



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:46 am 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 X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

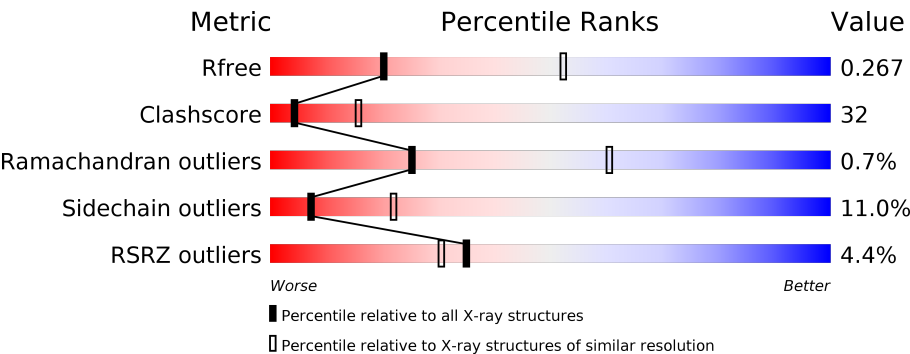
MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	324	<div><div>2%</div><div><div></div><div>44%</div><div>35%</div><div>5%</div><div>15%</div></div></div>
1	B	324	<div><div>2%</div><div><div></div><div>40%</div><div>40%</div><div>5%</div><div>15%</div></div></div>
1	C	324	<div><div>4%</div><div><div></div><div>40%</div><div>35%</div><div>9%</div><div>16%</div></div></div>
1	D	324	<div><div>3%</div><div><div></div><div>46%</div><div>33%</div><div>6%</div><div>15%</div></div></div>
1	E	324	<div><div>2%</div><div><div></div><div>47%</div><div>32%</div><div>6%</div><div>15%</div></div></div>
1	F	324	<div><div>4%</div><div><div></div><div>47%</div><div>37%</div><div>•</div><div>11%</div></div></div>

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Mol	Chain	Length	Quality of chain
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, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PDY	A	2	-	-	-	X
2	PDY	C	2	-	-	X	-
2	PDY	D	2	-	-	-	X
2	PDY	E	1	-	-	X	X
2	PDY	E	2	-	-	X	X
2	PDY	F	2	-	-	X	-
2	PDY	G	1	-	-	X	-
2	PDY	G	2	-	-	X	X
2	PDY	H	1	-	-	X	-
2	PDY	H	2	-	-	X	-
2	PDY	I	1	-	-	X	-
2	PDY	I	2	-	-	X	X
2	PDY	J	1	-	-	X	-
2	PDY	K	1	-	-	X	-
2	PDY	K	2	-	-	X	-
2	PDY	L	1	-	-	X	-
2	PDY	L	2	-	-	X	X

2 Entry composition

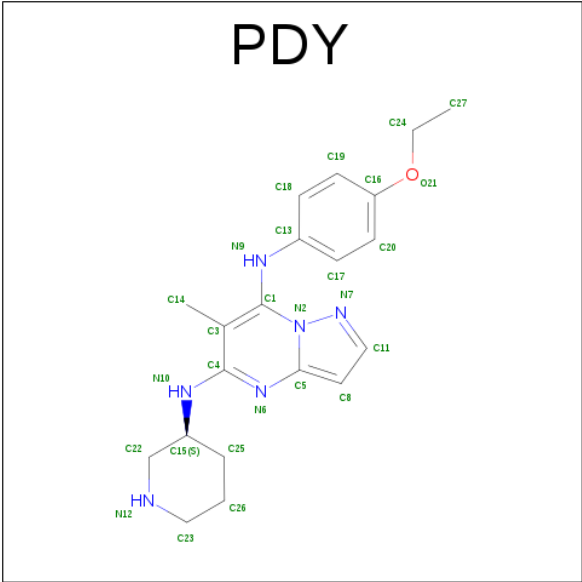
There are 3 unique types of molecules in this entry. The entry contains 27440 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 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: C₂₀H₂₆N₆O).



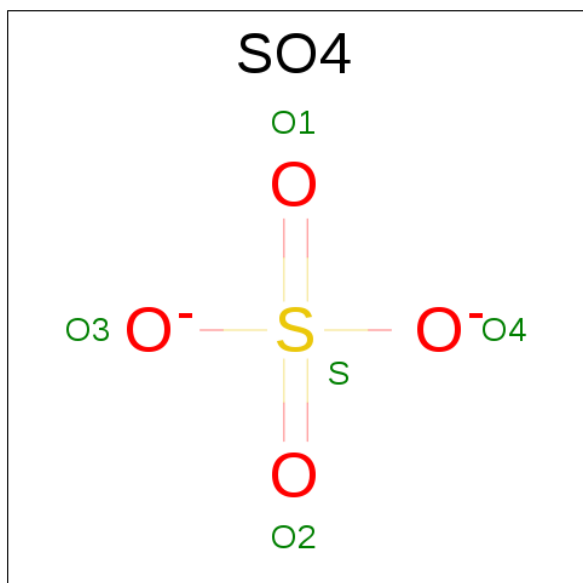
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			27	20	6	1		
2	A	1	Total	C	N	O	0	0
			27	20	6	1		
2	B	1	Total	C	N	O	0	0
			27	20	6	1		
2	B	1	Total	C	N	O	0	0
			27	20	6	1		
2	C	1	Total	C	N	O	0	0
			27	20	6	1		
2	C	1	Total	C	N	O	0	0
			27	20	6	1		
2	D	1	Total	C	N	O	0	0
			27	20	6	1		
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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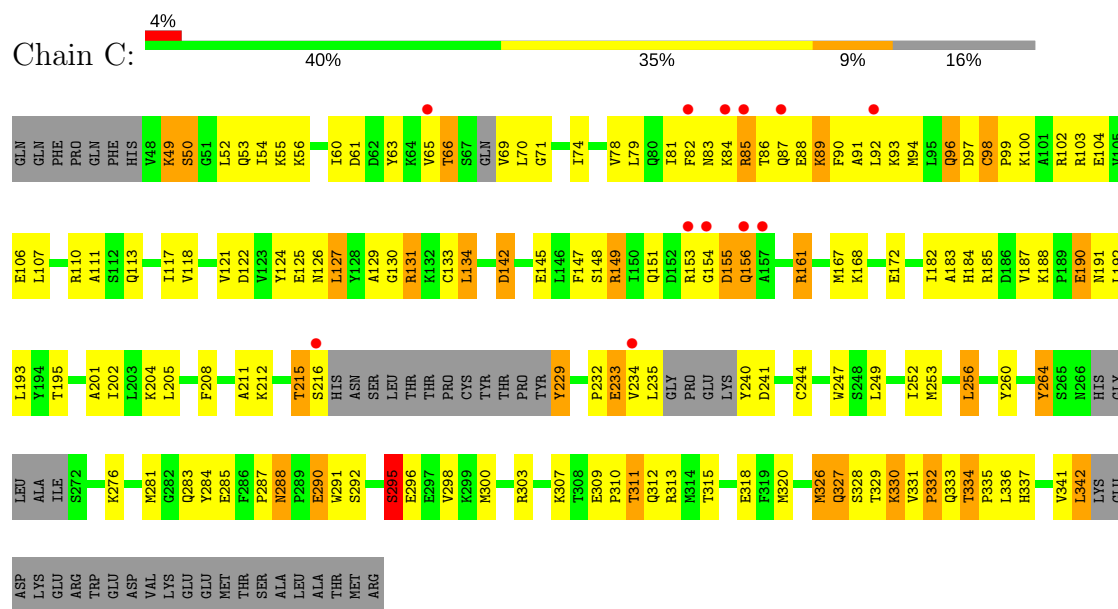
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	H	1	Total	C	N	O	0	0
			27	20	6	1		
2	H	1	Total	C	N	O	0	0
			27	20	6	1		
2	I	1	Total	C	N	O	0	0
			27	20	6	1		
2	I	1	Total	C	N	O	0	0
			27	20	6	1		
2	J	1	Total	C	N	O	0	0
			27	20	6	1		
2	J	1	Total	C	N	O	0	0
			27	20	6	1		
2	K	1	Total	C	N	O	0	0
			27	20	6	1		
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: O₄S).

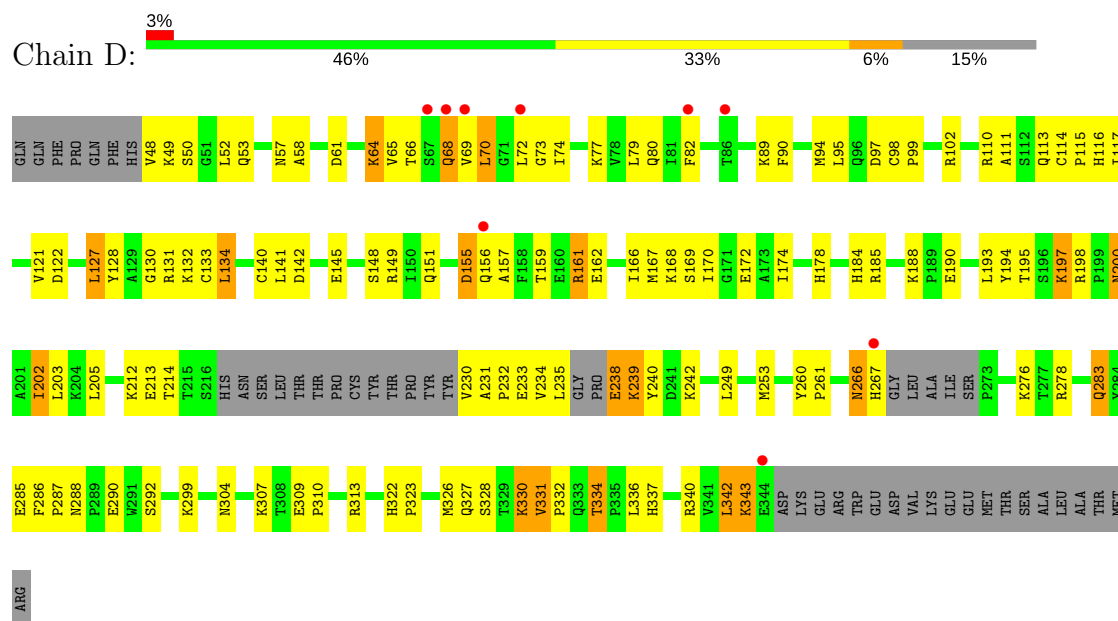


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	O	S	0	0
			5	4	1		

• Molecule 1: MAP kinase-activated protein kinase 2

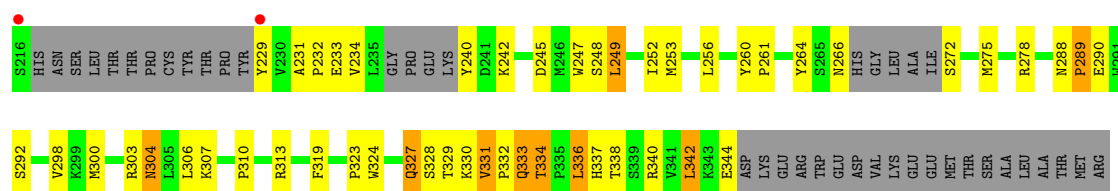


• Molecule 1: MAP kinase-activated protein kinase 2



• Molecule 1: MAP kinase-activated protein kinase 2

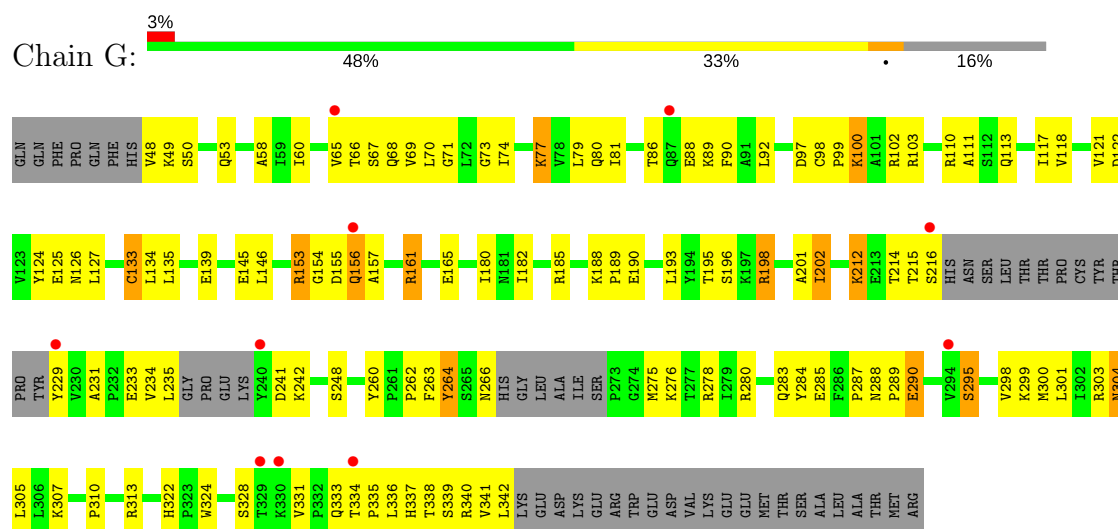




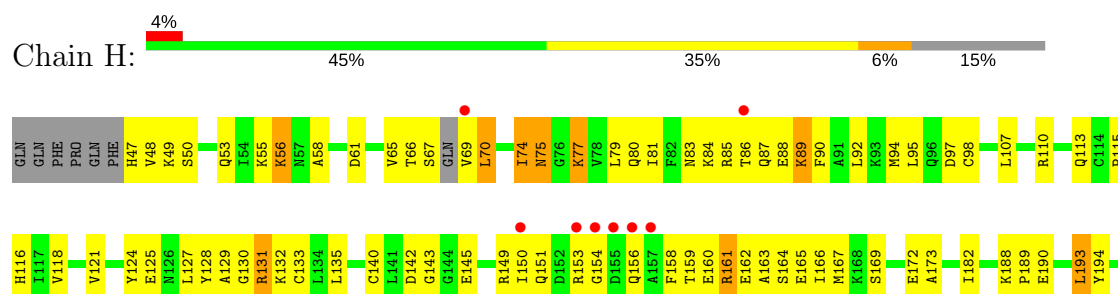
• Molecule 1: MAP kinase-activated protein kinase 2

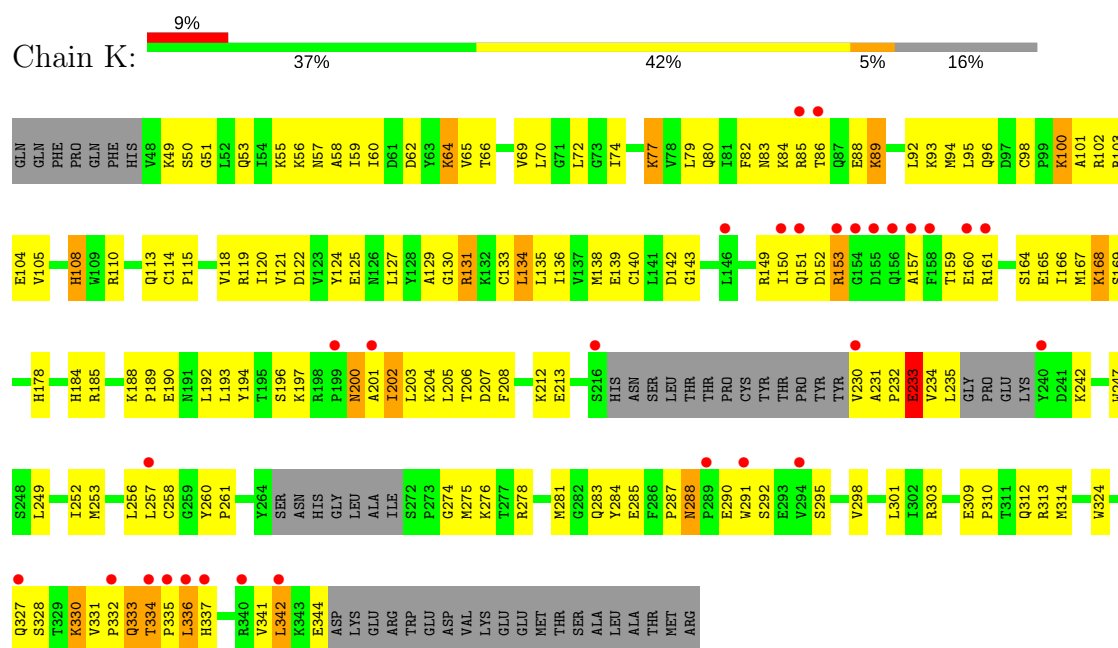


• Molecule 1: MAP kinase-activated protein kinase 2

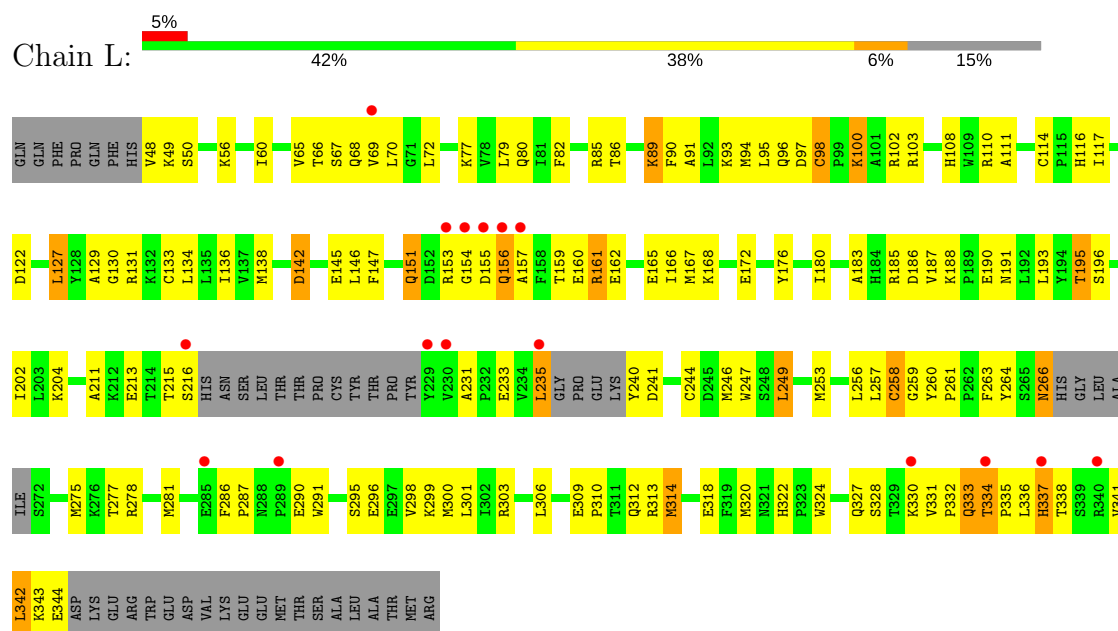


• Molecule 1: MAP kinase-activated protein kinase 2





- Molecule 1: MAP kinase-activated protein kinase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	4.84 (at 2.91Å)	Xtriage
Refinement program	CNX 2005	Depositor
R, R_{free}	0.288 , 0.335 0.213 , 0.267	Depositor DCC
R_{free} test set	6088 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	55.2	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 70.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	27440	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 32.

All (1767) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:H:264:TYR:CE2	2:H:2:PDY:H20	1.79	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H18	2:H:1:PDY:C14	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:D:2:PDY:H14	2:D:2:PDY:H18	1.03	1.00
2:I:2:PDY:H14	2:I:2:PDY:H18	1.02	1.00
2:K:1:PDY:H14	2:K:1:PDY:C18	1.91	1.00
1:K:332:PRO:HB2	1:K:334:THR:HG22	1.43	1.00
1:H:264:TYR:CD2	2:H:2:PDY:H17	1.95	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:K:230:VAL:HG22	1:K:231:ALA:H	1.27	0.98
1:L:111:ALA:HB1	1:L:117:ILE:HD13	1.42	0.98
2:E:1:PDY:C18	2:E:1:PDY:H14	1.94	0.98
1:I:264:TYR:HB2	2:I:2:PDY:H17	1.45	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	Interatomic distance (Å)	Clash overlap (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
2:E:2:PDY:C18	2:E:2:PDY:H14	1.98	0.93
1:H:264:TYR:CE1	2:H:2:PDY:C20	2.51	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:C14	2:F:1:PDY:C18	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
1:A:332:PRO:HB2	1:A:334:THR:HG22	1.51	0.91
2:F:1:PDY:H14	2:F:1:PDY:C18	2.01	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:C18	2:D:1:PDY:H14	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:C18	2:D:1:PDY:C14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:PDY:C18	2:B:2:PDY:C14	2.52	0.87
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:B:161:ARG:NH2	1:B:333:GLN:HE21	1.73	0.86
1:H:264:TYR:CD2	2:H:2:PDY:C17	2.59	0.86
1:H:332:PRO:HB2	1:H:334:THR:HG23	1.56	0.86
2:J:2:PDY:C14	2:J:2:PDY:C18	2.53	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:H18	2:H:1:PDY:C3	2.05	0.84
1:E:49:LYS:HD2	1:E:50:SER:H	1.42	0.84
2:F:2:PDY:C3	2:F:2:PDY:H18	2.05	0.84
2:J:2:PDY:H14	2:J:2:PDY:C18	2.08	0.84
1:G:67:SER:HA	1:G:70:LEU:HD23	1.57	0.84
2:K:1:PDY:C3	2:K:1:PDY:H18	1.99	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:H14	2:G:2:PDY:C18	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
1:A:49:LYS:HG3	1:A:113:GLN:OE1	1.79	0.83
1:G:301:LEU:HD13	1:G:322:HIS:CD2	2.13	0.83
2:J:1:PDY:H18	2:J:1:PDY:C3	2.09	0.83
1:A:185:ARG:NH2	1:A:212:LYS:HE2	1.92	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:C:1:PDY:H18	2:C:1:PDY:C14	2.09	0.81
1:I:332:PRO:HB2	1:I:334:THR:HG22	1.61	0.81
1:L:66:THR:HG23	1:L:69:VAL:N	1.94	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
1:B:161:ARG:HH21	1:B:333:GLN:NE2	1.78	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:K:83:ASN:HB3	1:K:86:THR:HB	1.64	0.80
1:L:337:HIS:O	1:L:341:VAL:HG23	1.80	0.80
2:H:1:PDY:H18	2:H:1:PDY:H14A	1.63	0.79
1:C:83:ASN:HD21	1:C:85:ARG:HD2	1.47	0.79
1:I:69:VAL:HA	1:I:79:LEU:HD22	1.63	0.79
1:K:49:LYS:HD3	1:K:50:SER:N	1.95	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
2:L:1:PDY:C18	2:L:1:PDY:H14	2.12	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:A:156:GLN:H	1:A:156:GLN:NE2	1.80	0.78
1:F:86:THR:HG22	1:F:88:GLU:H	1.46	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:C:2:PDY:C14	2:C:2:PDY:C18	2.62	0.78
1:D:185:ARG:HH21	1:D:212:LYS:HG3	1.48	0.78
1:H:322:HIS:HD2	1:H:324:TRP:H	1.32	0.78
2:K:2:PDY:C14	2:K:2:PDY:H18	2.12	0.78
1:H:264:TYR:CD2	2:H:2:PDY:H20	2.19	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:100:LYS:HG3	1:F:103:ARG:HH21	1.48	0.78
2:J:2:PDY:H18	2:J:2:PDY:H14A	1.64	0.78
1:L:69:VAL:HG13	1:L:79:LEU:CD1	2.13	0.78
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
2:B:1:PDY:H14	2:B:1:PDY:C18	2.14	0.77
1:E:69:VAL:HB	1:E:79:LEU:HD13	1.65	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
1:A:327:GLN:NE2	1:A:330:LYS:HD3	2.01	0.76
2:E:1:PDY:C3	2:E:1:PDY:H18	2.15	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:B:73:GLY:HA3	1:B:94:MET:SD	2.26	0.75
1:C:66:THR:OG1	1:C:69:VAL:HG13	1.86	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:B:77:LYS:HB3	1:B:77:LYS:HZ2	1.52	0.75
1:K:70:LEU:HD23	1:K:94:MET:CE	2.17	0.75
1:G:185:ARG:HH21	1:G:212:LYS:CG	1.89	0.75
1:L:66:THR:HG22	1:L:69:VAL:HG23	1.69	0.75
1:B:48:VAL:HB	1:L:70:LEU:HD21	1.69	0.74
1:E:80:GLN:HE21	1:E:89:LYS:HD3	1.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:49:LYS:HE2	1:A:113:GLN:HG2	1.71	0.73
1:G:100:LYS:HE2	1:G:103:ARG:CZ	2.18	0.73
2:K:1:PDY:H18	2:K:1:PDY:H14A	1.70	0.73
1:L:95:LEU:O	1:L:133:CYS:HB2	1.88	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
2:A:1:PDY:H14	2:A:1:PDY:C18	2.19	0.72
1:F:47:HIS:CD2	1:G:67:SER:HB3	2.24	0.72
1:H:264:TYR:CE2	2:H:2:PDY:C20	2.67	0.72
1:B:285:GLU:HG3	1:B:287:PRO:HD3	1.70	0.72
1:D:49:LYS:CD	1:D:113:GLN:HG2	2.19	0.72
2:B:2:PDY:H14	2:B:2:PDY:C18	2.18	0.72
1:B:72:LEU:HB3	1:B:77:LYS:HG3	1.71	0.72
1:G:66:THR:O	1:G:69:VAL:HG22	1.90	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
1:J:327:GLN:HG2	1:J:330:LYS:HD3	1.70	0.72
1:J:159:THR:CG2	1:J:333:GLN:HA	2.20	0.72
2:L:2:PDY:C18	2:L:2:PDY:C14	2.35	0.72
1:E:70:LEU:HD23	1:E:94:MET:HE2	1.71	0.72
1:H:61:ASP:O	1:H:84:LYS:HD2	1.90	0.72
1:D:167:MET:HG3	1:D:253:MET:HE2	1.72	0.71
1:H:261:PRO:HD3	2:H:2:PDY:H25	1.71	0.71
2:K:2:PDY:H14	2:K:2:PDY:C13	2.18	0.71
2:C:2:PDY:H14	2:C:2:PDY:C18	2.21	0.71
1:H:264:TYR:CD2	2:H:2:PDY:C20	2.72	0.71
1:F:185:ARG:HD3	1:F:241:ASP:HB3	1.71	0.71
1:F:71:GLY:HA2	1:F:74:ILE:HD11	1.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:TYR:O	1:A:275:MET:HG3	1.91	0.71
1:D:66:THR:HB	1:D:69:VAL:HG23	1.71	0.70
1:I:264:TYR:CD1	2:I:2:PDY:H20	2.25	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
1:B:266:ASN:CG	1:B:278:ARG:HH22	1.94	0.70
1:D:69:VAL:HG13	1:D:79:LEU:HD13	1.72	0.70
1:F:196:SER:OG	1:F:198:ARG:HB2	1.92	0.70
1:I:140:CYS:SG	2:I:1:PDY:H17	2.32	0.70
1:L:159:THR:HG21	1:L:161:ARG:HB3	1.73	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
1:A:70:LEU:HD13	1:G:48:VAL:HG23	1.73	0.70
2:H:2:PDY:C14	2:H:2:PDY:C18	2.62	0.70
1:F:327:GLN:HE21	1:F:330:LYS:HD2	1.57	0.70
1:K:96:GLN:HE22	1:K:131:ARG:NE	1.90	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:H14	2:I:1:PDY:C13	2.22	0.69
2:I:1:PDY:H14A	2:I:1:PDY:H18	1.73	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:C:185:ARG:CZ	1:C:212:LYS:HD2	2.21	0.69
1:F:97:ASP:H	1:F:133:CYS:HA	1.58	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:304:ASN:O	1:A:307:LYS:HG2	1.93	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: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:A:145:GLU:HG3	1:A:193:LEU:CD2	2.24	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:E:333:GLN:HA	1:E:333:GLN:HE21	1.58	0.68
1:H:322:HIS:CD2	1:H:324:TRP:H	2.12	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:70:LEU:HD23	1:K:94:MET:HE2	1.74	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
2:G:2:PDY:C13	2:G:2:PDY:H14	2.24	0.68
1:J:145:GLU:HG2	1:J:193:LEU:CD2	2.24	0.67
1:J:332:PRO:HB2	1:J:334:THR:HG22	1.75	0.67
1:K:80:GLN:HE21	2:K:1:PDY:C24	2.05	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
1:L:66:THR:CG2	1:L:69:VAL:H	1.99	0.67
2:G:1:PDY:H18	2:G:1:PDY:C3	2.22	0.67
1:F:272:SER:HB3	1:F:275:MET:HB2	1.77	0.67
1:H:65:VAL:HG11	1:H:70:LEU:HD13	1.75	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:B:231:ALA:HB1	1:B:233:GLU:HG3	1.77	0.67
1:I:284:TYR:OH	1:I:303:ARG:HG2	1.94	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:J:145:GLU:HG2	1:J:193:LEU:HD21	1.77	0.67
1:L:153:ARG:HB2	1:L:156:GLN:HG2	1.76	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:C:188:LYS:HG3	1:C:190:GLU:HG2	1.76	0.66
1:K:89:LYS:H	1:K:89:LYS:CD	2.08	0.66
1:A:328:SER:O	1:A:331:VAL:HG13	1.95	0.66
2:F:2:PDY:H14A	2:F:2:PDY:H18	1.77	0.66
1:I:186:ASP:OD1	1:I:188:LYS:HE3	1.95	0.66
2:J:2:PDY:H18	2:J:2:PDY:C3	2.23	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
1:C:55:LYS:HD3	1:C:124:TYR:CE2	2.30	0.66
1:C:287:PRO:O	1:C:291:TRP:HB2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:161:ARG:HD3	1:G:331:VAL:O	1.95	0.66
1:J:198:ARG:HH11	1:J:200:ASN:H	1.42	0.66
1:J:72:LEU:HB2	1:J:79:LEU:CD1	2.26	0.66
1:J:337:HIS:O	1:J:341:VAL:HG23	1.96	0.66
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
1:L:66:THR:CG2	1:L:69:VAL:HG23	2.24	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
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:K:105:VAL:HG22	1:K:136:ILE:HD11	1.77	0.65
1:L:161:ARG:HD3	1:L:331:VAL:O	1.95	0.65
1:L:97:ASP:H	1:L:133:CYS:HA	1.60	0.65
1:A:49:LYS:HE2	1:A:113:GLN:CD	2.16	0.65
1:F:230:VAL:HG21	1:F:235:LEU:HD21	1.78	0.65
1:F:73:GLY:HA3	1:F:94:MET:HE1	1.78	0.65
2:G:2:PDY:C18	2:G:2:PDY:C3	2.73	0.65
1:H:56:LYS:HE2	1:H:125:GLU:HB3	1.77	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:A:102:ARG:NH2	1:A:125:GLU:OE1	2.29	0.65
1:B:107:LEU:HD21	1:B:213:GLU:HG3	1.79	0.65
1:E:161:ARG:HA	1:E:331:VAL:CG2	2.27	0.65
1:E:86:THR:HG21	1:E:88:GLU:CD	2.17	0.65
1:I:94:MET:O	1:I:95:LEU:HD23	1.97	0.65
1:K:83:ASN:CB	1:K:86:THR:HB	2.27	0.65
1:L:264:TYR:HB2	2:L:2:PDY:C17	2.26	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:D:327:GLN:HB3	1:D:330:LYS:HD2	1.78	0.64
1:J:168:LYS:O	1:J:172:GLU:HG3	1.97	0.64
1:J:83:ASN:HD21	1:J:85:ARG:HH11	1.43	0.64
1:K:114:CYS:SG	1:K:115:PRO:HD2	2.36	0.64
1:K:62:ASP:HA	1:K:85:ARG:NH2	2.10	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:153:ARG:O	1:A:154:GLY:O	2.15	0.64
2:C:2:PDY:H18	2:C:2:PDY:C3	2.26	0.64
1:B:188:LYS:HD2	1:B:190:GLU:HB2	1.80	0.64
2:E:2:PDY:H18	2:E:2:PDY:C14	2.28	0.64
1:I:60:ILE:HG22	1:I:65:VAL:HB	1.79	0.64
1:J:329:THR:C	1:J:331:VAL:H	2.00	0.64
1:I:150:ILE:O	1:I:153:ARG:HG3	1.98	0.64
1:B:69:VAL:O	1:B:73:GLY:N	2.28	0.64
1:L:70:LEU:HA	1:L:94:MET:CE	2.23	0.64
1:B:98:CYS:HB2	1:B:99:PRO:HD2	1.78	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:H:161:ARG:HD3	1:H:331:VAL:O	1.98	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:K:96:GLN:NE2	1:K:131:ARG:HE	1.94	0.64
1:J:83:ASN:ND2	1:J:85:ARG:HH11	1.96	0.64
1:D:195:THR:HG23	1:D:202:ILE:O	1.98	0.64
1:H:188:LYS:HE2	1:H:190:GLU:CG	2.26	0.64
1:H:264:TYR:CB	2:H:2:PDY:H17	2.27	0.64
1:A:309:GLU:CD	1:C:311:THR:HG22	2.17	0.64
1:D:330:LYS:O	1:D:330:LYS:HG2	1.97	0.64
1:H:315:THR:OG1	1:H:318:GLU:HG3	1.98	0.64
1:H:86:THR:HG22	1:H:88:GLU:HB2	1.80	0.64
1:J:310:PRO:HB3	1:K:233:GLU:OE1	1.98	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:H:74:ILE:O	1:H:74:ILE:HD13	1.97	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:D:230:VAL:HG11	1:D:235:LEU:HD21	1.80	0.63
2:D:2:PDY:H14A	2:D:2:PDY:H18	1.69	0.63
1:J:143:GLY:O	1:J:149:ARG:HD3	1.98	0.63
1:J:69:VAL:HG23	1:J:79:LEU:CD1	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:64:LYS:HE3	1:D:64:LYS:HA	1.79	0.63
1:F:65:VAL:CG1	1:F:70:LEU:HD13	2.28	0.63
1:G:337:HIS:O	1:G:341:VAL:HG23	1.99	0.63
1:H:159:THR:OG1	1:H:162:GLU:HG3	1.99	0.63
1:L:114:CYS:HB2	1:L:176:TYR:CD2	2.34	0.63
1:L:266:ASN:HB2	1:L:278:ARG:NH2	2.14	0.63
1:L:72:LEU:HD23	1:L:77:LYS:HD3	1.81	0.63
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
1:A:151:GLN:O	1:A:343:LYS:HE2	2.00	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:66:THR:HG23	1:A:68:GLN:H	1.64	0.62
2:C:2:PDY:H14	2:C:2:PDY:C13	2.29	0.62
1:F:156:GLN:HA	1:F:156:GLN:HE21	1.64	0.62
1:L:246:MET:HA	1:L:246:MET:HE3	1.81	0.62
1:A:307:LYS:HB2	1:A:313:ARG:HG3	1.81	0.62
1:F:100:LYS:HZ2	1:F:103:ARG:HH22	1.47	0.62
1:G:153:ARG:HG3	1:G:157:ALA:HB3	1.81	0.62
1:B:109:TRP:O	1:B:112:SER:HB2	1.99	0.62
1:I:264:TYR:CD1	2:I:2:PDY:C20	2.83	0.62
1:B:74:ILE:HG23	1:B:94:MET:HE2	1.82	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:J:198:ARG:NH1	1:J:198:ARG:HG3	2.14	0.62
1:D:161:ARG:HD3	1:D:331:VAL:O	1.99	0.62
1:E:161:ARG:HA	1:E:331:VAL:HG21	1.82	0.62
1:L:258:CYS:O	1:L:341:VAL:HG21	1.99	0.62
1:C:85:ARG:HG2	1:C:85:ARG:O	2.00	0.61
1:H:70:LEU:HD12	1:H:94:MET:SD	2.39	0.61
1:I:100:LYS:HD2	1:I:103:ARG:NH2	2.14	0.61
1:C:290:GLU:HA	1:C:337:HIS:CD2	2.35	0.61
1:E:214:THR:HG21	1:E:242:LYS:HG3	1.82	0.61
1:E:49:LYS:HD2	1:E:50:SER:N	2.15	0.61
1:H:304:ASN:OD1	1:H:314:MET:HB2	1.97	0.61
1:L:69:VAL:CG1	1:L:79:LEU:HD13	2.27	0.61
1:J:233:GLU:HG2	1:L:310:PRO:HG3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:92:LEU:HD12	1:K:93:LYS:N	2.15	0.61
1:J:60:ILE:HD12	1:J:61:ASP:N	2.16	0.61
1:L:77:LYS:HE3	1:L:79:LEU:HD23	1.81	0.61
1:I:266:ASN:HD21	1:I:272:SER:CB	2.14	0.61
1:I:49:LYS:CG	1:I:50:SER:H	2.11	0.61
1:E:338:THR:HG22	1:E:342:LEU:HD23	1.83	0.61
1:E:66:THR:HG23	1:E:69:VAL:H	1.66	0.61
1:H:229:TYR:HD1	1:H:230:VAL:H	1.49	0.61
1:I:196:SER:O	1:I:201:ALA:HB2	2.01	0.61
1:L:85:ARG:HD2	1:L:85:ARG:O	2.01	0.61
1:D:231:ALA:HB1	1:D:233:GLU:OE2	2.00	0.61
1:H:69:VAL:CG2	1:H:79:LEU:HD13	2.29	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
1:C:65:VAL:CG1	1:C:70:LEU:HD11	2.31	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:F:156:GLN:HE21	1:F:156:GLN:CA	2.13	0.61
1:J:288:ASN:HD22	1:J:288:ASN:H	1.47	0.61
1:D:69:VAL:CG1	1:D:79:LEU:HD13	2.31	0.60
1:G:278:ARG:HG2	1:G:283:GLN:HG3	1.82	0.60
1:G:289:PRO:HG2	1:G:290:GLU:OE2	2.01	0.60
1:J:310:PRO:HA	1:J:313:ARG:HG3	1.80	0.60
1:K:143:GLY:HA3	1:K:194:TYR:HB2	1.82	0.60
1:J:276:LYS:HG3	1:K:235:LEU:CD1	2.31	0.60
1:K:66:THR:O	1:K:69:VAL:HG22	2.01	0.60
1:L:235:LEU:N	1:L:235:LEU:HD12	2.16	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:264:TYR:HB2	2:H:2:PDY:H17	1.83	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:A:327:GLN:HG2	1:A:330:LYS:HG2	1.82	0.60
1:B:48:VAL:HG11	1:L:60:ILE:HG23	1.84	0.60
1:A:127:LEU:HD23	1:G:113:GLN:OE1	2.02	0.60
1:I:264:TYR:HB2	2:I:2:PDY:C17	2.25	0.60
1:J:278:ARG:HG2	1:J:283:GLN:HB2	1.83	0.60
1:K:80:GLN:HE21	2:K:1:PDY:H24A	1.63	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:K:1:PDY:C13	2:K:1:PDY:H14	2.31	0.60
1:L:187:VAL:HG12	1:L:187:VAL:O	2.02	0.60
1:B:160:GLU:HB3	1:B:334:THR:HG23	1.83	0.60
1:B:266:ASN:O	1:B:266:ASN:OD1	2.19	0.60
1:C:327:GLN:HE21	1:C:330:LYS:CE	2.14	0.60
1:H:140:CYS:SG	2:H:1:PDY:H17	2.42	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
1:A:233:GLU:OE2	1:B:313:ARG:NH1	2.34	0.59
1:C:60:ILE:HD12	1:C:60:ILE:C	2.23	0.59
1:C:81:ILE:HD13	1:C:92:LEU:HB2	1.84	0.59
1:E:153:ARG:O	1:E:154:GLY:O	2.19	0.59
1:E:64:LYS:HD2	1:E:84:LYS:HE2	1.84	0.59
1:K:298:VAL:HG22	1:K:324:TRP:CD1	2.37	0.59
1:K:92:LEU:HD12	1:K:93:LYS:H	1.66	0.59
2:L:1:PDY:C13	2:L:1:PDY:H14	2.31	0.59
1:D:266:ASN:N	1:D:266:ASN:ND2	2.40	0.59
1:F:188:LYS:HD3	1:F:190:GLU:OE1	2.01	0.59
1:H:143:GLY:HA2	1:H:197:LYS:HD2	1.84	0.59
1:I:280:ARG:HH22	1:J:131:ARG:HH12	1.49	0.59
1:B:49:LYS:HD3	1:B:113:GLN:HG2	1.84	0.59
1:E:161:ARG:HD2	1:E:328:SER:O	2.01	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:J:66:THR:HG23	1:J:68:GLN:HB2	1.83	0.59
1:L:257:LEU:CD1	1:L:298:VAL:HG11	2.31	0.59
1:A:280:ARG:HH11	1:C:235:LEU:HD13	1.67	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: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:K:284:TYR:OH	1:K:303:ARG:HA	2.03	0.59
1:L:151:GLN:HB3	1:L:342:LEU:CD2	2.30	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:E:86:THR:HB	1:E:88:GLU:HG2	1.85	0.59
1:F:234:VAL:HG12	1:F:235:LEU:HD23	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:LEU:O	1:F:56:LYS:HD2	2.02	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:I:55:LYS:HD3	1:I:124:TYR:CZ	2.38	0.59
1:K:200:ASN:N	1:K:200:ASN:OD1	2.34	0.59
1:K:281:MET:HB2	1:K:283:GLN:HG3	1.85	0.59
1:L:168:LYS:O	1:L:172:GLU:HG3	2.02	0.59
1:D:72:LEU:HD22	1:D:77:LYS:HE3	1.85	0.59
1:H:200:ASN:N	1:H:200:ASN:HD22	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
2:C:1:PDY:H14	2:C:1:PDY:C13	2.32	0.59
2:E:2:PDY:C18	2:E:2:PDY:C3	2.75	0.59
1:F:295:SER:O	1:F:299:LYS:HD3	2.03	0.59
1:F:87:GLN:OE1	1:F:87:GLN:HA	2.03	0.59
1:G:100:LYS:HA	1:G:100:LYS:CE	2.20	0.59
1:H:337:HIS:HA	1:H:340:ARG:NH1	2.17	0.59
1:L:159:THR:HG22	1:L:161:ARG:N	2.16	0.59
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:E:49:LYS:CD	1:E:50:SER:H	2.12	0.58
1:F:151:GLN:HG3	1:F:152:ASP:N	2.18	0.58
1:I:264:TYR:HB2	2:I:2:PDY:HN9	1.68	0.58
1:A:188:LYS:HD2	1:A:191:ASN:ND2	2.18	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:I:58:ALA:HA	1:I:126:ASN:OD1	2.03	0.58
1:B:49:LYS:CD	1:B:113:GLN:HG2	2.33	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: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:A:278:ARG:HA	1:A:283:GLN:HG2	1.85	0.58
2:B:1:PDY:C3	2:B:1:PDY:H18	2.33	0.58
1:B:70:LEU:HD23	1:B:128:TYR:HE1	1.68	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:K:66:THR:H	1:K:69:VAL:CG2	2.16	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:93:LYS:HG2	1:L:136:ILE:HB	1.84	0.58
1:H:202:ILE:HD11	1:H:204:LYS:NZ	2.18	0.58
1:I:64:LYS:HD2	1:I:84:LYS:HE3	1.86	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:A:285:GLU:C	1:A:287:PRO:HD3	2.24	0.58
1:B:328:SER:O	1:B:331:VAL:HG13	2.03	0.58
1:E:57:ASN:HD22	1:E:57:ASN:H	1.51	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: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: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
1:H:264:TYR:CD1	2:H:2:PDY:H20	2.27	0.58
1:K:190:GLU:H	1:K:190:GLU:CD	2.06	0.58
1:B:184:HIS:HD2	1:B:186:ASP:N	1.98	0.58
1:G:264:TYR:O	1:G:275:MET:HG3	2.04	0.58
1:I:140:CYS:SG	2:I:1:PDY:C17	2.92	0.58
1:G:307:LYS:HB2	1:G:313:ARG:HG2	1.86	0.58
1:A:85:ARG:HH11	1:A:85:ARG:HG2	1.68	0.57
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:195:THR:HG23	1:A:202:ILE:O	2.04	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:E:156:GLN:HE21	1:E:156:GLN:N	2.01	0.57
1:E:229:TYR:OH	1:F:188:LYS:HE2	2.03	0.57
1:F:70:LEU:HD12	1:F:94:MET:CE	2.34	0.57
1:E:60:ILE:C	1:E:60:ILE:HD12	2.25	0.57
1:I:215:THR:OG1	1:I:216:SER:N	2.37	0.57
1:J:74:ILE:N	1:J:94:MET:HE3	2.19	0.57
1:L:48:VAL:O	1:L:48:VAL:HG12	2.02	0.57
1:A:295:SER:OG	1:A:298:VAL:HG23	2.04	0.57
1:B:108:HIS:CG	1:B:120:ILE:HD11	2.40	0.57
2:C:2:PDY:H18	2:C:2:PDY:C14	2.33	0.57
1:J:300:MET:SD	1:J:303:ARG:HD2	2.44	0.57
1:C:54:ILE:HG21	1:C:125:GLU:HB2	1.85	0.57
1:C:65:VAL:HG12	1:C:70:LEU:HD11	1.87	0.57
1:J:66:THR:CG2	1:J:68:GLN:HB2	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:73:GLY:C	1:J:94:MET:HE3	2.25	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:I:275:MET:O	1:I:279:ILE:HG13	2.05	0.57
1:J:147:PHE:HB3	1:J:342:LEU:HD21	1.86	0.57
1:J:156:GLN:HG3	1:J:340:ARG:HH11	1.69	0.57
1:B:108:HIS:HE1	1:B:138:MET:CE	2.16	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:I:200:ASN:N	1:I:200:ASN:HD22	2.03	0.57
1:K:288:ASN:H	1:K:288:ASN:HD22	1.52	0.57
1:D:49:LYS:HD2	1:D:113:GLN:CG	2.28	0.57
1:D:58:ALA:O	1:D:61:ASP:HB2	2.05	0.57
1:F:260:TYR:OH	1:F:287:PRO:HG2	2.05	0.57
1:J:140:CYS:SG	2:J:1:PDY:H17	2.45	0.57
1:J:187:VAL:O	1:J:187:VAL:HG12	2.04	0.57
1:K:102:ARG:HG3	1:K:134:LEU:HD21	1.87	0.57
1:D:278:ARG:HA	1:D:283:GLN:HG3	1.86	0.57
1:G:189:PRO:HG2	1:G:190:GLU:OE1	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:L:49:LYS:CD	1:L:50:SER:H	2.18	0.56
1:C:264:TYR:OH	2:C:2:PDY:H24	2.04	0.56
1:C:295:SER:CB	1:C:298:VAL:HG23	2.29	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
2:B:1:PDY:H18	2:B:1:PDY:C14	2.35	0.56
1:E:161:ARG:HB3	1:E:333:GLN:NE2	2.20	0.56
1:E:66:THR:HG22	1:E:69:VAL:HG13	1.85	0.56
1:G:310:PRO:HG3	1:I:233:GLU:HG2	1.87	0.56
1:K:129:ALA:C	1:K:131:ARG:H	2.09	0.56
1:A:327:GLN:CD	1:A:330:LYS:HD3	2.25	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
1:L:155:ASP:HA	1:L:157:ALA:N	2.20	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
2:F:2:PDY:H14	2:F:2:PDY:C13	2.35	0.56
1:F:288:ASN:OD1	1:F:292:SER:HB3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:110:ARG:HH22	1:E:213:GLU:CD	2.09	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:K:119:ARG:HB3	1:K:139:GLU:OE1	2.06	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
1:F:69:VAL:HB	1:F:79:LEU:HD13	1.87	0.56
1:H:328:SER:O	1:H:331:VAL:HG22	2.05	0.56
1:G:196:SER:OG	1:G:198:ARG:HG2	2.06	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: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:B:232:PRO:HD3	1:C:247:TRP:CZ2	2.41	0.56
1:E:260:TYR:HE2	1:E:290:GLU:OE1	1.88	0.56
1:F:338:THR:O	1:F:342:LEU:HB2	2.05	0.56
1:I:107:LEU:HD22	1:I:182:ILE:CD1	2.36	0.56
1:I:266:ASN:H	1:I:266:ASN:HD22	1.53	0.56
1:J:66:THR:CG2	1:J:69:VAL:HG12	2.36	0.56
1:J:71:GLY:O	1:J:74:ILE:HG22	2.06	0.56
2:A:2:PDY:C13	2:A:2:PDY:H14	2.36	0.56
1:H:66:THR:O	1:H:70:LEU:HB2	2.06	0.56
1:E:300:MET:SD	1:E:303:ARG:NE	2.70	0.55
1:H:295:SER:OG	1:H:298:VAL:HG23	2.07	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:L:49:LYS:HD2	1:L:50:SER:N	2.20	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:F:261:PRO:HD3	2:F:2:PDY:H25	1.87	0.55
1:H:300:MET:SD	1:H:303:ARG:NE	2.77	0.55
1:J:118:VAL:HG21	2:J:1:PDY:H11	1.88	0.55
1:A:175:GLN:NE2	1:A:320:MET:HG3	2.20	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:E:97:ASP:HB2	1:E:134:LEU:HD13	1.87	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:H:257:LEU:HD11	1:H:298:VAL:HG11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:322:HIS:ND1	1:I:323:PRO:HD2	2.20	0.55
1:L:97:ASP:O	1:L:98:CYS:HB3	2.05	0.55
1:C:82:PHE:HA	1:C:88:GLU:O	2.06	0.55
1:E:66:THR:O	1:E:69:VAL:HG22	2.05	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:300:MET:SD	1:L:303:ARG:NH2	2.75	0.55
1:A:280:ARG:HH11	1:C:235:LEU:CD1	2.20	0.55
1:G:97:ASP:OD2	1:G:102:ARG:NH2	2.37	0.55
1:L:70:LEU:HG	1:L:94:MET:HE1	1.88	0.55
1:B:296:GLU:OE2	1:B:303:ARG:NH2	2.39	0.55
1:C:252:ILE:O	1:C:256:LEU:HB2	2.07	0.55
1:C:66:THR:HG1	1:C:69:VAL:N	2.05	0.55
1:G:195:THR:HG23	1:G:202:ILE:O	2.06	0.55
1:J:254:TYR:CG	1:J:262:PRO:HG3	2.42	0.55
2:D:1:PDY:H14	2:D:1:PDY:C13	2.35	0.55
2:E:2:PDY:C18	2:E:2:PDY:H14A	2.36	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:D:184:HIS:CD2	1:D:205:LEU:HD21	2.42	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: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: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
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:E:111:ALA:HB1	1:E:117:ILE:CD1	2.38	0.54
1:F:202:ILE:CD1	1:F:204:LYS:HE2	2.37	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: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:B:58:ALA:O	1:B:61:ASP:HB2	2.08	0.54
1:H:264:TYR:CD1	2:H:2:PDY:C17	2.89	0.54
1:C:130:GLY:O	1:J:110:ARG:HD3	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:202:ILE:HD11	1:L:204:LYS:CE	2.36	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:E:178:HIS:HE1	1:E:245:ASP:OD2	1.91	0.54
1:G:190:GLU:H	1:G:190:GLU:CD	2.10	0.54
1:H:233:GLU:HG2	1:I:310:PRO:HG3	1.90	0.54
1:I:327:GLN:HE21	1:I:330:LYS:HZ1	1.54	0.54
1:J:327:GLN:HB3	1:J:330:LYS:HG2	1.90	0.54
1:K:150:ILE:O	1:K:153:ARG:HG3	2.07	0.54
1:A:190:GLU:CD	1:A:190:GLU:H	2.11	0.54
1:A:332:PRO:CB	1:A:334:THR:HG22	2.30	0.54
1:C:300:MET:SD	1:C:303:ARG:NE	2.80	0.54
1:E:145:GLU:HG2	1:E:193:LEU:HD21	1.90	0.54
1:I:72:LEU:CB	1:I:79:LEU:HD21	2.37	0.54
1:K:260:TYR:HB2	2:K:2:PDY:H19	1.90	0.54
1:A:159:THR:OG1	1:A:333:GLN:NE2	2.41	0.54
1:A:66:THR:O	1:A:69:VAL:HG22	2.07	0.54
1:C:327:GLN:HB3	1:C:330:LYS:HG3	1.90	0.54
1:C:161:ARG:HD3	1:C:331:VAL:HG13	1.90	0.54
1:F:214:THR:HG21	1:F:242:LYS:HE3	1.88	0.54
1:H:198:ARG:HG2	1:H:199:PRO:HD2	1.89	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
1:J:298:VAL:HG22	1:J:324:TRP:CD1	2.42	0.54
1:K:260:TYR:OH	1:K:287:PRO:HG2	2.07	0.54
1:L:235:LEU:H	1:L:235:LEU:HD12	1.73	0.54
1:I:202:ILE:HD11	1:I:204:LYS:HG2	1.89	0.54
1:K:261:PRO:HD3	2:K:2:PDY:H25	1.90	0.54
1:A:188:LYS:HE2	1:A:190:GLU:HB2	1.90	0.54
1:B:192:LEU:C	1:B:193:LEU:HD23	2.28	0.54
1:H:81:ILE:HD13	1:H:92:LEU:HB2	1.89	0.54
1:J:66:THR:HG22	1:J:69:VAL:HG12	1.89	0.54
1:K:49:LYS:HB3	1:K:113:GLN:NE2	2.23	0.54
1:L:147:PHE:CE2	1:L:256:LEU:HD23	2.43	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:B:146:LEU:HD11	1:B:166:ILE:HD13	1.89	0.53
1:D:188:LYS:HG3	1:D:190:GLU:HG2	1.91	0.53
1:J:159:THR:HG21	1:J:333:GLN:HG2	1.90	0.53
1:J:63:TYR:O	1:J:84:LYS:HE3	2.08	0.53
1:L:146:LEU:HD11	1:L:166:ILE:HD13	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ARG:HD2	1:A:328:SER:O	2.09	0.53
2:C:1:PDY:C3	2:C:1:PDY:H18	2.39	0.53
1:J:278:ARG:HG3	1:J:283:GLN:HE21	1.73	0.53
1:E:69:VAL:CB	1:E:79:LEU:HD13	2.38	0.53
1:H:150:ILE:O	1:H:153:ARG:HG2	2.08	0.53
1:K:309:GLU:OE2	1:K:310:PRO:HD2	2.07	0.53
1:K:80:GLN:NE2	2:K:1:PDY:H24	2.22	0.53
1:D:98:CYS:HB2	1:D:99:PRO:CD	2.39	0.53
1:G:285:GLU:C	1:G:287:PRO:HD3	2.29	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: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:A:288:ASN:HB3	1:A:289:PRO:HA	1.90	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:214:THR:HG21	1:A:242:LYS:HE3	1.90	0.53
1:B:155:ASP:N	1:B:156:GLN:OE1	2.41	0.53
1:C:60:ILE:HD12	1:C:61:ASP:N	2.24	0.53
1:K:234:VAL:O	1:K:234:VAL:HG12	2.09	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:E:332:PRO:HB2	1:E:334:THR:HG22	1.89	0.53
1:H:110:ARG:HH22	1:H:213:GLU:CD	2.12	0.53
1:J:276:LYS:CG	1:K:235:LEU:HD12	2.38	0.53
1:K:89:LYS:N	1:K:89:LYS:CD	2.72	0.53
1:L:260:TYR:OH	1:L:287:PRO:HG2	2.09	0.53
1:C:185:ARG:HD3	1:C:241:ASP:CG	2.29	0.53
1:E:87:GLN:NE2	1:E:87:GLN:N	2.57	0.53
1:H:212:LYS:HD3	1:H:213:GLU:N	2.23	0.53
1:J:185:ARG:CZ	1:J:212:LYS:HG3	2.38	0.53
1:J:198:ARG:CG	1:J:198:ARG:HH11	2.22	0.53
1:K:95:LEU:O	1:K:133:CYS:CB	2.56	0.53
1:C:148:SER:HA	1:C:151:GLN:HB3	1.91	0.52
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:A:107:LEU:HD21	1:A:213:GLU:HG3	1.90	0.52
1:D:328:SER:O	1:D:331:VAL:HG13	2.08	0.52
1:D:332:PRO:HB2	1:D:334:THR:HG22	1.91	0.52
1:H:115:PRO:O	1:H:204:LYS:NZ	2.40	0.52
1:H:154:GLY:HA2	1:H:156:GLN:H	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:129:ALA:HB3	1:C:131:ARG:NE	2.25	0.52
1:E:80:GLN:OE1	2:E:1:PDY:C24	2.58	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
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:C:260:TYR:OH	1:C:290:GLU:HG3	2.09	0.52
2:F:1:PDY:H18	2:F:1:PDY:H14A	1.91	0.52
1:I:160:GLU:HA	1:I:336:LEU:HD21	1.91	0.52
1:J:198:ARG:HH11	1:J:200:ASN:N	2.07	0.52
1:K:129:ALA:O	1:K:131:ARG:N	2.42	0.52
1:D:110:ARG:HH22	1:D:213:GLU:CD	2.12	0.52
1:E:161:ARG:HD3	1:E:331:VAL:O	2.09	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:K:140:CYS:SG	2:K:1:PDY:H17	2.50	0.52
1:K:104:GLU:HG3	1:K:208:PHE:O	2.10	0.52
1:E:160:GLU:HA	1:E:336:LEU:HD21	1.91	0.52
1:L:110:ARG:HH22	1:L:213:GLU:CD	2.12	0.52
1:B:290:GLU:HB2	1:B:291:TRP:CD1	2.44	0.52
1:H:154:GLY:CA	1:H:156:GLN:H	2.23	0.52
1:C:149:ARG:NH2	1:C:201:ALA:HB3	2.25	0.52
1:D:155:ASP:CG	1:D:156:GLN:H	2.12	0.52
1:D:286:PHE:CD1	1:D:299:LYS:HG2	2.44	0.52
1:D:73:GLY:HA3	1:D:94:MET:SD	2.50	0.52
1:I:108:HIS:HE1	1:I:138:MET:CE	2.23	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
2:G:1:PDY:H14A	2:G:1:PDY:H18	1.85	0.52
1:K:332:PRO:CB	1:K:334:THR:HG22	2.27	0.52
1:D:130:GLY:O	1:I:110:ARG:NH1	2.41	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:G:69:VAL:CB	1:G:79:LEU:HD13	2.34	0.51
1:K:60:ILE:HD12	1:K:60:ILE:C	2.30	0.51
1:L:159:THR:HG22	1:L:160:GLU:N	2.25	0.51
1:B:47:HIS:HD2	1:L:70:LEU:HD22	1.73	0.51
1:C:183:ALA:O	1:C:211:ALA:HA	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1:PDY:C3	2:I:1:PDY:H18	2.38	0.51
1:K:108:HIS:CG	1:K:120:ILE:HD11	2.45	0.51
1:B:189:PRO:HD2	1:B:190:GLU:OE1	2.10	0.51
1:B:339:SER:O	1:B:343:LYS:HG3	2.10	0.51
1:D:195:THR:HG21	1:D:202:ILE:HG23	1.92	0.51
1:E:98:CYS:HB2	1:E:99:PRO:HD2	1.91	0.51
1:J:332:PRO:HB2	1:J:334:THR:CG2	2.41	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: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:J:331:VAL:HG23	1:J:332:PRO:HD2	1.91	0.51
1:G:156:GLN:HE22	1:G:340:ARG:NH1	2.09	0.51
1:G:73:GLY:CA	1:G:79:LEU:HD11	2.40	0.51
1:J:293:GLU:HA	1:J:293:GLU:OE2	2.10	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:C:284:TYR:O	1:C:285:GLU:HG2	2.11	0.51
1:D:48:VAL:O	1:D:48:VAL:HG13	2.09	0.51
1:F:214:THR:HG21	1:F:242:LYS:HG3	1.93	0.51
1:F:161:ARG:HD3	1:F:331:VAL:O	2.09	0.51
1:I:168:LYS:O	1:I:172:GLU:HG3	2.10	0.51
1:J:185:ARG:NH2	1:J:212:LYS:HE2	2.26	0.51
1:J:110:ARG:HH22	1:J:213:GLU:CD	2.14	0.51
1:J:73:GLY:O	1:J:94:MET:HB2	2.10	0.51
1:K:188:LYS:NZ	1:K:190:GLU:HG3	2.25	0.51
1:A:168:LYS:HB2	1:A:325:ILE:HG23	1.93	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:C:102:ARG:NH2	1:C:134:LEU:HD11	2.26	0.51
1:D:110:ARG:O	1:D:113:GLN:HG3	2.11	0.51
1:E:115:PRO:O	1:E:202:ILE:HD11	2.11	0.51
1:E:260:TYR:HB2	2:E:2:PDY:H19	1.92	0.51
1:G:284:TYR:OH	1:G:303:ARG:HG2	2.11	0.51
1:H:341:VAL:C	1:H:343:LYS:H	2.14	0.51
1:I:100:LYS:CD	1:I:103:ARG:HH21	2.22	0.51
1:J:110:ARG:O	1:J:113:GLN:HG2	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:C:234:VAL:HG22	1:C:234:VAL:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:307:LYS:HG2	1:F:312:GLN:HB3	1.92	0.51
1:G:231:ALA:HB1	1:G:233:GLU:OE2	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:F:60:ILE:C	1:F:60:ILE:HD12	2.31	0.50
1:H:200:ASN:N	1:H:200:ASN:ND2	2.59	0.50
1:A:111:ALA:HB1	1:A:117:ILE:HD13	1.93	0.50
1:A:235:LEU:HD11	1:B:276:LYS:HE2	1.92	0.50
1:A:50:SER:HB2	1:F:56:LYS:O	2.11	0.50
1:G:86:THR:C	1:G:88:GLU:H	2.14	0.50
1:J:202:ILE:HD11	1:J:204:LYS:HE3	1.92	0.50
1:J:81:ILE:HD13	1:J:92:LEU:HB2	1.92	0.50
1:L:159:THR:CG2	1:L:161:ARG:HB3	2.40	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:B:69:VAL:CG2	1:B:70:LEU:N	2.73	0.50
1:D:239:LYS:O	1:D:240:TYR:HB2	2.11	0.50
1:E:260:TYR:HB2	1:E:261:PRO:HD2	1.92	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
1:L:264:TYR:CD2	2:L:2:PDY:H20	2.47	0.50
1:B:111:ALA:HB1	1:B:117:ILE:HD12	1.93	0.50
1:B:161:ARG:HD3	1:B:331:VAL:O	2.11	0.50
1:C:107:LEU:HD22	1:C:182:ILE:HG12	1.93	0.50
1:H:264:TYR:CG	2:H:2:PDY:H20	2.42	0.50
1:L:190:GLU:OE1	1:L:190:GLU:N	2.38	0.50
1:D:97:ASP:H	1:D:133:CYS:HA	1.76	0.50
1:J:114:CYS:SG	1:J:116:HIS:HB2	2.52	0.50
1:J:147:PHE:HE2	1:J:256:LEU:HD23	1.76	0.50
1:K:110:ARG:HH22	1:K:213:GLU:CD	2.15	0.50
1:K:164:SER:HA	1:K:324:TRP:CH2	2.46	0.50
1:L:66:THR:HG22	1:L:69:VAL:CG2	2.38	0.50
1:B:52:LEU:HD22	1:B:105:VAL:HG12	1.93	0.50
1:C:202:ILE:CD1	1:C:204:LYS:HE2	2.18	0.50
1:J:192:LEU:O	1:J:193:LEU:HD23	2.11	0.50
1:J:287:PRO:HD2	1:J:291:TRP:CD1	2.46	0.50
1:K:288:ASN:N	1:K:288:ASN:ND2	2.59	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:L:264:TYR:CB	2:L:2:PDY:C17	2.88	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:ILE:O	1:B:153:ARG:HG2	2.12	0.50
1:C:330:LYS:HB2	1:C:330:LYS:HZ3	1.77	0.50
1:D:116:HIS:CE1	1:D:169:SER:HB2	2.47	0.50
1:G:161:ARG:NH1	1:G:333:GLN:HG3	2.26	0.50
1:H:341:VAL:O	1:H:343:LYS:N	2.37	0.50
1:J:198:ARG:HG3	1:J:199:PRO:N	2.27	0.50
1:L:161:ARG:NH1	1:L:333:GLN:HG2	2.27	0.50
1:B:125:GLU:C	1:B:126:ASN:HD22	2.15	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:G:80:GLN:CD	1:G:89:LYS:HD2	2.31	0.50
1:B:145:GLU:O	1:B:148:SER:HB3	2.12	0.49
1:A:313:ARG:NH1	1:C:233:GLU:OE1	2.44	0.49
1:K:62:ASP:CA	1:K:85:ARG:HH21	2.22	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:D:151:GLN:HB3	1:D:342:LEU:HB3	1.94	0.49
1:G:180:ILE:HD11	1:G:182:ILE:HD12	1.94	0.49
1:C:127:LEU:O	1:J:48:VAL:HA	2.11	0.49
1:L:260:TYR:OH	1:L:290:GLU:HG3	2.12	0.49
1:E:214:THR:O	1:E:215:THR:HB	2.11	0.49
1:F:332:PRO:HB2	1:F:334:THR:HG22	1.93	0.49
1:G:49:LYS:HD2	1:G:113:GLN:CD	2.33	0.49
2:H:1:PDY:C18	2:H:1:PDY:C3	2.73	0.49
1:G:235:LEU:HD12	1:H:280:ARG:HG3	1.93	0.49
1:K:188:LYS:HZ1	1:K:190:GLU:CG	2.25	0.49
2:L:1:PDY:C14	2:L:1:PDY:H18	2.40	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:B:232:PRO:HD3	1:C:247:TRP:CH2	2.47	0.49
1:B:57:ASN:H	1:B:57:ASN:ND2	2.08	0.49
1:C:168:LYS:O	1:C:172:GLU:HG3	2.12	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:E:73:GLY:HA3	1:E:94:MET:CE	2.42	0.49
1:C:184:HIS:CD2	1:C:205:LEU:HD21	2.47	0.49
1:H:337:HIS:O	1:H:340:ARG:HG3	2.12	0.49
2:J:1:PDY:C18	2:J:1:PDY:C3	2.81	0.49
1:K:178:HIS:ND1	1:K:242:LYS:HG2	2.28	0.49
1:B:234:VAL:HG12	1:B:234:VAL:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:66:THR:OG1	1:I:69:VAL:HG23	2.12	0.49
2:L:2:PDY:H18	2:L:2:PDY:H14	0.64	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: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:235:LEU:CD1	1:B:276:LYS:HE2	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: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:I:107:LEU:HD22	1:I:182:ILE:HD13	1.93	0.49
1:J:198:ARG:HG2	1:J:201:ALA:N	2.27	0.49
1:K:247:TRP:HB2	1:K:313:ARG:NH1	2.28	0.49
1:L:266:ASN:HB2	1:L:278:ARG:HH22	1.77	0.49
1:A:97:ASP:HB3	1:A:132:LYS:O	2.13	0.49
1:A:280:ARG:NH1	1:C:235:LEU:HD13	2.28	0.49
1:B:202:ILE:CD1	1:B:204:LYS:HE2	2.30	0.49
1:F:145:GLU:HG2	1:F:193:LEU:HD22	1.95	0.49
1:F:156:GLN:NE2	1:F:156:GLN:CA	2.76	0.49
1:C:110:ARG:HD2	1:H:130:GLY:O	2.13	0.49
2:J:2:PDY:H14	2:J:2:PDY:C13	2.42	0.49
1:K:160:GLU:HB3	1:K:336:LEU:HD11	1.95	0.49
1:K:66:THR:OG1	1:K:69:VAL:HG13	2.12	0.49
1:C:264:TYR:CE1	2:C:2:PDY:C24	2.96	0.49
1:D:65:VAL:CG1	1:D:70:LEU:HD13	2.42	0.49
1:F:83:ASN:OD1	1:F:84:LYS:N	2.46	0.49
1:G:58:ALA:HB1	1:G:60:ILE:HG13	1.94	0.49
1:K:118:VAL:HG11	1:K:206:THR:HG22	1.94	0.49
1:K:274:GLY:O	1:K:278:ARG:HG3	2.12	0.49
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:C:161:ARG:HB2	1:C:332:PRO:O	2.13	0.48
1:D:77:LYS:HZ2	1:D:79:LEU:HD21	1.75	0.48
1:G:153:ARG:HB3	1:G:339:SER:OG	2.13	0.48
1:H:129:ALA:CB	1:H:131:ARG:HD3	2.34	0.48
1:I:264:TYR:CZ	2:I:2:PDY:H24	2.48	0.48
1:K:188:LYS:HZ1	1:K:190:GLU:HG3	1.77	0.48
1:K:188:LYS:NZ	1:K:190:GLU:CG	2.75	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:116:HIS:O	1:L:204:LYS:HA	2.12	0.48
1:D:162:GLU:O	1:D:166:ILE:HG13	2.13	0.48
1:E:332:PRO:HG2	1:E:334:THR:CG2	2.43	0.48
1:F:148:SER:HA	1:F:151:GLN:HG2	1.96	0.48
1:G:66:THR:HG23	1:G:68:GLN:HG2	1.95	0.48
1:G:188:LYS:HD3	1:I:229:TYR:CE1	2.48	0.48
1:I:69:VAL:HG13	1:I:79:LEU:CB	2.43	0.48
1:K:105:VAL:HG21	1:K:134:LEU:HD23	1.95	0.48
1:L:331:VAL:HG23	1:L:332:PRO:HD2	1.95	0.48
1:L:77:LYS:HE3	1:L:79:LEU:CD2	2.42	0.48
1:A:49:LYS:HG3	1:A:113:GLN:CD	2.33	0.48
1:B:52:LEU:CD2	1:B:105:VAL:HG12	2.43	0.48
1:B:65:VAL:HG12	1:B:70:LEU:CD1	2.43	0.48
1:D:74:ILE:HG13	1:D:128:TYR:CE2	2.48	0.48
1:D:151:GLN:HE21	1:D:343:LYS:HA	1.77	0.48
1:F:70:LEU:O	1:F:74:ILE:HD13	2.14	0.48
1:G:66:THR:HG21	1:G:68:GLN:OE1	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:K:56:LYS:NZ	1:K:125:GLU:OE1	2.46	0.48
1:L:295:SER:OG	1:L:298:VAL:HG23	2.13	0.48
1:L:301:LEU:HD13	1:L:322:HIS:CD2	2.48	0.48
1:A:233:GLU:HG2	1:B:310:PRO:HD3	1.95	0.48
1:B:48:VAL:HB	1:L:70:LEU:CD2	2.42	0.48
1:C:52:LEU:HG	1:C:53:GLN:N	2.28	0.48
1:E:298:VAL:HG22	1:E:324:TRP:NE1	2.28	0.48
1:G:290:GLU:OE2	1:G:337:HIS:HD2	1.96	0.48
1:G:295:SER:O	1:G:299:LYS:HG3	2.13	0.48
1:J:83:ASN:O	1:J:87:GLN:HA	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
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:A:230:VAL:HG13	1:A:230:VAL:O	2.14	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:J:69:VAL:HA	1:J:79:LEU:HD13	1.95	0.48
1:B:114:CYS:HB2	1:B:176:TYR:CD2	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:TYR:HB2	1:D:261:PRO:HD2	1.96	0.48
1:J:340:ARG:O	1:J:343:LYS:HD3	2.14	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:E:323:PRO:HA	1:E:327:GLN:NE2	2.28	0.48
1:F:149:ARG:NH1	1:F:196:SER:O	2.44	0.48
1:F:73:GLY:HA3	1:F:94:MET:HE3	1.94	0.48
1:F:86:THR:HG22	1:F:87:GLN:N	2.29	0.48
1:H:164:SER:HB3	1:H:328:SER:HB3	1.95	0.48
1:H:337:HIS:CG	1:H:340:ARG:NH1	2.82	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:I:83:ASN:OD1	1:I:84:LYS:N	2.47	0.48
1:H:110:ARG:HD3	1:J:127:LEU:HD11	1.96	0.48
1:J:159:THR:HG23	1:J:333:GLN:CA	2.42	0.48
1:J:65:VAL:HG12	1:J:70:LEU:HD22	1.96	0.48
1:K:327:GLN:HG2	1:K:330:LYS:NZ	2.29	0.48
1:B:110:ARG:NH2	1:B:213:GLU:OE2	2.47	0.48
1:B:85:ARG:HD2	1:B:86:THR:CG2	2.38	0.48
1:C:125:GLU:C	1:C:126:ASN:HD22	2.17	0.48
1:F:70:LEU:HA	1:F:94:MET:CE	2.44	0.48
1:I:56:LYS:O	1:K:51:GLY:N	2.44	0.48
1:J:57:ASN:HD22	1:J:57:ASN:H	1.61	0.48
1:K:161:ARG:NH2	1:K:333:GLN:HG3	2.29	0.48
1:L:82:PHE:CE1	1:L:89:LYS:HB2	2.49	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:I:172:GLU:HG2	1:I:320:MET:CE	2.44	0.48
1:J:311:THR:O	1:L:312:GLN:NE2	2.47	0.48
1:H:55:LYS:HD3	1:H:124:TYR:CE2	2.49	0.47
1:I:261:PRO:HG3	2:I:2:PDY:H25	1.95	0.47
1:B:64:LYS:HE3	1:B:84:LYS:HE3	1.96	0.47
1:C:300:MET:SD	1:C:303:ARG:NH2	2.86	0.47
1:E:97:ASP:H	1:E:133:CYS:HA	1.80	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:H:67:SER:C	1:H:69:VAL:N	2.67	0.47
1:I:149:ARG:HG3	1:I:194:TYR:CD2	2.49	0.47
1:I:207:ASP:OD2	2:I:1:PDY:N12	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ILE:HG13	1:B:124:TYR:CE1	2.50	0.47
1:B:330:LYS:HG3	1:B:330:LYS:O	2.14	0.47
1:L:296:GLU:O	1:L:300:MET:HB2	2.14	0.47
1:B:326:MET:HG3	1:B:326:MET:O	2.14	0.47
1:D:70:LEU:HD21	1:I:48:VAL:HG11	1.95	0.47
1:F:48:VAL:HG13	1:F:48:VAL:O	2.13	0.47
1:G:118:VAL:HG23	1:G:139:GLU:HG2	1.96	0.47
1:G:185:ARG:HD3	1:G:241:ASP:OD2	2.14	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
2:K:1:PDY:H24	2:K:1:PDY:H20	1.43	0.47
1:B:278:ARG:HG2	1:B:283:GLN:HG3	1.95	0.47
1:E:56:LYS:O	1:L:50:SER:HB2	2.15	0.47
1:F:160:GLU:O	1:F:163:ALA:HB3	2.14	0.47
1:F:235:LEU:HD23	1:F:235:LEU:N	2.29	0.47
1:G:231:ALA:HB3	1:G:234:VAL:CG2	2.35	0.47
1:G:90:PHE:HE2	1:G:121:VAL:HG21	1.77	0.47
1:H:162:GLU:O	1:H:166:ILE:HG13	2.15	0.47
1:I:254:TYR:CD1	1:I:262:PRO:HD3	2.48	0.47
1:I:266:ASN:N	1:I:266:ASN:ND2	2.49	0.47
1:A:66:THR:HG22	1:A:69:VAL:HG13	1.96	0.47
1:B:82:PHE:HA	1:B:88:GLU:O	2.15	0.47
1:C:60:ILE:O	1:C:84:LYS:HE3	2.15	0.47
1:D:276:LYS:HB2	1:D:276:LYS:HE3	1.45	0.47
1:F:272:SER:HB3	1:F:275:MET:H	1.79	0.47
1:F:304:ASN:C	1:F:304:ASN:OD1	2.53	0.47
1:G:198:ARG:HG3	1:G:201:ALA:N	2.30	0.47
1:G:49:LYS:HG2	1:G:50:SER:N	2.30	0.47
1:G:69:VAL:HG23	1:G:70:LEU:N	2.30	0.47
1:H:340:ARG:HG3	1:H:341:VAL:H	1.80	0.47
1:I:168:LYS:O	1:I:168:LYS:HG3	2.14	0.47
1:C:327:GLN:HG2	1:C:330:LYS:HD3	1.97	0.47
1:F:86:THR:HG22	1:F:88:GLU:N	2.23	0.47
1:I:89:LYS:NZ	1:I:142:ASP:OD2	2.48	0.47
1:A:185:ARG:HE	1:A:212:LYS:HG3	1.79	0.47
1:D:266:ASN:ND2	1:D:267:HIS:HD2	2.11	0.47
1:E:86:THR:O	1:E:87:GLN:HB2	2.13	0.47
1:G:145:GLU:HG2	1:G:193:LEU:CD2	2.45	0.47
1:A:90:PHE:CE2	1:A:121:VAL:HG21	2.50	0.47
1:F:322:HIS:ND1	1:F:323:PRO:HD2	2.30	0.47
1:K:288:ASN:ND2	1:K:288:ASN:H	2.11	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:161:ARG:O	1:L:165:GLU:HG3	2.15	0.47
1:A:185:ARG:HD3	1:A:241:ASP:HB3	1.97	0.47
1:C:129:ALA:O	1:C:131:ARG:HD3	2.14	0.47
1:C:154:GLY:HA2	1:C:155:ASP:HB3	1.97	0.47
1:C:330:LYS:HB2	1:C:330:LYS:NZ	2.28	0.47
1:D:307:LYS:HB2	1:D:313:ARG:HG3	1.97	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:J:70:LEU:HA	1:J:94:MET:CE	2.44	0.47
1:B:166:ILE:O	1:B:170:ILE:HG13	2.15	0.47
1:A:276:LYS:CG	1:C:235:LEU:HD11	2.45	0.47
1:D:140:CYS:SG	2:D:1:PDY:H17	2.55	0.47
1:E:310:PRO:O	1:E:313:ARG:HB2	2.15	0.47
1:E:70:LEU:HD23	1:E:94:MET:CE	2.43	0.47
1:G:229:TYR:CD1	1:H:251:VAL:HG11	2.47	0.47
1:L:215:THR:HG23	1:L:216:SER:N	2.29	0.47
1:L:89:LYS:HE2	1:L:142:ASP:OD2	2.15	0.47
1:E:261:PRO:HD3	2:E:2:PDY:H22A	1.97	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:H:199:PRO:HG2	1:H:200:ASN:HD22	1.80	0.46
1:I:124:TYR:HB2	1:I:135:LEU:HB2	1.97	0.46
1:J:116:HIS:HE1	1:J:169:SER:OG	1.97	0.46
1:J:327:GLN:HG2	1:J:330:LYS:CD	2.41	0.46
2:K:2:PDY:H14A	2:K:2:PDY:H18	1.96	0.46
1:B:233:GLU:OE2	1:C:313:ARG:NH1	2.44	0.46
1:D:151:GLN:NE2	1:D:343:LYS:HA	2.31	0.46
1:E:102:ARG:NH2	1:E:125:GLU:OE1	2.49	0.46
1:E:72:LEU:HB3	1:E:79:LEU:HD11	1.98	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
2:A:2:PDY:C17	2:A:2:PDY:C14	2.93	0.46
1:A:327:GLN:HG2	1:A:330:LYS:HD3	1.97	0.46
1:A:86:THR:HG22	1:A:86:THR:O	2.14	0.46
1:I:55:LYS:HD3	1:I:124:TYR:CE2	2.49	0.46
1:I:108:HIS:HE1	1:I:138:MET:HE3	1.79	0.46
1:I:167:MET:HG3	1:I:253:MET:HG2	1.97	0.46
1:K:185:ARG:NH2	1:K:212:LYS:HG3	2.25	0.46
1:K:59:ILE:HA	1:K:124:TYR:CE2	2.51	0.46
1:C:327:GLN:C	1:C:329:THR:H	2.17	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:80:GLN:HB2	2:D:1:PDY:H24A	1.97	0.46
1:E:187:VAL:HG12	1:E:252:ILE:HD11	1.97	0.46
1:H:322:HIS:HD2	1:H:324:TRP:N	2.06	0.46
1:I:202:ILE:HD12	1:I:203:LEU:N	2.30	0.46
1:K:232:PRO:C	1:K:234:VAL:H	2.17	0.46
1:K:281:MET:CB	1:K:283:GLN:HG3	2.45	0.46
1:K:257:LEU:HD11	1:K:298:VAL:HG11	1.98	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:A:331:VAL:HG23	1:A:332:PRO:HD2	1.97	0.46
1:A:180:ILE:HG22	1:F:130:GLY:HA3	1.97	0.46
1:F:98:CYS:HB2	1:F:99:PRO:CD	2.45	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:L:286:PHE:CE1	1:L:299:LYS:HB3	2.51	0.46
1:C:153:ARG:HD3	1:C:156:GLN:NE2	2.30	0.46
1:C:70:LEU:HD12	1:C:70:LEU:N	2.30	0.46
1:H:160:GLU:O	1:H:163:ALA:HB3	2.16	0.46
1:H:337:HIS:HA	1:H:340:ARG:HH11	1.79	0.46
1:I:286:PHE:CB	1:I:299:LYS:HE2	2.46	0.46
1:B:74:ILE:HG23	1:B:94:MET:CE	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:E:161:ARG:O	1:E:165:GLU:HG3	2.15	0.46
1:G:65:VAL:HG12	1:G:70:LEU:CD2	2.46	0.46
1:J:314:MET:CG	1:J:318:GLU:HB2	2.46	0.46
1:K:197:LYS:HA	1:K:197:LYS:HD2	1.77	0.46
1:L:79:LEU:O	1:L:91:ALA:HA	2.16	0.46
1:C:70:LEU:CD1	1:C:70:LEU:N	2.79	0.46
1:F:147:PHE:HE1	1:F:189:PRO:HG3	1.80	0.46
1:F:192:LEU:C	1:F:193:LEU:HD23	2.35	0.46
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:A:202:ILE:HD12	1:A:203:LEU:N	2.31	0.46
1:B:188:LYS:NZ	1:B:190:GLU:HB2	2.31	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:D:66:THR:HG21	1:D:68:GLN:CG	2.46	0.46
1:J:122:ASP:N	1:J:122:ASP:OD1	2.47	0.46
1:J:166:ILE:O	1:J:169:SER:HB3	2.15	0.46
1:L:264:TYR:CB	2:L:2:PDY:H17	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:ARG:O	1:B:154:GLY:C	2.54	0.46
1:C:241:ASP:O	1:C:244:CYS:HB3	2.16	0.46
1:F:147:PHE:CD1	1:F:189:PRO:HB3	2.51	0.46
1:F:310:PRO:O	1:F:313:ARG:HB2	2.16	0.46
1:J:155:ASP:OD2	1:J:340:ARG:HG3	2.16	0.46
1:K:55:LYS:HE2	1:K:57:ASN:HD21	1.81	0.46
1:A:332:PRO:HG2	1:A:334:THR:CG2	2.47	0.45
1:B:156:GLN:OE1	1:B:156:GLN:N	2.49	0.45
1:C:121:VAL:O	1:C:122:ASP:HB3	2.16	0.45
1:C:215:THR:HG23	1:C:216:SER:N	2.30	0.45
1:F:56:LYS:HE3	1:F:125:GLU:CD	2.36	0.45
1:G:125:GLU:O	1:G:126:ASN:ND2	2.43	0.45
1:I:97:ASP:HB2	1:I:134:LEU:HD13	1.98	0.45
1:J:48:VAL:O	1:J:48:VAL:HG13	2.16	0.45
1:J:70:LEU:O	1:J:94:MET:HE1	2.15	0.45
1:A:153:ARG:O	1:A:154:GLY:C	2.54	0.45
1:A:188:LYS:HB2	1:A:189:PRO:CD	2.46	0.45
1:C:145:GLU:HG2	1:C:193:LEU:CD2	2.47	0.45
1:C:327:GLN:O	1:C:329:THR:N	2.43	0.45
1:I:183:ALA:O	1:I:211:ALA:HA	2.16	0.45
1:K:80:GLN:HE21	2:K:1:PDY:H24	1.80	0.45
1:E:128:TYR:CD1	1:L:48:VAL:HG23	2.49	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:C:83:ASN:HD22	1:C:86:THR:HB	1.82	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
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:D:66:THR:HG21	1:D:68:GLN:HG3	1.97	0.45
1:E:66:THR:HG22	1:E:69:VAL:HG22	1.99	0.45
1:G:264:TYR:CE1	2:G:2:PDY:H24A	2.52	0.45
1:I:77:LYS:HA	1:I:77:LYS:HD3	1.79	0.45
1:J:186:ASP:OD1	1:J:188:LYS:HE3	2.16	0.45
1:J:278:ARG:HG3	1:J:283:GLN:NE2	2.31	0.45
1:A:52:LEU:HD21	1:A:105:VAL:HG12	1.98	0.45
1:A:185:ARG:NH2	1:A:212:LYS:HG3	2.31	0.45
1:A:298:VAL:O	1:A:302:ILE:HG13	2.16	0.45
1:B:151:GLN:HB2	1:B:342:LEU:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:GLU:HB3	1:C:312:GLN:HG3	1.98	0.45
1:D:111:ALA:HB1	1:D:117:ILE:HD13	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:H:290:GLU:H	1:H:290:GLU:CD	2.20	0.45
1:H:67:SER:O	1:H:69:VAL:N	2.49	0.45
1:L:188:LYS:HE2	1:L:190:GLU:HG2	1.98	0.45
1:A:52:LEU:HD21	1:A:105:VAL:CG1	2.46	0.45
1:A:69:VAL:HB	1:A:79:LEU:HD12	1.98	0.45
1:E:188:LYS:NZ	1:E:190:GLU:CG	2.79	0.45
1:H:94:MET:O	1:H:95:LEU:HD23	2.17	0.45
1:I:69:VAL:HG13	1:I:79:LEU:HD22	1.98	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:L:159:THR:HB	1:L:162:GLU:H	1.81	0.45
1:L:231:ALA:HB1	1:L:233:GLU:OE2	2.17	0.45
1:L:298:VAL:HG22	1:L:324:TRP:CD1	2.52	0.45
1:L:161:ARG:HD2	1:L:328:SER:O	2.16	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:F:260:TYR:CB	2:F:2:PDY:H19	2.47	0.45
1:H:233:GLU:HG3	1:H:233:GLU:H	1.35	0.45
1:J:240:TYR:HA	1:J:240:TYR:HD2	1.68	0.45
1:J:316:ILE:HG23	1:J:317:THR:N	2.31	0.45
1:K:310:PRO:HB3	1:L:233:GLU:OE1	2.17	0.45
1:L:249:LEU:HD12	1:L:249:LEU:HA	1.76	0.45
1:A:300:MET:SD	1:A:303:ARG:NH2	2.79	0.45
1:B:124:TYR:HB2	1:B:135:LEU:HB2	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:E:73:GLY:HA3	1:E:94:MET:HE3	1.98	0.45
1:G:118:VAL:HG21	2:G:1:PDY:H11	1.99	0.45
1:G:188:LYS:HB3	1:I:229:TYR:CD1	2.52	0.45
1:H:49:LYS:HB2	1:J:127:LEU:HB2	1.97	0.45
1:B:190:GLU:N	1:B:190:GLU:CD	2.70	0.45
1:B:327:GLN:NE2	1:B:330:LYS:NZ	2.65	0.45
1:B:70:LEU:O	1:B:74:ILE:HG13	2.16	0.45
1:F:265:SER:HB3	1:F:268:GLY:HA2	1.98	0.45
1:H:158:PHE:HZ	1:H:166:ILE:HD12	1.82	0.45
1:H:190:GLU:CD	1:H:190:GLU:H	2.21	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:298:VAL:HG22	1:H:324:TRP:CD1	2.52	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
2:C:1:PDY:H18	2:C:1:PDY:H14A	1.95	0.45
1:C:229:TYR:N	1:C:229:TYR:CD2	2.85	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:F:230:VAL:HG23	1:F:234:VAL:HG11	1.97	0.45
1:G:215:THR:OG1	1:G:216:SER:N	2.50	0.45
1:G:264:TYR:C	1:G:275:MET:HG3	2.38	0.45
1:G:305:LEU:O	1:G:313:ARG:HD3	2.16	0.45
1:H:90:PHE:CE2	1:H:121:VAL:HG21	2.51	0.45
1:J:160:GLU:O	1:J:163:ALA:HB3	2.16	0.45
1:L:344:GLU:N	1:L:344:GLU:OE1	2.50	0.45
1:C:145:GLU:HG2	1:C:193:LEU:HD22	1.99	0.44
1:E:95:LEU:O	1:E:133:CYS:HB2	2.16	0.44
1:F:125:GLU:OE2	1:F:132:LYS:HD2	2.17	0.44
1:I:167:MET:HE2	1:I:253:MET:HG3	1.99	0.44
1:A:88:GLU:HG2	1:A:89:LYS:N	2.31	0.44
1:C:233:GLU:HG3	1:C:233:GLU:H	1.47	0.44
1:E:100:LYS:HE2	1:E:100:LYS:HB2	1.84	0.44
1:E:155:ASP:N	1:E:155:ASP:OD2	2.49	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:202:ILE:HD11	1:H:204:LYS:CE	2.47	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:I:145:GLU:HG2	1:I:193:LEU:CD2	2.47	0.44
1:J:338:THR:O	1:J:342:LEU:HB2	2.17	0.44
1:L:259:GLY:HA3	1:L:341:VAL:HG11	1.98	0.44
1:A:161:ARG:HB3	1:A:333:GLN:NE2	2.31	0.44
2:A:2:PDY:C3	2:A:2:PDY:H17	2.47	0.44
1:A:253:MET:HE1	1:A:319:PHE:HE1	1.82	0.44
1:A:69:VAL:HB	1:A:79:LEU:HD13	1.98	0.44
1:C:104:GLU:HG3	1:C:208:PHE:C	2.37	0.44
1:E:275:MET:HA	1:E:278:ARG:NH1	2.31	0.44
1:L:154:GLY:C	1:L:156:GLN:HB3	2.37	0.44
1:L:258:CYS:HB3	1:L:291:TRP:CZ2	2.52	0.44
2:L:2:PDY:H24A	2:L:2:PDY:H20	1.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:GLY:O	1:C:74:ILE:HG22	2.18	0.44
1:D:113:GLN:O	1:D:115:PRO:HD3	2.17	0.44
1:G:161:ARG:NH1	1:G:331:VAL:O	2.46	0.44
1:H:332:PRO:HB2	1:H:334:THR:CG2	2.38	0.44
1:J:188:LYS:HB2	1:J:189:PRO:CD	2.48	0.44
1:J:254:TYR:CD1	1:J:262:PRO:HG3	2.52	0.44
1:K:161:ARG:O	1:K:165:GLU:HG3	2.18	0.44
1:K:188:LYS:HB2	1:K:189:PRO:HD2	1.99	0.44
1:A:134:LEU:HD12	1:A:134:LEU:HA	1.85	0.44
1:A:188:LYS:HB2	1:A:189:PRO:HD2	1.99	0.44
1:A:311:THR:O	1:B:312:GLN:NE2	2.50	0.44
1:C:147:PHE:O	1:C:151:GLN:N	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:H:233:GLU:OE2	1:I:313:ARG:NH1	2.41	0.44
1:H:97:ASP:H	1:H:133:CYS:HA	1.81	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: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:K:96:GLN:HE22	1:K:131:ARG:CD	2.30	0.44
1:J:313:ARG:NH2	1:K:233:GLU:HG2	2.14	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: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:F:49:LYS:HB2	1:F:113:GLN:NE2	2.32	0.44
1:H:65:VAL:CG1	1:H:70:LEU:HD13	2.45	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:A:97:ASP:OD2	1:A:102:ARG:NH2	2.33	0.44
1:B:58:ALA:HB1	1:B:60:ILE:HG13	2.00	0.44
1:C:94:MET:HE3	1:C:94:MET:HB3	1.90	0.44
1:D:148:SER:HA	1:D:151:GLN:HG2	2.00	0.44
1:D:309:GLU:OE2	1:D:310:PRO:HD2	2.18	0.44
1:F:233:GLU:HG2	1:F:234:VAL:N	2.33	0.44
1:G:81:ILE:HD13	1:G:92:LEU:HB2	1.99	0.44
1:H:200:ASN:HD22	1:H:200:ASN:H	1.63	0.44
1:H:158:PHE:O	1:H:336:LEU:HB2	2.17	0.44
1:I:285:GLU:O	1:I:287:PRO:HD3	2.17	0.44
1:I:304:ASN:O	1:I:307:LYS:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:165:GLU:O	1:K:168:LYS:HB3	2.17	0.44
1:K:103:ARG:NH1	1:K:212:LYS:HE2	2.33	0.44
1:L:336:LEU:HD22	1:L:336:LEU:N	2.32	0.44
1:B:80:GLN:NE2	2:B:1:PDY:H24A	2.32	0.44
2:B:2:PDY:C18	2:B:2:PDY:H14A	2.42	0.44
1:E:253:MET:HE1	1:E:319:PHE:HE1	1.83	0.44
1:F:97:ASP:HA	1:F:134:LEU:HD22	2.00	0.44
1:E:229:TYR:CE1	1:F:188:LYS:HG2	2.53	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
1:H:161:ARG:O	1:H:165:GLU:HG3	2.17	0.44
1:H:264:TYR:HB2	2:H:2:PDY:C17	2.47	0.44
1:H:86:THR:C	1:H:88:GLU:H	2.19	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:A:233:GLU:H	1:A:233:GLU:HG3	1.50	0.43
1:C:90:PHE:CE2	1:C:121:VAL:HG21	2.53	0.43
1:C:288:ASN:ND2	1:C:288:ASN:N	2.66	0.43
1:C:65:VAL:HG12	1:C:70:LEU:CD1	2.48	0.43
1:D:230:VAL:CG2	1:D:234:VAL:HB	2.47	0.43
1:D:161:ARG:HA	1:D:331:VAL:CG2	2.48	0.43
1:D:70:LEU:HD21	1:I:48:VAL:CG1	2.48	0.43
1:E:232:PRO:C	1:E:234:VAL:H	2.21	0.43
1:F:308:THR:HG22	1:F:309:GLU:N	2.33	0.43
1:G:288:ASN:HB3	1:G:289:PRO:HA	1.99	0.43
1:K:167:MET:SD	1:K:256:LEU:HD12	2.58	0.43
1:K:334:THR:HA	1:K:335:PRO:HD3	1.76	0.43
1:L:108:HIS:HE1	1:L:138:MET:HE3	1.83	0.43
1:B:266:ASN:C	1:B:266:ASN:OD1	2.56	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:J:192:LEU:HD11	1:J:252:ILE:HD13	1.99	0.43
1:B:327:GLN:HE22	1:B:330:LYS:HZ2	1.66	0.43
1:D:155:ASP:OD1	1:D:156:GLN:HG2	2.18	0.43
1:E:337:HIS:CG	1:E:340:ARG:NH2	2.86	0.43
1:G:70:LEU:H	1:G:70:LEU:HD22	1.83	0.43
1:I:126:ASN:HD22	1:I:126:ASN:N	2.11	0.43
1:L:215:THR:OG1	1:L:216:SER:N	2.50	0.43
1:A:130:GLY:O	1:G:110:ARG:HD2	2.17	0.43
1:A:83:ASN:O	1:A:87:GLN:N	2.51	0.43
1:C:235:LEU:O	1:C:235:LEU:HD13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:TYR:OH	1:D:287:PRO:HG2	2.17	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:G:337:HIS:ND1	1:G:340:ARG:NH1	2.66	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:J:311:THR:HG22	1:L:309:GLU:CD	2.38	0.43
1:L:93:LYS:HE3	1:L:93:LYS:HB2	1.76	0.43
1:A:135:LEU:N	1:A:135:LEU:HD12	2.33	0.43
1:B:56:LYS:O	1:E:50:SER:HB2	2.19	0.43
1:C:260:TYR:HD2	1:C:341:VAL:HG11	1.83	0.43
1:C:96:GLN:HE21	1:C:96:GLN:HB3	1.59	0.43
1:D:57:ASN:H	1:D:57:ASN:HD22	1.66	0.43
1:E:149:ARG:NH1	1:E:196:SER:O	2.51	0.43
1:G:278:ARG:HA	1:G:283:GLN:HG2	1.99	0.43
1:G:98:CYS:HB2	1:G:99:PRO:CD	2.48	0.43
1:I:285:GLU:C	1:I:287:PRO:HD3	2.39	0.43
1:J:89:LYS:HZ2	1:J:140:CYS:HB3	1.83	0.43
1:J:141:LEU:HD13	1:J:193:LEU:HB2	2.00	0.43
1:B:264:TYR:CZ	2:B:2:PDY:H24	2.53	0.43
1:B:80:GLN:CD	2:B:1:PDY:H24A	2.39	0.43
1:D:230:VAL:HG22	1:D:234:VAL:HB	1.99	0.43
1:D:167:MET:HE3	1:D:249:LEU:HG	2.00	0.43
1:E:249:LEU:HA	1:E:249:LEU:HD12	1.71	0.43
1:J:48:VAL:O	1:J:48:VAL:HG22	2.18	0.43
1:K:58:ALA:HB1	1:K:60:ILE:HG13	2.00	0.43
1:L:342:LEU:CD1	1:L:342:LEU:N	2.82	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:B:289:PRO:O	1:B:290:GLU:C	2.57	0.43
2:E:1:PDY:H24	2:E:1:PDY:H20	1.57	0.43
1:E:337:HIS:CD2	1:E:340:ARG:HH21	2.36	0.43
1:F:81:ILE:CD1	1:F:92:LEU:HB2	2.45	0.43
1:G:60:ILE:C	1:G:60:ILE:HD12	2.39	0.43
1:H:149:ARG:HG3	1:H:194:TYR:CD2	2.54	0.43
1:I:255:ILE:O	1:I:259:GLY:N	2.46	0.43
1:J:107:LEU:HD21	1:J:213:GLU:HG2	2.00	0.43
1:K:159:THR:C	1:K:161:ARG:H	2.22	0.43
1:K:230:VAL:HG13	1:K:231:ALA:N	2.33	0.43
1:K:344:GLU:O	1:K:344:GLU:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:TYR:HE1	1:A:124:TYR:OH	2.02	0.43
1:B:180:ILE:HG21	1:L:130:GLY:HA3	2.01	0.43
1:B:215:THR:HG22	1:B:216:SER:N	2.33	0.43
1:B:246:MET:CE	1:B:316:ILE:HA	2.49	0.43
1:D:198:ARG:HD2	1:D:200:ASN:OD1	2.19	0.43
1:F:54:ILE:HD13	1:F:102:ARG:NH1	2.34	0.43
1:G:298:VAL:HG22	1:G:324:TRP:CD1	2.54	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:J:160:GLU:HG2	1:J:331:VAL:CG2	2.49	0.43
1:J:111:ALA:HB2	1:J:177:LEU:HD21	2.01	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:K:56:LYS:NZ	1:K:125:GLU:CD	2.71	0.43
1:K:184:HIS:CD2	1:K:205:LEU:HD21	2.54	0.43
1:K:230:VAL:CG2	1:K:231:ALA:H	2.09	0.43
1:A:156:GLN:NE2	1:A:156:GLN:N	2.58	0.43
1:C:111:ALA:HB1	1:C:117:ILE:HD13	2.01	0.43
1:C:121:VAL:O	1:C:122:ASP:CB	2.67	0.43
1:C:172:GLU:HG2	1:C:320:MET:CE	2.49	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:D:134:LEU:HD12	1:D:134:LEU:HA	1.87	0.43
1:E:70:LEU:HA	1:E:70:LEU:HD23	1.89	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:I:160:GLU:CA	1:I:336:LEU:HD21	2.49	0.43
1:I:86:THR:C	1:I:88:GLU:H	2.22	0.43
1:J:336:LEU:HD22	1:J:336:LEU:N	2.34	0.43
1:C:88:GLU:CG	1:C:89:LYS:N	2.79	0.43
1:D:114:CYS:HB3	1:D:117:ILE:HD12	2.01	0.43
1:E:156:GLN:NE2	1:E:156:GLN:N	2.51	0.43
1:G:156:GLN:O	1:G:335:PRO:HB3	2.19	0.43
1:I:247:TRP:HZ3	1:I:306:LEU:O	2.02	0.43
1:I:96:GLN:OE1	1:I:131:ARG:HD2	2.19	0.43
1:K:102:ARG:NH2	1:K:125:GLU:OE1	2.51	0.43
1:A:185:ARG:CZ	1:A:212:LYS:HE2	2.49	0.42
1:D:90:PHE:CE2	1:D:121:VAL:HG21	2.53	0.42
1:D:285:GLU:HB2	1:D:287:PRO:HD3	2.01	0.42
1:E:340:ARG:O	1:E:344:GLU:HG3	2.19	0.42
1:G:156:GLN:HG3	1:G:335:PRO:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:189:PRO:HD2	1:H:190:GLU:OE1	2.19	0.42
1:I:69:VAL:HA	1:I:79:LEU:CD2	2.42	0.42
1:J:186:ASP:HB2	1:J:210:PHE:HD2	1.83	0.42
1:L:127:LEU:HD12	1:L:127:LEU:HA	1.85	0.42
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:D:149:ARG:NH1	1:D:197:LYS:HA	2.34	0.42
1:F:49:LYS:NZ	1:F:113:GLN:HG3	2.34	0.42
1:H:140:CYS:SG	2:H:1:PDY:C17	3.07	0.42
1:H:66:THR:OG1	1:H:69:VAL:HG12	2.20	0.42
1:K:157:ALA:HB1	1:K:335:PRO:HB3	2.01	0.42
1:A:247:TRP:CZ2	1:C:232:PRO:HD3	2.54	0.42
1:B:188:LYS:HE3	1:B:191:ASN:ND2	2.35	0.42
1:B:77:LYS:HZ2	1:B:79:LEU:HD21	1.83	0.42
1:E:187:VAL:HG12	1:E:252:ILE:CD1	2.49	0.42
1:E:231:ALA:HB1	1:E:233:GLU:CD	2.39	0.42
1:E:332:PRO:HG2	1:E:334:THR:HG22	2.00	0.42
1:E:97:ASP:OD2	1:E:102:ARG:NH2	2.34	0.42
2:H:1:PDY:H24	2:H:1:PDY:H20	1.40	0.42
1:H:331:VAL:HB	1:H:332:PRO:HD2	2.01	0.42
1:J:305:LEU:O	1:J:313:ARG:HD3	2.20	0.42
1:J:336:LEU:C	1:J:338:THR:H	2.23	0.42
1:L:68:GLN:O	1:L:72:LEU:HD13	2.19	0.42
1:A:234:VAL:O	1:A:234:VAL:HG12	2.19	0.42
1:A:287:PRO:O	1:A:291:TRP:HB2	2.18	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:H:151:GLN:HA	1:H:339:SER:OG	2.19	0.42
1:K:72:LEU:HB2	1:K:79:LEU:HD11	2.01	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:B:56:LYS:O	1:E:51:GLY:N	2.46	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:D:77:LYS:HB3	1:D:77:LYS:HZ2	1.84	0.42
1:F:278:ARG:NH2	3:F:3:SO4:O2	2.53	0.42
1:H:89:LYS:HG2	1:H:90:PHE:N	2.35	0.42
1:H:50:SER:O	1:J:127:LEU:HD23	2.19	0.42
1:J:66:THR:HG23	1:J:69:VAL:H	1.84	0.42
1:B:108:HIS:O	1:B:108:HIS:HD2	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:154:GLY:HA2	1:E:155:ASP:HA	1.72	0.42
1:F:307:LYS:HG2	1:F:312:GLN:CB	2.49	0.42
1:F:49:LYS:CG	1:G:127:LEU:HB2	2.49	0.42
1:H:161:ARG:HA	1:H:331:VAL:CG2	2.50	0.42
1:K:310:PRO:HG3	1:L:233:GLU:HG2	2.02	0.42
1:B:65:VAL:HG12	1:B:69:VAL:CG2	2.49	0.42
1:G:102:ARG:HH22	1:G:125:GLU:CD	2.23	0.42
1:I:60:ILE:HA	1:I:63:TYR:O	2.19	0.42
1:J:161:ARG:CZ	1:J:333:GLN:HG3	2.50	0.42
1:D:52:LEU:O	1:K:56:LYS:HE3	2.19	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: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: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:B:116:HIS:O	1:B:204:LYS:HA	2.20	0.42
1:C:142:ASP:N	1:C:195:THR:O	2.49	0.42
1:E:143:GLY:O	1:E:149:ARG:HD3	2.19	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:J:128:TYR:O	1:J:129:ALA:HB3	2.19	0.42
1:J:261:PRO:HD3	2:J:2:PDY:H25	2.02	0.42
1:J:327:GLN:HG2	1:J:330:LYS:CG	2.50	0.42
1:K:65:VAL:HG12	1:K:70:LEU:HG	2.00	0.42
1:B:113:GLN:HE21	1:B:113:GLN:HB3	1.55	0.42
1:B:62:ASP:OD2	1:B:62:ASP:N	2.53	0.42
1:D:127:LEU:HA	1:D:127:LEU:HD12	1.91	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:F:58:ALA:O	1:F:61:ASP:HB2	2.20	0.42
1:G:97:ASP:HA	1:G:134:LEU:HD22	2.02	0.42
1:H:260:TYR:OH	1:H:287:PRO:HG2	2.20	0.42
1:H:75:ASN:HA	1:H:75:ASN:HD22	1.66	0.42
1:K:69:VAL:HG23	1:K:70:LEU:N	2.35	0.42
1:J:233:GLU:CG	1:L:310:PRO:HG3	2.50	0.42
1:A:52:LEU:HB2	1:A:109:TRP:CD1	2.55	0.41
1:B:241:ASP:O	1:B:244:CYS:HB3	2.19	0.41
1:B:327:GLN:NE2	1:B:330:LYS:HZ2	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:TYR:N	1:C:229:TYR:HD2	2.17	0.41
1:C:147:PHE:CE2	1:C:256:LEU:HD23	2.47	0.41
1:E:247:TRP:HZ3	1:E:306:LEU:O	2.03	0.41
1:F:156:GLN:N	1:F:156:GLN:NE2	2.67	0.41
2:F:2:PDY:H14A	2:F:2:PDY:C18	2.38	0.41
1:J:143:GLY:CA	1:J:149:ARG:NH1	2.83	0.41
1:J:252:ILE:C	1:J:254:TYR:H	2.23	0.41
1:K:194:TYR:CZ	1:K:203:LEU:HD13	2.55	0.41
1:K:232:PRO:C	1:K:234:VAL:N	2.73	0.41
1:K:66:THR:N	1:K:69:VAL:HG22	2.33	0.41
1:L:195:THR:OG1	1:L:196:SER:N	2.53	0.41
1:A:113:GLN:HE21	1:A:113:GLN:HB3	1.62	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:E:304:ASN:HA	1:E:307:LYS:HG3	2.01	0.41
1:H:142:ASP:O	1:H:197:LYS:HE3	2.20	0.41
1:I:148:SER:O	1:I:152:ASP:HB2	2.20	0.41
1:I:322:HIS:HA	1:I:323:PRO:HD3	1.94	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:F:268:GLY:HA2	1:F:269:LEU:HA	1.70	0.41
1:H:154:GLY:O	1:H:156:GLN:NE2	2.53	0.41
1:J:141:LEU:HD12	1:J:193:LEU:HB2	2.00	0.41
1:J:188:LYS:HB2	1:J:189:PRO:HD2	2.03	0.41
1:C:104:GLU:HG3	1:C:208:PHE:O	2.21	0.41
1:D:65:VAL:HG12	1:D:70:LEU:HD13	2.00	0.41
1:E:147:PHE:HE2	1:E:256:LEU:HD23	1.85	0.41
1:J:172:GLU:HG2	1:J:320:MET:CE	2.51	0.41
1:J:337:HIS:ND1	1:J:337:HIS:N	2.68	0.41
1:K:143:GLY:HA3	1:K:194:TYR:CB	2.49	0.41
1:K:192:LEU:HD11	1:K:252:ILE:HD13	2.02	0.41
1:L:108:HIS:HE1	1:L:138:MET:CE	2.33	0.41
1:B:115:PRO:O	1:B:204:LYS:HD3	2.21	0.41
1:C:127:LEU:HA	1:C:127:LEU:HD12	1.87	0.41
1:C:185:ARG:HH21	1:C:212:LYS:HG3	1.85	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:K:275:MET:O	1:K:278:ARG:N	2.53	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:L:95:LEU:O	1:L:133:CYS:CB	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:LYS:HD3	1:B:307:LYS:HA	1.83	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:337:HIS:O	1:F:341:VAL:HG23	2.20	0.41
1:F:60:ILE:HA	1:F:63:TYR:O	2.21	0.41
1:F:49:LYS:HB3	1:G:127:LEU:HB2	2.01	0.41
1:H:133:CYS:SG	1:H:135:LEU:HD11	2.60	0.41
1:H:143:GLY:HA2	1:H:197:LYS:CD	2.50	0.41
1:H:340:ARG:O	1:H:343:LYS:HG2	2.20	0.41
1:I:71:GLY:O	1:I:75:ASN:HB2	2.20	0.41
1:J:260:TYR:OH	1:J:290:GLU:HG3	2.20	0.41
1:J:322:HIS:ND1	1:J:323:PRO:CD	2.83	0.41
1:K:118:VAL:CG1	1:K:206:THR:HG22	2.51	0.41
1:A:107:LEU:HD22	1:A:182:ILE:HG12	2.02	0.41
1:B:188:LYS:CD	1:B:190:GLU:HB2	2.50	0.41
1:D:141:LEU:HD13	1:D:193:LEU:HB2	2.03	0.41
1:D:170:ILE:O	1:D:174:ILE:HG12	2.20	0.41
1:E:167:MET:SD	1:E:256:LEU:HD12	2.61	0.41
1:H:314:MET:HG3	1:H:318:GLU:HB2	2.03	0.41
1:I:127:LEU:HD12	1:I:127:LEU:HA	1.87	0.41
1:I:65:VAL:HG11	1:I:70:LEU:HD21	2.03	0.41
1:J:245:ASP:O	1:J:248:SER:HB2	2.21	0.41
1:L:185:ARG:HD3	1:L:241:ASP:OD2	2.20	0.41
1:L:161:ARG:CZ	1:L:333:GLN:NE2	2.84	0.41
1:L:70:LEU:HD12	1:L:94:MET:CE	2.51	0.41
1:C:83:ASN:OD1	1:C:84:LYS:N	2.53	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:H:337:HIS:CB	1:H:340:ARG:HH11	2.34	0.41
1:I:100:LYS:HG3	1:I:103:ARG:HH21	1.85	0.41
1:J:107:LEU:HD21	1:J:213:GLU:CG	2.50	0.41
1:J:315:THR:OG1	1:J:318:GLU:HG3	2.20	0.41
1:K:121:VAL:C	1:K:122:ASP:OD1	2.59	0.41
1:K:129:ALA:C	1:K:131:ARG:N	2.74	0.41
1:K:151:GLN:HG3	1:K:152:ASP:N	2.36	0.41
1:A:66:THR:HG22	1:A:69:VAL:H	1.86	0.41
1:B:90:PHE:CE2	1:B:121:VAL:HG21	2.56	0.41
1:C:65:VAL:HG11	1:C:70:LEU:HD11	2.00	0.41
1:E:177:LEU:HD21	1:E:208:PHE:HE2	1.86	0.41
1:F:185:ARG:HD3	1:F:241:ASP:CB	2.47	0.41
2:F:2:PDY:C13	2:F:2:PDY:C14	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:304:ASN:OD1	1:F:304:ASN:O	2.37	0.41
1:H:107:LEU:HD22	1:H:182:ILE:CD1	2.51	0.41
1:I:172:GLU:HG2	1:I:320:MET:HE1	2.02	0.41
1:H:233:GLU:CG	1:I:310:PRO:HG3	2.51	0.41
1:J:111:ALA:CB	1:J:177:LEU:HD21	2.51	0.41
1:K:70:LEU:HD23	1:K:94:MET:HE1	2.00	0.41
1:L:309:GLU:OE2	1:L:310:PRO:HD2	2.21	0.41
1:L:336:LEU:C	1:L:338:THR:H	2.23	0.41
1:A:233:GLU:OE2	1:B:313:ARG:CZ	2.69	0.41
1:B:301:LEU:HD22	1:B:322:HIS:CE1	2.56	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:F:70:LEU:HA	1:F:94:MET:HE1	2.03	0.41
1:H:145:GLU:HG2	1:H:193:LEU:HD22	2.03	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:I:90:PHE:CE2	1:I:121:VAL:HG21	2.55	0.41
1:J:153:ARG:O	1:J:154:GLY:C	2.59	0.41
1:J:301:LEU:O	1:J:301:LEU:HD12	2.20	0.41
1:A:233:GLU:OE2	1:B:310:PRO:HB3	2.21	0.41
1:B:52:LEU:HB2	1:B:109:TRP:CG	2.57	0.41
1:C:332:PRO:HB2	1:C:334:THR:HG22	2.03	0.41
1:G:74:ILE:O	1:G:74:ILE:HG12	2.21	0.41
1:I:327:GLN:HE21	1:I:330:LYS:HZ2	1.67	0.41
1:J:82:PHE:HA	1:J:88:GLU:O	2.21	0.41
1:K:49:LYS:CD	1:K:50:SER:N	2.78	0.41
1:L:266:ASN:CB	1:L:278:ARG:NH2	2.82	0.41
1:L:264:TYR:CG	2:L:2:PDY:C17	3.04	0.41
1:A:233:GLU:OE2	1:B:313:ARG:NH2	2.54	0.40
1:A:313:ARG:HH22	1:C:233:GLU:CG	2.33	0.40
1:C:118:VAL:HG13	1:C:118:VAL:O	2.20	0.40
1:C:151:GLN:NE2	1:C:342:LEU:O	2.54	0.40
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: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:A:95:LEU:O	1:A:133:CYS:HB2	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:85:ARG:O	1:H:87:GLN:N	2.55	0.40
1:I:264:TYR:CE2	2:I:2:PDY:C20	2.99	0.40
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:L:97:ASP:CG	1:L:102:ARG:HH21	2.24	0.40
2:A:1:PDY:H18	2:A:1:PDY:C14	2.49	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
2:E:1:PDY:C3	2:E:1:PDY:C18	2.78	0.40
1:F:156:GLN:N	1:F:156:GLN:HE21	2.20	0.40
2:J:2:PDY:C18	2:J:2:PDY:C3	2.90	0.40
1:J:331:VAL:CG2	1:J:332:PRO:HD2	2.51	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:A:77:LYS:HB3	1:A:79:LEU:HD21	2.04	0.40
1:B:65:VAL:HG12	1:B:69:VAL:HG21	2.03	0.40
1:B:92:LEU:HD12	1:B:93:LYS:N	2.35	0.40
1:D:48:VAL:CG1	1:D:48:VAL:O	2.68	0.40
1:H:80:GLN:OE1	2:H:1:PDY:H24A	2.21	0.40
1:J:179:SER:HA	1:L:281:MET:SD	2.61	0.40
1:J:314:MET:HG3	1:J:318:GLU:OE1	2.21	0.40
1:K:330:LYS:HG3	1:K:330:LYS:O	2.21	0.40
1:L:277:THR:O	1:L:281:MET:HG2	2.21	0.40
1:A:247:TRP:HZ3	1:A:306:LEU:O	2.05	0.40
1:B:253:MET:CE	1:B:305:LEU:HD12	2.52	0.40
1:B:301:LEU:HD13	1:B:322:HIS:CD2	2.56	0.40
1:B:85:ARG:HH11	1:B:86:THR:CG2	2.34	0.40
1:C:281:MET:HB3	1:C:283:GLN:HG3	2.03	0.40
1:E:327:GLN:CD	1:E:330:LYS:HZ2	2.24	0.40
1:H:167:MET:HE3	1:H:167:MET:HB3	2.00	0.40
1:H:193:LEU:HD11	2:H:1:PDY:H22A	2.04	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: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: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%)	38	72
1	B	269/324 (83%)	252 (94%)	15 (6%)	2 (1%)	25	60
1	C	263/324 (81%)	237 (90%)	21 (8%)	5 (2%)	9	33
1	D	269/324 (83%)	249 (93%)	19 (7%)	1 (0%)	38	72
1	E	268/324 (83%)	249 (93%)	16 (6%)	3 (1%)	17	48
1	F	283/324 (87%)	262 (93%)	19 (7%)	2 (1%)	25	60
1	G	265/324 (82%)	240 (91%)	24 (9%)	1 (0%)	38	72
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%)	25	60
1	K	265/324 (82%)	238 (90%)	24 (9%)	3 (1%)	17	48
1	L	268/324 (83%)	241 (90%)	24 (9%)	3 (1%)	17	48
All	All	3215/3888 (83%)	2943 (92%)	249 (8%)	23 (1%)	25	60

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

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Mol	Chain	Res	Type
1	D	155	ASP
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%)	5	16
1	B	251/293 (86%)	228 (91%)	23 (9%)	11	32
1	C	247/293 (84%)	212 (86%)	35 (14%)	4	11
1	D	251/293 (86%)	223 (89%)	28 (11%)	7	21
1	E	250/293 (85%)	223 (89%)	27 (11%)	7	23
1	F	258/293 (88%)	225 (87%)	33 (13%)	5	15
1	G	247/293 (84%)	228 (92%)	19 (8%)	15	40
1	H	249/293 (85%)	224 (90%)	25 (10%)	9	27
1	I	249/293 (85%)	222 (89%)	27 (11%)	7	23
1	J	249/293 (85%)	219 (88%)	30 (12%)	6	17
1	K	247/293 (84%)	219 (89%)	28 (11%)	7	21
1	L	250/293 (85%)	226 (90%)	24 (10%)	10	29
All	All	2996/3516 (85%)	2666 (89%)	330 (11%)	7	22

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

Mol	Chain	Res	Type
1	A	47	HIS
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 molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	-	24,30,30	1.77	3 (12%)	30,41,41	2.69	6 (20%)
2	PDY	A	2	-	24,30,30	1.70	3 (12%)	30,41,41	2.75	9 (30%)
2	PDY	B	1	-	24,30,30	1.76	3 (12%)	30,41,41	2.71	5 (16%)
2	PDY	B	2	-	24,30,30	1.74	3 (12%)	30,41,41	2.76	5 (16%)
2	PDY	C	1	-	24,30,30	1.76	3 (12%)	30,41,41	2.69	6 (20%)
2	PDY	C	2	-	24,30,30	1.73	3 (12%)	30,41,41	2.80	5 (16%)
2	PDY	D	1	-	24,30,30	1.76	3 (12%)	30,41,41	2.76	6 (20%)
2	PDY	D	2	-	24,30,30	1.71	3 (12%)	30,41,41	2.55	7 (23%)
2	PDY	E	1	-	24,30,30	1.76	3 (12%)	30,41,41	2.56	7 (23%)
2	PDY	E	2	-	24,30,30	1.74	3 (12%)	30,41,41	2.72	5 (16%)
2	PDY	F	1	-	24,30,30	1.76	3 (12%)	30,41,41	2.84	7 (23%)
2	PDY	F	2	-	24,30,30	1.75	3 (12%)	30,41,41	2.82	6 (20%)
3	SO4	F	3	-	4,4,4	0.30	0	6,6,6	0.16	0
2	PDY	G	1	-	24,30,30	1.77	3 (12%)	30,41,41	2.71	6 (20%)
2	PDY	G	2	-	24,30,30	1.75	3 (12%)	30,41,41	2.66	5 (16%)
2	PDY	H	1	-	24,30,30	1.79	3 (12%)	30,41,41	2.69	8 (26%)
2	PDY	H	2	-	24,30,30	1.79	3 (12%)	30,41,41	2.59	14 (46%)
2	PDY	I	1	-	24,30,30	1.77	3 (12%)	30,41,41	2.58	6 (20%)
2	PDY	I	2	-	24,30,30	1.73	3 (12%)	30,41,41	2.38	13 (43%)
2	PDY	J	1	-	24,30,30	1.73	3 (12%)	30,41,41	2.62	4 (13%)
2	PDY	J	2	-	24,30,30	1.74	3 (12%)	30,41,41	2.61	5 (16%)
2	PDY	K	1	-	24,30,30	1.75	3 (12%)	30,41,41	2.61	6 (20%)
2	PDY	K	2	-	24,30,30	1.75	3 (12%)	30,41,41	2.73	6 (20%)
2	PDY	L	1	-	24,30,30	1.78	3 (12%)	30,41,41	2.59	6 (20%)
2	PDY	L	2	-	24,30,30	1.73	3 (12%)	30,41,41	2.21	7 (23%)

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	-	-	0/11/19/19	0/4/4/4
2	PDY	A	2	-	-	0/11/19/19	0/4/4/4
2	PDY	B	1	-	-	0/11/19/19	0/4/4/4
2	PDY	B	2	-	-	0/11/19/19	0/4/4/4
2	PDY	C	1	-	-	0/11/19/19	0/4/4/4
2	PDY	C	2	-	-	0/11/19/19	0/4/4/4
2	PDY	D	1	-	-	0/11/19/19	0/4/4/4
2	PDY	D	2	-	-	1/11/19/19	0/4/4/4
2	PDY	E	1	-	-	0/11/19/19	0/4/4/4
2	PDY	E	2	-	-	0/11/19/19	0/4/4/4
2	PDY	F	1	-	-	0/11/19/19	0/4/4/4
2	PDY	F	2	-	-	0/11/19/19	0/4/4/4
3	SO4	F	3	-	-	0/0/0/0	0/0/0/0
2	PDY	G	1	-	-	0/11/19/19	0/4/4/4
2	PDY	G	2	-	-	0/11/19/19	0/4/4/4
2	PDY	H	1	-	-	0/11/19/19	0/4/4/4
2	PDY	H	2	-	-	1/11/19/19	0/4/4/4
2	PDY	I	1	-	-	0/11/19/19	0/4/4/4
2	PDY	I	2	-	-	0/11/19/19	0/4/4/4
2	PDY	J	1	-	-	0/11/19/19	0/4/4/4
2	PDY	J	2	-	-	0/11/19/19	0/4/4/4
2	PDY	K	1	-	-	0/11/19/19	0/4/4/4
2	PDY	K	2	-	-	0/11/19/19	0/4/4/4
2	PDY	L	1	-	-	0/11/19/19	0/4/4/4
2	PDY	L	2	-	-	1/11/19/19	0/4/4/4

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	PDY	C13-N9	-3.79	1.32	1.40
2	F	1	PDY	C13-N9	-3.68	1.32	1.40
2	K	1	PDY	C13-N9	-3.67	1.33	1.40
2	E	1	PDY	C13-N9	-3.66	1.33	1.40
2	A	1	PDY	C13-N9	-3.63	1.33	1.40
2	B	1	PDY	C13-N9	-3.58	1.33	1.40
2	I	1	PDY	C13-N9	-3.58	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	-3.56	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1	PDY	C13-N9	-3.55	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	-3.33	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	-3.18	1.34	1.40
2	F	2	PDY	C4-N6	2.41	1.34	1.31
2	B	2	PDY	C4-N6	2.44	1.34	1.31
2	G	1	PDY	C4-N6	2.48	1.34	1.31
2	D	1	PDY	C4-N6	2.50	1.34	1.31
2	J	2	PDY	C4-N6	2.50	1.34	1.31
2	L	2	PDY	C4-N6	2.50	1.34	1.31
2	I	2	PDY	C4-N6	2.51	1.34	1.31
2	H	2	PDY	C4-N6	2.54	1.34	1.31
2	F	1	PDY	C4-N6	2.55	1.34	1.31
2	I	1	PDY	C4-N6	2.56	1.34	1.31
2	E	1	PDY	C4-N6	2.56	1.34	1.31
2	B	1	PDY	C4-N6	2.57	1.34	1.31
2	K	1	PDY	C4-N6	2.59	1.34	1.31
2	K	2	PDY	C4-N6	2.60	1.34	1.31
2	C	2	PDY	C4-N6	2.62	1.34	1.31
2	C	1	PDY	C4-N6	2.62	1.34	1.31
2	A	1	PDY	C4-N6	2.62	1.34	1.31
2	J	1	PDY	C4-N6	2.63	1.34	1.31
2	H	1	PDY	C4-N6	2.64	1.34	1.31
2	E	2	PDY	C4-N6	2.64	1.34	1.31
2	L	1	PDY	C4-N6	2.69	1.34	1.31
2	G	2	PDY	C4-N6	2.72	1.35	1.31
2	D	2	PDY	C4-N6	2.73	1.35	1.31
2	A	2	PDY	C4-N6	2.82	1.35	1.31
2	A	2	PDY	C11-N7	6.49	1.47	1.33
2	H	1	PDY	C11-N7	6.53	1.47	1.33
2	D	2	PDY	C11-N7	6.54	1.47	1.33
2	L	2	PDY	C11-N7	6.54	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	1	PDY	C11-N7	6.54	1.47	1.33
2	J	1	PDY	C11-N7	6.55	1.47	1.33
2	I	2	PDY	C11-N7	6.55	1.47	1.33
2	I	1	PDY	C11-N7	6.58	1.47	1.33
2	C	1	PDY	C11-N7	6.58	1.47	1.33
2	J	2	PDY	C11-N7	6.59	1.47	1.33
2	F	1	PDY	C11-N7	6.59	1.47	1.33
2	D	1	PDY	C11-N7	6.59	1.47	1.33
2	E	1	PDY	C11-N7	6.60	1.47	1.33
2	A	1	PDY	C11-N7	6.60	1.47	1.33
2	F	2	PDY	C11-N7	6.60	1.47	1.33
2	B	2	PDY	C11-N7	6.60	1.47	1.33
2	B	1	PDY	C11-N7	6.62	1.47	1.33
2	G	2	PDY	C11-N7	6.63	1.47	1.33
2	C	2	PDY	C11-N7	6.64	1.47	1.33
2	G	1	PDY	C11-N7	6.65	1.47	1.33
2	H	2	PDY	C11-N7	6.66	1.47	1.33
2	L	1	PDY	C11-N7	6.66	1.47	1.33
2	K	2	PDY	C11-N7	6.67	1.47	1.33
2	E	2	PDY	C11-N7	6.70	1.47	1.33

All (160) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1	PDY	C14-C3-C4	-5.16	116.33	121.84
2	L	2	PDY	C14-C3-C4	-5.05	116.45	121.84
2	H	1	PDY	C24-O21-C16	-4.57	105.36	117.93
2	F	1	PDY	C8-C11-N7	-4.52	100.08	111.35
2	F	1	PDY	C14-C3-C4	-4.51	117.03	121.84
2	B	1	PDY	C8-C11-N7	-4.48	100.18	111.35
2	L	1	PDY	C8-C11-N7	-4.45	100.25	111.35
2	C	1	PDY	C8-C11-N7	-4.43	100.30	111.35
2	D	2	PDY	C14-C3-C4	-4.42	117.12	121.84
2	F	2	PDY	C14-C3-C4	-4.42	117.12	121.84
2	A	1	PDY	C8-C11-N7	-4.40	100.37	111.35
2	D	1	PDY	C8-C11-N7	-4.35	100.50	111.35
2	H	1	PDY	C14-C3-C4	-4.34	117.20	121.84
2	H	1	PDY	C8-C11-N7	-4.34	100.53	111.35
2	B	2	PDY	C4-N10-C15	-4.33	116.16	124.10
2	A	2	PDY	C8-C11-N7	-4.32	100.57	111.35
2	G	1	PDY	C8-C11-N7	-4.30	100.62	111.35
2	C	2	PDY	C8-C11-N7	-4.29	100.65	111.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1	PDY	C8-C11-N7	-4.28	100.67	111.35
2	K	1	PDY	C8-C11-N7	-4.27	100.69	111.35
2	B	2	PDY	C8-C11-N7	-4.26	100.73	111.35
2	F	2	PDY	C8-C11-N7	-4.26	100.74	111.35
2	E	1	PDY	C8-C11-N7	-4.25	100.75	111.35
2	I	1	PDY	C8-C11-N7	-4.25	100.76	111.35
2	F	2	PDY	C4-N10-C15	-4.19	116.42	124.10
2	K	1	PDY	C14-C3-C4	-4.17	117.38	121.84
2	D	1	PDY	C14-C3-C4	-4.17	117.38	121.84
2	J	2	PDY	C8-C11-N7	-4.17	100.97	111.35
2	K	2	PDY	C8-C11-N7	-4.16	100.99	111.35
2	E	2	PDY	C8-C11-N7	-4.15	101.01	111.35
2	G	2	PDY	C8-C11-N7	-4.14	101.03	111.35
2	K	2	PDY	C4-N10-C15	-4.06	116.66	124.10
2	G	2	PDY	C14-C3-C4	-4.02	117.55	121.84
2	H	2	PDY	C19-C16-C20	-3.99	113.91	120.19
2	K	2	PDY	C14-C3-C4	-3.98	117.59	121.84
2	D	2	PDY	C8-C11-N7	-3.95	101.51	111.35
2	B	1	PDY	C14-C3-C4	-3.86	117.72	121.84
2	G	1	PDY	C14-C3-C4	-3.84	117.73	121.84
2	L	2	PDY	C8-C11-N7	-3.79	101.91	111.35
2	I	2	PDY	C8-C11-N7	-3.78	101.93	111.35
2	H	2	PDY	C8-C11-N7	-3.73	102.05	111.35
2	I	2	PDY	C14-C3-C4	-3.65	117.94	121.84
2	D	2	PDY	C25-C15-C22	-3.64	105.19	109.75
2	C	2	PDY	C14-C3-C4	-3.60	118.00	121.84
2	A	1	PDY	C25-C15-N10	-3.45	104.63	110.55
2	A	2	PDY	C14-C3-C4	-3.45	118.15	121.84
2	E	2	PDY	C14-C3-C4	-3.45	118.15	121.84
2	F	1	PDY	C24-O21-C16	-3.45	108.44	117.93
2	H	2	PDY	C17-C13-N9	-3.43	109.38	120.67
2	J	2	PDY	C14-C3-C4	-3.41	118.20	121.84
2	G	1	PDY	C25-C15-N10	-3.36	104.79	110.55
2	G	1	PDY	C4-N10-C15	-3.32	118.00	124.10
2	C	1	PDY	C14-C3-C4	-3.29	118.32	121.84
2	B	2	PDY	C14-C3-C4	-3.28	118.33	121.84
2	I	1	PDY	C14-C3-C4	-3.24	118.38	121.84
2	C	1	PDY	C22-C15-N10	-3.21	105.76	109.96
2	I	2	PDY	C4-N10-C15	-3.16	118.31	124.10
2	H	2	PDY	C14-C3-C4	-3.07	118.56	121.84
2	E	1	PDY	C14-C3-C4	-3.06	118.57	121.84
2	D	1	PDY	C24-O21-C16	-2.94	109.85	117.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2	PDY	C4-N10-C15	-2.92	118.74	124.10
2	K	1	PDY	C24-O21-C16	-2.92	109.90	117.93
2	C	2	PDY	C4-N10-C15	-2.89	118.80	124.10
2	H	2	PDY	C4-N10-C15	-2.87	118.84	124.10
2	A	1	PDY	C14-C3-C4	-2.86	118.79	121.84
2	D	1	PDY	C25-C15-N10	-2.85	105.67	110.55
2	E	1	PDY	C24-O21-C16	-2.74	110.40	117.93
2	C	1	PDY	C4-N10-C15	-2.71	119.12	124.10
2	J	2	PDY	C4-N10-C15	-2.71	119.13	124.10
2	I	2	PDY	C25-C15-C22	-2.68	106.40	109.75
2	H	2	PDY	C24-O21-C16	-2.63	110.69	117.93
2	L	1	PDY	C4-N10-C15	-2.61	119.32	124.10
2	H	1	PDY	C20-C17-C13	-2.58	117.28	120.30
2	E	1	PDY	C4-N10-C15	-2.58	119.38	124.10
2	I	1	PDY	C4-N10-C15	-2.53	119.46	124.10
2	A	2	PDY	C25-C15-C22	-2.52	106.59	109.75
2	I	2	PDY	C17-C13-N9	-2.46	112.57	120.67
2	E	1	PDY	C25-C15-N10	-2.45	106.36	110.55
2	F	2	PDY	C25-C15-N10	-2.39	106.46	110.55
2	F	1	PDY	C4-N10-C15	-2.37	119.76	124.10
2	H	2	PDY	C25-C15-C22	-2.35	106.80	109.75
2	H	1	PDY	C4-N10-C15	-2.33	119.82	124.10
2	H	2	PDY	N10-C4-N6	-2.28	113.10	118.42
2	I	2	PDY	C19-C16-C20	-2.26	116.62	120.19
2	F	1	PDY	C22-C15-N10	-2.26	107.00	109.96
2	K	1	PDY	C4-N10-C15	-2.24	119.98	124.10
2	K	2	PDY	C24-O21-C16	-2.23	111.78	117.93
2	B	1	PDY	C4-N10-C15	-2.18	120.10	124.10
2	L	2	PDY	C25-C15-C22	-2.13	107.09	109.75
2	I	1	PDY	C25-C15-N10	-2.09	106.97	110.55
2	I	2	PDY	C18-C13-C17	-2.07	116.15	119.04
2	A	2	PDY	C18-C13-C17	-2.03	116.20	119.04
2	L	1	PDY	C14-C3-C4	-2.01	119.69	121.84
2	A	2	PDY	C19-C18-C13	2.01	122.65	120.30
2	I	2	PDY	C18-C19-C16	2.08	122.35	119.74
2	L	2	PDY	C22-C15-N10	2.23	112.88	109.96
2	H	1	PDY	C18-C13-C17	2.25	122.17	119.04
2	I	2	PDY	C14-C3-C1	2.28	125.01	121.72
2	I	2	PDY	C20-C17-C13	2.42	123.13	120.30
2	D	2	PDY	C3-C1-N9	2.43	129.07	122.91
2	A	1	PDY	C13-N9-C1	2.45	132.81	126.76
2	H	2	PDY	C14-C3-C1	2.46	125.26	121.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	2	PDY	C13-N9-C1	2.67	133.36	126.76
2	H	2	PDY	C18-C13-N9	2.70	129.56	120.67
2	L	1	PDY	C13-N9-C1	2.84	133.77	126.76
2	L	2	PDY	C14-C3-C1	2.88	125.88	121.72
2	D	2	PDY	C13-N9-C1	2.92	133.98	126.76
2	E	2	PDY	C25-C15-N10	2.96	115.63	110.55
2	H	2	PDY	C22-C15-N10	3.03	113.92	109.96
2	I	2	PDY	C13-N9-C1	3.22	134.72	126.76
2	A	2	PDY	C3-C1-N9	3.31	131.28	122.91
2	A	2	PDY	C22-C15-N10	3.44	114.46	109.96
2	I	2	PDY	C22-C15-N10	3.60	114.67	109.96
2	I	1	PDY	C1-C3-C4	3.63	118.71	115.78
2	G	1	PDY	C1-C3-C4	4.06	119.06	115.78
2	A	1	PDY	C1-C3-C4	4.16	119.14	115.78
2	H	1	PDY	C1-C3-C4	4.16	119.14	115.78
2	H	2	PDY	C13-N9-C1	4.34	137.48	126.76
2	C	1	PDY	C1-C3-C4	4.39	119.32	115.78
2	L	1	PDY	C1-C3-C4	4.40	119.33	115.78
2	E	1	PDY	C1-C3-C4	4.40	119.33	115.78
2	H	2	PDY	C17-C20-C16	4.96	125.96	119.74
2	B	1	PDY	C1-C3-C4	5.03	119.84	115.78
2	K	1	PDY	C1-C3-C4	5.22	119.99	115.78
2	K	2	PDY	C1-C3-C4	5.24	120.01	115.78
2	J	2	PDY	C1-C3-C4	5.28	120.04	115.78
2	D	1	PDY	C1-C3-C4	5.31	120.06	115.78
2	F	1	PDY	C1-C3-C4	5.31	120.06	115.78
2	J	1	PDY	C1-C3-C4	5.33	120.08	115.78
2	F	2	PDY	C1-C3-C4	5.35	120.10	115.78
2	D	2	PDY	C1-C3-C4	5.40	120.14	115.78
2	B	2	PDY	C1-C3-C4	5.52	120.23	115.78
2	G	2	PDY	C1-C3-C4	6.06	120.67	115.78
2	C	2	PDY	C1-C3-C4	6.26	120.83	115.78
2	H	2	PDY	C11-N7-N2	6.74	108.51	103.70
2	A	2	PDY	C1-C3-C4	6.80	121.27	115.78
2	E	2	PDY	C1-C3-C4	6.87	121.32	115.78
2	I	2	PDY	C11-N7-N2	7.72	109.21	103.70
2	L	2	PDY	C11-N7-N2	7.92	109.35	103.70
2	D	2	PDY	C11-N7-N2	9.07	110.17	103.70
2	A	2	PDY	C11-N7-N2	9.99	110.83	103.70
2	H	1	PDY	C11-N7-N2	10.48	111.17	103.70
2	K	1	PDY	C11-N7-N2	10.61	111.27	103.70
2	G	2	PDY	C11-N7-N2	10.65	111.30	103.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1	PDY	C11-N7-N2	10.68	111.31	103.70
2	J	2	PDY	C11-N7-N2	10.70	111.33	103.70
2	E	2	PDY	C11-N7-N2	10.73	111.35	103.70
2	I	1	PDY	C11-N7-N2	10.87	111.45	103.70
2	E	1	PDY	C11-N7-N2	10.88	111.46	103.70
2	K	2	PDY	C11-N7-N2	10.89	111.47	103.70
2	L	1	PDY	C11-N7-N2	11.38	111.81	103.70
2	F	2	PDY	C11-N7-N2	11.44	111.86	103.70
2	B	2	PDY	C11-N7-N2	11.45	111.87	103.70
2	G	1	PDY	C11-N7-N2	11.48	111.89	103.70
2	C	1	PDY	C11-N7-N2	11.51	111.91	103.70
2	F	1	PDY	C11-N7-N2	11.59	111.97	103.70
2	D	1	PDY	C11-N7-N2	11.61	111.98	103.70
2	A	1	PDY	C11-N7-N2	11.79	112.11	103.70
2	C	2	PDY	C11-N7-N2	11.81	112.12	103.70
2	B	1	PDY	C11-N7-N2	11.91	112.20	103.70

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	2	PDY	C3-C1-N9-C13
2	L	2	PDY	C3-C1-N9-C13
2	H	2	PDY	C3-C1-N9-C13

There are no ring outliers.

25 monomers are involved in 243 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	PDY	4	0
2	A	2	PDY	3	0
2	B	1	PDY	8	0
2	B	2	PDY	8	0
2	C	1	PDY	6	0
2	C	2	PDY	10	0
2	D	1	PDY	8	0
2	D	2	PDY	5	0
2	E	1	PDY	10	0
2	E	2	PDY	9	0
2	F	1	PDY	6	0
2	F	2	PDY	12	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	3	SO4	1	0
2	G	1	PDY	9	0
2	G	2	PDY	9	0
2	H	1	PDY	13	0
2	H	2	PDY	26	0
2	I	1	PDY	9	0
2	I	2	PDY	25	0
2	J	1	PDY	10	0
2	J	2	PDY	8	0
2	K	1	PDY	14	0
2	K	2	PDY	10	0
2	L	1	PDY	9	0
2	L	2	PDY	11	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q<0.9
1	A	274/324 (84%)	0.14	8 (2%) 52 46	8, 24, 56, 81	0
1	B	277/324 (85%)	0.21	5 (1%) 69 66	7, 29, 71, 80	0
1	C	273/324 (84%)	0.29	12 (4%) 35 30	15, 40, 73, 83	0
1	D	277/324 (85%)	0.27	9 (3%) 48 42	8, 32, 70, 81	0
1	E	276/324 (85%)	0.21	7 (2%) 58 53	10, 28, 58, 76	0
1	F	287/324 (88%)	0.15	13 (4%) 34 29	4, 25, 70, 86	0
1	G	273/324 (84%)	0.35	10 (3%) 42 37	16, 38, 67, 79	0
1	H	275/324 (84%)	0.28	14 (5%) 29 24	13, 39, 68, 84	0
1	I	275/324 (84%)	0.17	8 (2%) 52 46	14, 30, 66, 97	0
1	J	275/324 (84%)	0.51	15 (5%) 26 21	27, 52, 81, 100	0
1	K	273/324 (84%)	0.59	30 (10%) 6 4	25, 49, 76, 98	0
1	L	276/324 (85%)	0.43	16 (5%) 24 19	15, 46, 83, 110	0
All	All	3311/3888 (85%)	0.30	147 (4%) 35 30	4, 37, 73, 110	0

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	216	SER	6.7
1	J	155	ASP	6.6
1	K	157	ALA	6.1
1	I	229	TYR	5.9
1	H	155	ASP	5.8
1	C	154	GLY	4.7
1	B	157	ALA	4.4
1	E	229	TYR	4.4
1	G	229	TYR	4.2
1	K	155	ASP	4.2
1	B	155	ASP	4.1

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Mol	Chain	Res	Type	RSRZ
1	L	154	GLY	4.0
1	K	156	GLN	4.0
1	K	216	SER	3.9
1	F	229	TYR	3.9
1	K	240	TYR	3.7
1	I	216	SER	3.7
1	D	86	THR	3.7
1	K	289	PRO	3.7
1	H	230	VAL	3.7
1	K	342	LEU	3.7
1	J	294	VAL	3.6
1	L	155	ASP	3.6
1	F	155	ASP	3.6
1	C	216	SER	3.6
1	B	47	HIS	3.5
1	J	69	VAL	3.5
1	J	156	GLN	3.5
1	A	216	SER	3.5
1	I	230	VAL	3.5
1	H	215	THR	3.4
1	G	156	GLN	3.4
1	K	201	ALA	3.4
1	L	235	LEU	3.4
1	L	216	SER	3.3
1	H	216	SER	3.3
1	K	334	THR	3.3
1	D	72	LEU	3.3
1	F	236	GLY	3.3
1	G	329	THR	3.3
1	H	340	ARG	3.3
1	K	151	GLN	3.2
1	C	82	PHE	3.2
1	G	330	LYS	3.1
1	K	150	ILE	3.1
1	H	154	GLY	3.1
1	D	156	GLN	3.1
1	G	87	GLN	3.1
1	L	337	HIS	3.1
1	K	335	PRO	3.1
1	L	69	VAL	3.1
1	G	216	SER	3.1
1	D	69	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	J	229	TYR	3.1
1	K	85	ARG	3.1
1	F	216	SER	3.0
1	D	267	HIS	3.0
1	C	156	GLN	3.0
1	H	69	VAL	3.0
1	H	157	ALA	3.0
1	H	229	TYR	3.0
1	L	156	GLN	3.0
1	L	229	TYR	3.0
1	L	340	ARG	2.9
1	A	289	PRO	2.9
1	G	334	THR	2.8
1	D	82	PHE	2.8
1	J	337	HIS	2.8
1	J	75	ASN	2.7
1	H	156	GLN	2.7
1	L	334	THR	2.7
1	K	154	GLY	2.7
1	G	65	VAL	2.7
1	J	335	PRO	2.7
1	A	235	LEU	2.7
1	D	344	GLU	2.7
1	G	240	TYR	2.7
1	L	289	PRO	2.6
1	H	86	THR	2.6
1	H	265	SER	2.6
1	K	332	PRO	2.6
1	K	336	LEU	2.6
1	L	157	ALA	2.6
1	F	234	VAL	2.6
1	C	87	GLN	2.6
1	K	158	PHE	2.6
1	J	99	PRO	2.6
1	A	65	VAL	2.5
1	A	85	ARG	2.5
1	K	337	HIS	2.5
1	J	260	TYR	2.5
1	F	235	LEU	2.5
1	K	86	THR	2.5
1	H	150	ILE	2.5
1	J	215	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	L	330	LYS	2.4
1	K	153	ARG	2.4
1	G	294	VAL	2.4
1	K	257	LEU	2.4
1	J	79	LEU	2.4
1	K	160	GLU	2.3
1	A	343	LYS	2.3
1	F	48	VAL	2.3
1	I	155	ASP	2.3
1	C	65	VAL	2.3
1	C	85	ARG	2.3
1	F	151	GLN	2.3
1	C	157	ALA	2.3
1	I	72	LEU	2.3
1	I	79	LEU	2.2
1	J	72	LEU	2.2
1	L	153	ARG	2.2
1	F	238	GLU	2.2
1	C	234	VAL	2.2
1	A	68	GLN	2.2
1	K	294	VAL	2.2
1	D	67	SER	2.2
1	K	146	LEU	2.2
1	B	231	ALA	2.2
1	D	68	GLN	2.2
1	I	70	LEU	2.1
1	E	150	ILE	2.1
1	J	330	LYS	2.1
1	C	92	LEU	2.1
1	K	230	VAL	2.1
1	K	327	GLN	2.1
1	K	340	ARG	2.1
1	A	47	HIS	2.1
1	E	65	VAL	2.1
1	I	69	VAL	2.1
1	L	230	VAL	2.1
1	C	84	LYS	2.1
1	K	161	ARG	2.1
1	E	155	ASP	2.1
1	J	234	VAL	2.1
1	K	199	PRO	2.1
1	K	291	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	151	GLN	2.1
1	B	216	SER	2.1
1	F	240	TYR	2.1
1	F	154	GLY	2.0
1	F	156	GLN	2.0
1	F	47	HIS	2.0
1	L	285	GLU	2.0
1	C	153	ARG	2.0
1	E	86	THR	2.0
1	H	153	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	PDY	D	2	27/27	0.69	0.42	7.76	65,74,80,81	0
2	PDY	L	2	27/27	0.82	0.43	5.01	71,75,77,77	0
2	PDY	E	2	27/27	0.82	0.43	3.98	60,67,69,69	0
2	PDY	G	2	27/27	0.90	0.37	2.95	52,56,64,64	0
2	PDY	A	2	27/27	0.82	0.37	2.61	60,65,69,71	0
2	PDY	E	1	27/27	0.97	0.28	2.25	7,23,37,38	0
2	PDY	I	2	27/27	0.80	0.38	2.24	53,61,74,75	0
3	SO4	F	3	5/5	0.87	0.26	1.30	61,62,64,65	0
2	PDY	K	2	27/27	0.85	0.40	1.24	61,67,79,80	0
2	PDY	C	2	27/27	0.91	0.25	0.89	48,50,62,63	0
2	PDY	H	2	27/27	0.90	0.33	0.83	52,55,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	PDY	J	2	27/27	0.90	0.33	0.80	59,62,67,68	0
2	PDY	K	1	27/27	0.94	0.24	0.75	27,44,54,55	0
2	PDY	B	2	27/27	0.95	0.21	0.66	20,29,34,35	0
2	PDY	C	1	27/27	0.92	0.23	0.49	18,32,56,58	0
2	PDY	A	1	27/27	0.97	0.22	0.45	2,11,31,32	0
2	PDY	H	1	27/27	0.96	0.22	0.43	22,31,54,55	0
2	PDY	J	1	27/27	0.96	0.23	0.38	31,39,54,55	0
2	PDY	D	1	27/27	0.95	0.23	0.17	16,23,43,44	0
2	PDY	L	1	27/27	0.95	0.21	0.07	30,34,47,50	0
2	PDY	F	2	27/27	0.96	0.17	-0.37	20,24,28,29	0
2	PDY	I	1	27/27	0.96	0.19	-0.39	5,19,43,45	0
2	PDY	B	1	27/27	0.96	0.21	-0.40	6,16,37,38	0
2	PDY	F	1	27/27	0.96	0.17	-0.46	5,15,32,34	0
2	PDY	G	1	27/27	0.96	0.16	-0.58	4,20,38,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.