



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 05:50 PM GMT

PDB ID : 3A2C  
Title : Crystal structure of a pyrazolopyrimidine inhibitor complex bound to MAP-KAP Kinase-2 (MK2)  
Authors : Fujino, A.; Takimoto-Kamimura, M.  
Deposited on : 2009-05-12  
Resolution : 2.90 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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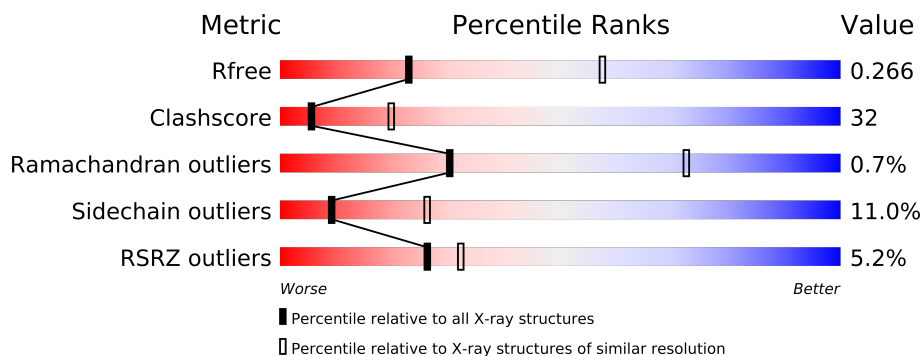
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	324	
1	B	324	
1	C	324	
1	D	324	
1	E	324	
1	F	324	
1	G	324	
1	H	324	
1	I	324	
1	J	324	
1	K	324	
1	L	324	

The following table lists non-polymeric compounds that are outliers for geometric or electron-

density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	PDY	A	2	-	X
2	PDY	D	2	-	X
2	PDY	E	1	-	X
2	PDY	E	2	-	X
2	PDY	G	2	-	X
2	PDY	L	2	-	X

## 2 Entry composition

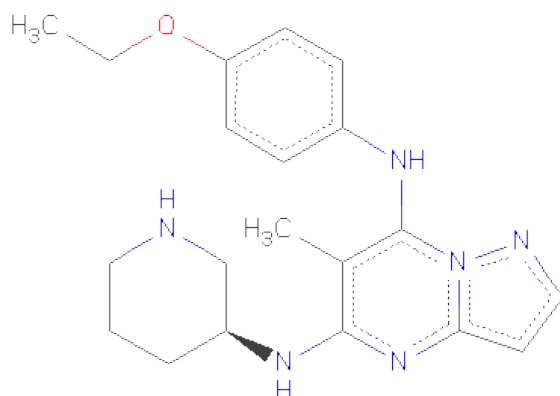
There are 3 unique types of molecules in this entry. The entry contains 27440 atoms, of which 0 are hydrogen and 0 are deuterium.

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 MAP kinase-activated protein kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2218	1415	384	402	17			
1	B	277	Total	C	N	O	S	0	0	0
			2240	1426	388	409	17			
1	C	273	Total	C	N	O	S	0	0	0
			2207	1409	380	401	17			
1	D	277	Total	C	N	O	S	0	0	0
			2244	1430	389	408	17			
1	E	276	Total	C	N	O	S	0	0	0
			2234	1425	385	407	17			
1	F	287	Total	C	N	O	S	0	0	0
			2316	1476	401	422	17			
1	G	273	Total	C	N	O	S	0	0	0
			2210	1411	381	401	17			
1	H	275	Total	C	N	O	S	0	0	0
			2226	1421	385	403	17			
1	I	275	Total	C	N	O	S	0	0	0
			2225	1420	384	404	17			
1	J	275	Total	C	N	O	S	0	0	0
			2225	1420	384	404	17			
1	K	273	Total	C	N	O	S	0	0	0
			2208	1409	381	401	17			
1	L	276	Total	C	N	O	S	0	0	0
			2234	1425	385	407	17			

- Molecule 2 is N 7 -(4-ETHOXYPHENYL)-6-METHYL-N 5 -[(3S)-PIPERIDIN-3-YL]PYRAZOLO[1,5-A]PYRIMIDINE-5,7-DIAMINE (three-letter code: PDY) (formula: C<sub>20</sub>H<sub>26</sub>N<sub>6</sub>O).



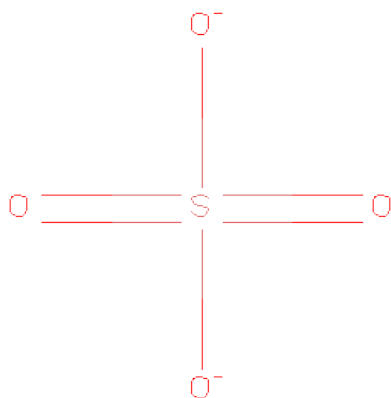
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			27	20	6	1		
2	A	1	Total	C	N	O	0	0
			27	20	6	1		
2	B	1	Total	C	N	O	0	0
			27	20	6	1		
2	B	1	Total	C	N	O	0	0
			27	20	6	1		
2	C	1	Total	C	N	O	0	0
			27	20	6	1		
2	C	1	Total	C	N	O	0	0
			27	20	6	1		
2	D	1	Total	C	N	O	0	0
			27	20	6	1		
2	D	1	Total	C	N	O	0	0
			27	20	6	1		
2	E	1	Total	C	N	O	0	0
			27	20	6	1		
2	E	1	Total	C	N	O	0	0
			27	20	6	1		
2	F	1	Total	C	N	O	0	0
			27	20	6	1		
2	F	1	Total	C	N	O	0	0
			27	20	6	1		
2	G	1	Total	C	N	O	0	0
			27	20	6	1		
2	G	1	Total	C	N	O	0	0
			27	20	6	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	H	1	Total	C	N	O	0	0
			27	20	6	1		
2	H	1	Total	C	N	O	0	0
			27	20	6	1		
2	I	1	Total	C	N	O	0	0
			27	20	6	1		
2	I	1	Total	C	N	O	0	0
			27	20	6	1		
2	J	1	Total	C	N	O	0	0
			27	20	6	1		
2	J	1	Total	C	N	O	0	0
			27	20	6	1		
2	K	1	Total	C	N	O	0	0
			27	20	6	1		
2	K	1	Total	C	N	O	0	0
			27	20	6	1		
2	L	1	Total	C	N	O	0	0
			27	20	6	1		
2	L	1	Total	C	N	O	0	0
			27	20	6	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



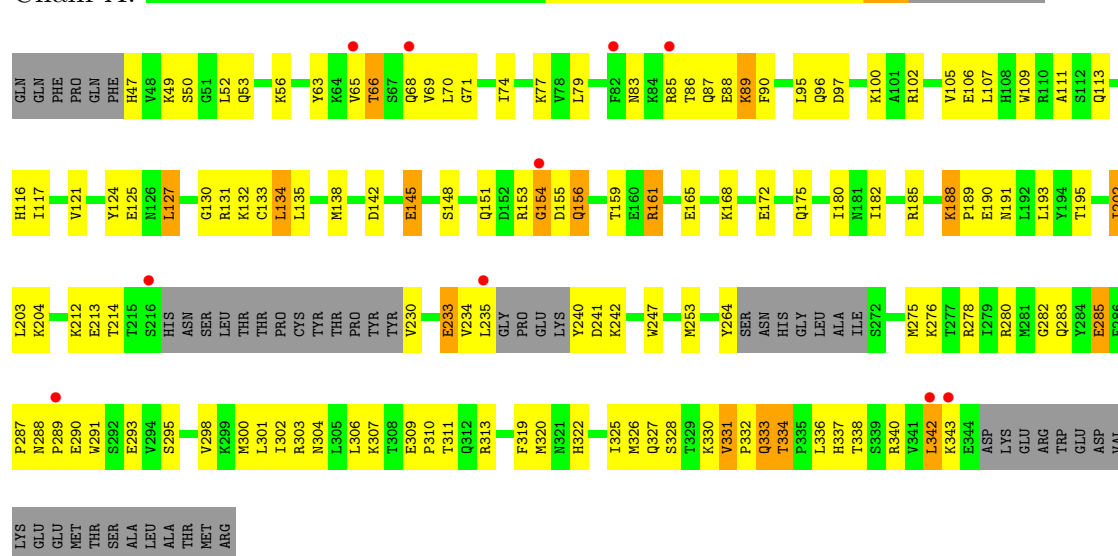
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	O	S	0	0
			5	4	1		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

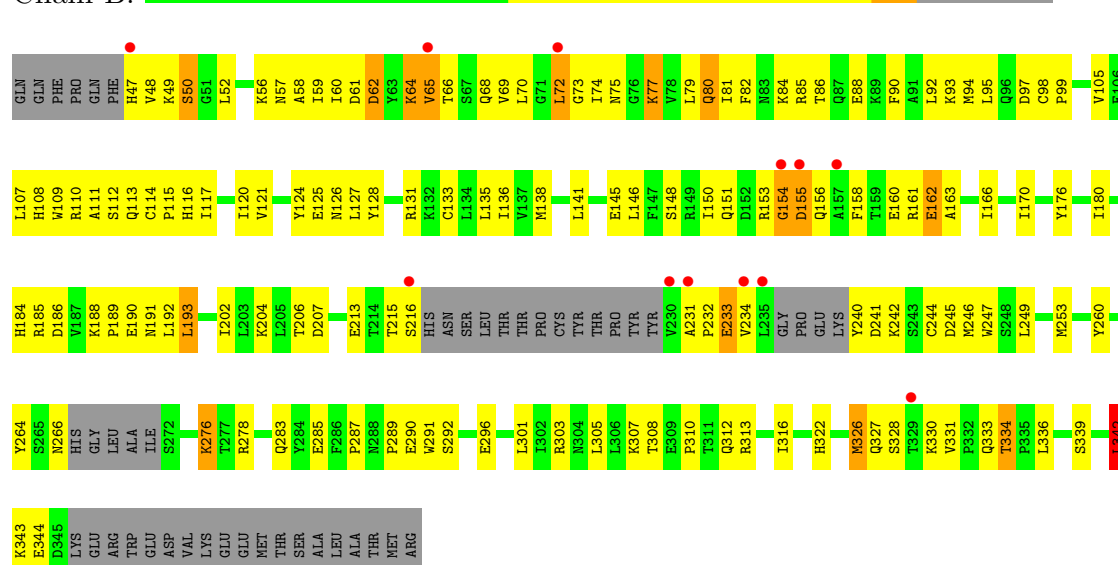
#### • Molecule 1: MAP kinase-activated protein kinase 2

Chain A:

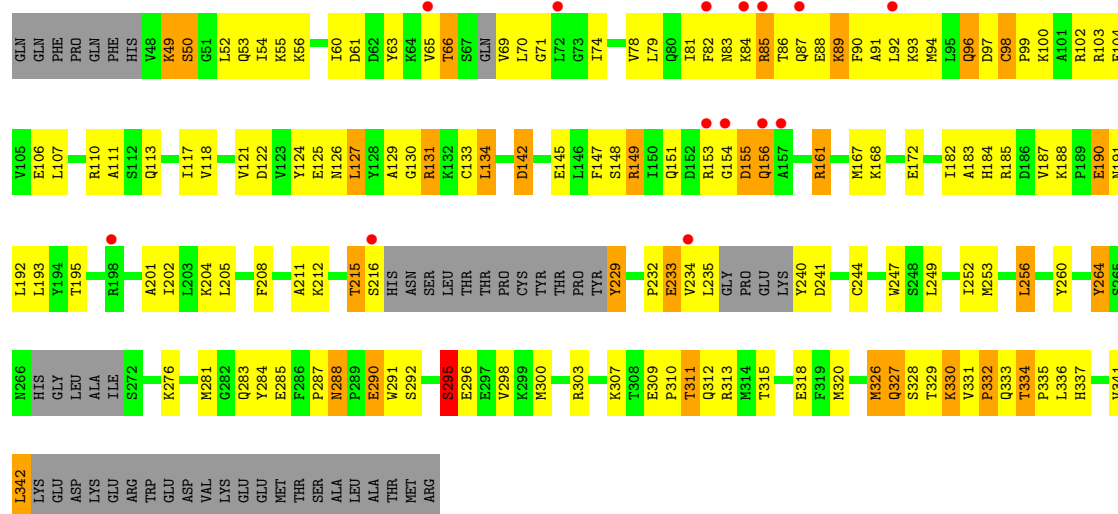


#### • Molecule 1: MAP kinase-activated protein kinase 2

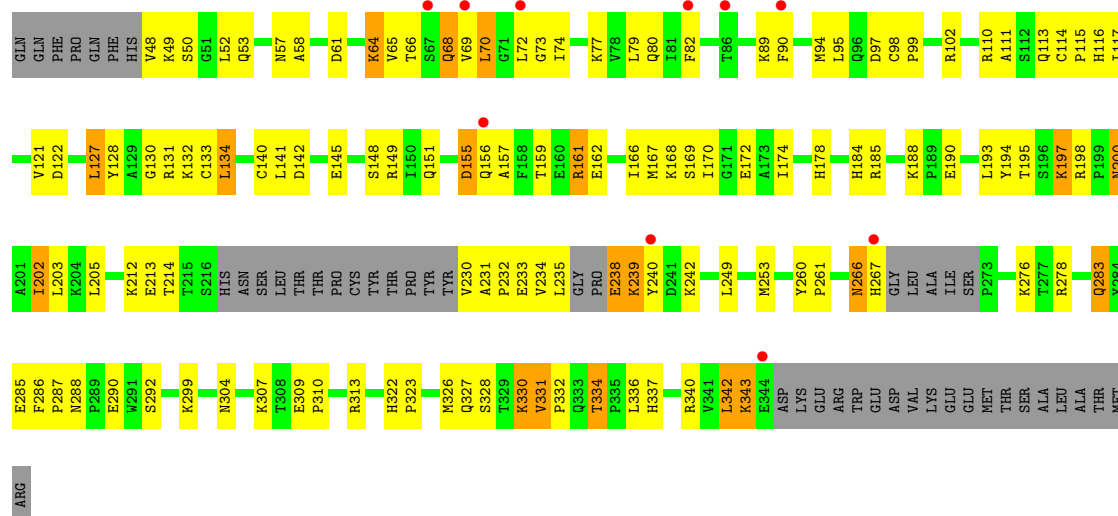
Chain B:



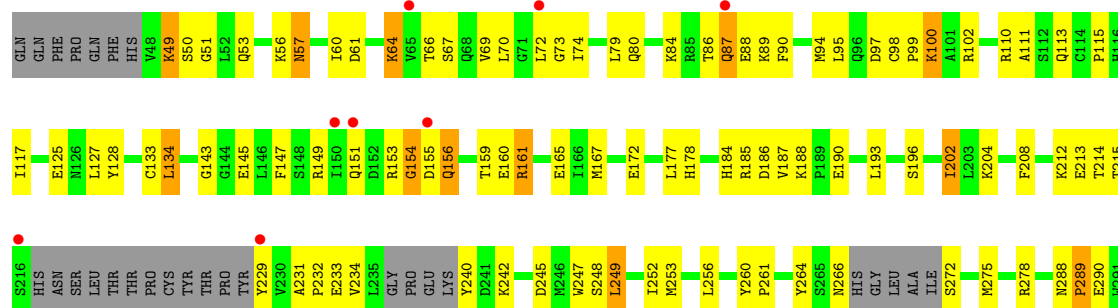
Chain C:



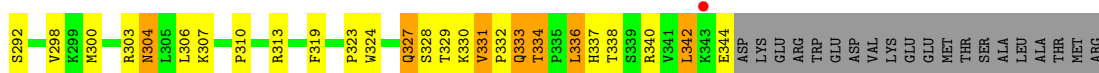
Chain D:



Chain E:

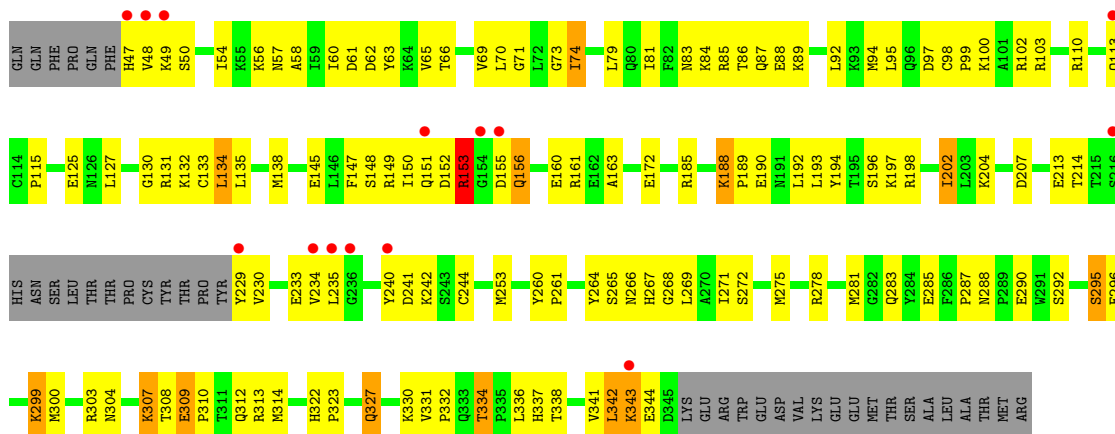






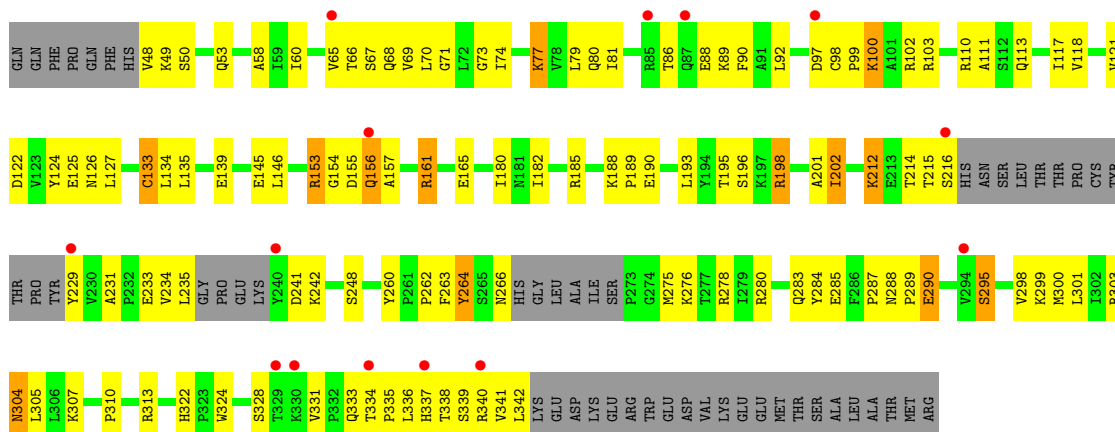
• Molecule 1: MAP kinase-activated protein kinase 2

Chain F:



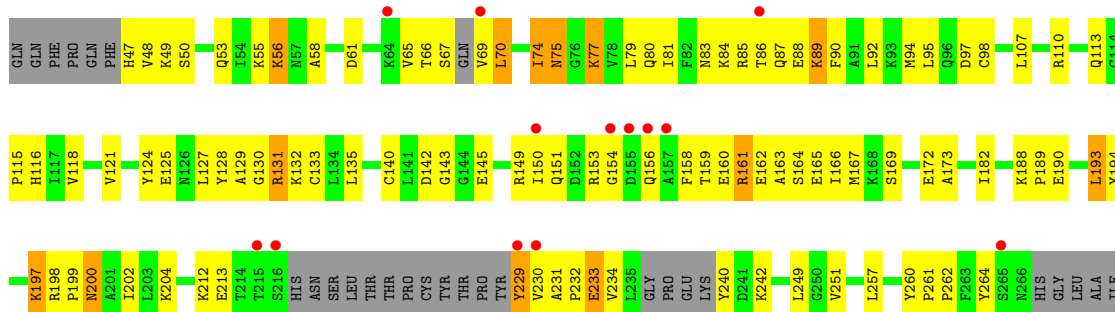
• Molecule 1: MAP kinase-activated protein kinase 2

Chain G:



• Molecule 1: MAP kinase-activated protein kinase 2

Chain H:







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.16Å 180.96Å 216.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.90 49.26 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.99-2.90) 99.6 (49.26-2.90)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.84 (at 2.91Å)	Xtriage
Refinement program	CNX 2005	Depositor
R, $R_{free}$	0.288 , 0.335 0.214 , 0.266	Depositor DCC
$R_{free}$ test set	6091 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	55.2	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 36.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 121020 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	27440	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.22% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, PDY

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	0.42	0/2262	0.58	0/3048
1	B	0.40	0/2284	0.57	1/3078 (0.0%)
1	C	0.36	0/2250	0.53	0/3032
1	D	0.40	0/2288	0.55	0/3081
1	E	0.42	0/2278	0.57	0/3070
1	F	0.44	0/2365	0.59	0/3191
1	G	0.36	0/2254	0.54	0/3038
1	H	0.38	0/2270	0.53	0/3058
1	I	0.41	0/2269	0.55	0/3058
1	J	0.31	0/2269	0.48	0/3058
1	K	0.33	0/2251	0.51	0/3033
1	L	0.33	0/2278	0.51	0/3070
All	All	0.38	0/27318	0.54	1/36815 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	342	LEU	CA-CB-CG	5.02	126.85	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2218	0	2255	134	0
1	B	2240	0	2270	153	0
1	C	2207	0	2240	156	0
1	D	2244	0	2281	113	0
1	E	2234	0	2268	127	0
1	F	2316	0	2347	123	0
1	G	2210	0	2245	119	0
1	H	2226	0	2260	160	0
1	I	2225	0	2262	147	0
1	J	2225	0	2262	173	0
1	K	2208	0	2248	160	0
1	L	2234	0	2268	149	0
2	A	54	0	52	7	0
2	B	54	0	52	16	0
2	C	54	0	52	16	0
2	D	54	0	52	13	0
2	E	54	0	52	19	0
2	F	54	0	52	18	0
2	G	54	0	52	18	0
2	H	54	0	51	39	0
2	I	54	0	52	34	0
2	J	54	0	52	18	0
2	K	54	0	52	24	0
2	L	54	0	52	20	0
3	F	5	0	0	1	0
All	All	27440	0	27829	1767	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 32.

All (1767) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:I:2:PDY:C18	2:I:2:PDY:H14	1.44	1.48
2:L:2:PDY:C14	2:L:2:PDY:H18	1.53	1.38
1:H:264:TYR:CZ	2:H:2:PDY:H20	1.61	1.32
1:I:264:TYR:CG	2:I:2:PDY:H17	1.65	1.32
2:L:2:PDY:C18	2:L:2:PDY:H14	1.58	1.32
2:D:2:PDY:H18	2:D:2:PDY:C14	1.60	1.29
2:J:1:PDY:H18	2:J:1:PDY:C14	1.60	1.29
2:I:1:PDY:C18	2:I:1:PDY:H14	1.75	1.17

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:264:TYR:CE2	2:H:2:PDY:H20	1.79	1.16
2:J:1:PDY:C18	2:J:1:PDY:H14	1.74	1.16
1:D:66:THR:HG22	1:D:68:GLN:H	1.06	1.15
1:C:202:ILE:HD11	1:C:204:LYS:HE2	1.26	1.14
1:I:264:TYR:CB	2:I:2:PDY:H17	1.77	1.13
2:H:2:PDY:H14	2:H:2:PDY:C18	1.80	1.11
2:H:1:PDY:C14	2:H:1:PDY:H18	1.80	1.10
2:L:1:PDY:H19	2:L:1:PDY:H27A	1.13	1.08
2:D:2:PDY:H14	2:D:2:PDY:C18	1.83	1.07
1:L:66:THR:HG23	1:L:69:VAL:H	1.10	1.07
2:K:1:PDY:C14	2:K:1:PDY:H18	1.83	1.07
1:I:264:TYR:CG	2:I:2:PDY:C17	2.38	1.06
1:G:100:LYS:HA	1:G:100:LYS:HE3	1.36	1.05
1:H:264:TYR:CE1	2:H:2:PDY:H20	1.90	1.05
1:G:185:ARG:HH21	1:G:212:LYS:HG3	0.95	1.04
2:I:1:PDY:C14	2:I:1:PDY:H18	1.88	1.04
2:J:2:PDY:H18	2:J:2:PDY:C14	1.88	1.03
2:H:2:PDY:H14	2:H:2:PDY:H18	1.04	1.03
1:H:264:TYR:CG	2:H:2:PDY:C17	2.42	1.02
2:G:1:PDY:H14	2:G:1:PDY:C18	1.89	1.02
2:K:1:PDY:C14	2:K:1:PDY:C18	2.37	1.02
2:I:2:PDY:C14	2:I:2:PDY:C18	2.37	1.02
2:K:2:PDY:C18	2:K:2:PDY:C14	2.39	1.01
2:I:2:PDY:H14	2:I:2:PDY:H18	1.02	1.00
2:D:2:PDY:H14	2:D:2:PDY:H18	1.03	1.00
2:K:1:PDY:H14	2:K:1:PDY:C18	1.91	1.00
1:H:264:TYR:CD2	2:H:2:PDY:H17	1.95	1.00
1:K:332:PRO:HB2	1:K:334:THR:HG22	1.43	1.00
2:H:1:PDY:C14	2:H:1:PDY:C18	2.39	1.00
1:I:264:TYR:CD2	2:I:2:PDY:H17	1.97	1.00
1:L:69:VAL:HG13	1:L:79:LEU:HD13	1.44	1.00
1:H:264:TYR:CG	2:H:2:PDY:H17	1.97	0.99
2:H:1:PDY:H14	2:H:1:PDY:C18	1.92	0.99
1:L:111:ALA:HB1	1:L:117:ILE:HD13	1.42	0.98
1:K:230:VAL:HG22	1:K:231:ALA:H	1.27	0.98
1:I:264:TYR:HB2	2:I:2:PDY:H17	1.45	0.98
2:E:1:PDY:C18	2:E:1:PDY:H14	1.94	0.98
2:E:2:PDY:C14	2:E:2:PDY:C18	2.41	0.98
1:B:202:ILE:HD11	1:B:204:LYS:HE2	1.43	0.97
2:G:1:PDY:C14	2:G:1:PDY:C18	2.41	0.97
1:C:69:VAL:HB	1:C:79:LEU:HD13	1.47	0.97
2:E:1:PDY:C14	2:E:1:PDY:C18	2.43	0.96

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:328:SER:O	1:G:331:VAL:HG12	1.65	0.96
1:D:49:LYS:HD2	1:D:113:GLN:HG2	1.45	0.96
1:G:185:ARG:NH2	1:G:212:LYS:HG3	1.81	0.96
2:I:2:PDY:C14	2:I:2:PDY:H18	1.94	0.95
2:I:1:PDY:C18	2:I:1:PDY:C14	2.42	0.94
1:K:80:GLN:NE2	2:K:1:PDY:H24A	1.82	0.94
2:F:2:PDY:C14	2:F:2:PDY:H18	1.97	0.94
2:F:2:PDY:C18	2:F:2:PDY:C14	2.46	0.94
2:L:1:PDY:C19	2:L:1:PDY:H27A	1.98	0.94
2:J:1:PDY:C14	2:J:1:PDY:C18	2.36	0.94
1:L:70:LEU:HA	1:L:94:MET:HE3	1.47	0.94
2:H:2:PDY:H18	2:H:2:PDY:C14	1.97	0.94
2:C:1:PDY:C18	2:C:1:PDY:H14	1.98	0.93
1:H:264:TYR:CE1	2:H:2:PDY:C20	2.51	0.93
2:E:2:PDY:C18	2:E:2:PDY:H14	1.98	0.93
1:K:167:MET:HG3	1:K:253:MET:HE2	1.50	0.93
1:B:161:ARG:HH21	1:B:333:GLN:HE21	0.93	0.93
2:E:1:PDY:C14	2:E:1:PDY:H18	1.99	0.93
1:J:313:ARG:HH22	1:K:233:GLU:HG2	1.32	0.93
1:K:49:LYS:HD3	1:K:50:SER:H	1.31	0.93
2:F:1:PDY:C18	2:F:1:PDY:C14	2.47	0.92
2:K:2:PDY:H14	2:K:2:PDY:C18	1.97	0.91
1:D:266:ASN:HD22	1:D:266:ASN:H	1.10	0.91
2:L:1:PDY:H19	2:L:1:PDY:C27	2.00	0.91
2:G:2:PDY:C18	2:G:2:PDY:C14	2.49	0.91
2:D:1:PDY:C14	2:D:1:PDY:H18	2.01	0.91
2:F:1:PDY:H14	2:F:1:PDY:C18	2.01	0.91
1:A:332:PRO:HB2	1:A:334:THR:HG22	1.51	0.91
1:K:70:LEU:HA	1:K:94:MET:HE1	1.53	0.91
1:H:69:VAL:HG23	1:H:79:LEU:HD13	1.52	0.90
1:E:156:GLN:NE2	1:E:156:GLN:H	1.69	0.90
1:I:49:LYS:HG3	1:I:50:SER:H	1.37	0.90
2:D:1:PDY:H14	2:D:1:PDY:C18	2.02	0.89
1:J:156:GLN:HE21	1:J:340:ARG:HD2	1.37	0.89
1:H:264:TYR:CD1	2:H:2:PDY:C20	2.56	0.89
2:D:1:PDY:C14	2:D:1:PDY:C18	2.51	0.89
2:G:1:PDY:H18	2:G:1:PDY:C14	2.02	0.88
1:H:129:ALA:HB3	1:H:131:ARG:HD3	1.52	0.88
1:D:66:THR:HG22	1:D:68:GLN:N	1.87	0.88
2:J:1:PDY:H18	2:J:1:PDY:H14	1.37	0.88
1:L:264:TYR:HB2	2:L:2:PDY:H17	1.56	0.88
2:B:2:PDY:C18	2:B:2:PDY:C14	2.52	0.87

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:264:TYR:CZ	2:H:2:PDY:C20	2.55	0.87
1:H:188:LYS:HG3	1:H:190:GLU:HG2	1.56	0.87
1:C:295:SER:HB2	1:C:298:VAL:HG23	1.54	0.86
1:B:85:ARG:HD2	1:B:86:THR:HG23	1.56	0.86
2:E:2:PDY:C13	2:E:2:PDY:H14	2.05	0.86
2:F:1:PDY:H18	2:F:1:PDY:C14	2.04	0.86
1:J:69:VAL:HG23	1:J:79:LEU:HD12	1.57	0.86
1:E:80:GLN:NE2	1:E:89:LYS:HD3	1.88	0.86
1:L:151:GLN:HB3	1:L:342:LEU:HD23	1.56	0.86
1:D:266:ASN:N	1:D:266:ASN:HD22	1.73	0.86
1:G:69:VAL:HB	1:G:79:LEU:HD13	1.58	0.86
1:H:264:TYR:CD2	2:H:2:PDY:C17	2.59	0.86
1:B:161:ARG:NH2	1:B:333:GLN:HE21	1.73	0.86
2:J:2:PDY:C14	2:J:2:PDY:C18	2.53	0.86
1:H:332:PRO:HB2	1:H:334:THR:HG23	1.56	0.86
1:F:74:ILE:HD13	1:F:74:ILE:H	1.39	0.85
1:B:94:MET:HG2	1:B:135:LEU:HD23	1.58	0.85
1:C:100:LYS:HE3	1:C:103:ARG:HH22	1.39	0.85
1:F:100:LYS:HG3	1:F:103:ARG:NH2	1.91	0.85
1:G:231:ALA:HB3	1:G:234:VAL:HG23	1.57	0.85
1:B:184:HIS:HD2	1:B:186:ASP:H	1.22	0.85
1:D:266:ASN:ND2	1:D:266:ASN:H	1.70	0.85
1:H:240:TYR:OH	1:H:242:LYS:HD2	1.77	0.84
2:H:1:PDY:C3	2:H:1:PDY:H18	2.05	0.84
2:J:2:PDY:H14	2:J:2:PDY:C18	2.08	0.84
2:F:2:PDY:C3	2:F:2:PDY:H18	2.05	0.84
1:E:49:LYS:HD2	1:E:50:SER:H	1.42	0.84
2:K:1:PDY:C3	2:K:1:PDY:H18	1.99	0.84
1:G:67:SER:HA	1:G:70:LEU:HD23	1.57	0.84
1:C:153:ARG:O	1:C:155:ASP:HA	1.77	0.84
1:I:266:ASN:H	1:I:266:ASN:ND2	1.72	0.84
1:H:80:GLN:HE21	1:H:89:LYS:HG3	1.43	0.84
1:F:65:VAL:HG11	1:F:70:LEU:HD13	1.59	0.84
2:G:2:PDY:C18	2:G:2:PDY:H14	2.08	0.83
1:J:159:THR:HG22	1:J:161:ARG:H	1.42	0.83
2:F:1:PDY:H18	2:F:1:PDY:C3	2.09	0.83
2:J:1:PDY:H18	2:J:1:PDY:C3	2.09	0.83
1:G:301:LEU:HD13	1:G:322:HIS:CD2	2.13	0.83
1:A:49:LYS:HG3	1:A:113:GLN:OE1	1.79	0.83
1:A:185:ARG:NH2	1:A:212:LYS:HE2	1.92	0.82
1:I:264:TYR:CD2	2:I:2:PDY:C17	2.62	0.82
1:L:159:THR:HG22	1:L:161:ARG:H	1.44	0.82

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:115:PRO:O	1:I:204:LYS:HE2	1.79	0.82
1:I:264:TYR:CE1	2:I:2:PDY:H20	2.14	0.82
2:F:2:PDY:H14	2:F:2:PDY:C18	2.07	0.82
2:C:1:PDY:C14	2:C:1:PDY:C18	2.58	0.82
1:I:264:TYR:CZ	2:I:2:PDY:H20	2.15	0.81
1:I:278:ARG:HG2	1:I:283:GLN:HB2	1.59	0.81
1:L:66:THR:HG23	1:L:69:VAL:N	1.94	0.81
2:C:1:PDY:C14	2:C:1:PDY:H18	2.09	0.81
1:I:332:PRO:HB2	1:I:334:THR:HG22	1.61	0.81
1:E:156:GLN:HE21	1:E:156:GLN:H	1.27	0.81
1:K:62:ASP:HA	1:K:85:ARG:HH21	1.46	0.81
1:F:95:LEU:O	1:F:133:CYS:HB2	1.80	0.81
1:K:80:GLN:NE2	2:K:1:PDY:C24	2.43	0.81
1:K:96:GLN:HE22	1:K:131:ARG:HE	1.28	0.80
2:B:2:PDY:C3	2:B:2:PDY:H18	2.10	0.80
2:J:1:PDY:H18	2:J:1:PDY:H14A	1.58	0.80
2:K:2:PDY:C3	2:K:2:PDY:H18	2.10	0.80
1:B:161:ARG:HH21	1:B:333:GLN:NE2	1.78	0.80
1:L:337:HIS:O	1:L:341:VAL:HG23	1.80	0.80
1:K:83:ASN:HB3	1:K:86:THR:HB	1.64	0.80
2:H:1:PDY:H14A	2:H:1:PDY:H18	1.63	0.79
1:K:49:LYS:HD3	1:K:50:SER:N	1.95	0.79
1:I:69:VAL:HA	1:I:79:LEU:HD22	1.63	0.79
1:C:83:ASN:HD21	1:C:85:ARG:HD2	1.47	0.79
2:L:1:PDY:C18	2:L:1:PDY:H14	2.12	0.79
1:I:70:LEU:HA	1:I:94:MET:HE1	1.62	0.79
1:J:276:LYS:HG3	1:K:235:LEU:HD12	1.64	0.79
1:K:115:PRO:O	1:K:204:LYS:HE2	1.82	0.79
1:H:80:GLN:NE2	1:H:89:LYS:HG3	1.97	0.79
1:F:86:THR:HG22	1:F:88:GLU:H	1.46	0.78
1:A:156:GLN:NE2	1:A:156:GLN:H	1.80	0.78
1:I:125:GLU:C	1:I:126:ASN:HD22	1.86	0.78
1:G:80:GLN:HB2	2:G:1:PDY:H24A	1.65	0.78
2:D:2:PDY:C14	2:D:2:PDY:C18	2.52	0.78
2:K:2:PDY:C14	2:K:2:PDY:H18	2.12	0.78
1:H:322:HIS:HD2	1:H:324:TRP:H	1.32	0.78
1:D:185:ARG:HH21	1:D:212:LYS:HG3	1.48	0.78
2:C:2:PDY:C14	2:C:2:PDY:C18	2.62	0.78
1:H:264:TYR:CD2	2:H:2:PDY:H20	2.19	0.78
1:L:69:VAL:HG13	1:L:79:LEU:CD1	2.13	0.78
2:J:2:PDY:H18	2:J:2:PDY:H14A	1.64	0.78
1:F:100:LYS:HG3	1:F:103:ARG:HH21	1.48	0.78

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:2:PDY:C14	2:B:2:PDY:H18	2.13	0.78
1:K:94:MET:HG2	1:K:135:LEU:HD23	1.67	0.77
1:F:73:GLY:HA3	1:F:94:MET:CE	2.15	0.77
1:E:69:VAL:HB	1:E:79:LEU:HD13	1.65	0.77
2:B:1:PDY:H14	2:B:1:PDY:C18	2.14	0.77
1:J:156:GLN:NE2	1:J:340:ARG:HD2	1.99	0.77
1:J:115:PRO:O	1:J:204:LYS:HE2	1.85	0.77
1:H:264:TYR:CG	2:H:2:PDY:C20	2.67	0.77
1:I:264:TYR:CB	2:I:2:PDY:C17	2.61	0.76
1:K:95:LEU:O	1:K:133:CYS:HB2	1.85	0.76
1:J:72:LEU:HB2	1:J:79:LEU:HD11	1.66	0.76
2:E:1:PDY:C3	2:E:1:PDY:H18	2.15	0.76
1:A:327:GLN:NE2	1:A:330:LYS:HD3	2.01	0.76
2:B:1:PDY:C18	2:B:1:PDY:C14	2.64	0.76
1:E:202:ILE:HD11	1:E:204:LYS:HE2	1.68	0.76
1:H:49:LYS:HG3	1:H:113:GLN:NE2	2.01	0.76
1:C:66:THR:OG1	1:C:69:VAL:HG13	1.86	0.75
1:B:73:GLY:HA3	1:B:94:MET:SD	2.26	0.75
1:H:128:TYR:O	1:H:131:ARG:HG2	1.85	0.75
1:C:327:GLN:HB2	1:C:330:LYS:HZ2	1.50	0.75
1:K:98:CYS:HB2	1:K:101:ALA:H	1.52	0.75
1:L:155:ASP:HA	1:L:156:GLN:C	2.07	0.75
1:K:70:LEU:HD23	1:K:94:MET:CE	2.17	0.75
1:B:77:LYS:HB3	1:B:77:LYS:HZ2	1.52	0.75
1:L:66:THR:HG22	1:L:69:VAL:HG23	1.69	0.75
1:G:185:ARG:HH21	1:G:212:LYS:CG	1.89	0.75
1:E:80:GLN:HE21	1:E:89:LYS:HD3	1.47	0.74
1:B:48:VAL:HB	1:L:70:LEU:HD21	1.69	0.74
2:G:2:PDY:H18	2:G:2:PDY:C3	2.16	0.74
1:J:198:ARG:NH1	1:J:200:ASN:H	1.85	0.74
1:A:156:GLN:H	1:A:156:GLN:HE21	1.33	0.74
1:J:161:ARG:HD2	1:J:329:THR:HA	1.69	0.74
1:D:66:THR:CG2	1:D:68:GLN:H	1.95	0.74
1:E:188:LYS:HZ2	1:E:190:GLU:HG2	1.52	0.74
1:G:304:ASN:O	1:G:307:LYS:HG2	1.88	0.74
1:G:80:GLN:OE1	1:G:89:LYS:HD2	1.87	0.74
1:I:49:LYS:HG3	1:I:50:SER:N	2.01	0.74
1:H:188:LYS:HE2	1:H:190:GLU:HG3	1.70	0.74
1:K:185:ARG:HH21	1:K:212:LYS:HG3	1.50	0.74
1:C:100:LYS:HE3	1:C:103:ARG:NH2	2.03	0.73
1:L:49:LYS:HD2	1:L:50:SER:H	1.53	0.73
1:D:337:HIS:HA	1:D:340:ARG:NH1	2.02	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:K:1:PDY:H18	2:K:1:PDY:H14A	1.70	0.73
1:G:100:LYS:HE2	1:G:103:ARG:CZ	2.18	0.73
1:L:95:LEU:O	1:L:133:CYS:HB2	1.88	0.73
1:A:49:LYS:HE2	1:A:113:GLN:HG2	1.71	0.73
1:I:98:CYS:HB2	1:I:99:PRO:HD2	1.70	0.73
1:F:81:ILE:HD13	1:F:92:LEU:HB2	1.69	0.73
1:I:100:LYS:HD2	1:I:103:ARG:HH21	1.53	0.73
1:G:161:ARG:O	1:G:165:GLU:HG3	1.88	0.73
1:H:264:TYR:CE2	2:H:2:PDY:C20	2.67	0.72
1:F:47:HIS:CD2	1:G:67:SER:HB3	2.24	0.72
2:A:1:PDY:H14	2:A:1:PDY:C18	2.19	0.72
1:D:49:LYS:CD	1:D:113:GLN:HG2	2.19	0.72
1:B:285:GLU:HG3	1:B:287:PRO:HD3	1.70	0.72
2:B:2:PDY:H14	2:B:2:PDY:C18	2.18	0.72
1:G:66:THR:O	1:G:69:VAL:HG22	1.90	0.72
1:B:72:LEU:HB3	1:B:77:LYS:HG3	1.71	0.72
1:I:264:TYR:CG	2:I:2:PDY:C20	2.72	0.72
1:F:278:ARG:HG2	1:F:283:GLN:HB2	1.68	0.72
1:G:190:GLU:OE1	1:G:190:GLU:N	2.22	0.72
1:G:260:TYR:HB2	2:G:2:PDY:H19	1.72	0.72
1:K:328:SER:O	1:K:331:VAL:HG22	1.89	0.72
2:L:2:PDY:C18	2:L:2:PDY:C14	2.35	0.72
1:J:159:THR:CG2	1:J:333:GLN:HA	2.20	0.72
1:J:327:GLN:HG2	1:J:330:LYS:HD3	1.70	0.72
1:H:61:ASP:O	1:H:84:LYS:HD2	1.90	0.72
1:E:70:LEU:HD23	1:E:94:MET:HE2	1.71	0.72
1:H:261:PRO:HD3	2:H:2:PDY:H25	1.71	0.71
1:D:167:MET:HG3	1:D:253:MET:HE2	1.72	0.71
2:K:2:PDY:H14	2:K:2:PDY:C13	2.18	0.71
1:H:264:TYR:CD2	2:H:2:PDY:C20	2.72	0.71
2:C:2:PDY:H14	2:C:2:PDY:C18	2.21	0.71
1:F:71:GLY:HA2	1:F:74:ILE:HD11	1.72	0.71
1:F:185:ARG:HD3	1:F:241:ASP:HB3	1.71	0.71
1:E:70:LEU:HA	1:E:94:MET:CE	2.20	0.71
1:B:185:ARG:HD3	1:B:241:ASP:HB3	1.72	0.71
1:J:231:ALA:O	1:J:234:VAL:HG12	1.90	0.71
2:D:1:PDY:H18	2:D:1:PDY:C3	2.19	0.71
1:A:264:TYR:O	1:A:275:MET:HG3	1.91	0.71
1:I:264:TYR:CD1	2:I:2:PDY:H20	2.25	0.70
1:D:66:THR:HB	1:D:69:VAL:HG23	1.71	0.70
1:I:70:LEU:HD23	1:I:94:MET:HE2	1.72	0.70
1:I:97:ASP:OD2	1:I:102:ARG:NH2	2.22	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:266:ASN:CG	1:B:278:ARG:HH22	1.94	0.70
1:I:140:CYS:SG	2:I:1:PDY:H17	2.32	0.70
1:D:69:VAL:HG13	1:D:79:LEU:HD13	1.72	0.70
1:L:159:THR:HG21	1:L:161:ARG:HB3	1.73	0.70
1:F:196:SER:OG	1:F:198:ARG:HB2	1.92	0.70
1:K:288:ASN:OD1	1:K:292:SER:HB3	1.91	0.70
1:A:71:GLY:O	1:A:74:ILE:HG22	1.91	0.70
2:H:2:PDY:C14	2:H:2:PDY:C18	2.62	0.70
1:A:70:LEU:HD13	1:G:48:VAL:HG23	1.73	0.70
1:K:96:GLN:HE22	1:K:131:ARG:NE	1.90	0.70
1:F:327:GLN:HE21	1:F:330:LYS:HD2	1.57	0.70
1:B:97:ASP:H	1:B:133:CYS:HA	1.56	0.69
1:E:185:ARG:HE	1:E:212:LYS:HG3	1.55	0.69
1:E:327:GLN:HB2	1:E:330:LYS:NZ	2.06	0.69
2:I:1:PDY:H18	2:I:1:PDY:H14A	1.73	0.69
2:I:1:PDY:H14	2:I:1:PDY:C13	2.22	0.69
1:I:264:TYR:CE2	2:I:2:PDY:H20	2.28	0.69
1:A:66:THR:H	1:A:69:VAL:CG2	2.06	0.69
1:F:150:ILE:O	1:F:153:ARG:HG2	1.92	0.69
1:F:97:ASP:H	1:F:133:CYS:HA	1.58	0.69
1:C:185:ARG:CZ	1:C:212:LYS:HD2	2.21	0.69
1:G:49:LYS:HD2	1:G:113:GLN:OE1	1.92	0.69
1:K:89:LYS:H	1:K:89:LYS:HD2	1.55	0.69
1:E:327:GLN:HB2	1:E:330:LYS:HZ2	1.57	0.69
1:A:66:THR:H	1:A:69:VAL:HG22	1.57	0.69
1:B:68:GLN:NE2	1:F:267:HIS:HB3	2.08	0.69
1:A:304:ASN:O	1:A:307:LYS:HG2	1.93	0.69
1:E:70:LEU:HA	1:E:94:MET:HE1	1.75	0.68
1:L:257:LEU:HD11	1:L:298:VAL:HG11	1.74	0.68
1:B:141:LEU:HD13	1:B:193:LEU:HB2	1.74	0.68
1:E:145:GLU:HG2	1:E:193:LEU:CD2	2.23	0.68
1:C:88:GLU:HG2	1:C:89:LYS:N	2.07	0.68
1:I:328:SER:O	1:I:331:VAL:HG13	1.94	0.68
1:A:145:GLU:HG3	1:A:193:LEU:CD2	2.24	0.68
1:H:322:HIS:CD2	1:H:324:TRP:H	2.12	0.68
1:E:333:GLN:HA	1:E:333:GLN:HE21	1.58	0.68
1:K:70:LEU:HD23	1:K:94:MET:HE2	1.74	0.68
2:G:2:PDY:C13	2:G:2:PDY:H14	2.24	0.68
1:C:161:ARG:NH1	1:C:331:VAL:O	2.27	0.68
1:D:190:GLU:CD	1:D:190:GLU:H	1.97	0.68
1:K:80:GLN:HE21	2:K:1:PDY:C24	2.05	0.67
1:J:332:PRO:HB2	1:J:334:THR:HG22	1.75	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:145:GLU:HG2	1:J:193:LEU:CD2	2.24	0.67
1:L:66:THR:CG2	1:L:69:VAL:H	1.99	0.67
2:G:1:PDY:C13	2:G:1:PDY:H14	2.23	0.67
1:H:231:ALA:HB3	1:H:234:VAL:HG23	1.75	0.67
1:I:327:GLN:HE21	1:I:330:LYS:NZ	1.92	0.67
2:G:1:PDY:H18	2:G:1:PDY:C3	2.22	0.67
1:H:65:VAL:HG11	1:H:70:LEU:HD13	1.75	0.67
1:F:272:SER:HB3	1:F:275:MET:HB2	1.77	0.67
1:E:188:LYS:NZ	1:E:190:GLU:HG2	2.09	0.67
1:E:60:ILE:HD12	1:E:61:ASP:N	2.10	0.67
1:K:166:ILE:O	1:K:169:SER:HB3	1.94	0.67
1:L:129:ALA:O	1:L:131:ARG:HG3	1.94	0.67
1:I:284:TYR:OH	1:I:303:ARG:HG2	1.94	0.67
1:B:231:ALA:HB1	1:B:233:GLU:HG3	1.77	0.67
1:G:80:GLN:CB	2:G:1:PDY:H24A	2.24	0.67
1:G:260:TYR:CB	2:G:2:PDY:H19	2.25	0.67
1:G:69:VAL:HB	1:G:79:LEU:CD1	2.24	0.67
1:L:153:ARG:HB2	1:L:156:GLN:HG2	1.76	0.67
1:J:145:GLU:HG2	1:J:193:LEU:HD21	1.77	0.67
1:L:202:ILE:HD11	1:L:204:LYS:HE2	1.76	0.67
1:A:49:LYS:HE2	1:A:113:GLN:CG	2.24	0.67
1:F:202:ILE:HD11	1:F:204:LYS:HE2	1.76	0.67
1:C:327:GLN:CB	1:C:330:LYS:HZ2	2.06	0.67
1:G:66:THR:HG23	1:G:69:VAL:HG13	1.76	0.67
1:K:89:LYS:H	1:K:89:LYS:CD	2.08	0.66
1:C:188:LYS:HG3	1:C:190:GLU:HG2	1.76	0.66
2:J:2:PDY:H18	2:J:2:PDY:C3	2.23	0.66
2:F:2:PDY:H14A	2:F:2:PDY:H18	1.77	0.66
1:A:328:SER:O	1:A:331:VAL:HG13	1.95	0.66
1:I:186:ASP:OD1	1:I:188:LYS:HE3	1.95	0.66
1:J:198:ARG:HG3	1:J:198:ARG:HH11	1.60	0.66
1:L:167:MET:HG3	1:L:253:MET:HG3	1.77	0.66
1:G:71:GLY:O	1:G:74:ILE:HG22	1.95	0.66
2:E:2:PDY:H18	2:E:2:PDY:C3	2.25	0.66
1:I:148:SER:HA	1:I:151:GLN:HG2	1.76	0.66
1:C:287:PRO:O	1:C:291:TRP:HB2	1.95	0.66
1:C:55:LYS:HD3	1:C:124:TYR:CE2	2.30	0.66
1:G:161:ARG:HD3	1:G:331:VAL:O	1.95	0.66
1:J:72:LEU:HB2	1:J:79:LEU:CD1	2.26	0.66
1:J:198:ARG:HH11	1:J:200:ASN:H	1.42	0.66
1:J:337:HIS:O	1:J:341:VAL:HG23	1.96	0.66
1:L:66:THR:CG2	1:L:69:VAL:HG23	2.24	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:147:PHE:HE2	1:C:256:LEU:HD23	1.60	0.66
1:D:233:GLU:HG2	1:E:310:PRO:HG3	1.76	0.66
2:G:2:PDY:H18	2:G:2:PDY:C14	2.23	0.66
1:I:72:LEU:HB2	1:I:79:LEU:HD21	1.77	0.66
1:B:81:ILE:HD13	1:B:92:LEU:HB2	1.77	0.66
1:G:229:TYR:HD1	1:H:251:VAL:HG11	1.61	0.66
1:L:97:ASP:H	1:L:133:CYS:HA	1.60	0.65
1:L:161:ARG:HD3	1:L:331:VAL:O	1.95	0.65
1:K:105:VAL:HG22	1:K:136:ILE:HD11	1.77	0.65
1:A:49:LYS:HE2	1:A:113:GLN:CD	2.16	0.65
2:G:2:PDY:C18	2:G:2:PDY:C3	2.73	0.65
1:F:73:GLY:HA3	1:F:94:MET:HE1	1.78	0.65
1:H:56:LYS:HE2	1:H:125:GLU:HB3	1.77	0.65
1:F:230:VAL:HG21	1:F:235:LEU:HD21	1.78	0.65
1:K:121:VAL:HG12	1:K:122:ASP:OD1	1.96	0.65
1:E:110:ARG:O	1:E:113:GLN:HG3	1.97	0.65
1:J:185:ARG:NE	1:J:212:LYS:HG3	2.11	0.65
1:F:296:GLU:OE2	1:F:300:MET:HG2	1.96	0.65
1:L:264:TYR:HB2	2:L:2:PDY:C17	2.26	0.65
1:K:83:ASN:CB	1:K:86:THR:HB	2.27	0.65
1:I:94:MET:O	1:I:95:LEU:HD23	1.97	0.65
1:E:161:ARG:HA	1:E:331:VAL:CG2	2.27	0.65
1:B:107:LEU:HD21	1:B:213:GLU:HG3	1.79	0.65
1:E:86:THR:HG21	1:E:88:GLU:CD	2.17	0.65
1:A:102:ARG:NH2	1:A:125:GLU:OE1	2.29	0.65
2:L:1:PDY:C14	2:L:1:PDY:C18	2.75	0.65
1:L:314:MET:HG3	1:L:318:GLU:HB2	1.78	0.65
1:I:307:LYS:HB2	1:I:313:ARG:HG3	1.79	0.65
1:K:72:LEU:HD12	1:K:77:LYS:HD2	1.78	0.65
1:K:62:ASP:HA	1:K:85:ARG:NH2	2.10	0.64
1:K:114:CYS:SG	1:K:115:PRO:HD2	2.36	0.64
1:J:83:ASN:HD21	1:J:85:ARG:HH11	1.43	0.64
1:J:168:LYS:O	1:J:172:GLU:HG3	1.97	0.64
1:D:327:GLN:HB3	1:D:330:LYS:HD2	1.78	0.64
1:F:296:GLU:OE2	1:F:303:ARG:NH2	2.30	0.64
1:H:83:ASN:HB3	1:H:86:THR:HB	1.80	0.64
2:C:2:PDY:H18	2:C:2:PDY:C3	2.26	0.64
1:A:153:ARG:O	1:A:154:GLY:O	2.15	0.64
2:E:2:PDY:H18	2:E:2:PDY:C14	2.28	0.64
1:J:329:THR:C	1:J:331:VAL:H	2.00	0.64
1:I:60:ILE:HG22	1:I:65:VAL:HB	1.79	0.64
1:B:188:LYS:HD2	1:B:190:GLU:HB2	1.80	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:150:ILE:O	1:I:153:ARG:HG3	1.98	0.64
1:L:70:LEU:HA	1:L:94:MET:CE	2.23	0.64
1:B:69:VAL:O	1:B:73:GLY:N	2.28	0.64
1:I:264:TYR:CD2	2:I:2:PDY:C20	2.81	0.64
1:J:118:VAL:HG21	1:J:138:MET:HE2	1.77	0.64
1:H:161:ARG:HD3	1:H:331:VAL:O	1.98	0.64
1:K:96:GLN:NE2	1:K:131:ARG:HE	1.94	0.64
1:A:310:PRO:HG3	1:C:233:GLU:HG2	1.80	0.64
1:F:49:LYS:HG3	1:G:127:LEU:HD23	1.79	0.64
1:B:98:CYS:HB2	1:B:99:PRO:HD2	1.78	0.64
1:J:83:ASN:ND2	1:J:85:ARG:HH11	1.96	0.64
1:H:264:TYR:CB	2:H:2:PDY:H17	2.27	0.64
1:H:188:LYS:HE2	1:H:190:GLU:CG	2.26	0.64
1:D:195:THR:HG23	1:D:202:ILE:O	1.98	0.64
1:J:310:PRO:HB3	1:K:233:GLU:OE1	1.98	0.64
1:D:330:LYS:O	1:D:330:LYS:HG2	1.97	0.64
1:H:86:THR:HG22	1:H:88:GLU:HB2	1.80	0.64
1:H:315:THR:OG1	1:H:318:GLU:HG3	1.98	0.64
1:A:309:GLU:CD	1:C:311:THR:HG22	2.17	0.64
2:E:1:PDY:C13	2:E:1:PDY:H14	2.28	0.63
1:H:107:LEU:HD21	1:H:213:GLU:HG3	1.79	0.63
1:G:276:LYS:HG3	1:I:235:LEU:HD22	1.80	0.63
1:I:280:ARG:NH2	1:J:131:ARG:HH12	1.95	0.63
1:H:74:ILE:O	1:H:74:ILE:HD13	1.97	0.63
2:D:2:PDY:H14A	2:D:2:PDY:H18	1.69	0.63
1:J:69:VAL:HG23	1:J:79:LEU:CD1	2.28	0.63
1:J:143:GLY:O	1:J:149:ARG:HD3	1.98	0.63
1:D:230:VAL:HG11	1:D:235:LEU:HD21	1.80	0.63
1:K:230:VAL:HG22	1:K:231:ALA:N	2.07	0.63
1:B:188:LYS:HD2	1:B:190:GLU:OE1	1.98	0.63
1:C:315:THR:OG1	1:C:318:GLU:HG3	1.99	0.63
1:A:333:GLN:HE21	1:A:333:GLN:HA	1.63	0.63
1:J:149:ARG:HG3	1:J:194:TYR:CD2	2.34	0.63
1:B:69:VAL:HG23	1:B:70:LEU:N	2.12	0.63
1:C:185:ARG:NH2	1:C:212:LYS:HD2	2.14	0.63
1:L:72:LEU:HD23	1:L:77:LYS:HD3	1.81	0.63
1:L:114:CYS:HB2	1:L:176:TYR:CD2	2.34	0.63
1:F:65:VAL:CG1	1:F:70:LEU:HD13	2.28	0.63
1:L:266:ASN:HB2	1:L:278:ARG:NH2	2.14	0.63
1:H:159:THR:OG1	1:H:162:GLU:HG3	1.99	0.63
1:G:337:HIS:O	1:G:341:VAL:HG23	1.99	0.63
1:D:64:LYS:HE3	1:D:64:LYS:HA	1.79	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:290:GLU:HA	1:G:337:HIS:CD2	2.34	0.63
1:J:304:ASN:OD1	1:J:314:MET:HB2	1.99	0.63
1:I:83:ASN:HB3	1:I:86:THR:O	1.99	0.62
1:J:288:ASN:N	1:J:288:ASN:HD22	1.96	0.62
2:A:1:PDY:C14	2:A:1:PDY:C18	2.77	0.62
1:E:88:GLU:HG3	1:E:90:PHE:HE1	1.63	0.62
1:A:151:GLN:O	1:A:343:LYS:HE2	2.00	0.62
2:C:2:PDY:H14	2:C:2:PDY:C13	2.29	0.62
1:A:66:THR:HG23	1:A:68:GLN:H	1.64	0.62
1:L:246:MET:HA	1:L:246:MET:HE3	1.81	0.62
1:F:156:GLN:HA	1:F:156:GLN:HE21	1.64	0.62
1:F:100:LYS:HZ2	1:F:103:ARG:HH22	1.47	0.62
1:A:307:LYS:HB2	1:A:313:ARG:HG3	1.81	0.62
1:G:153:ARG:HG3	1:G:157:ALA:HB3	1.81	0.62
1:I:264:TYR:CD1	2:I:2:PDY:C20	2.83	0.62
1:B:109:TRP:O	1:B:112:SER:HB2	1.99	0.62
1:B:74:ILE:HG23	1:B:94:MET:HE2	1.82	0.62
1:J:198:ARG:NH1	1:J:198:ARG:HG3	2.14	0.62
1:F:271:ILE:HG23	1:F:275:MET:HE2	1.80	0.62
1:G:97:ASP:HB2	1:G:133:CYS:HA	1.81	0.62
1:L:258:CYS:O	1:L:341:VAL:HG21	1.99	0.62
1:E:161:ARG:HA	1:E:331:VAL:HG21	1.82	0.62
1:D:161:ARG:HD3	1:D:331:VAL:O	1.99	0.62
1:H:70:LEU:HD12	1:H:94:MET:SD	2.39	0.61
1:C:85:ARG:HG2	1:C:85:ARG:O	2.00	0.61
1:I:100:LYS:HD2	1:I:103:ARG:NH2	2.14	0.61
1:L:69:VAL:CG1	1:L:79:LEU:HD13	2.27	0.61
1:E:49:LYS:HD2	1:E:50:SER:N	2.15	0.61
1:E:214:THR:HG21	1:E:242:LYS:HG3	1.82	0.61
1:H:304:ASN:OD1	1:H:314:MET:HB2	1.97	0.61
1:C:290:GLU:HA	1:C:337:HIS:CD2	2.35	0.61
1:K:92:LEU:HD12	1:K:93:LYS:N	2.15	0.61
1:J:233:GLU:HG2	1:L:310:PRO:HG3	1.81	0.61
1:L:77:LYS:HE3	1:L:79:LEU:HD23	1.81	0.61
1:J:60:ILE:HD12	1:J:61:ASP:N	2.16	0.61
1:I:49:LYS:CG	1:I:50:SER:H	2.11	0.61
1:I:266:ASN:HD21	1:I:272:SER:CB	2.14	0.61
1:E:66:THR:HG23	1:E:69:VAL:H	1.66	0.61
1:I:196:SER:O	1:I:201:ALA:HB2	2.01	0.61
1:H:229:TYR:HD1	1:H:230:VAL:H	1.49	0.61
1:E:338:THR:HG22	1:E:342:LEU:HD23	1.83	0.61
1:L:85:ARG:HD2	1:L:85:ARG:O	2.01	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:69:VAL:CG2	1:H:79:LEU:HD13	2.29	0.61
1:D:231:ALA:HB1	1:D:233:GLU:OE2	2.00	0.61
1:I:231:ALA:HB1	1:I:233:GLU:OE2	2.00	0.61
1:C:264:TYR:CZ	2:C:2:PDY:H24	2.36	0.61
1:D:327:GLN:CB	1:D:330:LYS:HD2	2.29	0.61
2:E:1:PDY:H14A	2:E:1:PDY:H18	1.83	0.61
1:E:80:GLN:OE1	2:E:1:PDY:H24A	2.01	0.61
1:J:288:ASN:HD22	1:J:288:ASN:H	1.47	0.61
1:F:156:GLN:HE21	1:F:156:GLN:CA	2.13	0.61
1:C:65:VAL:CG1	1:C:70:LEU:HD11	2.31	0.61
1:D:69:VAL:CG1	1:D:79:LEU:HD13	2.31	0.60
1:J:310:PRO:HA	1:J:313:ARG:HG3	1.80	0.60
1:K:66:THR:O	1:K:69:VAL:HG22	2.01	0.60
1:J:276:LYS:HG3	1:K:235:LEU:CD1	2.31	0.60
1:G:289:PRO:HG2	1:G:290:GLU:OE2	2.01	0.60
1:K:143:GLY:HA3	1:K:194:TYR:HB2	1.82	0.60
1:G:278:ARG:HG2	1:G:283:GLN:HG3	1.82	0.60
1:L:235:LEU:N	1:L:235:LEU:HD12	2.16	0.60
1:H:264:TYR:HB2	2:H:2:PDY:H17	1.83	0.60
1:D:77:LYS:HB3	1:D:77:LYS:NZ	2.16	0.60
1:H:154:GLY:HA2	1:H:156:GLN:N	2.15	0.60
1:H:342:LEU:O	1:H:343:LYS:HD2	2.01	0.60
1:C:49:LYS:HD2	1:C:50:SER:N	2.15	0.60
1:D:82:PHE:CE1	1:D:89:LYS:HB3	2.36	0.60
1:F:161:ARG:HA	1:F:331:VAL:CG2	2.32	0.60
1:I:264:TYR:HB2	2:I:2:PDY:C17	2.25	0.60
1:K:80:GLN:HE21	2:K:1:PDY:H24A	1.63	0.60
1:B:48:VAL:HG11	1:L:60:ILE:HG23	1.84	0.60
1:A:327:GLN:HG2	1:A:330:LYS:HG2	1.82	0.60
1:A:127:LEU:HD23	1:G:113:GLN:OE1	2.02	0.60
1:J:278:ARG:HG2	1:J:283:GLN:HB2	1.83	0.60
2:K:1:PDY:C13	2:K:1:PDY:H14	2.31	0.60
1:F:70:LEU:HD12	1:F:94:MET:HE2	1.82	0.60
1:K:188:LYS:HG3	1:K:190:GLU:HG2	1.84	0.60
1:L:187:VAL:O	1:L:187:VAL:HG12	2.02	0.60
1:H:140:CYS:SG	2:H:1:PDY:H17	2.42	0.60
1:C:327:GLN:HE21	1:C:330:LYS:CE	2.14	0.60
1:B:266:ASN:O	1:B:266:ASN:OD1	2.19	0.60
1:B:160:GLU:HB3	1:B:334:THR:HG23	1.83	0.60
2:D:1:PDY:H18	2:D:1:PDY:H14A	1.83	0.60
1:J:66:THR:O	1:J:69:VAL:HG13	2.02	0.60
1:K:202:ILE:HD12	1:K:203:LEU:N	2.16	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:1:PDY:C13	2:L:1:PDY:H14	2.31	0.59
1:C:60:ILE:HD12	1:C:60:ILE:C	2.23	0.59
1:K:92:LEU:HD12	1:K:93:LYS:H	1.66	0.59
1:A:233:GLU:OE2	1:B:313:ARG:NH1	2.34	0.59
1:K:298:VAL:HG22	1:K:324:TRP:CD1	2.37	0.59
1:C:81:ILE:HD13	1:C:92:LEU:HB2	1.84	0.59
1:E:64:LYS:HD2	1:E:84:LYS:HE2	1.84	0.59
1:E:153:ARG:O	1:E:154:GLY:O	2.19	0.59
1:D:266:ASN:N	1:D:266:ASN:ND2	2.40	0.59
1:I:280:ARG:HH22	1:J:131:ARG:HH12	1.49	0.59
1:H:143:GLY:HA2	1:H:197:LYS:HD2	1.84	0.59
1:F:188:LYS:HD3	1:F:190:GLU:OE1	2.01	0.59
1:J:66:THR:HG23	1:J:68:GLN:HB2	1.83	0.59
1:E:161:ARG:HD2	1:E:328:SER:O	2.01	0.59
1:L:257:LEU:CD1	1:L:298:VAL:HG11	2.31	0.59
1:I:80:GLN:OE1	1:I:89:LYS:HG3	2.02	0.59
1:J:124:TYR:HB2	1:J:135:LEU:HB2	1.84	0.59
1:B:49:LYS:HD3	1:B:113:GLN:HG2	1.84	0.59
1:A:66:THR:HG23	1:A:68:GLN:N	2.17	0.59
1:L:202:ILE:CD1	1:L:204:LYS:HE2	2.31	0.59
1:A:280:ARG:HH11	1:C:235:LEU:HD13	1.67	0.59
1:A:161:ARG:HD3	1:A:331:VAL:O	2.02	0.59
1:L:155:ASP:CA	1:L:156:GLN:C	2.70	0.59
2:B:2:PDY:H14	2:B:2:PDY:C13	2.32	0.59
1:L:151:GLN:HB3	1:L:342:LEU:CD2	2.30	0.59
1:K:284:TYR:OH	1:K:303:ARG:HA	2.03	0.59
1:E:128:TYR:HD1	1:L:48:VAL:HG23	1.67	0.59
1:B:70:LEU:HD23	1:B:128:TYR:CE1	2.38	0.59
1:A:70:LEU:HD13	1:G:48:VAL:CG2	2.32	0.59
1:I:327:GLN:HB3	1:I:330:LYS:HG2	1.85	0.59
1:F:234:VAL:HG12	1:F:235:LEU:HD23	1.85	0.59
1:E:86:THR:HB	1:E:88:GLU:HG2	1.85	0.59
1:L:168:LYS:O	1:L:172:GLU:HG3	2.02	0.59
1:K:281:MET:HB2	1:K:283:GLN:HG3	1.85	0.59
1:I:55:LYS:HD3	1:I:124:TYR:CZ	2.38	0.59
1:A:52:LEU:O	1:F:56:LYS:HD2	2.02	0.59
1:K:200:ASN:N	1:K:200:ASN:OD1	2.34	0.59
1:D:72:LEU:HD22	1:D:77:LYS:HE3	1.85	0.59
1:H:200:ASN:HD22	1:H:200:ASN:N	2.00	0.59
2:F:1:PDY:H14	2:F:1:PDY:C13	2.33	0.59
1:G:77:LYS:HB3	1:G:79:LEU:HD21	1.85	0.59
1:K:309:GLU:HB3	1:K:312:GLN:HG3	1.85	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:100:LYS:HA	1:G:100:LYS:CE	2.20	0.59
2:E:2:PDY:C3	2:E:2:PDY:C18	2.75	0.59
2:C:1:PDY:H14	2:C:1:PDY:C13	2.32	0.59
1:L:159:THR:HG22	1:L:161:ARG:N	2.16	0.59
1:F:87:GLN:OE1	1:F:87:GLN:HA	2.03	0.59
1:H:337:HIS:HA	1:H:340:ARG:NH1	2.17	0.59
1:F:295:SER:O	1:F:299:LYS:HD3	2.03	0.59
1:I:264:TYR:HB2	2:I:2:PDY:HN9	1.68	0.58
1:E:49:LYS:CD	1:E:50:SER:H	2.12	0.58
1:A:50:SER:HB2	1:F:57:ASN:HA	1.85	0.58
1:E:111:ALA:HB1	1:E:117:ILE:HD13	1.85	0.58
1:F:151:GLN:HG3	1:F:152:ASP:N	2.18	0.58
1:I:58:ALA:HA	1:I:126:ASN:OD1	2.03	0.58
2:B:1:PDY:C13	2:B:1:PDY:H14	2.33	0.58
1:C:55:LYS:HD3	1:C:124:TYR:CZ	2.38	0.58
1:A:188:LYS:HD2	1:A:191:ASN:ND2	2.18	0.58
1:B:66:THR:OG1	1:B:69:VAL:HG13	2.02	0.58
1:B:74:ILE:HD12	1:B:75:ASN:N	2.18	0.58
1:B:49:LYS:CD	1:B:113:GLN:HG2	2.33	0.58
1:C:129:ALA:HB3	1:C:131:ARG:HE	1.68	0.58
1:G:90:PHE:CE2	1:G:121:VAL:HG21	2.39	0.58
1:K:66:THR:H	1:K:69:VAL:CG2	2.16	0.58
1:B:70:LEU:HD23	1:B:128:TYR:HE1	1.68	0.58
2:B:1:PDY:C3	2:B:1:PDY:H18	2.33	0.58
1:C:88:GLU:HG2	1:C:89:LYS:H	1.69	0.58
1:E:88:GLU:HG3	1:E:90:PHE:CE1	2.38	0.58
1:F:151:GLN:O	1:F:343:LYS:HE3	2.03	0.58
1:J:97:ASP:O	1:J:98:CYS:HB3	2.03	0.58
1:A:278:ARG:HA	1:A:283:GLN:HG2	1.85	0.58
1:L:93:LYS:HG2	1:L:136:ILE:HB	1.84	0.58
1:I:64:LYS:HD2	1:I:84:LYS:HE3	1.86	0.58
1:H:202:ILE:HD11	1:H:204:LYS:NZ	2.18	0.58
1:I:264:TYR:CD2	2:I:2:PDY:H20	2.39	0.58
1:J:159:THR:HG22	1:J:161:ARG:N	2.16	0.58
1:B:328:SER:O	1:B:331:VAL:HG13	2.03	0.58
1:K:295:SER:OG	1:K:298:VAL:HG23	2.04	0.58
1:K:290:GLU:HA	1:K:337:HIS:HD2	1.68	0.58
1:A:285:GLU:C	1:A:287:PRO:HD3	2.24	0.58
1:E:57:ASN:HD22	1:E:57:ASN:H	1.51	0.58
1:H:264:TYR:CD1	2:H:2:PDY:H20	2.27	0.58
1:D:77:LYS:NZ	1:D:79:LEU:HD21	2.17	0.58
1:F:66:THR:O	1:F:70:LEU:HB2	2.04	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:77:LYS:HB3	1:B:77:LYS:NZ	2.18	0.58
1:C:161:ARG:NH1	1:C:333:GLN:HG2	2.18	0.58
1:K:190:GLU:H	1:K:190:GLU:CD	2.06	0.58
1:I:140:CYS:SG	2:I:1:PDY:C17	2.92	0.58
1:G:264:TYR:O	1:G:275:MET:HG3	2.04	0.58
1:B:184:HIS:HD2	1:B:186:ASP:N	1.98	0.58
1:G:307:LYS:HB2	1:G:313:ARG:HG2	1.86	0.58
1:I:58:ALA:O	1:I:61:ASP:HB2	2.04	0.57
1:J:288:ASN:N	1:J:288:ASN:ND2	2.52	0.57
1:J:322:HIS:ND1	1:J:323:PRO:HD2	2.19	0.57
1:A:85:ARG:HH11	1:A:85:ARG:HG2	1.68	0.57
1:E:156:GLN:HE21	1:E:156:GLN:N	2.01	0.57
1:B:49:LYS:HD3	1:B:113:GLN:CG	2.34	0.57
1:D:214:THR:O	1:D:238:GLU:HB3	2.04	0.57
1:A:195:THR:HG23	1:A:202:ILE:O	2.04	0.57
1:F:70:LEU:HD12	1:F:94:MET:CE	2.34	0.57
1:E:229:TYR:OH	1:F:188:LYS:HE2	2.03	0.57
1:J:74:ILE:N	1:J:94:MET:HE3	2.19	0.57
1:E:60:ILE:C	1:E:60:ILE:HD12	2.25	0.57
1:L:48:VAL:O	1:L:48:VAL:HG12	2.02	0.57
1:I:215:THR:OG1	1:I:216:SER:N	2.37	0.57
2:C:2:PDY:H18	2:C:2:PDY:C14	2.33	0.57
1:B:108:HIS:CG	1:B:120:ILE:HD11	2.40	0.57
1:J:300:MET:SD	1:J:303:ARG:HD2	2.44	0.57
1:A:295:SER:OG	1:A:298:VAL:HG23	2.04	0.57
1:J:66:THR:CG2	1:J:68:GLN:HB2	2.33	0.57
1:J:73:GLY:C	1:J:94:MET:HE3	2.25	0.57
1:C:65:VAL:HG12	1:C:70:LEU:HD11	1.87	0.57
1:C:54:ILE:HG21	1:C:125:GLU:HB2	1.85	0.57
1:J:156:GLN:HG3	1:J:340:ARG:HH11	1.69	0.57
1:C:97:ASP:H	1:C:133:CYS:HA	1.70	0.57
1:G:300:MET:SD	1:G:303:ARG:NH2	2.75	0.57
1:J:147:PHE:HB3	1:J:342:LEU:HD21	1.86	0.57
1:I:275:MET:O	1:I:279:ILE:HG13	2.05	0.57
1:F:264:TYR:CZ	2:F:2:PDY:H24	2.40	0.57
1:H:240:TYR:CE1	1:H:242:LYS:HB2	2.40	0.57
1:K:288:ASN:H	1:K:288:ASN:HD22	1.52	0.57
1:B:108:HIS:HE1	1:B:138:MET:CE	2.16	0.57
1:I:200:ASN:N	1:I:200:ASN:HD22	2.03	0.57
1:J:140:CYS:SG	2:J:1:PDY:H17	2.45	0.57
1:D:49:LYS:HD2	1:D:113:GLN:CG	2.28	0.57
1:F:260:TYR:OH	1:F:287:PRO:HG2	2.05	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:102:ARG:HG3	1:K:134:LEU:HD21	1.87	0.57
1:D:58:ALA:O	1:D:61:ASP:HB2	2.05	0.57
1:J:187:VAL:O	1:J:187:VAL:HG12	2.04	0.57
1:I:264:TYR:CG	2:I:2:PDY:H20	2.39	0.57
1:K:66:THR:H	1:K:69:VAL:HG22	1.69	0.57
1:G:189:PRO:HG2	1:G:190:GLU:OE1	2.04	0.57
1:D:278:ARG:HA	1:D:283:GLN:HG3	1.86	0.57
1:L:49:LYS:CD	1:L:50:SER:H	2.18	0.56
1:C:295:SER:CB	1:C:298:VAL:HG23	2.29	0.56
1:C:264:TYR:OH	2:C:2:PDY:H24	2.04	0.56
1:E:202:ILE:CD1	1:E:204:LYS:HE2	2.34	0.56
1:J:278:ARG:CG	1:J:283:GLN:HE21	2.18	0.56
1:K:129:ALA:C	1:K:131:ARG:H	2.09	0.56
1:E:66:THR:HG22	1:E:69:VAL:HG13	1.85	0.56
2:B:1:PDY:H18	2:B:1:PDY:C14	2.35	0.56
1:A:327:GLN:CD	1:A:330:LYS:HD3	2.25	0.56
1:L:155:ASP:HA	1:L:157:ALA:N	2.20	0.56
1:E:161:ARG:HB3	1:E:333:GLN:NE2	2.20	0.56
1:G:310:PRO:HG3	1:I:233:GLU:HG2	1.87	0.56
1:C:63:TYR:O	1:C:65:VAL:HG23	2.04	0.56
1:E:184:HIS:HD2	1:E:186:ASP:H	1.53	0.56
1:I:121:VAL:HB	1:I:137:VAL:HG12	1.87	0.56
2:F:2:PDY:H14	2:F:2:PDY:C13	2.35	0.56
1:D:202:ILE:HD12	1:D:203:LEU:N	2.20	0.56
1:E:304:ASN:C	1:E:304:ASN:OD1	2.43	0.56
1:F:110:ARG:HH22	1:F:213:GLU:CD	2.09	0.56
1:G:188:LYS:HB2	1:G:189:PRO:HD2	1.87	0.56
1:K:56:LYS:HZ1	1:K:125:GLU:CD	2.08	0.56
1:F:288:ASN:OD1	1:F:292:SER:HB3	2.05	0.56
1:F:100:LYS:NZ	1:F:103:ARG:HH22	2.04	0.56
1:F:281:MET:HB2	1:F:283:GLN:HG3	1.88	0.56
1:E:110:ARG:HH22	1:E:213:GLU:CD	2.09	0.56
1:K:119:ARG:HB3	1:K:139:GLU:OE1	2.06	0.56
1:H:328:SER:O	1:H:331:VAL:HG22	2.05	0.56
1:F:69:VAL:HB	1:F:79:LEU:HD13	1.87	0.56
1:A:276:LYS:HD3	1:A:280:ARG:HH12	1.70	0.56
1:B:60:ILE:HD12	1:B:61:ASP:N	2.21	0.56
2:H:1:PDY:H14	2:H:1:PDY:C13	2.34	0.56
1:I:69:VAL:CA	1:I:79:LEU:HD22	2.34	0.56
1:G:196:SER:OG	1:G:198:ARG:HG2	2.06	0.56
1:E:260:TYR:HE2	1:E:290:GLU:OE1	1.88	0.56
1:J:66:THR:CG2	1:J:69:VAL:HG12	2.36	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:71:GLY:O	1:J:74:ILE:HG22	2.06	0.56
1:I:266:ASN:H	1:I:266:ASN:HD22	1.53	0.56
1:B:233:GLU:HB3	1:C:310:PRO:HG3	1.88	0.56
1:C:188:LYS:HE3	1:C:191:ASN:HD21	1.70	0.56
1:F:338:THR:O	1:F:342:LEU:HB2	2.05	0.56
1:B:232:PRO:HD3	1:C:247:TRP:CZ2	2.41	0.56
1:I:107:LEU:HD22	1:I:182:ILE:CD1	2.36	0.56
1:H:66:THR:O	1:H:70:LEU:HB2	2.06	0.56
2:A:2:PDY:C13	2:A:2:PDY:H14	2.36	0.56
1:H:295:SER:OG	1:H:298:VAL:HG23	2.07	0.55
1:L:49:LYS:HD2	1:L:50:SER:N	2.20	0.55
1:E:300:MET:SD	1:E:303:ARG:NE	2.70	0.55
1:I:185:ARG:HH21	1:I:212:LYS:HG3	1.72	0.55
1:L:327:GLN:NE2	1:L:330:LYS:HD3	2.21	0.55
1:J:118:VAL:HG21	2:J:1:PDY:H11	1.88	0.55
1:F:261:PRO:HD3	2:F:2:PDY:H25	1.87	0.55
2:A:1:PDY:C13	2:A:1:PDY:H14	2.37	0.55
1:D:290:GLU:CD	1:D:290:GLU:H	2.10	0.55
1:H:300:MET:SD	1:H:303:ARG:NE	2.77	0.55
1:L:97:ASP:O	1:L:98:CYS:HB3	2.05	0.55
1:B:184:HIS:HE1	1:B:206:THR:O	1.89	0.55
1:C:83:ASN:ND2	1:C:86:THR:HB	2.22	0.55
1:H:257:LEU:HD11	1:H:298:VAL:HG11	1.88	0.55
1:E:327:GLN:CB	1:E:330:LYS:HZ2	2.18	0.55
1:G:338:THR:O	1:G:342:LEU:HB2	2.06	0.55
1:I:322:HIS:ND1	1:I:323:PRO:HD2	2.20	0.55
1:A:175:GLN:NE2	1:A:320:MET:HG3	2.20	0.55
1:E:97:ASP:HB2	1:E:134:LEU:HD13	1.87	0.55
1:E:66:THR:O	1:E:69:VAL:HG22	2.05	0.55
1:C:82:PHE:HA	1:C:88:GLU:O	2.06	0.55
1:L:300:MET:SD	1:L:303:ARG:NH2	2.75	0.55
1:F:304:ASN:OD1	1:F:314:MET:HB2	2.06	0.55
1:H:48:VAL:HG13	1:H:48:VAL:O	2.07	0.55
1:L:70:LEU:HG	1:L:94:MET:HE1	1.88	0.55
1:G:97:ASP:OD2	1:G:102:ARG:NH2	2.37	0.55
1:A:280:ARG:HH11	1:C:235:LEU:CD1	2.20	0.55
1:C:66:THR:HG1	1:C:69:VAL:N	2.05	0.55
1:J:254:TYR:CG	1:J:262:PRO:HG3	2.42	0.55
1:C:252:ILE:O	1:C:256:LEU:HB2	2.07	0.55
1:G:195:THR:HG23	1:G:202:ILE:O	2.06	0.55
1:B:296:GLU:OE2	1:B:303:ARG:NH2	2.39	0.55
2:E:2:PDY:C18	2:E:2:PDY:H14A	2.36	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:1:PDY:H14	2:D:1:PDY:C13	2.35	0.55
1:C:307:LYS:HD2	1:C:312:GLN:OE1	2.06	0.55
1:J:60:ILE:HD12	1:J:60:ILE:C	2.26	0.55
1:K:258:CYS:HB3	1:K:291:TRP:NE1	2.22	0.55
1:K:82:PHE:HA	1:K:88:GLU:O	2.07	0.55
1:A:69:VAL:HB	1:A:79:LEU:CD1	2.37	0.55
1:F:304:ASN:CG	1:F:314:MET:HB2	2.26	0.55
1:L:147:PHE:HE2	1:L:256:LEU:HD23	1.71	0.55
1:D:184:HIS:CD2	1:D:205:LEU:HD21	2.42	0.55
2:K:2:PDY:C18	2:K:2:PDY:H14A	2.35	0.55
1:L:94:MET:O	1:L:95:LEU:HD23	2.06	0.55
1:J:329:THR:C	1:J:331:VAL:N	2.60	0.55
1:J:159:THR:HG23	1:J:333:GLN:HA	1.89	0.55
1:C:264:TYR:CE1	2:C:2:PDY:H24A	2.42	0.55
2:C:2:PDY:C3	2:C:2:PDY:C18	2.84	0.55
1:F:202:ILE:CD1	1:F:204:LYS:HE2	2.37	0.54
1:E:111:ALA:HB1	1:E:117:ILE:CD1	2.38	0.54
1:C:153:ARG:HB2	1:C:156:GLN:HE22	1.72	0.54
1:J:116:HIS:CE1	1:J:169:SER:OG	2.60	0.54
1:J:287:PRO:O	1:J:291:TRP:HB2	2.06	0.54
1:H:264:TYR:CD1	2:H:2:PDY:C17	2.89	0.54
1:L:202:ILE:HD11	1:L:204:LYS:CE	2.36	0.54
1:B:58:ALA:O	1:B:61:ASP:HB2	2.08	0.54
1:C:130:GLY:O	1:J:110:ARG:HD3	2.06	0.54
1:B:155:ASP:HA	1:B:343:LYS:NZ	2.22	0.54
1:B:158:PHE:CE1	1:B:162:GLU:HB3	2.43	0.54
1:C:167:MET:HG3	1:C:253:MET:HE2	1.90	0.54
1:L:142:ASP:N	1:L:195:THR:O	2.41	0.54
1:G:190:GLU:H	1:G:190:GLU:CD	2.10	0.54
1:J:327:GLN:HB3	1:J:330:LYS:HG2	1.90	0.54
1:I:327:GLN:HE21	1:I:330:LYS:HZ1	1.54	0.54
1:H:233:GLU:HG2	1:I:310:PRO:HG3	1.90	0.54
1:K:150:ILE:O	1:K:153:ARG:HG3	2.07	0.54
1:E:178:HIS:HE1	1:E:245:ASP:OD2	1.91	0.54
1:K:260:TYR:HB2	2:K:2:PDY:H19	1.90	0.54
1:A:332:PRO:CB	1:A:334:THR:HG22	2.30	0.54
1:I:72:LEU:CB	1:I:79:LEU:HD21	2.37	0.54
1:E:145:GLU:HG2	1:E:193:LEU:HD21	1.90	0.54
1:A:190:GLU:CD	1:A:190:GLU:H	2.11	0.54
1:C:300:MET:SD	1:C:303:ARG:NE	2.80	0.54
1:H:264:TYR:CB	2:H:2:PDY:C17	2.85	0.54
1:H:90:PHE:HE2	1:H:121:VAL:HG21	1.71	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:260:TYR:OH	1:K:287:PRO:HG2	2.07	0.54
1:A:159:THR:OG1	1:A:333:GLN:NE2	2.41	0.54
1:C:327:GLN:HB3	1:C:330:LYS:HG3	1.90	0.54
1:A:66:THR:O	1:A:69:VAL:HG22	2.07	0.54
1:C:161:ARG:HD3	1:C:331:VAL:HG13	1.90	0.54
1:L:235:LEU:HD12	1:L:235:LEU:H	1.73	0.54
1:H:198:ARG:HG2	1:H:199:PRO:HD2	1.89	0.54
1:J:298:VAL:HG22	1:J:324:TRP:CD1	2.42	0.54
1:F:214:THR:HG21	1:F:242:LYS:HE3	1.88	0.54
1:K:261:PRO:HD3	2:K:2:PDY:H25	1.90	0.54
1:I:202:ILE:HD11	1:I:204:LYS:HG2	1.89	0.54
1:K:49:LYS:HB3	1:K:113:GLN:NE2	2.23	0.54
1:J:66:THR:HG22	1:J:69:VAL:HG12	1.89	0.54
1:B:192:LEU:C	1:B:193:LEU:HD23	2.28	0.54
1:A:188:LYS:HE2	1:A:190:GLU:HB2	1.90	0.54
1:L:147:PHE:CE2	1:L:256:LEU:HD23	2.43	0.54
1:H:81:ILE:HD13	1:H:92:LEU:HB2	1.89	0.54
1:H:97:ASP:OD1	1:H:98:CYS:N	2.41	0.53
1:B:60:ILE:C	1:B:60:ILE:HD12	2.28	0.53
1:J:159:THR:HG21	1:J:333:GLN:HG2	1.90	0.53
1:D:188:LYS:HG3	1:D:190:GLU:HG2	1.91	0.53
1:L:146:LEU:HD11	1:L:166:ILE:HD13	1.89	0.53
1:B:146:LEU:HD11	1:B:166:ILE:HD13	1.89	0.53
1:J:63:TYR:O	1:J:84:LYS:HE3	2.08	0.53
2:C:1:PDY:C3	2:C:1:PDY:H18	2.39	0.53
1:A:161:ARG:HD2	1:A:328:SER:O	2.09	0.53
1:J:278:ARG:HG3	1:J:283:GLN:HE21	1.73	0.53
1:K:80:GLN:NE2	2:K:1:PDY:H24	2.22	0.53
1:E:69:VAL:CB	1:E:79:LEU:HD13	2.38	0.53
1:K:309:GLU:OE2	1:K:310:PRO:HD2	2.07	0.53
1:H:150:ILE:O	1:H:153:ARG:HG2	2.08	0.53
1:K:332:PRO:HB2	1:K:334:THR:CG2	2.26	0.53
1:L:159:THR:HB	1:L:162:GLU:HG3	1.90	0.53
1:H:151:GLN:NE2	1:H:342:LEU:O	2.42	0.53
1:I:154:GLY:C	1:I:156:GLN:H	2.12	0.53
1:G:285:GLU:C	1:G:287:PRO:HD3	2.29	0.53
1:D:98:CYS:HB2	1:D:99:PRO:CD	2.39	0.53
1:G:264:TYR:CD2	1:G:264:TYR:C	2.82	0.53
1:H:69:VAL:HG13	1:H:70:LEU:H	1.74	0.53
1:A:288:ASN:HB3	1:A:289:PRO:HA	1.90	0.53
1:C:60:ILE:HD12	1:C:61:ASP:N	2.24	0.53
1:B:155:ASP:N	1:B:156:GLN:OE1	2.41	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:214:THR:HG21	1:A:242:LYS:HE3	1.90	0.53
1:K:234:VAL:O	1:K:234:VAL:HG12	2.09	0.53
1:J:276:LYS:CG	1:K:235:LEU:HD12	2.38	0.53
1:H:110:ARG:HH22	1:H:213:GLU:CD	2.12	0.53
1:K:89:LYS:N	1:K:89:LYS:CD	2.72	0.53
1:B:247:TRP:HB2	1:B:313:ARG:NH1	2.24	0.53
1:E:275:MET:HA	1:E:278:ARG:HH11	1.74	0.53
1:L:260:TYR:OH	1:L:287:PRO:HG2	2.09	0.53
1:E:332:PRO:HB2	1:E:334:THR:HG22	1.89	0.53
1:K:95:LEU:O	1:K:133:CYS:CB	2.56	0.53
1:H:212:LYS:HD3	1:H:213:GLU:N	2.23	0.53
1:J:198:ARG:CG	1:J:198:ARG:HH11	2.22	0.53
1:C:185:ARG:HD3	1:C:241:ASP:CG	2.29	0.53
1:J:185:ARG:CZ	1:J:212:LYS:HG3	2.38	0.53
1:E:87:GLN:NE2	1:E:87:GLN:N	2.57	0.53
1:J:255:ILE:HG12	1:J:261:PRO:HA	1.91	0.52
1:J:156:GLN:HG3	1:J:340:ARG:NH1	2.23	0.52
1:C:148:SER:HA	1:C:151:GLN:HB3	1.91	0.52
1:D:328:SER:O	1:D:331:VAL:HG13	2.08	0.52
1:H:154:GLY:HA2	1:H:156:GLN:H	1.75	0.52
1:H:115:PRO:O	1:H:204:LYS:NZ	2.40	0.52
1:D:332:PRO:HB2	1:D:334:THR:HG22	1.91	0.52
1:A:107:LEU:HD21	1:A:213:GLU:HG3	1.90	0.52
1:C:78:VAL:CG1	1:C:91:ALA:HB1	2.38	0.52
1:K:178:HIS:CE1	1:K:242:LYS:HG2	2.45	0.52
1:E:80:GLN:OE1	2:E:1:PDY:C24	2.58	0.52
1:C:129:ALA:HB3	1:C:131:ARG:NE	2.25	0.52
1:I:338:THR:O	1:I:342:LEU:HB2	2.09	0.52
1:J:241:ASP:O	1:J:244:CYS:HB3	2.10	0.52
1:L:241:ASP:O	1:L:244:CYS:HB3	2.09	0.52
2:F:1:PDY:H18	2:F:1:PDY:H14A	1.91	0.52
1:K:129:ALA:O	1:K:131:ARG:N	2.42	0.52
1:J:198:ARG:HH11	1:J:200:ASN:N	2.07	0.52
1:C:260:TYR:OH	1:C:290:GLU:HG3	2.09	0.52
1:A:278:ARG:O	1:A:282:GLY:N	2.43	0.52
1:A:285:GLU:O	1:A:287:PRO:HD3	2.09	0.52
1:I:160:GLU:HA	1:I:336:LEU:HD21	1.91	0.52
1:K:140:CYS:SG	2:K:1:PDY:H17	2.50	0.52
1:D:110:ARG:HH22	1:D:213:GLU:CD	2.12	0.52
1:I:70:LEU:HD23	1:I:94:MET:CE	2.38	0.52
1:J:276:LYS:HA	1:J:279:ILE:HD12	1.92	0.52
1:E:161:ARG:HD3	1:E:331:VAL:O	2.09	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:104:GLU:HG3	1:K:208:PHE:O	2.10	0.52
1:L:110:ARG:HH22	1:L:213:GLU:CD	2.12	0.52
1:E:160:GLU:HA	1:E:336:LEU:HD21	1.91	0.52
1:H:154:GLY:CA	1:H:156:GLN:H	2.23	0.52
1:B:290:GLU:HB2	1:B:291:TRP:CD1	2.44	0.52
1:C:149:ARG:NH2	1:C:201:ALA:HB3	2.25	0.52
1:D:286:PHE:CD1	1:D:299:LYS:HG2	2.44	0.52
1:I:108:HIS:HE1	1:I:138:MET:CE	2.23	0.52
1:D:73:GLY:HA3	1:D:94:MET:SD	2.50	0.52
1:D:155:ASP:CG	1:D:156:GLN:H	2.12	0.52
2:G:1:PDY:H18	2:G:1:PDY:H14A	1.85	0.52
1:K:332:PRO:CB	1:K:334:THR:HG22	2.27	0.52
1:D:49:LYS:HG2	1:D:50:SER:N	2.25	0.52
1:F:70:LEU:HD12	1:F:94:MET:SD	2.50	0.52
1:B:47:HIS:HD2	1:L:70:LEU:HD22	1.73	0.51
1:G:69:VAL:CB	1:G:79:LEU:HD13	2.34	0.51
1:L:159:THR:HG22	1:L:160:GLU:N	2.25	0.51
1:E:185:ARG:NE	1:E:212:LYS:HG3	2.25	0.51
1:G:214:THR:HG21	1:G:242:LYS:HG3	1.91	0.51
1:K:60:ILE:HD12	1:K:60:ILE:C	2.30	0.51
1:D:130:GLY:O	1:I:110:ARG:NH1	2.41	0.51
2:I:1:PDY:C3	2:I:1:PDY:H18	2.38	0.51
1:C:183:ALA:O	1:C:211:ALA:HA	2.09	0.51
1:K:108:HIS:CG	1:K:120:ILE:HD11	2.45	0.51
1:J:332:PRO:HB2	1:J:334:THR:CG2	2.41	0.51
1:B:189:PRO:HD2	1:B:190:GLU:OE1	2.10	0.51
1:D:195:THR:HG21	1:D:202:ILE:HG23	1.92	0.51
1:B:339:SER:O	1:B:343:LYS:HG3	2.10	0.51
1:E:98:CYS:HB2	1:E:99:PRO:HD2	1.91	0.51
1:F:260:TYR:HB2	2:F:2:PDY:H19	1.92	0.51
1:K:337:HIS:O	1:K:341:VAL:HG23	2.10	0.51
2:B:2:PDY:H14A	2:B:2:PDY:H18	1.92	0.51
1:J:331:VAL:HG23	1:J:332:PRO:HD2	1.91	0.51
1:I:202:ILE:HD11	1:I:204:LYS:CG	2.40	0.51
1:J:141:LEU:CD1	1:J:193:LEU:HB2	2.40	0.51
1:G:73:GLY:CA	1:G:79:LEU:HD11	2.40	0.51
1:G:156:GLN:HE22	1:G:340:ARG:NH1	2.09	0.51
1:K:164:SER:HB2	1:K:324:TRP:CZ2	2.46	0.51
1:L:261:PRO:HB2	1:L:263:PHE:O	2.11	0.51
1:J:293:GLU:HA	1:J:293:GLU:OE2	2.10	0.51
1:F:161:ARG:HD3	1:F:331:VAL:O	2.09	0.51
1:F:214:THR:HG21	1:F:242:LYS:HG3	1.93	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:284:TYR:O	1:C:285:GLU:HG2	2.11	0.51
1:I:168:LYS:O	1:I:172:GLU:HG3	2.10	0.51
1:D:48:VAL:O	1:D:48:VAL:HG13	2.09	0.51
1:J:73:GLY:O	1:J:94:MET:HB2	2.10	0.51
1:J:185:ARG:NH2	1:J:212:LYS:HE2	2.26	0.51
1:K:188:LYS:NZ	1:K:190:GLU:HG3	2.25	0.51
1:J:110:ARG:HH22	1:J:213:GLU:CD	2.14	0.51
1:E:260:TYR:HB2	2:E:2:PDY:H19	1.92	0.51
1:D:110:ARG:O	1:D:113:GLN:HG3	2.11	0.51
1:B:66:THR:O	1:B:69:VAL:HG22	2.10	0.51
1:B:69:VAL:HG23	1:B:70:LEU:H	1.74	0.51
1:E:115:PRO:O	1:E:202:ILE:HD11	2.11	0.51
1:I:100:LYS:CD	1:I:103:ARG:HH21	2.22	0.51
1:H:341:VAL:C	1:H:343:LYS:H	2.14	0.51
1:G:284:TYR:OH	1:G:303:ARG:HG2	2.11	0.51
1:J:110:ARG:O	1:J:113:GLN:HG2	2.11	0.51
1:A:168:LYS:HB2	1:A:325:ILE:HG23	1.93	0.51
1:C:102:ARG:NH2	1:C:134:LEU:HD11	2.26	0.51
1:G:231:ALA:HB1	1:G:233:GLU:OE2	2.11	0.51
1:A:185:ARG:NE	1:A:212:LYS:HG3	2.26	0.51
1:B:155:ASP:HA	1:B:343:LYS:HZ1	1.76	0.51
1:F:307:LYS:HG2	1:F:312:GLN:HB3	1.92	0.51
1:C:234:VAL:HG22	1:C:234:VAL:O	2.11	0.51
1:B:184:HIS:CD2	1:B:186:ASP:H	2.14	0.50
1:B:77:LYS:HZ2	1:B:79:LEU:CD2	2.24	0.50
1:F:149:ARG:HG3	1:F:194:TYR:CD2	2.46	0.50
1:H:200:ASN:ND2	1:H:200:ASN:N	2.59	0.50
1:F:60:ILE:C	1:F:60:ILE:HD12	2.31	0.50
1:L:80:GLN:HB2	2:L:1:PDY:H24A	1.92	0.50
1:L:97:ASP:N	1:L:133:CYS:HA	2.26	0.50
1:L:159:THR:CG2	1:L:161:ARG:HB3	2.40	0.50
1:J:202:ILE:HD11	1:J:204:LYS:HE3	1.92	0.50
1:A:50:SER:HB2	1:F:56:LYS:O	2.11	0.50
1:J:81:ILE:HD13	1:J:92:LEU:HB2	1.92	0.50
1:A:235:LEU:HD11	1:B:276:LYS:HE2	1.92	0.50
1:G:86:THR:C	1:G:88:GLU:H	2.14	0.50
1:A:111:ALA:HB1	1:A:117:ILE:HD13	1.93	0.50
1:L:264:TYR:CD2	2:L:2:PDY:H20	2.47	0.50
1:E:260:TYR:HB2	1:E:261:PRO:HD2	1.92	0.50
1:B:69:VAL:CG2	1:B:70:LEU:N	2.73	0.50
1:G:234:VAL:O	1:G:234:VAL:HG12	2.11	0.50
1:J:185:ARG:CZ	1:J:212:LYS:HE2	2.41	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:239:LYS:O	1:D:240:TYR:HB2	2.11	0.50
1:H:264:TYR:CG	2:H:2:PDY:H2O	2.42	0.50
1:B:161:ARG:HD3	1:B:331:VAL:O	2.11	0.50
1:L:190:GLU:OE1	1:L:190:GLU:N	2.38	0.50
1:C:107:LEU:HD22	1:C:182:ILE:HG12	1.93	0.50
1:B:111:ALA:HB1	1:B:117:ILE:HD12	1.93	0.50
1:L:66:THR:HG22	1:L:69:VAL:CG2	2.38	0.50
1:K:164:SER:HA	1:K:324:TRP:CH2	2.46	0.50
1:J:147:PHE:HE2	1:J:256:LEU:HD23	1.76	0.50
1:J:114:CYS:SG	1:J:116:HIS:HB2	2.52	0.50
1:K:110:ARG:HH22	1:K:213:GLU:CD	2.15	0.50
1:D:97:ASP:H	1:D:133:CYS:HA	1.76	0.50
1:C:202:ILE:CD1	1:C:204:LYS:HE2	2.18	0.50
1:K:288:ASN:N	1:K:288:ASN:ND2	2.59	0.50
1:J:192:LEU:O	1:J:193:LEU:HD23	2.11	0.50
1:B:52:LEU:HD22	1:B:105:VAL:HG12	1.93	0.50
1:J:287:PRO:HD2	1:J:291:TRP:CD1	2.46	0.50
1:L:264:TYR:CB	2:L:2:PDY:C17	2.88	0.50
1:F:69:VAL:HG23	1:F:70:LEU:N	2.26	0.50
1:K:108:HIS:CD2	1:K:120:ILE:HD11	2.47	0.50
1:G:161:ARG:NH1	1:G:333:GLN:HG3	2.26	0.50
1:L:161:ARG:NH1	1:L:333:GLN:HG2	2.27	0.50
1:C:330:LYS:HB2	1:C:330:LYS:HZ3	1.77	0.50
1:J:198:ARG:HG3	1:J:199:PRO:N	2.27	0.50
1:H:341:VAL:O	1:H:343:LYS:N	2.37	0.50
1:D:116:HIS:CE1	1:D:169:SER:HB2	2.47	0.50
1:B:150:ILE:O	1:B:153:ARG:HG2	2.12	0.50
1:G:80:GLN:CD	1:G:89:LYS:HD2	2.31	0.50
1:B:66:THR:O	1:B:70:LEU:HD13	2.12	0.50
1:D:232:PRO:HD2	1:D:233:GLU:OE2	2.11	0.50
1:B:125:GLU:C	1:B:126:ASN:HD22	2.15	0.50
1:K:62:ASP:CA	1:K:85:ARG:HH21	2.22	0.49
1:A:313:ARG:NH1	1:C:233:GLU:OE1	2.44	0.49
1:B:145:GLU:O	1:B:148:SER:HB3	2.12	0.49
1:L:247:TRP:HZ3	1:L:306:LEU:O	1.95	0.49
2:B:1:PDY:C3	2:B:1:PDY:C18	2.88	0.49
1:A:276:LYS:HG3	1:C:235:LEU:HD11	1.94	0.49
1:L:260:TYR:OH	1:L:290:GLU:HG3	2.12	0.49
1:C:127:LEU:O	1:J:48:VAL:HA	2.11	0.49
1:G:180:ILE:HD11	1:G:182:ILE:HD12	1.94	0.49
1:D:151:GLN:HB3	1:D:342:LEU:HB3	1.94	0.49
2:H:1:PDY:C18	2:H:1:PDY:C3	2.73	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:1:PDY:C14	2:L:1:PDY:H18	2.40	0.49
1:G:49:LYS:HD2	1:G:113:GLN:CD	2.33	0.49
1:E:214:THR:O	1:E:215:THR:HB	2.11	0.49
1:K:188:LYS:HZ1	1:K:190:GLU:CG	2.25	0.49
1:G:235:LEU:HD12	1:H:280:ARG:HG3	1.93	0.49
1:F:332:PRO:HB2	1:F:334:THR:HG22	1.93	0.49
1:A:161:ARG:O	1:A:165:GLU:HG3	2.12	0.49
1:A:328:SER:O	1:A:331:VAL:CG1	2.61	0.49
1:E:73:GLY:HA3	1:E:94:MET:CE	2.42	0.49
1:B:232:PRO:HD3	1:C:247:TRP:CH2	2.47	0.49
1:C:296:GLU:OE2	1:C:303:ARG:NH2	2.42	0.49
1:D:145:GLU:HG2	1:D:193:LEU:CD2	2.43	0.49
1:C:168:LYS:O	1:C:172:GLU:HG3	2.12	0.49
1:B:57:ASN:H	1:B:57:ASN:ND2	2.08	0.49
2:J:1:PDY:C18	2:J:1:PDY:C3	2.81	0.49
1:H:337:HIS:O	1:H:340:ARG:HG3	2.12	0.49
1:K:178:HIS:ND1	1:K:242:LYS:HG2	2.28	0.49
1:C:184:HIS:CD2	1:C:205:LEU:HD21	2.47	0.49
2:L:2:PDY:H18	2:L:2:PDY:H14	0.64	0.49
1:I:66:THR:OG1	1:I:69:VAL:HG23	2.12	0.49
1:E:159:THR:OG1	1:E:333:GLN:NE2	2.46	0.49
1:I:161:ARG:HD3	1:I:331:VAL:O	2.13	0.49
1:B:234:VAL:HG12	1:B:234:VAL:O	2.13	0.49
1:D:66:THR:HB	1:D:69:VAL:CG2	2.40	0.49
1:I:330:LYS:HG3	1:I:330:LYS:O	2.13	0.49
1:A:309:GLU:CG	1:C:311:THR:HG22	2.43	0.49
1:A:338:THR:HG22	1:A:342:LEU:CD2	2.42	0.49
1:B:69:VAL:CG2	1:B:70:LEU:H	2.26	0.49
1:C:327:GLN:NE2	1:C:330:LYS:NZ	2.61	0.49
1:J:198:ARG:HG2	1:J:201:ALA:N	2.27	0.49
1:L:266:ASN:HB2	1:L:278:ARG:HH22	1.77	0.49
1:I:107:LEU:HD22	1:I:182:ILE:HD13	1.93	0.49
1:A:235:LEU:CD1	1:B:276:LYS:HE2	2.42	0.49
1:D:239:LYS:HG2	1:D:240:TYR:CD1	2.48	0.49
1:G:124:TYR:HB2	1:G:135:LEU:HB2	1.95	0.49
1:K:247:TRP:HB2	1:K:313:ARG:NH1	2.28	0.49
2:J:2:PDY:H14	2:J:2:PDY:C13	2.42	0.49
1:B:202:ILE:CD1	1:B:204:LYS:HE2	2.30	0.49
1:K:66:THR:OG1	1:K:69:VAL:HG13	2.12	0.49
1:A:97:ASP:HB3	1:A:132:LYS:O	2.13	0.49
1:F:156:GLN:NE2	1:F:156:GLN:CA	2.76	0.49
1:A:280:ARG:NH1	1:C:235:LEU:HD13	2.28	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:110:ARG:HD2	1:H:130:GLY:O	2.13	0.49
1:F:145:GLU:HG2	1:F:193:LEU:HD22	1.95	0.49
1:K:160:GLU:HB3	1:K:336:LEU:HD11	1.95	0.49
1:C:264:TYR:CE1	2:C:2:PDY:C24	2.96	0.49
1:K:274:GLY:O	1:K:278:ARG:HG3	2.12	0.49
1:D:65:VAL:CG1	1:D:70:LEU:HD13	2.42	0.49
1:K:118:VAL:HG11	1:K:206:THR:HG22	1.94	0.49
1:G:58:ALA:HB1	1:G:60:ILE:HG13	1.94	0.49
1:F:83:ASN:OD1	1:F:84:LYS:N	2.46	0.49
1:I:264:TYR:CZ	2:I:2:PDY:H24	2.48	0.48
1:D:77:LYS:HZ2	1:D:79:LEU:HD21	1.75	0.48
1:H:129:ALA:CB	1:H:131:ARG:HD3	2.34	0.48
1:C:161:ARG:HB2	1:C:332:PRO:O	2.13	0.48
1:L:116:HIS:O	1:L:204:LYS:HA	2.12	0.48
1:G:153:ARG:HB3	1:G:339:SER:OG	2.13	0.48
1:K:188:LYS:NZ	1:K:190:GLU:CG	2.75	0.48
1:K:188:LYS:HZ1	1:K:190:GLU:HG3	1.77	0.48
1:A:116:HIS:O	1:A:204:LYS:HA	2.12	0.48
1:A:290:GLU:CD	1:A:290:GLU:H	2.16	0.48
1:L:77:LYS:HE3	1:L:79:LEU:CD2	2.42	0.48
1:G:66:THR:HG23	1:G:68:GLN:HG2	1.95	0.48
1:L:331:VAL:HG23	1:L:332:PRO:HD2	1.95	0.48
1:I:69:VAL:HG13	1:I:79:LEU:CB	2.43	0.48
1:G:188:LYS:HD3	1:I:229:TYR:CE1	2.48	0.48
1:K:105:VAL:HG21	1:K:134:LEU:HD23	1.95	0.48
1:F:148:SER:HA	1:F:151:GLN:HG2	1.96	0.48
1:E:332:PRO:HG2	1:E:334:THR:CG2	2.43	0.48
1:D:162:GLU:O	1:D:166:ILE:HG13	2.13	0.48
1:H:69:VAL:HG13	1:H:70:LEU:N	2.28	0.48
1:J:73:GLY:N	1:J:79:LEU:HD11	2.29	0.48
1:G:66:THR:HG21	1:G:68:GLN:OE1	2.13	0.48
1:F:70:LEU:O	1:F:74:ILE:HD13	2.14	0.48
1:B:65:VAL:HG12	1:B:70:LEU:CD1	2.43	0.48
1:A:49:LYS:HG3	1:A:113:GLN:CD	2.33	0.48
1:L:295:SER:OG	1:L:298:VAL:HG23	2.13	0.48
1:K:56:LYS:NZ	1:K:125:GLU:OE1	2.46	0.48
1:B:52:LEU:CD2	1:B:105:VAL:HG12	2.43	0.48
1:D:151:GLN:HE21	1:D:343:LYS:HA	1.77	0.48
1:D:74:ILE:HG13	1:D:128:TYR:CE2	2.48	0.48
1:L:301:LEU:HD13	1:L:322:HIS:CD2	2.48	0.48
1:B:48:VAL:HB	1:L:70:LEU:CD2	2.42	0.48
1:J:83:ASN:O	1:J:87:GLN:HA	2.13	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:290:GLU:OE2	1:G:337:HIS:HD2	1.96	0.48
1:A:233:GLU:HG2	1:B:310:PRO:HD3	1.95	0.48
1:E:298:VAL:HG22	1:E:324:TRP:NE1	2.28	0.48
1:G:295:SER:O	1:G:299:LYS:HG3	2.13	0.48
1:C:52:LEU:HG	1:C:53:GLN:N	2.28	0.48
2:J:1:PDY:C13	2:J:1:PDY:H14	2.38	0.48
1:K:70:LEU:O	1:K:74:ILE:HG12	2.13	0.48
1:E:66:THR:CG2	1:E:69:VAL:HG13	2.44	0.48
1:G:215:THR:HG23	1:G:216:SER:N	2.29	0.48
1:J:69:VAL:HA	1:J:79:LEU:HD13	1.95	0.48
1:B:260:TYR:OH	1:B:290:GLU:HG3	2.13	0.48
1:G:145:GLU:HG2	1:G:193:LEU:HD21	1.94	0.48
1:H:116:HIS:HB3	1:H:173:ALA:HB2	1.95	0.48
1:A:230:VAL:HG13	1:A:230:VAL:O	2.14	0.48
1:J:340:ARG:O	1:J:343:LYS:HD3	2.14	0.48
1:B:49:LYS:HG3	1:B:50:SER:N	2.28	0.48
1:C:284:TYR:C	1:C:285:GLU:HG2	2.34	0.48
1:D:260:TYR:HB2	1:D:261:PRO:HD2	1.96	0.48
1:B:114:CYS:HB2	1:B:176:TYR:CD2	2.49	0.48
1:H:66:THR:H	1:H:69:VAL:CG1	2.26	0.48
1:H:77:LYS:HD3	1:H:79:LEU:HD21	1.96	0.48
1:J:65:VAL:HG12	1:J:70:LEU:HD22	1.96	0.48
1:H:164:SER:HB3	1:H:328:SER:HB3	1.95	0.48
1:F:73:GLY:HA3	1:F:94:MET:HE3	1.94	0.48
1:J:159:THR:HG23	1:J:333:GLN:CA	2.42	0.48
1:F:86:THR:HG22	1:F:87:GLN:N	2.29	0.48
1:H:110:ARG:HD3	1:J:127:LEU:HD11	1.96	0.48
1:F:149:ARG:NH1	1:F:196:SER:O	2.44	0.48
1:E:323:PRO:HA	1:E:327:GLN:NE2	2.28	0.48
1:I:83:ASN:OD1	1:I:84:LYS:N	2.47	0.48
1:H:337:HIS:CG	1:H:340:ARG:NH1	2.82	0.48
1:A:52:LEU:C	1:F:56:LYS:HD2	2.34	0.48
1:A:85:ARG:NH1	1:A:85:ARG:HG2	2.28	0.48
1:B:242:LYS:O	1:B:245:ASP:HB2	2.13	0.48
1:D:157:ALA:O	1:D:159:THR:HG23	2.13	0.48
1:K:327:GLN:HG2	1:K:330:LYS:NZ	2.29	0.48
1:B:85:ARG:HD2	1:B:86:THR:CG2	2.38	0.48
1:F:70:LEU:HA	1:F:94:MET:CE	2.44	0.48
1:B:110:ARG:NH2	1:B:213:GLU:OE2	2.47	0.48
1:C:125:GLU:C	1:C:126:ASN:HD22	2.17	0.48
1:L:82:PHE:CE1	1:L:89:LYS:HB2	2.49	0.48
1:I:56:LYS:O	1:K:51:GLY:N	2.44	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:161:ARG:NH2	1:K:333:GLN:HG3	2.29	0.48
1:J:57:ASN:HD22	1:J:57:ASN:H	1.61	0.48
1:B:231:ALA:HB1	1:B:233:GLU:CG	2.43	0.48
1:G:156:GLN:HG3	1:G:335:PRO:CB	2.44	0.48
1:J:311:THR:O	1:L:312:GLN:NE2	2.47	0.48
1:I:172:GLU:HG2	1:I:320:MET:CE	2.44	0.48
1:I:261:PRO:HG3	2:I:2:PDY:H25	1.95	0.47
1:H:55:LYS:HD3	1:H:124:TYR:CE2	2.49	0.47
1:I:207:ASP:OD2	2:I:1:PDY:N12	2.43	0.47
1:H:67:SER:C	1:H:69:VAL:N	2.67	0.47
1:C:106:GLU:OE2	1:H:132:LYS:HE2	2.13	0.47
1:H:125:GLU:OE2	1:H:132:LYS:HE3	2.14	0.47
1:E:97:ASP:H	1:E:133:CYS:HA	1.80	0.47
1:C:300:MET:SD	1:C:303:ARG:NH2	2.86	0.47
1:B:64:LYS:HE3	1:B:84:LYS:HE3	1.96	0.47
1:I:149:ARG:HG3	1:I:194:TYR:CD2	2.49	0.47
1:B:59:ILE:HG13	1:B:124:TYR:CE1	2.50	0.47
1:L:296:GLU:O	1:L:300:MET:HB2	2.14	0.47
1:B:330:LYS:HG3	1:B:330:LYS:O	2.14	0.47
2:K:1:PDY:H24	2:K:1:PDY:H20	1.43	0.47
1:G:185:ARG:HD3	1:G:241:ASP:OD2	2.14	0.47
1:G:118:VAL:HG23	1:G:139:GLU:HG2	1.96	0.47
1:G:73:GLY:N	1:G:79:LEU:HD11	2.29	0.47
1:J:83:ASN:OD1	1:J:85:ARG:N	2.46	0.47
1:D:70:LEU:HD21	1:I:48:VAL:HG11	1.95	0.47
1:B:326:MET:HG3	1:B:326:MET:O	2.14	0.47
1:F:48:VAL:HG13	1:F:48:VAL:O	2.13	0.47
1:G:231:ALA:HB3	1:G:234:VAL:CG2	2.35	0.47
1:I:266:ASN:N	1:I:266:ASN:ND2	2.49	0.47
1:E:56:LYS:O	1:L:50:SER:HB2	2.15	0.47
1:B:278:ARG:HG2	1:B:283:GLN:HG3	1.95	0.47
1:F:235:LEU:N	1:F:235:LEU:HD23	2.29	0.47
1:H:162:GLU:O	1:H:166:ILE:HG13	2.15	0.47
1:G:90:PHE:HE2	1:G:121:VAL:HG21	1.77	0.47
1:F:160:GLU:O	1:F:163:ALA:HB3	2.14	0.47
1:I:254:TYR:CD1	1:I:262:PRO:HD3	2.48	0.47
1:G:69:VAL:HG23	1:G:70:LEU:N	2.30	0.47
1:C:60:ILE:O	1:C:84:LYS:HE3	2.15	0.47
1:A:66:THR:HG22	1:A:69:VAL:HG13	1.96	0.47
1:G:49:LYS:HG2	1:G:50:SER:N	2.30	0.47
1:F:272:SER:HB3	1:F:275:MET:H	1.79	0.47
1:H:340:ARG:HG3	1:H:341:VAL:H	1.80	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:198:ARG:HG3	1:G:201:ALA:N	2.30	0.47
1:F:304:ASN:C	1:F:304:ASN:OD1	2.53	0.47
1:I:168:LYS:O	1:I:168:LYS:HG3	2.14	0.47
1:B:82:PHE:HA	1:B:88:GLU:O	2.15	0.47
1:D:276:LYS:HB2	1:D:276:LYS:HE3	1.45	0.47
1:D:266:ASN:ND2	1:D:267:HIS:HD2	2.11	0.47
1:A:185:ARG:HE	1:A:212:LYS:HG3	1.79	0.47
1:F:86:THR:HG22	1:F:88:GLU:N	2.23	0.47
1:C:327:GLN:HG2	1:C:330:LYS:HD3	1.97	0.47
1:E:86:THR:O	1:E:87:GLN:HB2	2.13	0.47
1:I:89:LYS:NZ	1:I:142:ASP:OD2	2.48	0.47
1:G:145:GLU:HG2	1:G:193:LEU:CD2	2.45	0.47
1:L:161:ARG:O	1:L:165:GLU:HG3	2.15	0.47
1:K:288:ASN:ND2	1:K:288:ASN:H	2.11	0.47
1:F:322:HIS:ND1	1:F:323:PRO:HD2	2.30	0.47
1:A:90:PHE:CE2	1:A:121:VAL:HG21	2.50	0.47
1:J:70:LEU:HA	1:J:94:MET:CE	2.44	0.47
1:C:154:GLY:HA2	1:C:155:ASP:HB3	1.97	0.47
1:A:185:ARG:HD3	1:A:241:ASP:HB3	1.97	0.47
1:C:330:LYS:HB2	1:C:330:LYS:NZ	2.28	0.47
1:I:151:GLN:C	1:I:153:ARG:H	2.18	0.47
1:I:307:LYS:HB2	1:I:313:ARG:CG	2.45	0.47
1:C:129:ALA:O	1:C:131:ARG:HD3	2.14	0.47
1:D:307:LYS:HB2	1:D:313:ARG:HG3	1.97	0.47
1:D:140:CYS:SG	2:D:1:PDY:H17	2.55	0.47
1:E:70:LEU:HD23	1:E:94:MET:CE	2.43	0.47
1:E:310:PRO:O	1:E:313:ARG:HB2	2.15	0.47
1:G:229:TYR:CD1	1:H:251:VAL:HG11	2.47	0.47
1:A:276:LYS:CG	1:C:235:LEU:HD11	2.45	0.47
1:L:89:LYS:HE2	1:L:142:ASP:OD2	2.15	0.47
1:B:166:ILE:O	1:B:170:ILE:HG13	2.15	0.47
1:L:215:THR:HG23	1:L:216:SER:N	2.29	0.47
2:K:2:PDY:H14A	2:K:2:PDY:H18	1.96	0.46
1:E:261:PRO:HD3	2:E:2:PDY:H22A	1.97	0.46
1:J:327:GLN:HG2	1:J:330:LYS:CD	2.41	0.46
1:E:328:SER:C	1:E:330:LYS:H	2.18	0.46
1:F:190:GLU:H	1:F:190:GLU:CD	2.18	0.46
1:I:124:TYR:HB2	1:I:135:LEU:HB2	1.97	0.46
1:H:199:PRO:HG2	1:H:200:ASN:HD22	1.80	0.46
1:J:116:HIS:HE1	1:J:169:SER:OG	1.97	0.46
1:E:72:LEU:HB3	1:E:79:LEU:HD11	1.98	0.46
1:B:233:GLU:OE2	1:C:313:ARG:NH1	2.44	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:102:ARG:NH2	1:E:125:GLU:OE1	2.49	0.46
1:D:151:GLN:NE2	1:D:343:LYS:HA	2.31	0.46
1:G:154:GLY:O	1:G:155:ASP:C	2.54	0.46
1:G:262:PRO:HG2	1:G:263:PHE:CD1	2.50	0.46
1:L:183:ALA:O	1:L:211:ALA:HA	2.15	0.46
1:A:327:GLN:HG2	1:A:330:LYS:HD3	1.97	0.46
1:K:185:ARG:NH2	1:K:212:LYS:HG3	2.25	0.46
1:I:55:LYS:HD3	1:I:124:TYR:CE2	2.49	0.46
2:A:2:PDY:C17	2:A:2:PDY:C14	2.93	0.46
1:I:108:HIS:HE1	1:I:138:MET:HE3	1.79	0.46
1:K:59:ILE:HA	1:K:124:TYR:CE2	2.51	0.46
1:I:167:MET:HG3	1:I:253:MET:HG2	1.97	0.46
1:A:86:THR:HG22	1:A:86:THR:O	2.14	0.46
1:D:80:GLN:HB2	2:D:1:PDY:H24A	1.97	0.46
1:I:202:ILE:HD12	1:I:203:LEU:N	2.30	0.46
1:H:322:HIS:HD2	1:H:324:TRP:N	2.06	0.46
1:C:327:GLN:C	1:C:329:THR:H	2.17	0.46
1:K:72:LEU:HB3	1:K:77:LYS:HB3	1.96	0.46
1:K:77:LYS:HB3	1:K:79:LEU:HD21	1.98	0.46
1:K:257:LEU:HD11	1:K:298:VAL:HG11	1.98	0.46
1:K:281:MET:CB	1:K:283:GLN:HG3	2.45	0.46
1:K:232:PRO:C	1:K:234:VAL:H	2.17	0.46
1:E:187:VAL:HG12	1:E:252:ILE:HD11	1.97	0.46
1:A:331:VAL:HG23	1:A:332:PRO:HD2	1.97	0.46
1:H:135:LEU:HD12	1:H:135:LEU:N	2.30	0.46
1:J:57:ASN:ND2	1:J:57:ASN:H	2.13	0.46
1:F:98:CYS:HB2	1:F:99:PRO:CD	2.45	0.46
1:L:286:PHE:CE1	1:L:299:LYS:HB3	2.51	0.46
1:A:180:ILE:HG22	1:F:130:GLY:HA3	1.97	0.46
1:C:153:ARG:HD3	1:C:156:GLN:NE2	2.30	0.46
1:C:70:LEU:N	1:C:70:LEU:HD12	2.30	0.46
1:H:337:HIS:HA	1:H:340:ARG:HH11	1.79	0.46
1:H:160:GLU:O	1:H:163:ALA:HB3	2.16	0.46
1:I:286:PHE:CB	1:I:299:LYS:HE2	2.46	0.46
1:L:79:LEU:O	1:L:91:ALA:HA	2.16	0.46
1:G:65:VAL:HG12	1:G:70:LEU:CD2	2.46	0.46
1:B:74:ILE:HG23	1:B:94:MET:CE	2.46	0.46
1:E:161:ARG:O	1:E:165:GLU:HG3	2.15	0.46
1:J:314:MET:CG	1:J:318:GLU:HB2	2.46	0.46
1:C:187:VAL:HG22	1:C:205:LEU:HD11	1.98	0.46
1:D:288:ASN:OD1	1:D:292:SER:HB3	2.16	0.46
1:K:197:LYS:HA	1:K:197:LYS:HD2	1.77	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:118:VAL:HG21	2:H:1:PDY:H11	1.97	0.46
1:H:251:VAL:HG13	1:H:262:PRO:HD2	1.97	0.46
1:C:70:LEU:N	1:C:70:LEU:CD1	2.79	0.46
1:F:192:LEU:C	1:F:193:LEU:HD23	2.35	0.46
1:F:147:PHE:HE1	1:F:189:PRO:HG3	1.80	0.46
1:L:264:TYR:CB	2:L:2:PDY:H17	2.34	0.46
1:D:66:THR:HG21	1:D:68:GLN:CG	2.46	0.46
1:B:95:LEU:O	1:B:133:CYS:HB2	2.16	0.46
1:D:233:GLU:HG2	1:E:310:PRO:CG	2.43	0.46
1:B:188:LYS:NZ	1:B:190:GLU:HB2	2.31	0.46
1:A:202:ILE:HD12	1:A:203:LEU:N	2.31	0.46
1:J:166:ILE:O	1:J:169:SER:HB3	2.15	0.46
1:J:122:ASP:N	1:J:122:ASP:OD1	2.47	0.46
1:J:155:ASP:OD2	1:J:340:ARG:HG3	2.16	0.46
1:C:241:ASP:O	1:C:244:CYS:HB3	2.16	0.46
1:B:153:ARG:O	1:B:154:GLY:C	2.54	0.46
1:F:147:PHE:CD1	1:F:189:PRO:HB3	2.51	0.46
1:K:55:LYS:HE2	1:K:57:ASN:HD21	1.81	0.46
1:F:310:PRO:O	1:F:313:ARG:HB2	2.16	0.46
1:A:332:PRO:HG2	1:A:334:THR:CG2	2.47	0.45
1:J:70:LEU:O	1:J:94:MET:HE1	2.15	0.45
1:I:97:ASP:HB2	1:I:134:LEU:HD13	1.98	0.45
1:G:125:GLU:O	1:G:126:ASN:ND2	2.43	0.45
1:F:56:LYS:HE3	1:F:125:GLU:CD	2.36	0.45
1:B:156:GLN:OE1	1:B:156:GLN:N	2.49	0.45
1:J:48:VAL:O	1:J:48:VAL:HG13	2.16	0.45
1:C:215:THR:HG23	1:C:216:SER:N	2.30	0.45
1:C:121:VAL:O	1:C:122:ASP:HB3	2.16	0.45
1:K:80:GLN:HE21	2:K:1:PDY:H24	1.80	0.45
1:C:327:GLN:O	1:C:329:THR:N	2.43	0.45
1:A:153:ARG:O	1:A:154:GLY:C	2.54	0.45
1:E:128:TYR:CD1	1:L:48:VAL:HG23	2.49	0.45
1:A:188:LYS:HB2	1:A:189:PRO:CD	2.46	0.45
1:I:183:ALA:O	1:I:211:ALA:HA	2.16	0.45
1:C:145:GLU:HG2	1:C:193:LEU:CD2	2.47	0.45
1:C:83:ASN:HD22	1:C:86:THR:HB	1.82	0.45
1:B:266:ASN:CG	1:B:278:ARG:NH2	2.68	0.45
1:C:188:LYS:HE3	1:C:191:ASN:ND2	2.31	0.45
1:E:338:THR:HG22	1:E:342:LEU:CD2	2.46	0.45
1:H:202:ILE:HD11	1:H:204:LYS:HE2	1.98	0.45
1:I:185:ARG:NH2	1:I:212:LYS:HG3	2.32	0.45
1:I:286:PHE:HB3	1:I:299:LYS:HE2	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:66:THR:HG21	1:D:68:GLN:HG3	1.97	0.45
1:G:264:TYR:CE1	2:G:2:PDY:H24A	2.52	0.45
1:E:66:THR:HG22	1:E:69:VAL:HG22	1.99	0.45
1:J:278:ARG:HG3	1:J:283:GLN:NE2	2.31	0.45
1:B:160:GLU:O	1:B:163:ALA:HB3	2.17	0.45
1:D:322:HIS:ND1	1:D:323:PRO:HD2	2.31	0.45
1:J:186:ASP:OD1	1:J:188:LYS:HE3	2.16	0.45
1:I:77:LYS:HA	1:I:77:LYS:HD3	1.79	0.45
1:H:67:SER:O	1:H:69:VAL:N	2.49	0.45
1:A:185:ARG:NH2	1:A:212:LYS:HG3	2.31	0.45
1:C:309:GLU:HB3	1:C:312:GLN:HG3	1.98	0.45
1:A:52:LEU:HD21	1:A:105:VAL:HG12	1.98	0.45
1:A:298:VAL:O	1:A:302:ILE:HG13	2.16	0.45
1:L:188:LYS:HE2	1:L:190:GLU:HG2	1.98	0.45
1:D:97:ASP:HA	1:D:134:LEU:HD22	1.99	0.45
1:D:97:ASP:OD1	1:D:102:ARG:NE	2.42	0.45
1:E:288:ASN:HA	1:E:289:PRO:C	2.36	0.45
1:D:111:ALA:HB1	1:D:117:ILE:HD13	1.98	0.45
1:B:151:GLN:HB2	1:B:342:LEU:HB3	1.99	0.45
1:H:290:GLU:H	1:H:290:GLU:CD	2.20	0.45
1:H:94:MET:O	1:H:95:LEU:HD23	2.17	0.45
1:L:159:THR:HB	1:L:162:GLU:H	1.81	0.45
1:L:161:ARG:HD2	1:L:328:SER:O	2.16	0.45
1:I:69:VAL:HG13	1:I:79:LEU:HD22	1.98	0.45
1:E:188:LYS:NZ	1:E:190:GLU:CG	2.79	0.45
1:A:69:VAL:HB	1:A:79:LEU:HD12	1.98	0.45
1:L:298:VAL:HG22	1:L:324:TRP:CD1	2.52	0.45
1:A:52:LEU:HD21	1:A:105:VAL:CG1	2.46	0.45
1:L:231:ALA:HB1	1:L:233:GLU:OE2	2.17	0.45
1:K:160:GLU:HG3	1:K:160:GLU:O	2.17	0.45
1:L:100:LYS:O	1:L:103:ARG:HB3	2.17	0.45
1:F:260:TYR:CB	2:F:2:PDY:H19	2.47	0.45
1:A:65:VAL:HG12	1:A:70:LEU:HG	1.97	0.45
1:D:188:LYS:NZ	1:D:190:GLU:HG3	2.32	0.45
1:H:233:GLU:HG3	1:H:233:GLU:H	1.35	0.45
1:K:310:PRO:HB3	1:L:233:GLU:OE1	2.17	0.45
1:J:316:ILE:HG23	1:J:317:THR:N	2.31	0.45
1:L:249:LEU:HD12	1:L:249:LEU:HA	1.76	0.45
1:J:240:TYR:HA	1:J:240:TYR:HD2	1.68	0.45
1:G:118:VAL:HG21	2:G:1:PDY:H11	1.99	0.45
1:B:124:TYR:HB2	1:B:135:LEU:HB2	1.98	0.45
1:H:49:LYS:HB2	1:J:127:LEU:HB2	1.97	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:188:LYS:HB3	1:I:229:TYR:CD1	2.52	0.45
1:E:73:GLY:HA3	1:E:94:MET:HE3	1.98	0.45
1:C:161:ARG:NH1	1:C:333:GLN:CG	2.80	0.45
1:C:49:LYS:HB2	1:C:113:GLN:NE2	2.32	0.45
1:A:300:MET:SD	1:A:303:ARG:NH2	2.79	0.45
1:H:190:GLU:CD	1:H:190:GLU:H	2.21	0.45
1:B:70:LEU:O	1:B:74:ILE:HG13	2.16	0.45
1:H:298:VAL:HG22	1:H:324:TRP:CD1	2.52	0.45
1:B:190:GLU:N	1:B:190:GLU:CD	2.70	0.45
1:H:158:PHE:HZ	1:H:166:ILE:HD12	1.82	0.45
1:B:327:GLN:NE2	1:B:330:LYS:NZ	2.65	0.45
1:F:265:SER:HB3	1:F:268:GLY:HA2	1.98	0.45
1:H:90:PHE:CE2	1:H:121:VAL:HG21	2.51	0.45
2:C:1:PDY:H14A	2:C:1:PDY:H18	1.95	0.45
1:G:264:TYR:C	1:G:275:MET:HG3	2.38	0.45
1:J:160:GLU:O	1:J:163:ALA:HB3	2.16	0.45
1:G:305:LEU:O	1:G:313:ARG:HD3	2.16	0.45
1:F:230:VAL:HG23	1:F:234:VAL:HG11	1.97	0.45
1:A:309:GLU:HG2	1:C:311:THR:HG22	1.98	0.45
1:B:108:HIS:HE1	1:B:138:MET:HE2	1.82	0.45
1:G:215:THR:OG1	1:G:216:SER:N	2.50	0.45
1:L:344:GLU:N	1:L:344:GLU:OE1	2.50	0.45
1:D:178:HIS:CG	1:D:242:LYS:HG2	2.52	0.45
1:D:57:ASN:H	1:D:57:ASN:ND2	2.14	0.45
1:C:229:TYR:N	1:C:229:TYR:CD2	2.85	0.45
1:F:125:GLU:OE2	1:F:132:LYS:HD2	2.17	0.44
1:E:95:LEU:O	1:E:133:CYS:HB2	2.16	0.44
1:I:167:MET:HE2	1:I:253:MET:HG3	1.99	0.44
1:C:145:GLU:HG2	1:C:193:LEU:HD22	1.99	0.44
1:L:259:GLY:HA3	1:L:341:VAL:HG11	1.98	0.44
1:C:233:GLU:HG3	1:C:233:GLU:H	1.47	0.44
1:E:213:GLU:HB3	1:E:215:THR:HG22	2.00	0.44
1:F:49:LYS:HD3	1:F:113:GLN:HG2	1.99	0.44
1:H:342:LEU:HA	1:H:342:LEU:HD12	1.84	0.44
1:H:342:LEU:C	1:H:343:LYS:HD2	2.37	0.44
1:E:155:ASP:N	1:E:155:ASP:OD2	2.49	0.44
1:H:202:ILE:HD11	1:H:204:LYS:CE	2.47	0.44
1:J:338:THR:O	1:J:342:LEU:HB2	2.17	0.44
1:I:145:GLU:HG2	1:I:193:LEU:CD2	2.47	0.44
1:E:100:LYS:HE2	1:E:100:LYS:HB2	1.84	0.44
1:A:88:GLU:HG2	1:A:89:LYS:N	2.31	0.44
2:L:2:PDY:H24A	2:L:2:PDY:H20	1.72	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:161:ARG:HB3	1:A:333:GLN:NE2	2.31	0.44
1:L:258:CYS:HB3	1:L:291:TRP:CZ2	2.52	0.44
1:L:154:GLY:C	1:L:156:GLN:HB3	2.37	0.44
1:A:69:VAL:HB	1:A:79:LEU:HD13	1.98	0.44
2:A:2:PDY:C3	2:A:2:PDY:H17	2.47	0.44
1:E:275:MET:HA	1:E:278:ARG:NH1	2.31	0.44
1:C:104:GLU:HG3	1:C:208:PHE:C	2.37	0.44
1:A:253:MET:HE1	1:A:319:PHE:HE1	1.82	0.44
1:G:161:ARG:NH1	1:G:331:VAL:O	2.46	0.44
1:D:113:GLN:O	1:D:115:PRO:HD3	2.17	0.44
1:H:332:PRO:HB2	1:H:334:THR:CG2	2.38	0.44
1:A:327:GLN:CD	1:A:330:LYS:HZ2	2.20	0.44
1:C:331:VAL:HG23	1:C:332:PRO:HD2	2.00	0.44
1:J:254:TYR:CD1	1:J:262:PRO:HG3	2.52	0.44
1:K:188:LYS:HB2	1:K:189:PRO:HD2	1.99	0.44
1:K:161:ARG:O	1:K:165:GLU:HG3	2.18	0.44
1:J:188:LYS:HB2	1:J:189:PRO:CD	2.48	0.44
1:C:71:GLY:O	1:C:74:ILE:HG22	2.18	0.44
1:C:147:PHE:O	1:C:151:GLN:N	2.50	0.44
1:H:233:GLU:OE2	1:I:313:ARG:NH1	2.41	0.44
1:J:58:ALA:O	1:J:61:ASP:OD2	2.36	0.44
1:K:202:ILE:HD12	1:K:203:LEU:H	1.82	0.44
1:A:188:LYS:HB2	1:A:189:PRO:HD2	1.99	0.44
1:H:97:ASP:H	1:H:133:CYS:HA	1.81	0.44
1:A:311:THR:O	1:B:312:GLN:NE2	2.50	0.44
1:D:198:ARG:HB3	1:D:200:ASN:OD1	2.18	0.44
1:G:111:ALA:O	1:G:117:ILE:HG13	2.17	0.44
1:A:134:LEU:HD12	1:A:134:LEU:HA	1.85	0.44
1:J:313:ARG:NH2	1:K:233:GLU:HG2	2.14	0.44
1:K:96:GLN:HE22	1:K:131:ARG:CD	2.30	0.44
1:A:304:ASN:OD1	1:A:304:ASN:C	2.56	0.44
1:J:311:THR:HG22	1:L:309:GLU:CG	2.48	0.44
1:H:65:VAL:CG1	1:H:70:LEU:HD13	2.45	0.44
1:D:185:ARG:HH21	1:D:212:LYS:CG	2.24	0.44
1:E:145:GLU:HG2	1:E:193:LEU:HD23	1.99	0.44
1:A:97:ASP:H	1:A:133:CYS:HA	1.80	0.44
1:B:190:GLU:CD	1:B:190:GLU:H	2.20	0.44
1:F:49:LYS:HB2	1:F:113:GLN:NE2	2.32	0.44
1:K:258:CYS:HG	1:K:291:TRP:HZ2	1.62	0.44
1:K:276:LYS:HB2	1:K:276:LYS:HE3	1.73	0.44
1:K:103:ARG:NH1	1:K:212:LYS:HE2	2.33	0.44
1:F:233:GLU:HG2	1:F:234:VAL:N	2.33	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:97:ASP:OD2	1:A:102:ARG:NH2	2.33	0.44
1:I:304:ASN:O	1:I:307:LYS:HG2	2.18	0.44
1:H:158:PHE:O	1:H:336:LEU:HB2	2.17	0.44
1:H:200:ASN:HD22	1:H:200:ASN:H	1.63	0.44
1:B:58:ALA:HB1	1:B:60:ILE:HG13	2.00	0.44
1:D:148:SER:HA	1:D:151:GLN:HG2	2.00	0.44
1:K:165:GLU:O	1:K:168:LYS:HB3	2.17	0.44
1:D:309:GLU:OE2	1:D:310:PRO:HD2	2.18	0.44
1:C:94:MET:HE3	1:C:94:MET:HB3	1.90	0.44
1:L:336:LEU:HD22	1:L:336:LEU:N	2.32	0.44
1:G:81:ILE:HD13	1:G:92:LEU:HB2	1.99	0.44
1:I:285:GLU:O	1:I:287:PRO:HD3	2.17	0.44
1:H:264:TYR:HB2	2:H:2:PDY:C17	2.47	0.44
1:G:185:ARG:NH2	1:G:212:LYS:HE2	2.32	0.44
1:G:264:TYR:C	1:G:264:TYR:HD2	2.21	0.44
2:B:2:PDY:C18	2:B:2:PDY:H14A	2.42	0.44
1:H:161:ARG:O	1:H:165:GLU:HG3	2.17	0.44
1:F:97:ASP:HA	1:F:134:LEU:HD22	2.00	0.44
1:B:80:GLN:NE2	2:B:1:PDY:H24A	2.32	0.44
1:H:86:THR:C	1:H:88:GLU:H	2.19	0.44
1:E:229:TYR:CE1	1:F:188:LYS:HG2	2.53	0.44
1:I:121:VAL:HB	1:I:137:VAL:O	2.17	0.44
1:L:145:GLU:HG2	1:L:193:LEU:CD2	2.48	0.44
1:E:253:MET:HE1	1:E:319:PHE:HE1	1.83	0.44
1:K:334:THR:HA	1:K:335:PRO:HD3	1.76	0.43
1:K:167:MET:SD	1:K:256:LEU:HD12	2.58	0.43
1:D:230:VAL:CG2	1:D:234:VAL:HB	2.47	0.43
1:G:288:ASN:HB3	1:G:289:PRO:HA	1.99	0.43
1:D:161:ARG:HA	1:D:331:VAL:CG2	2.48	0.43
1:C:65:VAL:HG12	1:C:70:LEU:CD1	2.48	0.43
1:A:233:GLU:H	1:A:233:GLU:HG3	1.50	0.43
1:D:70:LEU:HD21	1:I:48:VAL:CG1	2.48	0.43
1:C:90:PHE:CE2	1:C:121:VAL:HG21	2.53	0.43
1:L:108:HIS:HE1	1:L:138:MET:HE3	1.83	0.43
1:F:308:THR:HG22	1:F:309:GLU:N	2.33	0.43
1:E:232:PRO:C	1:E:234:VAL:H	2.21	0.43
1:C:288:ASN:ND2	1:C:288:ASN:N	2.66	0.43
1:B:266:ASN:C	1:B:266:ASN:OD1	2.56	0.43
1:J:192:LEU:HD11	1:J:252:ILE:HD13	1.99	0.43
1:C:190:GLU:H	1:C:190:GLU:CD	2.21	0.43
1:C:192:LEU:C	1:C:193:LEU:HD23	2.38	0.43
1:G:70:LEU:H	1:G:70:LEU:HD22	1.83	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:126:ASN:HD22	1:I:126:ASN:N	2.11	0.43
1:D:155:ASP:OD1	1:D:156:GLN:HG2	2.18	0.43
1:B:327:GLN:HE22	1:B:330:LYS:HZ2	1.66	0.43
1:L:215:THR:OG1	1:L:216:SER:N	2.50	0.43
1:E:337:HIS:CG	1:E:340:ARG:NH2	2.86	0.43
1:H:129:ALA:C	1:H:131:ARG:H	2.20	0.43
1:I:70:LEU:HA	1:I:94:MET:CE	2.43	0.43
1:I:98:CYS:HB2	1:I:99:PRO:CD	2.45	0.43
1:G:337:HIS:ND1	1:G:340:ARG:NH1	2.66	0.43
1:J:311:THR:HG22	1:L:309:GLU:CD	2.38	0.43
1:C:235:LEU:HD13	1:C:235:LEU:O	2.19	0.43
1:L:93:LYS:HE3	1:L:93:LYS:HB2	1.76	0.43
1:D:95:LEU:O	1:D:133:CYS:HB2	2.18	0.43
1:D:95:LEU:O	1:D:134:LEU:N	2.48	0.43
1:D:260:TYR:OH	1:D:287:PRO:HG2	2.17	0.43
1:A:83:ASN:O	1:A:87:GLN:N	2.51	0.43
1:A:130:GLY:O	1:G:110:ARG:HD2	2.17	0.43
1:J:89:LYS:HZ2	1:J:140:CYS:HB3	1.83	0.43
1:B:56:LYS:O	1:E:50:SER:HB2	2.19	0.43
1:J:141:LEU:HD13	1:J:193:LEU:HB2	2.00	0.43
1:C:260:TYR:HD2	1:C:341:VAL:HG11	1.83	0.43
1:G:278:ARG:HA	1:G:283:GLN:HG2	1.99	0.43
1:D:57:ASN:H	1:D:57:ASN:HD22	1.66	0.43
1:I:285:GLU:C	1:I:287:PRO:HD3	2.39	0.43
1:E:149:ARG:NH1	1:E:196:SER:O	2.51	0.43
1:A:135:LEU:N	1:A:135:LEU:HD12	2.33	0.43
1:C:96:GLN:HE21	1:C:96:GLN:HB3	1.59	0.43
1:G:98:CYS:HB2	1:G:99:PRO:CD	2.48	0.43
1:B:264:TYR:CZ	2:B:2:PDY:H24	2.53	0.43
1:L:342:LEU:CD1	1:L:342:LEU:N	2.82	0.43
1:B:80:GLN:CD	2:B:1:PDY:H24A	2.39	0.43
1:D:167:MET:HE3	1:D:249:LEU:HG	2.00	0.43
1:D:230:VAL:HG22	1:D:234:VAL:HB	1.99	0.43
1:K:58:ALA:HB1	1:K:60:ILE:HG13	2.00	0.43
1:J:48:VAL:O	1:J:48:VAL:HG22	2.18	0.43
1:E:249:LEU:HA	1:E:249:LEU:HD12	1.71	0.43
1:K:230:VAL:HG13	1:K:231:ALA:N	2.33	0.43
2:E:1:PDY:H24	2:E:1:PDY:H20	1.57	0.43
1:F:81:ILE:CD1	1:F:92:LEU:HB2	2.45	0.43
1:J:107:LEU:HD21	1:J:213:GLU:HG2	2.00	0.43
1:B:289:PRO:O	1:B:290:GLU:C	2.57	0.43
1:G:60:ILE:C	1:G:60:ILE:HD12	2.39	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:159:THR:C	1:K:161:ARG:H	2.22	0.43
1:E:337:HIS:CD2	1:E:340:ARG:HH21	2.36	0.43
1:A:301:LEU:HD13	1:A:322:HIS:CD2	2.54	0.43
1:A:337:HIS:ND1	1:A:340:ARG:NH2	2.67	0.43
1:I:255:ILE:O	1:I:259:GLY:N	2.46	0.43
1:H:149:ARG:HG3	1:H:194:TYR:CD2	2.54	0.43
1:K:344:GLU:O	1:K:344:GLU:HG2	2.18	0.43
1:K:230:VAL:CG2	1:K:231:ALA:H	2.09	0.43
1:J:341:VAL:O	1:J:343:LYS:N	2.47	0.43
1:J:78:VAL:O	1:J:79:LEU:HD23	2.19	0.43
1:J:160:GLU:HG2	1:J:331:VAL:CG2	2.49	0.43
1:K:56:LYS:NZ	1:K:125:GLU:CD	2.71	0.43
1:H:154:GLY:C	1:H:156:GLN:H	2.22	0.43
1:I:80:GLN:HB3	1:I:80:GLN:HE21	1.61	0.43
1:D:198:ARG:HD2	1:D:200:ASN:OD1	2.19	0.43
1:G:298:VAL:HG22	1:G:324:TRP:CD1	2.54	0.43
1:B:215:THR:HG22	1:B:216:SER:N	2.33	0.43
1:K:184:HIS:CD2	1:K:205:LEU:HD21	2.54	0.43
1:B:246:MET:CE	1:B:316:ILE:HA	2.49	0.43
1:J:111:ALA:HB2	1:J:177:LEU:HD21	2.01	0.43
1:A:63:TYR:HE1	1:A:124:TYR:OH	2.02	0.43
1:F:54:ILE:HD13	1:F:102:ARG:NH1	2.34	0.43
1:B:180:ILE:HG21	1:L:130:GLY:HA3	2.01	0.43
1:A:156:GLN:NE2	1:A:156:GLN:N	2.58	0.43
1:E:70:LEU:HA	1:E:70:LEU:HD23	1.89	0.43
1:C:307:LYS:O	1:C:313:ARG:NE	2.50	0.43
1:C:307:LYS:O	1:C:313:ARG:NH2	2.46	0.43
1:I:86:THR:C	1:I:88:GLU:H	2.22	0.43
1:H:337:HIS:CG	1:H:340:ARG:HH11	2.37	0.43
1:H:340:ARG:O	1:H:343:LYS:HD3	2.19	0.43
1:J:336:LEU:HD22	1:J:336:LEU:N	2.34	0.43
1:I:160:GLU:CA	1:I:336:LEU:HD21	2.49	0.43
1:D:134:LEU:HD12	1:D:134:LEU:HA	1.87	0.43
1:C:172:GLU:HG2	1:C:320:MET:CE	2.49	0.43
1:C:121:VAL:O	1:C:122:ASP:CB	2.67	0.43
1:C:111:ALA:HB1	1:C:117:ILE:HD13	2.01	0.43
1:E:156:GLN:NE2	1:E:156:GLN:N	2.51	0.43
1:C:88:GLU:CG	1:C:89:LYS:N	2.79	0.43
1:K:102:ARG:NH2	1:K:125:GLU:OE1	2.51	0.43
1:G:156:GLN:O	1:G:335:PRO:HB3	2.19	0.43
1:D:114:CYS:HB3	1:D:117:ILE:HD12	2.01	0.43
1:I:96:GLN:OE1	1:I:131:ARG:HD2	2.19	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:247:TRP:HZ3	1:I:306:LEU:O	2.02	0.43
1:L:80:GLN:CB	2:L:1:PDY:H24A	2.49	0.42
1:L:80:GLN:HA	1:L:90:PHE:O	2.19	0.42
1:H:189:PRO:HD2	1:H:190:GLU:OE1	2.19	0.42
1:A:185:ARG:CZ	1:A:212:LYS:HE2	2.49	0.42
1:I:69:VAL:HA	1:I:79:LEU:CD2	2.42	0.42
1:G:156:GLN:HG3	1:G:335:PRO:HB2	2.01	0.42
1:D:285:GLU:HB2	1:D:287:PRO:HD3	2.01	0.42
1:J:186:ASP:HB2	1:J:210:PHE:HD2	1.83	0.42
1:E:340:ARG:O	1:E:344:GLU:HG3	2.19	0.42
1:D:90:PHE:CE2	1:D:121:VAL:HG21	2.53	0.42
1:L:127:LEU:HD12	1:L:127:LEU:HA	1.85	0.42
1:H:140:CYS:SG	2:H:1:PDY:C17	3.07	0.42
1:K:157:ALA:HB1	1:K:335:PRO:HB3	2.01	0.42
1:H:66:THR:OG1	1:H:69:VAL:HG12	2.20	0.42
1:F:49:LYS:NZ	1:F:113:GLN:HG3	2.34	0.42
1:D:149:ARG:NH1	1:D:197:LYS:HA	2.34	0.42
2:H:1:PDY:H24	2:H:1:PDY:H20	1.40	0.42
1:L:68:GLN:O	1:L:72:LEU:HD13	2.19	0.42
1:J:305:LEU:O	1:J:313:ARG:HD3	2.20	0.42
1:H:331:VAL:HB	1:H:332:PRO:HD2	2.01	0.42
1:B:77:LYS:HZ2	1:B:79:LEU:HD21	1.83	0.42
1:B:188:LYS:HE3	1:B:191:ASN:ND2	2.35	0.42
1:J:336:LEU:C	1:J:338:THR:H	2.23	0.42
1:E:97:ASP:OD2	1:E:102:ARG:NH2	2.34	0.42
1:E:332:PRO:HG2	1:E:334:THR:HG22	2.00	0.42
1:E:187:VAL:HG12	1:E:252:ILE:CD1	2.49	0.42
1:A:247:TRP:CZ2	1:C:232:PRO:HD3	2.54	0.42
1:E:231:ALA:HB1	1:E:233:GLU:CD	2.39	0.42
1:L:176:TYR:O	1:L:180:ILE:HG12	2.20	0.42
1:L:259:GLY:HA3	1:L:341:VAL:CG1	2.49	0.42
1:A:327:GLN:CG	1:A:330:LYS:HD3	2.50	0.42
1:B:77:LYS:NZ	1:B:79:LEU:HD23	2.33	0.42
1:F:115:PRO:O	1:F:202:ILE:HD11	2.19	0.42
1:K:72:LEU:HB2	1:K:79:LEU:HD11	2.01	0.42
1:H:151:GLN:HA	1:H:339:SER:OG	2.19	0.42
1:A:287:PRO:O	1:A:291:TRP:HB2	2.18	0.42
1:A:234:VAL:O	1:A:234:VAL:HG12	2.19	0.42
1:D:77:LYS:HB3	1:D:77:LYS:HZ2	1.84	0.42
1:H:89:LYS:HG2	1:H:90:PHE:N	2.35	0.42
1:J:66:THR:HG23	1:J:69:VAL:H	1.84	0.42
1:B:56:LYS:O	1:E:51:GLY:N	2.46	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:50:SER:O	1:J:127:LEU:HD23	2.19	0.42
1:F:278:ARG:NH2	3:F:3:SO4:O2	2.53	0.42
1:C:125:GLU:O	1:C:126:ASN:ND2	2.42	0.42
1:C:98:CYS:SG	1:C:99:PRO:HD2	2.60	0.42
1:H:161:ARG:HA	1:H:331:VAL:CG2	2.50	0.42
1:F:49:LYS:CG	1:G:127:LEU:HB2	2.49	0.42
1:E:154:GLY:HA2	1:E:155:ASP:HA	1.72	0.42
1:K:310:PRO:HG3	1:L:233:GLU:HG2	2.02	0.42
1:B:108:HIS:O	1:B:108:HIS:HD2	2.03	0.42
1:F:307:LYS:HG2	1:F:312:GLN:CB	2.49	0.42
1:B:65:VAL:HG12	1:B:69:VAL:CG2	2.49	0.42
1:J:161:ARG:CZ	1:J:333:GLN:HG3	2.50	0.42
1:I:60:ILE:HA	1:I:63:TYR:O	2.19	0.42
1:D:52:LEU:O	1:K:56:LYS:HE3	2.19	0.42
1:G:102:ARG:HH22	1:G:125:GLU:CD	2.23	0.42
1:L:343:LYS:N	1:L:344:GLU:OE1	2.53	0.42
1:C:153:ARG:O	1:C:153:ARG:HG3	2.19	0.42
1:C:327:GLN:HE21	1:C:330:LYS:HE3	1.82	0.42
1:K:77:LYS:HG2	1:K:79:LEU:CD2	2.49	0.42
1:J:233:GLU:OE2	1:L:313:ARG:NH1	2.53	0.42
1:F:304:ASN:ND2	1:F:314:MET:HB2	2.35	0.42
1:G:145:GLU:O	1:G:146:LEU:C	2.57	0.42
1:H:116:HIS:CE1	1:H:169:SER:HB2	2.55	0.42
1:J:261:PRO:HD3	2:J:2:PDY:H25	2.02	0.42
1:B:116:HIS:O	1:B:204:LYS:HA	2.20	0.42
1:K:65:VAL:HG12	1:K:70:LEU:HG	2.00	0.42
1:J:327:GLN:HG2	1:J:330:LYS:CG	2.50	0.42
1:F:300:MET:SD	1:F:303:ARG:NE	2.91	0.42
1:F:49:LYS:O	1:G:127:LEU:N	2.52	0.42
1:E:143:GLY:O	1:E:149:ARG:HD3	2.19	0.42
1:J:128:TYR:O	1:J:129:ALA:HB3	2.19	0.42
1:C:142:ASP:N	1:C:195:THR:O	2.49	0.42
1:K:69:VAL:HG23	1:K:70:LEU:N	2.35	0.42
1:G:97:ASP:HA	1:G:134:LEU:HD22	2.02	0.42
1:J:233:GLU:CG	1:L:310:PRO:HG3	2.50	0.42
1:B:113:GLN:HE21	1:B:113:GLN:HB3	1.55	0.42
1:D:240:TYR:CD1	1:D:240:TYR:N	2.88	0.42
1:F:266:ASN:C	1:F:268:GLY:N	2.73	0.42
1:H:260:TYR:OH	1:H:287:PRO:HG2	2.20	0.42
1:F:58:ALA:O	1:F:61:ASP:HB2	2.20	0.42
1:B:62:ASP:OD2	1:B:62:ASP:N	2.53	0.42
1:H:75:ASN:HA	1:H:75:ASN:HD22	1.66	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:127:LEU:HA	1:D:127:LEU:HD12	1.91	0.42
2:F:2:PDY:H14A	2:F:2:PDY:C18	2.38	0.41
1:K:66:THR:N	1:K:69:VAL:HG22	2.33	0.41
1:B:241:ASP:O	1:B:244:CYS:HB3	2.19	0.41
1:J:252:ILE:C	1:J:254:TYR:H	2.23	0.41
1:C:147:PHE:CE2	1:C:256:LEU:HD23	2.47	0.41
1:J:143:GLY:CA	1:J:149:ARG:NH1	2.83	0.41
1:F:156:GLN:N	1:F:156:GLN:NE2	2.67	0.41
1:K:194:TYR:CZ	1:K:203:LEU:HD13	2.55	0.41
1:A:52:LEU:HB2	1:A:109:TRP:CD1	2.55	0.41
1:L:195:THR:OG1	1:L:196:SER:N	2.53	0.41
1:K:232:PRO:C	1:K:234:VAL:N	2.73	0.41
1:B:327:GLN:NE2	1:B:330:LYS:HZ2	2.18	0.41
1:C:229:TYR:N	1:C:229:TYR:HD2	2.17	0.41
1:E:247:TRP:HZ3	1:E:306:LEU:O	2.03	0.41
1:A:113:GLN:HE21	1:A:113:GLN:HB3	1.62	0.41
1:I:148:SER:O	1:I:152:ASP:HB2	2.20	0.41
1:B:105:VAL:HG22	1:B:136:ILE:HD11	2.02	0.41
1:C:50:SER:HB2	1:H:58:ALA:N	2.35	0.41
1:H:142:ASP:O	1:H:197:LYS:HE3	2.20	0.41
1:E:304:ASN:HA	1:E:307:LYS:HG3	2.01	0.41
1:I:322:HIS:HA	1:I:323:PRO:HD3	1.94	0.41
1:J:141:LEU:HD12	1:J:193:LEU:HB2	2.00	0.41
1:H:154:GLY:O	1:H:156:GLN:NE2	2.53	0.41
1:C:92:LEU:HD12	1:C:93:LYS:H	1.86	0.41
1:E:245:ASP:O	1:E:248:SER:HB2	2.21	0.41
1:J:188:LYS:HB2	1:J:189:PRO:HD2	2.03	0.41
1:F:268:GLY:HA2	1:F:269:LEU:HA	1.70	0.41
1:J:337:HIS:ND1	1:J:337:HIS:N	2.68	0.41
1:J:172:GLU:HG2	1:J:320:MET:CE	2.51	0.41
1:K:143:GLY:HA3	1:K:194:TYR:CB	2.49	0.41
1:D:65:VAL:HG12	1:D:70:LEU:HD13	2.00	0.41
1:C:104:GLU:HG3	1:C:208:PHE:O	2.21	0.41
1:L:108:HIS:HE1	1:L:138:MET:CE	2.33	0.41
1:K:192:LEU:HD11	1:K:252:ILE:HD13	2.02	0.41
1:E:147:PHE:HE2	1:E:256:LEU:HD23	1.85	0.41
1:K:260:TYR:CB	2:K:2:PDY:H19	2.50	0.41
1:L:114:CYS:HB3	1:L:117:ILE:HD12	2.03	0.41
1:B:115:PRO:O	1:B:204:LYS:HD3	2.21	0.41
1:L:95:LEU:O	1:L:133:CYS:CB	2.63	0.41
1:C:185:ARG:HH21	1:C:212:LYS:HG3	1.85	0.41
1:C:127:LEU:HA	1:C:127:LEU:HD12	1.87	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:275:MET:O	1:K:278:ARG:N	2.53	0.41
1:I:167:MET:HG3	1:I:253:MET:CG	2.49	0.41
1:I:258:CYS:HB2	1:I:290:GLU:HG3	2.03	0.41
1:B:85:ARG:HH11	1:B:86:THR:HG21	1.84	0.41
1:C:188:LYS:HG2	1:C:191:ASN:ND2	2.35	0.41
1:F:49:LYS:HB3	1:G:127:LEU:HB2	2.01	0.41
1:H:340:ARG:O	1:H:343:LYS:HG2	2.20	0.41
1:H:143:GLY:HA2	1:H:197:LYS:CD	2.50	0.41
1:J:322:HIS:ND1	1:J:323:PRO:CD	2.83	0.41
1:H:133:CYS:SG	1:H:135:LEU:HD11	2.60	0.41
1:F:60:ILE:HA	1:F:63:TYR:O	2.21	0.41
1:K:118:VAL:CG1	1:K:206:THR:HG22	2.51	0.41
1:F:337:HIS:O	1:F:341:VAL:HG23	2.20	0.41
1:J:260:TYR:OH	1:J:290:GLU:HG3	2.20	0.41
1:I:71:GLY:O	1:I:75:ASN:HB2	2.20	0.41
1:B:307:LYS:HD3	1:B:307:LYS:HA	1.83	0.41
1:L:70:LEU:HD12	1:L:94:MET:CE	2.51	0.41
1:L:161:ARG:CZ	1:L:333:GLN:NE2	2.84	0.41
1:I:65:VAL:HG11	1:I:70:LEU:HD21	2.03	0.41
1:B:188:LYS:CD	1:B:190:GLU:HB2	2.50	0.41
1:H:314:MET:HG3	1:H:318:GLU:HB2	2.03	0.41
1:A:107:LEU:HD22	1:A:182:ILE:HG12	2.02	0.41
1:L:185:ARG:HD3	1:L:241:ASP:OD2	2.20	0.41
1:D:141:LEU:HD13	1:D:193:LEU:HB2	2.03	0.41
1:E:167:MET:SD	1:E:256:LEU:HD12	2.61	0.41
1:J:245:ASP:O	1:J:248:SER:HB2	2.21	0.41
1:I:127:LEU:HA	1:I:127:LEU:HD12	1.87	0.41
1:D:170:ILE:O	1:D:174:ILE:HG12	2.20	0.41
1:K:129:ALA:C	1:K:131:ARG:N	2.74	0.41
1:C:83:ASN:OD1	1:C:84:LYS:N	2.53	0.41
1:I:100:LYS:HG3	1:I:103:ARG:HH21	1.85	0.41
1:D:167:MET:HE1	1:D:253:MET:HB2	2.03	0.41
1:H:231:ALA:HB1	1:H:232:PRO:HD2	2.02	0.41
1:K:121:VAL:C	1:K:122:ASP:OD1	2.59	0.41
1:J:315:THR:OG1	1:J:318:GLU:HG3	2.20	0.41
1:H:337:HIS:CB	1:H:340:ARG:HH11	2.34	0.41
1:J:107:LEU:HD21	1:J:213:GLU:CG	2.50	0.41
1:K:151:GLN:HG3	1:K:152:ASP:N	2.36	0.41
1:H:145:GLU:HG2	1:H:193:LEU:HD22	2.03	0.41
2:F:2:PDY:C13	2:F:2:PDY:C14	2.98	0.41
1:K:70:LEU:HD23	1:K:94:MET:HE1	2.00	0.41
1:F:70:LEU:HA	1:F:94:MET:HE1	2.03	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:107:LEU:HD22	1:H:182:ILE:CD1	2.51	0.41
1:F:185:ARG:HD3	1:F:241:ASP:CB	2.47	0.41
1:E:212:LYS:HE3	1:E:212:LYS:HB3	1.83	0.41
1:E:328:SER:HA	1:E:331:VAL:HG13	2.03	0.41
1:A:66:THR:HG22	1:A:69:VAL:H	1.86	0.41
1:H:233:GLU:CG	1:I:310:PRO:HG3	2.51	0.41
1:L:309:GLU:OE2	1:L:310:PRO:HD2	2.21	0.41
1:C:65:VAL:HG11	1:C:70:LEU:HD11	2.00	0.41
1:A:233:GLU:OE2	1:B:313:ARG:CZ	2.69	0.41
1:I:90:PHE:CE2	1:I:121:VAL:HG21	2.55	0.41
1:F:304:ASN:OD1	1:F:304:ASN:O	2.37	0.41
1:I:172:GLU:HG2	1:I:320:MET:HE1	2.02	0.41
1:L:336:LEU:C	1:L:338:THR:H	2.23	0.41
1:J:111:ALA:CB	1:J:177:LEU:HD21	2.51	0.41
1:B:90:PHE:CE2	1:B:121:VAL:HG21	2.56	0.41
1:E:177:LEU:HD21	1:E:208:PHE:HE2	1.86	0.41
1:B:301:LEU:HD22	1:B:322:HIS:CE1	2.56	0.41
1:J:153:ARG:O	1:J:154:GLY:C	2.59	0.41
1:H:281:MET:HB2	1:H:283:GLN:HG3	2.02	0.41
1:I:139:GLU:HG3	1:I:139:GLU:O	2.20	0.41
1:J:301:LEU:O	1:J:301:LEU:HD12	2.20	0.41
1:L:264:TYR:CG	2:L:2:PDY:C17	3.04	0.41
1:K:49:LYS:CD	1:K:50:SER:N	2.78	0.41
1:C:332:PRO:HB2	1:C:334:THR:HG22	2.03	0.41
1:I:327:GLN:HE21	1:I:330:LYS:HZ2	1.67	0.41
1:G:74:ILE:O	1:G:74:ILE:HG12	2.21	0.41
1:L:266:ASN:CB	1:L:278:ARG:NH2	2.82	0.41
1:B:52:LEU:HB2	1:B:109:TRP:CG	2.57	0.41
1:A:233:GLU:OE2	1:B:310:PRO:HB3	2.21	0.41
1:J:82:PHE:HA	1:J:88:GLU:O	2.21	0.41
1:C:86:THR:O	1:C:87:GLN:CB	2.68	0.40
1:E:69:VAL:HB	1:E:79:LEU:CD1	2.45	0.40
1:F:281:MET:CB	1:F:283:GLN:HG3	2.51	0.40
1:F:327:GLN:HG2	1:F:330:LYS:HD2	2.02	0.40
1:A:313:ARG:HH22	1:C:233:GLU:CG	2.33	0.40
1:C:151:GLN:NE2	1:C:342:LEU:O	2.54	0.40
1:A:233:GLU:OE2	1:B:313:ARG:NH2	2.54	0.40
1:K:151:GLN:HB3	1:K:342:LEU:HB3	2.02	0.40
1:L:186:ASP:O	1:L:191:ASN:ND2	2.53	0.40
1:C:118:VAL:HG13	1:C:118:VAL:O	2.20	0.40
1:I:264:TYR:CE2	2:I:2:PDY:C20	2.99	0.40
1:L:97:ASP:CG	1:L:102:ARG:HH21	2.24	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:155:ASP:CG	1:J:156:GLN:HE22	2.25	0.40
1:K:98:CYS:C	1:K:100:LYS:N	2.74	0.40
1:A:145:GLU:HG3	1:A:193:LEU:HD23	2.02	0.40
1:C:334:THR:HA	1:C:335:PRO:HD3	1.92	0.40
1:A:95:LEU:O	1:A:133:CYS:HB2	2.21	0.40
1:H:85:ARG:O	1:H:87:GLN:N	2.55	0.40
2:J:2:PDY:C18	2:J:2:PDY:C3	2.90	0.40
2:E:1:PDY:C3	2:E:1:PDY:C18	2.78	0.40
1:J:331:VAL:CG2	1:J:332:PRO:HD2	2.51	0.40
2:A:1:PDY:H18	2:A:1:PDY:C14	2.49	0.40
1:F:156:GLN:HE21	1:F:156:GLN:N	2.20	0.40
1:B:64:LYS:CE	1:B:84:LYS:HE3	2.51	0.40
1:D:149:ARG:HG3	1:D:194:TYR:CD2	2.57	0.40
1:K:196:SER:H	1:K:201:ALA:HB1	1.86	0.40
1:L:334:THR:HA	1:L:335:PRO:HD3	1.87	0.40
1:H:80:GLN:OE1	2:H:1:PDY:H24A	2.21	0.40
1:B:65:VAL:HG12	1:B:69:VAL:HG21	2.03	0.40
1:A:77:LYS:HB3	1:A:79:LEU:HD21	2.04	0.40
1:B:92:LEU:HD12	1:B:93:LYS:N	2.35	0.40
1:J:314:MET:HG3	1:J:318:GLU:OE1	2.21	0.40
1:D:48:VAL:CG1	1:D:48:VAL:O	2.68	0.40
1:K:330:LYS:HG3	1:K:330:LYS:O	2.21	0.40
1:J:179:SER:HA	1:L:281:MET:SD	2.61	0.40
1:L:277:THR:O	1:L:281:MET:HG2	2.21	0.40
1:H:193:LEU:HD11	2:H:1:PDY:H22A	2.04	0.40
1:B:85:ARG:HH11	1:B:86:THR:CG2	2.34	0.40
1:L:331:VAL:CG2	1:L:332:PRO:HD2	2.51	0.40
1:E:127:LEU:HD23	1:L:50:SER:O	2.22	0.40
1:E:327:GLN:CD	1:E:330:LYS:HZ2	2.24	0.40
1:A:247:TRP:HZ3	1:A:306:LEU:O	2.05	0.40
1:B:301:LEU:HD13	1:B:322:HIS:CD2	2.56	0.40
1:C:281:MET:HB3	1:C:283:GLN:HG3	2.03	0.40
1:J:206:THR:OG1	1:J:207:ASP:OD2	2.33	0.40
1:K:64:LYS:HZ1	1:K:84:LYS:HE3	1.85	0.40
1:B:253:MET:CE	1:B:305:LEU:HD12	2.52	0.40
1:H:167:MET:HE3	1:H:167:MET:HB3	2.00	0.40
1:L:86:THR:O	1:L:86:THR:HG22	2.21	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	266/324 (82%)	251 (94%)	14 (5%)	1 (0%)	43	82
1	B	269/324 (83%)	252 (94%)	15 (6%)	2 (1%)	30	72
1	C	263/324 (81%)	237 (90%)	21 (8%)	5 (2%)	12	42
1	D	269/324 (83%)	249 (93%)	19 (7%)	1 (0%)	43	82
1	E	268/324 (83%)	249 (93%)	16 (6%)	3 (1%)	21	60
1	F	283/324 (87%)	262 (93%)	19 (7%)	2 (1%)	30	72
1	G	265/324 (82%)	240 (91%)	24 (9%)	1 (0%)	43	82
1	H	265/324 (82%)	242 (91%)	23 (9%)	0	100	100
1	I	267/324 (82%)	251 (94%)	16 (6%)	0	100	100
1	J	267/324 (82%)	231 (86%)	34 (13%)	2 (1%)	30	72
1	K	265/324 (82%)	238 (90%)	24 (9%)	3 (1%)	21	60
1	L	268/324 (83%)	241 (90%)	24 (9%)	3 (1%)	21	60
All	All	3215/3888 (83%)	2943 (92%)	249 (8%)	23 (1%)	30	72

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	154	GLY
1	A	154	GLY
1	C	328	SER
1	G	295	SER
1	L	156	GLN
1	C	66	THR
1	C	295	SER
1	C	332	PRO
1	F	153	ARG
1	J	85	ARG
1	J	199	PRO
1	K	207	ASP
1	D	155	ASP

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Mol	Chain	Res	Type
1	E	329	THR
1	F	207	ASP
1	K	233	GLU
1	L	195	THR
1	B	154	GLY
1	B	207	ASP
1	C	326	MET
1	K	130	GLY
1	L	98	CYS
1	E	289	PRO

### 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	248/293 (85%)	217 (88%)	31 (12%)	7	19
1	B	251/293 (86%)	228 (91%)	23 (9%)	13	38
1	C	247/293 (84%)	212 (86%)	35 (14%)	5	13
1	D	251/293 (86%)	223 (89%)	28 (11%)	9	25
1	E	250/293 (85%)	223 (89%)	27 (11%)	9	27
1	F	258/293 (88%)	225 (87%)	33 (13%)	6	18
1	G	247/293 (84%)	228 (92%)	19 (8%)	18	47
1	H	249/293 (85%)	224 (90%)	25 (10%)	11	32
1	I	249/293 (85%)	222 (89%)	27 (11%)	9	27
1	J	249/293 (85%)	219 (88%)	30 (12%)	7	21
1	K	247/293 (84%)	219 (89%)	28 (11%)	9	25
1	L	250/293 (85%)	226 (90%)	24 (10%)	12	35
All	All	2996/3516 (85%)	2666 (89%)	330 (11%)	9	26

All (330) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	HIS

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Mol	Chain	Res	Type
1	A	53	GLN
1	A	56	LYS
1	A	66	THR
1	A	89	LYS
1	A	96	GLN
1	A	100	LYS
1	A	106	GLU
1	A	127	LEU
1	A	131	ARG
1	A	134	LEU
1	A	138	MET
1	A	142	ASP
1	A	145	GLU
1	A	148	SER
1	A	155	ASP
1	A	156	GLN
1	A	161	ARG
1	A	172	GLU
1	A	188	LYS
1	A	202	ILE
1	A	233	GLU
1	A	240	TYR
1	A	285	GLU
1	A	293	GLU
1	A	326	MET
1	A	331	VAL
1	A	333	GLN
1	A	334	THR
1	A	336	LEU
1	A	342	LEU
1	B	50	SER
1	B	62	ASP
1	B	64	LYS
1	B	65	VAL
1	B	72	LEU
1	B	77	LYS
1	B	80	GLN
1	B	127	LEU
1	B	131	ARG
1	B	155	ASP
1	B	162	GLU
1	B	193	LEU

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Mol	Chain	Res	Type
1	B	233	GLU
1	B	240	TYR
1	B	249	LEU
1	B	276	LYS
1	B	292	SER
1	B	308	THR
1	B	326	MET
1	B	334	THR
1	B	336	LEU
1	B	342	LEU
1	B	344	GLU
1	C	49	LYS
1	C	50	SER
1	C	56	LYS
1	C	85	ARG
1	C	89	LYS
1	C	96	GLN
1	C	98	CYS
1	C	127	LEU
1	C	131	ARG
1	C	134	LEU
1	C	142	ASP
1	C	149	ARG
1	C	155	ASP
1	C	156	GLN
1	C	161	ARG
1	C	190	GLU
1	C	215	THR
1	C	229	TYR
1	C	233	GLU
1	C	240	TYR
1	C	249	LEU
1	C	256	LEU
1	C	264	TYR
1	C	276	LYS
1	C	288	ASN
1	C	290	GLU
1	C	292	SER
1	C	295	SER
1	C	311	THR
1	C	326	MET
1	C	327	GLN

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Mol	Chain	Res	Type
1	C	330	LYS
1	C	334	THR
1	C	336	LEU
1	C	342	LEU
1	D	53	GLN
1	D	64	LYS
1	D	68	GLN
1	D	70	LEU
1	D	122	ASP
1	D	127	LEU
1	D	131	ARG
1	D	132	LYS
1	D	134	LEU
1	D	142	ASP
1	D	161	ARG
1	D	168	LYS
1	D	172	GLU
1	D	197	LYS
1	D	200	ASN
1	D	202	ILE
1	D	238	GLU
1	D	239	LYS
1	D	266	ASN
1	D	283	GLN
1	D	304	ASN
1	D	326	MET
1	D	330	LYS
1	D	331	VAL
1	D	334	THR
1	D	336	LEU
1	D	342	LEU
1	D	343	LYS
1	E	49	LYS
1	E	53	GLN
1	E	57	ASN
1	E	64	LYS
1	E	67	SER
1	E	74	ILE
1	E	87	GLN
1	E	100	LYS
1	E	134	LEU
1	E	151	GLN

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Mol	Chain	Res	Type
1	E	156	GLN
1	E	161	ARG
1	E	172	GLU
1	E	202	ILE
1	E	240	TYR
1	E	249	LEU
1	E	264	TYR
1	E	266	ASN
1	E	272	SER
1	E	292	SER
1	E	304	ASN
1	E	327	GLN
1	E	331	VAL
1	E	333	GLN
1	E	334	THR
1	E	336	LEU
1	E	342	LEU
1	F	50	SER
1	F	62	ASP
1	F	74	ILE
1	F	85	ARG
1	F	89	LYS
1	F	127	LEU
1	F	131	ARG
1	F	134	LEU
1	F	135	LEU
1	F	138	MET
1	F	153	ARG
1	F	155	ASP
1	F	156	GLN
1	F	172	GLU
1	F	188	LYS
1	F	197	LYS
1	F	202	ILE
1	F	229	TYR
1	F	240	TYR
1	F	244	CYS
1	F	253	MET
1	F	285	GLU
1	F	290	GLU
1	F	295	SER
1	F	299	LYS

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Mol	Chain	Res	Type
1	F	307	LYS
1	F	309	GLU
1	F	327	GLN
1	F	334	THR
1	F	336	LEU
1	F	342	LEU
1	F	343	LYS
1	F	344	GLU
1	G	53	GLN
1	G	77	LYS
1	G	100	LYS
1	G	122	ASP
1	G	133	CYS
1	G	153	ARG
1	G	156	GLN
1	G	161	ARG
1	G	198	ARG
1	G	202	ILE
1	G	212	LYS
1	G	248	SER
1	G	264	TYR
1	G	266	ASN
1	G	280	ARG
1	G	290	GLU
1	G	304	ASN
1	G	334	THR
1	G	336	LEU
1	H	47	HIS
1	H	53	GLN
1	H	56	LYS
1	H	70	LEU
1	H	74	ILE
1	H	75	ASN
1	H	77	LYS
1	H	89	LYS
1	H	127	LEU
1	H	131	ARG
1	H	161	ARG
1	H	172	GLU
1	H	193	LEU
1	H	197	LYS
1	H	200	ASN

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Mol	Chain	Res	Type
1	H	229	TYR
1	H	233	GLU
1	H	249	LEU
1	H	275	MET
1	H	328	SER
1	H	330	LYS
1	H	336	LEU
1	H	337	HIS
1	H	340	ARG
1	H	343	LYS
1	I	64	LYS
1	I	89	LYS
1	I	96	GLN
1	I	100	LYS
1	I	113	GLN
1	I	122	ASP
1	I	127	LEU
1	I	134	LEU
1	I	149	ARG
1	I	153	ARG
1	I	155	ASP
1	I	161	ARG
1	I	168	LYS
1	I	169	SER
1	I	200	ASN
1	I	202	ILE
1	I	253	MET
1	I	266	ASN
1	I	297	GLU
1	I	308	THR
1	I	327	GLN
1	I	330	LYS
1	I	331	VAL
1	I	333	GLN
1	I	334	THR
1	I	336	LEU
1	I	342	LEU
1	J	53	GLN
1	J	56	LYS
1	J	68	GLN
1	J	69	VAL
1	J	70	LEU

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Mol	Chain	Res	Type
1	J	89	LYS
1	J	113	GLN
1	J	122	ASP
1	J	131	ARG
1	J	142	ASP
1	J	151	GLN
1	J	153	ARG
1	J	165	GLU
1	J	198	ARG
1	J	233	GLU
1	J	240	TYR
1	J	253	MET
1	J	266	ASN
1	J	285	GLU
1	J	288	ASN
1	J	290	GLU
1	J	293	GLU
1	J	295	SER
1	J	311	THR
1	J	326	MET
1	J	327	GLN
1	J	334	THR
1	J	337	HIS
1	J	340	ARG
1	J	343	LYS
1	K	53	GLN
1	K	64	LYS
1	K	77	LYS
1	K	89	LYS
1	K	100	LYS
1	K	108	HIS
1	K	127	LEU
1	K	131	ARG
1	K	134	LEU
1	K	138	MET
1	K	142	ASP
1	K	149	ARG
1	K	153	ARG
1	K	168	LYS
1	K	193	LEU
1	K	200	ASN
1	K	202	ILE

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Mol	Chain	Res	Type
1	K	233	GLU
1	K	249	LEU
1	K	285	GLU
1	K	288	ASN
1	K	301	LEU
1	K	314	MET
1	K	330	LYS
1	K	333	GLN
1	K	334	THR
1	K	336	LEU
1	K	342	LEU
1	L	56	LYS
1	L	65	VAL
1	L	67	SER
1	L	89	LYS
1	L	96	GLN
1	L	100	LYS
1	L	122	ASP
1	L	127	LEU
1	L	134	LEU
1	L	142	ASP
1	L	151	GLN
1	L	161	ARG
1	L	235	LEU
1	L	240	TYR
1	L	249	LEU
1	L	258	CYS
1	L	266	ASN
1	L	275	MET
1	L	314	MET
1	L	320	MET
1	L	333	GLN
1	L	334	THR
1	L	337	HIS
1	L	342	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (113) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	57	ASN
1	A	68	GLN

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Mol	Chain	Res	Type
1	A	80	GLN
1	A	87	GLN
1	A	113	GLN
1	A	116	HIS
1	A	151	GLN
1	A	156	GLN
1	A	175	GLN
1	A	333	GLN
1	B	47	HIS
1	B	57	ASN
1	B	108	HIS
1	B	181	ASN
1	B	184	HIS
1	B	283	GLN
1	B	327	GLN
1	B	333	GLN
1	C	53	GLN
1	C	57	ASN
1	C	113	GLN
1	C	116	HIS
1	C	151	GLN
1	C	156	GLN
1	C	175	GLN
1	C	200	ASN
1	C	288	ASN
1	C	327	GLN
1	C	337	HIS
1	D	57	ASN
1	D	68	GLN
1	D	87	GLN
1	D	96	GLN
1	D	151	GLN
1	D	266	ASN
1	D	267	HIS
1	D	283	GLN
1	E	53	GLN
1	E	57	ASN
1	E	87	GLN
1	E	116	HIS
1	E	151	GLN
1	E	156	GLN
1	E	178	HIS

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Mol	Chain	Res	Type
1	E	181	ASN
1	E	184	HIS
1	E	321	ASN
1	E	327	GLN
1	E	333	GLN
1	F	68	GLN
1	F	108	HIS
1	F	116	HIS
1	F	156	GLN
1	F	175	GLN
1	F	181	ASN
1	F	283	GLN
1	F	327	GLN
1	G	53	GLN
1	G	57	ASN
1	G	87	GLN
1	G	96	GLN
1	G	108	HIS
1	G	116	HIS
1	G	156	GLN
1	G	175	GLN
1	G	266	ASN
1	G	283	GLN
1	G	337	HIS
1	H	75	ASN
1	H	80	GLN
1	H	113	GLN
1	H	116	HIS
1	H	151	GLN
1	H	175	GLN
1	H	200	ASN
1	H	322	HIS
1	I	108	HIS
1	I	113	GLN
1	I	126	ASN
1	I	151	GLN
1	I	181	ASN
1	I	200	ASN
1	I	266	ASN
1	I	321	ASN
1	I	327	GLN
1	I	333	GLN

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Mol	Chain	Res	Type
1	J	57	ASN
1	J	68	GLN
1	J	87	GLN
1	J	116	HIS
1	J	151	GLN
1	J	156	GLN
1	J	191	ASN
1	J	283	GLN
1	J	288	ASN
1	K	53	GLN
1	K	57	ASN
1	K	80	GLN
1	K	87	GLN
1	K	96	GLN
1	K	113	GLN
1	K	116	HIS
1	K	151	GLN
1	K	337	HIS
1	L	57	ASN
1	L	68	GLN
1	L	80	GLN
1	L	96	GLN
1	L	108	HIS
1	L	113	GLN
1	L	327	GLN
1	L	333	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

25 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	PDY	A	1	-	30,30,30	9.23	6 (20%)	37,41,41	2.39	8 (21%)
2	PDY	A	2	-	30,30,30	9.47	6 (20%)	37,41,41	2.43	13 (35%)
2	PDY	B	1	-	30,30,30	9.18	6 (20%)	37,41,41	2.35	7 (18%)
2	PDY	B	2	-	30,30,30	9.35	6 (20%)	37,41,41	2.48	6 (16%)
2	PDY	C	1	-	30,30,30	9.33	6 (20%)	37,41,41	2.39	7 (18%)
2	PDY	C	2	-	30,30,30	9.21	6 (20%)	37,41,41	2.37	7 (18%)
2	PDY	D	1	-	30,30,30	9.33	6 (20%)	37,41,41	2.38	9 (24%)
2	PDY	D	2	-	30,30,30	9.38	6 (20%)	37,41,41	2.18	10 (27%)
2	PDY	E	1	-	30,30,30	9.16	6 (20%)	37,41,41	2.30	8 (21%)
2	PDY	E	2	-	30,30,30	9.26	6 (20%)	37,41,41	2.31	6 (16%)
2	PDY	F	1	-	30,30,30	9.24	6 (20%)	37,41,41	2.47	9 (24%)
2	PDY	F	2	-	30,30,30	9.21	6 (20%)	37,41,41	2.49	9 (24%)
3	SO4	F	3	-	4,4,4	0.24	0	6,6,6	0.19	0
2	PDY	G	1	-	30,30,30	9.16	6 (20%)	37,41,41	2.43	8 (21%)
2	PDY	G	2	-	30,30,30	9.24	6 (20%)	37,41,41	2.25	7 (18%)
2	PDY	H	1	-	30,30,30	9.36	6 (20%)	37,41,41	2.43	10 (27%)
2	PDY	H	2	-	30,30,30	9.38	6 (20%)	37,41,41	2.65	17 (45%)
2	PDY	I	1	-	30,30,30	9.16	6 (20%)	37,41,41	2.34	6 (16%)
2	PDY	I	2	-	30,30,30	9.54	6 (20%)	37,41,41	2.38	16 (43%)
2	PDY	J	1	-	30,30,30	9.18	6 (20%)	37,41,41	2.19	8 (21%)
2	PDY	J	2	-	30,30,30	9.38	6 (20%)	37,41,41	2.30	7 (18%)
2	PDY	K	1	-	30,30,30	9.31	6 (20%)	37,41,41	2.29	8 (21%)
2	PDY	K	2	-	30,30,30	9.27	6 (20%)	37,41,41	2.43	9 (24%)
2	PDY	L	1	-	30,30,30	9.27	6 (20%)	37,41,41	2.33	7 (18%)
2	PDY	L	2	-	30,30,30	9.28	6 (20%)	37,41,41	1.99	10 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PDY	A	1	-	-	1/11/19/19	0/2/4/4
2	PDY	A	2	-	-	1/11/19/19	0/2/4/4
2	PDY	B	1	-	-	1/11/19/19	0/2/4/4
2	PDY	B	2	-	-	1/11/19/19	0/2/4/4
2	PDY	C	1	-	-	1/11/19/19	0/2/4/4
2	PDY	C	2	-	-	1/11/19/19	0/2/4/4
2	PDY	D	1	-	-	1/11/19/19	0/2/4/4
2	PDY	D	2	-	-	1/11/19/19	0/2/4/4
2	PDY	E	1	-	-	1/11/19/19	0/2/4/4
2	PDY	E	2	-	-	1/11/19/19	0/2/4/4
2	PDY	F	1	-	-	1/11/19/19	0/2/4/4
2	PDY	F	2	-	-	1/11/19/19	0/2/4/4
3	SO4	F	3	-	-	0/0/0/0	0/0/0/0
2	PDY	G	1	-	-	1/11/19/19	0/2/4/4
2	PDY	G	2	-	-	1/11/19/19	0/2/4/4
2	PDY	H	1	-	-	1/11/19/19	0/2/4/4
2	PDY	H	2	-	-	1/11/19/19	0/2/4/4
2	PDY	I	1	-	-	1/11/19/19	0/2/4/4
2	PDY	I	2	-	-	1/11/19/19	0/2/4/4
2	PDY	J	1	-	-	1/11/19/19	0/2/4/4
2	PDY	J	2	-	-	1/11/19/19	0/2/4/4
2	PDY	K	1	-	-	1/11/19/19	0/2/4/4
2	PDY	K	2	-	-	1/11/19/19	0/2/4/4
2	PDY	L	1	-	-	1/11/19/19	0/2/4/4
2	PDY	L	2	-	-	1/11/19/19	0/2/4/4

All (144) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	2	PDY	C8-C5	-48.57	1.33	1.39
2	A	2	PDY	C8-C5	-48.20	1.33	1.39
2	D	2	PDY	C8-C5	-47.69	1.33	1.39
2	J	2	PDY	C8-C5	-47.64	1.33	1.39
2	H	2	PDY	C8-C5	-47.55	1.33	1.39
2	H	1	PDY	C8-C5	-47.51	1.33	1.39
2	B	2	PDY	C8-C5	-47.50	1.33	1.39
2	C	1	PDY	C8-C5	-47.36	1.33	1.39
2	D	1	PDY	C8-C5	-47.35	1.33	1.39
2	K	1	PDY	C8-C5	-47.27	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	2	PDY	C8-C5	-47.06	1.33	1.39
2	K	2	PDY	C8-C5	-46.99	1.33	1.39
2	E	2	PDY	C8-C5	-46.94	1.33	1.39
2	L	1	PDY	C8-C5	-46.93	1.33	1.39
2	G	2	PDY	C8-C5	-46.86	1.33	1.39
2	F	1	PDY	C8-C5	-46.80	1.33	1.39
2	A	1	PDY	C8-C5	-46.72	1.33	1.39
2	C	2	PDY	C8-C5	-46.67	1.33	1.39
2	F	2	PDY	C8-C5	-46.61	1.33	1.39
2	B	1	PDY	C8-C5	-46.48	1.33	1.39
2	J	1	PDY	C8-C5	-46.45	1.33	1.39
2	E	1	PDY	C8-C5	-46.35	1.33	1.39
2	G	1	PDY	C8-C5	-46.32	1.33	1.39
2	I	1	PDY	C8-C5	-46.29	1.33	1.39
2	L	2	PDY	C8-C11	14.94	1.53	1.38
2	I	2	PDY	C8-C11	14.90	1.53	1.38
2	D	2	PDY	C8-C11	14.89	1.53	1.38
2	H	2	PDY	C8-C11	14.81	1.53	1.38
2	L	1	PDY	C8-C11	14.76	1.53	1.38
2	J	1	PDY	C8-C11	14.74	1.53	1.38
2	I	1	PDY	C8-C11	14.73	1.53	1.38
2	E	2	PDY	C8-C11	14.73	1.53	1.38
2	J	2	PDY	C8-C11	14.72	1.53	1.38
2	H	1	PDY	C8-C11	14.71	1.53	1.38
2	F	1	PDY	C8-C11	14.70	1.53	1.38
2	D	1	PDY	C8-C11	14.69	1.53	1.38
2	A	1	PDY	C8-C11	14.69	1.53	1.38
2	G	1	PDY	C8-C11	14.68	1.53	1.38
2	B	1	PDY	C8-C11	14.67	1.53	1.38
2	C	2	PDY	C8-C11	14.66	1.53	1.38
2	F	2	PDY	C8-C11	14.65	1.53	1.38
2	K	1	PDY	C8-C11	14.65	1.53	1.38
2	A	2	PDY	C8-C11	14.65	1.53	1.38
2	G	2	PDY	C8-C11	14.65	1.53	1.38
2	K	2	PDY	C8-C11	14.64	1.53	1.38
2	B	2	PDY	C8-C11	14.62	1.53	1.38
2	C	1	PDY	C8-C11	14.62	1.53	1.38
2	E	1	PDY	C8-C11	14.60	1.53	1.38
2	A	2	PDY	N7-N2	-9.08	1.23	1.36
2	H	2	PDY	N7-N2	-8.96	1.23	1.36
2	D	1	PDY	N7-N2	-8.91	1.23	1.36
2	F	2	PDY	N7-N2	-8.90	1.23	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	PDY	N7-N2	-8.88	1.23	1.36
2	J	1	PDY	N7-N2	-8.86	1.23	1.36
2	H	1	PDY	N7-N2	-8.86	1.23	1.36
2	B	1	PDY	N7-N2	-8.84	1.23	1.36
2	F	1	PDY	N7-N2	-8.83	1.23	1.36
2	A	1	PDY	N7-N2	-8.83	1.23	1.36
2	C	1	PDY	N7-N2	-8.82	1.23	1.36
2	I	1	PDY	N7-N2	-8.82	1.23	1.36
2	G	1	PDY	N7-N2	-8.82	1.23	1.36
2	E	1	PDY	N7-N2	-8.82	1.23	1.36
2	L	1	PDY	N7-N2	-8.80	1.23	1.36
2	K	1	PDY	N7-N2	-8.79	1.23	1.36
2	J	2	PDY	N7-N2	-8.79	1.23	1.36
2	C	2	PDY	N7-N2	-8.78	1.23	1.36
2	K	2	PDY	N7-N2	-8.76	1.23	1.36
2	G	2	PDY	N7-N2	-8.75	1.23	1.36
2	E	2	PDY	N7-N2	-8.69	1.23	1.36
2	L	2	PDY	N7-N2	-8.57	1.24	1.36
2	I	2	PDY	N7-N2	-8.55	1.24	1.36
2	D	2	PDY	N7-N2	-8.51	1.24	1.36
2	E	2	PDY	C11-N7	6.71	1.47	1.33
2	K	2	PDY	C11-N7	6.68	1.47	1.33
2	L	1	PDY	C11-N7	6.68	1.47	1.33
2	H	2	PDY	C11-N7	6.68	1.47	1.33
2	G	1	PDY	C11-N7	6.66	1.47	1.33
2	C	2	PDY	C11-N7	6.66	1.47	1.33
2	G	2	PDY	C11-N7	6.65	1.47	1.33
2	B	1	PDY	C11-N7	6.63	1.47	1.33
2	F	2	PDY	C11-N7	6.62	1.47	1.33
2	B	2	PDY	C11-N7	6.62	1.47	1.33
2	A	1	PDY	C11-N7	6.62	1.47	1.33
2	E	1	PDY	C11-N7	6.61	1.47	1.33
2	D	1	PDY	C11-N7	6.61	1.47	1.33
2	J	2	PDY	C11-N7	6.61	1.47	1.33
2	F	1	PDY	C11-N7	6.61	1.47	1.33
2	C	1	PDY	C11-N7	6.60	1.47	1.33
2	I	1	PDY	C11-N7	6.59	1.47	1.33
2	J	1	PDY	C11-N7	6.56	1.47	1.33
2	I	2	PDY	C11-N7	6.56	1.47	1.33
2	D	2	PDY	C11-N7	6.56	1.47	1.33
2	L	2	PDY	C11-N7	6.56	1.47	1.33
2	K	1	PDY	C11-N7	6.56	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	PDY	C11-N7	6.55	1.47	1.33
2	A	2	PDY	C11-N7	6.50	1.47	1.33
2	H	1	PDY	C13-N9	-3.78	1.32	1.40
2	F	1	PDY	C13-N9	-3.68	1.32	1.40
2	K	1	PDY	C13-N9	-3.66	1.33	1.40
2	E	1	PDY	C13-N9	-3.65	1.33	1.40
2	A	1	PDY	C13-N9	-3.62	1.33	1.40
2	B	1	PDY	C13-N9	-3.57	1.33	1.40
2	I	1	PDY	C13-N9	-3.57	1.33	1.40
2	F	2	PDY	C13-N9	-3.57	1.33	1.40
2	D	1	PDY	C13-N9	-3.56	1.33	1.40
2	L	1	PDY	C13-N9	-3.55	1.33	1.40
2	G	1	PDY	C13-N9	-3.54	1.33	1.40
2	B	2	PDY	C13-N9	-3.53	1.33	1.40
2	J	1	PDY	C13-N9	-3.53	1.33	1.40
2	J	2	PDY	C13-N9	-3.52	1.33	1.40
2	C	1	PDY	C13-N9	-3.52	1.33	1.40
2	G	2	PDY	C13-N9	-3.46	1.33	1.40
2	A	2	PDY	C13-N9	-3.44	1.33	1.40
2	K	2	PDY	C13-N9	-3.40	1.33	1.40
2	C	2	PDY	C13-N9	-3.38	1.33	1.40
2	L	2	PDY	C13-N9	-3.32	1.33	1.40
2	H	2	PDY	C13-N9	-3.32	1.33	1.40
2	E	2	PDY	C13-N9	-3.21	1.33	1.40
2	D	2	PDY	C13-N9	-3.21	1.33	1.40
2	I	2	PDY	C13-N9	-3.17	1.34	1.40
2	A	2	PDY	C4-N6	2.66	1.35	1.31
2	D	2	PDY	C4-N6	2.56	1.35	1.31
2	G	2	PDY	C4-N6	2.55	1.35	1.31
2	L	1	PDY	C4-N6	2.51	1.34	1.31
2	E	2	PDY	C4-N6	2.46	1.34	1.31
2	H	1	PDY	C4-N6	2.46	1.34	1.31
2	J	1	PDY	C4-N6	2.45	1.34	1.31
2	A	1	PDY	C4-N6	2.44	1.34	1.31
2	C	1	PDY	C4-N6	2.44	1.34	1.31
2	C	2	PDY	C4-N6	2.43	1.34	1.31
2	K	2	PDY	C4-N6	2.42	1.34	1.31
2	K	1	PDY	C4-N6	2.40	1.34	1.31
2	B	1	PDY	C4-N6	2.39	1.34	1.31
2	I	1	PDY	C4-N6	2.37	1.34	1.31
2	E	1	PDY	C4-N6	2.37	1.34	1.31
2	F	1	PDY	C4-N6	2.36	1.34	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	2	PDY	C4-N6	2.35	1.34	1.31
2	I	2	PDY	C4-N6	2.32	1.34	1.31
2	L	2	PDY	C4-N6	2.31	1.34	1.31
2	J	2	PDY	C4-N6	2.30	1.34	1.31
2	D	1	PDY	C4-N6	2.30	1.34	1.31
2	G	1	PDY	C4-N6	2.28	1.34	1.31
2	B	2	PDY	C4-N6	2.23	1.34	1.31
2	F	2	PDY	C4-N6	2.21	1.34	1.31

All (212) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	PDY	C11-N7-N2	11.07	112.20	103.79
2	C	2	PDY	C11-N7-N2	10.98	112.12	103.79
2	A	1	PDY	C11-N7-N2	10.96	112.11	103.79
2	D	1	PDY	C11-N7-N2	10.79	111.98	103.79
2	F	1	PDY	C11-N7-N2	10.77	111.97	103.79
2	C	1	PDY	C11-N7-N2	10.70	111.91	103.79
2	G	1	PDY	C11-N7-N2	10.67	111.89	103.79
2	B	2	PDY	C11-N7-N2	10.64	111.87	103.79
2	F	2	PDY	C11-N7-N2	10.63	111.86	103.79
2	L	1	PDY	C11-N7-N2	10.57	111.81	103.79
2	K	2	PDY	C11-N7-N2	10.11	111.47	103.79
2	E	1	PDY	C11-N7-N2	10.11	111.46	103.79
2	I	1	PDY	C11-N7-N2	10.10	111.45	103.79
2	E	2	PDY	C11-N7-N2	9.96	111.35	103.79
2	J	2	PDY	C11-N7-N2	9.93	111.33	103.79
2	J	1	PDY	C11-N7-N2	9.91	111.31	103.79
2	G	2	PDY	C11-N7-N2	9.89	111.30	103.79
2	K	1	PDY	C11-N7-N2	9.85	111.27	103.79
2	H	1	PDY	C11-N7-N2	9.73	111.17	103.79
2	A	2	PDY	C11-N7-N2	9.27	110.83	103.79
2	D	2	PDY	C11-N7-N2	8.40	110.17	103.79
2	L	2	PDY	C11-N7-N2	7.32	109.35	103.79
2	I	2	PDY	C11-N7-N2	7.14	109.21	103.79
2	H	2	PDY	C11-N7-N2	6.21	108.51	103.79
2	B	2	PDY	C4-N10-C15	-6.17	116.16	123.84
2	F	2	PDY	C4-N10-C15	-5.97	116.42	123.84
2	K	2	PDY	C4-N10-C15	-5.77	116.66	123.84
2	H	1	PDY	C24-O21-C16	-5.61	105.36	117.97
2	G	1	PDY	C4-N10-C15	-4.69	118.00	123.84
2	H	2	PDY	C13-N9-C1	4.67	137.48	126.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	2	PDY	C17-C20-C16	4.64	125.96	119.76
2	F	1	PDY	C8-C11-N7	-4.53	100.08	111.36
2	B	1	PDY	C8-C11-N7	-4.49	100.18	111.36
2	L	1	PDY	C8-C11-N7	-4.46	100.25	111.36
2	I	2	PDY	C4-N10-C15	-4.45	118.31	123.84
2	C	1	PDY	C8-C11-N7	-4.44	100.30	111.36
2	A	1	PDY	C8-C11-N7	-4.41	100.37	111.36
2	D	1	PDY	C8-C11-N7	-4.36	100.50	111.36
2	H	1	PDY	C8-C11-N7	-4.35	100.53	111.36
2	A	2	PDY	C8-C11-N7	-4.33	100.57	111.36
2	G	1	PDY	C8-C11-N7	-4.31	100.62	111.36
2	C	2	PDY	C8-C11-N7	-4.30	100.65	111.36
2	J	1	PDY	C8-C11-N7	-4.29	100.67	111.36
2	K	1	PDY	C8-C11-N7	-4.28	100.69	111.36
2	B	2	PDY	C8-C11-N7	-4.27	100.73	111.36
2	F	2	PDY	C8-C11-N7	-4.27	100.74	111.36
2	E	1	PDY	C8-C11-N7	-4.26	100.75	111.36
2	I	1	PDY	C8-C11-N7	-4.26	100.76	111.36
2	F	1	PDY	C24-O21-C16	-4.24	108.44	117.97
2	J	2	PDY	C8-C11-N7	-4.17	100.97	111.36
2	K	2	PDY	C8-C11-N7	-4.16	100.99	111.36
2	I	2	PDY	C4-N6-C5	4.16	122.67	117.24
2	E	2	PDY	C8-C11-N7	-4.15	101.01	111.36
2	G	2	PDY	C8-C11-N7	-4.15	101.03	111.36
2	G	2	PDY	C4-N10-C15	-4.10	118.74	123.84
2	A	2	PDY	C3-C1-N9	4.08	131.28	123.07
2	C	2	PDY	C4-N10-C15	-4.05	118.80	123.84
2	H	2	PDY	C4-N10-C15	-4.02	118.84	123.84
2	I	1	PDY	C4-N6-C5	4.01	122.47	117.24
2	D	2	PDY	C8-C11-N7	-3.95	101.51	111.36
2	L	1	PDY	C4-N6-C5	3.92	122.35	117.24
2	A	1	PDY	C25-C15-N10	-3.80	104.63	110.55
2	C	1	PDY	C4-N10-C15	-3.79	119.12	123.84
2	L	2	PDY	C8-C11-N7	-3.79	101.91	111.36
2	I	2	PDY	C8-C11-N7	-3.79	101.93	111.36
2	J	2	PDY	C4-N10-C15	-3.78	119.13	123.84
2	E	2	PDY	N9-C1-N2	3.77	119.42	113.55
2	H	2	PDY	C4-N6-C5	3.76	122.14	117.24
2	K	1	PDY	C4-N6-C5	3.75	122.13	117.24
2	H	2	PDY	C8-C11-N7	-3.74	102.05	111.36
2	E	2	PDY	C1-C3-C4	3.73	121.32	116.38
2	I	2	PDY	C22-C15-N10	3.70	114.67	109.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1	PDY	C25-C15-N10	-3.70	104.79	110.55
2	A	2	PDY	C1-C3-C4	3.69	121.27	116.38
2	H	2	PDY	C19-C16-C20	-3.67	113.91	120.21
2	L	1	PDY	C4-N10-C15	-3.63	119.32	123.84
2	H	2	PDY	C5-N2-N7	3.63	115.15	111.08
2	E	1	PDY	C4-N6-C5	3.62	121.96	117.24
2	D	1	PDY	C24-O21-C16	-3.61	109.85	117.97
2	H	1	PDY	C4-N6-C5	3.61	121.94	117.24
2	E	1	PDY	C4-N10-C15	-3.59	119.38	123.84
2	K	1	PDY	C24-O21-C16	-3.59	109.90	117.97
2	I	1	PDY	N6-C5-N2	-3.55	118.94	122.20
2	A	2	PDY	C22-C15-N10	3.54	114.46	109.78
2	I	1	PDY	C4-N10-C15	-3.52	119.46	123.84
2	H	2	PDY	C17-C13-N9	-3.51	109.38	120.67
2	G	1	PDY	C4-N6-C5	3.51	121.82	117.24
2	I	2	PDY	C13-N9-C1	3.50	134.72	126.47
2	C	1	PDY	C4-N6-C5	3.48	121.78	117.24
2	B	1	PDY	C4-N6-C5	3.46	121.75	117.24
2	C	1	PDY	N6-C5-N2	-3.41	119.07	122.20
2	E	1	PDY	C24-O21-C16	-3.37	110.40	117.97
2	A	1	PDY	C4-N6-C5	3.36	121.63	117.24
2	C	2	PDY	C1-C3-C4	3.36	120.83	116.38
2	H	1	PDY	N6-C5-N2	-3.35	119.13	122.20
2	F	1	PDY	C4-N6-C5	3.34	121.60	117.24
2	H	2	PDY	C3-C4-N10	3.34	124.30	119.22
2	E	2	PDY	C4-N6-C5	3.34	121.59	117.24
2	F	1	PDY	C4-N10-C15	-3.29	119.76	123.84
2	I	2	PDY	C3-C1-N2	3.29	122.99	119.31
2	A	2	PDY	C4-N6-C5	3.28	121.51	117.24
2	E	2	PDY	C25-C15-N10	3.26	115.63	110.55
2	J	1	PDY	C4-N6-C5	3.25	121.48	117.24
2	A	1	PDY	N6-C5-N2	-3.24	119.23	122.20
2	G	2	PDY	C1-C3-C4	3.24	120.67	116.38
2	H	2	PDY	C24-O21-C16	-3.24	110.69	117.97
2	G	1	PDY	N6-C5-N2	-3.23	119.23	122.20
2	H	1	PDY	C4-N10-C15	-3.23	119.82	123.84
2	D	2	PDY	C13-N9-C1	3.18	133.98	126.47
2	F	1	PDY	N6-C5-N2	-3.18	119.28	122.20
2	G	2	PDY	C4-N6-C5	3.17	121.38	117.24
2	K	2	PDY	C4-N6-C5	3.17	121.38	117.24
2	J	2	PDY	C4-N6-C5	3.17	121.37	117.24
2	B	2	PDY	C4-N6-C5	3.16	121.36	117.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	PDY	C4-N6-C5	3.14	121.34	117.24
2	D	1	PDY	C25-C15-N10	-3.14	105.67	110.55
2	L	2	PDY	C4-N6-C5	3.13	121.32	117.24
2	H	2	PDY	C22-C15-N10	3.13	113.92	109.78
2	H	2	PDY	C3-C1-N2	3.11	122.80	119.31
2	K	1	PDY	C4-N10-C15	-3.10	119.98	123.84
2	D	2	PDY	C25-C15-C22	-3.10	105.19	109.59
2	D	2	PDY	C4-N6-C5	3.09	121.27	117.24
2	L	1	PDY	C13-N9-C1	3.09	133.77	126.47
2	B	1	PDY	N6-C5-N2	-3.08	119.38	122.20
2	F	2	PDY	C4-N6-C5	3.04	121.21	117.24
2	L	1	PDY	N6-C5-N2	-3.04	119.41	122.20
2	C	1	PDY	C22-C15-N10	-3.04	105.76	109.78
2	E	1	PDY	N6-C5-N2	-3.02	119.43	122.20
2	B	1	PDY	C4-N10-C15	-3.01	120.10	123.84
2	D	2	PDY	C3-C1-N9	2.98	129.07	123.07
2	I	2	PDY	N6-C5-N2	-2.98	119.47	122.20
2	H	2	PDY	N6-C5-N2	-2.97	119.48	122.20
2	H	2	PDY	N9-C1-N2	-2.95	108.96	113.55
2	F	2	PDY	N6-C5-N2	-2.93	119.51	122.20
2	J	1	PDY	C14-C3-C4	-2.92	116.33	121.45
2	L	2	PDY	C13-N9-C1	2.92	133.36	126.47
2	B	2	PDY	C1-C3-C4	2.91	120.23	116.38
2	C	2	PDY	C4-N6-C5	2.86	120.97	117.24
2	L	2	PDY	C14-C3-C4	-2.85	116.45	121.45
2	D	2	PDY	C1-C3-C4	2.84	120.14	116.38
2	F	2	PDY	C1-C3-C4	2.81	120.10	116.38
2	J	1	PDY	C1-C3-C4	2.79	120.08	116.38
2	K	1	PDY	N6-C5-N2	-2.79	119.64	122.20
2	D	1	PDY	C1-C3-C4	2.78	120.06	116.38
2	F	1	PDY	C1-C3-C4	2.78	120.06	116.38
2	D	1	PDY	N6-C5-N2	-2.77	119.66	122.20
2	J	2	PDY	C1-C3-C4	2.76	120.04	116.38
2	H	2	PDY	C18-C13-N9	2.76	129.56	120.67
2	K	2	PDY	C24-O21-C16	-2.75	111.78	117.97
2	K	2	PDY	C1-C3-C4	2.74	120.01	116.38
2	K	1	PDY	C1-C3-C4	2.73	119.99	116.38
2	E	1	PDY	C25-C15-N10	-2.70	106.36	110.55
2	J	1	PDY	N6-C5-N2	-2.69	119.73	122.20
2	A	1	PDY	C13-N9-C1	2.69	132.81	126.47
2	J	2	PDY	N6-C5-N2	-2.68	119.74	122.20
2	I	2	PDY	C5-N2-N7	2.67	114.07	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2	PDY	C3-C4-N10	2.65	123.24	119.22
2	F	2	PDY	C25-C15-N10	-2.63	106.46	110.55
2	B	2	PDY	N6-C5-N2	-2.62	119.79	122.20
2	A	2	PDY	C3-C1-N2	-2.62	116.37	119.31
2	B	1	PDY	C1-C3-C4	2.61	119.84	116.38
2	H	1	PDY	C20-C17-C13	-2.58	117.28	120.27
2	L	2	PDY	C5-N2-N7	2.57	113.97	111.08
2	A	2	PDY	N9-C1-N2	-2.56	109.57	113.55
2	F	1	PDY	C14-C3-C4	-2.52	117.03	121.45
2	L	2	PDY	N6-C5-N2	-2.52	119.89	122.20
2	I	2	PDY	C17-C13-N9	-2.52	112.57	120.67
2	D	2	PDY	C14-C3-C4	-2.47	117.12	121.45
2	F	2	PDY	C14-C3-C4	-2.47	117.12	121.45
2	I	2	PDY	C20-C17-C13	2.46	123.13	120.27
2	H	1	PDY	C14-C3-C4	-2.42	117.20	121.45
2	D	2	PDY	N9-C1-N2	-2.41	109.81	113.55
2	C	2	PDY	C3-C1-N2	-2.40	116.63	119.31
2	L	2	PDY	N9-C1-N2	-2.38	109.86	113.55
2	J	1	PDY	C24-O21-C16	-2.37	112.64	117.97
2	I	2	PDY	C3-C4-N10	2.36	122.81	119.22
2	L	2	PDY	C22-C15-N10	2.35	112.88	109.78
2	J	1	PDY	C3-C1-N9	2.32	127.74	123.07
2	K	1	PDY	C14-C3-C4	-2.32	117.38	121.45
2	D	1	PDY	C14-C3-C4	-2.32	117.38	121.45
2	I	1	PDY	C25-C15-N10	-2.30	106.97	110.55
2	I	2	PDY	C25-C15-C22	-2.25	106.40	109.59
2	L	2	PDY	C14-C3-C1	2.23	125.88	121.81
2	L	1	PDY	C1-C3-C4	2.23	119.33	116.38
2	G	2	PDY	C14-C3-C4	-2.23	117.55	121.45
2	E	1	PDY	C1-C3-C4	2.23	119.33	116.38
2	C	1	PDY	C1-C3-C4	2.22	119.32	116.38
2	D	1	PDY	C4-N10-C15	-2.22	121.08	123.84
2	K	2	PDY	C14-C3-C4	-2.20	117.59	121.45
2	D	2	PDY	N6-C5-N2	-2.20	120.18	122.20
2	K	2	PDY	N6-C5-N2	-2.19	120.19	122.20
2	H	1	PDY	C18-C13-C17	2.19	122.17	119.10
2	F	2	PDY	C3-C1-N2	-2.18	116.86	119.31
2	A	1	PDY	C4-N10-C15	-2.14	121.18	123.84
2	A	2	PDY	N6-C5-N2	-2.13	120.24	122.20
2	B	1	PDY	C14-C3-C4	-2.13	117.72	121.45
2	G	1	PDY	C14-C3-C4	-2.12	117.73	121.45
2	A	2	PDY	C25-C15-C22	-2.11	106.59	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	PDY	C22-C15-N10	-2.10	107.00	109.78
2	I	2	PDY	C18-C13-C17	-2.10	116.15	119.10
2	J	2	PDY	C24-O21-C16	-2.09	113.26	117.97
2	I	2	PDY	C19-C16-C20	-2.09	116.62	120.21
2	A	1	PDY	C1-C3-C4	2.08	119.14	116.38
2	H	1	PDY	C1-C3-C4	2.08	119.14	116.38
2	C	2	PDY	N6-C5-N2	-2.07	120.30	122.20
2	H	2	PDY	N10-C4-N6	-2.06	113.10	118.39
2	A	2	PDY	C18-C13-C17	-2.06	116.20	119.10
2	A	2	PDY	C19-C18-C13	2.05	122.65	120.27
2	K	2	PDY	N9-C1-N2	2.04	116.72	113.55
2	G	1	PDY	C1-C3-C4	2.02	119.06	116.38
2	G	2	PDY	C24-O21-C16	-2.02	113.43	117.97
2	I	2	PDY	C14-C3-C4	-2.00	117.94	121.45

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	2	PDY	C3-C1-N9-C13
2	L	2	PDY	C3-C1-N9-C13
2	D	2	PDY	C3-C1-N9-C13
2	I	2	PDY	C3-C1-N9-C13
2	J	1	PDY	C3-C1-N9-C13
2	A	2	PDY	C3-C1-N9-C13
2	H	1	PDY	C3-C1-N9-C13
2	I	1	PDY	C3-C1-N9-C13
2	J	2	PDY	C3-C1-N9-C13
2	K	1	PDY	C3-C1-N9-C13
2	D	1	PDY	C3-C1-N9-C13
2	C	1	PDY	C3-C1-N9-C13
2	E	1	PDY	C3-C1-N9-C13
2	G	1	PDY	C3-C1-N9-C13
2	F	2	PDY	C3-C1-N9-C13
2	F	1	PDY	C3-C1-N9-C13
2	L	1	PDY	C3-C1-N9-C13
2	B	2	PDY	C3-C1-N9-C13
2	K	2	PDY	C3-C1-N9-C13
2	G	2	PDY	C3-C1-N9-C13
2	B	1	PDY	C3-C1-N9-C13
2	A	1	PDY	C3-C1-N9-C13
2	C	2	PDY	C3-C1-N9-C13

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Mol	Chain	Res	Type	Atoms
2	E	2	PDY	C3-C1-N9-C13

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	274/324 (84%)	0.17	10 (3%) 41 48	8, 24, 56, 81	0
1	B	277/324 (85%)	0.27	12 (4%) 34 40	7, 29, 71, 80	0
1	C	273/324 (84%)	0.34	14 (5%) 27 33	15, 40, 73, 83	0
1	D	277/324 (85%)	0.31	10 (3%) 41 48	8, 32, 70, 81	0
1	E	276/324 (85%)	0.27	9 (3%) 44 53	10, 28, 58, 76	0
1	F	287/324 (88%)	0.19	14 (4%) 28 34	4, 25, 70, 86	0
1	G	273/324 (84%)	0.43	14 (5%) 27 33	16, 38, 67, 79	0
1	H	275/324 (84%)	0.33	14 (5%) 27 33	13, 39, 68, 84	0
1	I	275/324 (84%)	0.20	8 (2%) 49 58	14, 30, 66, 97	0
1	J	275/324 (84%)	0.56	18 (6%) 18 22	27, 52, 81, 100	0
1	K	273/324 (84%)	0.69	32 (11%) 5 7	25, 49, 76, 98	0
1	L	276/324 (85%)	0.52	18 (6%) 18 22	15, 46, 83, 110	0
All	All	3311/3888 (85%)	0.36	173 (5%) 26 32	4, 37, 73, 110	0

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	157	ALA	7.5
1	E	216	SER	7.3
1	J	155	ASP	6.9
1	I	229	TYR	6.6
1	B	157	ALA	6.2
1	H	155	ASP	5.5
1	C	154	GLY	5.2
1	E	229	TYR	5.0
1	K	155	ASP	4.9
1	G	229	TYR	4.7
1	K	216	SER	4.4

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Mol	Chain	Res	Type	RSRZ
1	F	229	TYR	4.3
1	B	155	ASP	4.2
1	K	156	GLN	4.2
1	D	72	LEU	4.2
1	K	342	LEU	4.2
1	I	230	VAL	4.0
1	L	154	GLY	4.0
1	B	47	HIS	4.0
1	J	294	VAL	3.8
1	K	240	TYR	3.7
1	J	156	GLN	3.7
1	L	155	ASP	3.7
1	A	216	SER	3.7
1	H	230	VAL	3.7
1	C	216	SER	3.6
1	G	65	VAL	3.6
1	H	340	ARG	3.6
1	K	85	ARG	3.5
1	H	216	SER	3.5
1	G	330	LYS	3.4
1	B	216	SER	3.4
1	F	236	GLY	3.4
1	J	229	TYR	3.4
1	C	82	PHE	3.4
1	L	337	HIS	3.4
1	I	216	SER	3.3
1	H	215	THR	3.3
1	D	82	PHE	3.3
1	L	216	SER	3.3
1	K	289	PRO	3.3
1	G	329	THR	3.3
1	L	235	LEU	3.3
1	H	154	GLY	3.3
1	H	229	TYR	3.3
1	J	99	PRO	3.2
1	G	156	GLN	3.2
1	D	344	GLU	3.1
1	H	69	VAL	3.1
1	I	72	LEU	3.1
1	K	150	ILE	3.1
1	G	87	GLN	3.1
1	F	234	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	K	158	PHE	3.1
1	D	69	VAL	3.1
1	F	48	VAL	3.1
1	L	69	VAL	3.1
1	L	156	GLN	3.1
1	G	216	SER	3.1
1	K	335	PRO	3.0
1	B	234	VAL	3.0
1	J	335	PRO	3.0
1	D	86	THR	3.0
1	K	154	GLY	3.0
1	K	334	THR	3.0
1	D	267	HIS	3.0
1	L	289	PRO	3.0
1	F	155	ASP	3.0
1	K	151	GLN	3.0
1	J	337	HIS	3.0
1	H	157	ALA	3.0
1	K	146	LEU	2.9
1	K	201	ALA	2.9
1	A	289	PRO	2.9
1	K	336	LEU	2.9
1	L	340	ARG	2.9
1	K	160	GLU	2.8
1	L	157	ALA	2.8
1	G	294	VAL	2.8
1	C	156	GLN	2.8
1	K	332	PRO	2.8
1	G	240	TYR	2.8
1	F	235	LEU	2.8
1	L	230	VAL	2.7
1	J	79	LEU	2.7
1	J	330	LYS	2.7
1	L	334	THR	2.7
1	J	260	TYR	2.7
1	C	87	GLN	2.7
1	D	156	GLN	2.7
1	L	229	TYR	2.7
1	B	235	LEU	2.7
1	C	92	LEU	2.7
1	K	291	TRP	2.6
1	F	216	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	240	TYR	2.6
1	A	85	ARG	2.6
1	K	161	ARG	2.6
1	E	87	GLN	2.6
1	H	150	ILE	2.6
1	K	257	LEU	2.6
1	K	294	VAL	2.6
1	E	72	LEU	2.6
1	I	74	ILE	2.6
1	K	153	ARG	2.6
1	J	69	VAL	2.6
1	H	156	GLN	2.5
1	K	337	HIS	2.5
1	C	234	VAL	2.5
1	I	79	LEU	2.5
1	K	331	VAL	2.5
1	K	340	ARG	2.5
1	D	240	TYR	2.4
1	H	86	THR	2.4
1	I	70	LEU	2.4
1	C	84	LYS	2.4
1	J	75	ASN	2.4
1	B	231	ALA	2.4
1	C	153	ARG	2.4
1	A	65	VAL	2.4
1	C	72	LEU	2.4
1	A	68	GLN	2.4
1	F	47	HIS	2.4
1	L	48	VAL	2.4
1	H	64	LYS	2.4
1	E	151	GLN	2.4
1	G	334	THR	2.4
1	L	65	VAL	2.3
1	F	343	LYS	2.3
1	J	324	TRP	2.3
1	K	86	THR	2.3
1	C	157	ALA	2.3
1	K	333	GLN	2.3
1	E	155	ASP	2.3
1	C	85	ARG	2.3
1	G	97	ASP	2.3
1	L	153	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	154	GLY	2.3
1	F	113	GLN	2.2
1	H	265	SER	2.2
1	G	85	ARG	2.2
1	A	82	PHE	2.2
1	B	329	THR	2.2
1	B	230	VAL	2.2
1	G	337	HIS	2.2
1	A	343	LYS	2.2
1	L	330	LYS	2.2
1	A	342	LEU	2.2
1	G	340	ARG	2.2
1	J	215	THR	2.2
1	C	198	ARG	2.2
1	K	235	LEU	2.2
1	E	150	ILE	2.2
1	K	199	PRO	2.1
1	C	65	VAL	2.1
1	D	90	PHE	2.1
1	B	154	GLY	2.1
1	J	234	VAL	2.1
1	I	75	ASN	2.1
1	E	65	VAL	2.1
1	E	343	LYS	2.1
1	A	235	LEU	2.1
1	J	72	LEU	2.1
1	F	151	GLN	2.1
1	J	158	PHE	2.1
1	D	67	SER	2.1
1	J	338	THR	2.0
1	F	49	LYS	2.0
1	A	154	GLY	2.0
1	B	65	VAL	2.0
1	K	99	PRO	2.0
1	L	294	VAL	2.0
1	B	72	LEU	2.0

## 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	PDY	D	2	27/27	0.40	8.03	65,74,80,81	0
2	PDY	L	2	27/27	0.42	4.68	71,75,77,77	0
2	PDY	E	2	27/27	0.43	3.70	60,67,69,69	0
2	PDY	G	2	27/27	0.41	3.46	52,56,64,64	0
2	PDY	E	1	27/27	0.29	2.46	7,23,37,38	0
2	PDY	A	2	27/27	0.36	2.40	60,65,69,71	0
2	PDY	I	2	27/27	0.33	1.66	53,61,74,75	0
3	SO4	F	3	5/5	0.25	1.27	61,62,64,65	0
2	PDY	K	2	27/27	0.41	1.22	61,67,79,80	0
2	PDY	H	2	27/27	0.35	1.00	52,55,60,60	0
2	PDY	J	2	27/27	0.34	0.95	59,62,67,68	0
2	PDY	A	1	27/27	0.23	0.74	2,11,31,32	0
2	PDY	H	1	27/27	0.21	0.54	22,31,54,55	0
2	PDY	C	1	27/27	0.23	0.53	18,32,56,58	0
2	PDY	B	2	27/27	0.20	0.52	20,29,34,35	0
2	PDY	J	1	27/27	0.23	0.49	31,39,54,55	0
2	PDY	C	2	27/27	0.24	0.49	48,50,62,63	0
2	PDY	K	1	27/27	0.22	0.46	27,44,54,55	0
2	PDY	D	1	27/27	0.23	0.27	16,23,43,44	0
2	PDY	L	1	27/27	0.22	0.13	30,34,47,50	0
2	PDY	I	1	27/27	0.20	-0.17	5,19,43,45	0
2	PDY	F	2	27/27	0.17	-0.37	20,24,28,29	0
2	PDY	F	1	27/27	0.18	-0.37	5,15,32,34	0
2	PDY	B	1	27/27	0.20	-0.42	6,16,37,38	0
2	PDY	G	1	27/27	0.16	-0.52	4,20,38,43	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.