



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:57 AM GMT

PDB ID : 3GPD
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

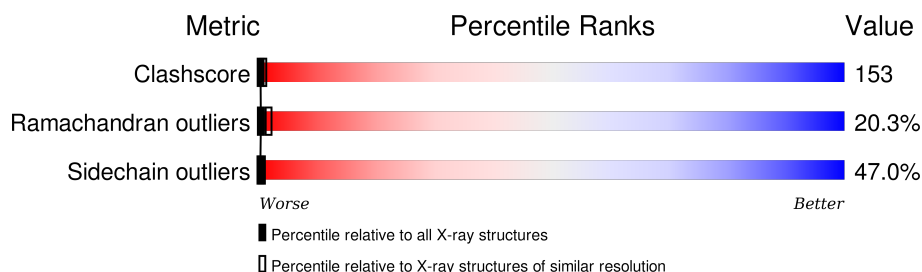
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	G	334	<div> <div>7%</div> <div>37%</div> <div>36%</div> <div>20%</div> </div>
1	R	334	<div> <div>5%</div> <div>46%</div> <div>34%</div> <div>15%</div> </div>

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	-

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

2 Entry composition [i](#)

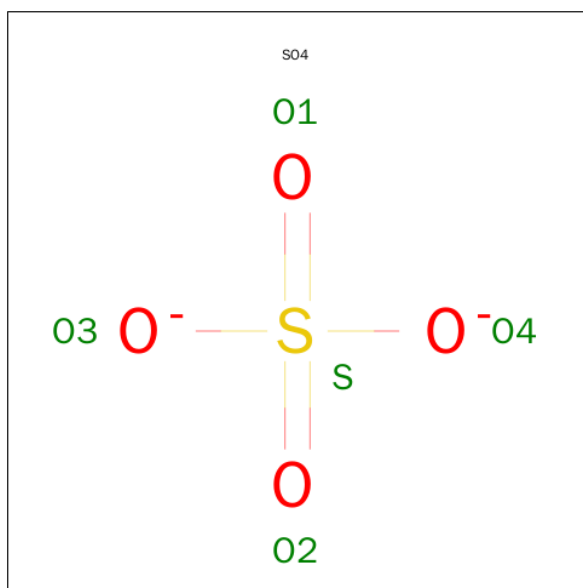
There are 3 unique types of molecules in this entry. The entry contains 5154 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

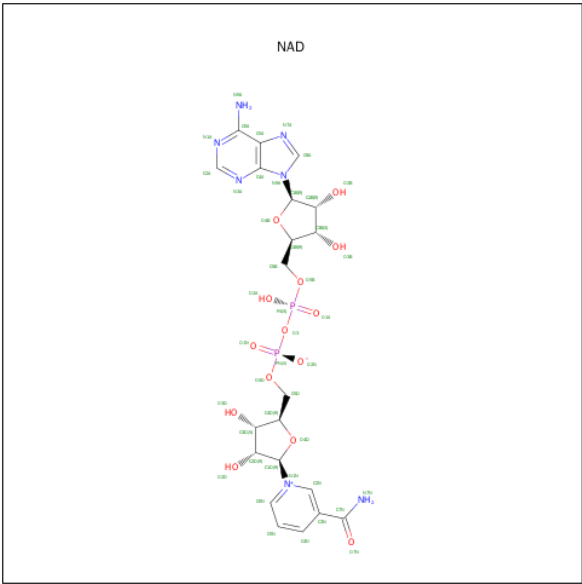
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	334	Total	C	N	O	S	0	0	0
			2523	1601	431	479	12			
1	G	334	Total	C	N	O	S	0	0	0
			2523	1601	431	479	12			

- Molecule 2 is SULFATE ION (three-letter code: 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 (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



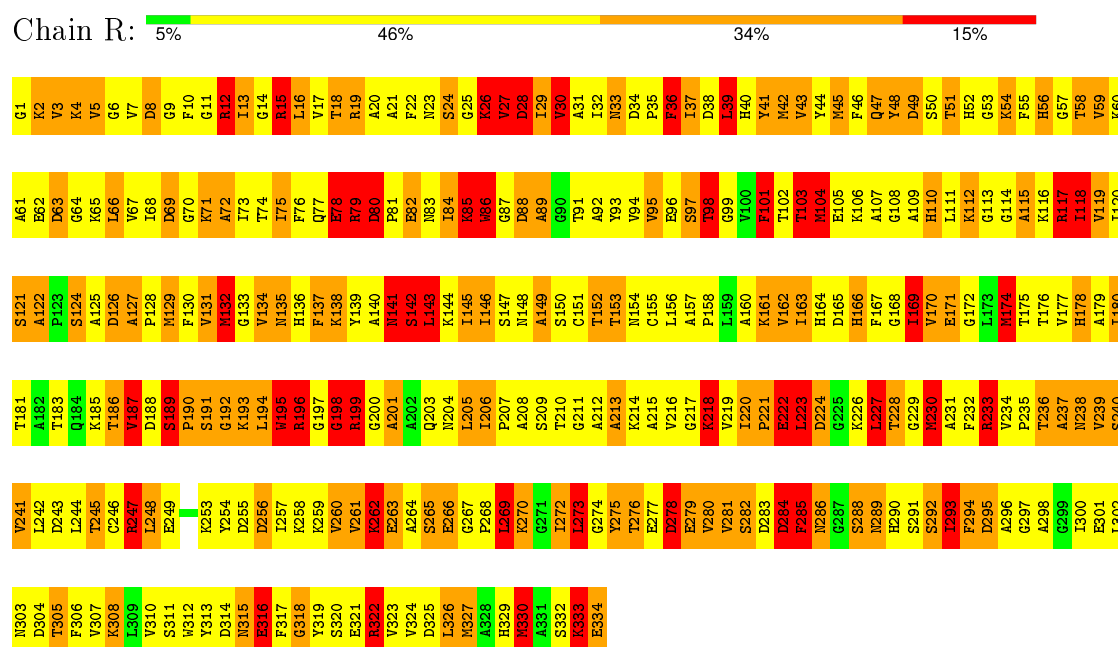
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	R	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

3 Residue-property plots

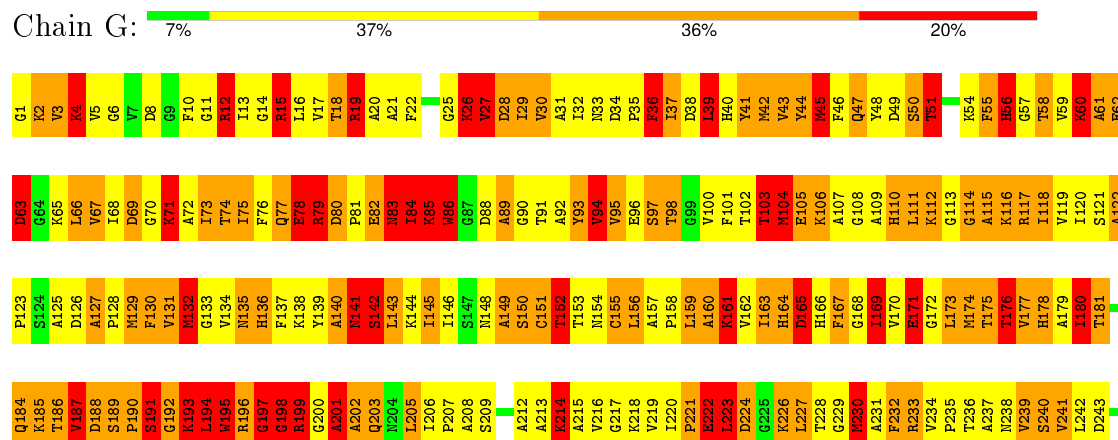
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

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



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



C246	F306
R247	V307
I248	K308
E249	I309
K250	V310
P251	S311
A252	K312
K253	Y313
Y254	D314
D255	R315
D256	E316
I257	F317
K258	G318
K259	Y319
V260	S320
V261	E321
K262	R322
E263	V323
A264	V324
S265	D325
E266	L326
G267	M327
P268	A328
I269	H329
K270	R330
G271	A331
I272	S332
L273	K333
G274	E334
Y275	
T276	
E277	
D278	
E279	
V280	
V281	
S282	
D283	
D284	
F285	
I286	
G287	
S288	
I288	
H290	
S291	
S292	
L293	
F294	
D295	
A296	
G297	
A298	
G299	
I300	
F301	
L302	
R303	
D304	
T305	

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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	1.40	11/2573 (0.4%)	2.06	121/3479 (3.5%)
1	R	1.12	3/2573 (0.1%)	1.67	54/3479 (1.6%)
All	All	1.27	14/5146 (0.3%)	1.87	175/6958 (2.5%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	198	GLY	N-CA	8.67	1.59	1.46
1	G	195	TRP	CB-CG	7.61	1.64	1.50
1	G	329	HIS	CB-CG	6.51	1.61	1.50
1	G	70	GLY	N-CA	6.48	1.55	1.46
1	G	279	GLU	N-CA	6.37	1.59	1.46
1	G	197	GLY	C-N	6.13	1.44	1.33
1	G	195	TRP	N-CA	6.09	1.58	1.46
1	G	194	LEU	N-CA	5.71	1.57	1.46
1	G	271	GLY	N-CA	5.63	1.54	1.46
1	G	86	TRP	NE1-CE2	-5.45	1.30	1.37
1	R	86	TRP	NE1-CE2	-5.40	1.30	1.37
1	R	195	TRP	NE1-CE2	-5.38	1.30	1.37
1	G	164	HIS	CB-CG	5.34	1.59	1.50
1	R	195	TRP	CB-CG	5.33	1.59	1.50

All (175) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	279	GLU	O-C-N	10.67	139.77	122.70
1	G	278	ASP	O-C-N	-10.53	105.85	122.70
1	G	196	ARG	O-C-N	10.25	140.63	123.20
1	G	196	ARG	CB-CA-C	9.98	130.36	110.40
1	R	27	VAL	O-C-N	9.88	138.50	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	177	VAL	O-C-N	9.34	137.64	122.70
1	G	304	ASP	O-C-N	9.22	137.45	122.70
1	G	290	HIS	CB-CA-C	-9.08	92.25	110.40
1	G	223	LEU	O-C-N	-8.97	108.34	122.70
1	G	334	GLU	CA-C-O	8.89	138.76	120.10
1	R	36	PHE	CB-CA-C	-8.87	92.65	110.40
1	G	196	ARG	CA-C-N	-8.87	98.46	116.20
1	R	28	ASP	O-C-N	8.63	136.51	122.70
1	G	201	ALA	O-C-N	8.48	136.28	122.70
1	G	313	TYR	CB-CA-C	-8.43	93.55	110.40
1	R	278	ASP	CB-CA-C	8.40	127.20	110.40
1	G	293	ILE	O-C-N	8.34	136.05	122.70
1	G	313	TYR	CB-CG-CD1	-8.32	116.01	121.00
1	G	314	ASP	CB-CA-C	8.30	127.01	110.40
1	G	303	ASN	N-CA-CB	-8.27	95.71	110.60
1	R	143	LEU	O-C-N	8.22	135.85	122.70
1	G	279	GLU	CA-C-N	-8.15	99.28	117.20
1	G	85	LYS	O-C-N	8.04	135.56	122.70
1	R	36	PHE	N-CA-CB	7.93	124.87	110.60
1	G	83	ASN	C-N-CA	-7.87	102.02	121.70
1	R	278	ASP	O-C-N	-7.79	110.23	122.70
1	G	36	PHE	CB-CG-CD2	7.75	126.23	120.80
1	G	198	GLY	O-C-N	7.61	134.87	122.70
1	R	27	VAL	CA-C-N	-7.58	100.53	117.20
1	G	238	ASN	O-C-N	7.50	134.70	122.70
1	G	222	GLU	CB-CA-C	7.49	125.37	110.40
1	R	322	ARG	NE-CZ-NH2	7.42	124.01	120.30
1	R	15	ARG	NE-CZ-NH2	7.41	124.01	120.30
1	G	78	GLU	O-C-N	7.39	134.52	122.70
1	R	12	ARG	NE-CZ-NH2	7.38	123.99	120.30
1	G	180	ILE	O-C-N	7.37	134.49	122.70
1	R	247	ARG	NE-CZ-NH2	7.36	123.98	120.30
1	R	19	ARG	NE-CZ-NH2	7.36	123.98	120.30
1	G	15	ARG	NE-CZ-NH2	7.34	123.97	120.30
1	R	233	ARG	NE-CZ-NH2	7.33	123.97	120.30
1	G	12	ARG	NE-CZ-NH2	7.33	123.96	120.30
1	G	196	ARG	NE-CZ-NH2	7.29	123.95	120.30
1	R	79	ARG	NE-CZ-NH2	7.28	123.94	120.30
1	G	233	ARG	NE-CZ-NH2	7.25	123.92	120.30
1	R	196	ARG	NE-CZ-NH2	7.23	123.91	120.30
1	R	199	ARG	NE-CZ-NH2	7.19	123.89	120.30
1	R	117	ARG	NE-CZ-NH2	7.17	123.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	63	ASP	O-C-N	7.14	135.34	123.20
1	G	278	ASP	CA-C-N	7.13	132.90	117.20
1	G	199	ARG	NE-CZ-NH2	7.12	123.86	120.30
1	G	186	THR	O-C-N	7.11	134.08	122.70
1	G	177	VAL	CA-C-N	-7.11	101.56	117.20
1	G	333	LYS	O-C-N	-7.11	111.33	122.70
1	G	304	ASP	CA-C-N	-7.10	101.58	117.20
1	G	280	VAL	O-C-N	7.09	134.05	122.70
1	G	19	ARG	NE-CZ-NH2	7.04	123.82	120.30
1	G	79	ARG	NE-CZ-NH2	6.97	123.78	120.30
1	G	247	ARG	NE-CZ-NH2	6.92	123.76	120.30
1	G	322	ARG	NE-CZ-NH2	6.79	123.69	120.30
1	G	333	LYS	CB-CA-C	6.77	123.94	110.40
1	G	117	ARG	NE-CZ-NH2	6.70	123.65	120.30
1	G	169	ILE	O-C-N	6.68	133.39	122.70
1	R	28	ASP	CA-C-N	-6.67	102.53	117.20
1	R	26	LYS	O-C-N	6.65	133.34	122.70
1	G	191	SER	O-C-N	6.63	134.47	123.20
1	G	253	LYS	CB-CA-C	-6.61	97.18	110.40
1	G	294	PHE	O-C-N	6.52	133.14	122.70
1	G	197	GLY	C-N-CA	6.51	135.97	122.30
1	R	88	ASP	O-C-N	6.48	133.07	122.70
1	G	85	LYS	CA-C-N	-6.46	102.98	117.20
1	R	198	GLY	O-C-N	6.41	132.96	122.70
1	G	229	GLY	O-C-N	6.41	132.95	122.70
1	G	79	ARG	O-C-N	6.40	132.93	122.70
1	G	304	ASP	C-N-CA	6.39	137.69	121.70
1	G	275	TYR	O-C-N	6.39	132.93	122.70
1	G	60	LYS	O-C-N	6.36	132.88	122.70
1	G	165	ASP	N-CA-CB	6.36	122.05	110.60
1	R	27	VAL	CB-CA-C	6.33	123.42	111.40
1	G	169	ILE	CB-CA-C	-6.33	98.95	111.60
1	G	142	SER	CB-CA-C	6.32	122.10	110.10
1	G	201	ALA	CA-C-N	-6.32	103.31	117.20
1	R	143	LEU	CA-C-N	-6.31	103.32	117.20
1	G	63	ASP	CA-C-N	-6.31	103.58	116.20
1	G	104	MET	CG-SD-CE	6.30	110.27	100.20
1	G	27	VAL	O-C-N	6.29	132.77	122.70
1	G	293	ILE	CA-C-N	-6.29	103.37	117.20
1	G	174	MET	CG-SD-CE	6.25	110.19	100.20
1	R	180	ILE	O-C-N	6.24	132.68	122.70
1	G	202	ALA	O-C-N	6.23	132.67	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	174	MET	CG-SD-CE	6.22	110.15	100.20
1	G	165	ASP	CB-CA-C	-6.22	97.96	110.40
1	G	326	LEU	CB-CA-C	6.18	121.94	110.20
1	R	42	MET	CG-SD-CE	6.15	110.04	100.20
1	R	101	PHE	O-C-N	6.13	132.50	122.70
1	G	36	PHE	CB-CG-CD1	-6.12	116.51	120.80
1	R	129	MET	CG-SD-CE	6.12	109.99	100.20
1	R	104	MET	CG-SD-CE	6.12	109.98	100.20
1	R	327	MET	CG-SD-CE	6.12	109.98	100.20
1	G	129	MET	CG-SD-CE	6.11	109.97	100.20
1	G	305	THR	N-CA-CB	-6.11	98.70	110.30
1	G	304	ASP	N-CA-CB	-6.09	99.63	110.60
1	R	230	MET	CG-SD-CE	6.09	109.95	100.20
1	G	42	MET	CG-SD-CE	6.09	109.94	100.20
1	R	330	MET	CG-SD-CE	6.08	109.94	100.20
1	G	192	GLY	O-C-N	6.08	132.44	122.70
1	G	230	MET	CG-SD-CE	6.08	109.93	100.20
1	G	327	MET	CG-SD-CE	6.08	109.93	100.20
1	R	132	MET	CG-SD-CE	6.06	109.90	100.20
1	R	334	GLU	N-CA-C	6.06	127.35	111.00
1	G	330	MET	CG-SD-CE	6.05	109.88	100.20
1	G	132	MET	CG-SD-CE	6.03	109.85	100.20
1	G	45	MET	CG-SD-CE	6.03	109.84	100.20
1	R	45	MET	CG-SD-CE	6.02	109.83	100.20
1	G	223	LEU	CA-C-N	5.98	130.36	117.20
1	G	167	PHE	CB-CA-C	-5.96	98.47	110.40
1	G	94	VAL	O-C-N	-5.94	113.20	122.70
1	G	209	SER	O-C-N	5.92	132.17	122.70
1	G	214	LYS	O-C-N	5.85	132.06	122.70
1	G	185	LYS	CB-CA-C	-5.85	98.70	110.40
1	G	198	GLY	CA-C-N	-5.83	104.37	117.20
1	G	78	GLU	CA-C-N	-5.83	104.38	117.20
1	G	199	ARG	N-CA-CB	-5.81	100.15	110.60
1	G	180	ILE	CA-C-N	-5.78	104.48	117.20
1	G	280	VAL	CA-C-N	-5.75	104.56	117.20
1	G	238	ASN	CA-C-N	-5.72	104.61	117.20
1	G	319	TYR	CB-CG-CD1	-5.70	117.58	121.00
1	G	69	ASP	N-CA-CB	-5.69	100.36	110.60
1	R	293	ILE	O-C-N	5.68	131.79	122.70
1	R	142	SER	O-C-N	5.66	131.75	122.70
1	G	285	PHE	O-C-N	-5.65	113.67	122.70
1	G	254	TYR	CB-CG-CD1	-5.63	117.62	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	191	SER	CA-C-N	-5.63	104.94	116.20
1	G	196	ARG	C-N-CA	5.60	134.07	122.30
1	G	186	THR	N-CA-CB	5.59	120.92	110.30
1	R	169	ILE	CB-CA-C	-5.56	100.47	111.60
1	G	186	THR	CA-C-N	-5.56	104.97	117.20
1	G	176	THR	O-C-N	5.54	131.57	122.70
1	G	193	LYS	CB-CA-C	5.49	121.37	110.40
1	G	141	ASN	O-C-N	5.38	131.30	122.70
1	R	223	LEU	O-C-N	-5.38	114.10	122.70
1	R	79	ARG	O-C-N	5.37	131.28	122.70
1	R	118	ILE	O-C-N	-5.34	114.16	122.70
1	R	238	ASN	O-C-N	5.32	131.21	122.70
1	R	227	LEU	CB-CA-C	-5.32	100.10	110.20
1	G	130	PHE	O-C-N	5.32	131.21	122.70
1	R	48	TYR	CB-CG-CD2	-5.29	117.82	121.00
1	G	83	ASN	O-C-N	-5.29	114.24	122.70
1	R	269	LEU	CB-CA-C	-5.26	100.20	110.20
1	G	229	GLY	CA-C-N	-5.26	105.62	117.20
1	G	26	LYS	O-C-N	5.25	131.11	122.70
1	G	174	MET	CB-CA-C	-5.25	99.89	110.40
1	G	310	VAL	O-C-N	5.25	131.11	122.70
1	G	169	ILE	CA-C-N	-5.25	105.65	117.20
1	R	192	GLY	O-C-N	5.24	131.08	122.70
1	R	177	VAL	O-C-N	5.24	131.08	122.70
1	R	278	ASP	CA-C-N	5.20	128.65	117.20
1	R	26	LYS	CA-C-N	-5.18	105.80	117.20
1	G	104	MET	N-CA-CB	5.18	119.92	110.60
1	G	219	VAL	CB-CA-C	5.17	121.22	111.40
1	G	289	ASN	O-C-N	5.14	130.92	122.70
1	R	88	ASP	CA-C-N	-5.13	105.90	117.20
1	G	140	ALA	O-C-N	5.10	130.87	122.70
1	G	222	GLU	N-CA-CB	-5.10	101.42	110.60
1	R	198	GLY	CA-C-N	-5.09	106.00	117.20
1	G	125	ALA	O-C-N	5.08	130.83	122.70
1	G	247	ARG	CD-NE-CZ	5.08	130.71	123.60
1	G	275	TYR	CA-C-N	-5.08	106.03	117.20
1	R	218	LYS	O-C-N	5.07	130.82	122.70
1	G	51	THR	CB-CA-C	5.07	125.28	111.60
1	G	61	ALA	O-C-N	5.06	130.79	122.70
1	G	280	VAL	CB-CA-C	5.06	121.01	111.40
1	R	87	GLY	O-C-N	5.03	130.74	122.70
1	G	60	LYS	CA-C-N	-5.02	106.15	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	304	ASP	CA-CB-CG	5.01	124.43	113.40
1	G	79	ARG	CA-C-N	-5.01	106.18	117.20

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	794	25
1	R	2523	0	2518	780	20
2	G	10	0	0	6	0
2	R	10	0	0	3	0
3	G	44	0	24	14	0
3	R	44	0	26	8	0
All	All	5154	0	5083	1561	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 153.

All (1561) 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	1.49
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:2:LYS:HB2	1:G:26:LYS:CD	1.66	1.26
1:R:223:LEU:O	1:R:224:ASP:CB	1.78	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
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:R:1:GLY:HA2	1:R:28:ASP:C	1.59	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:37:ILE:O	1:R:42:MET:HE3	1.38	1.20
1:R:39:LEU:H	1:R:39:LEU:CD1	1.54	1.20
1:G:291:SER:HB2	1:G:322:ARG:HD3	1.24	1.19
1:G:196:ARG:HH21	1:G:208:ALA:CB	1.55	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:191:SER:OG	1:G:192:GLY:N	1.71	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: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:80:ASP:O	1:G:83:ASN:HB2	1.39	1.16
1:G:65:LYS:HG3	1:G:73:ILE:O	1.31	1.16
1:R:156:LEU:HD13	1:R:242:LEU:HD21	1.23	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1:GLY:C	1:R:28:ASP:CA	2.08	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: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: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
1:R:3:VAL:HG23	1:R:27:VAL:HG22	1.18	1.12
1:R:2:LYS:N	1:R:28:ASP:H	1.41	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:HD22	1:G:269:LEU:H	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:259:LYS:HG2	1:R:262:LYS:CE	1.81	1.11
1:R:111:LEU:HA	1:R:115:ALA:HB3	1.31	1.11
1:G:16:LEU:HD12	1:G:320:SER:HB3	1.12	1.10
1:G:2:LYS:HZ2	1:G:25:GLY:HA3	1.14	1.10
1:G:35:PRO:O	1:G:36:PHE:HB2	1.41	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: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:R:223:LEU:O	1:R:224:ASP:HB2	1.28	1.10
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:156:LEU:HD13	1:R:242:LEU:HD23	1.17	1.07
1:R:26:LYS:CE	1:R:28:ASP:H	1.62	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:134:VAL:HG21	1:R:219:VAL:HG12	1.36	1.06
1:R:2:LYS:CD	1:R:27:VAL:N	2.08	1.06
1:R:176:THR:HG22	1:R:231:ALA:HB2	1.07	1.06
1:R:85:LYS:O	1:R:86:TRP:HB2	1.53	1.06
1:R:196:ARG:HH21	1:R:208:ALA:CB	1.67	1.06
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: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:G:65:LYS:CD	1:G:73:ILE:O	2.04	1.04
1:R:276:THR:HG23	1:R:295:ASP:HB3	1.06	1.04
1:R:152:THR:HA	1:R:313:TYR:CE2	1.93	1.04
1:R:39:LEU:N	1:R:39:LEU:HD12	1.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:28:ASP:CB	1:R:29:ILE:HG13	1.90	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:G:178:HIS:HA	1:G:240:SER:HB3	1.42	1.02
1:R:189:SER:CB	1:R:190:PRO:HD2	1.89	1.02
1:R:284:ASP:O	1:R:286:ASN:HB2	1.59	1.02
1:R:43:VAL:O	1:R:47:GLN:HB2	1.58	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:G:26:LYS:CD	1:G:27:VAL:N	2.22	1.01
1:R:189:SER:HB3	1:R:190:PRO:CD	1.89	1.01
1:G:223:LEU:O	1:G:224:ASP:HB3	1.20	1.01
1:G:39:LEU:HG	1:G:40:HIS:H	0.98	1.01
1:G:4:LYS:O	1:G:4:LYS:HG2	1.60	1.01
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:176:THR:HG23	1:R:231:ALA:HB1	1.42	1.00
1:G:275:TYR:CE2	1:G:277:GLU:HG2	1.97	1.00
1:R:260:VAL:HG13	1:R:261:VAL:H	1.24	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: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:153:THR:CG2	1:G:215:ALA:HB1	1.92	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: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:R:259:LYS:HG2	1:R:262:LYS:HE2	0.97	0.97
1:R:108:GLY:O	1:R:111:LEU:HB2	1.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:R:2:LYS:HD2	1:R:25:GLY:C	1.87	0.95
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: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:G:12:ARG:N	1:G:15:ARG:NH1	2.15	0.94
1:R:300:ILE:O	1:R:300:ILE:HD12	1.68	0.94
1:G:123:PRO:HA	1:G:129:MET:HE3	1.46	0.94
1:G:98:THR:HA	3:G:336:NAD:C8A	1.96	0.94
1:R:196:ARG:NH2	1:R:208:ALA:HB2	1.80	0.94
1:R:185:LYS:O	1:R:201:ALA:HB2	1.67	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:205:LEU:HD22	1:R:205:LEU:C	1.89	0.93
1:G:2:LYS:HB2	1:G:26:LYS:HD2	0.96	0.93
1:G:37:ILE:HG22	1:G:42:MET:HE2	1.49	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:G:85:LYS:O	1:G:113:GLY:C	2.08	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:G:195:TRP:CD1	1:G:197:GLY:HA2	2.02	0.92
1:R:78:GLU:HA	1:R:78:GLU:OE2	1.64	0.92
1:G:2:LYS:O	1:G:28:ASP:CG	2.08	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:174:MET:HG2	1:R:175:THR:N	1.84	0.92
1:R:2:LYS:H	1:R:28:ASP:CA	1.72	0.92
1:R:141:ASN:ND2	1:R:141:ASN:H	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:1:GLY:HA2	1:G:28:ASP:C	1.89	0.92
1:G:156:LEU:CD2	1:G:242:LEU:CD2	2.48	0.92
1:G:257:ILE:O	1:G:260:VAL:CG1	2.19	0.91
1:R:278:ASP:O	1:R:279:GLU:HB2	1.71	0.91
1:R:141:ASN:C	1:R:143:LEU:H	1.70	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:G:1:GLY:CA	1:G:28:ASP:CA	2.48	0.91
1:R:117:ARG:NH1	1:R:144:LYS:HD2	1.85	0.91
1:R:39:LEU:H	1:R:39:LEU:HD12	0.76	0.91
1:R:65:LYS:HB2	1:R:74:THR:CA	1.97	0.90
1:G:131:VAL:HG23	1:G:133:GLY:H	1.34	0.90
1:G:1:GLY:HA2	1:G:28:ASP:HA	1.44	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:191:SER:HG	1:G:192:GLY:H	1.20	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:28:ASP:HB3	1:R:29:ILE:CG1	1.99	0.89
1:R:2:LYS:NZ	1:R:25:GLY:CA	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1:GLY:C	1:R:28:ASP:H	1.75	0.88
1:G:305:THR:CG2	1:G:306:PHE:H	1.86	0.88
1:R:166:HIS:CD2	1:R:260:VAL:HG23	2.07	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: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:119:VAL:CG2	1:R:326:LEU:CD1	2.50	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
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: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:16:LEU:CD2	1:G:20:ALA:HB2	2.04	0.87
1:G:276:THR:HG23	1:G:295:ASP:CB	2.03	0.87
1:G:214:LYS:O	1:G:218:LYS:HG2	1.74	0.87
1:G:22:PHE:CE2	1:G:71:LYS:HD3	2.08	0.87
1:R:39:LEU:N	1:R:39:LEU:CD1	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:R:47:GLN:HG3	1:R:59:VAL:HG11	0.90	0.86
1:R:37:ILE:O	1:R:42:MET:CE	2.21	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:126:ASP:O	1:G:127:ALA:HB2	1.71	0.86
1:G:65:LYS:CB	1:G:73:ILE:O	2.23	0.86
1:G:117:ARG:HH11	1:G:144:LYS:HD3	1.37	0.86
1:G:16:LEU:HA	1:G:19:ARG:HB3	1.57	0.86
1:R:3:VAL:CG2	1:R:27:VAL:HG11	2.04	0.86
1:G:297:GLY:O	1:G:300:ILE:HG13	1.73	0.86
1:R:223:LEU:O	1:R:224:ASP:HB3	1.73	0.86
1:R:1:GLY:C	1:R:28:ASP:N	2.24	0.86
1:G:5:VAL:O	1:G:30:VAL:HA	1.74	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:141:ASN:C	1:R:143:LEU:N	2.26	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: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:230:MET:SD	1:R:232:PHE:CZ	2.70	0.84
1:R:22:PHE:HZ	1:R:69:ASP:HB3	1.42	0.84
1:G:15:ARG:HA	1:G:18:THR:HG23	1.57	0.84
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:G:258:LYS:HD2	1:G:275:TYR:OH	1.77	0.84
1:R:174:MET:HG3	1:R:242:LEU:HD11	1.59	0.84
1:R:2:LYS:CA	1:R:28:ASP:N	2.30	0.84
1:R:3:VAL:N	1:R:27:VAL:HA	1.88	0.83
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:250:LYS:HZ2	1:G:251:PRO:HD2	1.40	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:G:37:ILE:HG22	1:G:42:MET:CE	2.07	0.83
1:R:280:VAL:HG23	1:R:280:VAL:O	1.79	0.83
1:R:129:MET:C	1:R:130:PHE:HD1	1.82	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:G:221:PRO:O	1:G:222:GLU:C	2.16	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2:LYS:HB2	1:G:26:LYS:CE	2.08	0.81
1:R:163:ILE:CG2	1:R:169:ILE:HD11	2.10	0.81
1:R:272:ILE:O	1:R:273:LEU:HB2	1.79	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
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:208:ALA:N	1:G:231:ALA:O	2.14	0.81
1:G:84:ILE:C	1:G:85:LYS:HD3	2.00	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:156:LEU:HD22	1:R:174:MET:HE2	1.61	0.80
1:R:196:ARG:HH11	1:R:196:ARG:HA	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: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: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:R:117:ARG:HD2	1:R:144:LYS:HA	1.64	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:G:141:ASN:ND2	1:G:141:ASN:H	1.79	0.79
1:G:322:ARG:HH21	1:G:325:ASP:CG	1.85	0.79
1:R:205:LEU:O	1:R:205:LEU:HD13	1.82	0.79
1:G:26:LYS:C	1:G:26:LYS:HD2	2.02	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:269:LEU:CB	1:R:272:ILE:HD13	2.03	0.79
1:R:66:LEU:O	1:R:73:ILE:HG22	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:R:221:PRO:O	1:R:222:GLU:C	2.21	0.78
1:G:317:PHE:O	1:G:318:GLY:C	2.21	0.78
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: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:G:30:VAL:HG23	1:G:31:ALA:N	1.98	0.77
1:R:276:THR:OG1	1:R:278:ASP:HB2	1.83	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:G:15:ARG:NH2	1:G:45:MET:HE1	2.00	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:HG3	1:R:15:ARG:NH1	2.00	0.77
1:R:97:SER:O	1:R:98:THR:HB	1.84	0.77
1:R:2:LYS:H	1:R:28:ASP:CG	1.87	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:G:26:LYS:HD3	1:G:28:ASP:N	2.00	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:26:LYS:C	1:G:26:LYS:CD	2.53	0.76
1:G:300:ILE:O	1:G:300:ILE:HD12	1.85	0.76
1:R:135:ASN:ND2	1:R:136:HIS:N	2.34	0.76
1:G:174:MET:CE	1:G:212:ALA:HB2	2.14	0.76
1:G:195:TRP:HD1	1:G:197:GLY:HA2	1.47	0.76
1:R:239:VAL:HG22	1:R:314:ASP:HA	1.67	0.76
1:R:35:PRO:CD	1:R:77:GLN:O	2.34	0.76
1:R:79:ARG:O	1:R:80:ASP:HB2	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:29:ILE:C	1:R:30:VAL:HG12	2.05	0.75
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:243:ASP:OD1	1:G:308:LYS:HE3	1.84	0.75
1:R:174:MET:HE2	1:R:242:LEU:HD21	1.69	0.75
1:R:284:ASP:O	1:R:285:PHE:C	2.24	0.75
1:G:15:ARG:NH2	1:G:45:MET:CE	2.50	0.75
1:R:119:VAL:CG2	1:R:326:LEU:HD11	2.16	0.75
1:R:156:LEU:CD1	1:R:242:LEU:HD21	2.10	0.75
1:G:220:ILE:HG22	1:G:223:LEU:HB2	1.68	0.75
1:G:196:ARG:CA	1:G:196:ARG:HH11	1.95	0.75
1:G:269:LEU:N	1:G:269:LEU:HD22	1.99	0.75
1:R:195:TRP:O	1:R:196:ARG:HB2	1.86	0.75
1:G:106:LYS:O	1:G:109:ALA:HB3	1.86	0.74
1:G:71:LYS:O	1:G:73:ILE:HD12	1.87	0.74
1:G:122:ALA:HB2	3:G:336:NAD:O2D	1.87	0.74
1:G:65:LYS:CD	1:G:73:ILE:C	2.54	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:G:2:LYS:O	1:G:28:ASP:CB	2.36	0.74
1:G:128:PRO:HG3	1:G:143:LEU:HD21	1.68	0.74
1:R:197:GLY:O	1:R:199:ARG:CB	2.34	0.74
1:G:197:GLY:O	1:G:199:ARG:CB	2.33	0.74
1:G:322:ARG:HE	1:G:322:ARG:CA	1.96	0.74
1:R:186:THR:C	1:R:187:VAL:CG2	2.54	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:G:132:MET:HG3	1:G:322:ARG:HB3	1.69	0.74
1:R:15:ARG:HH11	1:R:15:ARG:HG3	1.52	0.73
1:G:239:VAL:HG22	1:G:314:ASP:HA	1.70	0.73
1:R:156:LEU:HD22	1:R:174:MET:CE	2.17	0.73
1:R:36:PHE:O	1:R:37:ILE:CG1	2.35	0.73
1:G:317:PHE:O	1:G:320:SER:N	2.20	0.73
1:G:291:SER:CB	1:G:322:ARG:HD3	2.12	0.73
1:R:119:VAL:HG21	1:R:326:LEU:HD11	1.65	0.73
1:G:156:LEU:HD21	1:G:242:LEU:HD21	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:R:3:VAL:H	1:R:27:VAL:CA	1.94	0.73
1:G:276:THR:HG1	1:G:278:ASP:HB2	1.53	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:176:THR:CG2	1:R:231:ALA:HB1	2.07	0.73
1:R:40:HIS:ND1	1:R:43:VAL:HG13	2.03	0.73
1:R:240:SER:O	1:R:313:TYR:HB2	1.89	0.73
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:174:MET:HE2	1:R:242:LEU:HD11	1.72	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:140:ALA:HA	1:R:333:LYS:HZ1	1.53	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:135:ASN:CG	1:R:136:HIS:N	2.43	0.71
1:G:216:VAL:HG13	1:G:223:LEU:HD23	1.72	0.71
1:R:205:LEU:HD22	1:R:205:LEU:O	1.90	0.71
1:G:26:LYS:HD2	1:G:27:VAL:H	1.48	0.71
1:G:213:ALA:HB2	1:G:228:THR:HA	1.72	0.71
1:R:134:VAL:HG23	1:R:219:VAL:HG12	1.72	0.71
1:R:84:ILE:HD12	1:R:85:LYS:HE3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:283:ASP:O	1:G:284:ASP:C	2.27	0.71
1:R:76:PHE:CE2	1:R:85:LYS:HD2	2.25	0.71
1:G:155:CYS:O	1:G:158:PRO:HD2	1.90	0.71
1:G:247:ARG:HB3	1:G:247:ARG:HH11	1.54	0.71
1:G:269:LEU:CD2	1:G:269:LEU:H	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:205:LEU:C	1:G:205:LEU:HD22	2.11	0.71
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
1:R:55:PHE:O	1:R:56:HIS:CB	2.39	0.70
1:R:197:GLY:O	1:R:198:GLY:C	2.26	0.70
1:G:175:THR:HB	1:G:230:MET:HE3	1.73	0.70
1:G:185:LYS:O	1:G:201:ALA:HB2	1.92	0.70
1:R:333:LYS:NZ	1:R:333:LYS:CB	2.53	0.70
1:G:141:ASN:N	1:G:333:LYS:HZ1	1.89	0.70
1:R:91:THR:O	1:R:91:THR:HG23	1.92	0.70
1:R:3:VAL:HG21	1:R:27:VAL:HG11	1.71	0.70
1:R:259:LYS:C	1:R:262:LYS:HG3	2.10	0.70
1:R:261:VAL:O	1:R:265:SER:HB3	1.90	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: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:35:PRO:HG3	1:R:78:GLU:C	2.13	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:85:LYS:O	1:G:113:GLY:O	2.12	0.68
1:R:120:ILE:HD12	1:R:146:ILE:O	1.93	0.68
1:R:38:ASP:OD2	1:R:39:LEU:N	2.24	0.68
1:R:174:MET:SD	1:R:242:LEU:HD11	2.33	0.68
1:G:4:LYS:HE3	1:G:92:ALA:HB2	1.74	0.68
1:R:197:GLY:O	1:R:199:ARG:N	2.26	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: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:174:MET:HE2	1:G:212:ALA:HB2	1.74	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:86:TRP:HE1	1:R:110:HIS:CE1	2.12	0.67
1:R:121:SER:O	1:R:122:ALA:HB2	1.94	0.67
1:R:85:LYS:H	1:R:85:LYS:HE3	1.59	0.67
1:R:98:THR:CG2	1:R:99:GLY:N	2.57	0.67
1:R:152:THR:HA	1:R:313:TYR:CZ	2.29	0.67
1:R:25:GLY:O	1:R:26:LYS:HB3	1.94	0.67
1:G:320:SER:HA	1:G:323:VAL:CG2	2.25	0.67
1:G:86:TRP:CD1	1:G:110:HIS:CD2	2.82	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:84:ILE:HB	1:G:85:LYS:HZ2	1.57	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:2:LYS:HG2	1:R:3:VAL:N	2.08	0.67
1:G:107:ALA:HB2	1:G:120:ILE:HD11	1.76	0.67
1:G:78:GLU:CB	1:G:84:ILE:CG2	2.71	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:14:GLY:O	1:G:18:THR:HG22	1.94	0.66
1:G:16:LEU:O	1:G:16:LEU:HD22	1.95	0.66
1:G:47:GLN:HB2	1:G:59:VAL:HG11	1.76	0.66
1:R:197:GLY:C	1:R:199:ARG:N	2.42	0.66
1:G:220:ILE:O	1:G:221:PRO:O	2.14	0.66
1:R:257:ILE:HG23	1:R:258:LYS:N	2.10	0.66
1:R:81:PRO:HA	1:R:84:ILE:CG2	2.26	0.66
1:G:65:LYS:HD2	1:G:73:ILE:C	2.15	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:R:3:VAL:HB	1:R:27:VAL:HG13	0.68	0.66
1:G:47:GLN:HA	1:G:55:PHE:HB2	1.77	0.66
1:G:275:TYR:C	1:G:275:TYR:HD2	1.98	0.66
1:R:103:THR:HG23	1:R:105:GLU:H	1.61	0.66
1:R:280:VAL:CG2	1:R:280:VAL:O	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:264:ALA:O	1:R:269:LEU:HD23	1.96	0.66
1:R:29:ILE:C	1:R:30:VAL:CG1	2.65	0.66
1:R:10:PHE:CE1	1:R:32:ILE:CD1	2.79	0.66
1:G:16:LEU:CA	1:G:19:ARG:HB3	2.25	0.66
1:G:190:PRO:O	1:G:191:SER:HB3	1.94	0.66
1:R:276:THR:HG23	1:R:295:ASP:CB	2.02	0.66
1:R:85:LYS:H	1:R:85:LYS:CE	2.09	0.65
1:G:141:ASN:N	1:G:333:LYS:NZ	2.43	0.65
1:G:21:ALA:O	1:G:26:LYS:CA	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:2:LYS:HD2	1:G:25:GLY:C	2.16	0.65
1:G:319:TYR:O	1:G:323:VAL:HG22	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:250:LYS:NZ	1:G:251:PRO:HD2	2.11	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:G:199:ARG:O	1:G:199:ARG:HG3	1.97	0.65
1:G:128:PRO:HG2	1:G:145:ILE:O	1.96	0.65
1:G:29:ILE:C	1:G:30:VAL:HG13	2.16	0.65
1:R:200:GLY:O	1:R:201:ALA:CB	2.44	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:G:130:PHE:CE1	1:G:138:LYS:HD3	2.32	0.65
1:R:196:ARG:NH2	1:R:208:ALA:CA	2.60	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:275:TYR:C	1:R:275:TYR:CD2	2.69	0.65
1:G:284:ASP:O	1:G:286:ASN:HB2	1.97	0.65
1:G:214:LYS:O	1:G:218:LYS:NZ	2.27	0.65
1:G:117:ARG:HH11	1:G:144:LYS:CD	2.08	0.64
1:R:291:SER:OG	1:R:322:ARG:CD	2.44	0.64
1:R:266:GLU:HG2	1:R:267:GLY:N	2.12	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:205:LEU:CD2	1:R:205:LEU:C	2.65	0.64
1:G:104:MET:O	1:G:105:GLU:C	2.32	0.64
1:G:131:VAL:O	1:G:135:ASN:HB3	1.97	0.64
1:G:42:MET:CE	1:G:75:ILE:HD13	2.27	0.64
1:R:170:VAL:O	1:R:247:ARG:HB3	1.98	0.64
1:R:67:VAL:CG2	1:R:67:VAL:O	2.44	0.64
1:G:153:THR:HG23	1:G:215:ALA:CB	2.21	0.64
1:G:78:GLU:HG3	1:G:84:ILE:CB	2.26	0.64
1:R:317:PHE:O	1:R:318:GLY:C	2.34	0.64
1:G:106:LYS:O	1:G:109:ALA:N	2.29	0.64
1:R:190:PRO:O	1:R:191:SER:OG	2.14	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:G:29:ILE:O	1:G:30:VAL:HG13	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:189:SER:O	1:R:190:PRO:O	2.15	0.64
1:R:247:ARG:HA	1:R:305:THR:O	1.97	0.64
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:CB	1:G:247:ARG:HH11	2.10	0.64
1:R:129:MET:C	1:R:130:PHE:CD1	2.68	0.64
1:R:16:LEU:HG	1:R:317:PHE:CD2	2.33	0.64
1:R:110:HIS:O	1:R:113:GLY:N	2.31	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:163:ILE:CG2	1:R:164:HIS:N	2.61	0.63
1:R:333:LYS:HZ3	1:R:333:LYS:HB3	1.61	0.63
1:R:174:MET:HG3	1:R:242:LEU:CD1	2.26	0.63
1:R:17:VAL:O	1:R:21:ALA:HB2	1.98	0.63
1:G:129:MET:HE1	1:G:149:ALA:HA	1.80	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:CA	1:R:78:GLU:OE2	2.43	0.63
1:G:254:TYR:CE2	1:G:300:ILE:HG12	2.33	0.63
1:R:315:ASN:O	1:R:316:GLU:C	2.36	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:R:254:TYR:OH	1:R:300:ILE:HG12	1.98	0.63
1:R:291:SER:CB	1:R:322:ARG:HD2	2.27	0.63
1:G:62:GLU:O	1:G:65:LYS:O	2.15	0.63
1:R:186:THR:O	1:R:187:VAL:HG22	1.93	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:273:LEU:O	1:G:293:ILE:HA	1.99	0.63
1:G:159:LEU:HD11	1:G:309:LEU:HD23	1.81	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:4:LYS:CE	1:G:92:ALA:HB3	2.29	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:326:LEU:HD22	1:R:326:LEU:C	2.19	0.62
1:R:317:PHE:O	1:R:319:TYR:N	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:81:PRO:O	1:R:84:ILE:HG23	1.99	0.62
1:R:8:ASP:HB2	1:R:96:GLU:HA	1.81	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:196:ARG:HG3	1:R:233:ARG:HH21	1.64	0.62
1:R:54:LYS:HE2	1:R:56:HIS:CE1	2.35	0.62
1:G:180:ILE:HG23	1:G:237:ALA:HA	1.80	0.62
1:G:159:LEU:O	1:G:163:ILE:HD13	2.00	0.62
1:G:257:ILE:HG22	1:G:258:LYS:H	1.64	0.62
1:G:161:LYS:C	1:G:165:ASP:OD2	2.37	0.62
1:G:297:GLY:O	1:G:300:ILE:CG1	2.47	0.62
1:G:86:TRP:CD1	1:G:110:HIS:NE2	2.67	0.62
1:R:37:ILE:HG23	1:R:41:TYR:HB3	1.82	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:275:TYR:CD2	1:G:275:TYR:C	2.69	0.62
1:R:257:ILE:CG2	1:R:258:LYS:H	2.12	0.62
1:G:213:ALA:HB1	1:G:227:LEU:O	2.00	0.62
1:R:238:ASN:OD1	1:R:239:VAL:N	2.33	0.62
1:G:139:TYR:HD2	1:G:333:LYS:HD3	1.65	0.62
1:G:78:GLU:CB	1:G:84:ILE:HG22	2.29	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:166:HIS:HD2	1:R:260:VAL:HG23	1.62	0.62
1:G:322:ARG:HE	1:G:322:ARG:HA	1.63	0.61
1:R:116:LYS:O	1:R:144:LYS:HG3	1.99	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: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: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:G:4:LYS:CG	1:G:4:LYS:O	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:317:PHE:O	1:G:319:TYR:N	2.33	0.61
1:G:171:GLU:H	1:G:226:LYS:HG3	1.65	0.61
1:G:86:TRP:NE1	1:G:110:HIS:CE1	2.68	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:O	1:R:194:LEU:HD12	2.00	0.61
1:G:151:CYS:SG	1:G:152:THR:N	2.71	0.61
1:R:186:THR:C	1:R:187:VAL:HG22	2.21	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:111:LEU:HA	1:G:115:ALA:HB3	1.81	0.61
1:G:326:LEU:C	1:G:326:LEU:HD12	2.21	0.61
1:G:129:MET:CE	1:G:149:ALA:HA	2.30	0.61
1:R:294:PHE:CD2	1:R:295:ASP:N	2.68	0.61
1:G:2:LYS:O	1:G:28:ASP:HB2	2.01	0.61
1:G:93:TYR:HD2	1:G:330:MET:HE3	1.65	0.61
1:R:323:VAL:O	1:R:326:LEU:HB3	2.00	0.61
1:R:141:ASN:O	1:R:143:LEU:O	2.18	0.60
1:R:68:ILE:HG13	1:R:73:ILE:HD12	1.82	0.60
1:G:315:ASN:O	1:G:316:GLU:C	2.40	0.60
1:R:1:GLY:HA2	1:R:29:ILE:N	2.13	0.60
1:R:47:GLN:NE2	1:R:48:TYR:CD1	2.69	0.60
1:G:326:LEU:HD12	1:G:327:MET:N	2.16	0.60
1:G:43:VAL:HG12	1:G:66:LEU:CD1	2.19	0.60
1:G:5:VAL:HG12	1:G:6:GLY:O	2.00	0.60
1:R:16:LEU:HD12	1:R:320:SER:HB3	0.68	0.60
1:R:98:THR:HG1	1:R:101:PHE:HD2	1.49	0.60
1:G:247:ARG:HB3	1:G:247:ARG:NH1	2.16	0.60
1:G:168:GLY:CA	1:G:249:GLU:HB3	2.30	0.60
1:G:65:LYS:HG3	1:G:66:LEU:N	2.17	0.60
1:G:189:SER:CB	1:G:190:PRO:HD2	2.32	0.60
1:R:3:VAL:H	1:R:27:VAL:HG22	1.66	0.60
1:G:55:PHE:C	1:G:55:PHE:CD2	2.74	0.60
1:R:156:LEU:C	1:R:158:PRO:HD2	2.22	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: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:G:140:ALA:HA	1:G:333:LYS:HZ2	1.67	0.59
1:G:155:CYS:C	1:G:158:PRO:HD2	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:275:TYR:HE2	1:R:277:GLU:CG	2.08	0.59
1:R:135:ASN:CG	1:R:136:HIS:H	2.04	0.59
1:G:91:THR:HG23	1:G:91:THR:O	2.02	0.59
1:G:98:THR:CB	3:G:336:NAD:H8A	2.32	0.59
1:G:196:ARG:C	1:G:198:GLY:H	2.04	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: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:65:LYS:HG3	1:G:66:LEU:O	2.03	0.59
1:R:5:VAL:C	1:R:91:THR:OG1	2.41	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:R:178:HIS:O	1:R:234:VAL:HG22	2.03	0.58
1:G:315:ASN:HB2	3:G:336:NAD:H4N	1.85	0.58
1:G:97:SER:O	1:G:98:THR:HB	2.03	0.58
1:R:258:LYS:HE3	1:R:296:ALA:HB1	1.85	0.58
1:R:121:SER:O	1:R:121:SER:OG	2.17	0.58
1:G:189:SER:HB2	1:G:190:PRO:HD2	1.85	0.58
1:R:86:TRP:CZ2	1:R:94:VAL:HG13	2.39	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:R:275:TYR:C	1:R:275:TYR:HD2	2.07	0.58
1:G:8:ASP:OD1	1:G:96:GLU:OE1	2.12	0.58
1:R:322:ARG:HA	1:R:325:ASP:HB2	1.85	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:G:79:ARG:HA	3:G:336:NAD:H62A	1.68	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:R:131:VAL:HG23	1:R:133:GLY:H	1.67	0.58
1:R:41:TYR:CE1	1:G:190:PRO:HA	2.39	0.58
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:G:86:TRP:O	1:G:91:THR:HG22	2.04	0.58
1:G:263:GLU:O	1:G:266:GLU:HB3	2.04	0.58
1:R:162:VAL:HG13	1:R:260:VAL:HG22	1.85	0.58
1:G:16:LEU:HD23	1:G:317:PHE:CE2	2.39	0.58
1:G:29:ILE:C	1:G:30:VAL:CG1	2.72	0.58
1:G:37:ILE:HG13	1:G:41:TYR:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:266:GLU:O	1:G:270:LYS:HE3	2.04	0.58
1:G:47:GLN:HG3	1:G:48:TYR:N	2.18	0.58
1:G:257:ILE:C	1:G:260:VAL:HG12	2.20	0.58
1:R:151:CYS:HB3	3:R:336:NAD:C5N	2.34	0.57
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:G:101:PHE:O	1:G:102:THR:HB	2.03	0.57
1:G:65:LYS:HD2	1:G:73:ILE:O	2.00	0.57
1:G:37:ILE:CG2	1:G:42:MET:HE2	2.30	0.57
1:G:106:LYS:HB2	1:G:106:LYS:NZ	2.19	0.57
1:G:186:THR:O	1:G:187:VAL:HG23	2.05	0.57
1:R:258:LYS:O	1:R:275:TYR:HE1	1.88	0.57
1:G:132:MET:O	1:G:135:ASN:OD1	2.21	0.57
1:G:130:PHE:CZ	1:G:138:LYS:HB3	2.40	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:R:163:ILE:HG23	1:R:169:ILE:CD1	2.35	0.57
1:G:65:LYS:HB2	1:G:74:THR:CA	2.12	0.57
1:G:30:VAL:CG2	1:G:73:ILE:CG1	2.81	0.57
1:G:260:VAL:HG13	1:G:261:VAL:H	1.70	0.57
1:R:117:ARG:CA	1:R:144:LYS:O	2.51	0.57
1:R:239:VAL:HG21	1:R:286:ASN:H	1.70	0.57
1:R:3:VAL:O	1:R:4:LYS:HG2	2.03	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:G:35:PRO:CB	1:G:79:ARG:HG2	2.32	0.57
1:R:313:TYR:HB3	1:R:315:ASN:H	1.70	0.57
1:G:148:ASN:O	1:G:319:TYR:OH	2.19	0.57
1:R:14:GLY:O	1:R:18:THR:CG2	2.53	0.56
1:G:163:ILE:N	1:G:163:ILE:CD1	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
1:G:10:PHE:CB	1:G:34:ASP:OD2	2.53	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:G:38:ASP:CG	1:G:39:LEU:HD23	2.25	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:285:PHE:CD2	1:R:285:PHE:N	2.73	0.56
1:R:241:VAL:HB	1:R:312:TRP:CE3	2.41	0.56
1:G:2:LYS:HZ1	1:G:25:GLY:HA3	1.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:160:ALA:O	1:G:161:LYS:C	2.44	0.56
1:R:44:TYR:OH	1:G:199:ARG:NE	2.38	0.56
1:G:30:VAL:HG23	1:G:31:ALA:H	1.69	0.56
1:R:196:ARG:HG3	1:R:233:ARG:NH2	2.21	0.56
1:R:197:GLY:C	1:R:199:ARG:CB	2.73	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:120:ILE:HG22	1:G:121:SER:N	2.18	0.56
1:G:85:LYS:CD	1:G:85:LYS:N	2.57	0.56
1:G:16:LEU:HD13	1:G:16:LEU:C	2.26	0.56
1:G:317:PHE:C	1:G:319:TYR:N	2.58	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:234:VAL:HB	1:R:235:PRO:CD	2.33	0.56
1:R:65:LYS:CG	1:R:66:LEU:N	2.69	0.56
1:G:157:ALA:HB3	1:G:158:PRO:HD3	1.88	0.56
1:G:322:ARG:CA	1:G:322:ARG:NE	2.67	0.56
1:G:196:ARG:NE	1:G:208:ALA:CB	2.68	0.56
1:R:19:ARG:HH21	1:R:55:PHE:HB2	1.69	0.55
1:R:12:ARG:NH2	1:R:51:THR:HG21	2.20	0.55
1:G:282:SER:O	1:G:312:TRP:CH2	2.59	0.55
1:R:146:ILE:HG21	1:R:330:MET:SD	2.46	0.55
1:R:137:PHE:O	1:R:138:LYS:C	2.44	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:G:222:GLU:C	1:G:223:LEU:O	2.44	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:G:81:PRO:O	1:G:82:GLU:C	2.45	0.55
1:G:8:ASP:OD2	1:G:33:ASN:CG	2.44	0.55
1:R:129:MET:O	1:R:130:PHE:HD1	1.88	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:G:98:THR:OG1	3:G:336:NAD:C8A	2.54	0.55
1:G:11:GLY:HA2	1:G:15:ARG:CZ	2.37	0.55
1:G:15:ARG:CA	1:G:18:THR:HG23	2.33	0.55
1:R:122:ALA:HB2	3:R:336:NAD:HO2N	1.70	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:13:ILE:CG2	1:G:97:SER:HB3	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:188:ASP:OD2	1:G:50:SER:OG	2.24	0.55
1:G:257:ILE:CG2	1:G:258:LYS:H	2.17	0.55
1:R:15:ARG:HH21	1:R:45:MET:CE	2.20	0.55
1:R:20:ALA:O	1:R:21:ALA:C	2.44	0.55
1:G:139:TYR:CD2	1:G:333:LYS:NZ	2.65	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:R:11:GLY:N	1:R:15:ARG:HD3	2.22	0.55
1:G:152:THR:HG22	1:G:153:THR:H	1.70	0.55
1:G:150:SER:HB3	2:G:340:SO4:O1	2.07	0.55
1:R:211:GLY:O	1:R:215:ALA:CB	2.55	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:213:ALA:HB2	1:R:228:THR:CA	2.27	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: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:4:LYS:CG	1:G:92:ALA:HB3	2.37	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:G:230:MET:HG2	1:G:231:ALA:H	1.72	0.54
1:R:323:VAL:O	1:R:327:MET:N	2.34	0.54
1:G:2:LYS:CB	1:G:26:LYS:CE	2.73	0.54
1:G:230:MET:SD	1:G:232:PHE:HE1	2.31	0.54
1:R:139:TYR:CE1	1:R:143:LEU:HD22	2.43	0.54
1:G:320:SER:C	1:G:323:VAL:HG23	2.27	0.54
1:G:169:ILE:H	1:G:248:LEU:HB3	1.71	0.54
1:G:285:PHE:CD2	1:G:285:PHE:N	2.75	0.54
1:R:160:ALA:HB1	1:R:223:LEU:CD1	2.37	0.54
1:R:174:MET:CE	1:R:242:LEU:CD1	2.85	0.54
1:R:211:GLY:O	1:R:215:ALA:HB2	2.07	0.54
1:R:98:THR:HG22	1:R:99:GLY:H	1.72	0.54
1:G:13:ILE:HB	3:G:336:NAD:O2N	2.08	0.54
1:G:326:LEU:O	1:G:330:MET:HG3	2.07	0.54
1:G:247:ARG:HG2	1:G:306:PHE:CD1	2.42	0.54
1:R:26:LYS:CG	1:R:27:VAL:N	2.67	0.54
1:R:1:GLY:CA	1:R:28:ASP:C	2.52	0.54
1:G:140:ALA:CA	1:G:333:LYS:HZ2	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:22:PHE:CE1	1:G:69:ASP:HB3	2.42	0.54
1:R:146:ILE:HG13	1:R:147:SER:H	1.70	0.54
1:R:12:ARG:HA	1:R:12:ARG:HE	1.73	0.54
1:R:157:ALA:N	1:R:158:PRO:CD	2.70	0.54
1:R:3:VAL:H	1:R:27:VAL:CG2	2.19	0.54
1:R:59:VAL:CG2	1:R:59:VAL:O	2.56	0.54
1:G:65:LYS:CG	1:G:66:LEU:N	2.69	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:G:192:GLY:O	1:G:195:TRP:HA	2.08	0.54
1:R:43:VAL:O	1:R:59:VAL:HG21	2.08	0.54
1:G:98:THR:OG1	3:G:336:NAD:H8A	2.07	0.53
1:R:254:TYR:CB	1:R:302:LEU:HD22	2.36	0.53
1:G:153:THR:HG21	1:G:215:ALA:HB1	1.83	0.53
1:G:25:GLY:O	1:G:26:LYS:HB3	2.07	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:R:172:GLY:HA2	1:R:245:THR:O	2.08	0.53
1:R:285:PHE:O	1:R:286:ASN:C	2.45	0.53
1:R:16:LEU:CD1	1:R:320:SER:CB	2.39	0.53
1:G:139:TYR:CE2	1:G:330:MET:HB3	2.43	0.53
1:G:16:LEU:HD22	1:G:20:ALA:H	1.73	0.53
1:G:93:TYR:N	1:G:93:TYR:CD1	2.76	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:G:76:PHE:HB3	1:G:85:LYS:NZ	2.23	0.53
1:R:196:ARG:NH1	1:R:196:ARG:CA	2.33	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:R:131:VAL:CG2	1:R:133:GLY:H	2.22	0.53
1:R:130:PHE:O	1:R:148:ASN:HA	2.09	0.53
1:G:239:VAL:CG1	1:G:240:SER:N	2.71	0.53
1:G:2:LYS:C	1:G:28:ASP:HB2	2.29	0.53
1:G:304:ASP:OD2	1:G:305:THR:HB	2.09	0.53
1:R:255:ASP:HA	1:R:258:LYS:HD3	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:283:ASP:O	1:R:284:ASP:C	2.47	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:R:285:PHE:O	1:R:286:ASN:CB	2.55	0.53
1:R:121:SER:HA	1:R:319:TYR:OH	2.08	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:G:180:ILE:HG13	1:G:181:THR:N	2.23	0.53
1:R:128:PRO:HG2	1:R:145:ILE:O	2.09	0.52
1:R:5:VAL:O	1:R:30:VAL:CA	2.56	0.52
1:G:323:VAL:HB	1:G:327:MET:CE	2.40	0.52
1:R:199:ARG:O	1:R:199:ARG:CG	2.57	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:148:ASN:OD1	1:G:326:LEU:HD23	2.09	0.52
1:G:8:ASP:HB2	1:G:96:GLU:HG2	1.92	0.52
1:R:106:LYS:O	1:R:109:ALA:N	2.42	0.52
1:R:15:ARG:CD	1:R:15:ARG:H	2.22	0.52
1:G:151:CYS:C	1:G:313:TYR:HE2	2.13	0.52
1:G:16:LEU:HA	1:G:19:ARG:CB	2.37	0.52
1:G:222:GLU:O	1:G:223:LEU:O	2.27	0.52
1:G:199:ARG:O	1:G:199:ARG:CG	2.57	0.52
1:R:176:THR:O	1:R:176:THR:HG23	2.09	0.52
1:R:47:GLN:O	1:R:55:PHE:N	2.42	0.52
1:G:273:LEU:O	1:G:292:SER:O	2.27	0.52
1:R:212:ALA:O	1:R:216:VAL:HG23	2.10	0.52
1:G:330:MET:O	1:G:334:GLU:CG	2.56	0.52
1:G:42:MET:HE1	1:G:75:ILE:HD13	1.90	0.52
1:G:298:ALA:HB1	1:G:310:VAL:CG1	2.40	0.52
1:G:316:GLU:O	1:G:319:TYR:HB3	2.10	0.52
1:G:20:ALA:O	1:G:21:ALA:C	2.48	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:124:SER:OG	1:R:127:ALA:HB3	2.10	0.52
1:R:12:ARG:HA	1:R:12:ARG:NE	2.24	0.52
1:R:155:CYS:SG	1:R:292:SER:HB2	2.50	0.52
1:G:148:ASN:O	1:G:149:ALA:O	2.27	0.52
1:G:29:ILE:CG2	1:G:72:ALA:O	2.58	0.52
1:G:34:ASP:HB3	1:G:42:MET:CE	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:109:ALA:O	1:R:112:LYS:N	2.38	0.52
1:R:14:GLY:O	1:R:18:THR:HG22	2.10	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:1:GLY:CA	1:R:28:ASP:OD2	2.48	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: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:R:152:THR:HA	1:R:313:TYR:OH	2.09	0.51
1:G:149:ALA:HB1	1:G:153:THR:HG21	1.86	0.51
1:R:200:GLY:O	1:R:201:ALA:HB2	2.10	0.51
1:R:157:ALA:HB3	1:R:158:PRO:HD3	1.93	0.51
1:G:265:SER:O	1:G:266:GLU:C	2.49	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:269:LEU:N	1:R:269:LEU:CD2	2.56	0.51
1:R:78:GLU:HG3	1:R:84:ILE:HB	1.75	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:102:THR:HG23	1:R:124:SER:HB2	1.93	0.51
1:R:37:ILE:HD11	1:G:190:PRO:HB3	1.93	0.51
1:G:322:ARG:HA	1:G:325:ASP:HB2	1.92	0.51
1:G:272:ILE:O	1:G:273:LEU:CB	2.43	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:3:VAL:C	1:R:4:LYS:HG2	2.31	0.51
1:R:86:TRP:HE1	1:R:94:VAL:HG11	1.74	0.51
1:G:276:THR:C	1:G:278:ASP:N	2.63	0.51
1:R:10:PHE:HB2	1:R:34:ASP:OD2	2.10	0.51
1:R:9:GLY:HA2	3:R:336:NAD:H8A	1.93	0.51
1:G:315:ASN:O	1:G:317:PHE:N	2.43	0.51
1:R:6:GLY:O	1:R:7:VAL:CG2	2.59	0.51
1:R:40:HIS:O	1:R:40:HIS:ND1	2.43	0.51
1:R:81:PRO:O	1:R:82:GLU:C	2.49	0.51
1:G:36:PHE:O	1:G:37:ILE:HD13	2.11	0.51
1:G:176:THR:O	1:G:231:ALA:HB1	2.09	0.51
1:G:156:LEU:HD11	1:G:242:LEU:CD2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:103:THR:HG22	1:G:106:LYS:H	1.75	0.51
1:G:82:GLU:HG2	1:G:83:ASN:H	1.76	0.51
1:R:155:CYS:C	1:R:158:PRO:HD2	2.32	0.50
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:130:PHE:C	1:G:131:VAL:CG1	2.80	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:G:195:TRP:C	1:G:197:GLY:N	2.62	0.50
1:R:78:GLU:HB3	1:R:84:ILE:HG22	1.93	0.50
1:G:141:ASN:C	1:G:143:LEU:H	2.14	0.50
1:G:164:HIS:CB	1:G:169:ILE:HD12	2.37	0.50
1:R:132:MET:O	1:R:133:GLY:C	2.49	0.50
1:R:75:ILE:HG13	1:R:75:ILE:O	2.11	0.50
1:G:174:MET:HE1	1:G:212:ALA:HB2	1.91	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:189:SER:CB	1:G:190:PRO:CD	2.89	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:139:TYR:HE1	1:R:143:LEU:HD22	1.77	0.50
1:R:22:PHE:CZ	1:R:69:ASP:HB3	2.31	0.50
1:G:106:LYS:HZ2	1:G:106:LYS:HB2	1.76	0.50
1:R:92:ALA:O	1:R:116:LYS:HB2	2.11	0.50
1:G:250:LYS:HZ2	1:G:251:PRO:CD	2.17	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:163:ILE:HG21	1:R:169:ILE:HD11	1.89	0.50
1:R:139:TYR:O	1:R:333:LYS:HE3	2.11	0.50
1:R:34:ASP:N	1:R:76:PHE:O	2.43	0.50
1:G:43:VAL:O	1:G:47:GLN:HB3	2.12	0.50
1:G:16:LEU:HG	1:G:317:PHE:CE2	2.47	0.50
1:G:4:LYS:CE	1:G:92:ALA:CB	2.81	0.50
1:R:118:ILE:O	1:R:118:ILE:HG22	2.12	0.49
1:R:37:ILE:HD12	1:R:41:TYR:CD1	2.47	0.49
1:G:323:VAL:HB	1:G:327:MET:HE1	1.93	0.49
1:G:320:SER:HA	1:G:323:VAL:HG21	1.94	0.49
1:R:222:GLU:C	1:R:223:LEU:O	2.49	0.49
1:G:8:ASP:HB2	1:G:96:GLU:CG	2.41	0.49
1:R:169:ILE:H	1:R:248:LEU:HA	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:118:ILE:O	1:R:118:ILE:CG2	2.60	0.49
1:G:141:ASN:ND2	1:G:333:LYS:HE3	2.26	0.49
1:G:42:MET:HE3	1:G:75:ILE:HD13	1.93	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:153:THR:HG21	1:R:215:ALA:HB1	1.94	0.49
1:R:51:THR:CG2	1:R:52:HIS:N	2.75	0.49
1:G:152:THR:HA	1:G:313:TYR:CE2	2.47	0.49
1:G:5:VAL:HA	1:G:93:TYR:O	2.11	0.49
1:R:261:VAL:O	1:R:262:LYS:C	2.51	0.49
1:R:104:MET:HA	1:R:145:ILE:CD1	2.43	0.49
1:R:2:LYS:HD2	1:R:25:GLY:O	2.10	0.49
1:G:153:THR:CG2	1:G:215:ALA:CB	2.79	0.49
1:G:16:LEU:HB3	1:G:320:SER:CB	2.43	0.49
1:G:179:ALA:HA	1:G:236:THR:O	2.13	0.49
1:G:284:ASP:O	1:G:285:PHE:C	2.50	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:104:MET:HA	1:R:145:ILE:HD11	1.95	0.49
1:R:12:ARG:H	1:R:15:ARG:NH1	2.11	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:257:ILE:HG22	1:R:258:LYS:H	1.76	0.49
1:R:126:ASP:O	1:R:127:ALA:HB3	2.11	0.49
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:163:ILE:HG22	1:R:164:HIS:N	2.27	0.49
1:R:80:ASP:O	1:R:83:ASN:HB2	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:6:GLY:O	1:R:7:VAL:HG22	2.13	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:320:SER:O	1:G:323:VAL:HG23	2.13	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:R:3:VAL:N	1:R:27:VAL:HG13	2.28	0.48
1:R:2:LYS:HD2	1:R:27:VAL:N	2.01	0.48
1:R:149:ALA:O	1:R:319:TYR:HE1	1.95	0.48
1:G:107:ALA:HB1	1:G:118:ILE:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:253:LYS:O	1:R:256:ASP:N	2.46	0.48
1:R:92:ALA:HB1	1:R:116:LYS:HB2	1.94	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:G:86:TRP:HD1	1:G:110:HIS:CD2	2.31	0.48
1:G:331:ALA:O	1:G:332:SER:C	2.51	0.48
1:G:186:THR:C	1:G:187:VAL:HG23	2.34	0.48
1:G:173:LEU:CD2	1:G:228:THR:HG22	2.42	0.48
1:G:188:ASP:O	1:G:189:SER:CB	2.58	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:R:333:LYS:HZ2	1:R:333:LYS:CB	2.26	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:217:GLY:CA	1:G:224:ASP:HB2	2.43	0.48
1:R:38:ASP:O	1:R:39:LEU:C	2.51	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:180:ILE:HD12	1:G:186:THR:HB	1.95	0.48
1:R:33:ASN:O	1:R:33:ASN:ND2	2.45	0.48
1:R:84:ILE:CD1	1:R:85:LYS:HE3	2.41	0.48
1:G:5:VAL:HG12	1:G:6:GLY:N	2.28	0.48
1:G:77:GLN:O	1:G:78:GLU:C	2.51	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:G:94:VAL:HG22	1:G:118:ILE:HG13	1.96	0.48
1:G:239:VAL:HG12	1:G:240:SER:N	2.28	0.48
1:G:196:ARG:NH2	1:G:207:PRO:O	2.47	0.48
1:R:68:ILE:CD1	1:R:73:ILE:HG21	2.37	0.48
1:G:326:LEU:C	1:G:326:LEU:CD1	2.82	0.48
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:5:VAL:HG12	1:G:6:GLY:H	1.79	0.47
1:G:220:ILE:CG2	1:G:220:ILE:O	2.62	0.47
1:R:6:GLY:C	1:R:7:VAL:HG23	2.34	0.47
1:R:180:ILE:HG23	1:R:235:PRO:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:141:ASN:C	1:G:143:LEU:N	2.67	0.47
1:G:2:LYS:HZ1	1:G:25:GLY:CA	2.24	0.47
1:G:63:ASP:C	1:G:65:LYS:H	2.17	0.47
1:G:273:LEU:HA	1:G:273:LEU:HD23	1.71	0.47
1:R:259:LYS:HA	1:R:262:LYS:HD3	1.95	0.47
1:R:163:ILE:HG22	1:R:164:HIS:H	1.79	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:G:294:PHE:CD2	1:G:294:PHE:C	2.88	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:R:317:PHE:C	1:R:319:TYR:N	2.66	0.47
1:G:68:ILE:O	1:G:69:ASP:HB3	2.14	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: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:G:10:PHE:HD1	1:G:32:ILE:HG23	1.79	0.47
1:G:167:PHE:O	1:G:248:LEU:HB2	2.13	0.47
1:R:92:ALA:CA	1:R:116:LYS:HB2	2.44	0.47
1:G:67:VAL:CG2	1:G:67:VAL:O	2.62	0.47
1:R:44:TYR:OH	1:G:199:ARG:HD3	2.14	0.47
1:G:16:LEU:CD1	1:G:20:ALA:HB2	2.44	0.47
1:G:196:ARG:HH21	1:G:208:ALA:HB2	0.60	0.47
1:G:285:PHE:O	1:G:286:ASN:CB	2.60	0.47
1:G:282:SER:O	1:G:312:TRP:CZ3	2.68	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:R:170:VAL:O	1:R:171:GLU:O	2.33	0.47
1:R:10:PHE:CE2	1:R:46:PHE:CB	2.78	0.47
1:R:239:VAL:HB	1:R:283:ASP:OD2	2.14	0.47
1:R:84:ILE:O	1:R:85:LYS:O	2.32	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:R:16:LEU:O	1:R:17:VAL:C	2.52	0.47
1:G:293:ILE:O	1:G:312:TRP:N	2.48	0.47
1:R:240:SER:C	1:R:313:TYR:HD1	2.18	0.47
1:R:37:ILE:HG22	1:R:42:MET:HG3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:65:LYS:HG3	1:G:66:LEU:H	1.80	0.46
1:R:192:GLY:O	1:R:195:TRP:CA	2.63	0.46
1:G:33:ASN:O	1:G:33:ASN:ND2	2.48	0.46
1:G:8:ASP:CB	1:G:96:GLU:CG	2.92	0.46
1:G:213:ALA:HB2	1:G:227:LEU:C	2.34	0.46
1:R:140:ALA:O	1:R:143:LEU:HB2	2.14	0.46
1:R:28:ASP:CG	1:R:29:ILE:CG1	2.83	0.46
1:G:240:SER:O	1:G:313:TYR:HD1	1.97	0.46
1:R:254:TYR:HB3	1:R:302:LEU:HD22	1.96	0.46
1:R:86:TRP:HA	1:R:86:TRP:CE3	2.50	0.46
1:R:8:ASP:CB	1:R:96:GLU:HA	2.45	0.46
1:G:117:ARG:HH11	1:G:144:LYS:CG	2.28	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:R:199:ARG:HG3	1:R:199:ARG:O	2.14	0.46
1:R:196:ARG:NH2	1:R:208:ALA:HA	2.28	0.46
1:R:88:ASP:O	1:R:89:ALA:CB	2.63	0.46
1:G:112:LYS:HA	1:G:112:LYS:HD2	1.73	0.46
1:R:152:THR:OG1	1:R:313:TYR:OH	2.32	0.46
1:R:241:VAL:HA	1:R:312:TRP:HA	1.98	0.46
1:R:240:SER:O	1:R:313:TYR:HD1	1.97	0.46
1:R:154:ASN:O	1:R:158:PRO:HD3	2.15	0.46
1:R:16:LEU:CD2	1:R:317:PHE:CE2	2.99	0.46
1:G:168:GLY:HA3	1:G:249:GLU:CB	2.45	0.46
1:G:174:MET:HG3	1:G:174:MET:O	2.07	0.46
1:G:38:ASP:O	1:G:39:LEU:C	2.53	0.46
1:R:96:GLU:OE1	1:R:101:PHE:HB3	2.16	0.46
1:R:15:ARG:O	1:R:18:THR:HG23	2.15	0.46
1:R:12:ARG:NH2	1:R:49:ASP:OD1	2.48	0.46
1:G:29:ILE:HG22	1:G:30:VAL:H	1.80	0.46
1:R:111:LEU:HD21	1:R:116:LYS:C	2.36	0.46
1:G:55:PHE:CD1	1:G:56:HIS:O	2.69	0.46
1:G:174:MET:HE3	1:G:176:THR:HG22	1.98	0.46
1:G:185:LYS:O	1:G:200:GLY:O	2.34	0.46
1:R:6:GLY:C	1:R:7:VAL:CG2	2.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:42:MET:SD	1:G:75:ILE:HB	2.56	0.46
1:R:256:ASP:O	1:R:259:LYS:CB	2.64	0.46
1:G:86:TRP:HA	1:G:86:TRP:CE3	2.51	0.46
1:R:41:TYR:HE1	1:G:190:PRO:HA	1.81	0.46
1:R:16:LEU:HB3	1:R:320:SER:CB	2.46	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:R:62:GLU:HB3	1:R:63:ASP:H	1.57	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:322:ARG:N	1:G:322:ARG:NE	2.64	0.46
1:R:197:GLY:C	1:R:199:ARG:HB3	2.36	0.46
1:G:174:MET:HB2	1:G:243:ASP:O	2.15	0.46
1:G:273:LEU:HB3	1:G:274:GLY:H	1.55	0.46
1:G:234:VAL:CB	1:G:235:PRO:HD2	2.38	0.46
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:210:THR:HG23	2:R:340:SO4:O2	2.15	0.45
1:R:78:GLU:HG2	1:R:84:ILE:HB	1.92	0.45
1:G:320:SER:HA	1:G:323:VAL:HG23	1.97	0.45
1:G:37:ILE:HG22	1:G:42:MET:HE3	1.95	0.45
1:G:281:VAL:HG23	1:G:285:PHE:CE2	2.50	0.45
1:R:256:ASP:O	1:R:259:LYS:HB3	2.16	0.45
1:R:107:ALA:HB3	1:R:145:ILE:HD12	1.99	0.45
1:R:74:THR:HG22	1:R:75:ILE:N	2.30	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:G:140:ALA:C	1:G:142:SER:N	2.68	0.45
1:G:16:LEU:HD12	1:G:320:SER:C	2.37	0.45
1:G:16:LEU:HD22	1:G:20:ALA:N	2.31	0.45
1:G:84:ILE:H	1:G:84:ILE:HG13	1.45	0.45
1:R:303:ASN:O	1:R:306:PHE:N	2.49	0.45
1:R:94:VAL:HB	1:R:118:ILE:HG13	1.99	0.45
1:R:230:MET:CE	1:R:232:PHE:CE2	3.00	0.45
1:R:81:PRO:O	1:R:84:ILE:N	2.49	0.45
1:G:76:PHE:CD2	1:G:85:LYS:NZ	2.78	0.45
1:R:220:ILE:O	1:R:221:PRO:O	2.35	0.45
1:G:180:ILE:HD12	1:G:184:GLN:HB3	1.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:2:LYS:CG	1:R:3:VAL:H	2.09	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:181:THR:HG22	2:R:338:SO4:O1	2.16	0.45
1:R:155:CYS:O	1:R:158:PRO:HD2	2.17	0.45
1:R:15:ARG:CA	1:R:18:THR:HG23	2.46	0.45
1:G:257:ILE:HG21	1:G:309:LEU:HD11	1.99	0.45
1:R:222:GLU:O	1:R:223:LEU:O	2.35	0.45
1:G:16:LEU:HG	1:G:317:PHE:CD2	2.52	0.45
1:G:324:VAL:HA	1:G:327:MET:SD	2.56	0.45
1:G:273:LEU:O	1:G:293:ILE:HB	2.17	0.45
1:G:303:ASN:O	1:G:304:ASP:C	2.55	0.45
1:G:88:ASP:O	1:G:89:ALA:HB3	2.17	0.45
1:R:14:GLY:O	1:R:18:THR:HG23	2.17	0.45
1:G:55:PHE:O	1:G:56:HIS:CB	2.65	0.45
1:G:196:ARG:CA	1:G:196:ARG:NH1	2.60	0.45
1:R:179:ALA:HA	1:R:236:THR:O	2.17	0.44
1:G:34:ASP:HB3	1:G:42:MET:HE2	1.97	0.44
1:R:188:ASP:O	1:R:189:SER:CB	2.64	0.44
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:17:VAL:O	1:R:21:ALA:CB	2.63	0.44
1:R:34:ASP:HB3	1:R:42:MET:HE2	1.99	0.44
1:R:55:PHE:CG	1:R:56:HIS:N	2.86	0.44
1:R:42:MET:CE	1:R:75:ILE:HD13	2.46	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:G:191:SER:HG	1:G:192:GLY:N	1.86	0.44
1:R:131:VAL:O	1:R:135:ASN:HB3	2.18	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:R:43:VAL:HG12	1:R:66:LEU:HD11	1.99	0.44
1:G:117:ARG:HA	1:G:144:LYS:O	2.18	0.44
1:R:193:LYS:HE3	1:R:193:LYS:HB2	1.38	0.44
1:R:248:LEU:HG	1:R:248:LEU:H	1.70	0.44
1:R:156:LEU:HD22	1:R:174:MET:HE3	1.99	0.44
1:G:108:GLY:O	1:G:111:LEU:HD11	2.18	0.44
1:G:3:VAL:C	1:G:28:ASP:HB2	2.38	0.44
1:G:170:VAL:O	1:G:171:GLU:O	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:254:TYR:CZ	1:R:300:ILE:CG1	3.01	0.44
1:G:186:THR:C	1:G:187:VAL:CG2	2.85	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:257:ILE:O	1:R:258:LYS:C	2.56	0.44
1:R:22:PHE:HE2	1:R:71:LYS:CD	2.28	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:R:197:GLY:CA	1:R:199:ARG:HB3	2.48	0.43
1:G:166:HIS:HD2	1:G:260:VAL:HG23	1.82	0.43
1:R:15:ARG:C	1:R:18:THR:HG23	2.38	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:G:117:ARG:HG3	1:G:334:GLU:CD	2.26	0.43
1:G:261:VAL:O	1:G:262:LYS:C	2.57	0.43
1:G:298:ALA:CB	1:G:310:VAL:CG1	2.96	0.43
1:R:218:LYS:H	1:R:218:LYS:HG2	1.57	0.43
1:G:191:SER:OG	1:G:192:GLY:O	2.36	0.43
1:R:156:LEU:HA	1:R:156:LEU:HD12	1.88	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:1:GLY:HA3	1:G:28:ASP:HA	1.87	0.43
1:R:13:ILE:HA	1:R:13:ILE:HD13	1.85	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: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:HG13	1:G:59:VAL:O	2.19	0.43
1:R:160:ALA:O	1:R:161:LYS:C	2.55	0.43
1:R:28:ASP:CG	1:R:29:ILE:HG12	2.39	0.43
1:G:135:ASN:O	1:G:138:LYS:CB	2.67	0.43
1:G:2:LYS:C	1:G:28:ASP:CB	2.85	0.43
1:G:98:THR:HG1	1:G:101:PHE:HD2	1.67	0.43
1:G:269:LEU:HB3	1:G:272:ILE:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:102:THR:CG2	1:R:124:SER:HA	2.47	0.43
1:G:43:VAL:HA	1:G:59:VAL:HG22	2.01	0.43
1:R:220:ILE:O	1:R:221:PRO:C	2.55	0.43
1:G:2:LYS:O	1:G:28:ASP:OD1	2.37	0.43
1:G:208:ALA:O	1:G:230:MET:CG	2.56	0.43
1:G:158:PRO:HG2	1:G:292:SER:CB	2.49	0.43
1:G:188:ASP:O	1:G:189:SER:HB3	2.17	0.43
1:R:174:MET:HA	1:R:243:ASP:O	2.19	0.43
1:R:111:LEU:HD21	1:R:116:LYS:CA	2.48	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:269:LEU:HB3	1:G:272:ILE:CD1	2.49	0.42
1:G:193:LYS:HG3	1:G:193:LYS:O	2.19	0.42
1:R:269:LEU:HB3	1:R:272:ILE:O	2.19	0.42
1:G:139:TYR:HB3	1:G:333:LYS:HD3	2.00	0.42
1:G:60:LYS:HD3	1:G:62:GLU:HG3	2.01	0.42
1:G:162:VAL:HB	1:G:163:ILE:CD1	2.49	0.42
1:G:205:LEU:O	1:G:205:LEU:HD22	2.19	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:162:VAL:HG11	1:R:261:VAL:HB	2.01	0.42
1:R:330:MET:O	1:R:334:GLU:CG	2.67	0.42
1:R:141:ASN:O	1:R:142:SER:C	2.54	0.42
1:R:44:TYR:O	1:R:48:TYR:HB2	2.19	0.42
1:G:140:ALA:O	1:G:143:LEU:CB	2.52	0.42
1:G:60:LYS:CG	1:G:61:ALA:N	2.60	0.42
1:R:98:THR:OG1	1:R:101:PHE:HD2	2.02	0.42
1:R:106:LYS:O	1:R:107:ALA:C	2.57	0.42
1:R:3:VAL:N	1:R:27:VAL:CA	2.63	0.42
1:R:2:LYS:HD2	1:R:26:LYS:N	2.32	0.42
1:G:115:ALA:O	1:G:116:LYS:CD	2.64	0.42
1:G:44:TYR:HB3	1:G:45:MET:H	1.68	0.42
1:R:160:ALA:HB1	1:R:223:LEU:HD13	2.00	0.42
1:R:95:VAL:HG11	1:R:327:MET:HE2	2.01	0.42
1:G:190:PRO:O	1:G:191:SER:CB	2.63	0.42
1:R:153:THR:HG23	1:R:215:ALA:HB1	2.00	0.42
1:R:24:SER:HB2	1:R:321:GLU:OE1	2.19	0.42
1:R:241:VAL:HB	1:R:312:TRP:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:317:PHE:HA	1:R:320:SER:HB2	2.02	0.42
1:R:51:THR:HG22	1:R:52:HIS:N	2.34	0.42
1:G:141:ASN:HD22	1:G:333:LYS:CE	2.32	0.42
1:G:16:LEU:O	1:G:17:VAL:C	2.56	0.42
1:G:76:PHE:CB	1:G:85:LYS:HZ3	2.32	0.42
1:G:194:LEU:O	1:G:196:ARG:HG2	2.19	0.42
1:G:162:VAL:HG11	1:G:261:VAL:HA	2.02	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: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:45:MET:HE3	1:G:189:SER:O	2.19	0.42
1:G:141:ASN:HA	1:G:334:GLU:HB3	2.02	0.42
1:G:41:TYR:O	1:G:42:MET:C	2.57	0.42
1:G:196:ARG:CZ	1:G:207:PRO:O	2.68	0.42
1:G:276:THR:C	1:G:278:ASP:H	2.20	0.42
1:R:288:SER:O	1:R:289:ASN:HB2	2.19	0.42
1:R:56:HIS:O	1:R:58:THR:N	2.53	0.42
1:G:126:ASP:O	1:G:127:ALA:HB3	2.12	0.42
1:G:119:VAL:HG21	1:G:326:LEU:HD11	2.02	0.42
1:R:187:VAL:HB	1:R:188:ASP:H	1.72	0.42
1:G:161:LYS:HD3	1:G:165:ASP:OD1	2.20	0.42
1:R:117:ARG:CG	1:R:334:GLU:OE2	2.68	0.42
1:R:228:THR:HG23	1:R:229:GLY:N	2.34	0.42
1:G:203:GLN:HE21	1:G:203:GLN:HB3	1.64	0.42
1:R:137:PHE:HA	1:R:137:PHE:HD1	1.70	0.42
1:R:74:THR:HG23	1:R:75:ILE:N	2.34	0.42
1:R:97:SER:OG	1:R:98:THR:N	2.51	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:168:GLY:HA3	1:R:249:GLU:H	1.85	0.42
1:R:210:THR:CG2	1:R:211:GLY:N	2.82	0.41
1:G:240:SER:O	1:G:313:TYR:N	2.53	0.41
1:G:201:ALA:HB3	1:G:202:ALA:H	1.32	0.41
1:R:16:LEU:HD22	1:R:19:ARG:HG2	2.00	0.41
1:G:135:ASN:O	1:G:138:LYS:HB3	2.20	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:R:308:LYS:HB2	1:R:308:LYS:HE3	1.93	0.41
1:G:187:VAL:HB	1:G:188:ASP:H	1.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2:LYS:CG	1:G:26:LYS:HZ2	2.31	0.41
1:G:156:LEU:HD13	1:G:156:LEU:HA	1.79	0.41
1:R:68:ILE:HG13	1:R:73:ILE:HB	2.02	0.41
1:G:2:LYS:HD2	1:G:25:GLY:O	2.19	0.41
1:R:193:LYS:C	1:R:195:TRP:H	2.21	0.41
1:R:288:SER:O	1:R:289:ASN:CB	2.68	0.41
1:R:98:THR:HG21	1:R:101:PHE:H	1.86	0.41
1:R:66:LEU:HB3	1:R:73:ILE:CG2	2.50	0.41
1:R:86:TRP:HE3	1:R:86:TRP:HA	1.86	0.41
1:G:111:LEU:HG	1:G:111:LEU:H	1.58	0.41
1:G:178:HIS:CE1	1:G:240:SER:HG	2.38	0.41
1:G:266:GLU:HG2	1:G:267:GLY:N	2.35	0.41
1:G:276:THR:OG1	1:G:278:ASP:CG	2.59	0.41
1:R:162:VAL:HG13	1:R:260:VAL:CG2	2.50	0.41
1:R:272:ILE:O	1:R:272:ILE:HD13	2.20	0.41
1:G:127:ALA:HB1	1:G:128:PRO:HD2	2.02	0.41
1:G:141:ASN:N	1:G:141:ASN:HD22	2.02	0.41
1:G:181:THR:CB	2:G:338:SO4:O1	2.68	0.41
1:R:190:PRO:HB2	1:R:191:SER:H	1.76	0.41
1:R:143:LEU:HD23	1:R:145:ILE:O	2.21	0.41
1:R:174:MET:HE3	1:R:212:ALA:CB	2.51	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:R:196:ARG:HD2	1:R:196:ARG:N	2.33	0.41
1:R:297:GLY:O	1:R:300:ILE:HG12	2.10	0.41
1:R:300:ILE:H	1:R:300:ILE:HG13	1.73	0.41
1:R:330:MET:O	1:R:334:GLU:HG3	2.21	0.41
1:G:86:TRP:HE3	1:G:86:TRP:HA	1.85	0.41
1:R:303:ASN:O	1:R:306:PHE:O	2.39	0.41
1:G:46:PHE:HD2	1:G:59:VAL:HG21	1.85	0.41
1:G:5:VAL:O	1:G:30:VAL:CB	2.69	0.41
1:G:295:ASP:OD2	1:G:298:ALA:HB2	2.21	0.41
1:R:205:LEU:CD1	1:R:205:LEU:O	2.61	0.41
1:R:180:ILE:CG2	1:R:235:PRO:O	2.69	0.41
1:R:22:PHE:CZ	1:R:69:ASP:CG	2.94	0.41
1:R:104:MET:O	1:R:105:GLU:C	2.59	0.41
1:R:3:VAL:O	1:R:4:LYS:CG	2.69	0.41
1:G:32:ILE:O	1:G:76:PHE:N	2.38	0.41
1:G:156:LEU:CG	1:G:242:LEU:CD2	2.80	0.41
1:R:221:PRO:O	1:R:224:ASP:CB	2.61	0.41
1:R:217:GLY:O	1:R:220:ILE:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:191:SER:HB2	1:G:195:TRP:O	2.21	0.41
1:R:29:ILE:O	1:R:30:VAL:CG1	2.64	0.41
1:G:129:MET:C	1:G:130:PHE:HD1	2.24	0.41
1:G:129:MET:O	1:G:130:PHE:CD1	2.74	0.41
1:G:129:MET:O	1:G:130:PHE:HD1	2.04	0.41
1:G:240:SER:O	1:G:313:TYR:HB2	2.21	0.41
1:R:254:TYR:HH	1:R:296:ALA:HA	1.86	0.41
1:R:61:ALA:HB2	1:R:66:LEU:CD1	2.45	0.40
1:R:224:ASP:H	1:R:227:LEU:HD11	1.86	0.40
1:R:205:LEU:CD2	1:R:205:LEU:O	2.66	0.40
1:R:239:VAL:HG12	1:R:240:SER:N	2.36	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:G:167:PHE:HE1	1:G:260:VAL:HG11	1.87	0.40
1:R:291:SER:HB2	1:R:322:ARG:HD2	2.02	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: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: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:HA	1:R:273:LEU:HD13	1.67	0.40
1:R:82:GLU:H	1:R:82:GLU:HG2	1.70	0.40
1:G:106:LYS:O	1:G:107:ALA:C	2.57	0.40
1:G:76:PHE:HB3	1:G:85:LYS:HZ3	1.85	0.40
1:G:164:HIS:O	1:G:165:ASP:C	2.58	0.40
1:R:116:LYS:O	1:R:144:LYS:HE2	2.21	0.40
1:G:108:GLY:O	1:G:111:LEU:HG	2.22	0.40
1:G:148:ASN:C	1:G:149:ALA:O	2.59	0.40
1:G:4:LYS:HG3	1:G:92:ALA:HB3	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:112:LYS:CE	1:G:145:ILE:CG2[2_556]	1.89	0.31
1:R:268:PRO:N	1:G:166:HIS:CE1[3_545]	1.89	0.31
1:R:267:GLY:C	1:G:166:HIS:CE1[3_545]	1.92	0.28
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%)		
1	R	332/334 (99%)	205 (62%)	58 (18%)	69 (21%)		
All	All	664/668 (99%)	403 (61%)	126 (19%)	135 (20%)		

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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%)	140 (52%)	127 (48%)	0	0
1	R	267/267 (100%)	143 (54%)	124 (46%)	0	0
All	All	534/534 (100%)	283 (53%)	251 (47%)	0	0

All (251) 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	23	ASN
1	R	24	SER
1	R	26	LYS
1	R	28	ASP
1	R	29	ILE
1	R	30	VAL
1	R	33	ASN
1	R	36	PHE

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Mol	Chain	Res	Type
1	R	39	LEU
1	R	41	TYR
1	R	43	VAL
1	R	47	GLN
1	R	49	ASP
1	R	51	THR
1	R	54	LYS
1	R	59	VAL
1	R	63	ASP
1	R	66	LEU
1	R	69	ASP
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	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	137	PHE
1	R	138	LYS
1	R	141	ASN
1	R	143	LEU
1	R	145	ILE
1	R	146	ILE
1	R	152	THR

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Mol	Chain	Res	Type
1	R	153	THR
1	R	161	LYS
1	R	162	VAL
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	199	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	256	ASP
1	R	261	VAL
1	R	262	LYS
1	R	263	GLU
1	R	265	SER
1	R	266	GLU
1	R	269	LEU

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Mol	Chain	Res	Type
1	R	270	LYS
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	326	LEU
1	R	330	MET
1	R	333	LYS
1	G	4	LYS
1	G	12	ARG
1	G	15	ARG
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	43	VAL
1	G	45	MET
1	G	47	GLN
1	G	50	SER
1	G	51	THR
1	G	55	PHE
1	G	56	HIS

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Mol	Chain	Res	Type
1	G	60	LYS
1	G	62	GLU
1	G	63	ASP
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	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	106	LYS
1	G	110	HIS
1	G	111	LEU
1	G	112	LYS
1	G	116	LYS
1	G	118	ILE
1	G	131	VAL
1	G	132	MET
1	G	134	VAL
1	G	135	ASN
1	G	137	PHE
1	G	141	ASN
1	G	142	SER
1	G	143	LEU
1	G	145	ILE
1	G	146	ILE
1	G	150	SER
1	G	152	THR
1	G	155	CYS
1	G	156	LEU

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Mol	Chain	Res	Type
1	G	159	LEU
1	G	161	LYS
1	G	163	ILE
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	214	LYS
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	255	ASP
1	G	256	ASP
1	G	257	ILE
1	G	258	LYS
1	G	261	VAL
1	G	262	LYS
1	G	266	GLU
1	G	269	LEU

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Mol	Chain	Res	Type
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	303	ASN
1	G	306	PHE
1	G	309	LEU
1	G	314	ASP
1	G	315	ASN
1	G	316	GLU
1	G	317	PHE
1	G	322	ARG
1	G	323	VAL
1	G	326	LEU
1	G	330	MET
1	G	333	LYS
1	G	334	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
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	289	ASN
1	R	303	ASN
1	R	315	ASN
1	R	329	HIS
1	G	33	ASN

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Mol	Chain	Res	Type
1	G	110	HIS
1	G	135	ASN
1	G	141	ASN
1	G	154	ASN
1	G	166	HIS
1	G	289	ASN
1	G	315	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
3	NAD	G	336	-	38,48,48	2.76	10 (26%)	47,73,73	2.68	14 (29%)
2	SO4	G	338	-	4,4,4	0.51	0	6,6,6	0.11	0
2	SO4	G	340	1	4,4,4	0.52	0	6,6,6	0.10	0
3	NAD	R	336	-	38,48,48	1.40	4 (10%)	47,73,73	2.14	8 (17%)
2	SO4	R	338	-	4,4,4	0.51	0	6,6,6	0.11	0
2	SO4	R	340	1	4,4,4	0.52	0	6,6,6	0.10	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	G	336	-	1/1/11/11	0/22/62/62	0/5/5/5
2	SO4	G	338	-	-	0/0/0/0	0/0/0/0
2	SO4	G	340	1	-	0/0/0/0	0/0/0/0
3	NAD	R	336	-	-	0/22/62/62	0/5/5/5
2	SO4	R	338	-	-	0/0/0/0	0/0/0/0
2	SO4	R	340	1	-	0/0/0/0	0/0/0/0

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	336	NAD	C2B-C3B	-7.73	1.32	1.53
3	G	336	NAD	C3B-C4B	-6.08	1.36	1.53
3	G	336	NAD	O2B-C2B	-5.74	1.29	1.43
3	R	336	NAD	C6N-N1N	2.08	1.41	1.35
3	G	336	NAD	O4D-C4D	2.10	1.49	1.45
3	R	336	NAD	C2A-N1A	2.48	1.38	1.33
3	G	336	NAD	C6N-N1N	3.02	1.43	1.35
3	G	336	NAD	O4D-C1D	3.09	1.45	1.41
3	G	336	NAD	C4A-N3A	3.16	1.40	1.35
3	R	336	NAD	O4B-C1B	3.21	1.45	1.41
3	G	336	NAD	C5A-N7A	4.33	1.54	1.39
3	R	336	NAD	C3N-C7N	4.54	1.57	1.50
3	G	336	NAD	C8A-N7A	6.13	1.46	1.34
3	G	336	NAD	C3N-C7N	6.75	1.61	1.50

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	336	NAD	C1B-N9A-C4A	-9.61	112.44	126.94
3	G	336	NAD	C5N-C4N-C3N	-6.28	112.44	120.33
3	R	336	NAD	C5N-C4N-C3N	-5.94	112.86	120.33
3	G	336	NAD	C4A-C5A-N7A	-4.23	105.59	109.48
3	G	336	NAD	C2B-C1B-N9A	-3.91	108.33	114.29
3	G	336	NAD	C2N-C3N-C7N	-3.67	108.66	119.31
3	G	336	NAD	C2B-C3B-C4B	-2.99	96.47	102.61
3	R	336	NAD	C5N-C6N-N1N	-2.66	115.86	120.47
3	R	336	NAD	C2B-C3B-C4B	-2.14	98.21	102.61
3	G	336	NAD	C5N-C6N-N1N	-2.00	117.01	120.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	336	NAD	O2A-PA-O3	2.37	115.85	105.09
3	R	336	NAD	C4B-O4B-C1B	2.43	112.38	109.72
3	G	336	NAD	C4N-C3N-C7N	2.52	127.73	121.09
3	G	336	NAD	O4D-C1D-N1N	3.10	111.54	108.13
3	G	336	NAD	C4D-O4D-C1D	3.88	113.98	109.72
3	G	336	NAD	O4B-C1B-N9A	3.96	116.39	108.10
3	G	336	NAD	C2N-C3N-C4N	4.14	122.90	118.29
3	R	336	NAD	C2N-C3N-C4N	4.23	123.00	118.29
3	R	336	NAD	O4B-C1B-N9A	5.47	119.55	108.10
3	R	336	NAD	C6N-C5N-C4N	6.05	128.59	119.44
3	R	336	NAD	C1B-N9A-C4A	6.31	136.46	126.94
3	G	336	NAD	C6N-C5N-C4N	6.49	129.25	119.44

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	G	336	NAD	C2B

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	336	NAD	14	0
2	G	338	SO4	4	0
2	G	340	SO4	2	0
3	R	336	NAD	8	0
2	R	338	SO4	2	0
2	R	340	SO4	1	0

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 will therefore be empty.

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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