H	1.41	1.12
1:R:3:VAL:HG23	1:R:27:VAL:HG22	1.18	1.12
1:G:1:GLY:CA	1:G:28:ASP:HA	1.74	1.12
1:G:39:LEU:HG	1:G:40:HIS:N	1.48	1.12
1:G:269:LEU:H	1:G:269:LEU:HD22	1.15	1.11
1:R:119:VAL:HG21	1:R:326:LEU:HD12	1.15	1.11
1:G:2:LYS:HA	1:G:26:LYS:HZ3	0.96	1.11
1:R:111:LEU:HA	1:R:115:ALA:HB3	1.31	1.11
1:R:259:LYS:HG2	1:R:262:LYS:CE	1.81	1.11
1:G:2:LYS:HZ2	1:G:25:GLY:HA3	1.14	1.10
1:G:16:LEU:HD12	1:G:320:SER:HB3	1.12	1.10
1:G:35:PRO:O	1:G:36:PHE:HB2	1.41	1.10
1:G:174:MET:HE2	1:G:212:ALA:HB2	1.25	1.10
1:G:305:THR:HG23	1:G:306:PHE:H	1.15	1.10
1:G:174:MET:SD	1:G:242:LEU:HD11	1.92	1.10
1:R:223:LEU:O	1:R:224:ASP:HB2	1.28	1.10
1:G:2:LYS:HA	1:G:26:LYS:NZ	1.66	1.10
1:G:43:VAL:HG12	1:G:66:LEU:HD11	1.31	1.10
1:G:37:ILE:HG22	1:G:42:MET:HE3	1.31	1.09
1:G:276:THR:HG23	1:G:295:ASP:HB3	1.27	1.09
1:R:22:PHE:HZ	1:R:69:ASP:CB	1.63	1.09
1:G:98:THR:HA	3:G:336:NAD:H8A	1.27	1.09
1:R:176:THR:CG2	1:R:231:ALA:CB	2.30	1.09
1:R:10:PHE:CE2	1:R:46:PHE:HB2	1.88	1.08
1:G:156:LEU:CD2	1:G:242:LEU:HD21	1.83	1.08
1:G:16:LEU:CD2	1:G:19:ARG:HG2	1.80	1.08
1:G:149:ALA:HB1	1:G:153:THR:HG22	1.20	1.08
1:R:189:SER:HB3	1:R:190:PRO:HD2	1.20	1.08
1:R:102:THR:O	1:R:103:THR:HB	1.40	1.07
1:R:269:LEU:HD22	1:R:269:LEU:H	1.11	1.07
1:R:3:VAL:CG2	1:R:27:VAL:CG1	2.31	1.07
1:R:26:LYS:CE	1:R:28:ASP:H	1.62	1.07
1:R:156:LEU:HD13	1:R:242:LEU:HD23	1.17	1.07
1:G:153:THR:HG23	1:G:215:ALA:HB1	1.35	1.07
1:R:3:VAL:HG23	1:R:27:VAL:HG21	1.31	1.07
1:R:188:ASP:OD1	1:R:199:ARG:NH1	1.89	1.06
1:R:2:LYS:CD	1:R:27:VAL:N	2.08	1.06
1:R:85:LYS:O	1:R:86:TRP:HB2	1.53	1.06
1:R:134:VAL:HG21	1:R:219:VAL:HG12	1.36	1.06
1:R:176:THR:HG22	1:R:231:ALA:HB2	1.07	1.06
1:R:196:ARG:HH21	1:R:208:ALA:CB	1.67	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:297:GLY:O	1:R:300:ILE:CG1	2.04	1.06
1:R:135:ASN:O	1:R:138:LYS:HB2	1.55	1.06
1:G:196:ARG:HA	1:G:196:ARG:NH1	1.70	1.06
1:G:16:LEU:HD23	1:G:19:ARG:HG2	1.33	1.05
1:G:2:LYS:NZ	1:G:25:GLY:HA3	1.72	1.05
1:R:78:GLU:HG3	1:R:84:ILE:CA	1.87	1.05
1:R:275:TYR:HE2	1:R:277:GLU:HG2	1.22	1.05
1:R:30:VAL:CG2	1:R:31:ALA:N	2.07	1.05
1:R:176:THR:HG22	1:R:231:ALA:CB	1.85	1.04
1:G:149:ALA:HB1	1:G:153:THR:CG2	1.87	1.04
1:G:42:MET:HE1	1:G:75:ILE:HD13	1.35	1.04
1:R:134:VAL:CG2	1:R:219:VAL:HG12	1.88	1.04
1:R:21:ALA:O	1:R:26:LYS:N	1.90	1.04
1:R:276:THR:HG23	1:R:295:ASP:HB3	1.06	1.04
1:G:65:LYS:CD	1:G:73:ILE:O	2.04	1.04
1:R:39:LEU:HD12	1:R:39:LEU:N	1.60	1.04
1:R:152:THR:HA	1:R:313:TYR:CE2	1.93	1.04
1:R:213:ALA:HB2	1:R:228:THR:HA	1.40	1.04
1:R:269:LEU:HB3	1:R:272:ILE:HD13	1.08	1.03
1:G:16:LEU:CD1	1:G:320:SER:HB3	1.86	1.03
1:R:22:PHE:CZ	1:R:69:ASP:HB2	1.93	1.03
1:G:272:ILE:O	1:G:273:LEU:HB2	1.56	1.03
1:G:2:LYS:CA	1:G:26:LYS:NZ	2.21	1.03
1:G:26:LYS:HD2	1:G:27:VAL:CA	1.89	1.02
1:R:28:ASP:CB	1:R:29:ILE:HG13	1.90	1.02
1:G:191:SER:OG	1:G:192:GLY:N	1.71	1.02
1:R:28:ASP:HB3	1:R:29:ILE:HG13	1.05	1.02
1:R:269:LEU:HB3	1:R:272:ILE:CD1	1.89	1.02
1:R:189:SER:CB	1:R:190:PRO:HD2	1.89	1.02
1:G:178:HIS:HA	1:G:240:SER:HB3	1.42	1.02
1:R:43:VAL:O	1:R:47:GLN:HB2	1.58	1.02
1:R:284:ASP:O	1:R:286:ASN:HB2	1.59	1.02
1:G:156:LEU:HD13	1:G:242:LEU:HD23	1.07	1.02
1:G:22:PHE:HE2	1:G:71:LYS:HD3	1.25	1.01
1:G:98:THR:CA	3:G:336:NAD:H8A	1.89	1.01
1:R:3:VAL:CG2	1:R:27:VAL:CG2	2.38	1.01
1:R:189:SER:HB3	1:R:190:PRO:CD	1.89	1.01
1:G:26:LYS:CD	1:G:27:VAL:N	2.22	1.01
1:G:39:LEU:HG	1:G:40:HIS:H	0.98	1.01
1:G:223:LEU:O	1:G:224:ASP:HB3	1.20	1.01
1:G:4:LYS:O	1:G:4:LYS:HG2	1.60	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:156:LEU:HD11	1:G:242:LEU:HD21	1.37	1.01
1:G:3:VAL:N	1:G:27:VAL:CG1	1.91	1.00
1:R:2:LYS:HD2	1:R:25:GLY:C	1.87	1.00
1:R:176:THR:HG23	1:R:231:ALA:HB1	1.42	1.00
1:R:260:VAL:HG13	1:R:261:VAL:H	1.24	1.00
1:G:275:TYR:CE2	1:G:277:GLU:HG2	1.97	1.00
1:R:36:PHE:O	1:R:37:ILE:HG12	1.60	1.00
1:R:65:LYS:HB2	1:R:74:THR:HA	1.01	0.99
1:R:150:SER:OG	2:R:340:SO4:O1	1.80	0.99
1:G:169:ILE:HG12	1:G:246:CYS:SG	2.02	0.99
1:R:2:LYS:HZ2	1:R:25:GLY:HA3	0.85	0.99
1:R:22:PHE:CZ	1:R:69:ASP:CB	2.44	0.98
1:R:156:LEU:CD1	1:R:242:LEU:CD2	2.41	0.98
1:R:156:LEU:CD1	1:R:242:LEU:HD23	1.93	0.98
1:R:259:LYS:CG	1:R:262:LYS:HE2	1.93	0.98
1:R:180:ILE:HG12	1:R:237:ALA:HA	1.45	0.98
1:G:2:LYS:CB	1:G:26:LYS:HZ2	1.77	0.98
1:G:2:LYS:HG2	1:G:3:VAL:H	1.27	0.98
1:G:153:THR:CG2	1:G:215:ALA:HB1	1.92	0.98
1:R:205:LEU:C	1:R:205:LEU:HD22	1.89	0.98
1:R:273:LEU:O	1:R:293:ILE:HA	1.64	0.98
1:G:60:LYS:HG2	1:G:61:ALA:N	1.78	0.98
1:R:141:ASN:HD22	1:R:141:ASN:H	0.98	0.98
1:G:85:LYS:O	1:G:113:GLY:C	2.08	0.97
1:R:108:GLY:O	1:R:111:LEU:HB2	1.62	0.97
1:R:259:LYS:HG2	1:R:262:LYS:HE2	0.97	0.97
1:R:276:THR:CG2	1:R:295:ASP:HB3	1.93	0.97
1:G:1:GLY:HA2	1:G:28:ASP:CA	1.94	0.97
1:G:4:LYS:HE3	1:G:92:ALA:CB	1.94	0.97
1:G:78:GLU:HG3	1:G:84:ILE:CG2	1.94	0.97
1:G:30:VAL:HG22	1:G:73:ILE:HG13	1.44	0.97
1:G:2:LYS:O	1:G:28:ASP:CG	2.08	0.97
1:R:30:VAL:HG22	1:R:73:ILE:HG13	1.44	0.96
1:G:2:LYS:CB	1:G:26:LYS:CD	2.38	0.96
1:G:278:ASP:O	1:G:279:GLU:HB2	1.63	0.96
1:G:117:ARG:NH1	1:G:144:LYS:HD3	1.80	0.96
1:G:318:GLY:O	1:G:322:ARG:HD2	1.65	0.96
1:R:78:GLU:HG3	1:R:84:ILE:HA	1.47	0.96
1:G:140:ALA:O	1:G:143:LEU:HB2	1.66	0.96
1:G:16:LEU:HD21	1:G:20:ALA:HB2	1.48	0.96
1:G:275:TYR:HE2	1:G:277:GLU:HG2	1.25	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:102:THR:O	1:G:103:THR:HB	1.65	0.95
1:R:35:PRO:HD3	1:R:77:GLN:O	1.65	0.95
1:G:1:GLY:HA2	1:G:28:ASP:C	1.89	0.95
1:G:60:LYS:HG2	1:G:61:ALA:H	1.32	0.95
1:R:178:HIS:HA	1:R:240:SER:HB3	1.48	0.94
1:R:2:LYS:CD	1:R:27:VAL:H	1.70	0.94
1:G:2:LYS:CA	1:G:26:LYS:HZ3	1.77	0.94
1:R:2:LYS:H	1:R:28:ASP:CB	1.79	0.94
1:R:300:ILE:O	1:R:300:ILE:HD12	1.68	0.94
1:G:12:ARG:N	1:G:15:ARG:NH1	2.15	0.94
1:G:98:THR:HA	3:G:336:NAD:C8A	1.96	0.94
1:R:185:LYS:O	1:R:201:ALA:HB2	1.67	0.94
1:R:196:ARG:NH2	1:R:208:ALA:HB2	1.80	0.94
1:R:141:ASN:C	1:R:143:LEU:H	1.70	0.94
1:G:80:ASP:O	1:G:83:ASN:CB	2.16	0.94
1:G:221:PRO:O	1:G:223:LEU:O	1.86	0.94
1:R:313:TYR:O	1:R:314:ASP:CB	2.14	0.94
1:R:65:LYS:CB	1:R:74:THR:HA	1.95	0.93
1:R:1:GLY:C	1:R:28:ASP:H	1.75	0.93
1:G:2:LYS:HB2	1:G:26:LYS:HD2	0.96	0.93
1:G:65:LYS:CB	1:G:74:THR:HA	1.98	0.93
1:R:3:VAL:CG2	1:R:27:VAL:HG13	1.97	0.93
1:R:269:LEU:H	1:R:269:LEU:CD2	1.80	0.93
1:R:152:THR:HA	1:R:313:TYR:HE2	1.31	0.93
1:R:293:ILE:O	1:R:312:TRP:HB2	1.69	0.92
1:R:78:GLU:OE2	1:R:78:GLU:HA	1.64	0.92
1:G:195:TRP:CD1	1:G:197:GLY:HA2	2.02	0.92
1:G:212:ALA:O	1:G:216:VAL:HB	1.70	0.92
1:G:152:THR:HA	1:G:313:TYR:OH	1.70	0.92
1:R:2:LYS:H	1:R:28:ASP:CA	1.72	0.92
1:R:174:MET:HG2	1:R:175:THR:N	1.84	0.92
1:R:141:ASN:H	1:R:141:ASN:ND2	1.60	0.92
1:R:207:PRO:HA	1:R:232:PHE:HD1	1.33	0.92
1:G:126:ASP:O	1:G:127:ALA:CB	2.17	0.92
1:G:156:LEU:CD2	1:G:242:LEU:CD2	2.48	0.92
1:R:278:ASP:O	1:R:279:GLU:HB2	1.71	0.91
1:G:257:ILE:O	1:G:260:VAL:CG1	2.19	0.91
1:G:178:HIS:HB3	1:G:233:ARG:HG2	1.51	0.91
1:R:3:VAL:H	1:R:27:VAL:HA	1.30	0.91
1:R:117:ARG:NH1	1:R:144:LYS:HD2	1.85	0.91
1:G:1:GLY:CA	1:G:28:ASP:CA	2.48	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:174:MET:HE2	1:R:242:LEU:HD11	1.49	0.91
1:R:39:LEU:H	1:R:39:LEU:HD12	0.76	0.91
1:R:1:GLY:C	1:R:28:ASP:N	2.24	0.90
1:R:65:LYS:HB2	1:R:74:THR:CA	1.97	0.90
1:G:1:GLY:HA2	1:G:28:ASP:HA	1.44	0.90
1:G:131:VAL:HG23	1:G:133:GLY:H	1.34	0.90
1:R:10:PHE:HE2	1:R:46:PHE:HB2	1.30	0.90
1:R:98:THR:HG22	1:R:99:GLY:N	1.87	0.90
1:G:156:LEU:HD22	1:G:242:LEU:CD2	2.01	0.90
1:G:78:GLU:HB2	1:G:84:ILE:HG23	1.54	0.90
1:G:208:ALA:O	1:G:230:MET:HG2	1.71	0.90
1:R:117:ARG:HA	1:R:144:LYS:O	1.72	0.90
1:G:161:LYS:O	1:G:165:ASP:OD2	1.90	0.90
1:G:2:LYS:CB	1:G:26:LYS:NZ	2.35	0.89
1:R:179:ALA:HB2	1:R:239:VAL:O	1.72	0.89
1:G:78:GLU:HG3	1:G:84:ILE:HA	1.52	0.89
1:G:213:ALA:HB2	1:G:227:LEU:O	1.72	0.89
1:R:40:HIS:O	1:R:43:VAL:CG1	2.20	0.89
1:G:35:PRO:HB3	1:G:79:ARG:HG2	1.55	0.89
1:G:85:LYS:HD3	1:G:85:LYS:N	1.84	0.89
1:R:2:LYS:NZ	1:R:25:GLY:CA	2.35	0.89
1:R:28:ASP:HB3	1:R:29:ILE:CG1	1.99	0.89
1:G:15:ARG:O	1:G:19:ARG:HB3	1.72	0.89
1:G:10:PHE:CE2	1:G:46:PHE:HB2	2.08	0.89
1:R:8:ASP:O	1:R:97:SER:HB3	1.73	0.89
1:R:197:GLY:O	1:R:199:ARG:HB2	1.71	0.89
1:R:2:LYS:HD2	1:R:27:VAL:H	1.36	0.89
1:G:141:ASN:H	1:G:141:ASN:HD22	1.21	0.89
1:G:78:GLU:CG	1:G:84:ILE:CG2	2.49	0.89
1:R:37:ILE:O	1:R:42:MET:CE	2.21	0.88
1:R:166:HIS:CD2	1:R:260:VAL:HG23	2.07	0.88
1:G:305:THR:CG2	1:G:306:PHE:H	1.86	0.88
1:R:60:LYS:HG3	1:R:61:ALA:N	1.87	0.88
1:G:2:LYS:HB2	1:G:26:LYS:HZ2	1.31	0.88
1:G:39:LEU:CG	1:G:40:HIS:H	1.85	0.88
1:R:1:GLY:HA3	1:R:28:ASP:OD2	1.72	0.88
1:R:119:VAL:CG2	1:R:326:LEU:CD1	2.50	0.88
1:R:149:ALA:HB1	1:R:153:THR:CG2	2.03	0.88
1:G:156:LEU:HD22	1:G:242:LEU:HD22	1.56	0.88
1:R:2:LYS:HZ2	1:R:25:GLY:CA	1.81	0.88
1:R:189:SER:CB	1:R:190:PRO:CD	2.50	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:195:TRP:HD1	1:R:197:GLY:H	1.18	0.88
1:G:276:THR:OG1	1:G:278:ASP:CB	2.21	0.88
1:R:129:MET:C	1:R:130:PHE:HD1	1.82	0.88
1:R:269:LEU:HD22	1:R:269:LEU:N	1.87	0.88
1:G:234:VAL:HB	1:G:235:PRO:HD2	1.55	0.88
1:R:326:LEU:HD22	1:R:326:LEU:O	1.74	0.88
1:G:221:PRO:O	1:G:222:GLU:C	2.16	0.88
1:G:16:LEU:CD2	1:G:20:ALA:HB2	2.04	0.87
1:G:214:LYS:O	1:G:218:LYS:HG2	1.74	0.87
1:G:276:THR:HG23	1:G:295:ASP:CB	2.03	0.87
1:G:22:PHE:CE2	1:G:71:LYS:HD3	2.08	0.87
1:R:39:LEU:CD1	1:R:39:LEU:N	2.22	0.87
1:R:16:LEU:HA	1:R:19:ARG:HB3	1.57	0.86
1:R:22:PHE:HA	1:R:26:LYS:HA	1.57	0.86
1:G:129:MET:HE2	1:G:149:ALA:HA	1.56	0.86
1:R:47:GLN:HG3	1:R:59:VAL:HG11	0.90	0.86
1:G:16:LEU:HD12	1:G:320:SER:HB2	1.55	0.86
1:G:83:ASN:O	1:G:84:ILE:O	1.93	0.86
1:G:253:LYS:HB2	1:G:256:ASP:HB2	1.58	0.86
1:G:65:LYS:CB	1:G:73:ILE:O	2.23	0.86
1:G:126:ASP:O	1:G:127:ALA:HB2	1.71	0.86
1:G:16:LEU:HA	1:G:19:ARG:HB3	1.57	0.86
1:G:117:ARG:HH11	1:G:144:LYS:HD3	1.37	0.86
1:R:3:VAL:CG2	1:R:27:VAL:HG11	2.04	0.86
1:R:174:MET:HE2	1:R:242:LEU:CD1	2.05	0.86
1:R:223:LEU:O	1:R:224:ASP:HB3	1.73	0.86
1:G:297:GLY:O	1:G:300:ILE:HG13	1.73	0.86
1:G:5:VAL:O	1:G:30:VAL:HA	1.74	0.86
1:G:191:SER:HG	1:G:192:GLY:H	1.24	0.85
1:G:2:LYS:HB2	1:G:26:LYS:NZ	1.90	0.85
1:G:21:ALA:O	1:G:26:LYS:N	2.08	0.85
1:G:84:ILE:C	1:G:85:LYS:HD3	2.00	0.85
1:G:305:THR:HG23	1:G:306:PHE:N	1.90	0.85
1:R:30:VAL:HG23	1:R:31:ALA:H	0.70	0.85
1:R:141:ASN:O	1:R:143:LEU:N	2.08	0.85
1:R:207:PRO:HA	1:R:232:PHE:CD1	2.11	0.85
1:R:2:LYS:CA	1:R:28:ASP:H	1.71	0.84
1:G:213:ALA:CB	1:G:227:LEU:O	2.24	0.84
1:R:22:PHE:HZ	1:R:69:ASP:HB3	1.42	0.84
1:R:230:MET:SD	1:R:232:PHE:CZ	2.70	0.84
1:G:15:ARG:HA	1:G:18:THR:HG23	1.57	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:2:LYS:HG2	1:R:3:VAL:H	1.43	0.84
1:R:174:MET:CE	1:R:242:LEU:HD11	2.07	0.84
1:R:3:VAL:CG2	1:R:27:VAL:HG22	2.05	0.84
1:R:141:ASN:C	1:R:143:LEU:N	2.26	0.84
1:G:258:LYS:HD2	1:G:275:TYR:OH	1.77	0.84
1:G:322:ARG:HH21	1:G:325:ASP:CG	1.85	0.84
1:R:2:LYS:CA	1:R:28:ASP:N	2.30	0.84
1:R:174:MET:HG3	1:R:242:LEU:HD11	1.59	0.84
1:G:26:LYS:HD2	1:G:26:LYS:C	2.02	0.84
1:R:68:ILE:HD11	1:R:73:ILE:HG21	1.58	0.83
1:G:156:LEU:CG	1:G:242:LEU:HD21	2.07	0.83
1:G:16:LEU:CD1	1:G:320:SER:CB	2.49	0.83
1:R:150:SER:HB3	1:R:153:THR:HB	1.60	0.83
1:G:86:TRP:HE1	1:G:110:HIS:CE1	1.96	0.83
1:R:280:VAL:HG23	1:R:280:VAL:O	1.79	0.83
1:R:176:THR:HG23	1:R:231:ALA:CB	2.03	0.83
1:R:11:GLY:O	1:R:14:GLY:N	2.11	0.83
1:R:221:PRO:O	1:R:222:GLU:C	2.21	0.83
1:G:123:PRO:HA	1:G:129:MET:HE1	1.61	0.83
1:G:317:PHE:O	1:G:318:GLY:C	2.21	0.83
1:G:10:PHE:HE2	1:G:46:PHE:HB2	1.42	0.83
1:G:15:ARG:O	1:G:19:ARG:N	2.12	0.83
1:R:193:LYS:O	1:R:194:LEU:HB3	1.76	0.82
1:G:37:ILE:HG22	1:G:42:MET:CE	2.07	0.82
1:G:35:PRO:HG3	1:G:78:GLU:O	1.79	0.82
1:R:35:PRO:CG	1:R:78:GLU:O	2.24	0.82
1:G:269:LEU:O	1:G:271:GLY:N	2.12	0.82
1:G:241:VAL:HB	1:G:312:TRP:CE3	2.15	0.82
1:R:55:PHE:O	1:R:56:HIS:CG	2.33	0.82
1:R:15:ARG:HH21	1:R:45:MET:HE2	1.42	0.82
1:G:57:GLY:O	1:G:58:THR:HB	1.79	0.82
1:G:265:SER:HA	1:G:269:LEU:HD23	1.59	0.82
1:R:163:ILE:CG2	1:R:169:ILE:HD11	2.10	0.81
1:G:2:LYS:HB2	1:G:26:LYS:CE	2.08	0.81
1:R:272:ILE:O	1:R:273:LEU:HB2	1.79	0.81
1:R:2:LYS:H	1:R:28:ASP:CG	1.87	0.81
1:R:13:ILE:O	1:R:17:VAL:HG23	1.79	0.81
1:R:257:ILE:O	1:R:260:VAL:CG1	2.26	0.81
1:R:275:TYR:CE2	1:R:277:GLU:HG2	2.10	0.81
1:R:50:SER:OG	1:G:188:ASP:OD2	1.97	0.81
1:G:180:ILE:HD12	1:G:184:GLN:HB2	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:135:ASN:ND2	1:G:136:HIS:N	2.29	0.81
1:G:78:GLU:HG2	1:G:84:ILE:HG22	1.60	0.81
1:G:92:ALA:O	1:G:116:LYS:HB2	1.81	0.81
1:R:126:ASP:O	1:R:127:ALA:CB	2.28	0.81
1:G:26:LYS:CD	1:G:26:LYS:C	2.53	0.81
1:G:208:ALA:N	1:G:231:ALA:O	2.14	0.81
1:R:273:LEU:O	1:R:292:SER:O	1.98	0.81
1:G:149:ALA:CB	1:G:153:THR:HG22	2.09	0.81
1:G:196:ARG:CZ	1:G:208:ALA:HB2	2.09	0.81
1:R:196:ARG:HA	1:R:196:ARG:HH11	0.70	0.80
1:R:146:ILE:HG13	1:R:147:SER:N	1.96	0.80
1:R:130:PHE:CE2	1:R:138:LYS:HB3	2.17	0.80
1:G:293:ILE:O	1:G:312:TRP:CD1	2.35	0.80
1:R:42:MET:HE1	1:R:75:ILE:HD13	1.62	0.80
1:R:284:ASP:O	1:R:285:PHE:C	2.24	0.80
1:R:322:ARG:NH2	1:R:325:ASP:OD1	2.15	0.80
1:R:149:ALA:CB	1:R:153:THR:HG22	2.07	0.80
1:R:117:ARG:HD2	1:R:144:LYS:HA	1.64	0.80
1:R:141:ASN:HD22	1:R:141:ASN:N	1.76	0.80
1:R:234:VAL:HB	1:R:235:PRO:HD2	1.62	0.80
1:G:13:ILE:O	1:G:17:VAL:HG23	1.81	0.80
1:G:29:ILE:O	1:G:30:VAL:CG1	2.29	0.80
1:G:30:VAL:CG2	1:G:73:ILE:HG13	2.11	0.79
1:R:78:GLU:CG	1:R:84:ILE:HB	2.11	0.79
1:R:205:LEU:HD13	1:R:205:LEU:O	1.82	0.79
1:G:65:LYS:CD	1:G:73:ILE:C	2.54	0.79
1:G:141:ASN:H	1:G:141:ASN:ND2	1.79	0.79
1:G:78:GLU:HG3	1:G:84:ILE:CA	2.13	0.79
1:G:154:ASN:O	1:G:158:PRO:HD3	1.82	0.79
1:R:29:ILE:C	1:R:30:VAL:HG12	2.05	0.79
1:R:66:LEU:O	1:R:73:ILE:HG22	1.82	0.79
1:R:269:LEU:CB	1:R:272:ILE:HD13	2.03	0.79
1:G:2:LYS:CA	1:G:26:LYS:CE	2.60	0.79
1:R:5:VAL:O	1:R:30:VAL:HA	1.83	0.79
1:R:186:THR:C	1:R:187:VAL:CG2	2.54	0.79
1:R:254:TYR:N	1:R:302:LEU:HD13	1.94	0.79
1:G:156:LEU:HD21	1:G:174:MET:SD	2.22	0.79
1:G:278:ASP:O	1:G:279:GLU:CB	2.28	0.79
1:G:4:LYS:HE3	1:G:92:ALA:HB3	1.63	0.79
1:G:254:TYR:CZ	1:G:300:ILE:CG2	2.66	0.79
1:G:164:HIS:HB2	1:G:169:ILE:HD12	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:317:PHE:O	1:R:320:SER:N	2.17	0.78
1:R:333:LYS:NZ	1:R:333:LYS:HB3	1.96	0.78
1:G:220:ILE:CG2	1:G:223:LEU:HB2	2.13	0.78
1:G:15:ARG:HH21	1:G:45:MET:CE	1.97	0.78
1:R:291:SER:OG	1:R:322:ARG:HD2	1.84	0.78
1:R:333:LYS:HZ2	1:R:333:LYS:CB	1.97	0.78
1:G:255:ASP:O	1:G:258:LYS:HG2	1.84	0.78
1:R:78:GLU:HG3	1:R:84:ILE:CB	2.13	0.77
1:R:276:THR:OG1	1:R:278:ASP:HB2	1.83	0.77
1:G:30:VAL:HG23	1:G:31:ALA:N	1.98	0.77
1:R:175:THR:HA	1:R:230:MET:O	1.84	0.77
1:G:16:LEU:HD22	1:G:19:ARG:HG2	1.65	0.77
1:R:59:VAL:HG22	1:R:59:VAL:O	1.85	0.77
1:G:35:PRO:O	1:G:36:PHE:CB	2.25	0.77
1:R:3:VAL:CG2	1:R:27:VAL:HG21	2.10	0.77
1:G:123:PRO:HA	1:G:129:MET:CE	2.13	0.77
1:G:47:GLN:CB	1:G:59:VAL:HG11	2.14	0.77
1:R:15:ARG:NH1	1:R:15:ARG:HG3	2.00	0.77
1:R:15:ARG:NH2	1:R:45:MET:HE2	1.99	0.77
1:R:97:SER:O	1:R:98:THR:HB	1.84	0.77
1:G:205:LEU:HD13	1:G:205:LEU:O	1.85	0.76
1:R:29:ILE:O	1:R:30:VAL:HG12	1.86	0.76
1:R:260:VAL:HG13	1:R:261:VAL:N	1.99	0.76
1:R:2:LYS:HD3	1:R:27:VAL:N	1.75	0.76
1:G:300:ILE:HD12	1:G:300:ILE:O	1.85	0.76
1:R:135:ASN:ND2	1:R:136:HIS:N	2.34	0.76
1:R:35:PRO:CD	1:R:77:GLN:O	2.34	0.76
1:R:135:ASN:CG	1:R:136:HIS:N	2.43	0.76
1:R:239:VAL:HG22	1:R:314:ASP:HA	1.67	0.76
1:G:195:TRP:HD1	1:G:197:GLY:HA2	1.47	0.76
1:R:79:ARG:O	1:R:80:ASP:HB2	1.86	0.76
1:G:283:ASP:O	1:G:284:ASP:C	2.27	0.76
1:G:3:VAL:O	1:G:4:LYS:HB3	1.83	0.75
1:R:122:ALA:HB2	3:R:336:NAD:O2D	1.87	0.75
1:R:274:GLY:HA3	1:R:293:ILE:HD12	1.68	0.75
1:G:196:ARG:HH22	1:G:206:ILE:HG22	1.50	0.75
1:R:84:ILE:HD12	1:R:85:LYS:N	2.01	0.75
1:G:205:LEU:HD22	1:G:205:LEU:C	2.11	0.75
1:G:243:ASP:OD1	1:G:308:LYS:HE3	1.84	0.75
1:R:119:VAL:CG2	1:R:326:LEU:HD11	2.16	0.75
1:G:15:ARG:NH2	1:G:45:MET:CE	2.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:156:LEU:CD1	1:R:242:LEU:HD21	2.10	0.75
1:R:197:GLY:O	1:R:198:GLY:C	2.26	0.75
1:G:220:ILE:HG22	1:G:223:LEU:HB2	1.68	0.75
1:G:196:ARG:HH11	1:G:196:ARG:CA	1.95	0.75
1:G:269:LEU:HD22	1:G:269:LEU:N	1.99	0.75
1:R:195:TRP:O	1:R:196:ARG:HB2	1.86	0.75
1:R:259:LYS:C	1:R:262:LYS:HG3	2.10	0.74
1:G:71:LYS:O	1:G:73:ILE:HD12	1.87	0.74
1:G:106:LYS:O	1:G:109:ALA:HB3	1.86	0.74
1:G:122:ALA:HB2	3:G:336:NAD:O2D	1.87	0.74
1:R:5:VAL:HA	1:R:93:TYR:O	1.87	0.74
1:G:98:THR:HG21	1:G:101:PHE:CD2	2.21	0.74
1:R:197:GLY:O	1:R:199:ARG:CB	2.34	0.74
1:G:128:PRO:HG3	1:G:143:LEU:HD21	1.68	0.74
1:G:197:GLY:O	1:G:199:ARG:CB	2.33	0.74
1:G:322:ARG:CA	1:G:322:ARG:HE	1.96	0.74
1:R:3:VAL:CA	1:R:27:VAL:HG13	2.17	0.74
1:R:33:ASN:OD1	1:R:84:ILE:HG21	1.87	0.74
1:R:282:SER:O	1:R:312:TRP:CH2	2.41	0.74
1:G:180:ILE:HD12	1:G:184:GLN:CB	2.17	0.74
1:R:35:PRO:HG3	1:R:78:GLU:C	2.13	0.74
1:G:132:MET:HG3	1:G:322:ARG:HB3	1.69	0.74
1:R:15:ARG:HG3	1:R:15:ARG:HH11	1.52	0.73
1:G:239:VAL:HG22	1:G:314:ASP:HA	1.70	0.73
1:R:36:PHE:O	1:R:37:ILE:CG1	2.35	0.73
1:R:119:VAL:HG21	1:R:326:LEU:HD11	1.65	0.73
1:G:291:SER:CB	1:G:322:ARG:HD3	2.12	0.73
1:G:317:PHE:O	1:G:320:SER:N	2.20	0.73
1:G:2:LYS:O	1:G:28:ASP:CB	2.36	0.73
1:G:156:LEU:HD21	1:G:242:LEU:HD21	1.69	0.73
1:R:163:ILE:HG23	1:R:169:ILE:HD11	1.69	0.73
1:R:10:PHE:CZ	1:R:46:PHE:HB2	2.23	0.73
1:G:196:ARG:NH2	1:G:208:ALA:CB	2.27	0.73
1:G:276:THR:HG1	1:G:278:ASP:HB2	1.53	0.73
1:R:3:VAL:H	1:R:27:VAL:CA	1.94	0.73
1:G:327:MET:HA	1:G:330:MET:HE2	1.71	0.73
1:R:102:THR:O	1:R:103:THR:CB	2.27	0.73
1:G:293:ILE:O	1:G:312:TRP:HD1	1.70	0.73
1:R:40:HIS:ND1	1:R:43:VAL:HG13	2.03	0.73
1:R:176:THR:CG2	1:R:231:ALA:HB1	2.07	0.73
1:R:240:SER:O	1:R:313:TYR:HB2	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:179:ALA:HB2	1:G:239:VAL:O	1.89	0.73
1:G:273:LEU:CA	1:G:292:SER:O	2.37	0.73
1:R:3:VAL:HG23	1:R:27:VAL:CB	2.19	0.72
1:G:78:GLU:OE1	1:G:85:LYS:HE3	1.89	0.72
1:R:230:MET:HG2	1:R:231:ALA:N	2.02	0.72
1:G:128:PRO:CG	1:G:143:LEU:HD21	2.18	0.72
1:G:86:TRP:NE1	1:G:110:HIS:NE2	2.38	0.72
1:R:15:ARG:HH11	1:R:15:ARG:CG	2.02	0.72
1:R:60:LYS:HG3	1:R:61:ALA:H	1.55	0.72
1:G:114:GLY:O	1:G:115:ALA:O	2.07	0.72
1:R:134:VAL:CG2	1:R:219:VAL:CG1	2.66	0.72
1:G:77:GLN:O	1:G:78:GLU:O	2.08	0.72
1:G:171:GLU:OE2	1:G:247:ARG:NH1	2.23	0.72
1:R:2:LYS:HB2	1:R:26:LYS:CG	2.16	0.72
1:G:2:LYS:NZ	1:G:25:GLY:CA	2.51	0.72
1:R:134:VAL:HG23	1:R:219:VAL:CG1	2.19	0.72
1:G:115:ALA:O	1:G:116:LYS:HD3	1.90	0.71
1:G:135:ASN:HD22	1:G:136:HIS:N	1.88	0.71
1:R:10:PHE:CB	1:R:34:ASP:OD2	2.37	0.71
1:R:191:SER:HB2	1:G:41:TYR:OH	1.89	0.71
1:R:10:PHE:CE1	1:R:32:ILE:HD13	2.25	0.71
1:R:76:PHE:HD2	1:R:85:LYS:HZ2	1.36	0.71
1:R:205:LEU:HD22	1:R:205:LEU:O	1.90	0.71
1:G:216:VAL:HG13	1:G:223:LEU:HD23	1.72	0.71
1:G:26:LYS:HD2	1:G:27:VAL:H	1.48	0.71
1:R:197:GLY:C	1:R:199:ARG:N	2.42	0.71
1:G:213:ALA:HB2	1:G:228:THR:HA	1.72	0.71
1:R:84:ILE:HD12	1:R:85:LYS:HE3	1.71	0.71
1:R:134:VAL:HG23	1:R:219:VAL:HG12	1.72	0.71
1:R:76:PHE:CE2	1:R:85:LYS:HD2	2.25	0.71
1:G:65:LYS:HD2	1:G:73:ILE:C	2.15	0.71
1:G:155:CYS:O	1:G:158:PRO:HD2	1.90	0.71
1:G:247:ARG:HH11	1:G:247:ARG:HB3	1.54	0.71
1:G:269:LEU:H	1:G:269:LEU:CD2	2.00	0.71
1:G:10:PHE:CD1	1:G:32:ILE:HG21	2.26	0.71
1:G:78:GLU:HB2	1:G:84:ILE:CG2	2.20	0.71
1:G:34:ASP:HB3	1:G:42:MET:HE2	1.73	0.70
1:R:2:LYS:HZ1	1:R:25:GLY:HA3	1.56	0.70
1:R:67:VAL:HG23	1:R:67:VAL:O	1.89	0.70
1:R:196:ARG:HH21	1:R:208:ALA:CA	2.02	0.70
1:G:314:ASP:O	1:G:315:ASN:O	2.09	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:55:PHE:O	1:R:56:HIS:CB	2.39	0.70
1:G:185:LYS:O	1:G:201:ALA:HB2	1.92	0.70
1:G:275:TYR:C	1:G:275:TYR:HD2	1.98	0.70
1:R:29:ILE:C	1:R:30:VAL:CG1	2.65	0.70
1:R:333:LYS:NZ	1:R:333:LYS:CB	2.53	0.70
1:G:2:LYS:HD2	1:G:25:GLY:C	2.16	0.70
1:R:91:THR:HG23	1:R:91:THR:O	1.92	0.70
1:R:3:VAL:HG21	1:R:27:VAL:HG11	1.71	0.70
1:R:261:VAL:O	1:R:265:SER:HB3	1.90	0.70
1:G:29:ILE:C	1:G:30:VAL:HG13	2.16	0.70
1:R:16:LEU:HD12	1:R:320:SER:HB2	1.68	0.70
1:G:130:PHE:O	1:G:131:VAL:HG12	1.92	0.70
1:R:175:THR:HG22	1:R:243:ASP:HB3	1.71	0.70
1:R:260:VAL:CG1	1:R:261:VAL:H	2.03	0.70
1:G:81:PRO:O	1:G:84:ILE:HG13	1.92	0.69
1:G:47:GLN:HB3	1:G:59:VAL:HG11	1.74	0.69
1:R:275:TYR:C	1:R:275:TYR:CD2	2.69	0.69
1:G:12:ARG:N	1:G:15:ARG:HH11	1.89	0.69
1:G:175:THR:HB	1:G:230:MET:CE	2.22	0.69
1:R:61:ALA:HB2	1:R:66:LEU:HD12	1.72	0.69
1:G:156:LEU:CD1	1:G:242:LEU:HD23	1.96	0.69
1:G:15:ARG:O	1:G:19:ARG:CB	2.40	0.69
1:R:193:LYS:O	1:R:194:LEU:CB	2.40	0.69
1:R:174:MET:CG	1:R:242:LEU:HD11	2.21	0.69
1:R:221:PRO:O	1:R:224:ASP:HB2	1.93	0.69
1:G:104:MET:O	1:G:105:GLU:C	2.32	0.69
1:R:129:MET:C	1:R:130:PHE:CD1	2.68	0.69
1:R:317:PHE:O	1:R:318:GLY:C	2.34	0.69
1:G:26:LYS:HD3	1:G:28:ASP:N	2.00	0.69
1:G:35:PRO:HG2	3:G:336:NAD:C6A	2.23	0.69
1:G:65:LYS:HB2	1:G:73:ILE:O	1.92	0.69
1:R:126:ASP:O	1:R:127:ALA:HB2	1.91	0.69
1:G:330:MET:O	1:G:334:GLU:HG3	1.93	0.69
1:R:10:PHE:HB3	1:R:34:ASP:OD2	1.93	0.69
1:R:117:ARG:HH11	1:R:144:LYS:HD2	1.56	0.69
1:R:111:LEU:HD21	1:R:116:LYS:O	1.92	0.68
1:R:269:LEU:HD12	1:R:272:ILE:HD11	1.75	0.68
1:G:22:PHE:O	1:G:26:LYS:HA	1.92	0.68
1:R:314:ASP:O	1:R:315:ASN:O	2.10	0.68
1:R:38:ASP:OD2	1:R:39:LEU:N	2.24	0.68
1:R:120:ILE:HD12	1:R:146:ILE:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:85:LYS:O	1:G:113:GLY:O	2.12	0.68
1:R:174:MET:SD	1:R:242:LEU:HD11	2.33	0.68
1:R:197:GLY:O	1:R:199:ARG:N	2.26	0.68
1:G:4:LYS:HE3	1:G:92:ALA:HB2	1.74	0.68
1:R:86:TRP:CZ2	1:R:94:VAL:CG1	2.77	0.68
1:G:30:VAL:HG22	1:G:73:ILE:CG1	2.21	0.68
1:R:315:ASN:O	1:R:316:GLU:C	2.36	0.68
1:R:26:LYS:HG2	1:R:28:ASP:N	2.08	0.68
1:R:40:HIS:ND1	1:R:43:VAL:CG1	2.57	0.68
1:G:38:ASP:OD2	1:G:39:LEU:N	2.25	0.68
1:G:234:VAL:HB	1:G:235:PRO:CD	2.23	0.68
1:R:22:PHE:HE2	1:R:71:LYS:HD2	1.59	0.67
1:R:196:ARG:HA	1:R:196:ARG:CZ	2.22	0.67
1:R:196:ARG:NH2	1:R:208:ALA:CB	2.49	0.67
1:G:257:ILE:CG2	1:G:258:LYS:N	2.56	0.67
1:R:85:LYS:HE3	1:R:85:LYS:H	1.59	0.67
1:R:86:TRP:HE1	1:R:110:HIS:CE1	2.12	0.67
1:R:98:THR:CG2	1:R:99:GLY:N	2.57	0.67
1:R:121:SER:O	1:R:122:ALA:HB2	1.94	0.67
1:R:25:GLY:O	1:R:26:LYS:HB3	1.94	0.67
1:R:152:THR:HA	1:R:313:TYR:CZ	2.29	0.67
1:G:86:TRP:CD1	1:G:110:HIS:CD2	2.82	0.67
1:G:320:SER:HA	1:G:323:VAL:CG2	2.25	0.67
1:R:16:LEU:HB3	1:R:320:SER:OG	1.94	0.67
1:G:121:SER:O	1:G:122:ALA:HB2	1.94	0.67
1:G:152:THR:HG22	1:G:153:THR:N	2.10	0.67
1:G:221:PRO:O	1:G:223:LEU:N	2.27	0.67
1:R:260:VAL:HG13	1:R:261:VAL:HG12	1.77	0.67
1:R:294:PHE:CG	1:R:295:ASP:N	2.63	0.67
1:R:326:LEU:HD22	1:R:326:LEU:C	2.19	0.67
1:G:84:ILE:HB	1:G:85:LYS:HZ2	1.58	0.67
1:R:2:LYS:HG2	1:R:3:VAL:N	2.08	0.67
1:G:78:GLU:CB	1:G:84:ILE:CG2	2.71	0.67
1:G:107:ALA:HB2	1:G:120:ILE:HD11	1.76	0.67
1:R:257:ILE:CG2	1:R:258:LYS:N	2.57	0.67
1:R:16:LEU:CD2	1:R:19:ARG:HG2	2.23	0.67
1:G:161:LYS:C	1:G:165:ASP:OD2	2.37	0.67
1:G:254:TYR:HH	1:G:300:ILE:HG21	1.57	0.67
1:G:140:ALA:O	1:G:143:LEU:N	2.26	0.67
1:G:178:HIS:HA	1:G:240:SER:CB	2.21	0.67
1:R:15:ARG:O	1:R:19:ARG:N	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:106:LYS:O	1:G:109:ALA:CB	2.43	0.66
1:G:261:VAL:HG23	1:G:273:LEU:HD13	1.77	0.66
1:R:49:ASP:O	1:R:53:GLY:O	2.12	0.66
1:G:29:ILE:O	1:G:30:VAL:HG12	1.94	0.66
1:G:196:ARG:HE	1:G:208:ALA:CB	2.08	0.66
1:G:250:LYS:NZ	1:G:251:PRO:HD2	2.11	0.66
1:G:14:GLY:O	1:G:18:THR:HG22	1.94	0.66
1:G:16:LEU:HD22	1:G:16:LEU:O	1.95	0.66
1:G:47:GLN:HB2	1:G:59:VAL:HG11	1.76	0.66
1:G:220:ILE:O	1:G:221:PRO:O	2.14	0.66
1:G:275:TYR:C	1:G:275:TYR:CD2	2.69	0.66
1:R:81:PRO:HA	1:R:84:ILE:CG2	2.26	0.66
1:R:3:VAL:HB	1:R:27:VAL:HG13	0.68	0.66
1:R:10:PHE:HE2	1:R:46:PHE:CB	2.05	0.66
1:R:153:THR:CG2	1:R:215:ALA:HB1	2.26	0.66
1:G:47:GLN:HA	1:G:55:PHE:HB2	1.77	0.66
1:R:103:THR:HG23	1:R:105:GLU:H	1.61	0.66
1:R:280:VAL:O	1:R:280:VAL:CG2	2.44	0.66
1:G:3:VAL:N	1:G:27:VAL:HG12	2.03	0.66
1:G:273:LEU:N	1:G:292:SER:O	2.29	0.66
1:R:45:MET:HE1	1:G:189:SER:O	1.95	0.66
1:G:174:MET:CE	1:G:212:ALA:HB2	2.14	0.66
1:R:10:PHE:CE1	1:R:32:ILE:CD1	2.79	0.66
1:R:264:ALA:O	1:R:269:LEU:HD23	1.96	0.66
1:G:16:LEU:CA	1:G:19:ARG:HB3	2.25	0.66
1:G:141:ASN:N	1:G:333:LYS:HZ1	1.93	0.66
1:R:186:THR:C	1:R:187:VAL:HG22	2.21	0.66
1:R:276:THR:HG23	1:R:295:ASP:CB	2.02	0.66
1:G:190:PRO:O	1:G:191:SER:HB3	1.94	0.66
1:G:326:LEU:C	1:G:326:LEU:HD12	2.21	0.66
1:R:85:LYS:H	1:R:85:LYS:CE	2.09	0.65
1:G:21:ALA:O	1:G:26:LYS:CA	2.43	0.65
1:G:141:ASN:N	1:G:333:LYS:NZ	2.43	0.65
1:R:21:ALA:O	1:R:26:LYS:CA	2.44	0.65
1:G:131:VAL:HG23	1:G:133:GLY:N	2.07	0.65
1:G:315:ASN:O	1:G:316:GLU:C	2.40	0.65
1:G:319:TYR:O	1:G:323:VAL:HG22	1.96	0.65
1:R:3:VAL:HG23	1:R:27:VAL:CG1	2.11	0.65
1:G:121:SER:O	1:G:122:ALA:CB	2.45	0.65
1:G:168:GLY:HA3	1:G:249:GLU:HB3	1.77	0.65
1:R:195:TRP:CD1	1:R:197:GLY:H	2.08	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:200:GLY:O	1:R:201:ALA:CB	2.44	0.65
1:G:128:PRO:HG2	1:G:145:ILE:O	1.96	0.65
1:G:199:ARG:HG3	1:G:199:ARG:O	1.97	0.65
1:R:3:VAL:H	1:R:27:VAL:CB	2.08	0.65
1:R:76:PHE:CD2	1:R:85:LYS:HD2	2.32	0.65
1:R:196:ARG:NH2	1:R:208:ALA:CA	2.60	0.65
1:G:130:PHE:CE1	1:G:138:LYS:HD3	2.32	0.65
1:G:299:GLY:O	1:G:308:LYS:HD3	1.96	0.65
1:R:110:HIS:ND1	1:R:118:ILE:HD11	2.11	0.65
1:R:190:PRO:O	1:R:191:SER:CB	2.44	0.65
1:R:192:GLY:O	1:R:195:TRP:HA	1.96	0.65
1:G:260:VAL:HG13	1:G:261:VAL:N	2.12	0.65
1:R:132:MET:HE2	1:R:325:ASP:O	1.97	0.65
1:R:156:LEU:C	1:R:158:PRO:HD2	2.22	0.65
1:R:257:ILE:HG23	1:R:258:LYS:N	2.10	0.65
1:G:15:ARG:NH2	1:G:45:MET:HE1	2.12	0.65
1:G:55:PHE:C	1:G:55:PHE:CD2	2.74	0.65
1:G:284:ASP:O	1:G:286:ASN:HB2	1.97	0.65
1:G:323:VAL:HB	1:G:327:MET:HE3	1.78	0.65
1:R:266:GLU:HG2	1:R:267:GLY:N	2.12	0.64
1:R:291:SER:OG	1:R:322:ARG:CD	2.44	0.64
1:G:117:ARG:HH11	1:G:144:LYS:CD	2.08	0.64
1:R:24:SER:OG	1:R:25:GLY:N	2.29	0.64
1:R:254:TYR:CE2	1:R:300:ILE:HD13	2.33	0.64
1:R:67:VAL:O	1:R:67:VAL:CG2	2.44	0.64
1:R:170:VAL:O	1:R:247:ARG:HB3	1.98	0.64
1:G:131:VAL:O	1:G:135:ASN:HB3	1.97	0.64
1:G:78:GLU:HG3	1:G:84:ILE:CB	2.26	0.64
1:G:129:MET:HE2	1:G:149:ALA:CA	2.27	0.64
1:G:153:THR:HG23	1:G:215:ALA:CB	2.21	0.64
1:R:190:PRO:O	1:R:191:SER:OG	2.14	0.64
1:G:106:LYS:O	1:G:109:ALA:N	2.29	0.64
1:G:155:CYS:C	1:G:158:PRO:HD2	2.22	0.64
1:R:86:TRP:NE1	1:R:110:HIS:NE2	2.45	0.64
1:G:168:GLY:O	1:G:169:ILE:O	2.15	0.64
1:R:30:VAL:HG22	1:R:31:ALA:N	2.11	0.64
1:R:74:THR:CG2	1:R:75:ILE:N	2.60	0.64
1:R:189:SER:O	1:R:190:PRO:O	2.15	0.64
1:G:29:ILE:O	1:G:30:VAL:HG13	1.97	0.64
1:R:135:ASN:CG	1:R:136:HIS:H	2.04	0.64
1:R:247:ARG:HA	1:R:305:THR:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:264:ALA:O	1:G:268:PRO:HD2	1.98	0.64
1:R:130:PHE:HE2	1:R:139:TYR:N	1.96	0.64
1:G:78:GLU:CG	1:G:84:ILE:HA	2.26	0.64
1:G:247:ARG:HH11	1:G:247:ARG:CB	2.10	0.64
1:R:5:VAL:C	1:R:91:THR:OG1	2.41	0.64
1:R:16:LEU:HG	1:R:317:PHE:CD2	2.33	0.64
1:G:196:ARG:C	1:G:198:GLY:H	2.04	0.64
1:R:110:HIS:O	1:R:113:GLY:N	2.31	0.63
1:R:163:ILE:CG2	1:R:164:HIS:N	2.61	0.63
1:R:315:ASN:O	1:R:317:PHE:N	2.31	0.63
1:G:13:ILE:HG22	1:G:97:SER:HB3	1.80	0.63
1:G:294:PHE:CG	1:G:295:ASP:N	2.64	0.63
1:R:17:VAL:O	1:R:21:ALA:HB2	1.98	0.63
1:R:174:MET:HG3	1:R:242:LEU:CD1	2.26	0.63
1:R:259:LYS:HA	1:R:262:LYS:CD	2.28	0.63
1:R:278:ASP:O	1:R:279:GLU:CB	2.41	0.63
1:R:78:GLU:OE2	1:R:78:GLU:CA	2.43	0.63
1:G:254:TYR:CE2	1:G:300:ILE:HG12	2.33	0.63
1:R:34:ASP:HB3	1:R:42:MET:HE2	1.81	0.63
1:R:254:TYR:OH	1:R:300:ILE:HG12	1.98	0.63
1:R:275:TYR:C	1:R:275:TYR:HD2	2.07	0.63
1:R:291:SER:CB	1:R:322:ARG:HD2	2.27	0.63
1:G:135:ASN:ND2	1:G:136:HIS:H	1.97	0.63
1:G:247:ARG:HG2	1:G:306:PHE:HD1	1.63	0.63
1:G:62:GLU:O	1:G:65:LYS:O	2.15	0.63
1:G:123:PRO:CA	1:G:129:MET:HE1	2.26	0.63
1:G:293:ILE:O	1:G:312:TRP:HB2	1.99	0.63
1:R:129:MET:O	1:R:130:PHE:CD1	2.52	0.63
1:R:47:GLN:HG2	1:R:55:PHE:HB3	1.80	0.63
1:G:159:LEU:HD11	1:G:309:LEU:HD23	1.81	0.63
1:G:273:LEU:O	1:G:293:ILE:HA	1.99	0.63
1:G:81:PRO:O	1:G:84:ILE:N	2.31	0.62
1:G:276:THR:HG22	1:G:295:ASP:HB3	1.76	0.62
1:G:29:ILE:C	1:G:30:VAL:CG1	2.72	0.62
1:G:4:LYS:CE	1:G:92:ALA:HB3	2.29	0.62
1:G:257:ILE:C	1:G:260:VAL:HG12	2.20	0.62
1:R:11:GLY:CA	1:R:15:ARG:HD3	2.29	0.62
1:R:22:PHE:CE2	1:R:71:LYS:HD2	2.35	0.62
1:G:313:TYR:O	1:G:314:ASP:CB	2.43	0.62
1:R:8:ASP:HB2	1:R:96:GLU:HA	1.81	0.62
1:R:81:PRO:O	1:R:84:ILE:HG23	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:196:ARG:HG3	1:R:233:ARG:HH21	1.64	0.62
1:R:317:PHE:O	1:R:319:TYR:N	2.33	0.62
1:G:5:VAL:O	1:G:30:VAL:CA	2.46	0.62
1:G:93:TYR:CE2	1:G:334:GLU:OE1	2.53	0.62
1:R:54:LYS:HE2	1:R:56:HIS:CE1	2.35	0.62
1:R:205:LEU:C	1:R:205:LEU:CD2	2.65	0.62
1:G:159:LEU:O	1:G:163:ILE:HD13	2.00	0.62
1:G:180:ILE:HG23	1:G:237:ALA:HA	1.80	0.62
1:G:257:ILE:HG22	1:G:258:LYS:H	1.64	0.62
1:G:86:TRP:CD1	1:G:110:HIS:NE2	2.67	0.62
1:G:297:GLY:O	1:G:300:ILE:CG1	2.47	0.62
1:R:37:ILE:HG23	1:R:41:TYR:HB3	1.82	0.62
1:R:257:ILE:CG2	1:R:258:LYS:H	2.12	0.62
1:G:117:ARG:NH1	1:G:144:LYS:CD	2.60	0.62
1:G:196:ARG:HE	1:G:208:ALA:HB1	1.65	0.62
1:G:213:ALA:HB1	1:G:227:LEU:O	2.00	0.62
1:R:186:THR:O	1:R:187:VAL:HG22	1.93	0.62
1:R:3:VAL:N	1:R:27:VAL:HA	1.88	0.62
1:R:166:HIS:HD2	1:R:260:VAL:HG23	1.62	0.62
1:R:238:ASN:OD1	1:R:239:VAL:N	2.33	0.62
1:G:78:GLU:CB	1:G:84:ILE:HG22	2.29	0.62
1:G:139:TYR:HD2	1:G:333:LYS:HD3	1.65	0.62
1:G:154:ASN:O	1:G:158:PRO:CD	2.47	0.62
1:G:175:THR:HA	1:G:230:MET:O	1.99	0.62
1:G:230:MET:SD	1:G:232:PHE:CE1	2.93	0.62
1:R:116:LYS:O	1:R:144:LYS:HG3	1.99	0.61
1:G:322:ARG:HE	1:G:322:ARG:HA	1.63	0.61
1:G:93:TYR:HA	1:G:117:ARG:O	2.00	0.61
1:R:86:TRP:NE1	1:R:94:VAL:HG11	2.15	0.61
1:G:103:THR:HG23	1:G:105:GLU:N	2.15	0.61
1:R:26:LYS:HG2	1:R:27:VAL:N	2.08	0.61
1:R:42:MET:O	1:R:46:PHE:HB3	2.01	0.61
1:R:47:GLN:NE2	1:R:48:TYR:CE1	2.68	0.61
1:R:106:LYS:O	1:R:109:ALA:HB3	2.01	0.61
1:R:179:ALA:HB1	1:R:237:ALA:O	2.00	0.61
1:G:4:LYS:O	1:G:4:LYS:CG	2.42	0.61
1:R:10:PHE:HE1	1:R:32:ILE:CD1	2.14	0.61
1:R:230:MET:SD	1:R:232:PHE:HZ	2.21	0.61
1:G:86:TRP:NE1	1:G:110:HIS:CE1	2.68	0.61
1:G:171:GLU:H	1:G:226:LYS:HG3	1.65	0.61
1:G:317:PHE:O	1:G:319:TYR:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:78:GLU:CG	1:R:84:ILE:HA	2.26	0.61
1:R:194:LEU:HD12	1:R:194:LEU:O	2.00	0.61
1:R:197:GLY:C	1:R:199:ARG:CB	2.73	0.61
1:G:38:ASP:CG	1:G:39:LEU:HD23	2.25	0.61
1:G:160:ALA:O	1:G:161:LYS:C	2.44	0.61
1:G:255:ASP:HA	1:G:258:LYS:HE2	1.81	0.61
1:R:131:VAL:HG13	1:R:219:VAL:HG13	1.80	0.61
1:G:37:ILE:CG2	1:G:42:MET:HE3	2.19	0.61
1:G:111:LEU:HA	1:G:115:ALA:HB3	1.81	0.61
1:R:294:PHE:CD2	1:R:295:ASP:N	2.68	0.61
1:R:156:LEU:HD22	1:R:174:MET:CE	2.17	0.61
1:R:323:VAL:O	1:R:326:LEU:HB3	2.00	0.61
1:G:2:LYS:O	1:G:28:ASP:HB2	2.01	0.61
1:R:68:ILE:HG13	1:R:73:ILE:HD12	1.82	0.60
1:R:141:ASN:O	1:R:143:LEU:O	2.18	0.60
1:R:1:GLY:HA2	1:R:29:ILE:N	2.13	0.60
1:G:175:THR:HB	1:G:230:MET:HE3	1.82	0.60
1:G:317:PHE:C	1:G:319:TYR:N	2.58	0.60
1:R:47:GLN:NE2	1:R:48:TYR:CD1	2.69	0.60
1:G:5:VAL:HG12	1:G:6:GLY:O	2.00	0.60
1:G:43:VAL:HG12	1:G:66:LEU:CD1	2.19	0.60
1:G:140:ALA:HA	1:G:333:LYS:HZ2	1.67	0.60
1:G:326:LEU:HD12	1:G:327:MET:N	2.16	0.60
1:R:16:LEU:HD12	1:R:320:SER:HB3	0.68	0.60
1:G:168:GLY:CA	1:G:249:GLU:HB3	2.30	0.60
1:G:247:ARG:NH1	1:G:247:ARG:HB3	2.16	0.60
1:G:65:LYS:HG3	1:G:66:LEU:N	2.17	0.60
1:R:137:PHE:O	1:R:138:LYS:C	2.44	0.60
1:G:8:ASP:OD2	1:G:33:ASN:CG	2.44	0.60
1:G:81:PRO:O	1:G:82:GLU:C	2.45	0.60
1:G:189:SER:CB	1:G:190:PRO:HD2	2.32	0.60
1:G:222:GLU:C	1:G:223:LEU:O	2.44	0.60
1:R:3:VAL:H	1:R:27:VAL:HG22	1.66	0.60
1:R:121:SER:O	1:R:121:SER:OG	2.17	0.60
1:G:16:LEU:C	1:G:16:LEU:HD13	2.26	0.60
1:G:98:THR:CA	3:G:336:NAD:C8A	2.68	0.60
1:G:15:ARG:HA	1:G:18:THR:CG2	2.28	0.60
1:R:121:SER:O	1:R:122:ALA:CB	2.50	0.60
1:R:261:VAL:HG22	1:R:275:TYR:HD1	1.65	0.60
1:G:129:MET:CE	1:G:149:ALA:HA	2.30	0.60
1:R:20:ALA:O	1:R:21:ALA:C	2.44	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:102:THR:HG23	1:R:124:SER:HA	1.84	0.59
1:G:10:PHE:HD1	1:G:32:ILE:CG2	2.14	0.59
1:R:157:ALA:N	1:R:158:PRO:HD2	2.17	0.59
1:R:275:TYR:HE2	1:R:277:GLU:CG	2.08	0.59
1:G:216:VAL:CG1	1:G:223:LEU:HD23	2.30	0.59
1:G:217:GLY:HA3	1:G:224:ASP:HA	1.85	0.59
1:G:91:THR:HG23	1:G:91:THR:O	2.02	0.59
1:G:117:ARG:HG3	1:G:334:GLU:CD	2.26	0.59
1:G:98:THR:CB	3:G:336:NAD:H8A	2.32	0.59
1:R:55:PHE:O	1:R:56:HIS:HB2	2.02	0.59
1:G:3:VAL:O	1:G:28:ASP:OD1	2.21	0.59
1:G:93:TYR:HD2	1:G:330:MET:HE3	1.66	0.59
1:G:242:LEU:O	1:G:310:VAL:HG23	2.02	0.59
1:G:152:THR:HA	1:G:313:TYR:CZ	2.38	0.59
1:G:34:ASP:CB	1:G:42:MET:HE2	2.33	0.59
1:G:65:LYS:HG3	1:G:66:LEU:O	2.03	0.59
1:G:88:ASP:O	1:G:89:ALA:CB	2.51	0.59
1:G:139:TYR:HE2	1:G:334:GLU:HG2	1.67	0.59
1:G:302:LEU:O	1:G:303:ASN:HB2	2.03	0.59
1:G:320:SER:C	1:G:323:VAL:HG23	2.27	0.59
1:R:178:HIS:O	1:R:234:VAL:HG22	2.03	0.58
1:R:258:LYS:HE3	1:R:296:ALA:HB1	1.85	0.58
1:G:97:SER:O	1:G:98:THR:HB	2.03	0.58
1:G:315:ASN:HB2	3:G:336:NAD:H4N	1.85	0.58
1:G:17:VAL:CG1	1:G:327:MET:HE1	2.33	0.58
1:R:86:TRP:CZ2	1:R:94:VAL:HG13	2.39	0.58
1:R:322:ARG:HA	1:R:325:ASP:HB2	1.85	0.58
1:G:8:ASP:OD1	1:G:96:GLU:OE1	2.12	0.58
1:G:10:PHE:HB3	1:G:34:ASP:OD2	2.03	0.58
1:G:54:LYS:HG2	1:G:55:PHE:H	1.68	0.58
1:G:189:SER:HB2	1:G:190:PRO:HD2	1.85	0.58
1:R:117:ARG:CD	1:R:144:LYS:HA	2.30	0.58
1:R:168:GLY:O	1:R:169:ILE:HB	2.04	0.58
1:G:79:ARG:HA	3:G:336:NAD:H62A	1.68	0.58
1:G:139:TYR:HD2	1:G:333:LYS:CD	2.15	0.58
1:G:179:ALA:HB1	1:G:237:ALA:O	2.03	0.58
1:R:45:MET:HE1	1:G:189:SER:C	2.28	0.58
1:R:41:TYR:CE1	1:G:190:PRO:HA	2.39	0.58
1:R:131:VAL:HG23	1:R:133:GLY:H	1.67	0.58
1:G:2:LYS:C	1:G:28:ASP:HB2	2.29	0.58
1:G:86:TRP:O	1:G:91:THR:HG22	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:156:LEU:HB3	1:G:216:VAL:CG2	2.33	0.58
1:G:254:TYR:HB2	1:G:302:LEU:HD22	1.84	0.58
1:R:162:VAL:HG13	1:R:260:VAL:HG22	1.85	0.58
1:G:214:LYS:O	1:G:218:LYS:NZ	2.27	0.58
1:G:263:GLU:O	1:G:266:GLU:HB3	2.04	0.58
1:R:285:PHE:O	1:R:286:ASN:C	2.45	0.58
1:G:16:LEU:HD23	1:G:317:PHE:CE2	2.39	0.58
1:G:37:ILE:HG13	1:G:41:TYR:HB3	1.85	0.58
1:G:266:GLU:O	1:G:270:LYS:HE3	2.04	0.58
1:R:81:PRO:HA	1:R:84:ILE:HG23	1.86	0.57
1:R:98:THR:HG21	1:R:101:PHE:HB2	1.86	0.57
1:R:151:CYS:HB3	3:R:336:NAD:C5N	2.34	0.57
1:G:65:LYS:HD2	1:G:73:ILE:O	2.00	0.57
1:G:101:PHE:O	1:G:102:THR:HB	2.03	0.57
1:R:283:ASP:O	1:R:284:ASP:C	2.47	0.57
1:G:106:LYS:HB2	1:G:106:LYS:NZ	2.19	0.57
1:R:258:LYS:O	1:R:275:TYR:HE1	1.88	0.57
1:G:186:THR:O	1:G:187:VAL:HG23	2.05	0.57
1:R:163:ILE:HG23	1:R:169:ILE:CD1	2.35	0.57
1:R:174:MET:HE2	1:R:242:LEU:HD21	1.87	0.57
1:G:3:VAL:H	1:G:27:VAL:HG13	0.44	0.57
1:G:48:TYR:CE2	1:G:54:LYS:HG3	2.40	0.57
1:G:130:PHE:CZ	1:G:138:LYS:HB3	2.40	0.57
1:G:132:MET:O	1:G:135:ASN:OD1	2.21	0.57
1:R:117:ARG:CA	1:R:144:LYS:O	2.51	0.57
1:G:30:VAL:CG2	1:G:73:ILE:CG1	2.81	0.57
1:G:65:LYS:HB2	1:G:74:THR:CA	2.12	0.57
1:G:151:CYS:C	1:G:313:TYR:HE2	2.13	0.57
1:G:260:VAL:HG13	1:G:261:VAL:H	1.70	0.57
1:R:3:VAL:O	1:R:4:LYS:HG2	2.03	0.57
1:R:239:VAL:HG21	1:R:286:ASN:H	1.70	0.57
1:G:35:PRO:CB	1:G:79:ARG:HG2	2.32	0.57
1:G:47:GLN:HG3	1:G:48:TYR:N	2.18	0.57
1:G:141:ASN:HD22	1:G:333:LYS:NZ	2.02	0.57
1:G:333:LYS:HE2	1:G:334:GLU:N	2.20	0.57
1:R:313:TYR:HB3	1:R:315:ASN:H	1.70	0.57
1:R:14:GLY:O	1:R:18:THR:CG2	2.53	0.56
1:R:174:MET:HE2	1:R:242:LEU:CD2	2.35	0.56
1:G:163:ILE:CD1	1:G:163:ILE:N	2.68	0.56
1:R:103:THR:OG1	1:R:126:ASP:OD2	2.22	0.56
1:R:240:SER:OG	1:R:315:ASN:ND2	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:10:PHE:CB	1:G:34:ASP:OD2	2.53	0.56
1:G:20:ALA:O	1:G:21:ALA:C	2.48	0.56
1:G:230:MET:HG2	1:G:231:ALA:N	2.20	0.56
1:G:294:PHE:CD2	1:G:295:ASP:N	2.73	0.56
1:R:103:THR:HG23	1:R:105:GLU:N	2.20	0.56
1:R:148:ASN:O	1:R:149:ALA:O	2.23	0.56
1:R:241:VAL:HB	1:R:312:TRP:CE3	2.41	0.56
1:R:285:PHE:N	1:R:285:PHE:CD2	2.73	0.56
1:G:2:LYS:HZ1	1:G:25:GLY:HA3	1.68	0.56
1:R:44:TYR:OH	1:G:199:ARG:NE	2.38	0.56
1:R:196:ARG:HG3	1:R:233:ARG:NH2	2.21	0.56
1:G:30:VAL:HG23	1:G:31:ALA:H	1.69	0.56
1:G:293:ILE:O	1:G:312:TRP:CB	2.54	0.56
1:R:215:ALA:O	1:R:219:VAL:HG23	2.06	0.56
1:G:85:LYS:N	1:G:85:LYS:CD	2.57	0.56
1:G:120:ILE:HG22	1:G:121:SER:N	2.18	0.56
1:G:265:SER:O	1:G:266:GLU:C	2.49	0.56
1:G:66:LEU:HB3	1:G:68:ILE:CD1	2.36	0.56
1:G:295:ASP:OD1	1:G:312:TRP:NE1	2.38	0.56
1:R:65:LYS:CG	1:R:66:LEU:N	2.69	0.56
1:R:234:VAL:HB	1:R:235:PRO:CD	2.33	0.56
1:G:157:ALA:HB3	1:G:158:PRO:HD3	1.88	0.56
1:R:3:VAL:C	1:R:4:LYS:HG2	2.31	0.56
1:G:196:ARG:NE	1:G:208:ALA:CB	2.68	0.56
1:G:322:ARG:CA	1:G:322:ARG:NE	2.67	0.56
1:R:12:ARG:NH2	1:R:51:THR:HG21	2.20	0.55
1:R:19:ARG:HH21	1:R:55:PHE:HB2	1.69	0.55
1:R:146:ILE:HG21	1:R:330:MET:SD	2.46	0.55
1:G:276:THR:C	1:G:278:ASP:N	2.63	0.55
1:G:282:SER:O	1:G:312:TRP:CH2	2.59	0.55
1:G:10:PHE:CD1	1:G:32:ILE:CG2	2.89	0.55
1:G:120:ILE:CG2	1:G:121:SER:N	2.68	0.55
1:R:30:VAL:HG22	1:R:73:ILE:CG1	2.29	0.55
1:R:54:LYS:HG2	1:R:55:PHE:N	2.21	0.55
1:G:139:TYR:CD2	1:G:333:LYS:HD3	2.42	0.55
1:R:77:GLN:O	1:R:78:GLU:O	2.24	0.55
1:R:86:TRP:NE1	1:R:110:HIS:CD2	2.73	0.55
1:R:155:CYS:C	1:R:158:PRO:HD2	2.32	0.55
1:G:98:THR:OG1	3:G:336:NAD:C8A	2.54	0.55
1:G:130:PHE:C	1:G:131:VAL:CG1	2.80	0.55
1:G:11:GLY:HA2	1:G:15:ARG:CZ	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:15:ARG:CA	1:G:18:THR:HG23	2.33	0.55
1:R:132:MET:O	1:R:133:GLY:C	2.49	0.55
1:R:188:ASP:OD2	1:G:50:SER:OG	2.24	0.55
1:G:13:ILE:CG2	1:G:97:SER:HB3	2.37	0.55
1:G:43:VAL:CG1	1:G:66:LEU:HD11	2.20	0.55
1:G:65:LYS:CE	1:G:73:ILE:O	2.54	0.55
1:G:257:ILE:CG2	1:G:258:LYS:H	2.17	0.55
1:R:181:THR:CG2	2:R:338:SO4:O1	2.55	0.55
1:R:214:LYS:O	1:R:218:LYS:HG2	2.07	0.55
1:G:139:TYR:CD2	1:G:333:LYS:NZ	2.65	0.55
1:G:195:TRP:C	1:G:197:GLY:N	2.62	0.55
1:R:11:GLY:N	1:R:15:ARG:HD3	2.22	0.55
1:G:150:SER:HB3	2:G:340:SO4:O1	2.07	0.55
1:G:152:THR:HG22	1:G:153:THR:H	1.70	0.55
1:R:129:MET:O	1:R:130:PHE:HD1	1.88	0.55
1:R:211:GLY:O	1:R:215:ALA:CB	2.55	0.55
1:R:213:ALA:HB2	1:R:228:THR:CA	2.27	0.55
1:G:148:ASN:HB3	1:G:319:TYR:OH	2.07	0.55
1:G:254:TYR:CD2	1:G:300:ILE:HD13	2.42	0.55
1:R:180:ILE:CG1	1:R:237:ALA:HA	2.28	0.55
1:R:285:PHE:HE1	1:R:293:ILE:HG12	1.72	0.55
1:G:4:LYS:CG	1:G:92:ALA:HB3	2.37	0.55
1:G:128:PRO:CG	1:G:143:LEU:CD2	2.85	0.55
1:G:239:VAL:HG22	1:G:314:ASP:CA	2.37	0.55
1:G:250:LYS:HZ3	1:G:251:PRO:HD2	1.72	0.55
1:R:3:VAL:N	1:R:27:VAL:HG22	2.22	0.54
1:R:34:ASP:HB3	1:R:42:MET:CE	2.37	0.54
1:R:263:GLU:O	1:R:266:GLU:OE1	2.25	0.54
1:R:239:VAL:HG21	1:R:286:ASN:N	2.22	0.54
1:R:323:VAL:O	1:R:327:MET:N	2.34	0.54
1:G:230:MET:HG2	1:G:231:ALA:H	1.72	0.54
1:R:222:GLU:C	1:R:223:LEU:O	2.49	0.54
1:G:2:LYS:CB	1:G:26:LYS:CE	2.73	0.54
1:G:15:ARG:NH2	1:G:45:MET:HE2	2.23	0.54
1:G:230:MET:SD	1:G:232:PHE:HE1	2.31	0.54
1:R:81:PRO:O	1:R:82:GLU:C	2.49	0.54
1:R:139:TYR:CE1	1:R:143:LEU:HD22	2.43	0.54
1:R:160:ALA:HB1	1:R:223:LEU:CD1	2.37	0.54
1:G:169:ILE:H	1:G:248:LEU:HB3	1.71	0.54
1:G:285:PHE:N	1:G:285:PHE:CD2	2.75	0.54
1:R:98:THR:HG22	1:R:99:GLY:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:211:GLY:O	1:R:215:ALA:HB2	2.07	0.54
1:G:13:ILE:HB	3:G:336:NAD:O2N	2.08	0.54
1:G:140:ALA:CA	1:G:333:LYS:HZ2	2.20	0.54
1:G:247:ARG:HG2	1:G:306:PHE:CD1	2.42	0.54
1:G:326:LEU:O	1:G:330:MET:HG3	2.07	0.54
1:R:26:LYS:CG	1:R:27:VAL:N	2.67	0.54
1:R:146:ILE:HG13	1:R:147:SER:H	1.70	0.54
1:G:22:PHE:CE1	1:G:69:ASP:HB3	2.42	0.54
1:G:141:ASN:C	1:G:143:LEU:H	2.14	0.54
1:G:284:ASP:O	1:G:285:PHE:C	2.50	0.54
1:R:3:VAL:H	1:R:27:VAL:CG2	2.19	0.54
1:R:12:ARG:HE	1:R:12:ARG:HA	1.73	0.54
1:R:59:VAL:O	1:R:59:VAL:CG2	2.56	0.54
1:R:157:ALA:N	1:R:158:PRO:CD	2.70	0.54
1:G:303:ASN:O	1:G:305:THR:N	2.40	0.54
1:R:98:THR:HG21	1:R:101:PHE:CB	2.38	0.54
1:G:11:GLY:O	1:G:13:ILE:N	2.41	0.54
1:R:43:VAL:O	1:R:59:VAL:HG21	2.08	0.54
1:G:192:GLY:O	1:G:195:TRP:HA	2.08	0.54
1:R:254:TYR:CB	1:R:302:LEU:HD22	2.36	0.53
1:G:98:THR:OG1	3:G:336:NAD:H8A	2.07	0.53
1:R:172:GLY:HA2	1:R:245:THR:O	2.08	0.53
1:G:10:PHE:CZ	1:G:46:PHE:HB2	2.42	0.53
1:G:65:LYS:CE	1:G:72:ALA:HB1	2.27	0.53
1:G:153:THR:HG21	1:G:215:ALA:HB1	1.83	0.53
1:R:16:LEU:CD1	1:R:320:SER:CB	2.39	0.53
1:G:16:LEU:HD22	1:G:20:ALA:H	1.73	0.53
1:G:93:TYR:CD1	1:G:93:TYR:N	2.76	0.53
1:G:139:TYR:CE2	1:G:330:MET:HB3	2.43	0.53
1:R:261:VAL:O	1:R:262:LYS:C	2.51	0.53
1:G:12:ARG:NH2	1:G:49:ASP:OD1	2.42	0.53
1:R:43:VAL:HG22	1:R:44:TYR:N	2.21	0.53
1:R:196:ARG:NH1	1:R:196:ARG:CA	2.33	0.53
1:G:76:PHE:HB3	1:G:85:LYS:NZ	2.23	0.53
1:G:186:THR:C	1:G:187:VAL:HG23	2.34	0.53
1:G:273:LEU:HA	1:G:292:SER:O	2.09	0.53
1:G:275:TYR:HE2	1:G:277:GLU:CG	2.12	0.53
1:G:285:PHE:HA	1:G:288:SER:HB2	1.91	0.53
1:G:331:ALA:O	1:G:332:SER:C	2.51	0.53
1:R:34:ASP:CB	1:R:42:MET:HE2	2.38	0.53
1:R:130:PHE:O	1:R:148:ASN:HA	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:131:VAL:CG2	1:R:133:GLY:H	2.22	0.53
1:R:255:ASP:HA	1:R:258:LYS:HD3	1.90	0.53
1:G:25:GLY:O	1:G:26:LYS:HB3	2.07	0.53
1:G:239:VAL:CG1	1:G:240:SER:N	2.71	0.53
1:G:304:ASP:OD2	1:G:305:THR:HB	2.09	0.53
1:R:38:ASP:O	1:R:39:LEU:C	2.51	0.53
1:R:65:LYS:HG3	1:R:66:LEU:N	2.23	0.53
1:R:86:TRP:CZ2	1:R:94:VAL:HG11	2.44	0.53
1:G:181:THR:HB	2:G:338:SO4:O1	2.08	0.53
1:R:22:PHE:CA	1:R:26:LYS:HA	2.34	0.53
1:R:70:GLY:O	1:R:72:ALA:N	2.42	0.53
1:R:11:GLY:O	1:R:13:ILE:N	2.42	0.53
1:R:155:CYS:O	1:R:158:PRO:HG2	2.09	0.53
1:R:204:ASN:HB3	1:R:206:ILE:HD13	1.90	0.53
1:G:148:ASN:O	1:G:319:TYR:OH	2.19	0.53
1:R:68:ILE:HG13	1:R:73:ILE:CD1	2.39	0.53
1:R:86:TRP:CE2	1:R:94:VAL:HG11	2.43	0.53
1:R:121:SER:HA	1:R:319:TYR:OH	2.08	0.53
1:G:77:GLN:O	1:G:78:GLU:C	2.51	0.53
1:G:180:ILE:HG13	1:G:181:THR:N	2.23	0.53
1:R:5:VAL:O	1:R:30:VAL:CA	2.56	0.52
1:R:128:PRO:HG2	1:R:145:ILE:O	2.09	0.52
1:R:199:ARG:CG	1:R:199:ARG:O	2.57	0.52
1:G:323:VAL:HB	1:G:327:MET:CE	2.40	0.52
1:R:6:GLY:C	1:R:7:VAL:HG23	2.34	0.52
1:R:28:ASP:CB	1:R:29:ILE:CG1	2.74	0.52
1:R:78:GLU:HG3	1:R:84:ILE:N	2.24	0.52
1:G:8:ASP:HB2	1:G:96:GLU:HG2	1.92	0.52
1:G:148:ASN:OD1	1:G:326:LEU:HD23	2.09	0.52
1:R:15:ARG:CD	1:R:15:ARG:H	2.22	0.52
1:R:106:LYS:O	1:R:109:ALA:N	2.42	0.52
1:G:16:LEU:HA	1:G:19:ARG:CB	2.37	0.52
1:G:174:MET:HE2	1:G:212:ALA:CB	2.16	0.52
1:G:222:GLU:O	1:G:223:LEU:O	2.27	0.52
1:R:47:GLN:O	1:R:55:PHE:N	2.42	0.52
1:R:176:THR:HG23	1:R:176:THR:O	2.09	0.52
1:G:199:ARG:O	1:G:199:ARG:CG	2.57	0.52
1:G:323:VAL:C	1:G:327:MET:HE3	2.33	0.52
1:R:28:ASP:CG	1:R:29:ILE:CG1	2.83	0.52
1:G:273:LEU:O	1:G:292:SER:O	2.27	0.52
1:G:294:PHE:CD2	1:G:294:PHE:C	2.88	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:212:ALA:O	1:R:216:VAL:HG23	2.10	0.52
1:G:298:ALA:HB1	1:G:310:VAL:CG1	2.40	0.52
1:G:330:MET:O	1:G:334:GLU:CG	2.56	0.52
1:R:317:PHE:C	1:R:319:TYR:N	2.66	0.52
1:G:316:GLU:O	1:G:319:TYR:HB3	2.10	0.52
1:G:326:LEU:C	1:G:326:LEU:CD1	2.82	0.52
1:R:333:LYS:HZ2	1:R:333:LYS:HB2	1.74	0.52
1:G:47:GLN:O	1:G:55:PHE:N	2.43	0.52
1:G:283:ASP:O	1:G:284:ASP:O	2.27	0.52
1:R:12:ARG:HA	1:R:12:ARG:NE	2.24	0.52
1:R:124:SER:OG	1:R:127:ALA:HB3	2.10	0.52
1:R:155:CYS:SG	1:R:292:SER:HB2	2.50	0.52
1:G:29:ILE:CG2	1:G:72:ALA:O	2.58	0.52
1:G:148:ASN:O	1:G:149:ALA:O	2.27	0.52
1:R:14:GLY:O	1:R:18:THR:HG22	2.10	0.52
1:R:109:ALA:O	1:R:112:LYS:N	2.38	0.52
1:G:65:LYS:CG	1:G:66:LEU:N	2.69	0.52
1:G:85:LYS:O	1:G:113:GLY:CA	2.57	0.52
1:G:155:CYS:HA	1:G:292:SER:HB2	1.91	0.52
1:R:16:LEU:HD21	1:R:317:PHE:CE2	2.44	0.51
1:R:167:PHE:CZ	1:R:257:ILE:HA	2.45	0.51
1:R:254:TYR:HH	1:R:297:GLY:H	1.57	0.51
1:R:1:GLY:CA	1:R:28:ASP:OD2	2.48	0.51
1:R:111:LEU:CA	1:R:115:ALA:HB3	2.22	0.51
1:R:146:ILE:CG1	1:R:147:SER:N	2.70	0.51
1:R:248:LEU:O	1:R:305:THR:OG1	2.27	0.51
1:G:205:LEU:O	1:G:207:PRO:HD3	2.10	0.51
1:G:254:TYR:CE1	1:G:300:ILE:HG21	2.42	0.51
1:R:152:THR:HA	1:R:313:TYR:OH	2.09	0.51
1:R:200:GLY:O	1:R:201:ALA:HB2	2.10	0.51
1:R:240:SER:C	1:R:313:TYR:HD1	2.18	0.51
1:G:149:ALA:HB1	1:G:153:THR:HG21	1.86	0.51
1:R:157:ALA:HB3	1:R:158:PRO:HD3	1.93	0.51
1:G:213:ALA:HB2	1:G:227:LEU:C	2.34	0.51
1:R:78:GLU:HG3	1:R:84:ILE:HB	1.75	0.51
1:R:141:ASN:ND2	1:R:141:ASN:N	2.37	0.51
1:R:174:MET:CG	1:R:175:THR:N	2.67	0.51
1:R:195:TRP:HD1	1:R:197:GLY:N	1.97	0.51
1:R:254:TYR:CE1	1:R:300:ILE:HB	2.46	0.51
1:R:269:LEU:CD2	1:R:269:LEU:N	2.56	0.51
1:G:123:PRO:HA	1:G:129:MET:HE3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:37:ILE:HD11	1:G:190:PRO:HB3	1.93	0.51
1:R:102:THR:HG23	1:R:124:SER:HB2	1.93	0.51
1:G:272:ILE:O	1:G:273:LEU:CB	2.43	0.51
1:G:322:ARG:HA	1:G:325:ASP:HB2	1.92	0.51
1:R:19:ARG:O	1:R:22:PHE:HB3	2.10	0.51
1:R:33:ASN:HA	1:R:76:PHE:O	2.11	0.51
1:R:86:TRP:HE1	1:R:94:VAL:HG11	1.74	0.51
1:R:6:GLY:O	1:R:7:VAL:CG2	2.59	0.51
1:R:9:GLY:HA2	3:R:336:NAD:H8A	1.93	0.51
1:R:10:PHE:HB2	1:R:34:ASP:OD2	2.10	0.51
1:G:38:ASP:O	1:G:39:LEU:C	2.53	0.51
1:G:315:ASN:O	1:G:317:PHE:N	2.43	0.51
1:R:40:HIS:O	1:R:40:HIS:ND1	2.43	0.51
1:R:111:LEU:HD21	1:R:116:LYS:C	2.36	0.51
1:G:36:PHE:O	1:G:37:ILE:HD13	2.11	0.51
1:G:63:ASP:C	1:G:65:LYS:H	2.17	0.51
1:G:156:LEU:HD11	1:G:242:LEU:CD2	2.10	0.51
1:G:176:THR:O	1:G:231:ALA:HB1	2.09	0.51
1:R:6:GLY:C	1:R:7:VAL:CG2	2.84	0.51
1:G:82:GLU:HG2	1:G:83:ASN:H	1.76	0.51
1:G:103:THR:HG22	1:G:106:LYS:H	1.75	0.51
1:R:239:VAL:CG1	1:R:283:ASP:OD2	2.59	0.50
1:G:95:VAL:HB	1:G:119:VAL:HG13	1.94	0.50
1:G:196:ARG:CZ	1:G:208:ALA:CB	2.79	0.50
1:G:248:LEU:N	1:G:305:THR:O	2.41	0.50
1:R:16:LEU:O	1:R:17:VAL:C	2.52	0.50
1:R:78:GLU:HB3	1:R:84:ILE:HG22	1.93	0.50
1:G:164:HIS:CB	1:G:169:ILE:HD12	2.37	0.50
1:R:75:ILE:HG13	1:R:75:ILE:O	2.11	0.50
1:R:197:GLY:C	1:R:199:ARG:HB3	2.36	0.50
1:R:254:TYR:CZ	1:R:300:ILE:HG12	2.46	0.50
1:G:39:LEU:CG	1:G:40:HIS:N	2.38	0.50
1:R:68:ILE:CG1	1:R:73:ILE:HB	2.42	0.50
1:G:141:ASN:C	1:G:143:LEU:N	2.67	0.50
1:R:13:ILE:HG22	1:R:97:SER:HB2	1.93	0.50
1:R:92:ALA:HB1	1:R:116:LYS:CB	2.41	0.50
1:R:285:PHE:O	1:R:286:ASN:CB	2.55	0.50
1:G:189:SER:CB	1:G:190:PRO:CD	2.89	0.50
1:R:22:PHE:CZ	1:R:69:ASP:HB3	2.31	0.50
1:R:92:ALA:O	1:R:116:LYS:HB2	2.11	0.50
1:R:139:TYR:HE1	1:R:143:LEU:HD22	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:106:LYS:HB2	1:G:106:LYS:HZ2	1.76	0.50
1:R:163:ILE:HG21	1:R:169:ILE:HD11	1.89	0.50
1:G:16:LEU:HD12	1:G:320:SER:C	2.37	0.50
1:G:34:ASP:HB3	1:G:42:MET:CE	2.40	0.50
1:G:140:ALA:C	1:G:142:SER:N	2.68	0.50
1:G:247:ARG:HH11	1:G:247:ARG:CG	2.24	0.50
1:G:305:THR:CG2	1:G:306:PHE:N	2.57	0.50
1:R:34:ASP:N	1:R:76:PHE:O	2.43	0.50
1:R:139:TYR:O	1:R:333:LYS:HE3	2.11	0.50
1:G:43:VAL:O	1:G:47:GLN:HB3	2.12	0.50
1:G:4:LYS:CE	1:G:92:ALA:CB	2.81	0.50
1:G:16:LEU:HG	1:G:317:PHE:CE2	2.47	0.50
1:R:37:ILE:HD12	1:R:41:TYR:CD1	2.47	0.49
1:R:118:ILE:HG22	1:R:118:ILE:O	2.12	0.49
1:R:169:ILE:H	1:R:248:LEU:HA	1.76	0.49
1:G:8:ASP:HB2	1:G:96:GLU:CG	2.41	0.49
1:G:320:SER:HA	1:G:323:VAL:HG21	1.94	0.49
1:G:141:ASN:ND2	1:G:333:LYS:HE3	2.26	0.49
1:G:303:ASN:O	1:G:304:ASP:C	2.55	0.49
1:R:12:ARG:HH22	1:R:51:THR:HG21	1.76	0.49
1:G:12:ARG:CA	1:G:15:ARG:NH1	2.75	0.49
1:R:51:THR:CG2	1:R:52:HIS:N	2.75	0.49
1:R:153:THR:HG21	1:R:215:ALA:HB1	1.94	0.49
1:G:5:VAL:HA	1:G:93:TYR:O	2.11	0.49
1:G:152:THR:HA	1:G:313:TYR:CE2	2.47	0.49
1:G:230:MET:HE1	1:G:232:PHE:CZ	2.48	0.49
1:R:2:LYS:HD2	1:R:25:GLY:O	2.10	0.49
1:R:104:MET:HA	1:R:145:ILE:CD1	2.43	0.49
1:G:16:LEU:HB3	1:G:320:SER:CB	2.43	0.49
1:G:153:THR:CG2	1:G:215:ALA:CB	2.79	0.49
1:G:179:ALA:HA	1:G:236:THR:O	2.13	0.49
1:R:86:TRP:CD1	1:R:110:HIS:CD2	3.00	0.49
1:R:194:LEU:HD11	1:R:209:SER:HB3	1.94	0.49
1:R:12:ARG:H	1:R:15:ARG:NH1	2.11	0.49
1:R:104:MET:HA	1:R:145:ILE:HD11	1.95	0.49
1:R:257:ILE:HG22	1:R:258:LYS:H	1.76	0.49
1:G:30:VAL:CG2	1:G:31:ALA:H	2.21	0.49
1:G:196:ARG:HA	1:G:196:ARG:CZ	2.38	0.49
1:R:80:ASP:O	1:R:83:ASN:HB2	2.13	0.49
1:R:126:ASP:O	1:R:127:ALA:HB3	2.11	0.49
1:R:163:ILE:HG22	1:R:164:HIS:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:71:LYS:O	1:G:73:ILE:CD1	2.59	0.49
1:G:173:LEU:HD21	1:G:228:THR:HG22	1.94	0.49
1:R:6:GLY:O	1:R:7:VAL:HG22	2.13	0.49
1:R:103:THR:CG2	1:R:105:GLU:HB2	2.42	0.49
1:R:206:ILE:O	1:R:232:PHE:HA	2.13	0.49
1:G:150:SER:CB	2:G:340:SO4:O1	2.61	0.49
1:R:44:TYR:OH	1:G:199:ARG:CD	2.61	0.48
1:R:47:GLN:HE22	1:R:48:TYR:HE1	1.59	0.48
1:G:3:VAL:C	1:G:28:ASP:HB2	2.38	0.48
1:G:206:ILE:O	1:G:232:PHE:HA	2.12	0.48
1:G:257:ILE:HG23	1:G:258:LYS:N	2.27	0.48
1:G:320:SER:O	1:G:323:VAL:HG23	2.13	0.48
1:R:2:LYS:HD2	1:R:27:VAL:N	2.01	0.48
1:R:3:VAL:N	1:R:27:VAL:HG13	2.28	0.48
1:R:37:ILE:HG22	1:R:42:MET:HE3	1.94	0.48
1:R:92:ALA:HB1	1:R:116:LYS:HB2	1.94	0.48
1:R:149:ALA:O	1:R:319:TYR:HE1	1.95	0.48
1:R:253:LYS:O	1:R:256:ASP:N	2.46	0.48
1:G:107:ALA:HB1	1:G:118:ILE:HG21	1.95	0.48
1:R:86:TRP:NE1	1:R:110:HIS:CE1	2.78	0.48
1:R:197:GLY:HA3	1:R:199:ARG:HB3	1.95	0.48
1:R:254:TYR:HB2	1:R:302:LEU:HD22	1.94	0.48
1:R:257:ILE:O	1:R:258:LYS:C	2.56	0.48
1:G:86:TRP:HD1	1:G:110:HIS:CD2	2.31	0.48
1:G:173:LEU:CD2	1:G:228:THR:HG22	2.42	0.48
1:R:15:ARG:C	1:R:18:THR:HG23	2.38	0.48
1:R:239:VAL:CG2	1:R:286:ASN:H	2.27	0.48
1:R:284:ASP:O	1:R:286:ASN:CB	2.48	0.48
1:G:78:GLU:CB	1:G:84:ILE:HG23	2.31	0.48
1:G:163:ILE:N	1:G:163:ILE:HD12	2.29	0.48
1:G:188:ASP:O	1:G:189:SER:CB	2.58	0.48
1:G:217:GLY:CA	1:G:224:ASP:HB2	2.43	0.48
1:G:261:VAL:O	1:G:262:LYS:C	2.57	0.48
1:G:321:GLU:O	1:G:321:GLU:HG3	2.14	0.48
1:R:151:CYS:SG	1:R:152:THR:N	2.86	0.48
1:R:155:CYS:SG	1:R:312:TRP:O	2.54	0.48
1:G:79:ARG:H	1:G:79:ARG:HG3	1.51	0.48
1:G:98:THR:CB	3:G:336:NAD:C8A	2.92	0.48
1:R:28:ASP:CG	1:R:29:ILE:HG12	2.39	0.48
1:R:33:ASN:ND2	1:R:33:ASN:O	2.45	0.48
1:R:84:ILE:CD1	1:R:85:LYS:HE3	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:180:ILE:HD12	1:G:186:THR:HB	1.95	0.48
1:G:5:VAL:HG12	1:G:6:GLY:N	2.28	0.48
1:G:186:THR:C	1:G:187:VAL:CG2	2.85	0.48
1:R:190:PRO:HA	1:G:37:ILE:HD11	1.96	0.48
1:R:259:LYS:HA	1:R:262:LYS:CG	2.44	0.48
1:R:160:ALA:O	1:R:161:LYS:C	2.55	0.48
1:G:94:VAL:HG22	1:G:118:ILE:HG13	1.96	0.48
1:G:196:ARG:NH2	1:G:207:PRO:O	2.47	0.48
1:G:239:VAL:HG12	1:G:240:SER:N	2.28	0.48
1:R:68:ILE:CD1	1:R:73:ILE:HG21	2.37	0.48
1:G:2:LYS:C	1:G:28:ASP:CB	2.85	0.48
1:R:193:LYS:C	1:R:195:TRP:H	2.21	0.47
1:R:220:ILE:O	1:R:221:PRO:C	2.55	0.47
1:G:5:VAL:HG12	1:G:6:GLY:H	1.79	0.47
1:G:11:GLY:O	1:G:14:GLY:N	2.35	0.47
1:G:16:LEU:HD12	1:G:320:SER:CA	2.36	0.47
1:G:181:THR:CG2	2:G:338:SO4:O1	2.62	0.47
1:G:220:ILE:CG2	1:G:220:ILE:O	2.62	0.47
1:R:163:ILE:HG22	1:R:164:HIS:H	1.79	0.47
1:R:180:ILE:HG23	1:R:235:PRO:O	2.14	0.47
1:R:259:LYS:HA	1:R:262:LYS:HD3	1.95	0.47
1:G:2:LYS:HZ1	1:G:25:GLY:CA	2.24	0.47
1:G:273:LEU:HA	1:G:273:LEU:HD23	1.71	0.47
1:R:91:THR:O	1:R:91:THR:CG2	2.62	0.47
1:G:152:THR:CG2	1:G:153:THR:N	2.75	0.47
1:R:10:PHE:HE1	1:R:32:ILE:HD11	1.79	0.47
1:G:22:PHE:HA	1:G:26:LYS:HA	1.96	0.47
1:G:79:ARG:O	1:G:80:ASP:HB2	2.14	0.47
1:R:176:THR:O	1:R:231:ALA:HB1	2.14	0.47
1:R:264:ALA:O	1:R:269:LEU:CD2	2.63	0.47
1:G:68:ILE:O	1:G:69:ASP:HB3	2.14	0.47
1:R:13:ILE:HD11	1:R:319:TYR:HD2	1.80	0.47
1:R:78:GLU:CG	1:R:84:ILE:CB	2.79	0.47
1:R:92:ALA:CA	1:R:116:LYS:HB2	2.44	0.47
1:R:106:LYS:O	1:R:109:ALA:CB	2.62	0.47
1:R:139:TYR:HB3	1:R:329:HIS:HE1	1.80	0.47
1:R:141:ASN:O	1:R:142:SER:C	2.54	0.47
1:G:10:PHE:HD1	1:G:32:ILE:HG23	1.79	0.47
1:G:67:VAL:O	1:G:67:VAL:CG2	2.62	0.47
1:G:167:PHE:O	1:G:248:LEU:HB2	2.13	0.47
1:R:44:TYR:OH	1:G:199:ARG:HD3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:106:LYS:O	1:R:107:ALA:C	2.57	0.47
1:R:170:VAL:O	1:R:171:GLU:O	2.33	0.47
1:R:326:LEU:O	1:R:330:MET:HB2	2.14	0.47
1:G:8:ASP:HB3	1:G:96:GLU:HA	1.97	0.47
1:G:16:LEU:CD1	1:G:20:ALA:HB2	2.44	0.47
1:G:16:LEU:O	1:G:17:VAL:C	2.56	0.47
1:G:196:ARG:HH21	1:G:208:ALA:HB2	0.60	0.47
1:G:282:SER:O	1:G:312:TRP:CZ3	2.68	0.47
1:G:285:PHE:O	1:G:286:ASN:CB	2.60	0.47
1:R:1:GLY:CA	1:R:28:ASP:C	2.52	0.47
1:R:10:PHE:CE2	1:R:46:PHE:CB	2.78	0.47
1:R:84:ILE:O	1:R:85:LYS:O	2.32	0.47
1:R:239:VAL:HB	1:R:283:ASP:OD2	2.14	0.47
1:G:141:ASN:H	1:G:333:LYS:NZ	2.12	0.47
1:G:217:GLY:HA3	1:G:224:ASP:CA	2.44	0.47
1:G:41:TYR:O	1:G:42:MET:C	2.57	0.47
1:G:293:ILE:O	1:G:312:TRP:N	2.48	0.47
1:R:37:ILE:HG22	1:R:42:MET:HG3	1.97	0.47
1:G:12:ARG:H	1:G:15:ARG:CZ	2.17	0.47
1:G:30:VAL:CG2	1:G:31:ALA:N	2.63	0.47
1:G:285:PHE:HE1	1:G:293:ILE:HG12	1.80	0.47
1:R:35:PRO:HG2	3:R:336:NAD:C6A	2.45	0.46
1:R:192:GLY:O	1:R:195:TRP:CA	2.63	0.46
1:G:8:ASP:CB	1:G:96:GLU:CG	2.92	0.46
1:G:33:ASN:ND2	1:G:33:ASN:O	2.48	0.46
1:G:65:LYS:HG3	1:G:66:LEU:H	1.80	0.46
1:R:140:ALA:O	1:R:143:LEU:HB2	2.14	0.46
1:R:140:ALA:HA	1:R:333:LYS:NZ	2.30	0.46
1:R:217:GLY:O	1:R:220:ILE:C	2.58	0.46
1:R:254:TYR:HB3	1:R:302:LEU:HD22	1.96	0.46
1:G:240:SER:O	1:G:313:TYR:HD1	1.97	0.46
1:G:276:THR:C	1:G:278:ASP:H	2.20	0.46
1:R:8:ASP:CB	1:R:96:GLU:HA	2.45	0.46
1:R:15:ARG:HH21	1:R:45:MET:CE	2.20	0.46
1:R:86:TRP:HA	1:R:86:TRP:CE3	2.50	0.46
1:R:88:ASP:O	1:R:89:ALA:CB	2.63	0.46
1:R:196:ARG:NH2	1:R:208:ALA:HA	2.28	0.46
1:R:199:ARG:O	1:R:199:ARG:HG3	2.14	0.46
1:G:4:LYS:CD	1:G:92:ALA:HB3	2.45	0.46
1:G:55:PHE:O	1:G:56:HIS:CG	2.69	0.46
1:G:112:LYS:HD2	1:G:112:LYS:HA	1.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:117:ARG:HH11	1:G:144:LYS:CG	2.28	0.46
1:R:240:SER:O	1:R:313:TYR:HD1	1.97	0.46
1:R:241:VAL:HA	1:R:312:TRP:HA	1.98	0.46
1:R:16:LEU:CD2	1:R:317:PHE:CE2	2.99	0.46
1:R:154:ASN:O	1:R:158:PRO:HD3	2.15	0.46
1:G:168:GLY:HA3	1:G:249:GLU:CB	2.45	0.46
1:G:174:MET:O	1:G:174:MET:HG3	2.07	0.46
1:R:12:ARG:NH2	1:R:49:ASP:OD1	2.48	0.46
1:R:15:ARG:O	1:R:18:THR:HG23	2.15	0.46
1:R:96:GLU:OE1	1:R:101:PHE:HB3	2.16	0.46
1:R:140:ALA:HA	1:R:333:LYS:HZ1	1.81	0.46
1:G:29:ILE:HG22	1:G:30:VAL:H	1.80	0.46
1:G:55:PHE:CD1	1:G:56:HIS:O	2.69	0.46
1:G:185:LYS:O	1:G:200:GLY:O	2.34	0.46
1:G:276:THR:OG1	1:G:278:ASP:CG	2.59	0.46
1:R:12:ARG:HH22	1:R:51:THR:CG2	2.28	0.46
1:R:68:ILE:HG12	1:R:73:ILE:HB	1.98	0.46
1:R:256:ASP:O	1:R:259:LYS:CB	2.64	0.46
1:G:42:MET:SD	1:G:75:ILE:HB	2.56	0.46
1:G:86:TRP:HA	1:G:86:TRP:CE3	2.51	0.46
1:G:117:ARG:HH11	1:G:144:LYS:HG2	1.81	0.46
1:G:128:PRO:HG3	1:G:143:LEU:CD2	2.42	0.46
1:R:16:LEU:HB3	1:R:320:SER:CB	2.46	0.46
1:R:41:TYR:HE1	1:G:190:PRO:HA	1.81	0.46
1:R:62:GLU:HB3	1:R:63:ASP:H	1.57	0.46
1:R:199:ARG:HD3	1:G:44:TYR:OH	2.16	0.46
1:G:260:VAL:CG1	1:G:261:VAL:N	2.77	0.46
1:G:261:VAL:HG23	1:G:273:LEU:CD1	2.44	0.46
1:G:16:LEU:CD2	1:G:317:PHE:CE2	2.99	0.46
1:G:16:LEU:HD11	1:G:20:ALA:HB2	1.98	0.46
1:G:151:CYS:SG	1:G:152:THR:N	2.71	0.46
1:G:174:MET:HB2	1:G:243:ASP:O	2.15	0.46
1:G:234:VAL:CB	1:G:235:PRO:HD2	2.38	0.46
1:G:273:LEU:HB3	1:G:274:GLY:H	1.55	0.46
1:G:322:ARG:NE	1:G:322:ARG:N	2.64	0.46
1:R:22:PHE:CZ	1:R:69:ASP:CG	2.94	0.45
1:R:118:ILE:O	1:R:118:ILE:CG2	2.60	0.45
1:G:254:TYR:CE1	1:G:300:ILE:CG2	2.99	0.45
1:R:2:LYS:CE	1:R:25:GLY:HA3	2.36	0.45
1:R:78:GLU:HG2	1:R:84:ILE:HB	1.92	0.45
1:R:104:MET:O	1:R:105:GLU:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:210:THR:HG23	2:R:340:SO4:O2	2.15	0.45
1:R:256:ASP:O	1:R:259:LYS:HB3	2.16	0.45
1:G:281:VAL:HG23	1:G:285:PHE:CE2	2.50	0.45
1:G:320:SER:HA	1:G:323:VAL:HG23	1.97	0.45
1:R:74:THR:HG22	1:R:75:ILE:N	2.30	0.45
1:R:107:ALA:HB3	1:R:145:ILE:HD12	1.99	0.45
1:G:128:PRO:CB	1:G:143:LEU:HD21	2.45	0.45
1:G:158:PRO:HG2	1:G:292:SER:HB3	1.98	0.45
1:R:303:ASN:O	1:R:306:PHE:N	2.49	0.45
1:G:16:LEU:HD22	1:G:20:ALA:N	2.31	0.45
1:G:84:ILE:HG13	1:G:84:ILE:H	1.45	0.45
1:R:81:PRO:O	1:R:84:ILE:N	2.49	0.45
1:R:94:VAL:HB	1:R:118:ILE:HG13	1.99	0.45
1:R:220:ILE:O	1:R:221:PRO:O	2.35	0.45
1:R:230:MET:CE	1:R:232:PHE:CE2	3.00	0.45
1:G:76:PHE:CD2	1:G:85:LYS:NZ	2.78	0.45
1:G:180:ILE:HD12	1:G:184:GLN:HB3	1.96	0.45
1:R:2:LYS:CG	1:R:3:VAL:H	2.09	0.45
1:R:181:THR:HG22	2:R:338:SO4:O1	2.16	0.45
1:G:106:LYS:O	1:G:107:ALA:C	2.57	0.45
1:G:181:THR:HG21	2:G:338:SO4:O1	2.17	0.45
1:G:254:TYR:H	1:G:302:LEU:HD13	1.81	0.45
1:R:15:ARG:CA	1:R:18:THR:HG23	2.46	0.45
1:R:155:CYS:O	1:R:158:PRO:HD2	2.17	0.45
1:R:222:GLU:O	1:R:223:LEU:O	2.35	0.45
1:G:164:HIS:O	1:G:165:ASP:C	2.58	0.45
1:G:257:ILE:HG21	1:G:309:LEU:HD11	1.99	0.45
1:R:174:MET:CE	1:R:242:LEU:HD21	2.46	0.45
1:G:16:LEU:HG	1:G:317:PHE:CD2	2.52	0.45
1:G:88:ASP:O	1:G:89:ALA:HB3	2.17	0.45
1:G:273:LEU:O	1:G:293:ILE:HB	2.17	0.45
1:G:324:VAL:HA	1:G:327:MET:SD	2.56	0.45
1:R:14:GLY:O	1:R:18:THR:HG23	2.17	0.45
1:R:326:LEU:C	1:R:326:LEU:CD2	2.89	0.45
1:G:55:PHE:O	1:G:56:HIS:CB	2.65	0.45
1:G:106:LYS:C	1:G:109:ALA:H	2.23	0.45
1:G:129:MET:C	1:G:130:PHE:HD1	2.24	0.45
1:G:196:ARG:NH1	1:G:196:ARG:CA	2.60	0.45
1:G:250:LYS:HZ2	1:G:251:PRO:HD2	1.82	0.45
1:R:179:ALA:HA	1:R:236:THR:O	2.17	0.44
1:G:115:ALA:C	1:G:116:LYS:HD3	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:156:LEU:HB3	1:G:216:VAL:HG21	1.98	0.44
1:R:15:ARG:HA	1:R:18:THR:HG23	1.99	0.44
1:R:22:PHE:HZ	1:R:69:ASP:CG	2.23	0.44
1:R:44:TYR:CD1	1:R:44:TYR:C	2.94	0.44
1:R:17:VAL:O	1:R:21:ALA:CB	2.63	0.44
1:R:55:PHE:CG	1:R:56:HIS:N	2.86	0.44
1:G:155:CYS:SG	1:G:312:TRP:O	2.63	0.44
1:G:172:GLY:O	1:G:227:LEU:HA	2.17	0.44
1:R:131:VAL:O	1:R:135:ASN:HB3	2.18	0.44
1:R:156:LEU:O	1:R:157:ALA:C	2.61	0.44
1:G:254:TYR:CE2	1:G:300:ILE:CG1	2.99	0.44
1:R:16:LEU:CA	1:R:19:ARG:HB3	2.38	0.44
1:R:151:CYS:HB3	3:R:336:NAD:H5N	1.99	0.44
1:R:324:VAL:HA	1:R:327:MET:HB2	1.99	0.44
1:G:148:ASN:C	1:G:149:ALA:O	2.59	0.44
1:R:43:VAL:HG12	1:R:66:LEU:HD11	1.99	0.44
1:R:193:LYS:HB2	1:R:193:LYS:HE3	1.38	0.44
1:R:248:LEU:H	1:R:248:LEU:HG	1.70	0.44
1:G:117:ARG:HA	1:G:144:LYS:O	2.18	0.44
1:R:254:TYR:CZ	1:R:300:ILE:CG1	3.01	0.44
1:G:108:GLY:O	1:G:111:LEU:HD11	2.18	0.44
1:G:170:VAL:O	1:G:171:GLU:O	2.35	0.44
1:R:28:ASP:CG	1:R:29:ILE:HG13	2.40	0.44
1:R:135:ASN:ND2	1:R:135:ASN:C	2.76	0.44
1:G:117:ARG:NH1	1:G:144:LYS:HG2	2.33	0.44
1:G:304:ASP:HB3	1:G:305:THR:HG22	1.98	0.44
1:R:16:LEU:HD22	1:R:19:ARG:HB3	2.00	0.44
1:G:184:GLN:HG3	1:G:233:ARG:HE	1.83	0.44
1:R:22:PHE:HE2	1:R:71:LYS:CD	2.28	0.43
1:R:197:GLY:CA	1:R:199:ARG:HB3	2.48	0.43
1:R:285:PHE:O	1:R:286:ASN:O	2.36	0.43
1:G:5:VAL:HG13	1:G:93:TYR:O	2.17	0.43
1:G:97:SER:HB2	1:G:98:THR:H	1.59	0.43
1:G:166:HIS:HD2	1:G:260:VAL:HG23	1.82	0.43
1:R:2:LYS:HB2	1:R:26:LYS:HG2	1.93	0.43
1:R:40:HIS:ND1	1:R:43:VAL:HG11	2.31	0.43
1:R:65:LYS:HG3	1:R:66:LEU:H	1.83	0.43
1:R:78:GLU:HG2	1:R:85:LYS:HZ1	1.83	0.43
1:R:218:LYS:HG2	1:R:218:LYS:H	1.57	0.43
1:G:140:ALA:C	1:G:142:SER:H	2.26	0.43
1:G:298:ALA:CB	1:G:310:VAL:CG1	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:16:LEU:HD22	1:G:16:LEU:C	2.43	0.43
1:R:156:LEU:HD12	1:R:156:LEU:HA	1.88	0.43
1:R:300:ILE:HD12	1:R:300:ILE:C	2.40	0.43
1:G:1:GLY:HA3	1:G:28:ASP:HA	1.87	0.43
1:G:16:LEU:HD23	1:G:19:ARG:CG	2.24	0.43
1:G:22:PHE:O	1:G:26:LYS:CA	2.64	0.43
1:G:191:SER:OG	1:G:192:GLY:O	2.36	0.43
1:G:221:PRO:O	1:G:223:LEU:C	2.58	0.43
1:R:13:ILE:HD13	1:R:13:ILE:HA	1.85	0.43
1:R:66:LEU:C	1:R:73:ILE:HG22	2.44	0.43
1:G:108:GLY:O	1:G:111:LEU:CD1	2.66	0.43
1:G:260:VAL:CG1	1:G:261:VAL:H	2.32	0.43
1:G:282:SER:HB2	1:G:283:ASP:H	1.55	0.43
1:R:12:ARG:N	1:R:15:ARG:NH1	2.67	0.43
1:R:277:GLU:O	1:R:278:ASP:C	2.61	0.43
1:G:35:PRO:HG3	1:G:78:GLU:C	2.42	0.43
1:G:35:PRO:HG2	3:G:336:NAD:N1A	2.33	0.43
1:G:54:LYS:HG2	1:G:55:PHE:N	2.32	0.43
1:G:59:VAL:O	1:G:59:VAL:HG13	2.19	0.43
1:G:76:PHE:CB	1:G:85:LYS:HZ3	2.31	0.43
1:G:135:ASN:O	1:G:138:LYS:CB	2.67	0.43
1:G:269:LEU:HB3	1:G:272:ILE:HD13	2.00	0.43
1:R:102:THR:CG2	1:R:124:SER:HA	2.47	0.43
1:R:222:GLU:O	1:R:223:LEU:C	2.62	0.43
1:G:43:VAL:HA	1:G:59:VAL:HG22	2.01	0.43
1:R:314:ASP:O	1:R:315:ASN:C	2.62	0.43
1:R:319:TYR:C	1:R:321:GLU:N	2.75	0.43
1:G:158:PRO:HG2	1:G:292:SER:CB	2.49	0.43
1:G:208:ALA:O	1:G:230:MET:CG	2.56	0.43
1:R:111:LEU:HD21	1:R:116:LYS:CA	2.48	0.43
1:R:174:MET:HA	1:R:243:ASP:O	2.19	0.43
1:G:200:GLY:O	1:G:201:ALA:HB2	2.19	0.43
1:G:12:ARG:NH2	1:G:51:THR:HG22	2.34	0.42
1:G:12:ARG:CA	1:G:15:ARG:HH11	2.32	0.42
1:G:16:LEU:O	1:G:20:ALA:N	2.34	0.42
1:G:178:HIS:ND1	1:G:240:SER:CB	2.82	0.42
1:G:193:LYS:HG3	1:G:193:LYS:O	2.19	0.42
1:G:269:LEU:HB3	1:G:272:ILE:CD1	2.49	0.42
1:R:162:VAL:HG11	1:R:261:VAL:HB	2.01	0.42
1:R:230:MET:HE3	1:R:232:PHE:CE2	2.54	0.42
1:R:269:LEU:HB3	1:R:272:ILE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:330:MET:O	1:R:334:GLU:CG	2.67	0.42
1:G:60:LYS:HD3	1:G:62:GLU:HG3	2.01	0.42
1:G:139:TYR:HB3	1:G:333:LYS:HD3	2.00	0.42
1:G:162:VAL:HB	1:G:163:ILE:CD1	2.49	0.42
1:G:269:LEU:O	1:G:270:LYS:C	2.62	0.42
1:G:293:ILE:O	1:G:312:TRP:CG	2.71	0.42
1:G:298:ALA:HB1	1:G:310:VAL:HG11	2.01	0.42
1:R:44:TYR:O	1:R:48:TYR:HB2	2.19	0.42
1:G:40:HIS:O	1:G:41:TYR:C	2.60	0.42
1:G:60:LYS:CG	1:G:61:ALA:N	2.60	0.42
1:G:140:ALA:O	1:G:143:LEU:CB	2.52	0.42
1:R:3:VAL:N	1:R:27:VAL:CA	2.63	0.42
1:R:98:THR:OG1	1:R:101:PHE:HD2	2.02	0.42
1:R:160:ALA:HB1	1:R:223:LEU:HD13	2.00	0.42
1:R:253:LYS:O	1:R:254:TYR:C	2.59	0.42
1:R:297:GLY:O	1:R:298:ALA:C	2.62	0.42
1:G:44:TYR:HB3	1:G:45:MET:H	1.68	0.42
1:G:115:ALA:O	1:G:116:LYS:CD	2.64	0.42
1:R:24:SER:HB2	1:R:321:GLU:OE1	2.19	0.42
1:R:51:THR:HG22	1:R:52:HIS:N	2.34	0.42
1:R:153:THR:HG23	1:R:215:ALA:HB1	2.00	0.42
1:R:241:VAL:HB	1:R:312:TRP:CD2	2.55	0.42
1:R:317:PHE:HA	1:R:320:SER:HB2	2.02	0.42
1:G:141:ASN:HD22	1:G:333:LYS:CE	2.32	0.42
1:G:162:VAL:HG11	1:G:261:VAL:HA	2.02	0.42
1:G:190:PRO:O	1:G:191:SER:CB	2.63	0.42
1:G:194:LEU:O	1:G:196:ARG:HG2	2.19	0.42
1:R:175:THR:CG2	1:R:243:ASP:HB3	2.44	0.42
1:R:239:VAL:HA	1:R:315:ASN:ND2	2.35	0.42
1:G:31:ALA:HB1	1:G:76:PHE:CE1	2.54	0.42
1:G:178:HIS:CE1	1:G:240:SER:HG	2.37	0.42
1:R:2:LYS:CB	1:R:26:LYS:HG2	2.49	0.42
1:R:3:VAL:O	1:R:4:LYS:CB	2.67	0.42
1:R:288:SER:O	1:R:289:ASN:HB2	2.19	0.42
1:G:141:ASN:HA	1:G:334:GLU:HB3	2.02	0.42
1:G:196:ARG:CZ	1:G:207:PRO:O	2.68	0.42
1:G:297:GLY:O	1:G:298:ALA:C	2.63	0.42
1:R:55:PHE:CD2	1:R:55:PHE:C	2.97	0.42
1:R:56:HIS:O	1:R:58:THR:N	2.53	0.42
1:R:117:ARG:CG	1:R:334:GLU:OE2	2.68	0.42
1:R:187:VAL:HB	1:R:188:ASP:H	1.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:228:THR:HG23	1:R:229:GLY:N	2.34	0.42
1:G:83:ASN:O	1:G:84:ILE:C	2.33	0.42
1:G:119:VAL:HG21	1:G:326:LEU:HD11	2.02	0.42
1:G:126:ASP:O	1:G:127:ALA:HB3	2.12	0.42
1:G:161:LYS:HD3	1:G:165:ASP:OD1	2.20	0.42
1:G:203:GLN:HE21	1:G:203:GLN:HB3	1.64	0.42
1:R:74:THR:HG23	1:R:75:ILE:N	2.34	0.42
1:R:137:PHE:HD1	1:R:137:PHE:HA	1.70	0.42
1:R:168:GLY:HA3	1:R:249:GLU:H	1.85	0.42
1:G:14:GLY:O	1:G:18:THR:CG2	2.67	0.42
1:G:95:VAL:HA	1:G:119:VAL:O	2.20	0.42
1:R:11:GLY:C	1:R:15:ARG:HD3	2.44	0.41
1:G:201:ALA:HB3	1:G:202:ALA:H	1.32	0.41
1:G:217:GLY:O	1:G:220:ILE:C	2.63	0.41
1:G:240:SER:O	1:G:313:TYR:N	2.53	0.41
1:R:16:LEU:HD22	1:R:19:ARG:HG2	2.00	0.41
1:R:210:THR:CG2	1:R:211:GLY:N	2.82	0.41
1:R:225:GLY:C	1:R:227:LEU:H	2.28	0.41
1:R:294:PHE:CD2	1:R:294:PHE:C	2.98	0.41
1:R:308:LYS:HB2	1:R:308:LYS:HE3	1.93	0.41
1:G:43:VAL:CG2	1:G:44:TYR:N	2.83	0.41
1:G:59:VAL:HG23	1:G:68:ILE:HG13	2.02	0.41
1:G:107:ALA:C	1:G:109:ALA:N	2.77	0.41
1:G:135:ASN:O	1:G:138:LYS:HB3	2.20	0.41
1:G:300:ILE:HD12	1:G:300:ILE:C	2.45	0.41
1:G:2:LYS:CG	1:G:26:LYS:HZ2	2.31	0.41
1:G:81:PRO:C	1:G:83:ASN:N	2.69	0.41
1:G:156:LEU:HD13	1:G:156:LEU:HA	1.79	0.41
1:G:187:VAL:HB	1:G:188:ASP:H	1.43	0.41
1:R:68:ILE:HG13	1:R:73:ILE:HB	2.02	0.41
1:R:288:SER:O	1:R:289:ASN:CB	2.68	0.41
1:G:2:LYS:HD2	1:G:25:GLY:O	2.19	0.41
1:R:17:VAL:CG1	1:R:327:MET:HE1	2.51	0.41
1:R:55:PHE:C	1:R:56:HIS:CG	2.98	0.41
1:R:66:LEU:HB3	1:R:73:ILE:CG2	2.50	0.41
1:R:86:TRP:HA	1:R:86:TRP:HE3	1.86	0.41
1:R:98:THR:HG21	1:R:101:PHE:H	1.86	0.41
1:R:148:ASN:O	1:R:149:ALA:C	2.62	0.41
1:R:162:VAL:HG13	1:R:260:VAL:CG2	2.50	0.41
1:G:42:MET:HE1	1:G:75:ILE:CD1	2.26	0.41
1:G:111:LEU:H	1:G:111:LEU:HG	1.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:266:GLU:HG2	1:G:267:GLY:N	2.35	0.41
1:R:190:PRO:HB2	1:R:191:SER:H	1.76	0.41
1:R:272:ILE:HD13	1:R:272:ILE:O	2.20	0.41
1:G:127:ALA:HB1	1:G:128:PRO:HD2	2.02	0.41
1:G:130:PHE:C	1:G:131:VAL:HG12	2.44	0.41
1:G:141:ASN:HD22	1:G:141:ASN:N	2.02	0.41
1:G:181:THR:CB	2:G:338:SO4:O1	2.68	0.41
1:R:143:LEU:HD23	1:R:145:ILE:O	2.21	0.41
1:R:196:ARG:N	1:R:196:ARG:HD2	2.33	0.41
1:R:297:GLY:O	1:R:300:ILE:HG12	2.10	0.41
1:R:300:ILE:HG13	1:R:300:ILE:H	1.73	0.41
1:R:303:ASN:O	1:R:306:PHE:O	2.39	0.41
1:R:330:MET:O	1:R:334:GLU:HG3	2.21	0.41
1:G:26:LYS:CD	1:G:27:VAL:CA	2.67	0.41
1:G:55:PHE:CG	1:G:56:HIS:N	2.86	0.41
1:G:86:TRP:HA	1:G:86:TRP:HE3	1.85	0.41
1:G:333:LYS:HE2	1:G:333:LYS:C	2.46	0.41
1:R:205:LEU:O	1:R:205:LEU:CD1	2.61	0.41
1:G:5:VAL:O	1:G:30:VAL:CB	2.69	0.41
1:G:46:PHE:HD2	1:G:59:VAL:HG21	1.85	0.41
1:G:295:ASP:OD2	1:G:298:ALA:HB2	2.21	0.41
1:R:3:VAL:O	1:R:4:LYS:CG	2.69	0.41
1:R:97:SER:OG	1:R:98:THR:N	2.51	0.41
1:R:180:ILE:CG2	1:R:235:PRO:O	2.69	0.41
1:R:221:PRO:O	1:R:224:ASP:CB	2.61	0.41
1:G:32:ILE:O	1:G:76:PHE:N	2.38	0.41
1:G:76:PHE:HB3	1:G:85:LYS:HZ3	1.85	0.41
1:G:135:ASN:CG	1:G:136:HIS:N	2.78	0.41
1:G:156:LEU:CG	1:G:242:LEU:CD2	2.80	0.41
1:G:205:LEU:O	1:G:205:LEU:HD22	2.19	0.41
1:G:314:ASP:O	1:G:315:ASN:C	2.64	0.41
1:R:29:ILE:O	1:R:30:VAL:CG1	2.64	0.41
1:G:107:ALA:O	1:G:108:GLY:C	2.64	0.41
1:G:129:MET:O	1:G:130:PHE:HD1	2.04	0.41
1:G:129:MET:O	1:G:130:PHE:CD1	2.74	0.41
1:G:191:SER:HB2	1:G:195:TRP:O	2.21	0.41
1:G:205:LEU:C	1:G:205:LEU:CD2	2.85	0.41
1:G:240:SER:O	1:G:313:TYR:HB2	2.21	0.41
1:R:61:ALA:HB2	1:R:66:LEU:CD1	2.45	0.40
1:R:86:TRP:C	1:R:88:ASP:N	2.79	0.40
1:R:224:ASP:H	1:R:227:LEU:HD11	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:141:ASN:N	1:G:333:LYS:HZ2	2.19	0.40
1:R:27:VAL:HG12	1:R:27:VAL:O	2.20	0.40
1:R:98:THR:O	3:R:336:NAD:H3B	2.21	0.40
1:R:239:VAL:HG12	1:R:240:SER:N	2.36	0.40
1:R:291:SER:HB2	1:R:322:ARG:HD2	2.02	0.40
1:G:123:PRO:CB	1:G:129:MET:HE1	2.50	0.40
1:G:167:PHE:HE1	1:G:260:VAL:HG11	1.87	0.40
1:R:19:ARG:NH2	1:R:55:PHE:HB2	2.36	0.40
1:G:103:THR:CG2	1:G:106:LYS:H	2.34	0.40
1:G:123:PRO:HB3	1:G:129:MET:HE1	2.03	0.40
1:G:130:PHE:CZ	1:G:139:TYR:N	2.90	0.40
1:G:184:GLN:OE1	1:G:233:ARG:HB3	2.21	0.40
1:G:281:VAL:HG23	1:G:285:PHE:CZ	2.57	0.40
1:G:307:VAL:HG22	1:G:308:LYS:N	2.36	0.40
1:R:82:GLU:H	1:R:82:GLU:HG2	1.70	0.40
1:R:116:LYS:O	1:R:144:LYS:HE2	2.21	0.40
1:R:139:TYR:HE1	1:R:143:LEU:CD2	2.34	0.40
1:R:153:THR:OG1	1:R:215:ALA:CB	2.68	0.40
1:R:273:LEU:HD13	1:R:273:LEU:HA	1.67	0.40
1:G:4:LYS:HG3	1:G:92:ALA:HB3	2.03	0.40
1:G:22:PHE:C	1:G:26:LYS:HA	2.47	0.40
1:G:108:GLY:O	1:G:111:LEU:HG	2.22	0.40

All (25) 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:R:267:GLY:CA	1:G:166:HIS:ND1[3_545]	1.06	1.14
1:R:263:GLU:OE1	1:G:260:VAL:CA[3_545]	1.27	0.93
1:R:308:LYS:CG	1:G:173:LEU:CD1[2_555]	1.33	0.87
1:R:260:VAL:CA	1:G:263:GLU:OE1[3_545]	1.45	0.75
1:R:263:GLU:OE2	1:G:259:LYS:O[3_545]	1.52	0.68
1:G:104:MET:CE	1:G:112:LYS:CB[2_556]	1.56	0.64
1:R:268:PRO:CD	1:G:166:HIS:CE1[3_545]	1.59	0.61
1:R:267:GLY:CA	1:G:166:HIS:CE1[3_545]	1.65	0.55
1:R:308:LYS:CD	1:G:173:LEU:CD1[2_555]	1.69	0.51
1:R:267:GLY:C	1:G:166:HIS:ND1[3_545]	1.75	0.45
1:R:268:PRO:N	1:G:166:HIS:CE1[3_545]	1.89	0.31
1:G:112:LYS:CE	1:G:145:ILE:CG2[2_556]	1.89	0.31
1:R:267:GLY:C	1:G:166:HIS:CE1[3_545]	1.92	0.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:104:MET:CE	1:G:112:LYS:CG[2_556]	1.98	0.22
1:G:111:LEU:O	1:G:144:LYS:NZ[2_556]	1.98	0.22
1:G:112:LYS:NZ	1:G:145:ILE:CG2[2_556]	2.04	0.16
1:R:260:VAL:C	1:G:263:GLU:OE1[3_545]	2.05	0.15
1:R:204:ASN:OD1	1:G:283:ASP:CB[2_555]	2.07	0.13
1:R:205:LEU:N	1:G:283:ASP:OD1[2_555]	2.10	0.10
1:R:267:GLY:CA	1:G:166:HIS:CG[3_545]	2.10	0.10
1:R:262:LYS:NZ	1:G:259:LYS:NZ[3_545]	2.11	0.09
1:R:263:GLU:OE1	1:G:260:VAL:N[3_545]	2.13	0.07
1:R:263:GLU:OE1	1:G:260:VAL:CB[3_545]	2.13	0.07
1:R:260:VAL:O	1:G:263:GLU:OE1[3_545]	2.15	0.05
1:R:268:PRO:CD	1:G:166:HIS:NE2[3_545]	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%)	198 (60%)	68 (20%)	66 (20%)	0	1
1	R	332/334 (99%)	205 (62%)	58 (18%)	69 (21%)	0	1
All	All	664/668 (99%)	403 (61%)	126 (19%)	135 (20%)	0	1

All (135) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	R	2	LYS
1	R	4	LYS
1	R	12	ARG
1	R	26	LYS
1	R	30	VAL
1	R	37	ILE
1	R	56	HIS
1	R	71	LYS

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Mol	Chain	Res	Type
1	R	78	GLU
1	R	80	ASP
1	R	85	LYS
1	R	103	THR
1	R	115	ALA
1	R	122	ALA
1	R	127	ALA
1	R	141	ASN
1	R	142	SER
1	R	149	ALA
1	R	171	GLU
1	R	190	PRO
1	R	191	SER
1	R	201	ALA
1	R	222	GLU
1	R	224	ASP
1	R	270	LYS
1	R	273	LEU
1	R	278	ASP
1	R	279	GLU
1	R	280	VAL
1	R	298	ALA
1	R	304	ASP
1	R	315	ASN
1	R	316	GLU
1	R	333	LYS
1	G	2	LYS
1	G	3	VAL
1	G	4	LYS
1	G	12	ARG
1	G	27	VAL
1	G	30	VAL
1	G	56	HIS
1	G	58	THR
1	G	78	GLU
1	G	80	ASP
1	G	84	ILE
1	G	103	THR
1	G	115	ALA
1	G	122	ALA
1	G	127	ALA
1	G	149	ALA

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Mol	Chain	Res	Type
1	G	161	LYS
1	G	169	ILE
1	G	171	GLU
1	G	190	PRO
1	G	191	SER
1	G	197	GLY
1	G	198	GLY
1	G	201	ALA
1	G	221	PRO
1	G	223	LEU
1	G	224	ASP
1	G	239	VAL
1	G	270	LYS
1	G	273	LEU
1	G	278	ASP
1	G	279	GLU
1	G	280	VAL
1	G	284	ASP
1	G	298	ALA
1	G	315	ASN
1	G	316	GLU
1	R	3	VAL
1	R	39	LEU
1	R	86	TRP
1	R	89	ALA
1	R	97	SER
1	R	98	THR
1	R	101	PHE
1	R	187	VAL
1	R	213	ALA
1	R	221	PRO
1	R	223	LEU
1	R	237	ALA
1	R	239	VAL
1	R	260	VAL
1	R	275	TYR
1	R	285	PHE
1	R	289	ASN
1	R	318	GLY
1	G	71	LYS
1	G	89	ALA
1	G	141	ASN

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Mol	Chain	Res	Type
1	G	152	THR
1	G	282	SER
1	G	289	ASN
1	G	303	ASN
1	R	57	GLY
1	R	125	ALA
1	R	236	THR
1	R	284	ASP
1	G	28	ASP
1	G	29	ILE
1	G	36	PHE
1	G	39	LEU
1	G	77	GLN
1	G	187	VAL
1	G	195	TRP
1	G	222	GLU
1	G	262	LYS
1	G	285	PHE
1	R	27	VAL
1	R	72	ALA
1	R	195	TRP
1	R	282	SER
1	R	332	SER
1	G	90	GLY
1	G	98	THR
1	G	105	GLU
1	G	136	HIS
1	G	194	LEU
1	G	318	GLY
1	R	58	THR
1	R	169	ILE
1	R	189	SER
1	R	262	LYS
1	G	151	CYS
1	G	160	ALA
1	G	275	TYR
1	R	198	GLY
1	G	44	TYR
1	G	100	VAL
1	G	114	GLY
1	R	114	GLY
1	R	281	VAL

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Mol	Chain	Res	Type
1	R	64	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	267/267 (100%)	137 (51%)	130 (49%)	0	0
1	R	267/267 (100%)	136 (51%)	131 (49%)	0	0
All	All	534/534 (100%)	273 (51%)	261 (49%)	0	0

All (261) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	5	VAL
1	R	8	ASP
1	R	12	ARG
1	R	13	ILE
1	R	15	ARG
1	R	16	LEU
1	R	18	THR
1	R	24	SER
1	R	26	LYS
1	R	27	VAL
1	R	28	ASP
1	R	29	ILE
1	R	30	VAL
1	R	33	ASN
1	R	36	PHE
1	R	39	LEU
1	R	41	TYR
1	R	42	MET
1	R	43	VAL
1	R	47	GLN
1	R	49	ASP
1	R	51	THR

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Mol	Chain	Res	Type
1	R	54	LYS
1	R	59	VAL
1	R	62	GLU
1	R	63	ASP
1	R	66	LEU
1	R	67	VAL
1	R	69	ASP
1	R	74	THR
1	R	75	ILE
1	R	78	GLU
1	R	79	ARG
1	R	80	ASP
1	R	82	GLU
1	R	84	ILE
1	R	85	LYS
1	R	86	TRP
1	R	95	VAL
1	R	98	THR
1	R	102	THR
1	R	103	THR
1	R	104	MET
1	R	110	HIS
1	R	112	LYS
1	R	117	ARG
1	R	118	ILE
1	R	119	VAL
1	R	121	SER
1	R	124	SER
1	R	126	ASP
1	R	131	VAL
1	R	132	MET
1	R	134	VAL
1	R	135	ASN
1	R	138	LYS
1	R	141	ASN
1	R	143	LEU
1	R	145	ILE
1	R	146	ILE
1	R	152	THR
1	R	153	THR
1	R	161	LYS
1	R	162	VAL

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Mol	Chain	Res	Type
1	R	163	ILE
1	R	165	ASP
1	R	166	HIS
1	R	170	VAL
1	R	174	MET
1	R	178	HIS
1	R	183	THR
1	R	186	THR
1	R	187	VAL
1	R	189	SER
1	R	193	LYS
1	R	194	LEU
1	R	196	ARG
1	R	203	GLN
1	R	205	LEU
1	R	206	ILE
1	R	218	LYS
1	R	220	ILE
1	R	222	GLU
1	R	226	LYS
1	R	227	LEU
1	R	228	THR
1	R	230	MET
1	R	233	ARG
1	R	240	SER
1	R	241	VAL
1	R	244	LEU
1	R	245	THR
1	R	246	CYS
1	R	247	ARG
1	R	248	LEU
1	R	250	LYS
1	R	253	LYS
1	R	256	ASP
1	R	259	LYS
1	R	261	VAL
1	R	262	LYS
1	R	263	GLU
1	R	265	SER
1	R	266	GLU
1	R	269	LEU
1	R	270	LYS

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Mol	Chain	Res	Type
1	R	272	ILE
1	R	273	LEU
1	R	276	THR
1	R	281	VAL
1	R	284	ASP
1	R	285	PHE
1	R	286	ASN
1	R	288	SER
1	R	290	HIS
1	R	292	SER
1	R	293	ILE
1	R	294	PHE
1	R	295	ASP
1	R	301	GLU
1	R	305	THR
1	R	307	VAL
1	R	308	LYS
1	R	310	VAL
1	R	311	SER
1	R	316	GLU
1	R	322	ARG
1	R	323	VAL
1	R	326	LEU
1	R	330	MET
1	R	333	LYS
1	G	4	LYS
1	G	5	VAL
1	G	12	ARG
1	G	13	ILE
1	G	17	VAL
1	G	18	THR
1	G	19	ARG
1	G	26	LYS
1	G	36	PHE
1	G	37	ILE
1	G	39	LEU
1	G	41	TYR
1	G	42	MET
1	G	43	VAL
1	G	45	MET
1	G	47	GLN
1	G	50	SER

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Mol	Chain	Res	Type
1	G	51	THR
1	G	54	LYS
1	G	60	LYS
1	G	62	GLU
1	G	66	LEU
1	G	67	VAL
1	G	71	LYS
1	G	73	ILE
1	G	74	THR
1	G	75	ILE
1	G	77	GLN
1	G	78	GLU
1	G	79	ARG
1	G	82	GLU
1	G	83	ASN
1	G	84	ILE
1	G	85	LYS
1	G	86	TRP
1	G	93	TYR
1	G	94	VAL
1	G	95	VAL
1	G	97	SER
1	G	103	THR
1	G	104	MET
1	G	105	GLU
1	G	106	LYS
1	G	110	HIS
1	G	111	LEU
1	G	112	LYS
1	G	116	LYS
1	G	118	ILE
1	G	129	MET
1	G	131	VAL
1	G	132	MET
1	G	134	VAL
1	G	141	ASN
1	G	142	SER
1	G	143	LEU
1	G	144	LYS
1	G	145	ILE
1	G	146	ILE
1	G	150	SER

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Mol	Chain	Res	Type
1	G	152	THR
1	G	155	CYS
1	G	156	LEU
1	G	159	LEU
1	G	161	LYS
1	G	163	ILE
1	G	164	HIS
1	G	165	ASP
1	G	171	GLU
1	G	173	LEU
1	G	175	THR
1	G	176	THR
1	G	177	VAL
1	G	178	HIS
1	G	180	ILE
1	G	181	THR
1	G	184	GLN
1	G	187	VAL
1	G	188	ASP
1	G	189	SER
1	G	191	SER
1	G	193	LYS
1	G	199	ARG
1	G	203	GLN
1	G	205	LEU
1	G	210	THR
1	G	214	LYS
1	G	216	VAL
1	G	220	ILE
1	G	223	LEU
1	G	226	LYS
1	G	227	LEU
1	G	230	MET
1	G	232	PHE
1	G	240	SER
1	G	241	VAL
1	G	246	CYS
1	G	247	ARG
1	G	248	LEU
1	G	249	GLU
1	G	250	LYS
1	G	256	ASP

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Mol	Chain	Res	Type
1	G	257	ILE
1	G	258	LYS
1	G	261	VAL
1	G	262	LYS
1	G	266	GLU
1	G	269	LEU
1	G	270	LYS
1	G	272	ILE
1	G	273	LEU
1	G	275	TYR
1	G	282	SER
1	G	283	ASP
1	G	284	ASP
1	G	285	PHE
1	G	286	ASN
1	G	293	ILE
1	G	294	PHE
1	G	301	GLU
1	G	302	LEU
1	G	309	LEU
1	G	314	ASP
1	G	315	ASN
1	G	316	GLU
1	G	322	ARG
1	G	323	VAL
1	G	326	LEU
1	G	330	MET
1	G	333	LYS
1	G	334	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	R	33	ASN
1	R	47	GLN
1	R	77	GLN
1	R	135	ASN
1	R	141	ASN
1	R	148	ASN
1	R	154	ASN
1	R	166	HIS
1	R	203	GLN

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Mol	Chain	Res	Type
1	R	289	ASN
1	R	303	ASN
1	R	315	ASN
1	G	33	ASN
1	G	110	HIS
1	G	135	ASN
1	G	141	ASN
1	G	154	ASN
1	G	166	HIS
1	G	203	GLN
1	G	289	ASN
1	G	315	ASN
1	G	329	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	G	340	-	4,4,4	0.24	0	6,6,6	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	G	338	-	4,4,4	0.25	0	6,6,6	0.11	0
3	NAD	R	336	-	46,48,48	2.36	8 (17%)	64,73,73	2.33	20 (31%)
2	SO4	R	340	-	4,4,4	0.24	0	6,6,6	0.11	0
2	SO4	R	338	-	4,4,4	0.24	0	6,6,6	0.11	0
3	NAD	G	336	-	46,48,48	3.59	16 (34%)	64,73,73	3.42	24 (37%)

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
3	NAD	G	336	-	1/1/11/11	10/30/62/62	0/5/5/5
3	NAD	R	336	-	-	11/30/62/62	0/5/5/5

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	336	NAD	C2N-N1N	9.43	1.45	1.35
3	R	336	NAD	PN-O3	8.63	1.68	1.59
3	G	336	NAD	C5A-N7A	8.22	1.54	1.39
3	G	336	NAD	PN-O3	8.10	1.68	1.59
3	G	336	NAD	C2B-C3B	-7.76	1.32	1.53
3	G	336	NAD	C8A-N7A	7.65	1.46	1.31
3	G	336	NAD	C3N-C7N	7.11	1.61	1.50
3	R	336	NAD	C2N-N1N	6.52	1.42	1.35
3	G	336	NAD	C3B-C4B	-6.46	1.36	1.53
3	R	336	NAD	C4A-N9A	6.44	1.51	1.37
3	G	336	NAD	C4A-N9A	5.74	1.49	1.37
3	G	336	NAD	O2B-C2B	-5.55	1.29	1.43
3	R	336	NAD	C3N-C7N	4.76	1.57	1.50
3	R	336	NAD	C1B-N9A	4.37	1.58	1.46
3	G	336	NAD	C6N-N1N	3.61	1.43	1.35
3	G	336	NAD	C1B-N9A	3.34	1.55	1.46
3	G	336	NAD	O4D-C1D	3.21	1.45	1.40
3	G	336	NAD	C5A-C6A	3.18	1.49	1.41
3	G	336	NAD	C4A-N3A	3.14	1.40	1.34
3	R	336	NAD	C2A-N1A	2.64	1.38	1.33
3	R	336	NAD	C6N-N1N	2.51	1.41	1.35
3	G	336	NAD	C2B-C1B	-2.44	1.45	1.53
3	G	336	NAD	O4D-C4D	2.20	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	336	NAD	C5A-N7A	-2.17	1.35	1.39

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	336	NAD	C3B-C2B-C1B	12.52	125.15	101.46
3	G	336	NAD	O4B-C1B-C2B	-8.68	88.03	106.62
3	G	336	NAD	N9A-C8A-N7A	-8.53	101.84	113.94
3	G	336	NAD	C5N-C4N-C3N	-8.06	112.44	120.36
3	R	336	NAD	C5N-C4N-C3N	-7.63	112.86	120.36
3	G	336	NAD	C6N-N1N-C2N	-6.98	115.94	121.88
3	G	336	NAD	C6N-C5N-C4N	6.80	129.25	119.45
3	R	336	NAD	C6N-C5N-C4N	6.34	128.59	119.45
3	R	336	NAD	C4A-N9A-C8A	-6.25	99.18	105.74
3	G	336	NAD	C4A-N9A-C1B	-6.07	112.44	126.63
3	R	336	NAD	O4B-C1B-N9A	5.97	119.55	108.09
3	G	336	NAD	C4A-N9A-C8A	5.73	111.76	105.74
3	G	336	NAD	C4D-O4D-C1D	4.43	113.98	109.92
3	G	336	NAD	C4A-C5A-N7A	-4.37	105.59	110.58
3	G	336	NAD	O4B-C1B-N9A	4.32	116.39	108.09
3	R	336	NAD	C4A-N9A-C1B	4.20	136.46	126.63
3	R	336	NAD	C2N-C3N-C4N	4.08	123.00	118.26
3	G	336	NAD	C2N-C3N-C4N	3.99	122.90	118.26
3	G	336	NAD	C2N-N1N-C1D	3.80	127.52	119.13
3	G	336	NAD	C2N-C3N-C7N	-3.74	108.66	119.46
3	G	336	NAD	C5A-N7A-C8A	3.64	109.18	103.45
3	R	336	NAD	C6A-C5A-C4A	3.63	122.14	117.18
3	R	336	NAD	C5A-C4A-N3A	-3.42	122.00	126.72
3	G	336	NAD	C6A-C5A-N7A	3.42	138.68	132.09
3	R	336	NAD	C5N-C6N-N1N	-3.31	115.86	120.38
3	G	336	NAD	C2B-C3B-C4B	-3.18	96.47	102.61
3	G	336	NAD	O2A-PA-O3	3.17	115.85	107.27
3	R	336	NAD	N3A-C4A-N9A	2.89	132.09	127.17
3	R	336	NAD	C2N-N1N-C1D	2.87	125.48	119.13
3	G	336	NAD	C1B-N9A-C8A	2.83	133.38	127.09
3	R	336	NAD	C6N-N1N-C1D	-2.76	114.32	119.73
3	R	336	NAD	C6A-C5A-N7A	-2.72	126.85	132.09
3	R	336	NAD	C3B-C2B-C1B	2.66	106.50	101.46
3	R	336	NAD	N9A-C8A-N7A	2.61	117.64	113.94
3	R	336	NAD	O4B-C1B-C2B	-2.50	101.26	106.62
3	G	336	NAD	C5N-C6N-N1N	-2.48	117.01	120.38
3	G	336	NAD	C4N-C3N-C7N	2.45	127.73	121.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	336	NAD	O2A-PA-O3	2.39	113.72	107.27
3	G	336	NAD	O2B-C2B-C1B	2.28	117.96	110.10
3	R	336	NAD	C2B-C3B-C4B	-2.27	98.21	102.61
3	R	336	NAD	O5D-C5D-C4D	2.14	116.27	108.99
3	R	336	NAD	C6N-N1N-C2N	-2.09	120.10	121.88
3	G	336	NAD	C2B-C1B-N9A	-2.00	108.33	113.30
3	G	336	NAD	C6A-C5A-C4A	-2.00	114.45	117.18

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	G	336	NAD	C2B

All (21) torsion outliers are listed below:

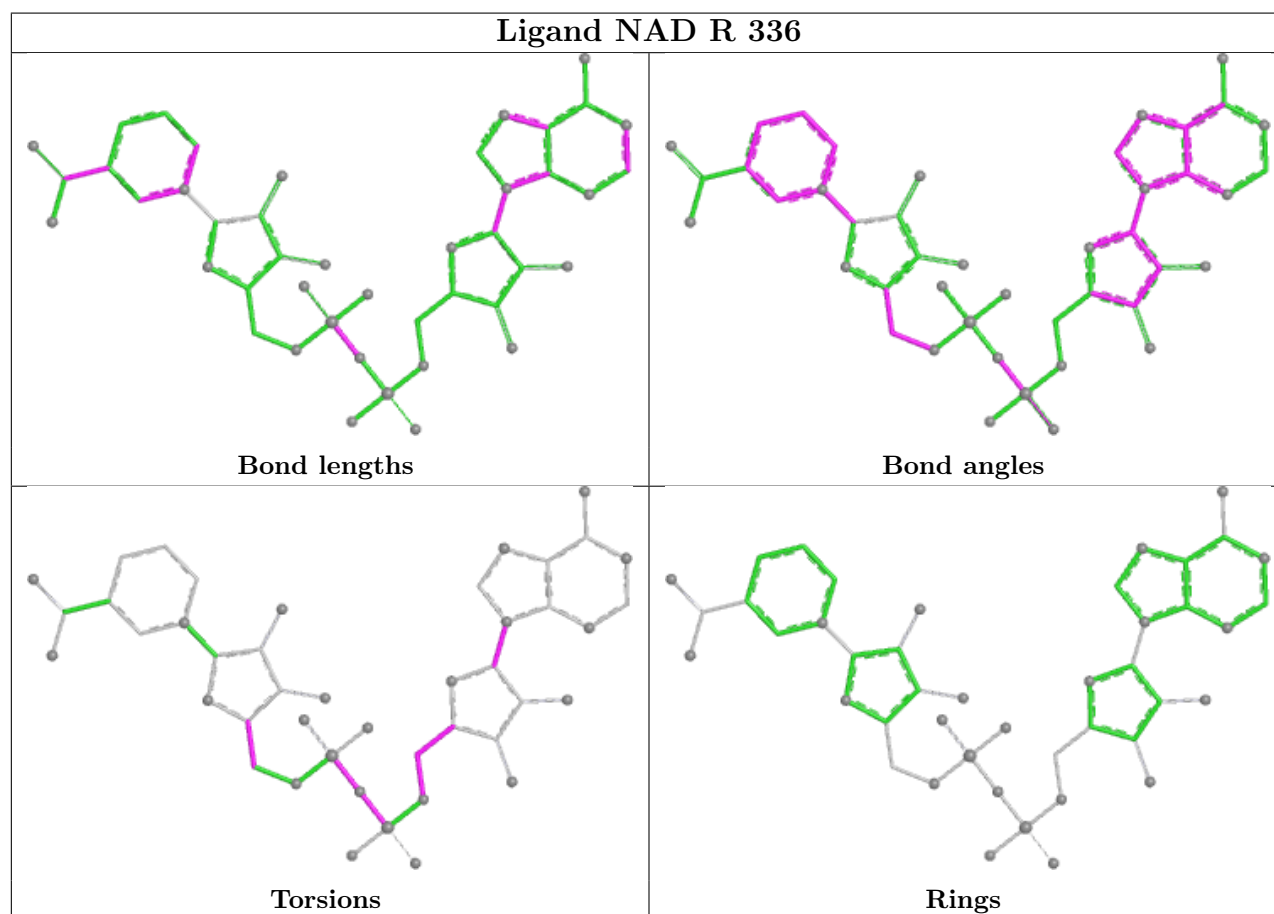
Mol	Chain	Res	Type	Atoms
3	G	336	NAD	C5D-O5D-PN-O3
3	G	336	NAD	C5D-O5D-PN-O1N
3	G	336	NAD	C5D-O5D-PN-O2N
3	G	336	NAD	O4D-C1D-N1N-C2N
3	G	336	NAD	O4D-C1D-N1N-C6N
3	R	336	NAD	C3B-C4B-C5B-O5B
3	R	336	NAD	O4D-C4D-C5D-O5D
3	R	336	NAD	C3D-C4D-C5D-O5D
3	G	336	NAD	C3D-C4D-C5D-O5D
3	G	336	NAD	O4B-C4B-C5B-O5B
3	G	336	NAD	O4D-C4D-C5D-O5D
3	G	336	NAD	C3B-C4B-C5B-O5B
3	R	336	NAD	O4B-C4B-C5B-O5B
3	R	336	NAD	PN-O3-PA-O1A
3	R	336	NAD	C4B-C5B-O5B-PA
3	R	336	NAD	C2B-C1B-N9A-C8A
3	G	336	NAD	C5B-O5B-PA-O1A
3	R	336	NAD	C2B-C1B-N9A-C4A
3	R	336	NAD	PN-O3-PA-O2A
3	R	336	NAD	PA-O3-PN-O2N
3	R	336	NAD	PA-O3-PN-O1N

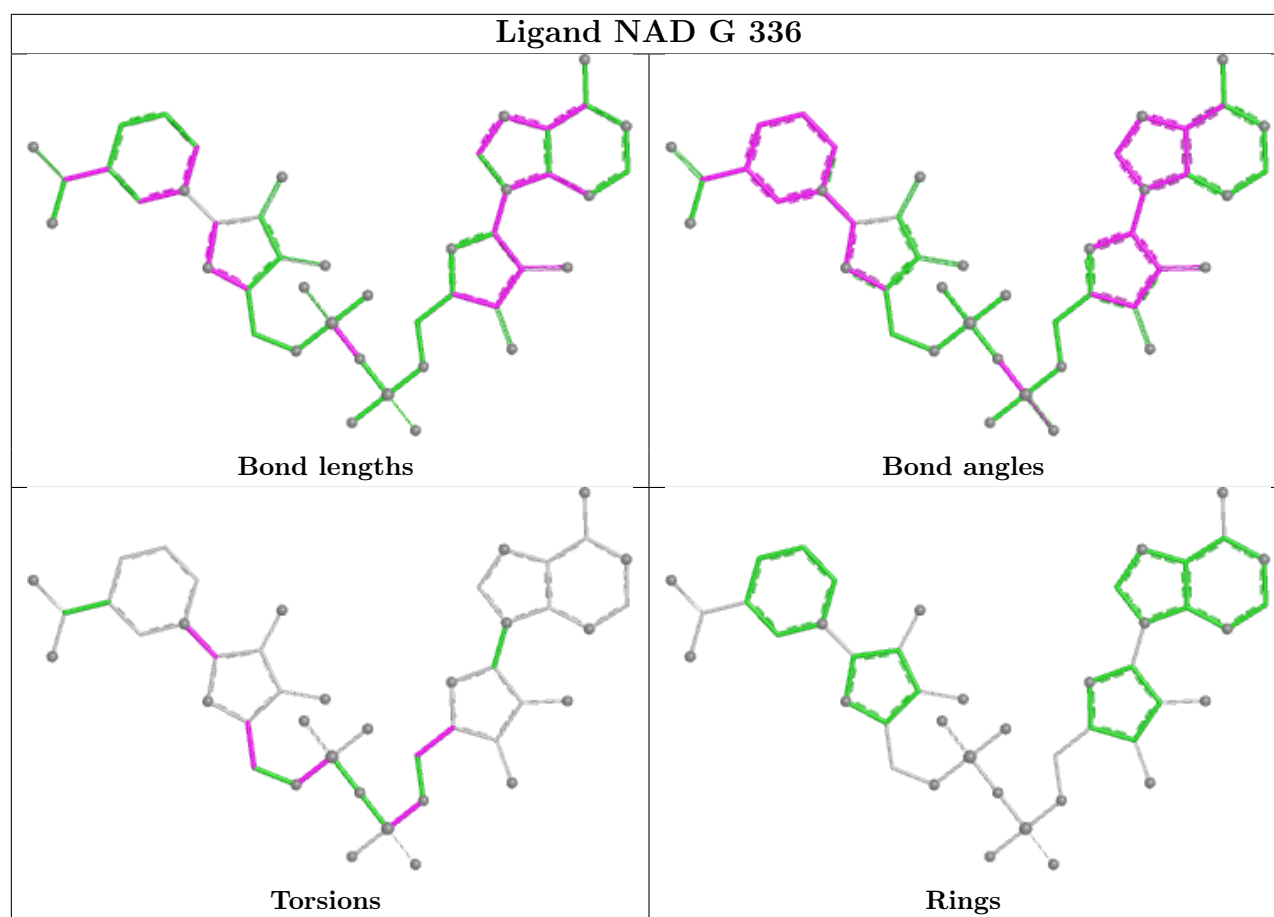
There are no ring outliers.

6 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	340	SO4	2	0
2	G	338	SO4	4	0
3	R	336	NAD	7	0
2	R	340	SO4	2	0
2	R	338	SO4	2	0
3	G	336	NAD	14	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.