



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:30 AM GMT

PDB ID : 3B1K  
Title : Crystal structure of Glyceraldehyde-3-Phosphate Dehydrogenase complexed with CP12 in the absence of copper from *Synechococcus elongatus*  
Authors : Matsumura, H.; Kai, A.; Inoue, T.  
Deposited on : 2011-07-04  
Resolution : 3.30 Å(reported)

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

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

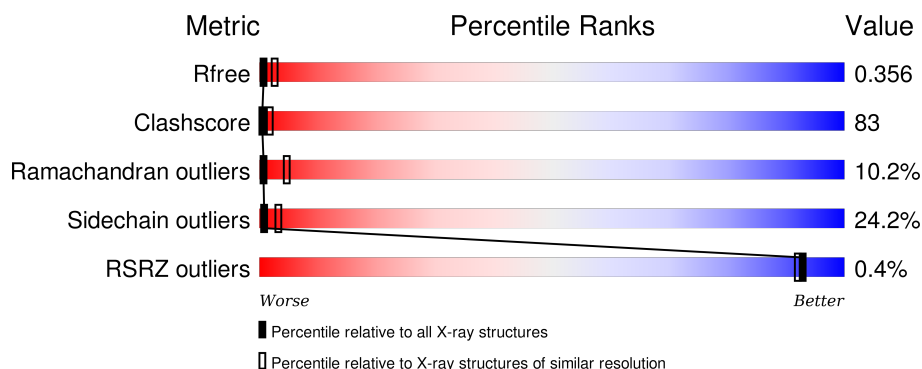
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

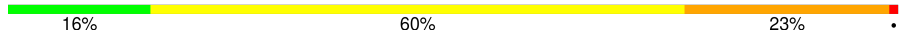
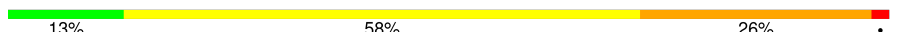
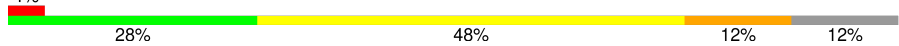
The reported resolution of this entry is 3.30 Å.

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



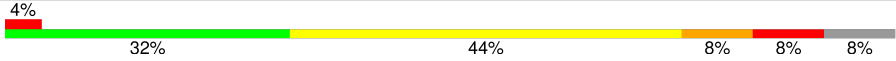
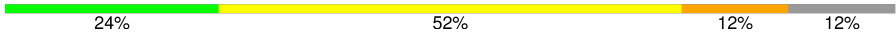

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	339	
1	B	339	
1	G	339	
1	H	339	
2	C	25	

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Mol	Chain	Length	Quality of chain
2	D	25	
2	I	25	
2	J	25	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAD	G	340	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11278 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 Glyceraldehyde 3-phosphate dehydrogenase (NADP+).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2596	1633	455	499	9			
1	B	338	Total	C	N	O	S	0	0	0
			2596	1633	455	499	9			
1	G	338	Total	C	N	O	S	0	0	0
			2596	1633	455	499	9			
1	H	338	Total	C	N	O	S	0	0	0
			2596	1633	455	499	9			

- Molecule 2 is a protein called CP12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	22	Total	C	N	O	S	0	0	0
			175	110	23	40	2			
2	D	23	Total	C	N	O	S	0	0	0
			182	114	24	42	2			
2	I	22	Total	C	N	O	S	0	0	0
			175	110	23	40	2			
2	J	23	Total	C	N	O	S	0	0	0
			182	114	24	42	2			

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	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	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

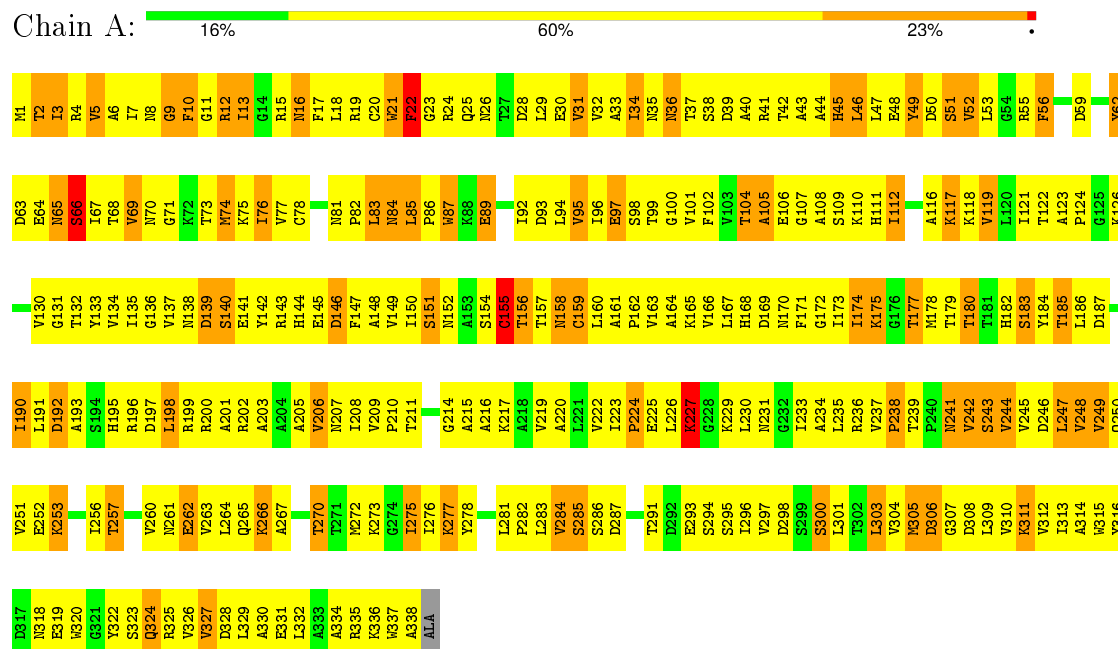
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	4	Total	O	0	0
			4	4		

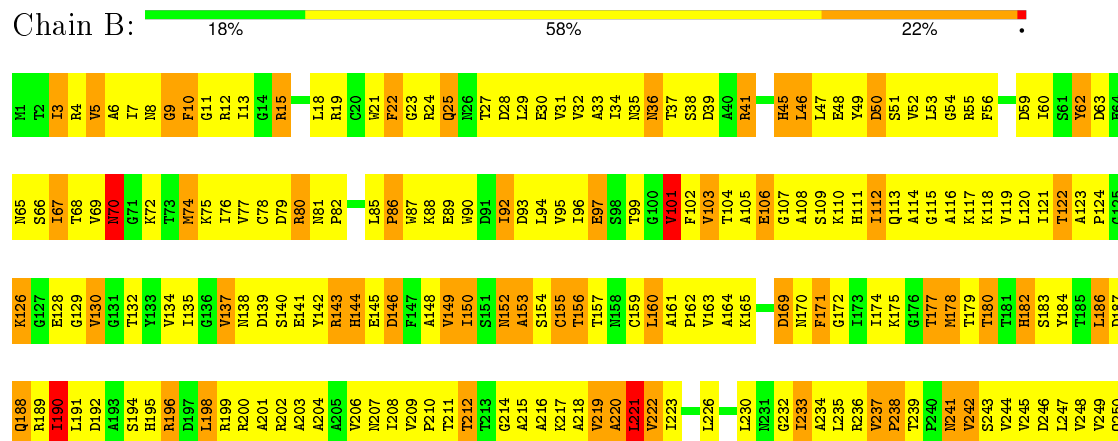
### 3 Residue-property plots

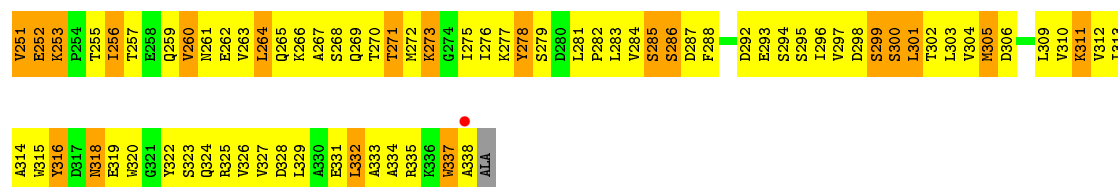
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

- Molecule 1: Glyceraldehyde 3-phosphate dehydrogenase (NADP+)



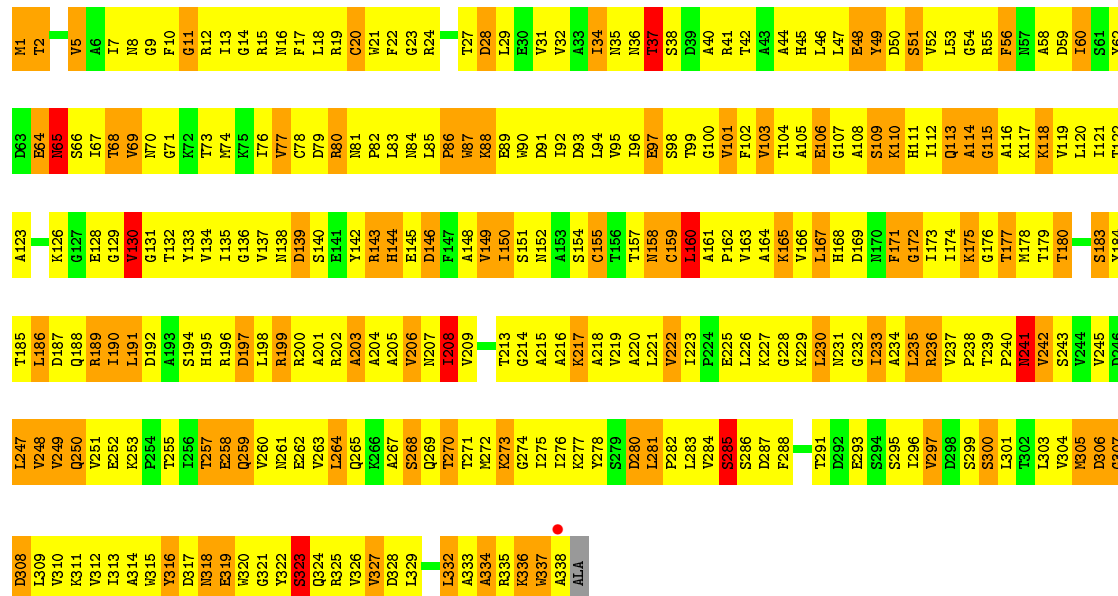
- Molecule 1: Glyceraldehyde 3-phosphate dehydrogenase (NADP+)





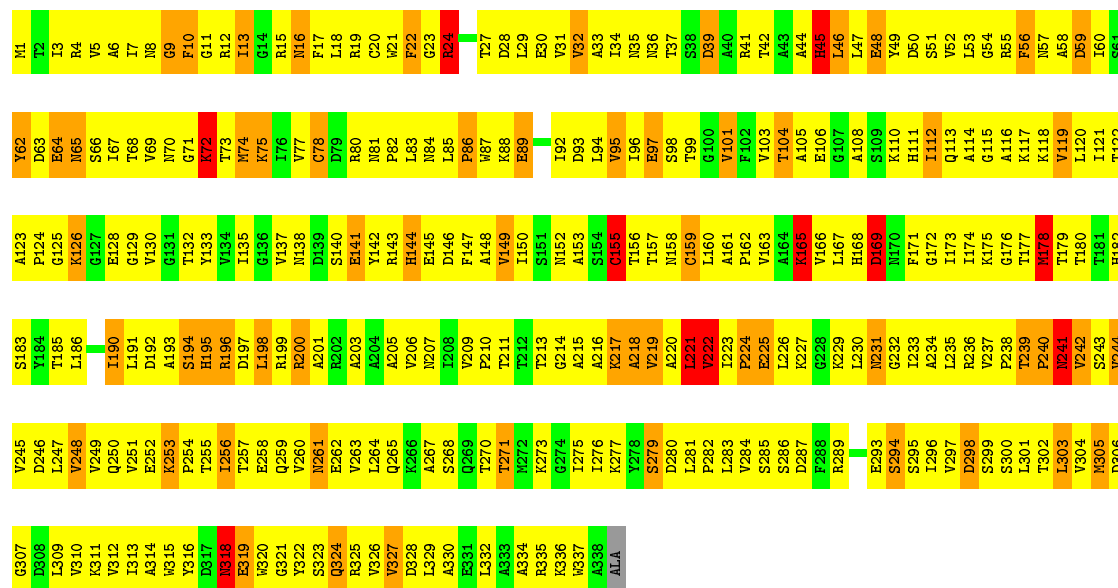
• Molecule 1: Glyceraldehyde 3-phosphate dehydrogenase (NADP+)

Chain G: 13% 58% 26%

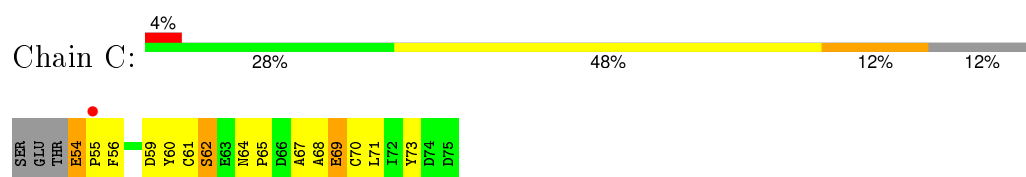


• Molecule 1: Glyceraldehyde 3-phosphate dehydrogenase (NADP+)

Chain H: 14% 65% 17%



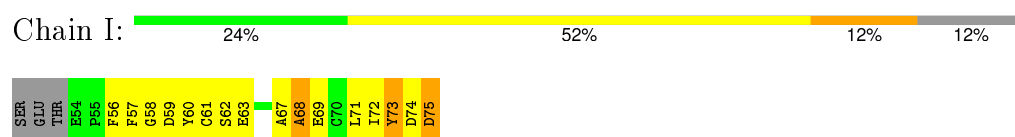
• Molecule 2: CP12



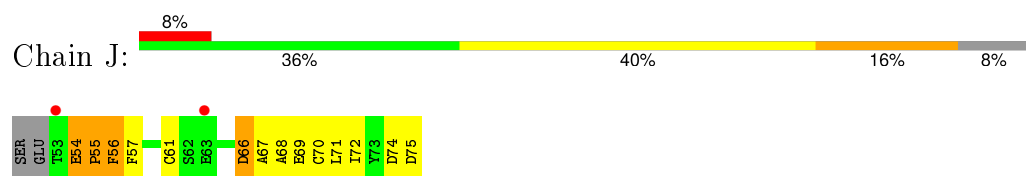
• Molecule 2: CP12



• Molecule 2: CP12



• Molecule 2: CP12





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.04Å 146.89Å 161.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.06 – 3.30 26.06 – 3.30	Depositor EDS
% Data completeness (in resolution range)	88.9 (26.06-3.30) 88.7 (26.06-3.30)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.46 (at 3.31Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, $R_{free}$	0.252 , 0.363 0.248 , 0.356	Depositor DCC
$R_{free}$ test set	1166 reflections (5.38%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.9	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 55.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.34$ , $\langle L^2 \rangle = 0.17$	Xtriage
Outliers	4 of 22927 reflections (0.017%)	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	11278	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 63.49 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.5976e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	A	0.51	0/2639	0.75	0/3590
1	B	0.51	0/2639	0.75	2/3590 (0.1%)
1	G	0.51	0/2639	0.74	1/3590 (0.0%)
1	H	0.49	0/2639	0.73	0/3590
2	C	0.50	0/180	0.63	0/245
2	D	0.46	0/187	0.60	0/255
2	I	0.72	0/180	0.67	0/245
2	J	0.41	0/187	0.64	0/255
All	All	0.51	0/11290	0.74	3/15360 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	190	ILE	CB-CA-C	-6.11	99.38	111.60
1	B	264	LEU	CA-CB-CG	-5.98	101.54	115.30
1	G	206	VAL	CB-CA-C	-5.71	100.55	111.40

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	A	2596	0	2620	503	0
1	B	2596	0	2620	427	0
1	G	2596	0	2620	488	0
1	H	2596	0	2620	485	0
2	C	175	0	137	19	0
2	D	182	0	144	30	0
2	I	175	0	137	23	0
2	J	182	0	144	25	0
3	A	44	0	26	18	0
3	B	44	0	26	20	0
3	G	44	0	26	30	0
3	H	44	0	26	17	0
4	H	4	0	0	0	0
All	All	11278	0	11146	1854	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 83.

All (1854) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:247:LEU:HD12	1:G:248:VAL:H	1.10	1.16
1:B:305:MET:HB3	1:H:175:LYS:HD2	1.22	1.15
1:G:144:HIS:CD2	1:G:337:TRP:HA	1.84	1.12
1:A:31:VAL:HG12	1:A:74:MET:HG2	1.23	1.11
1:A:305:MET:HE2	1:G:231:ASN:H	0.97	1.10
1:B:306:ASP:HB2	1:H:175:LYS:HE2	1.29	1.10
1:B:15:ARG:HH11	1:B:15:ARG:HG3	1.16	1.10
1:A:36:ASN:HD22	1:A:37:THR:N	1.51	1.08
1:A:198:LEU:HD22	1:A:198:LEU:H	1.19	1.07
1:H:20:CYS:HB3	1:H:327:VAL:HG21	1.34	1.07
1:B:36:ASN:HD22	1:B:37:THR:N	1.51	1.06
1:A:233:ILE:HD13	1:G:301:LEU:HD22	1.34	1.05
1:G:83:LEU:HA	1:G:114:ALA:HB2	1.41	1.03
1:H:324:GLN:HA	1:H:324:GLN:HE21	1.17	1.02
1:B:36:ASN:ND2	1:B:37:THR:H	1.57	1.02
1:G:155:CYS:H	3:G:340:NAD:H5N	1.25	1.00
1:G:104:THR:HB	1:G:107:GLY:H	1.19	1.00
1:A:16:ASN:ND2	1:A:53:LEU:HD11	1.77	0.98
1:B:284:VAL:HG11	1:H:209:VAL:HG13	1.42	0.98
1:A:283:LEU:H	1:G:199:ARG:HH21	1.08	0.97
1:B:155:CYS:HB3	3:B:340:NAD:H4N	1.46	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:167:LEU:HB3	1:G:173:ILE:HD11	1.46	0.97
1:B:190:ILE:HD12	1:B:190:ILE:H	1.30	0.96
1:A:305:MET:HE2	1:G:231:ASN:N	1.81	0.96
1:H:82:PRO:HA	1:H:85:LEU:HD12	1.45	0.96
1:G:118:LYS:HE2	1:G:148:ALA:HA	1.48	0.96
1:G:31:VAL:HG12	1:G:74:MET:SD	2.06	0.95
2:J:54:GLU:N	2:J:55:PRO:HD3	1.82	0.95
1:H:118:LYS:HG3	1:H:148:ALA:HA	1.48	0.94
2:I:68:ALA:HA	2:I:71:LEU:HD11	1.49	0.94
1:G:267:ALA:HA	1:G:270:THR:OG1	1.66	0.94
1:G:93:ASP:HB3	1:G:337:TRP:CZ2	2.03	0.94
1:B:306:ASP:CB	1:H:175:LYS:HE2	1.98	0.93
1:B:94:LEU:HD12	1:B:118:LYS:O	1.69	0.92
1:A:155:CYS:CB	3:A:340:NAD:H5N	1.99	0.92
1:G:67:ILE:HG12	1:G:76:ILE:HD11	1.48	0.92
1:H:48:GLU:HG3	1:H:60:ILE:HD12	1.48	0.91
1:A:155:CYS:HB3	3:A:340:NAD:H5N	1.53	0.90
1:A:324:GLN:HE21	1:A:324:GLN:HA	1.37	0.90
1:A:190:ILE:CD1	1:H:186:LEU:HD23	2.01	0.90
1:H:332:LEU:HD23	1:H:335:ARG:HH11	1.35	0.90
1:H:245:VAL:HG12	1:H:314:ALA:HB3	1.52	0.90
1:A:305:MET:CE	1:G:231:ASN:H	1.85	0.89
1:H:298:ASP:HB3	1:H:301:LEU:CD1	2.02	0.89
1:H:6:ALA:HB3	1:H:95:VAL:HG13	1.52	0.89
1:B:52:VAL:HG11	1:B:241:ASN:OD1	1.73	0.89
1:G:155:CYS:HB3	3:G:340:NAD:H4N	1.55	0.89
1:A:291:THR:HG21	1:A:296:ILE:HD11	1.52	0.88
1:B:89:GLU:O	1:B:90:TRP:HD1	1.56	0.88
1:A:283:LEU:H	1:G:199:ARG:NH2	1.72	0.88
1:B:117:LYS:HD2	1:B:337:TRP:CZ2	2.08	0.87
1:H:118:LYS:HA	1:H:148:ALA:HB1	1.55	0.87
1:H:216:ALA:HB1	1:H:231:ASN:HA	1.55	0.87
1:B:296:ILE:HB	1:B:315:TRP:HB2	1.56	0.87
1:A:223:ILE:HB	1:A:226:LEU:HD12	1.56	0.87
1:G:187:ASP:HB2	2:I:71:LEU:O	1.74	0.86
1:H:325:ARG:NE	1:H:325:ARG:HA	1.88	0.86
1:H:99:THR:OG1	1:H:101:VAL:HG13	1.75	0.86
1:B:18:LEU:O	1:B:22:PHE:HB2	1.74	0.86
1:A:156:THR:HA	1:A:316:TYR:CE2	2.11	0.86
1:G:264:LEU:O	1:G:268:SER:HB3	1.76	0.86
1:B:143:ARG:HB3	1:B:146:ASP:HB2	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:247:LEU:HD12	1:G:248:VAL:N	1.90	0.86
1:G:161:ALA:HB3	1:G:162:PRO:HD3	1.57	0.86
1:B:13:ILE:HG13	3:B:340:NAD:O4D	1.75	0.86
1:H:9:GLY:HA3	1:H:98:SER:C	1.96	0.85
1:A:135:ILE:HG13	1:A:328:ASP:HB3	1.56	0.85
1:B:198:LEU:H	1:B:198:LEU:HD22	1.41	0.85
1:A:168:HIS:CE1	1:A:173:ILE:H	1.94	0.85
1:G:143:ARG:CZ	1:G:145:GLU:HB2	2.07	0.85
1:B:206:VAL:HG11	1:G:240:PRO:HG3	1.57	0.84
1:A:190:ILE:HD13	1:A:190:ILE:H	1.43	0.84
1:H:160:LEU:HD23	1:H:219:VAL:HG21	1.57	0.84
1:H:214:GLY:C	1:H:216:ALA:H	1.79	0.84
1:A:190:ILE:HD11	1:H:186:LEU:HD23	1.57	0.84
1:A:175:LYS:HG2	1:A:250:GLN:HB3	1.59	0.84
1:A:281:LEU:HB3	1:A:283:LEU:HD21	1.57	0.84
1:G:159:CYS:SG	1:G:316:TYR:CD1	2.71	0.84
1:A:175:LYS:HG3	1:G:309:LEU:HD22	1.59	0.84
1:B:117:LYS:HD2	1:B:337:TRP:HZ2	1.42	0.84
1:B:180:THR:HG23	1:B:234:ALA:HB2	1.59	0.84
1:H:240:PRO:O	1:H:241:ASN:HB2	1.78	0.84
1:A:247:LEU:HD12	1:A:248:VAL:N	1.91	0.84
1:G:264:LEU:HD12	1:G:297:VAL:HG11	1.58	0.84
1:B:244:VAL:HG23	1:B:315:TRP:HA	1.59	0.84
1:B:11:GLY:HA3	3:B:340:NAD:O5B	1.78	0.84
1:B:143:ARG:HD3	1:B:146:ASP:OD1	1.77	0.84
1:H:67:ILE:O	1:H:73:THR:HG23	1.79	0.83
1:H:190:ILE:HD12	1:H:190:ILE:N	1.94	0.83
1:G:81:ASN:ND2	1:G:83:LEU:HD13	1.93	0.83
1:A:36:ASN:HD22	1:A:37:THR:H	1.23	0.83
1:H:304:VAL:HG12	1:H:305:MET:H	1.44	0.83
1:G:168:HIS:HA	1:G:172:GLY:HA2	1.58	0.83
1:A:5:VAL:HG23	1:A:94:LEU:HB3	1.61	0.83
1:A:35:ASN:HB2	1:A:77:VAL:HB	1.59	0.83
1:G:285:SER:O	1:G:287:ASP:N	2.12	0.83
1:G:142:TYR:CD2	1:G:332:LEU:HD13	2.14	0.83
1:B:285:SER:O	1:B:287:ASP:N	2.12	0.83
1:B:180:THR:HB	1:B:245:VAL:HG12	1.61	0.82
1:B:331:GLU:O	1:B:335:ARG:HG3	1.79	0.82
1:A:7:ILE:HB	1:A:34:ILE:HG12	1.62	0.82
1:B:186:LEU:HG	1:G:190:ILE:HD13	1.61	0.82
1:H:58:ALA:HB1	1:H:70:ASN:OD1	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:159:CYS:HG	1:G:316:TYR:HD1	1.24	0.82
1:A:168:HIS:CE1	1:A:173:ILE:N	2.48	0.82
1:B:191:LEU:HA	1:B:203:ALA:HB2	1.60	0.82
1:G:11:GLY:HA3	3:G:340:NAD:H4B	1.61	0.82
2:J:57:PHE:O	2:J:61:CYS:HB2	1.78	0.82
1:A:165:LYS:HG2	1:A:272:MET:HE1	1.62	0.82
1:G:55:ARG:HG2	1:G:56:PHE:N	1.94	0.81
1:G:50:ASP:OD1	1:G:52:VAL:N	2.13	0.81
1:B:10:PHE:CZ	1:B:15:ARG:HG2	2.15	0.81
1:B:15:ARG:CG	1:B:15:ARG:HH11	1.93	0.81
1:B:155:CYS:CB	3:B:340:NAD:H4N	2.10	0.81
1:B:118:LYS:HD3	1:B:148:ALA:HA	1.60	0.81
1:G:104:THR:HB	1:G:107:GLY:N	1.95	0.81
1:A:191:LEU:HB2	1:H:186:LEU:HD11	1.60	0.81
1:H:298:ASP:HB3	1:H:301:LEU:HD12	1.60	0.81
1:A:210:PRO:HB3	1:G:301:LEU:HD11	1.63	0.80
1:B:156:THR:HG21	1:B:180:THR:HG21	1.61	0.80
1:G:41:ARG:O	1:G:44:ALA:HB3	1.81	0.80
1:B:284:VAL:CG1	1:H:209:VAL:HG13	2.12	0.80
3:A:340:NAD:H3D	2:C:73:TYR:CD1	2.17	0.80
1:H:178:MET:HA	1:H:246:ASP:O	1.82	0.80
1:A:19:ARG:HG2	1:A:56:PHE:CE2	2.16	0.80
1:A:198:LEU:N	1:A:198:LEU:HD22	1.96	0.80
1:B:87:TRP:HB2	1:B:114:ALA:O	1.82	0.80
1:A:12:ARG:HD2	1:A:15:ARG:NH2	1.96	0.79
1:B:174:ILE:HD12	1:B:250:GLN:NE2	1.96	0.79
1:A:325:ARG:HA	1:A:325:ARG:NE	1.98	0.79
1:A:97:GLU:HB3	1:A:121:ILE:HA	1.63	0.79
1:B:272:MET:HB3	1:B:275:ILE:HB	1.64	0.79
1:A:183:SER:HB2	1:A:242:VAL:O	1.83	0.79
1:A:36:ASN:ND2	1:A:37:THR:N	2.31	0.79
1:A:174:ILE:HG22	1:A:175:LYS:HG2	1.65	0.79
1:A:182:HIS:HA	1:A:243:SER:HB3	1.65	0.79
1:G:83:LEU:HD12	1:G:83:LEU:H	1.48	0.79
1:A:39:ASP:HB3	2:J:56:PHE:HB3	1.65	0.78
1:A:10:PHE:HD2	1:A:43:ALA:HB1	1.47	0.78
1:H:20:CYS:CB	1:H:327:VAL:HG21	2.12	0.78
1:H:255:THR:OG1	1:H:259:GLN:HB3	1.84	0.78
1:H:171:PHE:CE1	1:H:255:THR:HB	2.19	0.78
1:G:178:MET:HB3	1:G:232:GLY:HA3	1.66	0.78
1:B:190:ILE:N	1:B:190:ILE:HD12	1.98	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:THR:OG1	1:B:304:VAL:HG23	1.83	0.78
1:A:39:ASP:HB3	2:J:56:PHE:CB	2.14	0.78
1:H:45:HIS:O	1:H:48:GLU:N	2.17	0.78
1:B:29:LEU:HD11	1:B:331:GLU:HG2	1.65	0.78
1:H:276:ILE:C	1:H:293:GLU:HG2	2.04	0.78
1:G:160:LEU:HD21	1:G:178:MET:HE3	1.65	0.78
1:B:284:VAL:HG12	1:H:209:VAL:HA	1.64	0.78
1:G:83:LEU:CA	1:G:114:ALA:HB2	2.13	0.78
1:B:175:LYS:NZ	1:H:306:ASP:OD1	2.17	0.77
1:A:172:GLY:O	1:A:251:VAL:HG13	1.85	0.77
1:H:214:GLY:HA2	1:H:217:LYS:NZ	1.98	0.77
1:G:167:LEU:CB	1:G:173:ILE:HD11	2.15	0.77
1:H:214:GLY:O	1:H:216:ALA:N	2.17	0.77
1:H:68:THR:HG23	1:H:73:THR:OG1	1.84	0.77
1:A:12:ARG:HH11	1:A:15:ARG:HH21	1.33	0.77
1:A:248:VAL:HG13	1:A:311:LYS:HG3	1.67	0.77
1:A:135:ILE:HA	1:A:139:ASP:HB3	1.67	0.77
1:H:50:ASP:HB3	1:H:54:GLY:H	1.50	0.77
1:H:226:LEU:HA	1:H:229:LYS:HD2	1.65	0.77
1:G:318:ASN:HD22	3:G:340:NAD:H72N	1.32	0.77
2:I:67:ALA:O	2:I:69:GLU:N	2.18	0.76
1:A:198:LEU:CD2	1:A:198:LEU:H	1.94	0.76
1:H:6:ALA:HB2	1:H:92:ILE:HG21	1.67	0.76
1:G:288:PHE:CE1	1:G:315:TRP:CD2	2.74	0.76
1:B:208:ILE:HG13	1:H:285:SER:HB3	1.68	0.76
1:B:296:ILE:O	1:B:314:ALA:HA	1.86	0.76
1:H:17:PHE:O	1:H:20:CYS:HB2	1.84	0.76
1:B:15:ARG:NH1	1:B:15:ARG:HG3	1.94	0.76
1:B:206:VAL:HG23	1:B:207:ASN:ND2	2.01	0.76
1:H:159:CYS:SG	1:H:316:TYR:HD1	2.08	0.76
1:B:263:VAL:O	1:B:266:LYS:HB2	1.86	0.76
1:G:245:VAL:HG23	1:G:316:TYR:HE1	1.49	0.76
1:H:152:ASN:ND2	1:H:326:VAL:HG22	2.00	0.76
1:G:190:ILE:H	1:G:190:ILE:HD12	1.50	0.76
1:G:195:HIS:HB3	1:G:201:ALA:HB2	1.68	0.75
1:H:159:CYS:HB2	1:H:316:TYR:CD1	2.21	0.75
1:G:177:THR:HG22	1:G:248:VAL:HB	1.69	0.75
1:G:261:ASN:HB3	1:G:278:TYR:OH	1.87	0.75
1:B:288:PHE:CE2	1:B:296:ILE:HG21	2.21	0.75
1:H:324:GLN:CA	1:H:324:GLN:HE21	1.97	0.75
1:H:18:LEU:HD23	1:H:47:LEU:HD13	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:PRO:C	1:A:283:LEU:HD23	2.07	0.75
1:G:155:CYS:CB	3:G:340:NAD:H4N	2.17	0.75
1:A:327:VAL:O	1:A:331:GLU:HG2	1.87	0.75
2:D:56:PHE:O	2:D:58:GLY:N	2.20	0.75
1:H:217:LYS:H	1:H:217:LYS:HD2	1.52	0.75
1:G:159:CYS:SG	1:G:316:TYR:HD1	2.10	0.74
1:G:318:ASN:HB2	3:G:340:NAD:H71N	1.52	0.74
1:A:10:PHE:CD2	1:A:43:ALA:HB1	2.22	0.74
1:B:322:TYR:O	1:B:326:VAL:HG23	1.88	0.74
1:B:22:PHE:CZ	1:B:69:VAL:HB	2.22	0.74
1:H:304:VAL:HG12	1:H:305:MET:N	2.02	0.74
1:H:88:LYS:HB2	1:H:115:GLY:HA3	1.70	0.74
1:H:161:ALA:HB3	1:H:162:PRO:HD3	1.69	0.74
1:B:172:GLY:O	1:B:251:VAL:HA	1.86	0.74
1:A:165:LYS:HG2	1:A:272:MET:CE	2.17	0.74
1:B:242:VAL:H	1:B:318:ASN:ND2	1.86	0.74
1:H:183:SER:HB3	1:H:239:THR:HB	1.70	0.74
1:A:196:ARG:HD2	2:C:70:CYS:HA	1.68	0.74
1:H:118:LYS:HE3	1:H:147:PHE:O	1.88	0.73
1:B:271:THR:HG23	1:B:272:MET:HG2	1.70	0.73
1:G:89:GLU:O	1:G:90:TRP:HD1	1.72	0.73
1:H:217:LYS:N	1:H:217:LYS:HD2	2.03	0.73
1:G:190:ILE:HD12	1:G:190:ILE:N	2.04	0.73
1:H:245:VAL:CG1	1:H:314:ALA:HB3	2.18	0.73
1:B:118:LYS:HG3	1:B:148:ALA:O	1.88	0.73
1:G:19:ARG:NH1	1:G:56:PHE:HB2	2.02	0.73
1:B:41:ARG:HA	1:B:62:TYR:CE2	2.24	0.73
1:A:186:LEU:HD11	1:H:191:LEU:HB2	1.70	0.73
1:B:120:LEU:HD12	1:B:121:ILE:H	1.52	0.73
1:A:312:VAL:HG12	1:A:313:ILE:N	2.03	0.73
1:G:155:CYS:SG	3:G:340:NAD:C4N	2.77	0.73
1:B:11:GLY:CA	3:B:340:NAD:O5B	2.37	0.73
1:B:298:ASP:OD2	1:B:301:LEU:HG	1.89	0.73
1:B:242:VAL:H	1:B:318:ASN:HD21	1.35	0.73
1:G:155:CYS:SG	3:G:340:NAD:H4N	2.29	0.73
1:H:180:THR:HG22	1:H:233:ILE:O	1.89	0.73
1:G:95:VAL:HG12	1:G:119:VAL:HG23	1.71	0.73
1:A:155:CYS:HB3	3:A:340:NAD:C5N	2.19	0.72
1:A:247:LEU:HD11	1:A:249:VAL:HG13	1.71	0.72
1:B:10:PHE:CE1	1:B:15:ARG:HG2	2.24	0.72
1:B:32:VAL:O	1:B:74:MET:HA	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ASN:ND2	1:A:37:THR:H	1.85	0.72
1:A:52:VAL:HG21	1:A:241:ASN:HB2	1.71	0.72
1:A:144:HIS:CD2	1:A:337:TRP:HA	2.23	0.72
1:B:155:CYS:SG	3:B:340:NAD:H4N	2.30	0.72
1:G:207:ASN:O	1:G:209:VAL:HG23	1.90	0.72
1:A:284:VAL:HB	1:G:207:ASN:OD1	1.89	0.72
1:G:322:TYR:C	1:G:324:GLN:H	1.93	0.72
1:G:48:GLU:HB3	1:G:49:TYR:CD2	2.25	0.72
1:A:322:TYR:O	1:A:325:ARG:N	2.23	0.72
1:G:283:LEU:HD22	1:G:287:ASP:OD2	1.90	0.71
1:B:311:LYS:HE3	1:H:179:THR:OG1	1.90	0.71
1:A:12:ARG:HB2	3:A:340:NAD:O2N	1.90	0.71
2:J:54:GLU:N	2:J:55:PRO:CD	2.53	0.71
1:H:195:HIS:CE1	1:H:197:ASP:H	2.07	0.71
1:B:305:MET:HB3	1:H:175:LYS:CD	2.12	0.71
1:A:246:ASP:HA	1:A:313:ILE:CD1	2.20	0.71
1:A:260:VAL:O	1:A:263:VAL:HG12	1.90	0.71
1:G:16:ASN:HB3	1:G:323:SER:OG	1.90	0.71
1:A:186:LEU:HG	1:H:190:ILE:HD13	1.72	0.71
1:B:174:ILE:HD12	1:B:250:GLN:CD	2.11	0.71
1:G:52:VAL:HG11	1:G:241:ASN:OD1	1.90	0.71
1:G:195:HIS:CE1	1:G:200:ARG:HB2	2.25	0.71
1:A:266:LYS:O	1:A:270:THR:N	2.20	0.71
1:B:180:THR:HG23	1:B:234:ALA:CB	2.19	0.71
1:A:18:LEU:HD23	1:A:47:LEU:HD21	1.71	0.71
1:B:198:LEU:HB2	1:H:282:PRO:HB2	1.73	0.71
1:A:152:ASN:HD22	1:A:326:VAL:CG2	2.04	0.71
1:G:83:LEU:HD11	1:G:110:LYS:HD3	1.72	0.71
1:G:10:PHE:CE1	1:G:15:ARG:HG2	2.26	0.71
1:A:277:LYS:HB3	1:A:296:ILE:HG13	1.73	0.71
1:A:7:ILE:HD12	1:A:34:ILE:HD11	1.72	0.71
1:B:245:VAL:CG2	1:B:314:ALA:HB3	2.20	0.70
1:A:242:VAL:H	1:A:318:ASN:ND2	1.89	0.70
1:H:316:TYR:CE2	1:H:318:ASN:HB3	2.25	0.70
1:A:31:VAL:CG1	1:A:74:MET:HG2	2.14	0.70
1:B:82:PRO:O	1:B:85:LEU:HB2	1.91	0.70
1:G:296:ILE:HD12	1:G:316:TYR:HA	1.73	0.70
1:A:284:VAL:O	1:A:287:ASP:HB2	1.89	0.70
1:B:22:PHE:CE2	1:B:69:VAL:HB	2.25	0.70
1:B:124:PRO:HG2	2:D:74:ASP:HB3	1.73	0.70
1:H:87:TRP:HE1	1:H:111:HIS:HD1	1.38	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:VAL:HG12	1:A:243:SER:N	2.05	0.70
1:B:250:GLN:O	1:B:251:VAL:HG23	1.90	0.70
1:H:11:GLY:HA3	3:H:340:NAD:H4B	1.74	0.70
3:B:340:NAD:H2D	2:D:73:TYR:CD2	2.27	0.70
1:B:182:HIS:HA	1:B:243:SER:HB3	1.72	0.70
1:A:191:LEU:HB2	1:H:186:LEU:CD1	2.20	0.70
2:I:67:ALA:O	2:I:71:LEU:HD21	1.92	0.70
1:A:51:SER:OG	1:H:192:ASP:OD1	2.09	0.70
1:G:216:ALA:C	1:G:218:ALA:H	1.93	0.70
1:A:158:ASN:ND2	1:A:325:ARG:HG3	2.06	0.69
1:G:152:ASN:HB3	1:G:322:TYR:OH	1.92	0.69
1:G:265:GLN:HA	1:G:268:SER:HB3	1.74	0.69
1:G:55:ARG:HG2	1:G:56:PHE:H	1.58	0.69
1:H:158:ASN:O	1:H:162:PRO:HD2	1.92	0.69
1:A:67:ILE:O	1:A:73:THR:HG23	1.93	0.69
1:H:241:ASN:ND2	1:H:242:VAL:H	1.91	0.69
1:A:134:VAL:O	1:A:137:VAL:HB	1.92	0.69
1:H:318:ASN:HD22	1:H:318:ASN:H	1.38	0.69
1:H:324:GLN:HA	1:H:324:GLN:NE2	2.00	0.69
1:A:282:PRO:HA	1:G:199:ARG:CZ	2.23	0.69
1:H:104:THR:OG1	1:H:106:GLU:HB2	1.93	0.69
1:H:190:ILE:HD12	1:H:190:ILE:H	1.57	0.69
1:A:45:HIS:CG	1:A:45:HIS:O	2.46	0.69
1:A:40:ALA:HB2	1:A:76:ILE:HG13	1.75	0.69
1:G:16:ASN:O	1:G:20:CYS:HB2	1.92	0.69
1:H:118:LYS:HG3	1:H:148:ALA:CA	2.21	0.69
1:B:112:ILE:HG23	1:B:116:ALA:O	1.92	0.69
1:B:199:ARG:O	1:B:202:ARG:HG2	1.94	0.69
1:G:241:ASN:HD22	1:G:242:VAL:H	1.39	0.69
1:H:183:SER:HB2	1:H:239:THR:O	1.93	0.69
1:A:283:LEU:N	1:A:283:LEU:HD23	2.07	0.69
1:B:89:GLU:O	1:B:90:TRP:CD1	2.45	0.69
1:G:312:VAL:C	1:G:313:ILE:HD13	2.12	0.69
1:H:19:ARG:NH1	1:H:47:LEU:O	2.26	0.68
1:B:32:VAL:C	1:B:74:MET:HB3	2.13	0.68
1:G:215:ALA:O	1:G:218:ALA:HB3	1.92	0.68
1:A:146:ASP:HB3	1:A:147:PHE:HD1	1.57	0.68
1:A:264:LEU:HD13	1:A:297:VAL:HG11	1.75	0.68
1:H:303:LEU:HD22	1:H:311:LYS:HB3	1.76	0.68
1:A:209:VAL:HG22	1:G:284:VAL:HG11	1.76	0.68
1:H:255:THR:O	1:H:307:GLY:HA2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:205:ALA:O	1:G:238:PRO:HB3	1.93	0.68
1:H:253:LYS:HE3	1:H:253:LYS:C	2.12	0.68
1:B:190:ILE:CD1	1:B:190:ILE:H	1.93	0.68
1:A:156:THR:HG23	1:A:316:TYR:OH	1.93	0.68
1:A:199:ARG:HB3	1:A:209:VAL:CG1	2.23	0.68
1:G:178:MET:HB3	1:G:232:GLY:CA	2.23	0.68
1:G:97:GLU:HA	1:G:97:GLU:OE2	1.94	0.68
1:A:246:ASP:HA	1:A:313:ILE:HD13	1.76	0.68
2:C:54:GLU:N	2:C:55:PRO:HD3	2.08	0.68
1:H:258:GLU:O	1:H:262:GLU:HB2	1.93	0.68
1:A:16:ASN:HD21	1:A:53:LEU:HD11	1.54	0.68
1:B:155:CYS:SG	3:B:340:NAD:C4N	2.81	0.67
1:A:311:LYS:HZ3	1:G:177:THR:CG2	2.06	0.67
1:G:19:ARG:HG2	1:G:56:PHE:CD2	2.29	0.67
1:H:11:GLY:CA	3:H:340:NAD:H4B	2.24	0.67
1:A:21:TRP:CZ3	1:A:31:VAL:HB	2.29	0.67
1:G:88:LYS:O	1:G:88:LYS:HE3	1.95	0.67
1:A:156:THR:HA	1:A:316:TYR:CZ	2.29	0.67
1:G:285:SER:C	1:G:287:ASP:H	1.98	0.67
1:G:86:PRO:O	1:G:89:GLU:HG2	1.93	0.67
1:G:165:LYS:O	1:G:168:HIS:N	2.27	0.67
1:B:263:VAL:HG13	1:B:264:LEU:HD22	1.76	0.67
1:A:49:TYR:HB3	1:B:287:ASP:OD1	1.94	0.67
1:B:155:CYS:N	3:B:340:NAD:H5N	2.10	0.67
1:B:118:LYS:CD	1:B:148:ALA:HA	2.24	0.67
1:B:134:VAL:HG23	1:B:222:VAL:HG11	1.77	0.67
1:G:132:THR:HG23	1:G:151:SER:OG	1.94	0.67
1:H:156:THR:HA	1:H:316:TYR:CZ	2.30	0.67
1:B:120:LEU:HD13	1:B:150:ILE:HG13	1.76	0.67
1:A:311:LYS:HZ3	1:G:177:THR:HG23	1.59	0.67
1:H:326:VAL:O	1:H:329:LEU:N	2.28	0.67
1:H:97:GLU:HB3	1:H:121:ILE:HA	1.77	0.67
1:A:168:HIS:C	1:A:170:ASN:H	1.97	0.67
1:A:276:ILE:HG12	1:A:295:SER:HB2	1.76	0.67
1:H:81:ASN:OD1	1:H:82:PRO:HD2	1.95	0.67
1:A:168:HIS:HE1	1:A:173:ILE:O	1.78	0.67
1:A:251:VAL:HG12	1:A:252:GLU:N	2.10	0.67
1:G:67:ILE:O	1:G:67:ILE:HD12	1.95	0.67
1:H:180:THR:HG23	1:H:234:ALA:HA	1.76	0.67
1:A:242:VAL:H	1:A:318:ASN:HD21	1.43	0.66
1:G:97:GLU:OE1	1:G:102:PHE:HB2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:89:GLU:C	1:G:90:TRP:HD1	1.99	0.66
1:B:48:GLU:HG2	1:B:49:TYR:CE1	2.31	0.66
1:G:257:THR:HG22	1:G:258:GLU:N	2.09	0.66
1:G:238:PRO:O	1:G:239:THR:HG23	1.95	0.66
1:A:257:THR:HG22	1:A:261:ASN:HD21	1.59	0.66
1:G:313:ILE:N	1:G:313:ILE:HD13	2.11	0.66
1:H:216:ALA:HB1	1:H:231:ASN:CA	2.26	0.66
1:B:112:ILE:C	1:B:114:ALA:H	1.98	0.66
3:G:340:NAD:O5D	2:I:73:TYR:CE2	2.48	0.66
1:H:72:LYS:H	1:H:72:LYS:HD2	1.60	0.66
1:B:152:ASN:HB3	1:B:322:TYR:OH	1.96	0.66
1:G:186:LEU:H	1:G:186:LEU:HD12	1.60	0.66
1:G:219:VAL:HG21	1:G:230:LEU:HD11	1.78	0.66
1:G:110:LYS:HA	1:G:113:GLN:HG3	1.76	0.66
1:A:10:PHE:CE1	1:A:15:ARG:HG2	2.30	0.66
1:G:102:PHE:HB3	1:G:107:GLY:O	1.96	0.66
1:G:135:ILE:HD12	1:G:328:ASP:HB3	1.78	0.66
1:B:45:HIS:CG	1:G:198:LEU:HD23	2.31	0.66
1:H:63:ASP:OD2	1:H:66:SER:O	2.14	0.66
1:G:20:CYS:SG	1:G:324:GLN:HG2	2.35	0.66
1:H:125:GLY:O	1:H:126:LYS:HD2	1.94	0.66
1:G:171:PHE:HB3	1:G:251:VAL:HG11	1.78	0.66
1:A:78:CYS:HB3	2:J:56:PHE:CE1	2.31	0.66
1:B:174:ILE:HG22	1:B:175:LYS:HE3	1.78	0.65
2:D:73:TYR:O	2:D:75:ASP:N	2.28	0.65
1:G:158:ASN:O	1:G:162:PRO:HD3	1.96	0.65
1:A:192:ASP:N	1:A:192:ASP:OD1	2.21	0.65
1:B:245:VAL:HG13	1:B:316:TYR:CE1	2.30	0.65
1:A:220:ALA:CB	1:A:227:LYS:HA	2.26	0.65
1:A:251:VAL:HG12	1:A:253:LYS:H	1.61	0.65
1:H:41:ARG:HA	1:H:62:TYR:CD1	2.31	0.65
1:G:264:LEU:N	1:G:264:LEU:HD23	2.11	0.65
1:B:245:VAL:HG22	1:B:314:ALA:HB3	1.78	0.65
1:G:174:ILE:HD11	1:G:252:GLU:OE1	1.97	0.65
1:A:293:GLU:N	1:A:293:GLU:OE2	2.30	0.65
1:H:214:GLY:HA2	1:H:217:LYS:HZ2	1.60	0.65
1:B:188:GLN:NE2	1:B:204:ALA:HB2	2.12	0.65
1:A:220:ALA:HB1	1:A:227:LYS:HA	1.77	0.65
1:A:312:VAL:CG1	1:A:313:ILE:N	2.59	0.65
1:G:235:LEU:HD12	1:G:235:LEU:N	2.12	0.65
1:B:45:HIS:ND1	1:G:198:LEU:HD23	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:195:HIS:HB3	1:H:201:ALA:HB2	1.79	0.65
1:B:214:GLY:O	1:B:218:ALA:HB2	1.96	0.65
1:H:11:GLY:N	3:H:340:NAD:H4B	2.11	0.65
1:B:13:ILE:HG21	1:B:122:THR:HG21	1.79	0.65
1:G:167:LEU:HB3	1:G:173:ILE:CD1	2.24	0.65
1:A:87:TRP:CD1	1:A:116:ALA:HB2	2.32	0.65
1:B:152:ASN:HB3	1:B:322:TYR:CZ	2.32	0.65
1:B:242:VAL:N	1:B:318:ASN:ND2	2.44	0.65
1:H:9:GLY:HA3	1:H:99:THR:N	2.11	0.65
1:A:18:LEU:HD23	1:A:47:LEU:CD2	2.25	0.65
1:B:155:CYS:H	3:B:340:NAD:H5N	1.62	0.65
1:A:34:ILE:HG22	1:A:34:ILE:O	1.97	0.65
1:A:99:THR:OG1	1:A:101:VAL:HG12	1.97	0.65
1:A:52:VAL:HG11	1:A:241:ASN:OD1	1.97	0.65
1:G:260:VAL:O	1:G:264:LEU:HD23	1.96	0.65
1:A:168:HIS:ND1	1:A:173:ILE:N	2.38	0.65
1:A:247:LEU:CD1	1:A:249:VAL:HG13	2.27	0.65
1:A:199:ARG:HD3	1:A:210:PRO:O	1.97	0.64
1:A:22:PHE:CE1	1:A:69:VAL:HB	2.32	0.64
1:A:199:ARG:HB3	1:A:209:VAL:HG13	1.78	0.64
1:G:264:LEU:HB2	1:G:278:TYR:CE1	2.33	0.64
1:A:324:GLN:NE2	1:A:324:GLN:HA	2.11	0.64
1:A:335:ARG:O	1:A:336:LYS:HG2	1.97	0.64
1:G:324:GLN:HB3	1:G:325:ARG:NH2	2.12	0.64
1:B:251:VAL:HG12	1:B:252:GLU:N	2.12	0.64
1:G:243:SER:HB2	1:G:316:TYR:CE2	2.33	0.64
1:A:224:PRO:C	1:A:226:LEU:H	2.00	0.64
1:B:155:CYS:HB3	3:B:340:NAD:C4N	2.24	0.64
1:H:144:HIS:CD2	1:H:337:TRP:HA	2.33	0.64
1:B:223:ILE:CG2	1:B:226:LEU:HG	2.27	0.64
1:B:232:GLY:O	1:B:233:ILE:HG23	1.98	0.64
1:H:33:ALA:HA	1:H:75:LYS:O	1.97	0.64
1:B:217:LYS:O	1:B:220:ALA:HB3	1.97	0.64
1:A:303:LEU:O	1:A:304:VAL:HG23	1.97	0.64
1:H:246:ASP:OD2	1:H:313:ILE:HD11	1.97	0.64
1:H:8:ASN:O	1:H:98:SER:N	2.28	0.64
1:A:291:THR:HG22	1:A:293:GLU:H	1.61	0.64
1:A:319:GLU:HG2	3:A:340:NAD:N7N	2.13	0.64
1:G:19:ARG:HG2	1:G:56:PHE:CE2	2.33	0.64
1:A:284:VAL:HG12	1:G:208:ILE:O	1.97	0.64
1:B:263:VAL:HG13	1:B:264:LEU:CD2	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:GLN:HG2	1:B:251:VAL:H	1.62	0.64
1:H:155:CYS:HB3	3:H:340:NAD:H4N	1.79	0.64
1:H:147:PHE:HB3	1:H:149:VAL:HG23	1.79	0.64
1:G:206:VAL:HG23	1:G:206:VAL:O	1.98	0.64
1:H:12:ARG:HH11	1:H:15:ARG:HH21	1.44	0.64
1:A:65:ASN:O	1:A:66:SER:HB3	1.98	0.64
1:A:3:ILE:HG21	1:A:334:ALA:HA	1.80	0.63
1:G:195:HIS:HE1	1:G:197:ASP:HB3	1.64	0.63
1:H:178:MET:HB2	1:H:247:LEU:HA	1.79	0.63
1:H:296:ILE:HB	1:H:315:TRP:HB2	1.80	0.63
1:G:209:VAL:O	1:G:236:ARG:N	2.29	0.63
2:C:67:ALA:HB1	2:C:69:GLU:OE2	1.98	0.63
1:A:49:TYR:N	1:A:49:TYR:CD2	2.66	0.63
1:B:315:TRP:O	1:B:316:TYR:HB3	1.98	0.63
1:A:152:ASN:HD22	1:A:326:VAL:HG23	1.62	0.63
1:B:162:PRO:O	1:B:276:ILE:HD11	1.98	0.63
1:B:270:THR:O	1:B:273:LYS:N	2.30	0.63
1:A:62:TYR:HB3	1:A:67:ILE:HG22	1.80	0.63
1:H:103:VAL:HA	1:H:121:ILE:HD13	1.81	0.63
1:G:174:ILE:HG22	1:G:175:LYS:HE2	1.81	0.63
1:B:59:ASP:HB2	1:B:70:ASN:HA	1.80	0.63
1:H:142:TYR:CE2	1:H:332:LEU:HB3	2.33	0.63
1:B:285:SER:C	1:B:287:ASP:H	1.98	0.63
1:G:152:ASN:HD22	1:G:326:VAL:CG2	2.11	0.63
1:H:263:VAL:HG12	1:H:264:LEU:N	2.13	0.63
1:G:35:ASN:OD1	1:G:77:VAL:HB	1.98	0.63
1:A:152:ASN:HB2	1:A:329:LEU:HD23	1.81	0.63
1:A:18:LEU:HD11	1:A:31:VAL:HG11	1.81	0.63
1:B:46:LEU:N	1:B:46:LEU:HD23	2.14	0.63
1:B:171:PHE:HB3	1:B:251:VAL:HG11	1.81	0.62
1:A:31:VAL:HG12	1:A:74:MET:CG	2.15	0.62
1:H:217:LYS:H	1:H:217:LYS:CD	2.09	0.62
1:B:165:LYS:O	1:B:169:ASP:OD1	2.17	0.62
1:G:129:GLY:O	1:G:130:VAL:HG13	1.99	0.62
1:A:241:ASN:ND2	1:A:318:ASN:OD1	2.31	0.62
1:H:241:ASN:HD22	1:H:242:VAL:H	1.45	0.62
1:G:88:LYS:H	1:G:115:GLY:HA3	1.64	0.62
1:B:93:ASP:HB3	1:B:337:TRP:CZ2	2.34	0.62
1:B:294:SER:OG	1:B:325:ARG:HD2	1.99	0.62
1:B:260:VAL:HG12	1:B:261:ASN:OD1	1.99	0.62
1:B:192:ASP:OD1	1:B:202:ARG:HA	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:152:ASN:HD22	1:G:326:VAL:HG22	1.64	0.62
1:G:54:GLY:HA2	1:H:289:ARG:NH2	2.14	0.62
1:B:242:VAL:N	1:B:318:ASN:HD21	1.98	0.62
1:H:159:CYS:HG	1:H:316:TYR:HD1	1.47	0.62
1:G:190:ILE:H	1:G:190:ILE:CD1	2.05	0.62
1:G:109:SER:O	1:G:112:ILE:HG12	2.00	0.62
1:A:177:THR:OG1	1:G:311:LYS:HD2	2.00	0.62
1:A:248:VAL:HG13	1:A:311:LYS:CG	2.29	0.62
1:G:12:ARG:HB2	3:G:340:NAD:O2A	2.00	0.62
1:B:241:ASN:ND2	1:B:319:GLU:HG3	2.15	0.62
1:B:251:VAL:CG1	1:B:252:GLU:N	2.62	0.62
1:A:66:SER:HB2	1:A:75:LYS:HA	1.80	0.62
1:B:241:ASN:HD22	1:B:318:ASN:HD21	1.45	0.62
1:H:325:ARG:HA	1:H:325:ARG:HE	1.65	0.62
1:A:48:GLU:OE1	1:A:49:TYR:CE2	2.52	0.62
1:B:241:ASN:HD21	1:B:319:GLU:HG3	1.64	0.62
1:B:265:GLN:HG3	1:B:269:GLN:HE22	1.63	0.62
1:A:12:ARG:HD2	1:A:15:ARG:HH22	1.63	0.61
1:G:85:LEU:HD13	1:G:87:TRP:CZ2	2.34	0.61
1:H:82:PRO:HA	1:H:85:LEU:CD1	2.25	0.61
1:H:81:ASN:OD1	1:H:83:LEU:HD12	2.00	0.61
1:G:216:ALA:C	1:G:218:ALA:N	2.50	0.61
1:B:306:ASP:CB	1:H:175:LYS:CE	2.78	0.61
1:G:259:GLN:O	1:G:262:GLU:HB2	2.00	0.61
1:H:179:THR:HG21	1:H:235:LEU:HD12	1.83	0.61
1:G:142:TYR:OH	1:G:333:ALA:HA	2.01	0.61
1:B:134:VAL:CG2	1:B:222:VAL:HG21	2.30	0.61
1:A:13:ILE:O	1:A:17:PHE:N	2.31	0.61
1:G:219:VAL:HG12	1:G:220:ALA:N	2.15	0.61
1:G:288:PHE:CD1	1:G:315:TRP:CE3	2.88	0.61
1:H:93:ASP:HB3	1:H:337:TRP:CZ2	2.36	0.61
1:B:255:THR:O	1:B:304:VAL:HG11	2.00	0.61
1:H:247:LEU:HD11	1:H:249:VAL:HG13	1.82	0.61
1:H:159:CYS:CB	1:H:316:TYR:HD1	2.13	0.61
1:A:168:HIS:ND1	1:A:173:ILE:HG13	2.15	0.61
1:B:165:LYS:HD3	1:B:272:MET:HE1	1.83	0.61
1:B:219:VAL:O	1:B:221:LEU:N	2.30	0.61
1:G:89:GLU:C	1:G:90:TRP:CD1	2.74	0.61
1:A:159:CYS:HB2	1:A:294:SER:O	2.00	0.61
1:G:48:GLU:HB3	1:G:49:TYR:HD2	1.64	0.61
1:B:288:PHE:HE2	1:B:296:ILE:HG21	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:251:VAL:HG12	1:H:252:GLU:N	2.15	0.61
1:H:158:ASN:O	1:H:162:PRO:CD	2.48	0.61
1:A:146:ASP:HB3	1:A:147:PHE:CD1	2.35	0.61
1:B:137:VAL:HG11	1:B:222:VAL:HG23	1.82	0.61
1:B:67:ILE:HG23	1:B:76:ILE:HD11	1.83	0.61
1:H:262:GLU:O	1:H:265:GLN:HB2	2.01	0.61
1:G:186:LEU:HD13	3:G:340:NAD:O3	2.01	0.61
1:B:252:GLU:OE2	1:B:252:GLU:HA	2.00	0.61
1:H:246:ASP:HA	1:H:313:ILE:CD1	2.30	0.60
1:G:87:TRP:O	1:G:88:LYS:C	2.38	0.60
1:A:310:VAL:HG12	1:A:311:LYS:N	2.16	0.60
1:H:10:PHE:HB2	1:H:34:ILE:HG21	1.83	0.60
1:G:191:LEU:HA	1:G:203:ALA:HB2	1.84	0.60
1:B:188:GLN:OE1	1:B:236:ARG:HD3	2.01	0.60
1:B:174:ILE:HD11	1:B:252:GLU:OE2	2.01	0.60
1:B:36:ASN:ND2	1:B:37:THR:N	2.30	0.60
1:G:128:GLU:HA	1:G:128:GLU:OE1	2.01	0.60
1:G:299:SER:C	1:G:301:LEU:H	2.04	0.60
1:B:318:ASN:HD22	1:B:318:ASN:H	1.50	0.60
1:H:242:VAL:O	1:H:243:SER:OG	2.15	0.60
1:B:159:CYS:O	1:B:162:PRO:HD2	2.00	0.60
1:B:196:ARG:HD2	2:D:72:ILE:HD11	1.81	0.60
1:B:208:ILE:O	1:B:210:PRO:HD3	2.01	0.60
1:B:95:VAL:HG13	1:B:119:VAL:HG23	1.83	0.60
1:H:225:GLU:O	1:H:226:LEU:HD23	2.01	0.60
1:H:195:HIS:ND1	1:H:196:ARG:N	2.50	0.60
1:A:160:LEU:O	1:A:160:LEU:HD12	2.01	0.60
1:B:207:ASN:HD21	1:G:51:SER:HB3	1.66	0.60
1:B:199:ARG:NH1	1:H:282:PRO:HA	2.16	0.60
1:H:121:ILE:HG22	1:H:123:ALA:N	2.16	0.60
1:G:143:ARG:HD3	1:G:146:ASP:N	2.17	0.60
1:G:144:HIS:NE2	1:G:337:TRP:CE3	2.64	0.60
1:G:81:ASN:HB3	1:G:84:ASN:OD1	2.02	0.60
1:B:270:THR:O	1:B:272:MET:N	2.35	0.60
1:B:134:VAL:HG21	1:B:222:VAL:HG21	1.83	0.60
1:G:138:ASN:CG	1:G:222:VAL:HG12	2.21	0.60
1:G:267:ALA:HA	1:G:270:THR:HG1	1.67	0.60
1:G:316:TYR:HE2	1:G:318:ASN:HB3	1.66	0.60
1:G:322:TYR:O	1:G:324:GLN:N	2.34	0.60
1:H:185:THR:HG21	2:J:75:ASP:OD1	2.01	0.60
1:A:144:HIS:HD2	1:A:337:TRP:HA	1.64	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:LEU:HD23	1:A:334:ALA:HB2	1.83	0.60
1:A:22:PHE:CZ	1:A:69:VAL:HB	2.36	0.60
1:A:74:MET:H	1:A:74:MET:CE	2.14	0.60
1:A:305:MET:O	1:A:307:GLY:N	2.35	0.60
1:H:95:VAL:HB	1:H:119:VAL:HG23	1.84	0.60
1:B:215:ALA:O	1:B:218:ALA:HB3	2.01	0.60
1:G:288:PHE:O	1:G:291:THR:HB	2.01	0.59
1:H:44:ALA:O	1:H:47:LEU:HB3	2.02	0.59
1:A:331:GLU:HA	1:A:331:GLU:OE2	2.02	0.59
1:B:206:VAL:HG23	1:B:207:ASN:HD22	1.66	0.59
1:B:246:ASP:OD2	1:B:311:LYS:HD3	2.02	0.59
1:H:171:PHE:HE1	1:H:255:THR:HB	1.63	0.59
1:B:15:ARG:HH21	1:B:46:LEU:HB3	1.67	0.59
1:B:178:MET:HG2	1:B:179:THR:N	2.17	0.59
1:G:34:ILE:O	1:G:77:VAL:HG23	2.03	0.59
1:G:87:TRP:HA	1:G:87:TRP:CE3	2.37	0.59
1:A:277:LYS:N	1:A:293:GLU:HG2	2.18	0.59
2:C:67:ALA:HB3	2:C:70:CYS:SG	2.42	0.59
1:G:295:SER:C	1:G:296:ILE:HG13	2.23	0.59
1:H:190:ILE:CD1	1:H:190:ILE:H	2.15	0.59
1:G:144:HIS:HD2	1:G:337:TRP:HA	1.59	0.59
1:A:193:ALA:O	1:A:201:ALA:HB1	2.02	0.59
1:G:305:MET:O	1:G:307:GLY:N	2.36	0.59
1:H:156:THR:HA	1:H:316:TYR:CE1	2.37	0.59
1:H:11:GLY:HA2	1:H:15:ARG:HH12	1.68	0.59
1:A:39:ASP:HB3	2:J:56:PHE:HB2	1.85	0.59
1:G:131:GLY:O	1:G:150:ILE:HG22	2.03	0.59
1:A:83:LEU:C	1:A:85:LEU:H	2.05	0.59
1:B:177:THR:OG1	1:B:178:MET:N	2.35	0.59
1:A:78:CYS:HB3	2:J:56:PHE:CD1	2.37	0.59
1:B:32:VAL:O	1:B:74:MET:CA	2.50	0.59
1:G:195:HIS:CE1	1:G:197:ASP:HB3	2.38	0.59
1:A:190:ILE:CG1	1:H:186:LEU:HD23	2.32	0.59
1:G:5:VAL:CG1	1:G:94:LEU:HD23	2.33	0.59
1:A:180:THR:HB	1:A:245:VAL:HG12	1.84	0.59
1:B:85:LEU:HD22	1:B:86:PRO:HD2	1.85	0.59
1:H:312:VAL:HG12	1:H:313:ILE:N	2.16	0.58
1:G:83:LEU:HD12	1:G:83:LEU:N	2.16	0.58
1:B:60:ILE:HA	1:B:68:THR:O	2.03	0.58
1:A:155:CYS:CA	3:A:340:NAD:H5N	2.33	0.58
1:A:242:VAL:N	1:A:318:ASN:HD21	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:318:ASN:ND2	3:G:340:NAD:H72N	1.99	0.58
1:H:20:CYS:SG	1:H:324:GLN:CD	2.81	0.58
1:B:54:GLY:O	1:B:55:ARG:C	2.39	0.58
1:G:240:PRO:O	1:G:241:ASN:HB2	2.01	0.58
1:H:140:SER:C	1:H:142:TYR:H	2.07	0.58
1:H:332:LEU:HD23	1:H:335:ARG:NH1	2.12	0.58
1:G:191:LEU:HA	1:G:203:ALA:CB	2.33	0.58
1:G:221:LEU:H	1:G:221:LEU:HD12	1.67	0.58
2:I:73:TYR:N	2:I:73:TYR:HD1	2.02	0.58
1:H:171:PHE:HB3	1:H:251:VAL:HG11	1.84	0.58
1:H:304:VAL:CG1	1:H:305:MET:H	2.16	0.58
1:A:170:ASN:HB3	1:A:171:PHE:CD2	2.38	0.58
1:G:180:THR:HG23	1:G:234:ALA:CB	2.33	0.58
3:A:340:NAD:O7N	3:A:340:NAD:O2N	2.21	0.58
1:A:48:GLU:HG2	1:A:49:TYR:CE2	2.38	0.58
1:H:244:VAL:HA	1:H:314:ALA:O	2.04	0.58
1:H:214:GLY:O	1:H:218:ALA:HB3	2.03	0.58
1:B:138:ASN:O	1:B:140:SER:N	2.37	0.58
2:C:59:ASP:HA	2:C:62:SER:HB3	1.85	0.58
1:A:4:ARG:HD2	1:A:32:VAL:HG11	1.84	0.58
1:H:10:PHE:CZ	1:H:15:ARG:HG2	2.38	0.58
1:H:37:THR:HG21	1:H:80:ARG:NH1	2.17	0.58
1:A:5:VAL:CG2	1:A:94:LEU:HB3	2.33	0.58
1:H:119:VAL:HG12	1:H:148:ALA:O	2.04	0.58
1:A:249:VAL:HG23	1:A:310:VAL:HB	1.84	0.58
1:G:245:VAL:HG23	1:G:316:TYR:CE1	2.37	0.58
1:G:304:VAL:HG22	1:G:310:VAL:HG22	1.85	0.58
1:B:306:ASP:HB3	1:H:175:LYS:NZ	2.18	0.58
1:H:260:VAL:HA	1:H:263:VAL:HB	1.85	0.58
1:H:194:SER:O	1:H:195:HIS:HB2	2.02	0.58
1:A:104:THR:O	1:A:126:LYS:O	2.21	0.58
1:H:316:TYR:HE2	1:H:318:ASN:HB3	1.65	0.58
2:J:54:GLU:H	2:J:55:PRO:HD3	1.65	0.58
1:B:303:LEU:HD21	1:H:231:ASN:ND2	2.18	0.58
1:B:85:LEU:CD2	1:B:86:PRO:HD2	2.34	0.58
1:B:184:TYR:OH	1:G:205:ALA:HB3	2.04	0.58
1:A:83:LEU:HD11	1:A:110:LYS:NZ	2.19	0.58
1:G:135:ILE:HG12	1:G:329:LEU:HD13	1.86	0.58
1:A:136:GLY:H	1:A:139:ASP:HB3	1.68	0.58
1:B:120:LEU:CD1	1:B:150:ILE:HG13	2.33	0.58
1:G:233:ILE:HG13	1:G:234:ALA:N	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:VAL:HG12	1:B:74:MET:HG2	1.85	0.58
1:B:161:ALA:C	1:B:163:VAL:H	2.05	0.58
1:A:154:SER:O	1:A:155:CYS:C	2.42	0.57
1:G:16:ASN:HB3	1:G:323:SER:CB	2.33	0.57
1:H:178:MET:SD	1:H:178:MET:O	2.62	0.57
1:H:21:TRP:CZ2	1:H:30:GLU:HA	2.38	0.57
1:A:306:ASP:HB2	1:G:175:LYS:HD3	1.85	0.57
1:H:223:ILE:O	1:H:225:GLU:N	2.37	0.57
1:H:171:PHE:HD1	1:H:253:LYS:O	1.86	0.57
1:H:117:LYS:O	1:H:118:LYS:HB2	2.03	0.57
1:H:32:VAL:N	1:H:74:MET:HG2	2.18	0.57
1:B:261:ASN:HB3	1:B:278:TYR:OH	2.03	0.57
2:C:59:ASP:O	2:C:62:SER:HB3	2.03	0.57
1:G:155:CYS:SG	3:G:340:NAD:C5N	2.92	0.57
1:A:202:ARG:NH2	1:H:51:SER:N	2.51	0.57
1:H:261:ASN:OD1	1:H:302:THR:HB	2.04	0.57
1:A:69:VAL:O	1:A:70:ASN:HB2	2.04	0.57
1:G:160:LEU:O	1:G:164:ALA:HB2	2.05	0.57
2:D:67:ALA:HB1	2:D:69:GLU:OE2	2.04	0.57
1:G:138:ASN:C	1:G:140:SER:N	2.56	0.57
1:G:221:LEU:CD1	1:G:221:LEU:H	2.17	0.57
1:A:152:ASN:ND2	1:A:326:VAL:CG2	2.68	0.57
2:D:54:GLU:N	2:D:55:PRO:CD	2.68	0.57
1:H:89:GLU:N	1:H:89:GLU:OE1	2.37	0.57
1:A:247:LEU:HD12	1:A:247:LEU:C	2.24	0.57
1:G:229:LYS:HB2	1:G:230:LEU:HD23	1.86	0.57
1:H:10:PHE:CD1	1:H:34:ILE:HD13	2.39	0.57
1:A:63:ASP:OD2	1:A:65:ASN:N	2.27	0.57
1:B:144:HIS:HD2	1:B:337:TRP:C	2.07	0.57
1:B:48:GLU:C	1:B:49:TYR:HD1	2.07	0.57
1:G:121:ILE:HB	1:G:151:SER:HA	1.87	0.57
1:B:305:MET:O	1:B:306:ASP:HB3	2.05	0.57
1:A:281:LEU:HB3	1:A:283:LEU:CD2	2.32	0.57
1:H:279:SER:O	1:H:298:ASP:HA	2.03	0.57
1:A:119:VAL:HG12	1:A:119:VAL:O	2.05	0.57
1:G:264:LEU:HB2	1:G:278:TYR:HE1	1.68	0.57
1:A:152:ASN:ND2	1:A:326:VAL:HG23	2.19	0.57
1:B:62:TYR:C	1:B:62:TYR:CD1	2.77	0.57
1:A:82:PRO:HG2	1:A:110:LYS:HB3	1.87	0.57
1:A:155:CYS:CB	3:A:340:NAD:C5N	2.80	0.57
1:H:39:ASP:O	1:H:42:THR:HB	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:180:THR:O	1:G:235:LEU:HD12	2.04	0.57
1:B:134:VAL:HG11	1:B:161:ALA:HB3	1.86	0.57
1:B:174:ILE:HD11	1:B:251:VAL:O	2.05	0.57
1:H:171:PHE:HB3	1:H:251:VAL:CG1	2.35	0.57
1:G:142:TYR:HD2	1:G:332:LEU:HD13	1.66	0.57
1:G:81:ASN:CG	1:G:83:LEU:HD13	2.25	0.57
1:A:161:ALA:C	1:A:163:VAL:H	2.06	0.57
1:G:41:ARG:HA	1:G:62:TYR:CZ	2.40	0.57
1:A:97:GLU:CD	1:A:97:GLU:C	2.62	0.57
1:A:196:ARG:HD2	2:C:70:CYS:CA	2.34	0.57
1:A:257:THR:HG22	1:A:261:ASN:ND2	2.20	0.57
1:G:277:LYS:N	1:G:293:GLU:HG2	2.19	0.57
1:G:269:GLN:O	1:G:273:LYS:HB2	2.04	0.57
1:A:138:ASN:O	1:A:140:SER:N	2.37	0.57
1:A:196:ARG:CD	2:C:70:CYS:HA	2.35	0.56
1:H:155:CYS:HB3	3:H:340:NAD:C4N	2.35	0.56
1:H:177:THR:OG1	1:H:178:MET:N	2.37	0.56
1:H:251:VAL:HG12	1:H:252:GLU:H	1.70	0.56
1:G:143:ARG:O	1:G:144:HIS:C	2.44	0.56
1:H:6:ALA:O	1:H:96:ILE:HG12	2.05	0.56
1:A:7:ILE:HB	1:A:34:ILE:CG1	2.33	0.56
1:A:196:ARG:HG3	2:C:69:GLU:O	2.05	0.56
1:G:184:TYR:HE2	1:G:239:THR:N	2.03	0.56
1:B:137:VAL:HG12	1:B:138:ASN:N	2.19	0.56
1:B:195:HIS:HD2	2:D:69:GLU:HA	1.70	0.56
1:B:97:GLU:OE2	1:B:97:GLU:HA	2.04	0.56
1:A:191:LEU:HA	1:A:203:ALA:HB2	1.87	0.56
1:H:159:CYS:CB	1:H:316:TYR:CD1	2.88	0.56
1:A:174:ILE:HG22	1:A:175:LYS:N	2.19	0.56
2:D:56:PHE:CE1	1:G:78:CYS:HB2	2.41	0.56
1:G:271:THR:OG1	1:G:272:MET:HG2	2.05	0.56
1:A:186:LEU:HD11	1:H:191:LEU:CB	2.34	0.56
1:B:305:MET:CB	1:H:175:LYS:HD2	2.15	0.56
1:H:199:ARG:HD3	1:H:210:PRO:O	2.05	0.56
1:B:101:VAL:HG13	1:B:102:PHE:CD1	2.41	0.56
1:G:13:ILE:HG21	1:G:122:THR:HG21	1.88	0.56
1:H:10:PHE:CE1	1:H:15:ARG:HG2	2.40	0.56
1:A:211:THR:OG1	1:A:236:ARG:NE	2.30	0.56
3:A:340:NAD:H3D	2:C:73:TYR:CE1	2.40	0.56
1:H:190:ILE:CD1	1:H:191:LEU:H	2.19	0.56
1:H:163:VAL:HG23	1:H:295:SER:OG	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:336:LYS:O	1:G:338:ALA:N	2.38	0.56
1:A:118:LYS:HB2	1:A:337:TRP:HH2	1.69	0.56
1:G:327:VAL:HG12	1:G:327:VAL:O	2.06	0.56
1:A:310:VAL:HG12	1:A:311:LYS:H	1.70	0.56
1:G:219:VAL:O	1:G:222:VAL:HG23	2.06	0.56
1:G:241:ASN:ND2	1:G:242:VAL:H	2.04	0.56
1:B:235:LEU:HD12	1:B:235:LEU:N	2.21	0.56
1:B:245:VAL:HG13	1:B:316:TYR:HE1	1.70	0.56
1:H:295:SER:C	1:H:296:ILE:HD12	2.26	0.56
1:A:324:GLN:CA	1:A:324:GLN:HE21	2.12	0.56
1:B:29:LEU:CD1	1:B:331:GLU:HG2	2.35	0.56
1:G:95:VAL:CG1	1:G:119:VAL:HG23	2.34	0.56
1:A:133:TYR:CE1	1:A:142:TYR:HD1	2.24	0.56
2:J:67:ALA:O	2:J:70:CYS:HB2	2.06	0.56
1:B:191:LEU:HB2	1:G:186:LEU:HG	1.88	0.56
1:G:284:VAL:O	1:G:285:SER:C	2.44	0.56
1:G:81:ASN:HD21	1:G:83:LEU:HD13	1.69	0.56
1:B:32:VAL:O	1:B:74:MET:HB3	2.06	0.56
1:G:178:MET:HE1	1:G:180:THR:HG22	1.88	0.56
1:B:216:ALA:HA	1:B:219:VAL:HG23	1.88	0.56
1:G:255:THR:O	1:G:307:GLY:HA2	2.06	0.56
1:B:12:ARG:HB2	3:B:340:NAD:O2N	2.06	0.55
1:G:190:ILE:CD1	1:G:190:ILE:N	2.68	0.55
1:H:279:SER:O	1:H:297:VAL:O	2.23	0.55
1:B:144:HIS:HD2	1:B:337:TRP:O	1.89	0.55
1:A:87:TRP:CE3	1:A:87:TRP:HA	2.41	0.55
2:I:60:TYR:HA	2:I:63:GLU:HG2	1.86	0.55
1:B:203:ALA:O	1:B:206:VAL:HG22	2.06	0.55
1:G:268:SER:HB2	1:G:278:TYR:HB2	1.89	0.55
2:I:73:TYR:N	2:I:73:TYR:CD1	2.71	0.55
1:B:172:GLY:O	1:B:251:VAL:HG13	2.04	0.55
1:G:5:VAL:HG21	1:G:29:LEU:HB3	1.87	0.55
1:A:159:CYS:HA	1:A:294:SER:O	2.05	0.55
1:B:301:LEU:HD23	1:B:301:LEU:N	2.20	0.55
1:B:223:ILE:HG22	1:B:226:LEU:HG	1.86	0.55
1:H:121:ILE:HG22	1:H:123:ALA:H	1.70	0.55
1:G:192:ASP:OD1	1:G:202:ARG:HA	2.06	0.55
1:B:30:GLU:O	1:B:32:VAL:HG13	2.07	0.55
1:H:57:ASN:O	1:H:58:ALA:HB2	2.04	0.55
1:A:145:GLU:O	1:A:146:ASP:O	2.23	0.55
1:G:269:GLN:O	1:G:270:THR:O	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:LEU:HB2	1:H:186:LEU:CG	2.37	0.55
1:B:284:VAL:HG12	1:H:210:PRO:HD3	1.88	0.55
1:H:303:LEU:HD23	1:H:303:LEU:C	2.26	0.55
1:A:7:ILE:HA	1:A:96:ILE:HB	1.89	0.55
1:H:158:ASN:O	1:H:162:PRO:HG2	2.06	0.55
1:H:158:ASN:HB3	1:H:294:SER:OG	2.06	0.55
1:G:220:ALA:HA	1:G:223:ILE:O	2.06	0.55
1:G:285:SER:H	1:G:315:TRP:HH2	1.55	0.55
1:H:175:LYS:HG3	1:H:176:GLY:N	2.22	0.55
1:A:216:ALA:O	1:A:219:VAL:HG23	2.06	0.55
1:B:41:ARG:HA	1:B:62:TYR:CD2	2.42	0.55
1:G:214:GLY:HA2	1:G:217:LYS:HE3	1.89	0.55
1:B:120:LEU:HD12	1:B:121:ILE:N	2.20	0.55
1:H:175:LYS:O	1:H:250:GLN:N	2.37	0.55
1:B:144:HIS:CD2	1:B:337:TRP:C	2.80	0.55
1:A:159:CYS:SG	1:A:316:TYR:CD1	2.97	0.55
1:G:58:ALA:HB1	1:G:70:ASN:OD1	2.05	0.55
1:G:189:ARG:HH21	2:I:69:GLU:HG3	1.72	0.55
1:G:83:LEU:CD1	1:G:83:LEU:H	2.17	0.55
1:A:86:PRO:C	1:A:87:TRP:HE3	2.10	0.55
1:G:317:ASP:OD1	1:G:320:TRP:N	2.38	0.55
1:A:15:ARG:NE	1:A:46:LEU:HD22	2.22	0.55
1:A:62:TYR:CB	1:A:67:ILE:HG22	2.36	0.55
1:G:295:SER:O	1:G:296:ILE:HG13	2.07	0.55
1:H:48:GLU:HG2	1:H:56:PHE:H	1.72	0.55
1:G:237:VAL:HB	1:G:238:PRO:CD	2.37	0.55
1:G:154:SER:O	1:G:155:CYS:C	2.44	0.55
1:H:24:ARG:NH1	1:H:24:ARG:HG3	2.21	0.55
1:H:62:TYR:O	1:H:62:TYR:CD2	2.60	0.55
1:G:24:ARG:HH21	1:G:324:GLN:NE2	2.05	0.54
1:A:48:GLU:HG2	1:A:49:TYR:CD2	2.42	0.54
1:H:253:LYS:O	1:H:253:LYS:HE3	2.07	0.54
1:A:306:ASP:CB	1:G:175:LYS:HD3	2.37	0.54
1:H:4:ARG:HB2	1:H:93:ASP:OD1	2.08	0.54
1:B:82:PRO:HB2	1:B:110:LYS:HB3	1.89	0.54
2:J:68:ALA:C	2:J:70:CYS:H	2.10	0.54
1:H:12:ARG:HG2	1:H:186:LEU:HD12	1.89	0.54
1:H:10:PHE:HB2	1:H:34:ILE:CG2	2.38	0.54
1:A:3:ILE:HD13	1:A:334:ALA:HB2	1.88	0.54
1:B:186:LEU:HD13	3:B:340:NAD:O2A	2.06	0.54
1:A:205:ALA:O	1:A:206:VAL:HG13	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:GLY:O	1:B:251:VAL:CA	2.54	0.54
1:H:155:CYS:SG	3:H:340:NAD:C5N	2.95	0.54
1:H:85:LEU:CD1	1:H:111:HIS:HE1	2.20	0.54
1:G:68:THR:HG23	1:G:73:THR:OG1	2.07	0.54
1:B:209:VAL:HA	1:H:284:VAL:HG12	1.89	0.54
1:H:318:ASN:N	1:H:318:ASN:HD22	2.05	0.54
1:H:152:ASN:HD21	1:H:326:VAL:HG22	1.71	0.54
1:A:175:LYS:HD2	1:A:250:GLN:NE2	2.22	0.54
1:H:142:TYR:HE2	1:H:332:LEU:HB3	1.71	0.54
1:H:276:ILE:O	1:H:293:GLU:HG2	2.07	0.54
1:B:50:ASP:HB3	1:B:53:LEU:H	1.71	0.54
1:B:311:LYS:HE2	1:H:177:THR:OG1	2.07	0.54
1:A:190:ILE:HG12	1:H:186:LEU:HD23	1.89	0.54
1:A:186:LEU:HD12	1:H:191:LEU:HD12	1.89	0.54
1:H:190:ILE:HD12	1:H:191:LEU:H	1.73	0.54
1:H:257:THR:HG23	1:H:302:THR:O	2.08	0.54
1:H:182:HIS:CD2	1:H:316:TYR:OH	2.61	0.54
1:G:174:ILE:HG22	1:G:175:LYS:CE	2.38	0.54
1:B:10:PHE:HB2	1:B:36:ASN:HB2	1.89	0.54
1:G:178:MET:HE1	1:G:180:THR:CG2	2.37	0.54
1:G:130:VAL:HA	1:G:149:VAL:O	2.07	0.54
2:I:59:ASP:O	2:I:62:SER:N	2.41	0.54
1:H:283:LEU:HD22	1:H:287:ASP:OD2	2.08	0.54
1:G:299:SER:O	1:G:301:LEU:N	2.37	0.54
1:A:191:LEU:H	1:H:186:LEU:HD21	1.72	0.54
1:A:24:ARG:HH21	1:A:324:GLN:NE2	2.05	0.54
1:G:250:GLN:HG3	1:G:308:ASP:OD1	2.06	0.54
1:B:36:ASN:HD22	1:B:37:THR:H	0.74	0.54
1:A:41:ARG:O	1:A:44:ALA:N	2.40	0.54
2:I:67:ALA:C	2:I:69:GLU:H	2.08	0.54
1:H:11:GLY:O	1:H:12:ARG:C	2.46	0.54
1:B:337:TRP:O	1:B:338:ALA:HB2	2.06	0.54
1:A:106:GLU:O	1:A:107:GLY:C	2.45	0.54
1:H:68:THR:HA	1:H:73:THR:HG23	1.89	0.54
1:A:93:ASP:HA	1:A:117:LYS:HG3	1.89	0.54
1:B:21:TRP:C	1:B:23:GLY:H	2.11	0.54
1:G:178:MET:CE	1:G:180:THR:HG22	2.38	0.54
1:H:220:ALA:HB2	1:H:226:LEU:O	2.08	0.54
1:G:69:VAL:C	1:G:71:GLY:H	2.09	0.54
1:G:264:LEU:N	1:G:264:LEU:CD2	2.70	0.54
1:H:15:ARG:O	1:H:16:ASN:C	2.45	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:THR:CG2	1:B:180:THR:HG21	2.37	0.53
1:A:186:LEU:HG	1:H:190:ILE:CD1	2.36	0.53
1:G:113:GLN:O	1:G:115:GLY:N	2.41	0.53
1:H:193:ALA:O	1:H:201:ALA:HB1	2.07	0.53
1:B:3:ILE:HG21	1:B:334:ALA:HA	1.90	0.53
1:G:50:ASP:CG	1:G:53:LEU:H	2.10	0.53
1:H:260:VAL:HG23	1:H:261:ASN:N	2.23	0.53
1:A:175:LYS:HD3	1:G:309:LEU:HB2	1.89	0.53
1:B:45:HIS:HB3	1:B:46:LEU:HD23	1.89	0.53
1:B:329:LEU:O	1:B:332:LEU:HB3	2.09	0.53
1:B:11:GLY:O	1:B:15:ARG:NH1	2.41	0.53
1:G:171:PHE:CB	1:G:251:VAL:HG11	2.38	0.53
1:A:184:TYR:CD2	1:A:238:PRO:HA	2.42	0.53
1:A:242:VAL:N	1:A:318:ASN:ND2	2.55	0.53
1:B:206:VAL:CG1	1:G:240:PRO:HG3	2.35	0.53
1:G:143:ARG:O	1:G:143:ARG:HD3	2.08	0.53
1:A:242:VAL:CG1	1:A:243:SER:N	2.71	0.53
1:G:19:ARG:NH1	1:G:56:PHE:CB	2.72	0.53
1:B:171:PHE:N	1:B:171:PHE:CD2	2.76	0.53
1:H:7:ILE:CG2	1:H:34:ILE:HG23	2.39	0.53
1:B:303:LEU:HD21	1:H:231:ASN:CG	2.29	0.53
1:B:123:ALA:HB1	1:B:124:PRO:HD2	1.91	0.53
1:B:48:GLU:C	1:B:49:TYR:CD1	2.82	0.53
1:B:126:LYS:HZ3	1:B:126:LYS:HB3	1.73	0.53
1:G:267:ALA:CA	1:G:270:THR:OG1	2.48	0.53
1:G:133:TYR:HB2	1:G:329:LEU:HD21	1.90	0.53
1:B:177:THR:HG22	1:H:309:LEU:HD21	1.91	0.53
1:B:175:LYS:HD3	1:H:305:MET:O	2.09	0.53
1:A:7:ILE:HG12	1:A:96:ILE:HG13	1.90	0.53
1:B:275:ILE:HG22	1:B:276:ILE:HG13	1.91	0.53
1:B:322:TYR:C	1:B:324:GLN:H	2.11	0.53
1:H:159:CYS:SG	1:H:316:TYR:CD1	2.97	0.53
1:H:171:PHE:HZ	1:H:259:GLN:HG2	1.73	0.53
1:G:333:ALA:O	1:G:335:ARG:N	2.41	0.53
1:B:22:PHE:HZ	1:B:69:VAL:O	1.92	0.53
1:A:112:ILE:HA	1:A:116:ALA:O	2.09	0.53
1:B:102:PHE:O	1:B:108:ALA:HB2	2.09	0.53
1:G:268:SER:OG	1:G:269:GLN:NE2	2.41	0.53
1:H:182:HIS:O	1:H:236:ARG:HA	2.08	0.53
1:H:63:ASP:O	1:H:65:ASN:N	2.41	0.53
1:B:216:ALA:O	1:B:219:VAL:HG23	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:TRP:HB3	1:A:116:ALA:N	2.24	0.53
1:A:30:GLU:O	1:A:32:VAL:HG22	2.07	0.53
1:H:120:LEU:HD12	1:H:121:ILE:N	2.24	0.53
1:H:121:ILE:N	1:H:150:ILE:O	2.31	0.53
1:H:319:GLU:O	1:H:320:TRP:C	2.46	0.53
1:G:150:ILE:H	1:G:150:ILE:HD12	1.74	0.53
1:A:104:THR:O	1:A:105:ALA:HB2	2.09	0.53
1:G:103:VAL:O	1:G:126:LYS:HB2	2.09	0.53
1:H:29:LEU:HD11	1:H:330:ALA:HB1	1.91	0.53
1:G:134:VAL:HG11	1:G:161:ALA:CB	2.39	0.53
1:G:276:ILE:HA	1:G:295:SER:O	2.09	0.53
1:B:247:LEU:HD12	1:B:248:VAL:H	1.72	0.53
1:H:120:LEU:HD13	1:H:150:ILE:HG13	1.91	0.53
1:A:326:VAL:C	1:A:328:ASP:N	2.62	0.53
1:B:60:ILE:HD11	1:B:69:VAL:HG13	1.90	0.53
1:G:120:LEU:HD13	1:G:150:ILE:HD13	1.89	0.53
1:B:101:VAL:C	1:B:103:VAL:H	2.12	0.53
1:G:15:ARG:HD2	1:G:47:LEU:HA	1.90	0.52
1:B:311:LYS:HG3	1:H:177:THR:OG1	2.09	0.52
1:H:82:PRO:O	1:H:85:LEU:HB2	2.09	0.52
1:A:312:VAL:O	1:A:313:ILE:HD13	2.08	0.52
1:A:241:ASN:O	1:A:242:VAL:HB	2.08	0.52
1:G:264:LEU:O	1:G:268:SER:CB	2.55	0.52
1:G:87:TRP:HA	1:G:87:TRP:HE3	1.72	0.52
2:C:68:ALA:HA	2:C:71:LEU:HD12	1.91	0.52
1:A:233:ILE:HD13	1:G:301:LEU:CD2	2.23	0.52
1:H:11:GLY:HA3	3:H:340:NAD:C4B	2.39	0.52
1:A:108:ALA:C	1:A:110:LYS:H	2.10	0.52
1:A:82:PRO:HA	1:A:85:LEU:HG	1.90	0.52
1:A:244:VAL:HA	1:A:314:ALA:O	2.09	0.52
1:G:9:GLY:HA3	1:G:98:SER:C	2.30	0.52
1:G:135:ILE:HD11	1:G:329:LEU:N	2.24	0.52
1:G:154:SER:OG	1:G:157:THR:OG1	2.28	0.52
1:G:5:VAL:HG13	1:G:94:LEU:HD23	1.91	0.52
1:B:94:LEU:HD12	1:B:118:LYS:C	2.30	0.52
1:H:213:THR:O	1:H:217:LYS:NZ	2.43	0.52
1:G:195:HIS:CE1	1:G:200:ARG:CB	2.93	0.52
1:H:161:ALA:HB3	1:H:162:PRO:CD	2.39	0.52
1:B:67:ILE:HG12	1:B:76:ILE:HD11	1.92	0.52
1:G:321:GLY:O	1:G:325:ARG:HG2	2.10	0.52
3:G:340:NAD:O5B	3:G:340:NAD:O1N	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:318:ASN:OD1	3:H:340:NAD:N7N	2.43	0.52
2:C:60:TYR:OH	1:H:80:ARG:NH2	2.40	0.52
1:G:333:ALA:C	1:G:335:ARG:H	2.13	0.52
1:G:113:GLN:O	1:G:114:ALA:C	2.47	0.52
1:H:83:LEU:HG	1:H:110:LYS:HB3	1.92	0.52
1:H:211:THR:O	1:H:234:ALA:HB3	2.10	0.52
1:H:62:TYR:HA	1:H:67:ILE:HA	1.92	0.52
1:G:214:GLY:CA	1:G:217:LYS:HE3	2.40	0.52
1:A:179:THR:HA	1:A:233:ILE:O	2.10	0.52
1:H:247:LEU:HD12	1:H:248:VAL:N	2.24	0.52
1:A:19:ARG:HG2	1:A:56:PHE:CZ	2.44	0.52
1:A:283:LEU:N	1:G:199:ARG:HH21	1.92	0.52
1:H:138:ASN:C	1:H:140:SER:H	2.11	0.52
1:A:12:ARG:HD3	1:H:192:ASP:O	2.09	0.52
1:G:138:ASN:C	1:G:140:SER:H	2.13	0.52
1:H:11:GLY:HA3	3:H:340:NAD:O5B	2.10	0.52
1:A:226:LEU:O	1:A:227:LYS:C	2.48	0.52
1:G:309:LEU:HG	1:G:309:LEU:O	2.10	0.52
1:G:7:ILE:HB	1:G:34:ILE:CG2	2.39	0.52
1:H:142:TYR:O	1:H:143:ARG:HG3	2.09	0.52
1:H:214:GLY:HA2	1:H:217:LYS:HZ3	1.72	0.52
1:A:82:PRO:O	1:A:85:LEU:HB2	2.10	0.52
1:H:267:ALA:HA	1:H:271:THR:HG23	1.92	0.52
1:G:134:VAL:HG23	1:G:222:VAL:HG11	1.91	0.52
1:G:288:PHE:CE1	1:G:315:TRP:CE3	2.98	0.52
1:G:50:ASP:OD1	1:G:51:SER:N	2.43	0.52
1:B:251:VAL:HG12	1:B:253:LYS:N	2.25	0.52
1:B:243:SER:HB2	1:B:316:TYR:CZ	2.44	0.52
1:B:12:ARG:NH1	1:G:192:ASP:HB2	2.24	0.52
1:H:214:GLY:C	1:H:216:ALA:N	2.51	0.52
1:B:152:ASN:O	1:B:153:ALA:HB3	2.09	0.52
1:G:134:VAL:HG11	1:G:161:ALA:HB1	1.92	0.52
1:H:304:VAL:HA	1:H:309:LEU:O	2.09	0.52
2:I:72:ILE:HG22	2:I:72:ILE:O	2.09	0.52
1:A:101:VAL:HG13	1:A:102:PHE:N	2.25	0.52
1:B:188:GLN:HE22	1:B:209:VAL:HG21	1.74	0.52
1:G:123:ALA:HB2	3:G:340:NAD:O2D	2.10	0.52
1:A:6:ALA:O	1:A:95:VAL:HA	2.10	0.52
1:B:36:ASN:HB3	1:B:38:SER:OG	2.09	0.52
1:B:22:PHE:HD1	1:B:22:PHE:O	1.93	0.52
1:H:270:THR:OG1	1:H:271:THR:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:158:ASN:O	1:G:161:ALA:HB3	2.10	0.51
1:G:159:CYS:O	1:G:162:PRO:HD2	2.10	0.51
1:B:257:THR:N	1:B:304:VAL:HG21	2.25	0.51
1:A:224:PRO:O	1:A:226:LEU:N	2.43	0.51
1:A:21:TRP:O	1:A:22:PHE:C	2.48	0.51
1:A:251:VAL:HG12	1:A:252:GLU:H	1.76	0.51
1:H:6:ALA:CB	1:H:95:VAL:HG13	2.31	0.51
1:H:216:ALA:O	1:H:219:VAL:HG23	2.10	0.51
1:B:138:ASN:O	1:B:141:GLU:HG3	2.09	0.51
1:G:324:GLN:HB3	1:G:325:ARG:HH21	1.76	0.51
1:H:92:ILE:O	1:H:116:ALA:HA	2.10	0.51
1:B:103:VAL:HG23	1:B:103:VAL:O	2.09	0.51
1:B:192:ASP:HA	1:B:201:ALA:O	2.10	0.51
1:B:177:THR:O	1:B:247:LEU:HD12	2.10	0.51
1:H:312:VAL:O	1:H:313:ILE:HD13	2.10	0.51
1:A:174:ILE:HG21	1:A:250:GLN:OE1	2.10	0.51
1:G:89:GLU:CD	1:G:89:GLU:H	2.11	0.51
1:H:118:LYS:HG3	1:H:148:ALA:CB	2.39	0.51
1:B:93:ASP:HB3	1:B:337:TRP:CH2	2.46	0.51
1:H:137:VAL:CG1	1:H:223:ILE:HG13	2.40	0.51
1:A:48:GLU:HB3	1:A:49:TYR:CD2	2.46	0.51
1:B:233:ILE:HD12	1:B:234:ALA:N	2.25	0.51
1:G:117:LYS:HB2	1:G:337:TRP:HH2	1.76	0.51
1:A:1:MET:HG2	1:A:28:ASP:HA	1.92	0.51
1:G:209:VAL:HB	1:G:236:ARG:HB2	1.92	0.51
1:G:5:VAL:HG13	1:G:94:LEU:HB3	1.91	0.51
1:A:277:LYS:HD2	1:A:293:GLU:OE1	2.11	0.51
1:H:232:GLY:O	1:H:233:ILE:HG23	2.11	0.51
1:A:159:CYS:HB2	1:A:316:TYR:CB	2.40	0.51
1:B:81:ASN:OD1	1:B:82:PRO:HD2	2.11	0.51
1:G:237:VAL:HB	1:G:238:PRO:HD3	1.92	0.51
1:B:48:GLU:O	1:B:49:TYR:HD1	1.93	0.51
1:A:84:ASN:C	1:A:85:LEU:HD23	2.30	0.51
1:B:189:ARG:NH1	2:D:68:ALA:HB1	2.25	0.51
1:A:179:THR:CG2	1:A:235:LEU:HD12	2.41	0.51
1:A:44:ALA:C	1:A:46:LEU:H	2.14	0.51
1:G:45:HIS:CE1	1:H:282:PRO:HG2	2.45	0.51
1:G:232:GLY:O	1:G:233:ILE:HG22	2.11	0.51
1:G:195:HIS:HB3	1:G:201:ALA:CB	2.37	0.51
1:A:30:GLU:O	1:A:32:VAL:HG13	2.11	0.51
1:A:300:SER:C	1:A:301:LEU:HD23	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:264:LEU:H	1:G:264:LEU:HD23	1.74	0.51
1:H:7:ILE:HG22	1:H:34:ILE:HG23	1.93	0.51
1:B:337:TRP:O	1:B:338:ALA:CB	2.59	0.51
1:B:300:SER:O	1:B:302:THR:N	2.44	0.51
1:B:66:SER:HB3	1:B:75:LYS:HA	1.93	0.51
1:G:318:ASN:HB2	3:G:340:NAD:N7N	2.23	0.51
1:H:324:GLN:O	1:H:325:ARG:NH2	2.44	0.51
1:H:155:CYS:SG	3:H:340:NAD:C4N	2.98	0.51
1:A:33:ALA:HA	1:A:75:LYS:H	1.75	0.51
1:B:260:VAL:HG12	1:B:261:ASN:N	2.26	0.51
1:G:183:SER:OG	1:G:239:THR:O	2.27	0.51
1:H:68:THR:CG2	1:H:73:THR:OG1	2.56	0.51
1:B:138:ASN:O	1:B:141:GLU:N	2.40	0.51
1:G:2:THR:O	1:G:2:THR:HG22	2.10	0.51
1:A:68:THR:CG2	1:A:71:GLY:HA2	2.41	0.51
1:A:37:THR:HG1	3:A:340:NAD:HO2A	1.59	0.51
1:H:21:TRP:CZ3	1:H:22:PHE:CE2	2.99	0.51
1:H:256:ILE:C	1:H:304:VAL:HG21	2.31	0.51
1:H:316:TYR:CD2	1:H:318:ASN:HB3	2.45	0.51
1:H:318:ASN:O	3:H:340:NAD:H4N	2.11	0.51
1:G:143:ARG:NH2	1:G:145:GLU:HB2	2.24	0.51
1:A:94:LEU:HD12	1:A:118:LYS:O	2.11	0.51
1:A:168:HIS:C	1:A:170:ASN:N	2.64	0.51
1:H:123:ALA:HB1	1:H:124:PRO:HD2	1.94	0.51
1:A:284:VAL:HG21	1:G:202:ARG:HG3	1.92	0.51
1:A:168:HIS:CE1	1:A:173:ILE:HB	2.46	0.51
1:A:165:LYS:HG3	1:A:166:VAL:N	2.26	0.51
1:A:133:TYR:HE1	1:A:142:TYR:HD1	1.58	0.51
1:B:191:LEU:HD12	1:G:186:LEU:HG	1.93	0.50
1:A:49:TYR:H	1:A:49:TYR:HD2	1.58	0.50
1:B:15:ARG:HE	1:B:46:LEU:CB	2.24	0.50
1:A:159:CYS:HB2	1:A:316:TYR:HB3	1.93	0.50
1:G:12:ARG:C	1:G:14:GLY:N	2.64	0.50
1:H:68:THR:HG23	1:H:71:GLY:O	2.11	0.50
1:B:29:LEU:HD23	1:B:334:ALA:HB2	1.93	0.50
1:B:320:TRP:C	1:B:322:TYR:H	2.15	0.50
1:G:243:SER:HB2	1:G:316:TYR:CZ	2.47	0.50
1:A:64:GLU:OE2	2:J:55:PRO:HG2	2.11	0.50
1:H:216:ALA:HB3	1:H:217:LYS:HD2	1.93	0.50
1:H:62:TYR:HB2	1:H:67:ILE:HG22	1.92	0.50
1:G:215:ALA:C	1:G:218:ALA:HB3	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:ASN:ND2	1:B:222:VAL:HB	2.26	0.50
1:A:236:ARG:C	1:A:237:VAL:HG13	2.31	0.50
1:B:304:VAL:O	1:B:305:MET:SD	2.69	0.50
1:H:10:PHE:HB3	1:H:36:ASN:CG	2.32	0.50
1:G:35:ASN:HB2	1:G:85:LEU:HD21	1.93	0.50
1:G:87:TRP:CE3	1:G:92:ILE:HG13	2.47	0.50
1:H:230:LEU:O	1:H:231:ASN:CB	2.59	0.50
1:B:112:ILE:C	1:B:114:ALA:N	2.62	0.50
1:H:276:ILE:HG22	1:H:277:LYS:N	2.27	0.50
1:B:49:TYR:N	1:B:49:TYR:CD1	2.77	0.50
1:B:315:TRP:O	1:B:316:TYR:CB	2.58	0.50
1:H:159:CYS:SG	1:H:316:TYR:HB3	2.52	0.50
1:A:17:PHE:CE2	1:A:326:VAL:HG12	2.47	0.50
1:B:186:LEU:HG	1:G:190:ILE:CD1	2.38	0.50
1:H:157:THR:HG23	1:H:219:VAL:HG22	1.93	0.50
1:A:46:LEU:O	1:A:46:LEU:HD23	2.12	0.50
1:G:315:TRP:O	1:G:316:TYR:HB3	2.12	0.50
1:H:182:HIS:HA	1:H:243:SER:OG	2.12	0.50
1:A:337:TRP:CD1	1:A:338:ALA:N	2.80	0.50
1:A:251:VAL:CG1	1:A:252:GLU:N	2.73	0.50
1:G:250:GLN:HG2	1:G:250:GLN:O	2.10	0.50
2:D:73:TYR:HB3	2:D:75:ASP:OD2	2.11	0.50
1:B:5:VAL:HA	1:B:94:LEU:O	2.12	0.50
2:C:65:PRO:C	2:C:67:ALA:H	2.15	0.50
1:G:184:TYR:CE2	1:G:239:THR:N	2.80	0.50
1:B:286:SER:HB3	1:H:207:ASN:HD21	1.75	0.50
1:G:227:LYS:O	1:G:228:GLY:C	2.50	0.50
1:A:9:GLY:O	1:A:98:SER:OG	2.29	0.50
1:A:138:ASN:C	1:A:140:SER:N	2.65	0.50
1:G:8:ASN:OD1	1:G:85:LEU:HD11	2.12	0.50
1:A:4:ARG:CD	1:A:32:VAL:HG11	2.41	0.50
1:B:244:VAL:HG23	1:B:315:TRP:CA	2.36	0.50
1:H:326:VAL:O	1:H:327:VAL:C	2.50	0.50
1:A:17:PHE:HA	1:A:323:SER:HB3	1.94	0.50
1:H:118:LYS:CG	1:H:148:ALA:HA	2.32	0.50
1:G:18:LEU:C	1:G:20:CYS:N	2.65	0.50
1:A:49:TYR:OH	1:B:281:LEU:HD11	2.12	0.50
1:H:82:PRO:CA	1:H:85:LEU:HD12	2.30	0.50
1:B:5:VAL:HG23	1:B:30:GLU:C	2.32	0.50
1:G:197:ASP:C	1:G:197:ASP:OD2	2.50	0.50
1:B:298:ASP:OD2	1:B:300:SER:OG	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:PHE:O	1:A:15:ARG:NH1	2.45	0.49
1:B:284:VAL:O	1:B:285:SER:C	2.48	0.49
1:H:183:SER:CB	1:H:241:ASN:H	2.25	0.49
1:H:178:MET:CA	1:H:246:ASP:O	2.58	0.49
1:H:24:ARG:HH11	1:H:24:ARG:CG	2.24	0.49
1:H:86:PRO:HA	1:H:89:GLU:HG2	1.94	0.49
1:H:195:HIS:ND1	1:H:197:ASP:N	2.59	0.49
1:A:40:ALA:CB	1:A:76:ILE:HG13	2.41	0.49
1:A:92:ILE:O	1:A:116:ALA:HA	2.11	0.49
1:G:14:GLY:O	1:G:17:PHE:HB3	2.12	0.49
1:G:99:THR:HG22	3:G:340:NAD:C4A	2.42	0.49
1:H:182:HIS:HD2	1:H:316:TYR:OH	1.94	0.49
1:H:248:VAL:HA	1:H:310:VAL:O	2.12	0.49
1:A:20:CYS:O	1:A:24:ARG:HG3	2.11	0.49
2:J:71:LEU:O	2:J:72:ILE:HG12	2.12	0.49
1:G:130:VAL:HG12	1:G:149:VAL:HB	1.93	0.49
1:G:325:ARG:HA	1:G:325:ARG:HE	1.77	0.49
1:B:143:ARG:O	1:B:146:ASP:HB2	2.12	0.49
1:A:186:LEU:CD1	1:H:191:LEU:HB2	2.41	0.49
1:H:239:THR:HG22	1:H:240:PRO:HD2	1.95	0.49
1:G:28:ASP:C	1:G:29:LEU:HD23	2.33	0.49
1:G:138:ASN:ND2	1:G:222:VAL:HG12	2.27	0.49
1:G:21:TRP:C	1:G:23:GLY:N	2.66	0.49
1:H:122:THR:O	3:H:340:NAD:H1D	2.12	0.49
1:H:256:ILE:O	1:H:259:GLN:HB3	2.12	0.49
1:H:256:ILE:HD11	1:H:258:GLU:HB3	1.93	0.49
2:D:73:TYR:HB2	2:D:75:ASP:OD1	2.13	0.49
1:B:199:ARG:O	1:B:202:ARG:CG	2.60	0.49
1:A:138:ASN:HD21	1:A:222:VAL:HG12	1.76	0.49
1:B:15:ARG:HE	1:B:46:LEU:HB3	1.77	0.49
1:B:93:ASP:O	1:B:117:LYS:HB2	2.13	0.49
2:D:66:ASP:C	2:D:71:LEU:HD21	2.33	0.49
1:A:301:LEU:N	1:A:301:LEU:HD23	2.26	0.49
1:G:15:ARG:O	1:G:16:ASN:C	2.50	0.49
1:A:78:CYS:SG	2:J:56:PHE:HD1	2.35	0.49
1:H:195:HIS:CE1	1:H:197:ASP:N	2.79	0.49
1:A:89:GLU:OE1	1:A:89:GLU:N	2.46	0.49
1:A:48:GLU:CG	1:A:49:TYR:CE2	2.95	0.49
1:B:171:PHE:CB	1:B:251:VAL:HG11	2.43	0.49
1:H:171:PHE:CD1	1:H:253:LYS:O	2.65	0.49
1:A:138:ASN:O	1:A:141:GLU:N	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ASN:HD22	1:A:325:ARG:HG3	1.76	0.49
1:H:137:VAL:HG11	1:H:222:VAL:HB	1.95	0.49
1:B:277:LYS:HG2	1:B:278:TYR:H	1.77	0.49
1:B:238:PRO:HB2	1:H:238:PRO:HB2	1.95	0.49
1:G:49:TYR:CD2	1:G:49:TYR:N	2.81	0.49
1:H:12:ARG:HH11	1:H:15:ARG:NH2	2.10	0.49
1:G:109:SER:C	1:G:111:HIS:H	2.16	0.49
1:B:80:ARG:HH22	2:D:66:ASP:CG	2.16	0.49
1:H:296:ILE:N	1:H:296:ILE:HD12	2.28	0.49
1:B:155:CYS:CB	3:B:340:NAD:C4N	2.87	0.49
1:B:285:SER:C	1:B:287:ASP:N	2.62	0.48
1:H:285:SER:HA	1:H:315:TRP:CZ3	2.48	0.48
1:G:335:ARG:O	1:G:336:LYS:HD3	2.13	0.48
3:B:340:NAD:H3D	2:D:73:TYR:CZ	2.47	0.48
1:B:8:ASN:ND2	1:B:97:GLU:OE2	2.40	0.48
1:G:18:LEU:O	1:G:19:ARG:C	2.51	0.48
1:B:210:PRO:HA	1:B:235:LEU:HA	1.95	0.48
1:B:260:VAL:O	1:B:263:VAL:HG12	2.14	0.48
1:H:166:VAL:O	1:H:169:ASP:HB2	2.13	0.48
1:G:185:THR:O	1:G:187:ASP:N	2.46	0.48
1:G:264:LEU:CD1	1:G:297:VAL:HG11	2.36	0.48
1:H:304:VAL:CG1	1:H:305:MET:N	2.72	0.48
1:A:19:ARG:HD3	1:A:53:LEU:CD1	2.43	0.48
1:G:188:GLN:NE2	1:G:204:ALA:CB	2.76	0.48
1:B:161:ALA:C	1:B:163:VAL:N	2.67	0.48
1:A:275:ILE:HA	1:A:275:ILE:HD13	1.64	0.48
1:A:108:ALA:O	1:A:110:LYS:N	2.46	0.48
1:A:82:PRO:CG	1:A:110:LYS:HB3	2.43	0.48
1:G:285:SER:N	1:G:315:TRP:CH2	2.80	0.48
1:H:124:PRO:HG2	2:J:74:ASP:HB3	1.94	0.48
1:H:16:ASN:OD1	1:H:320:TRP:N	2.46	0.48
1:H:255:THR:HG22	1:H:307:GLY:O	2.13	0.48
1:H:85:LEU:HD13	1:H:87:TRP:CZ2	2.48	0.48
1:A:85:LEU:HD12	1:A:87:TRP:CZ2	2.48	0.48
1:G:60:ILE:HA	1:G:68:THR:O	2.13	0.48
1:H:124:PRO:HA	1:H:153:ALA:HA	1.96	0.48
1:H:318:ASN:ND2	1:H:318:ASN:H	2.09	0.48
1:A:78:CYS:O	2:J:56:PHE:HE1	1.97	0.48
2:I:57:PHE:O	2:I:61:CYS:HB2	2.14	0.48
1:A:100:GLY:HA2	3:A:340:NAD:O3D	2.14	0.48
1:B:200:ARG:NH1	1:B:236:ARG:HH21	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:245:VAL:N	1:G:314:ALA:O	2.33	0.48
1:G:326:VAL:O	1:G:328:ASP:N	2.46	0.48
1:H:182:HIS:HA	1:H:243:SER:CB	2.43	0.48
1:H:48:GLU:OE2	1:H:49:TYR:CE2	2.67	0.48
1:G:144:HIS:HB2	1:G:336:LYS:O	2.14	0.48
1:A:152:ASN:HD22	1:A:326:VAL:HG22	1.77	0.48
1:A:159:CYS:CB	1:A:294:SER:O	2.60	0.48
1:H:62:TYR:CB	1:H:67:ILE:HG22	2.43	0.48
1:A:76:ILE:HA	1:A:76:ILE:HD13	1.53	0.48
1:A:87:TRP:HE3	1:A:87:TRP:HA	1.78	0.48
1:B:88:LYS:N	1:B:115:GLY:HA3	2.28	0.48
1:A:186:LEU:N	1:A:186:LEU:HD12	2.29	0.48
1:H:19:ARG:HH22	1:H:56:PHE:HA	1.79	0.48
1:A:6:ALA:HB2	1:A:33:ALA:HB3	1.95	0.48
1:B:117:LYS:CD	1:B:337:TRP:CZ2	2.90	0.48
1:B:143:ARG:HB3	1:B:146:ASP:CB	2.37	0.48
1:H:268:SER:O	1:H:273:LYS:HA	2.13	0.48
1:B:207:ASN:OD1	1:H:284:VAL:HG23	2.13	0.48
1:H:247:LEU:HD12	1:H:248:VAL:H	1.75	0.48
1:H:143:ARG:HB2	1:H:146:ASP:OD1	2.13	0.48
1:A:245:VAL:HG13	1:A:316:TYR:CE1	2.49	0.48
1:A:312:VAL:CG1	1:A:313:ILE:H	2.25	0.48
1:B:138:ASN:C	1:B:140:SER:N	2.67	0.48
1:B:106:GLU:O	1:B:108:ALA:N	2.47	0.48
1:A:197:ASP:HB3	1:A:200:ARG:HG3	1.96	0.48
1:H:55:ARG:HG3	1:H:56:PHE:N	2.29	0.48
1:H:7:ILE:HB	1:H:34:ILE:HG23	1.95	0.48
1:A:277:LYS:HB2	1:A:293:GLU:HG2	1.95	0.48
1:H:196:ARG:HD3	2:J:72:ILE:HD11	1.95	0.48
1:B:109:SER:HA	1:B:112:ILE:HG12	1.94	0.48
1:A:248:VAL:O	1:A:249:VAL:HG13	2.14	0.48
1:G:322:TYR:C	1:G:324:GLN:N	2.62	0.48
1:B:251:VAL:CG1	1:B:252:GLU:H	2.27	0.48
1:H:21:TRP:O	1:H:23:GLY:N	2.47	0.48
1:G:77:VAL:HG12	1:G:78:CYS:H	1.78	0.48
1:H:87:TRP:HA	1:H:92:ILE:HG12	1.95	0.48
1:H:105:ALA:HB2	1:H:130:VAL:HG13	1.95	0.47
1:H:155:CYS:H	3:H:340:NAD:H5N	1.79	0.47
1:H:18:LEU:HD23	1:H:47:LEU:CD1	2.41	0.47
1:A:305:MET:O	1:A:306:ASP:C	2.52	0.47
1:B:15:ARG:HD2	1:B:47:LEU:HA	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:ARG:HE	1:B:46:LEU:C	2.18	0.47
1:B:21:TRP:CH2	1:B:31:VAL:HB	2.49	0.47
1:H:62:TYR:C	1:H:62:TYR:CD2	2.84	0.47
1:A:187:ASP:O	1:A:200:ARG:HB3	2.14	0.47
1:H:159:CYS:O	1:H:163:VAL:HG23	2.14	0.47
1:H:318:ASN:N	1:H:318:ASN:ND2	2.60	0.47
1:A:175:LYS:HE2	1:G:306:ASP:HB3	1.96	0.47
2:D:56:PHE:HE1	1:G:78:CYS:HB2	1.78	0.47
1:G:83:LEU:O	1:G:114:ALA:CB	2.62	0.47
1:H:85:LEU:HD13	1:H:111:HIS:HE1	1.78	0.47
1:B:22:PHE:CD1	1:B:22:PHE:O	2.67	0.47
1:B:5:VAL:O	1:B:32:VAL:HG22	2.14	0.47
1:H:182:HIS:HA	1:H:243:SER:HB3	1.97	0.47
1:B:10:PHE:HB3	1:B:36:ASN:OD1	2.13	0.47
1:A:162:PRO:O	1:A:276:ILE:HD11	2.14	0.47
1:G:109:SER:HA	1:G:112:ILE:HG12	1.96	0.47
1:H:37:THR:HG23	3:H:340:NAD:C4A	2.44	0.47
1:A:123:ALA:O	1:A:124:PRO:C	2.51	0.47
1:H:280:ASP:OD1	1:H:281:LEU:HD23	2.15	0.47
1:A:241:ASN:O	1:A:242:VAL:CB	2.62	0.47
1:H:23:GLY:O	1:H:24:ARG:O	2.31	0.47
1:H:244:VAL:HG23	1:H:315:TRP:N	2.29	0.47
1:A:284:VAL:CG2	1:G:202:ARG:HG3	2.45	0.47
1:G:82:PRO:O	1:G:85:LEU:HB2	2.15	0.47
1:H:87:TRP:CE3	1:H:92:ILE:HG13	2.49	0.47
1:H:332:LEU:CD2	1:H:335:ARG:HH11	2.18	0.47
1:G:180:THR:HG23	1:G:234:ALA:HB2	1.96	0.47
1:H:221:LEU:O	1:H:222:VAL:HG13	2.14	0.47
1:A:155:CYS:SG	3:A:340:NAD:C5N	3.02	0.47
1:G:134:VAL:CG2	1:G:222:VAL:HG11	2.44	0.47
1:H:155:CYS:SG	2:J:75:ASP:OD2	2.72	0.47
1:H:20:CYS:O	1:H:24:ARG:HG2	2.14	0.47
1:H:251:VAL:HG12	1:H:253:LYS:H	1.80	0.47
1:H:66:SER:OG	1:H:74:MET:O	2.31	0.47
1:G:195:HIS:CE1	1:G:197:ASP:H	2.32	0.47
1:G:17:PHE:N	1:G:323:SER:HB3	2.29	0.47
1:A:41:ARG:O	1:A:42:THR:C	2.53	0.47
1:G:13:ILE:HG22	1:G:13:ILE:O	2.15	0.47
1:G:159:CYS:SG	1:G:316:TYR:HB3	2.54	0.47
1:G:280:ASP:HA	1:G:299:SER:OG	2.15	0.47
1:G:99:THR:HB	1:G:101:VAL:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:LYS:HE2	1:B:253:LYS:HB3	1.62	0.47
1:H:305:MET:O	1:H:306:ASP:HB3	2.15	0.47
1:A:137:VAL:HG12	1:A:138:ASN:N	2.29	0.47
1:G:83:LEU:CD1	1:G:110:LYS:HB3	2.44	0.47
1:G:36:ASN:C	1:G:38:SER:H	2.18	0.47
1:H:85:LEU:HD22	1:H:87:TRP:CH2	2.50	0.47
1:H:220:ALA:CB	1:H:227:LYS:HA	2.45	0.47
1:A:275:ILE:HG22	1:A:276:ILE:HG13	1.96	0.47
1:B:189:ARG:CZ	2:D:68:ALA:HB1	2.44	0.47
1:A:182:HIS:ND1	1:A:183:SER:O	2.46	0.47
1:A:138:ASN:C	1:A:140:SER:H	2.18	0.47
1:A:131:GLY:O	1:A:150:ILE:HG22	2.15	0.47
1:G:18:LEU:O	1:G:21:TRP:N	2.46	0.47
1:G:221:LEU:N	1:G:221:LEU:HD12	2.29	0.47
1:G:144:HIS:NE2	1:G:337:TRP:HA	2.28	0.47
1:A:245:VAL:O	1:A:313:ILE:HA	2.14	0.47
1:A:196:ARG:HD2	2:C:70:CYS:C	2.36	0.47
1:A:8:ASN:ND2	1:A:111:HIS:HE1	2.12	0.47
1:H:312:VAL:CG1	1:H:313:ILE:N	2.78	0.47
1:A:157:THR:HG23	1:A:219:VAL:HG22	1.96	0.47
1:G:7:ILE:HG23	1:G:96:ILE:CG2	2.45	0.47
1:A:97:GLU:HG3	1:A:121:ILE:HG23	1.97	0.47
2:D:67:ALA:C	2:D:69:GLU:H	2.17	0.47
1:B:286:SER:HB3	1:H:207:ASN:OD1	2.15	0.47
1:G:161:ALA:HB3	1:G:162:PRO:CD	2.39	0.46
1:G:19:ARG:HH12	1:G:56:PHE:HB2	1.74	0.46
1:A:190:ILE:H	1:A:190:ILE:CD1	2.21	0.46
1:H:104:THR:HG22	1:H:126:LYS:HB3	1.97	0.46
1:H:45:HIS:O	1:H:47:LEU:N	2.47	0.46
1:A:78:CYS:HB3	2:J:56:PHE:HE1	1.78	0.46
1:B:152:ASN:HB3	1:B:322:TYR:CE1	2.50	0.46
1:B:101:VAL:HG13	1:B:102:PHE:CE1	2.50	0.46
1:B:203:ALA:HB3	1:B:206:VAL:HG22	1.97	0.46
1:A:214:GLY:C	1:A:216:ALA:N	2.69	0.46
1:B:21:TRP:O	1:B:23:GLY:N	2.49	0.46
1:G:119:VAL:O	1:G:150:ILE:HD12	2.15	0.46
1:A:112:ILE:HD11	1:A:148:ALA:HB1	1.96	0.46
2:I:56:PHE:C	2:I:56:PHE:CD2	2.88	0.46
1:G:186:LEU:HD13	3:G:340:NAD:PA	2.55	0.46
1:G:155:CYS:N	3:G:340:NAD:H5N	2.10	0.46
1:A:31:VAL:HG12	1:A:31:VAL:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:MET:HE3	1:A:74:MET:H	1.81	0.46
1:B:263:VAL:O	1:B:266:LYS:CB	2.59	0.46
1:B:264:LEU:HD13	1:B:264:LEU:HA	1.50	0.46
1:B:11:GLY:CA	3:B:340:NAD:H4B	2.45	0.46
1:B:221:LEU:HD23	1:B:221:LEU:HA	1.81	0.46
1:A:87:TRP:CA	1:A:87:TRP:CE3	2.98	0.46
1:A:247:LEU:HD11	1:A:249:VAL:CG1	2.42	0.46
1:A:36:ASN:HB3	1:A:38:SER:OG	2.16	0.46
1:G:329:LEU:HD12	1:G:329:LEU:HA	1.58	0.46
1:G:37:THR:CG2	3:G:340:NAD:C4A	2.93	0.46
1:B:174:ILE:CD1	1:B:252:GLU:OE2	2.62	0.46
1:H:10:PHE:CE1	1:H:34:ILE:HD13	2.50	0.46
1:H:24:ARG:HH11	1:H:24:ARG:HG3	1.79	0.46
1:A:18:LEU:CD1	1:A:31:VAL:HG21	2.46	0.46
1:B:215:ALA:C	1:B:218:ALA:HB3	2.35	0.46
1:H:167:LEU:CD1	1:H:167:LEU:N	2.79	0.46
1:B:306:ASP:HB3	1:H:175:LYS:HE2	1.94	0.46
1:A:74:MET:H	1:A:74:MET:HE2	1.79	0.46
1:A:251:VAL:CG1	1:A:252:GLU:H	2.29	0.46
2:D:53:THR:C	2:D:55:PRO:HD2	2.35	0.46
1:G:81:ASN:HA	1:G:82:PRO:HD3	1.72	0.46
1:G:5:VAL:HG11	1:G:94:LEU:HD23	1.97	0.46
1:G:67:ILE:HG12	1:G:76:ILE:CD1	2.35	0.46
1:H:200:ARG:HG3	1:H:211:THR:HG22	1.96	0.46
1:B:275:ILE:HA	1:B:275:ILE:HD13	1.79	0.46
1:B:134:VAL:HG11	1:B:161:ALA:CB	2.46	0.46
1:B:63:ASP:OD2	1:B:66:SER:N	2.48	0.46
1:A:184:TYR:HD2	1:A:238:PRO:HA	1.81	0.46
1:H:10:PHE:HB3	1:H:36:ASN:OD1	2.15	0.46
1:A:5:VAL:HG12	1:A:31:VAL:HA	1.97	0.46
1:B:13:ILE:HG21	1:B:122:THR:CG2	2.43	0.46
1:B:120:LEU:HD13	1:B:150:ILE:CD1	2.46	0.46
1:G:28:ASP:HB3	1:G:334:ALA:HB3	1.98	0.46
1:B:21:TRP:CZ3	1:B:22:PHE:CD2	3.03	0.46
1:H:162:PRO:O	1:H:165:LYS:HB3	2.16	0.46
1:G:66:SER:HB2	1:G:73:THR:CG2	2.46	0.46
1:A:247:LEU:O	1:A:311:LYS:HA	2.16	0.46
1:B:200:ARG:HH11	1:B:236:ARG:NH2	2.14	0.46
1:G:10:PHE:CZ	1:G:15:ARG:HG2	2.51	0.46
1:G:261:ASN:OD1	1:G:299:SER:CB	2.64	0.46
1:B:15:ARG:NH2	1:B:46:LEU:HB3	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:ALA:HB1	1:B:129:GLY:O	2.16	0.46
1:A:12:ARG:HH12	1:A:50:ASP:CG	2.19	0.46
1:G:241:ASN:O	1:G:242:VAL:O	2.34	0.46
1:A:190:ILE:N	1:A:190:ILE:HD13	2.21	0.46
1:A:152:ASN:O	1:A:322:TYR:OH	2.34	0.46
1:A:3:ILE:HD13	1:A:334:ALA:CB	2.45	0.46
1:G:90:TRP:O	1:G:91:ASP:C	2.54	0.46
1:B:21:TRP:C	1:B:23:GLY:N	2.69	0.46
1:B:53:LEU:HD13	1:B:320:TRP:CZ3	2.51	0.46
1:B:216:ALA:C	1:B:218:ALA:N	2.65	0.46
1:G:24:ARG:HE	1:G:324:GLN:HE22	1.64	0.45
1:A:190:ILE:O	1:A:191:LEU:HD23	2.16	0.45
1:B:245:VAL:O	1:B:245:VAL:HG23	2.16	0.45
1:H:303:LEU:HD22	1:H:311:LYS:CB	2.45	0.45
1:G:174:ILE:HB	1:G:250:GLN:O	2.16	0.45
1:G:171:PHE:O	1:G:172:GLY:O	2.34	0.45
1:G:28:ASP:HB3	1:G:29:LEU:HD23	1.98	0.45
1:A:264:LEU:O	1:A:267:ALA:HB3	2.15	0.45
1:A:332:LEU:HD23	1:A:332:LEU:HA	1.59	0.45
1:B:194:SER:O	1:B:195:HIS:HB2	2.14	0.45
2:D:68:ALA:HB3	2:D:69:GLU:OE1	2.16	0.45
1:B:237:VAL:HB	1:B:238:PRO:HD2	1.97	0.45
1:B:7:ILE:O	1:B:34:ILE:HA	2.16	0.45
1:B:72:LYS:HB2	1:B:72:LYS:HE3	1.46	0.45
1:H:17:PHE:O	1:H:20:CYS:N	2.49	0.45
1:A:224:PRO:C	1:A:226:LEU:N	2.67	0.45
1:A:108:ALA:C	1:A:110:LYS:N	2.69	0.45
1:G:139:ASP:N	1:G:139:ASP:OD2	2.47	0.45
1:A:130:VAL:HG12	1:A:149:VAL:HB	1.98	0.45
1:B:174:ILE:HB	1:B:250:GLN:OE1	2.16	0.45
1:B:306:ASP:HB3	1:H:175:LYS:CE	2.45	0.45
1:H:12:ARG:HG2	1:H:186:LEU:CD1	2.47	0.45
1:A:168:HIS:ND1	1:A:173:ILE:CG1	2.79	0.45
1:H:68:THR:HG23	1:H:73:THR:HG1	1.81	0.45
1:B:85:LEU:HA	1:B:85:LEU:HD23	1.46	0.45
1:G:191:LEU:H	1:G:191:LEU:HD12	1.81	0.45
1:G:303:LEU:O	1:G:303:LEU:CD2	2.65	0.45
1:A:155:CYS:SG	3:A:340:NAD:H5N	2.57	0.45
1:G:306:ASP:C	1:G:308:ASP:H	2.20	0.45
1:B:6:ALA:HB1	1:B:87:TRP:CH2	2.51	0.45
1:B:299:SER:O	1:B:302:THR:OG1	2.27	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:60:ILE:CG1	1:G:69:VAL:HG13	2.46	0.45
1:B:9:GLY:HA3	1:B:99:THR:HG22	1.99	0.45
1:A:187:ASP:CG	2:C:73:TYR:HB2	2.37	0.45
2:I:73:TYR:O	2:I:74:ASP:C	2.54	0.45
1:H:244:VAL:HG23	1:H:314:ALA:C	2.37	0.45
1:B:120:LEU:HD13	1:B:150:ILE:CG1	2.42	0.45
2:D:56:PHE:HD2	2:D:57:PHE:N	2.15	0.45
1:G:5:VAL:CG2	1:G:29:LEU:HB3	2.47	0.45
1:H:158:ASN:O	1:H:162:PRO:CG	2.64	0.45
1:A:83:LEU:O	1:A:85:LEU:N	2.48	0.45
1:G:20:CYS:SG	1:G:323:SER:O	2.75	0.45
1:B:45:HIS:CG	1:G:198:LEU:CD2	2.99	0.45
1:B:69:VAL:O	1:B:70:ASN:C	2.54	0.45
1:B:6:ALA:HB2	1:B:92:ILE:HD12	1.99	0.45
1:B:265:GLN:HA	1:B:268:SER:OG	2.16	0.45
1:A:332:LEU:HD22	1:A:336:LYS:HD2	1.99	0.45
1:A:205:ALA:O	1:A:206:VAL:CG1	2.65	0.45
1:G:176:GLY:HA3	1:G:249:VAL:HG12	1.99	0.45
1:A:10:PHE:HE2	1:A:43:ALA:O	2.00	0.45
1:A:241:ASN:C	1:A:242:VAL:HG23	2.37	0.45
1:H:80:ARG:NH1	3:H:340:NAD:N7A	2.65	0.45
1:H:118:LYS:HD2	1:H:144:HIS:HE1	1.81	0.45
1:A:161:ALA:C	1:A:163:VAL:N	2.69	0.45
1:G:109:SER:O	1:G:111:HIS:N	2.50	0.45
1:A:184:TYR:CD1	1:A:184:TYR:O	2.70	0.45
1:B:19:ARG:CZ	1:B:56:PHE:HB2	2.47	0.45
1:G:121:ILE:HG22	1:G:123:ALA:O	2.17	0.45
1:B:247:LEU:HG	1:B:249:VAL:HG13	1.98	0.45
1:B:284:VAL:HG12	1:H:210:PRO:CD	2.46	0.45
1:H:176:GLY:HA3	1:H:249:VAL:HG12	1.98	0.45
1:G:175:LYS:HB3	1:G:175:LYS:HE2	1.60	0.45
1:B:51:SER:HG	1:G:192:ASP:CG	2.20	0.45
1:G:171:PHE:CD2	1:G:171:PHE:N	2.85	0.45
1:B:5:VAL:HG23	1:B:30:GLU:O	2.17	0.45
1:B:266:LYS:C	1:B:268:SER:H	2.20	0.45
1:A:49:TYR:HD2	1:A:49:TYR:N	2.11	0.45
1:H:242:VAL:HG11	1:H:285:SER:O	2.17	0.45
1:A:251:VAL:HG12	1:A:253:LYS:N	2.31	0.45
1:B:18:LEU:O	1:B:22:PHE:CB	2.57	0.45
1:G:194:SER:O	1:G:195:HIS:HB2	2.17	0.45
1:H:135:ILE:HG21	1:H:275:ILE:HD11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:GLY:O	1:A:12:ARG:C	2.55	0.45
1:G:310:VAL:CG1	1:G:311:LYS:N	2.80	0.45
1:B:121:ILE:HG22	1:B:122:THR:H	1.82	0.45
1:G:83:LEU:HD11	1:G:110:LYS:CD	2.44	0.45
1:A:156:THR:CA	1:A:316:TYR:CE2	2.94	0.45
1:B:272:MET:O	1:B:275:ILE:N	2.35	0.45
2:C:61:CYS:O	2:C:62:SER:O	2.34	0.45
1:B:195:HIS:CD2	2:D:69:GLU:O	2.69	0.45
1:G:17:PHE:O	1:G:20:CYS:CB	2.65	0.44
1:G:220:ALA:O	1:G:221:LEU:C	2.56	0.44
1:G:310:VAL:HG12	1:G:311:LYS:N	2.31	0.44
1:H:302:THR:HG23	1:H:312:VAL:HG22	1.98	0.44
1:A:29:LEU:CD2	1:A:334:ALA:HB2	2.48	0.44
1:A:29:LEU:HD11	1:A:330:ALA:HB3	1.98	0.44
1:H:142:TYR:CD1	1:H:143:ARG:N	2.86	0.44
1:G:232:GLY:O	1:G:233:ILE:CG2	2.65	0.44
1:B:300:SER:O	1:B:301:LEU:C	2.55	0.44
2:I:59:ASP:O	2:I:60:TYR:C	2.55	0.44
1:H:168:HIS:O	1:H:169:ASP:O	2.35	0.44
1:A:231:ASN:HB3	1:G:303:LEU:HD21	1.98	0.44
1:G:189:ARG:HH21	2:I:69:GLU:CG	2.31	0.44
1:A:48:GLU:OE1	1:A:49:TYR:CZ	2.71	0.44
1:H:85:LEU:HD13	1:H:87:TRP:HZ2	1.81	0.44
1:A:68:THR:HG22	1:A:71:GLY:HA2	1.98	0.44
1:H:206:VAL:HG23	1:H:206:VAL:O	2.18	0.44
1:A:195:HIS:CE1	1:A:200:ARG:HB2	2.52	0.44
1:G:12:ARG:HE	1:G:319:GLU:CD	2.20	0.44
1:A:202:ARG:HH21	1:H:51:SER:N	2.15	0.44
1:H:80:ARG:CZ	2:J:66:ASP:OD2	2.65	0.44
1:A:175:LYS:HD3	1:G:308:ASP:OD2	2.18	0.44
1:H:63:ASP:O	1:H:64:GLU:C	2.56	0.44
1:G:42:THR:O	1:G:44:ALA:N	2.50	0.44
1:B:6:ALA:O	1:B:96:ILE:N	2.48	0.44
1:A:177:THR:O	1:A:248:VAL:HG23	2.18	0.44
1:B:283:LEU:O	1:B:284:VAL:HG13	2.18	0.44
1:A:31:VAL:O	1:A:74:MET:HG2	2.17	0.44
1:G:235:LEU:CD1	1:G:235:LEU:N	2.78	0.44
1:A:107:GLY:O	1:A:110:LYS:HD2	2.18	0.44
1:H:205:ALA:O	1:H:238:PRO:CG	2.66	0.44
1:B:24:ARG:NH1	1:B:327:VAL:HG12	2.32	0.44
1:G:261:ASN:OD1	1:G:299:SER:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:THR:HG23	1:B:234:ALA:HA	1.99	0.44
1:H:323:SER:O	1:H:326:VAL:N	2.43	0.44
1:A:326:VAL:O	1:A:329:LEU:N	2.47	0.44
1:A:159:CYS:O	1:A:163:VAL:HG23	2.18	0.44
1:B:112:ILE:O	1:B:114:ALA:N	2.51	0.44
1:B:111:HIS:O	1:B:114:ALA:HB3	2.18	0.44
1:A:121:ILE:HB	1:A:151:SER:HB2	2.00	0.44
1:A:101:VAL:CG1	1:A:102:PHE:N	2.81	0.44
1:G:132:THR:HG21	1:G:221:LEU:HD23	2.00	0.44
1:G:155:CYS:HB3	3:G:340:NAD:C4N	2.37	0.44
1:G:316:TYR:CE2	1:G:318:ASN:HB3	2.51	0.44
1:G:99:THR:CG2	3:G:340:NAD:C5A	2.95	0.44
1:A:202:ARG:HD2	1:A:202:ARG:HA	1.75	0.44
1:B:11:GLY:HA2	3:B:340:NAD:O5B	2.14	0.44
1:G:168:HIS:CA	1:G:172:GLY:HA2	2.38	0.44
1:B:62:TYR:HD1	1:B:62:TYR:C	2.19	0.44
1:A:83:LEU:HD11	1:A:110:LYS:HZ2	1.83	0.44
1:B:195:HIS:CD2	2:D:69:GLU:HA	2.52	0.44
1:A:160:LEU:CD2	1:A:178:MET:HG3	2.48	0.44
1:G:241:ASN:HD22	1:G:242:VAL:N	2.11	0.44
1:G:301:LEU:HA	1:G:301:LEU:HD23	1.84	0.44
1:G:89:GLU:HB2	1:G:90:TRP:CD1	2.53	0.44
1:H:88:LYS:HB3	1:H:89:GLU:OE1	2.17	0.44
1:H:94:LEU:HD12	1:H:95:VAL:N	2.33	0.44
1:G:5:VAL:HB	1:G:31:VAL:CG2	2.48	0.44
1:A:40:ALA:HB2	1:A:76:ILE:HG21	1.99	0.44
1:G:66:SER:HB2	1:G:73:THR:HG22	2.00	0.44
1:G:136:GLY:N	1:G:139:ASP:OD2	2.50	0.44
1:B:200:ARG:C	1:B:202:ARG:H	2.21	0.44
1:A:281:LEU:CB	1:A:283:LEU:HD21	2.38	0.44
2:J:54:GLU:O	2:J:56:PHE:N	2.40	0.44
1:H:137:VAL:CG1	1:H:222:VAL:HB	2.47	0.44
1:A:196:ARG:HD2	2:C:70:CYS:O	2.17	0.44
1:A:248:VAL:HG11	1:G:248:VAL:HG11	2.00	0.44
1:G:50:ASP:N	1:G:54:GLY:O	2.47	0.44
1:H:175:LYS:CG	1:H:176:GLY:N	2.81	0.44
1:A:144:HIS:ND1	1:A:144:HIS:C	2.71	0.44
1:H:87:TRP:HB3	1:H:116:ALA:HB2	2.00	0.44
1:H:223:ILE:C	1:H:225:GLU:N	2.71	0.44
1:H:128:GLU:HB3	1:H:129:GLY:H	1.68	0.44
1:G:37:THR:HG22	3:G:340:NAD:C4A	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:19:ARG:CG	1:G:56:PHE:CE2	3.00	0.43
1:H:21:TRP:HZ2	1:H:30:GLU:HA	1.81	0.43
1:A:220:ALA:HB2	1:A:227:LYS:HA	1.99	0.43
1:A:324:GLN:O	1:A:326:VAL:N	2.51	0.43
1:A:78:CYS:HG	2:J:56:PHE:HD1	1.66	0.43
1:G:122:THR:O	1:G:123:ALA:HB2	2.18	0.43
1:G:12:ARG:C	1:G:14:GLY:H	2.20	0.43
1:G:161:ALA:CB	1:G:162:PRO:HD3	2.37	0.43
1:H:253:LYS:CE	1:H:254:PRO:O	2.65	0.43
1:H:9:GLY:HA3	1:H:98:SER:O	2.16	0.43
1:G:118:LYS:HB2	1:G:337:TRP:HZ3	1.82	0.43
1:H:112:ILE:HG12	1:H:116:ALA:O	2.18	0.43
1:B:95:VAL:HG22	1:B:96:ILE:N	2.33	0.43
1:A:132:THR:HA	1:A:151:SER:O	2.17	0.43
1:H:137:VAL:HG12	1:H:223:ILE:HG13	2.00	0.43
1:A:112:ILE:CD1	1:A:148:ALA:HB1	2.48	0.43
2:I:57:PHE:O	2:I:58:GLY:C	2.56	0.43
1:G:275:ILE:HA	1:G:275:ILE:HD13	1.79	0.43
1:H:85:LEU:HD13	1:H:111:HIS:CE1	2.53	0.43
1:H:69:VAL:O	1:H:70:ASN:C	2.56	0.43
1:H:104:THR:O	1:H:105:ALA:C	2.57	0.43
1:H:108:ALA:CB	1:H:149:VAL:HG12	2.49	0.43
1:H:140:SER:C	1:H:142:TYR:N	2.72	0.43
1:H:180:THR:CG2	1:H:234:ALA:HA	2.44	0.43
1:B:85:LEU:HA	1:B:86:PRO:HD2	1.58	0.43
1:A:86:PRO:C	1:A:87:TRP:CE3	2.90	0.43
1:A:237:VAL:O	1:A:239:THR:N	2.52	0.43
1:H:53:LEU:HA	1:H:53:LEU:HD23	1.87	0.43
1:A:197:ASP:OD2	1:A:199:ARG:HB2	2.18	0.43
1:H:286:SER:O	1:H:289:ARG:NE	2.47	0.43
1:B:255:THR:OG1	1:B:256:ILE:N	2.51	0.43
1:H:321:GLY:O	1:H:322:TYR:C	2.56	0.43
1:A:118:LYS:HB2	1:A:337:TRP:CH2	2.50	0.43
1:A:16:ASN:HD21	1:A:53:LEU:CD1	2.28	0.43
1:H:138:ASN:C	1:H:140:SER:N	2.72	0.43
1:A:10:PHE:HB3	1:A:36:ASN:OD1	2.18	0.43
1:G:15:ARG:CZ	1:G:46:LEU:HB3	2.48	0.43
1:G:99:THR:HG22	3:G:340:NAD:C5A	2.48	0.43
1:H:120:LEU:CD2	1:H:329:LEU:HD23	2.47	0.43
1:H:36:ASN:O	1:H:78:CYS:HA	2.19	0.43
1:A:138:ASN:ND2	1:A:222:VAL:HB	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:ILE:HD13	1:A:334:ALA:HA	2.01	0.43
1:B:320:TRP:CD1	1:B:320:TRP:C	2.92	0.43
1:A:2:THR:O	1:A:2:THR:HG22	2.19	0.43
1:A:177:THR:HG23	1:A:248:VAL:HG23	2.01	0.43
1:G:21:TRP:C	1:G:23:GLY:H	2.20	0.43
1:B:246:ASP:OD2	1:B:313:ILE:HD11	2.18	0.43
1:B:312:VAL:O	1:B:313:ILE:HD13	2.19	0.43
1:H:183:SER:HB2	1:H:241:ASN:H	1.83	0.43
1:A:29:LEU:HG	1:A:331:GLU:OE2	2.18	0.43
1:B:117:LYS:HD2	1:B:337:TRP:CE2	2.52	0.43
1:A:246:ASP:OD2	1:G:179:THR:HG21	2.19	0.43
1:B:66:SER:HA	1:B:76:ILE:HG13	2.01	0.43
1:A:9:GLY:C	1:A:11:GLY:H	2.22	0.43
1:A:283:LEU:N	1:G:199:ARG:NH2	2.54	0.43
1:G:40:ALA:O	1:G:41:ARG:C	2.56	0.43
1:A:191:LEU:O	1:A:192:ASP:C	2.57	0.43
1:B:315:TRP:O	1:B:316:TYR:HD1	2.02	0.43
1:H:176:GLY:HA3	1:H:248:VAL:O	2.19	0.43
1:A:247:LEU:HD12	1:A:248:VAL:O	2.19	0.43
1:A:310:VAL:CG1	1:A:311:LYS:H	2.32	0.43
1:A:37:THR:HG23	3:A:340:NAD:C4A	2.49	0.43
1:G:326:VAL:C	1:G:328:ASP:H	2.22	0.43
1:H:321:GLY:O	1:H:324:GLN:N	2.52	0.43
1:A:13:ILE:HA	1:A:16:ASN:HB2	2.00	0.43
1:A:327:VAL:O	1:A:331:GLU:CG	2.62	0.43
1:A:66:SER:HB2	1:A:74:MET:O	2.19	0.43
1:B:121:ILE:HG22	1:B:122:THR:N	2.34	0.43
1:H:6:ALA:N	1:H:94:LEU:O	2.48	0.43
1:G:325:ARG:CA	1:G:325:ARG:NE	2.82	0.42
1:A:191:LEU:HB2	1:H:186:LEU:HG	2.01	0.42
1:A:202:ARG:NH1	1:H:49:TYR:HB3	2.34	0.42
1:H:52:VAL:HG11	1:H:241:ASN:OD1	2.19	0.42
1:H:20:CYS:SG	1:H:324:GLN:NE2	2.92	0.42
1:A:152:ASN:ND2	1:A:326:VAL:HG22	2.33	0.42
1:A:175:LYS:CG	1:A:250:GLN:HB3	2.41	0.42
1:H:83:LEU:HD21	1:H:110:LYS:HG2	2.01	0.42
1:B:123:ALA:HB1	1:B:124:PRO:CD	2.49	0.42
1:G:257:THR:CG2	1:G:258:GLU:N	2.81	0.42
1:A:261:ASN:HB3	1:A:278:TYR:OH	2.19	0.42
1:G:64:GLU:C	1:G:65:ASN:CG	2.78	0.42
1:A:178:MET:O	1:G:311:LYS:HE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:THR:HG23	1:A:233:ILE:O	2.19	0.42
1:B:198:LEU:N	1:B:198:LEU:HD22	2.22	0.42
1:A:209:VAL:HA	1:G:284:VAL:HG12	2.01	0.42
1:H:12:ARG:N	3:H:340:NAD:O2A	2.48	0.42
1:G:163:VAL:O	1:G:167:LEU:HB2	2.19	0.42
1:H:3:ILE:HD13	1:H:337:TRP:CE3	2.54	0.42
1:H:217:LYS:O	1:H:219:VAL:N	2.41	0.42
1:A:262:GLU:HA	1:A:265:GLN:HB2	2.00	0.42
1:A:208:ILE:O	1:A:210:PRO:HD3	2.19	0.42
1:H:15:ARG:HD2	1:H:47:LEU:N	2.34	0.42
1:H:244:VAL:HG22	1:H:313:ILE:HG23	2.00	0.42
1:H:296:ILE:HD13	1:H:315:TRP:O	2.19	0.42
1:A:29:LEU:HD21	1:A:331:GLU:HA	2.01	0.42
1:B:11:GLY:HA2	3:B:340:NAD:H4B	2.01	0.42
2:D:56:PHE:CD2	2:D:57:PHE:N	2.86	0.42
1:B:93:ASP:CB	1:B:337:TRP:CZ2	3.02	0.42
1:G:42:THR:C	1:G:44:ALA:N	2.71	0.42
2:C:61:CYS:O	2:C:62:SER:C	2.57	0.42
1:B:332:LEU:C	1:B:332:LEU:CD2	2.87	0.42
1:H:299:SER:OG	1:H:300:SER:N	2.52	0.42
1:B:154:SER:OG	1:B:157:THR:CB	2.66	0.42
3:A:340:NAD:O5D	3:A:340:NAD:H2N	2.19	0.42
1:B:250:GLN:O	1:B:251:VAL:CG2	2.64	0.42
1:B:257:THR:N	1:B:304:VAL:CG2	2.83	0.42
1:G:80:ARG:O	1:G:82:PRO:HD3	2.19	0.42
1:H:144:HIS:CD2	1:H:336:LYS:O	2.72	0.42
1:A:159:CYS:CB	1:A:316:TYR:CG	3.03	0.42
1:H:41:ARG:HA	1:H:62:TYR:HD1	1.78	0.42
1:B:164:ALA:O	1:B:165:LYS:C	2.57	0.42
1:B:101:VAL:C	1:B:103:VAL:N	2.73	0.42
1:G:60:ILE:HG12	1:G:69:VAL:HG13	2.01	0.42
1:B:7:ILE:O	1:B:35:ASN:N	2.40	0.42
1:A:12:ARG:HG2	3:A:340:NAD:O2A	2.19	0.42
1:G:104:THR:HG22	1:G:106:GLU:H	1.85	0.42
1:B:309:LEU:HD12	1:B:310:VAL:H	1.84	0.42
1:G:188:GLN:OE1	1:G:236:ARG:HG2	2.19	0.42
1:H:6:ALA:CB	1:H:92:ILE:HG21	2.46	0.42
1:H:195:HIS:HE1	1:H:197:ASP:H	1.64	0.42
1:A:86:PRO:C	1:A:89:GLU:HG2	2.40	0.42
1:G:259:GLN:O	1:G:263:VAL:HG23	2.18	0.42
2:J:68:ALA:C	2:J:70:CYS:N	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:126:LYS:HA	1:G:126:LYS:HD2	1.91	0.42
1:H:168:HIS:O	1:H:172:GLY:N	2.53	0.42
1:A:309:LEU:C	1:A:309:LEU:HD23	2.40	0.42
1:A:310:VAL:CG1	1:A:311:LYS:N	2.81	0.42
1:B:180:THR:O	1:B:234:ALA:HB1	2.19	0.42
1:H:241:ASN:HD22	1:H:242:VAL:N	2.12	0.42
1:G:116:ALA:C	1:G:117:LYS:HD3	2.40	0.42
1:B:13:ILE:CG2	1:B:122:THR:HG21	2.48	0.42
1:H:200:ARG:CZ	2:J:72:ILE:HG23	2.50	0.42
1:G:215:ALA:HA	1:G:218:ALA:HB2	2.00	0.42
1:A:41:ARG:HB2	1:A:62:TYR:HE1	1.84	0.42
1:G:16:ASN:OD1	1:G:319:GLU:HB3	2.19	0.42
1:B:251:VAL:HG12	1:B:253:LYS:H	1.84	0.42
1:H:17:PHE:HA	1:H:20:CYS:HB2	2.02	0.42
1:B:95:VAL:HG11	1:B:111:HIS:ND1	2.35	0.42
1:H:223:ILE:O	1:H:223:ILE:HG22	2.20	0.42
1:A:206:VAL:HG23	1:A:207:ASN:CG	2.40	0.42
1:A:311:LYS:HZ3	1:G:177:THR:HG21	1.80	0.42
1:B:200:ARG:C	1:B:202:ARG:N	2.72	0.42
1:G:11:GLY:HA3	3:G:340:NAD:C4B	2.42	0.42
1:G:288:PHE:CE1	1:G:315:TRP:CE2	3.07	0.42
1:G:100:GLY:HA2	3:G:340:NAD:O3D	2.19	0.42
1:H:11:GLY:CA	1:H:15:ARG:HH12	2.32	0.42
1:G:174:ILE:CG2	1:G:175:LYS:HE2	2.49	0.42
1:G:29:LEU:N	1:G:29:LEU:HD23	2.35	0.42
1:A:97:GLU:HB3	1:A:121:ILE:HG23	2.02	0.42
1:G:237:VAL:CB	1:G:238:PRO:CD	2.97	0.42
1:H:133:TYR:CD1	1:H:133:TYR:N	2.88	0.42
1:B:259:GLN:O	1:B:262:GLU:N	2.52	0.42
1:A:44:ALA:O	1:A:46:LEU:N	2.51	0.42
1:G:101:VAL:HG22	1:G:102:PHE:N	2.34	0.42
1:G:155:CYS:SG	3:G:340:NAD:H5N	2.59	0.42
1:G:37:THR:HG22	3:G:340:NAD:N3A	2.35	0.42
1:G:99:THR:CB	1:G:101:VAL:HG13	2.50	0.42
1:B:233:ILE:CD1	1:B:234:ALA:N	2.83	0.42
1:B:242:VAL:HG13	1:B:316:TYR:O	2.19	0.42
1:H:177:THR:O	1:H:247:LEU:HD12	2.20	0.42
1:H:264:LEU:HD23	1:H:264:LEU:HA	1.73	0.42
3:B:340:NAD:H3D	2:D:73:TYR:CE2	2.55	0.42
1:H:112:ILE:HA	1:H:116:ALA:O	2.20	0.42
1:B:320:TRP:C	1:B:322:TYR:N	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:VAL:HG11	1:A:315:TRP:CZ3	2.54	0.42
1:A:233:ILE:HG22	1:A:234:ALA:N	2.34	0.42
1:G:138:ASN:O	1:G:140:SER:N	2.53	0.42
1:B:312:VAL:C	1:B:313:ILE:HD13	2.40	0.42
1:B:318:ASN:H	1:B:318:ASN:ND2	2.17	0.42
1:H:12:ARG:HB3	1:H:319:GLU:OE2	2.20	0.42
1:H:260:VAL:HG23	1:H:261:ASN:H	1.83	0.42
1:A:56:PHE:HD1	1:A:56:PHE:HA	1.68	0.42
1:B:46:LEU:N	1:B:46:LEU:CD2	2.82	0.42
1:H:111:HIS:O	1:H:114:ALA:HB3	2.20	0.42
1:B:89:GLU:N	1:B:89:GLU:OE1	2.52	0.42
1:H:41:ARG:CG	1:H:42:THR:N	2.82	0.42
1:B:277:LYS:HG2	1:B:278:TYR:N	2.35	0.42
1:G:272:MET:O	1:G:274:GLY:N	2.53	0.42
1:A:131:GLY:O	1:A:133:TYR:CG	2.72	0.42
1:B:142:TYR:CE2	1:B:333:ALA:HA	2.55	0.42
1:A:41:ARG:HG3	1:A:62:TYR:CZ	2.55	0.41
2:I:68:ALA:CA	2:I:71:LEU:HD11	2.35	0.41
1:G:187:ASP:HB3	2:I:73:TYR:CE1	2.55	0.41
1:A:185:THR:C	1:A:186:LEU:HD12	2.40	0.41
1:H:15:ARG:NE	1:H:46:LEU:HB2	2.34	0.41
1:H:318:ASN:O	1:H:322:TYR:HB3	2.19	0.41
1:A:29:LEU:HG	1:A:331:GLU:CD	2.40	0.41
1:A:326:VAL:C	1:A:328:ASP:H	2.23	0.41
1:A:337:TRP:CG	1:A:338:ALA:N	2.88	0.41
1:A:175:LYS:HE3	1:A:175:LYS:HB3	1.48	0.41
1:G:1:MET:CG	1:G:2:THR:H	2.32	0.41
1:A:247:LEU:HD12	1:A:248:VAL:C	2.40	0.41
1:A:41:ARG:HA	1:A:62:TYR:CE1	2.54	0.41
1:G:123:ALA:O	1:G:151:SER:HB2	2.20	0.41
1:G:159:CYS:O	1:G:161:ALA:N	2.53	0.41
1:G:223:ILE:HG21	1:G:226:LEU:HG	2.01	0.41
1:G:45:HIS:O	1:G:49:TYR:HD2	2.02	0.41
1:G:93:ASP:HB3	1:G:337:TRP:CE2	2.52	0.41
1:A:219:VAL:HG12	1:A:223:ILE:HD12	2.00	0.41
1:B:10:PHE:CE1	1:B:15:ARG:HA	2.55	0.41
1:A:285:SER:HB3	1:G:208:ILE:HB	2.02	0.41
1:H:231:ASN:OD1	1:H:232:GLY:N	2.53	0.41
1:B:6:ALA:O	1:B:95:VAL:HA	2.20	0.41
1:B:33:ALA:HB1	1:B:75:LYS:O	2.20	0.41
1:G:280:ASP:O	1:G:281:LEU:O	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ILE:HG12	1:H:186:LEU:CD2	2.50	0.41
1:B:183:SER:OG	1:B:241:ASN:C	2.59	0.41
1:B:247:LEU:HD12	1:B:248:VAL:N	2.35	0.41
1:A:28:ASP:HB2	1:A:334:ALA:HB1	2.02	0.41
1:A:13:ILE:HG23	1:A:323:SER:OG	2.21	0.41
1:A:24:ARG:CZ	1:A:327:VAL:HB	2.51	0.41
1:B:15:ARG:NH1	1:B:15:ARG:CG	2.60	0.41
1:H:59:ASP:O	1:H:70:ASN:OD1	2.38	0.41
1:B:263:VAL:HG13	1:B:264:LEU:N	2.34	0.41
2:D:67:ALA:O	2:D:71:LEU:HD21	2.19	0.41
1:H:7:ILE:CB	1:H:34:ILE:HG23	2.50	0.41
1:A:20:CYS:SG	1:A:320:TRP:CE2	3.14	0.41
3:B:340:NAD:C2D	2:D:73:TYR:CD2	3.00	0.41
2:D:54:GLU:C	2:D:56:PHE:N	2.73	0.41
1:A:272:MET:O	1:A:273:LYS:C	2.58	0.41
1:B:161:ALA:O	1:B:163:VAL:N	2.53	0.41
1:G:69:VAL:O	1:G:70:ASN:HB2	2.19	0.41
1:B:329:LEU:O	1:B:332:LEU:CB	2.69	0.41
1:B:154:SER:OG	1:B:157:THR:HB	2.19	0.41
1:A:178:MET:SD	1:A:179:THR:N	2.93	0.41
1:A:122:THR:O	3:A:340:NAD:H1D	2.21	0.41
1:G:12:ARG:HB3	3:G:340:NAD:O2N	2.20	0.41
1:B:305:MET:CB	1:B:309:LEU:HD23	2.51	0.41
1:H:21:TRP:C	1:H:23:GLY:H	2.23	0.41
1:H:31:VAL:HG12	1:H:74:MET:HG2	2.02	0.41
1:H:71:GLY:O	1:H:72:LYS:C	2.58	0.41
1:A:236:ARG:C	1:A:237:VAL:CG1	2.88	0.41
1:B:332:LEU:O	1:B:333:ALA:C	2.58	0.41
1:H:209:VAL:O	1:H:236:ARG:HB2	2.20	0.41
1:H:55:ARG:CG	1:H:56:PHE:N	2.84	0.41
1:A:222:VAL:C	1:A:224:PRO:HD3	2.40	0.41
1:A:325:ARG:HA	1:A:325:ARG:HE	1.81	0.41
1:A:250:GLN:HG2	1:A:251:VAL:N	2.36	0.41
1:G:236:ARG:NE	2:I:75:ASP:OD1	2.54	0.41
1:G:167:LEU:HD13	1:G:167:LEU:HA	1.57	0.41
1:H:94:LEU:HD12	1:H:95:VAL:H	1.86	0.41
1:G:120:LEU:CD1	1:G:150:ILE:HD13	2.51	0.41
1:A:266:LYS:HE2	1:A:266:LYS:HB3	1.66	0.41
1:A:45:HIS:HD2	1:H:198:LEU:HG	1.85	0.41
1:G:183:SER:CB	1:G:239:THR:O	2.69	0.41
1:H:299:SER:O	1:H:300:SER:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ARG:HA	1:A:62:TYR:CD1	2.55	0.41
1:G:285:SER:HA	1:G:315:TRP:CZ3	2.56	0.41
1:G:18:LEU:HD23	1:G:47:LEU:HD11	2.02	0.41
1:H:121:ILE:CG2	1:H:122:THR:N	2.82	0.41
1:H:247:LEU:HG	1:H:248:VAL:N	2.30	0.41
1:H:13:ILE:HB	3:H:340:NAD:O1N	2.20	0.41
1:G:83:LEU:C	1:G:114:ALA:HB2	2.41	0.41
1:H:85:LEU:HA	1:H:86:PRO:HD2	1.25	0.41
1:B:32:VAL:O	1:B:74:MET:CB	2.68	0.41
1:A:168:HIS:ND1	1:A:173:ILE:CB	2.83	0.41
1:H:66:SER:OG	1:H:67:ILE:N	2.53	0.41
1:B:170:ASN:ND2	1:B:263:VAL:HG21	2.35	0.41
1:A:184:TYR:CD1	1:A:184:TYR:C	2.93	0.41
1:B:130:VAL:HG23	1:B:149:VAL:O	2.21	0.41
1:B:241:ASN:HD22	1:B:242:VAL:H	1.68	0.41
1:H:103:VAL:HG23	1:H:104:THR:N	2.36	0.41
1:H:174:ILE:HG22	1:H:175:LYS:N	2.35	0.41
1:H:19:ARG:HA	1:H:56:PHE:HZ	1.84	0.41
1:G:306:ASP:O	1:G:308:ASP:N	2.49	0.41
1:H:224:PRO:C	1:H:226:LEU:H	2.23	0.41
1:A:45:HIS:O	1:A:45:HIS:CD2	2.74	0.41
1:A:262:GLU:HG3	1:A:265:GLN:OE1	2.20	0.41
1:G:276:ILE:HG12	1:G:295:SER:HB3	2.03	0.41
1:G:325:ARG:NE	1:G:325:ARG:HA	2.35	0.41
1:A:248:VAL:HG11	1:G:177:THR:HG21	2.03	0.41
1:G:325:ARG:CA	1:G:325:ARG:HE	2.34	0.41
1:G:19:ARG:HG3	1:G:47:LEU:HD11	2.02	0.41
1:B:233:ILE:O	1:B:234:ALA:HB2	2.21	0.41
1:H:121:ILE:HG22	1:H:123:ALA:O	2.21	0.41
1:A:190:ILE:HG22	1:H:190:ILE:HG23	2.02	0.41
1:H:247:LEU:CG	1:H:248:VAL:N	2.84	0.41
1:H:248:VAL:O	1:H:249:VAL:HG13	2.21	0.41
1:A:17:PHE:CE2	1:A:327:VAL:HG22	2.55	0.41
1:A:6:ALA:CB	1:A:33:ALA:HB3	2.50	0.41
1:A:226:LEU:O	1:A:229:LYS:CG	2.68	0.41
1:A:22:PHE:C	1:A:24:ARG:H	2.25	0.41
1:G:79:ASP:OD2	1:G:84:ASN:HB2	2.21	0.41
1:G:167:LEU:O	1:G:172:GLY:N	2.52	0.41
1:A:277:LYS:CB	1:A:296:ILE:HG13	2.45	0.41
1:A:156:THR:HB	1:A:215:ALA:HB1	2.02	0.41
1:A:163:VAL:O	1:A:164:ALA:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:VAL:HG13	1:A:316:TYR:HE1	1.83	0.41
1:H:32:VAL:O	1:H:33:ALA:HB2	2.21	0.41
1:B:159:CYS:O	1:B:295:SER:OG	2.39	0.41
1:B:265:GLN:HB2	1:B:278:TYR:CE2	2.56	0.41
1:G:200:ARG:CZ	2:I:72:ILE:HG12	2.51	0.41
1:G:103:VAL:HG23	1:G:103:VAL:O	2.20	0.41
1:H:168:HIS:HA	1:H:173:ILE:H	1.85	0.41
1:G:261:ASN:HD22	1:G:261:ASN:N	2.19	0.41
1:B:179:THR:HG22	1:B:180:THR:N	2.35	0.41
1:G:7:ILE:HB	1:G:34:ILE:HG22	2.02	0.41
1:A:281:LEU:CD2	1:A:282:PRO:HD2	2.50	0.41
1:H:142:TYR:HD1	1:H:143:ARG:N	2.19	0.41
1:A:147:PHE:CD1	1:A:147:PHE:N	2.89	0.41
1:A:237:VAL:HA	1:A:238:PRO:HD3	1.88	0.41
2:I:60:TYR:CA	2:I:63:GLU:HG2	2.50	0.41
1:B:286:SER:HB3	1:H:207:ASN:ND2	2.36	0.41
1:B:259:GLN:HA	1:B:262:GLU:HB2	2.02	0.41
1:G:326:VAL:C	1:G:328:ASP:N	2.74	0.40
1:G:318:ASN:ND2	3:G:340:NAD:N7N	2.64	0.40
1:H:250:GLN:CG	1:H:251:VAL:N	2.85	0.40
1:H:256:ILE:HG13	1:H:257:THR:N	2.30	0.40
1:H:9:GLY:O	1:H:11:GLY:N	2.45	0.40
1:G:332:LEU:HA	1:G:332:LEU:HD23	1.75	0.40
1:A:138:ASN:O	1:A:139:ASP:C	2.59	0.40
1:A:19:ARG:HG2	1:A:56:PHE:CD2	2.54	0.40
1:A:229:LYS:O	1:A:230:LEU:HD23	2.20	0.40
1:A:3:ILE:HD13	1:A:334:ALA:CA	2.51	0.40
1:A:306:ASP:O	1:A:308:ASP:N	2.52	0.40
1:A:284:VAL:HB	1:G:207:ASN:CG	2.41	0.40
1:H:41:ARG:CA	1:H:62:TYR:HD1	2.33	0.40
1:B:81:ASN:OD1	1:B:82:PRO:CD	2.69	0.40
1:A:81:ASN:OD1	1:A:83:LEU:HD12	2.21	0.40
1:H:105:ALA:HB2	1:H:130:VAL:CG1	2.51	0.40
1:B:175:LYS:HD3	1:H:306:ASP:HB3	2.03	0.40
1:A:65:ASN:O	1:A:66:SER:CB	2.66	0.40
1:G:113:GLN:C	1:G:115:GLY:N	2.74	0.40
1:B:187:ASP:HB2	2:D:71:LEU:O	2.21	0.40
1:B:142:TYR:CE2	1:B:332:LEU:HD22	2.56	0.40
1:H:35:ASN:HA	1:H:77:VAL:O	2.22	0.40
1:G:18:LEU:O	1:G:20:CYS:N	2.53	0.40
1:A:49:TYR:OH	1:B:281:LEU:CD1	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:TRP:O	1:A:24:ARG:N	2.50	0.40
1:B:143:ARG:CD	1:B:146:ASP:OD1	2.59	0.40
1:A:97:GLU:O	1:A:97:GLU:OE1	2.40	0.40
1:B:53:LEU:HD13	1:B:320:TRP:HZ3	1.87	0.40
1:A:83:LEU:HD11	1:A:110:LYS:HZ3	1.84	0.40
1:A:298:ASP:O	1:A:300:SER:N	2.55	0.40
1:G:159:CYS:C	1:G:161:ALA:H	2.25	0.40
1:A:48:GLU:HB3	1:A:49:TYR:HD2	1.84	0.40
1:B:234:ALA:C	1:B:235:LEU:HD12	2.41	0.40
1:H:175:LYS:HE3	1:H:175:LYS:HB2	1.79	0.40
1:H:247:LEU:O	1:H:311:LYS:HA	2.21	0.40
1:G:7:ILE:HB	1:G:34:ILE:HG23	2.02	0.40
1:B:298:ASP:O	1:B:299:SER:C	2.60	0.40
1:G:109:SER:C	1:G:111:HIS:N	2.74	0.40
1:B:54:GLY:O	1:B:55:ARG:O	2.38	0.40
1:H:280:ASP:HA	1:H:299:SER:OG	2.22	0.40
1:A:318:ASN:OD1	1:A:319:GLU:N	2.54	0.40
1:G:152:ASN:HD22	1:G:326:VAL:HG23	1.85	0.40
1:H:183:SER:HB2	1:H:239:THR:C	2.41	0.40
1:H:21:TRP:O	1:H:24:ARG:HG2	2.22	0.40
1:H:260:VAL:C	1:H:262:GLU:N	2.75	0.40
1:A:174:ILE:CG2	1:A:175:LYS:NZ	2.85	0.40
2:D:57:PHE:CZ	1:G:38:SER:HA	2.57	0.40
1:G:85:LEU:HA	1:G:86:PRO:HD2	1.64	0.40
1:H:6:ALA:O	1:H:96:ILE:N	2.41	0.40
1:A:156:THR:HG23	1:A:316:TYR:HH	1.85	0.40
1:H:41:ARG:CA	1:H:62:TYR:CD1	3.01	0.40
1:G:105:ALA:O	1:G:108:ALA:HB3	2.21	0.40
1:H:28:ASP:O	1:H:334:ALA:HB1	2.22	0.40

There are no symmetry-related clashes.

## 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	A	336/339 (99%)	234 (70%)	75 (22%)	27 (8%)	1	8
1	B	336/339 (99%)	231 (69%)	70 (21%)	35 (10%)	1	4
1	G	336/339 (99%)	220 (66%)	74 (22%)	42 (12%)	0	2
1	H	336/339 (99%)	222 (66%)	82 (24%)	32 (10%)	1	6
2	C	20/25 (80%)	12 (60%)	6 (30%)	2 (10%)	1	5
2	D	21/25 (84%)	15 (71%)	3 (14%)	3 (14%)	0	1
2	I	20/25 (80%)	14 (70%)	5 (25%)	1 (5%)	3	19
2	J	21/25 (84%)	13 (62%)	5 (24%)	3 (14%)	0	1
All	All	1426/1456 (98%)	961 (67%)	320 (22%)	145 (10%)	1	5

All (145) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	105	ALA
1	A	146	ASP
1	A	155	CYS
1	A	206	VAL
1	A	242	VAL
1	A	306	ASP
1	B	106	GLU
1	B	233	ILE
1	B	271	THR
1	B	282	PRO
1	B	285	SER
1	B	286	SER
1	B	337	TRP
2	C	56	PHE
2	C	62	SER
2	D	57	PHE
1	G	2	THR
1	G	113	GLN
1	G	250	GLN
1	G	257	THR
1	G	270	THR
1	G	273	LYS
1	G	285	SER
1	G	286	SER
1	G	306	ASP
1	G	337	TRP

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Mol	Chain	Res	Type
1	H	24	ARG
1	H	32	VAL
1	H	45	HIS
1	H	64	GLU
1	H	165	LYS
1	H	169	ASP
1	H	215	ALA
1	H	231	ASN
1	H	242	VAL
2	I	68	ALA
1	A	2	THR
1	A	45	HIS
1	A	51	SER
1	A	66	SER
1	A	139	ASP
1	A	225	GLU
1	B	25	GLN
1	B	107	GLY
1	B	139	ASP
1	B	153	ALA
1	B	220	ALA
1	B	238	PRO
1	B	273	LYS
1	B	300	SER
1	B	323	SER
2	D	74	ASP
1	G	86	PRO
1	G	110	LYS
1	G	114	ALA
1	G	144	HIS
1	G	160	LEU
1	G	172	GLY
1	G	203	ALA
1	G	233	ILE
1	G	241	ASN
1	G	242	VAL
1	G	248	VAL
1	G	300	SER
1	G	323	SER
1	H	22	PHE
1	H	72	LYS
1	H	155	CYS

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Mol	Chain	Res	Type
1	H	218	ALA
1	H	221	LEU
1	H	222	VAL
1	H	241	ASN
2	J	56	PHE
1	A	22	PHE
1	A	84	ASN
1	A	169	ASP
1	A	227	LYS
1	B	39	ASP
1	B	221	LEU
1	B	242	VAL
1	B	301	LEU
1	B	316	TYR
1	G	48	GLU
1	G	65	ASN
1	G	87	TRP
1	G	165	LYS
1	G	186	LEU
1	G	319	GLU
1	G	334	ALA
1	H	86	PRO
1	H	195	HIS
1	H	203	ALA
1	H	327	VAL
2	J	69	GLU
1	A	21	TRP
1	A	25	GLN
1	A	31	VAL
1	B	70	ASN
1	B	101	VAL
1	B	160	LEU
1	B	212	THR
1	B	292	ASP
1	G	37	THR
1	G	281	LEU
1	G	316	TYR
1	H	10	PHE
1	H	305	MET
1	H	319	GLU
1	A	9	GLY
1	A	177	THR

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Mol	Chain	Res	Type
1	A	224	PRO
1	A	238	PRO
1	B	9	GLY
1	B	22	PHE
1	B	86	PRO
1	B	267	ALA
1	G	11	GLY
1	G	208	ILE
1	G	282	PRO
1	H	178	MET
1	H	200	ARG
2	J	55	PRO
1	A	34	ILE
1	A	109	SER
1	B	113	GLN
1	B	299	SER
2	D	54	GLU
1	G	115	GLY
1	H	46	LEU
1	H	141	GLU
1	H	224	PRO
1	H	240	PRO
1	H	318	ASN
1	A	23	GLY
1	B	137	VAL
1	H	9	GLY
1	B	251	VAL
1	G	137	VAL
1	G	253	LYS
1	H	219	VAL
1	G	130	VAL
1	G	307	GLY
1	G	327	VAL
1	B	150	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	284/284 (100%)	213 (75%)	71 (25%)	1	3
1	B	284/284 (100%)	208 (73%)	76 (27%)	0	2
1	G	284/284 (100%)	208 (73%)	76 (27%)	0	2
1	H	284/284 (100%)	223 (78%)	61 (22%)	1	5
2	C	19/22 (86%)	16 (84%)	3 (16%)	3	15
2	D	20/22 (91%)	17 (85%)	3 (15%)	3	17
2	I	19/22 (86%)	17 (90%)	2 (10%)	8	33
2	J	20/22 (91%)	18 (90%)	2 (10%)	9	36
All	All	1214/1224 (99%)	920 (76%)	294 (24%)	1	3

All (294) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	5	VAL
1	A	10	PHE
1	A	13	ILE
1	A	16	ASN
1	A	22	PHE
1	A	26	ASN
1	A	36	ASN
1	A	46	LEU
1	A	49	TYR
1	A	52	VAL
1	A	55	ARG
1	A	56	PHE
1	A	59	ASP
1	A	62	TYR
1	A	65	ASN
1	A	66	SER
1	A	69	VAL
1	A	74	MET
1	A	76	ILE
1	A	83	LEU
1	A	85	LEU
1	A	87	TRP
1	A	89	GLU
1	A	95	VAL
1	A	97	GLU
1	A	104	THR

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Mol	Chain	Res	Type
1	A	112	ILE
1	A	117	LYS
1	A	119	VAL
1	A	140	SER
1	A	143	ARG
1	A	151	SER
1	A	155	CYS
1	A	156	THR
1	A	158	ASN
1	A	159	CYS
1	A	167	LEU
1	A	174	ILE
1	A	175	LYS
1	A	180	THR
1	A	183	SER
1	A	185	THR
1	A	190	ILE
1	A	192	ASP
1	A	198	LEU
1	A	217	LYS
1	A	227	LYS
1	A	241	ASN
1	A	243	SER
1	A	244	VAL
1	A	247	LEU
1	A	248	VAL
1	A	249	VAL
1	A	253	LYS
1	A	256	ILE
1	A	257	THR
1	A	262	GLU
1	A	266	LYS
1	A	270	THR
1	A	275	ILE
1	A	277	LYS
1	A	284	VAL
1	A	285	SER
1	A	286	SER
1	A	300	SER
1	A	303	LEU
1	A	305	MET
1	A	311	LYS

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Mol	Chain	Res	Type
1	A	324	GLN
1	A	327	VAL
1	B	3	ILE
1	B	4	ARG
1	B	5	VAL
1	B	10	PHE
1	B	15	ARG
1	B	25	GLN
1	B	27	THR
1	B	28	ASP
1	B	36	ASN
1	B	41	ARG
1	B	45	HIS
1	B	46	LEU
1	B	50	ASP
1	B	62	TYR
1	B	65	ASN
1	B	67	ILE
1	B	70	ASN
1	B	74	MET
1	B	77	VAL
1	B	78	CYS
1	B	79	ASP
1	B	80	ARG
1	B	92	ILE
1	B	97	GLU
1	B	101	VAL
1	B	103	VAL
1	B	104	THR
1	B	112	ILE
1	B	122	THR
1	B	126	LYS
1	B	128	GLU
1	B	130	VAL
1	B	132	THR
1	B	135	ILE
1	B	143	ARG
1	B	144	HIS
1	B	145	GLU
1	B	146	ASP
1	B	149	VAL
1	B	152	ASN

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Mol	Chain	Res	Type
1	B	155	CYS
1	B	156	THR
1	B	160	LEU
1	B	169	ASP
1	B	171	PHE
1	B	177	THR
1	B	178	MET
1	B	180	THR
1	B	182	HIS
1	B	186	LEU
1	B	188	GLN
1	B	190	ILE
1	B	196	ARG
1	B	198	LEU
1	B	211	THR
1	B	212	THR
1	B	219	VAL
1	B	221	LEU
1	B	222	VAL
1	B	230	LEU
1	B	237	VAL
1	B	239	THR
1	B	241	ASN
1	B	252	GLU
1	B	253	LYS
1	B	256	ILE
1	B	260	VAL
1	B	278	TYR
1	B	279	SER
1	B	293	GLU
1	B	297	VAL
1	B	305	MET
1	B	311	LYS
1	B	318	ASN
1	B	328	ASP
1	B	332	LEU
2	C	54	GLU
2	C	64	ASN
2	C	69	GLU
2	D	54	GLU
2	D	66	ASP
2	D	74	ASP

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Mol	Chain	Res	Type
1	G	1	MET
1	G	5	VAL
1	G	20	CYS
1	G	22	PHE
1	G	27	THR
1	G	28	ASP
1	G	32	VAL
1	G	34	ILE
1	G	37	THR
1	G	49	TYR
1	G	51	SER
1	G	56	PHE
1	G	59	ASP
1	G	60	ILE
1	G	64	GLU
1	G	65	ASN
1	G	68	THR
1	G	69	VAL
1	G	77	VAL
1	G	80	ARG
1	G	88	LYS
1	G	97	GLU
1	G	101	VAL
1	G	103	VAL
1	G	106	GLU
1	G	109	SER
1	G	118	LYS
1	G	130	VAL
1	G	139	ASP
1	G	143	ARG
1	G	146	ASP
1	G	149	VAL
1	G	150	ILE
1	G	155	CYS
1	G	158	ASN
1	G	159	CYS
1	G	160	LEU
1	G	166	VAL
1	G	167	LEU
1	G	169	ASP
1	G	171	PHE
1	G	175	LYS

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Mol	Chain	Res	Type
1	G	177	THR
1	G	180	THR
1	G	183	SER
1	G	189	ARG
1	G	190	ILE
1	G	191	LEU
1	G	196	ARG
1	G	197	ASP
1	G	199	ARG
1	G	208	ILE
1	G	213	THR
1	G	217	LYS
1	G	222	VAL
1	G	225	GLU
1	G	230	LEU
1	G	235	LEU
1	G	236	ARG
1	G	241	ASN
1	G	247	LEU
1	G	249	VAL
1	G	258	GLU
1	G	259	GLN
1	G	264	LEU
1	G	268	SER
1	G	280	ASP
1	G	285	SER
1	G	297	VAL
1	G	300	SER
1	G	305	MET
1	G	308	ASP
1	G	318	ASN
1	G	323	SER
1	G	332	LEU
1	G	336	LYS
1	H	1	MET
1	H	5	VAL
1	H	13	ILE
1	H	16	ASN
1	H	24	ARG
1	H	27	THR
1	H	39	ASP
1	H	45	HIS

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Mol	Chain	Res	Type
1	H	48	GLU
1	H	56	PHE
1	H	59	ASP
1	H	62	TYR
1	H	65	ASN
1	H	72	LYS
1	H	74	MET
1	H	75	LYS
1	H	78	CYS
1	H	84	ASN
1	H	89	GLU
1	H	95	VAL
1	H	97	GLU
1	H	101	VAL
1	H	104	THR
1	H	112	ILE
1	H	113	GLN
1	H	119	VAL
1	H	126	LYS
1	H	132	THR
1	H	141	GLU
1	H	144	HIS
1	H	145	GLU
1	H	149	VAL
1	H	155	CYS
1	H	159	CYS
1	H	165	LYS
1	H	169	ASP
1	H	178	MET
1	H	190	ILE
1	H	194	SER
1	H	196	ARG
1	H	198	LEU
1	H	217	LYS
1	H	221	LEU
1	H	222	VAL
1	H	225	GLU
1	H	237	VAL
1	H	239	THR
1	H	241	ASN
1	H	244	VAL
1	H	248	VAL

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Mol	Chain	Res	Type
1	H	253	LYS
1	H	256	ILE
1	H	261	ASN
1	H	271	THR
1	H	279	SER
1	H	294	SER
1	H	298	ASP
1	H	303	LEU
1	H	318	ASN
1	H	324	GLN
1	H	328	ASP
2	I	73	TYR
2	I	75	ASP
2	J	54	GLU
2	J	66	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	45	HIS
1	A	111	HIS
1	A	152	ASN
1	A	158	ASN
1	A	241	ASN
1	A	261	ASN
1	A	318	ASN
1	A	324	GLN
1	B	36	ASN
1	B	144	HIS
1	B	170	ASN
1	B	195	HIS
1	B	241	ASN
1	B	269	GLN
1	B	318	ASN
2	C	64	ASN
1	G	45	HIS
1	G	81	ASN
1	G	152	ASN
1	G	269	GLN
1	G	318	ASN
1	G	324	GLN

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Mol	Chain	Res	Type
1	H	65	ASN
1	H	152	ASN
1	H	182	HIS
1	H	241	ASN
1	H	259	GLN
1	H	324	GLN

### 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 ⓘ

4 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	A	340	-	38,48,48	1.02	2 (5%)	47,73,73	2.30	11 (23%)
3	NAD	B	340	-	38,48,48	1.01	2 (5%)	47,73,73	2.29	9 (19%)
3	NAD	G	340	-	38,48,48	1.07	4 (10%)	47,73,73	2.71	10 (21%)
3	NAD	H	340	-	38,48,48	1.02	3 (7%)	47,73,73	1.89	6 (12%)

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	A	340	-	-	0/22/62/62	0/5/5/5
3	NAD	B	340	-	-	0/22/62/62	0/5/5/5
3	NAD	G	340	-	-	0/22/62/62	0/5/5/5
3	NAD	H	340	-	-	0/22/62/62	0/5/5/5

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	340	NAD	C3N-C7N	-2.89	1.46	1.50
3	G	340	NAD	C8A-N7A	-2.21	1.30	1.34
3	B	340	NAD	C8A-N7A	-2.18	1.30	1.34
3	H	340	NAD	C8A-N7A	-2.07	1.30	1.34
3	G	340	NAD	O4B-C1B	2.39	1.44	1.41
3	A	340	NAD	O4B-C1B	2.59	1.44	1.41
3	H	340	NAD	O4D-C1D	2.65	1.44	1.41
3	H	340	NAD	O4B-C1B	2.84	1.44	1.41
3	A	340	NAD	O4D-C1D	3.14	1.45	1.41
3	G	340	NAD	O4D-C1D	3.23	1.45	1.41
3	B	340	NAD	O4B-C1B	3.52	1.45	1.41

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	340	NAD	C4D-O4D-C1D	-8.99	99.84	109.72
3	H	340	NAD	N3A-C2A-N1A	-8.93	122.05	128.89
3	B	340	NAD	PN-O3-PA	-8.07	110.05	132.73
3	A	340	NAD	PN-O3-PA	-7.64	111.28	132.73
3	G	340	NAD	PN-O3-PA	-7.59	111.42	132.73
3	B	340	NAD	N3A-C2A-N1A	-7.27	123.33	128.89
3	B	340	NAD	C4D-O4D-C1D	-6.80	102.25	109.72
3	A	340	NAD	N3A-C2A-N1A	-6.77	123.71	128.89
3	G	340	NAD	N3A-C2A-N1A	-6.49	123.92	128.89
3	A	340	NAD	O4D-C1D-N1N	-6.35	101.16	108.13
3	H	340	NAD	PN-O3-PA	-4.50	120.09	132.73
3	G	340	NAD	O7N-C7N-C3N	-4.32	114.87	119.59
3	G	340	NAD	C4A-C5A-N7A	-3.99	105.81	109.48
3	B	340	NAD	O4D-C1D-N1N	-3.96	103.78	108.13
3	A	340	NAD	C4A-C5A-N7A	-2.85	106.85	109.48
3	A	340	NAD	C5N-C4N-C3N	-2.81	116.80	120.33
3	B	340	NAD	O5D-C5D-C4D	-2.51	99.87	109.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	340	NAD	O7N-C7N-C3N	-2.43	116.94	119.59
3	A	340	NAD	O4D-C4D-C5D	-2.40	100.73	109.32
3	A	340	NAD	C1B-N9A-C4A	-2.31	123.45	126.94
3	H	340	NAD	C4A-C5A-N7A	-2.23	107.42	109.48
3	B	340	NAD	C4A-C5A-N7A	-2.10	107.55	109.48
3	G	340	NAD	C2B-C1B-N9A	2.11	117.52	114.29
3	A	340	NAD	C2D-C3D-C4D	2.20	107.14	102.61
3	B	340	NAD	O7N-C7N-C3N	2.26	122.06	119.59
3	H	340	NAD	O7N-C7N-C3N	2.34	122.14	119.59
3	G	340	NAD	O3-PA-O5B	2.35	109.18	102.94
3	A	340	NAD	O3-PN-O5D	2.46	109.45	102.94
3	B	340	NAD	O4B-C4B-C3B	2.49	110.17	105.15
3	H	340	NAD	O3-PN-O5D	2.50	109.56	102.94
3	B	340	NAD	O4B-C1B-N9A	2.95	114.27	108.10
3	G	340	NAD	O3-PN-O5D	3.68	112.70	102.94
3	A	340	NAD	C3N-C7N-N7N	4.11	122.32	117.82
3	H	340	NAD	O3-PA-O5B	4.13	113.90	102.94
3	G	340	NAD	C3N-C7N-N7N	4.53	122.78	117.82
3	G	340	NAD	O4D-C1D-N1N	6.94	115.76	108.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 85 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	340	NAD	18	0
3	B	340	NAD	20	0
3	G	340	NAD	30	0
3	H	340	NAD	17	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 ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	338/339 (99%)	-0.55	0 100 100	2, 20, 39, 58	0
1	B	338/339 (99%)	-0.48	1 (0%) 94 94	6, 25, 44, 68	0
1	G	338/339 (99%)	-0.52	1 (0%) 94 94	4, 22, 41, 69	0
1	H	338/339 (99%)	-0.43	0 100 100	5, 27, 52, 66	0
2	C	22/25 (88%)	-0.08	1 (4%) 37 30	10, 28, 49, 67	0
2	D	23/25 (92%)	0.27	1 (4%) 39 32	26, 46, 67, 95	0
2	I	22/25 (88%)	-0.31	0 100 100	9, 25, 51, 54	0
2	J	23/25 (92%)	0.03	2 (8%) 13 10	17, 40, 70, 86	0
All	All	1442/1456 (99%)	-0.46	6 (0%) 93 92	2, 24, 48, 95	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	53	THR	6.1
2	J	53	THR	3.0
2	C	55	PRO	2.3
2	J	63	GLU	2.3
1	G	338	ALA	2.2
1	B	338	ALA	2.2

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.



## 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAD	G	340	44/44	0.95	0.17	0.11	9,15,26,34	0
3	NAD	B	340	44/44	0.94	0.19	0.02	10,25,43,45	0
3	NAD	A	340	44/44	0.95	0.16	-0.20	10,17,29,33	0
3	NAD	H	340	44/44	0.96	0.14	-0.85	10,23,30,34	0

## 6.5 Other polymers

There are no such residues in this entry.