



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:47 PM GMT

PDB ID : 3S2C  
Title : Structure of the thermostable GH51 alpha-L-arabinofuranosidase from Thermotoga petrophila RKU-1  
Authors : Souza, T.A.C.B.; Santos, C.R.; Souza, A.R.; Oldiges, D.P.; Ruller, R.; Prade, R.A.; Squina, F.M.; Murakami, M.T.  
Deposited on : 2011-05-16  
Resolution : 3.00 Å(reported)

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

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

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

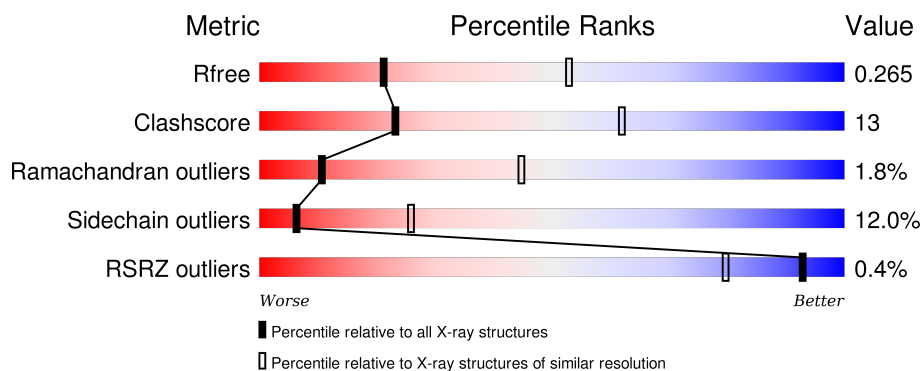
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	484	 66% 27% 6%
1	B	484	 70% 25% 5%
1	C	484	 69% 25% 6%
1	D	484	 65% 29% 5%
1	E	484	 68% 26% 5%

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Mol	Chain	Length	Quality of chain
1	F	484	<div><div></div><div>66%29%5%</div></div>
1	G	484	<div><div></div><div>66%26%8%</div></div>
1	H	484	<div><div>%<div></div></div><div>62%30%6%•</div></div>
1	I	484	<div><div>%<div></div></div><div>64%30%6%</div></div>
1	J	484	<div><div></div><div>68%26%5%•</div></div>
1	K	484	<div><div></div><div>69%25%6%</div></div>
1	L	484	<div><div>%<div></div></div><div>62%34%5%</div></div>

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 47152 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 Alpha-N-arabinofuranosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	483	Total	C	N	O	S	0	0	0
			3893	2499	649	730	15			
1	B	483	Total	C	N	O	S	0	0	0
			3893	2499	649	730	15			
1	C	483	Total	C	N	O	S	0	0	0
			3893	2499	649	730	15			
1	D	483	Total	C	N	O	S	0	0	0
			3893	2499	649	730	15			
1	E	483	Total	C	N	O	S	0	0	0
			3893	2499	649	730	15			
1	F	483	Total	C	N	O	S	0	0	0
			3893	2499	649	730	15			
1	G	483	Total	C	N	O	S	0	1	0
			3904	2505	653	731	15			
1	H	483	Total	C	N	O	S	0	0	0
			3893	2499	649	730	15			
1	I	483	Total	C	N	O	S	0	0	0
			3893	2499	649	730	15			
1	J	481	Total	C	N	O	S	0	0	0
			3876	2488	647	726	15			
1	K	483	Total	C	N	O	S	0	0	0
			3893	2499	649	730	15			
1	L	483	Total	C	N	O	S	0	1	0
			3902	2504	650	733	15			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	42	Total	O	0	0
			42	42		
2	B	43	Total	O	0	0
			43	43		

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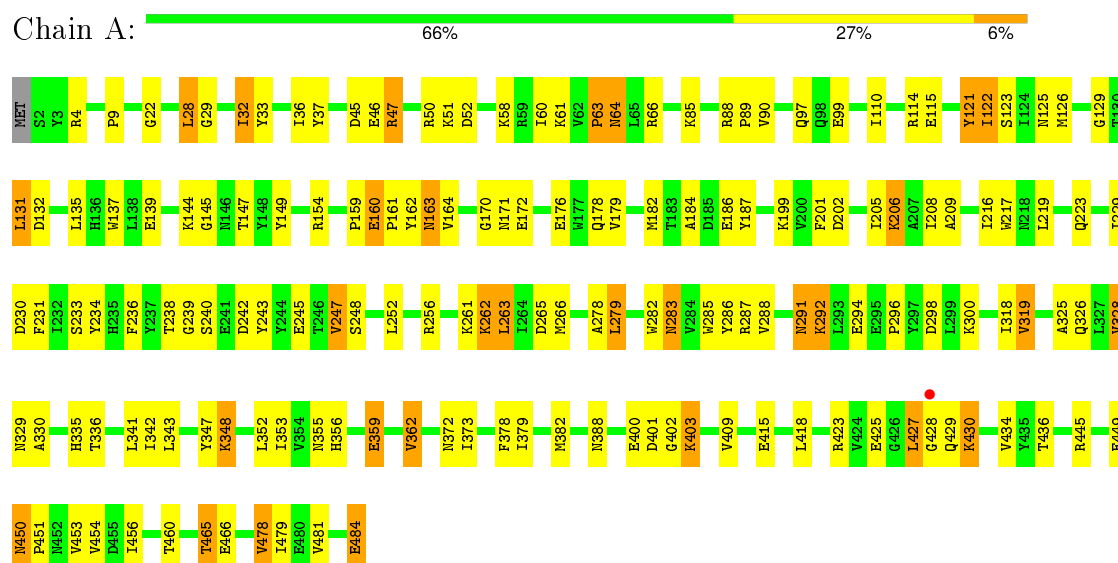
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	50	Total	O	0	0
			50	50		
2	D	54	Total	O	0	0
			54	54		
2	E	45	Total	O	0	0
			45	45		
2	F	39	Total	O	0	0
			39	39		
2	G	30	Total	O	0	0
			30	30		
2	H	28	Total	O	0	0
			28	28		
2	I	27	Total	O	0	0
			27	27		
2	J	23	Total	O	0	0
			23	23		
2	K	32	Total	O	0	0
			32	32		
2	L	20	Total	O	0	0
			20	20		

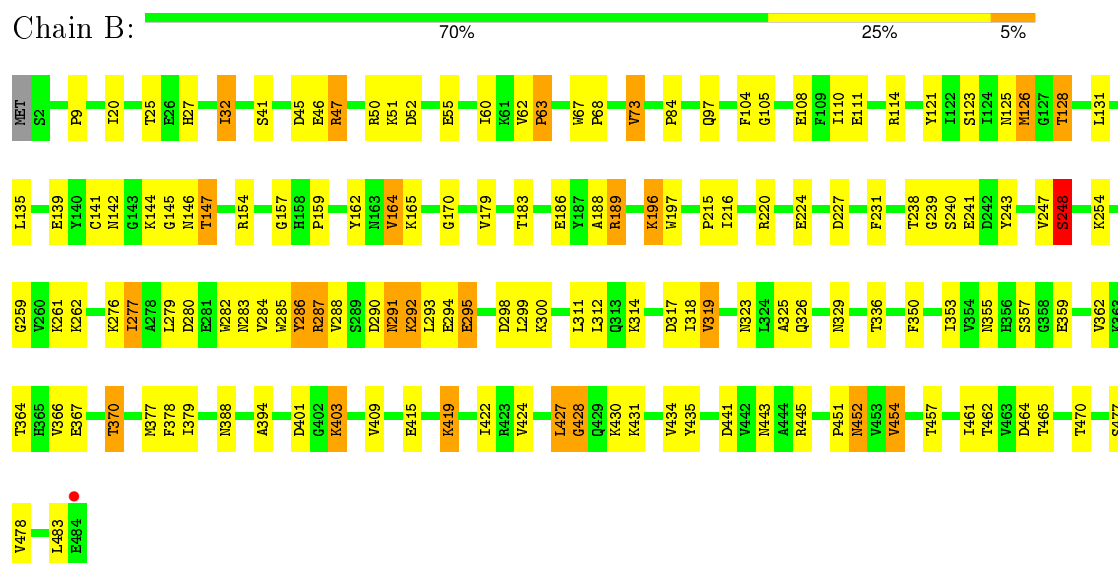
### 3 Residue-property plots

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

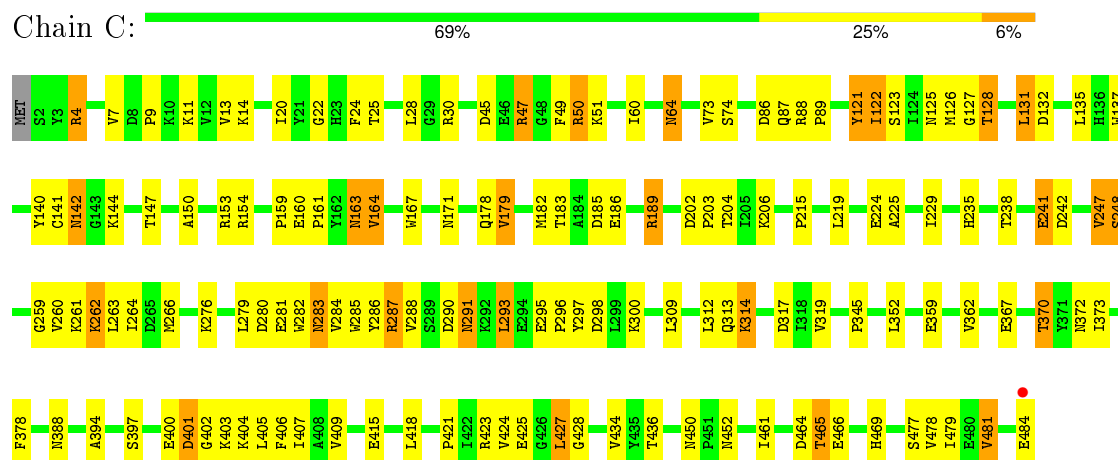
#### • Molecule 1: Alpha-N-arabinofuranosidase



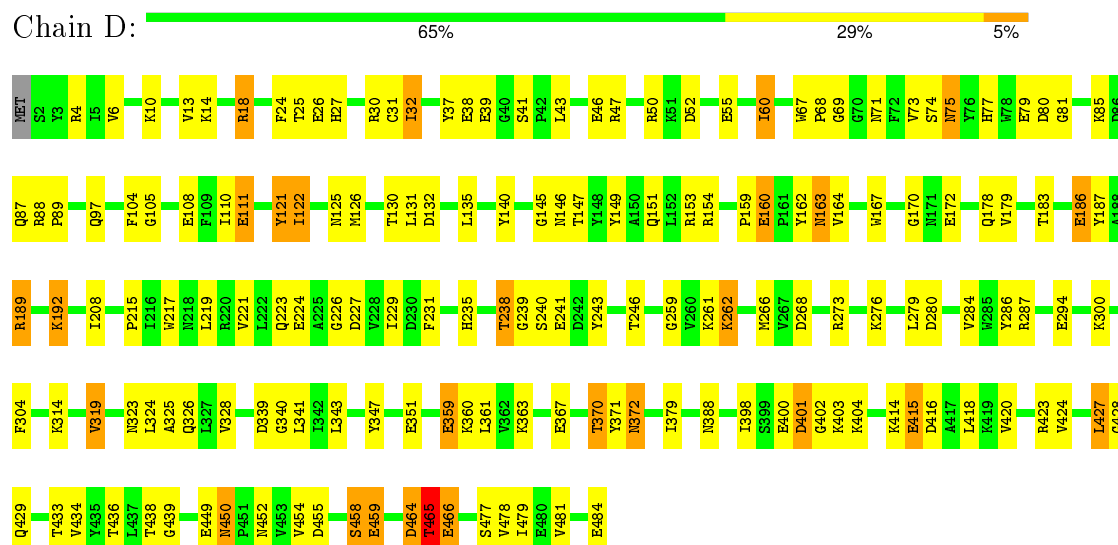
#### • Molecule 1: Alpha-N-arabinofuranosidase



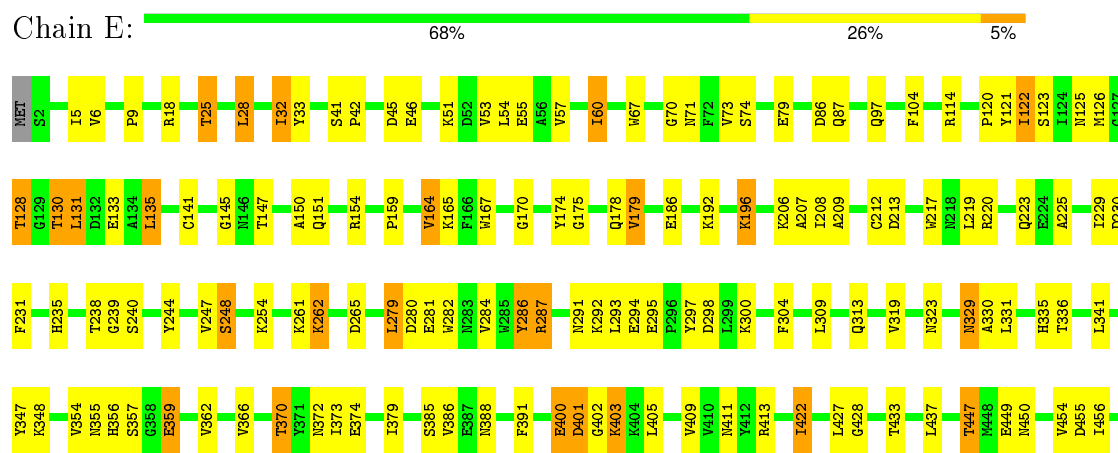
#### • Molecule 1: Alpha-N-arabinofuranosidase



• Molecule 1: Alpha-N-arabinofuranosidase



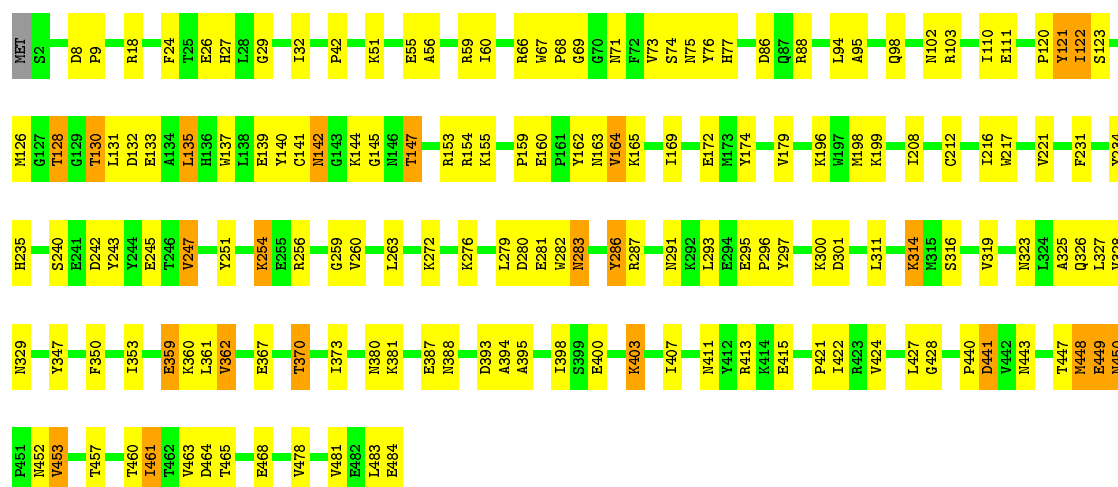
• Molecule 1: Alpha-N-arabinofuranosidase





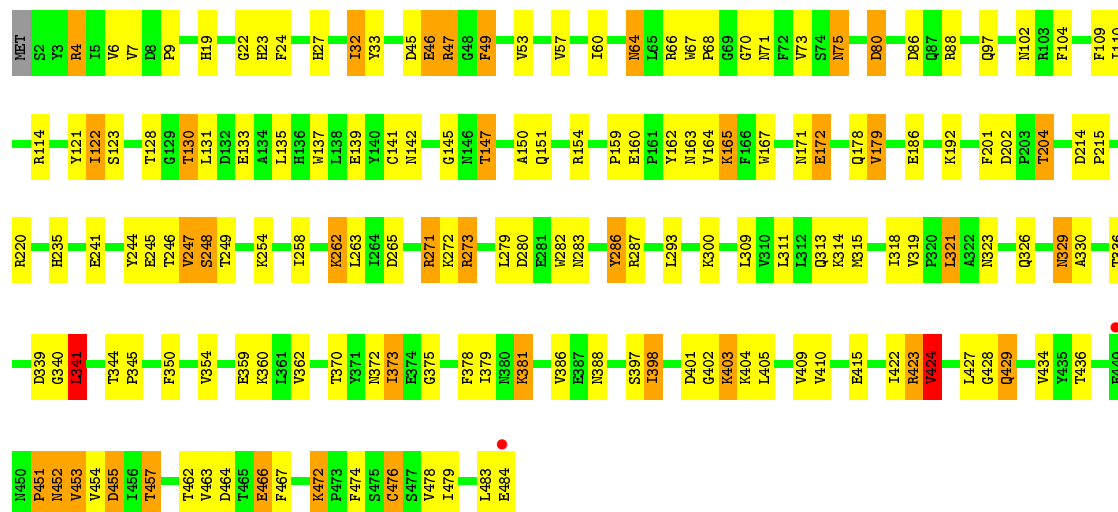
• Molecule 1: Alpha-N-arabinofuranosidase

Chain F: 66% 29% 5%



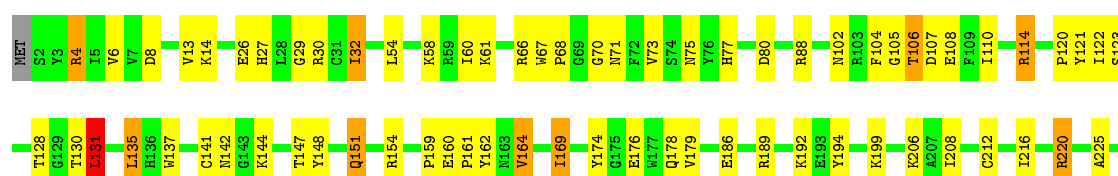
• Molecule 1: Alpha-N-arabinofuranosidase

Chain G: 66% 26% 8%

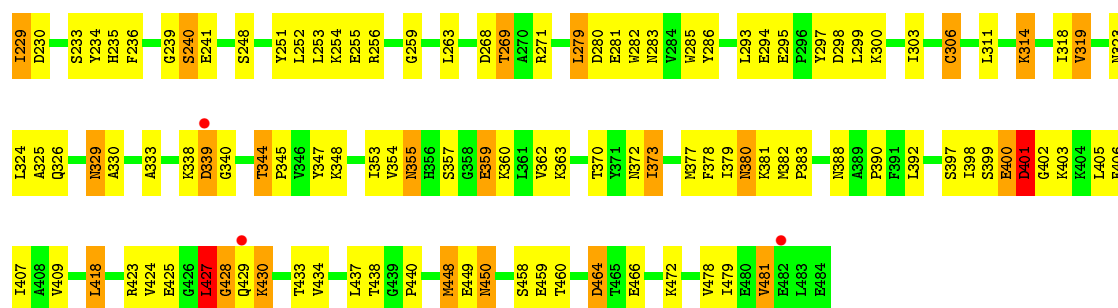


• Molecule 1: Alpha-N-arabinofuranosidase

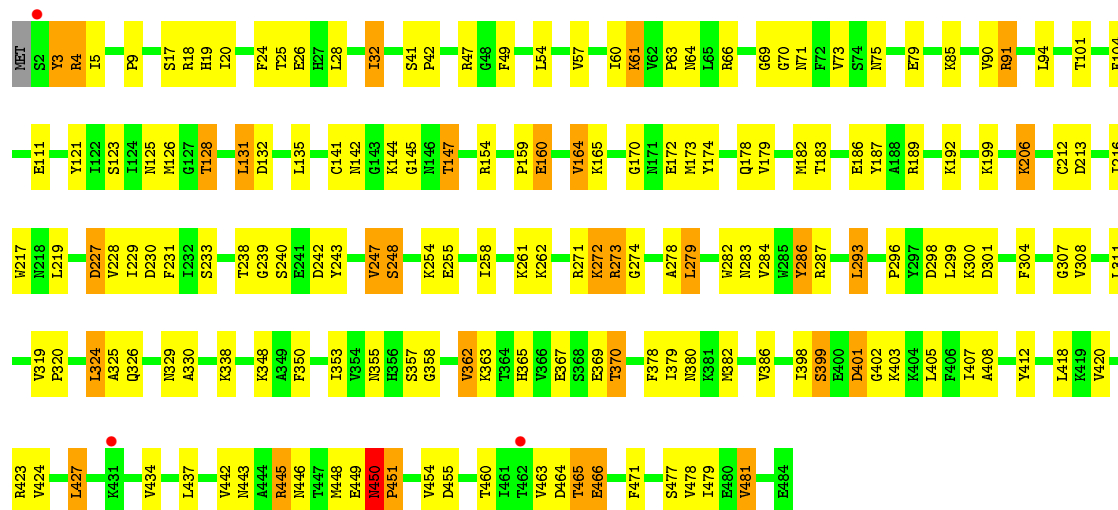
Chain H: 62% 30% 6%



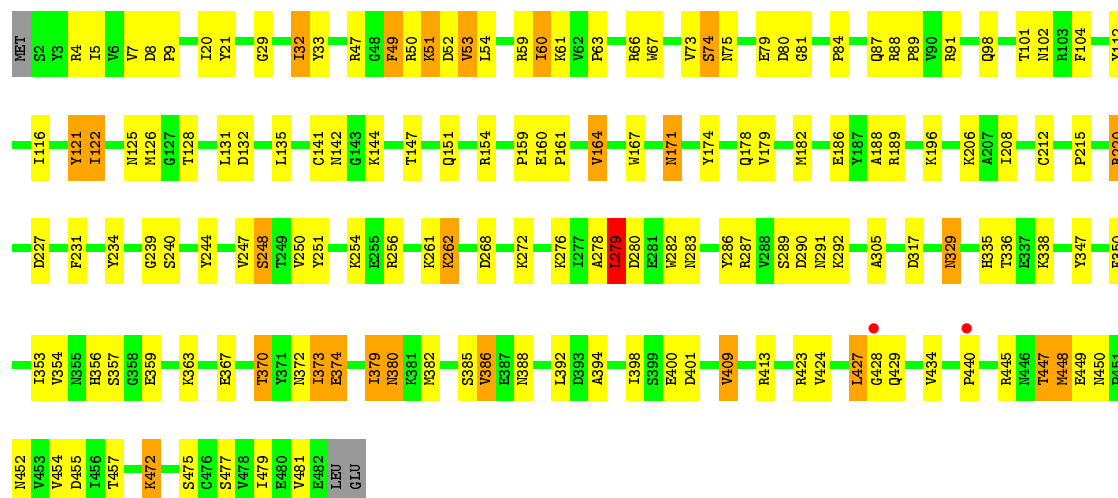




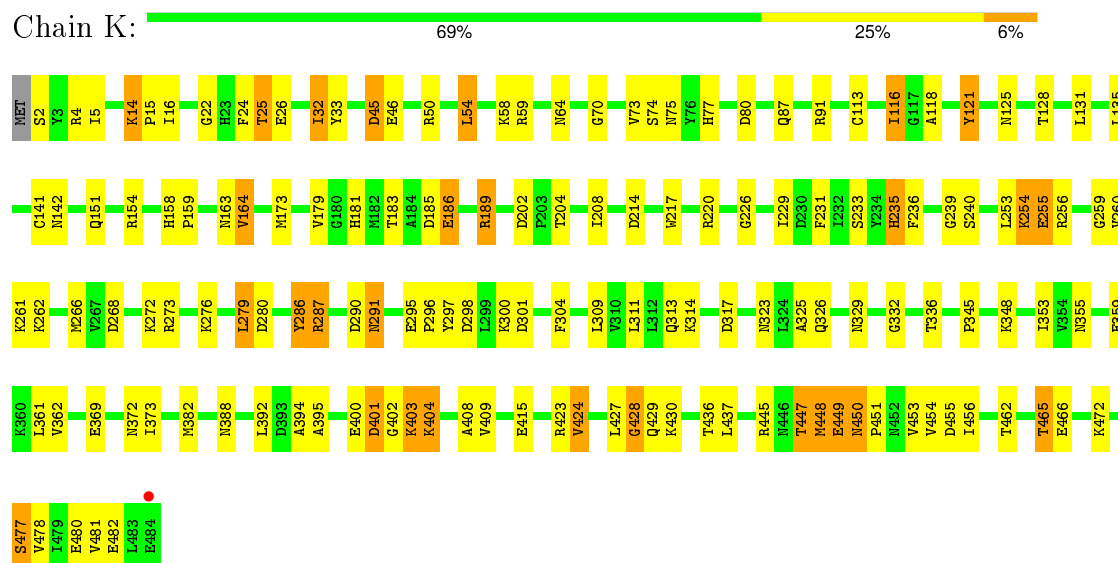
• Molecule 1: Alpha-N-arabinofuranosidase



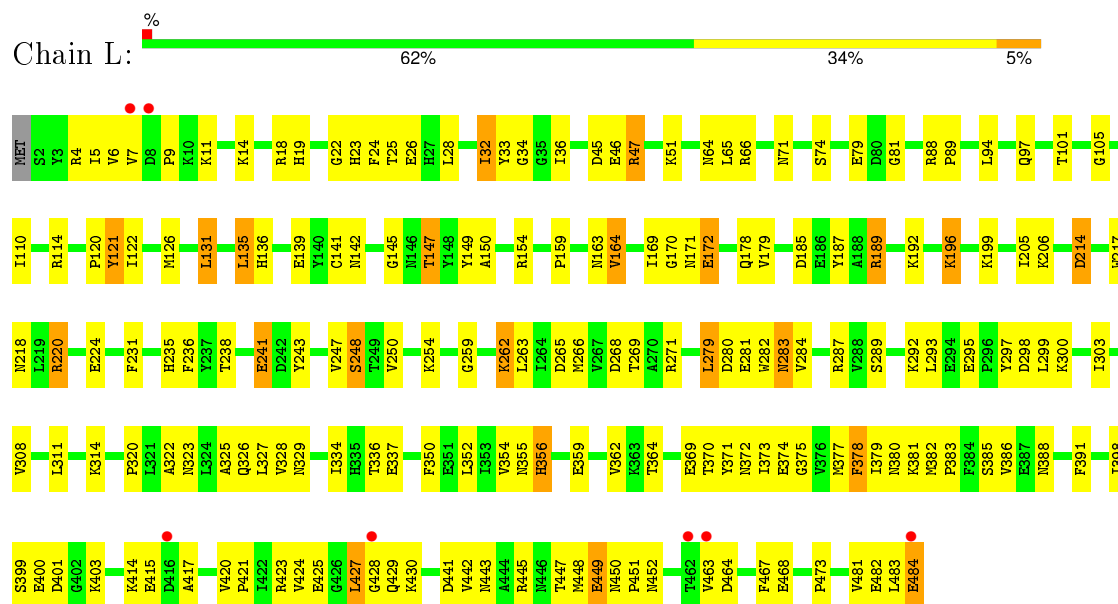
• Molecule 1: Alpha-N-arabinofuranosidase



• Molecule 1: Alpha-N-arabinofuranosidase



• Molecule 1: Alpha-N-arabinofuranosidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.95Å 187.29Å 180.64Å 90.00° 90.87° 90.00°	Depositor
Resolution (Å)	49.24 – 3.00 48.87 – 2.99	Depositor EDS
% Data completeness (in resolution range)	97.2 (49.24-3.00) 97.2 (48.87-2.99)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.01 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.195 , 0.268 0.195 , 0.265	Depositor DCC
$R_{free}$ test set	6906 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.9	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 51.6	EDS
Estimated twinning fraction	0.000 for -h,-l,-k 0.000 for -h,l,k 0.013 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 137481 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	47152	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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	0.52	0/3990	0.67	0/5413
1	B	0.55	0/3990	0.68	0/5413
1	C	0.55	0/3990	0.67	0/5413
1	D	0.54	0/3990	0.69	1/5413 (0.0%)
1	E	0.56	0/3990	0.69	0/5413
1	F	0.54	0/3990	0.68	0/5413
1	G	0.52	0/4001	0.69	1/5427 (0.0%)
1	H	0.53	0/3990	0.68	3/5413 (0.1%)
1	I	0.49	0/3990	0.64	1/5413 (0.0%)
1	J	0.48	0/3973	0.63	1/5390 (0.0%)
1	K	0.50	0/3990	0.66	0/5413
1	L	0.49	0/3999	0.66	0/5426
All	All	0.52	0/47883	0.67	7/64960 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	D	0	2
1	J	0	1
1	K	0	2
All	All	0	7

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	341	LEU	CA-CB-CG	6.25	129.68	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	239	GLY	N-CA-C	-6.21	97.58	113.10
1	H	131	LEU	CA-CB-CG	6.16	129.46	115.30
1	H	427	LEU	CA-CB-CG	5.86	128.78	115.30
1	J	279	LEU	CA-CB-CG	5.74	128.50	115.30
1	I	293	LEU	CA-CB-CG	5.33	127.56	115.30
1	H	269	THR	N-CA-C	-5.05	97.35	111.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	63	PRO	Peptide
1	B	63	PRO	Peptide
1	D	238	THR	Peptide
1	D	240	SER	Peptide
1	J	448	MET	Peptide
1	K	14	LYS	Peptide
1	K	15	PRO	Peptide

## 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	3893	0	3818	116	0
1	B	3893	0	3818	94	0
1	C	3893	0	3818	99	0
1	D	3893	0	3818	120	0
1	E	3893	0	3818	105	0
1	F	3893	0	3818	91	0
1	G	3904	0	3830	103	0
1	H	3893	0	3818	118	0
1	I	3893	0	3818	115	0
1	J	3876	0	3801	84	0
1	K	3893	0	3818	100	0
1	L	3902	0	3824	127	0
2	A	42	0	0	1	0
2	B	43	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	50	0	0	0	0
2	D	54	0	0	1	0
2	E	45	0	0	3	0
2	F	39	0	0	4	0
2	G	30	0	0	3	0
2	H	28	0	0	3	0
2	I	27	0	0	2	0
2	J	23	0	0	2	0
2	K	32	0	0	1	0
2	L	20	0	0	1	0
All	All	47152	0	45817	1236	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 13.

All (1236) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:ASN:HB3	2:B:495:HOH:O	1.43	1.19
1:E:125:ASN:HD21	1:E:128:THR:HG22	1.05	1.11
1:L:154:ARG:HG2	1:L:159:PRO:HA	1.36	1.05
1:G:4:ARG:HH11	1:G:4:ARG:HG3	1.21	1.02
1:F:154:ARG:HG2	1:F:159:PRO:HA	1.37	1.01
1:L:329:ASN:HD21	1:L:336:THR:H	1.07	1.00
1:L:428:GLY:HA3	1:L:464:ASP:HA	1.42	1.00
1:L:26:GLU:HG2	1:L:326:GLN:HE22	1.26	0.99
1:J:60:ILE:HD11	1:J:350:PHE:CB	1.93	0.99
1:I:60:ILE:HD11	1:I:350:PHE:CB	1.92	0.98
1:G:154:ARG:HG2	1:G:159:PRO:HA	1.43	0.98
1:J:60:ILE:HD11	1:J:350:PHE:HB3	0.99	0.97
1:I:60:ILE:HD11	1:I:350:PHE:HB2	1.46	0.97
1:B:247:VAL:O	1:B:248:SER:HB3	1.64	0.95
1:J:60:ILE:CD1	1:J:350:PHE:HB3	1.95	0.95
1:L:429:GLN:HG3	1:L:464:ASP:HB2	1.49	0.94
1:E:125:ASN:ND2	1:E:128:THR:HG22	1.82	0.94
1:H:372:ASN:ND2	1:H:388:ASN:H	1.64	0.93
1:L:370:THR:HG23	1:L:388:ASN:HA	1.50	0.92
1:I:450:ASN:H	1:I:451:PRO:HD3	1.33	0.92
1:L:220:ARG:HH11	1:L:220:ARG:HG3	1.34	0.92
1:F:126:MET:HE1	1:F:169:ILE:HG22	1.52	0.91
1:D:464:ASP:O	1:D:466:GLU:N	2.04	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:GLN:HE22	1:B:216:ILE:HD11	1.35	0.89
1:J:32:ILE:HG23	1:J:33:TYR:H	1.37	0.89
1:F:59:ARG:HD3	2:F:523:HOH:O	1.73	0.88
1:B:239:GLY:HA3	1:B:240:SER:OG	1.74	0.88
1:K:287:ARG:HD3	1:K:296:PRO:HD2	1.54	0.88
1:J:373:ILE:HD12	1:J:386:VAL:HG13	1.52	0.88
1:K:348:LYS:HB3	1:K:437:LEU:HD21	1.56	0.87
1:J:329:ASN:HD21	1:J:336:THR:H	1.22	0.87
1:L:189:ARG:HG3	1:L:189:ARG:HH11	1.38	0.87
1:H:372:ASN:HD21	1:H:388:ASN:H	1.21	0.87
1:C:287:ARG:HD3	1:C:296:PRO:HD2	1.56	0.87
1:H:4:ARG:HG3	1:H:4:ARG:HH11	1.41	0.86
1:J:142:ASN:HD21	1:J:164:VAL:H	1.20	0.85
1:A:449:GLU:O	1:A:450:ASN:HB2	1.75	0.85
1:B:292:LYS:HG3	1:B:294:GLU:HG3	1.58	0.85
1:A:32:ILE:HG23	1:A:33:TYR:H	1.42	0.85
1:C:125:ASN:HD21	1:C:128:THR:H	1.20	0.85
1:B:189:ARG:HG3	1:B:189:ARG:HH11	1.42	0.85
1:J:154:ARG:HG2	1:J:159:PRO:HA	1.57	0.84
1:K:262:LYS:HG2	1:L:259:GLY:HA2	1.59	0.83
1:A:359:GLU:HG3	1:A:400:GLU:HG2	1.59	0.83
1:D:126:MET:CE	1:D:187:TYR:HE1	1.89	0.83
1:I:449:GLU:O	1:I:450:ASN:HB2	1.76	0.82
1:F:126:MET:CE	1:F:169:ILE:HG22	2.09	0.82
1:J:424:VAL:HG13	1:J:427:LEU:HG	1.61	0.82
1:A:262:LYS:HB2	1:A:262:LYS:HZ2	1.44	0.81
1:B:139:GLU:HG2	1:B:147:THR:HG21	1.63	0.81
1:D:47:ARG:NH1	1:D:111:GLU:OE1	2.13	0.80
1:C:247:VAL:O	1:C:248:SER:HB3	1.80	0.80
1:D:449:GLU:O	1:D:450:ASN:HB2	1.80	0.80
1:L:398:ILE:HG22	1:L:399:SER:O	1.82	0.79
1:C:405:LEU:HB3	1:C:481:VAL:HG12	1.63	0.79
1:G:142:ASN:HD21	1:G:164:VAL:H	1.29	0.79
1:D:26:GLU:HG3	1:D:69:GLY:HA2	1.65	0.79
1:E:53:VAL:O	1:E:57:VAL:HG23	1.83	0.79
1:B:47:ARG:HB2	1:B:47:ARG:HH11	1.46	0.78
1:L:329:ASN:ND2	1:L:336:THR:H	1.80	0.78
1:F:359:GLU:HG3	1:F:400:GLU:HG2	1.65	0.78
1:D:415:GLU:HG2	1:D:416:ASP:OD1	1.84	0.78
1:L:126:MET:HE2	1:L:170:GLY:HA3	1.65	0.78
1:I:147:THR:HB	2:I:485:HOH:O	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:247:VAL:O	1:I:248:SER:HB3	1.85	0.77
1:C:291:ASN:HD22	1:C:291:ASN:H	1.30	0.77
1:H:268:ASP:HB3	1:H:271:ARG:NH1	2.00	0.77
1:E:147:THR:HG22	2:E:486:HOH:O	1.84	0.77
1:L:282:TRP:O	1:L:283:ASN:HB2	1.85	0.77
1:C:142:ASN:HD21	1:C:164:VAL:H	1.30	0.77
1:L:247:VAL:O	1:L:248:SER:HB3	1.83	0.77
1:I:131:LEU:HD22	1:I:135:LEU:HD23	1.66	0.76
1:F:142:ASN:HD21	1:F:164:VAL:H	1.33	0.76
1:B:68:PRO:HG2	1:B:73:VAL:HG23	1.68	0.76
1:C:436:THR:HG23	1:C:477:SER:HB3	1.68	0.76
1:L:26:GLU:HG2	1:L:326:GLN:NE2	2.01	0.76
1:I:60:ILE:HD11	1:I:350:PHE:HB3	1.65	0.76
1:J:220:ARG:HD2	2:J:852:HOH:O	1.86	0.76
1:I:464:ASP:O	1:I:466:GLU:N	2.19	0.76
1:J:50:ARG:HG3	1:J:52:ASP:OD1	1.85	0.75
1:H:269:THR:HG23	2:H:711:HOH:O	1.86	0.75
1:K:291:ASN:N	1:K:291:ASN:HD22	1.83	0.75
1:J:80:ASP:OD2	1:J:91:ARG:NE	2.19	0.75
1:A:372:ASN:HD22	1:A:388:ASN:H	1.32	0.75
1:H:283:ASN:ND2	1:H:324:LEU:HD11	2.02	0.75
1:G:7:VAL:O	1:G:424:VAL:HA	1.87	0.75
1:F:120:PRO:HG2	1:F:164:VAL:HB	1.69	0.74
1:G:329:ASN:HD21	1:G:336:THR:H	1.36	0.74
1:E:247:VAL:O	1:E:248:SER:HB3	1.86	0.74
1:A:262:LYS:HB2	1:A:262:LYS:NZ	2.03	0.74
1:I:154:ARG:HG2	1:I:159:PRO:HA	1.67	0.74
1:E:370:THR:HG23	1:E:388:ASN:HA	1.70	0.73
1:K:298:ASP:HB3	1:K:445:ARG:HH21	1.53	0.73
1:E:372:ASN:ND2	1:E:388:ASN:H	1.85	0.73
1:C:160:GLU:HG3	1:C:161:PRO:HD2	1.71	0.73
1:H:235:HIS:HD2	1:H:281:GLU:HB2	1.52	0.73
1:D:189:ARG:HH11	1:D:189:ARG:HG3	1.53	0.73
1:H:429:GLN:O	1:H:430:LYS:HD2	1.89	0.73
1:A:262:LYS:HG2	1:B:259:GLY:HA2	1.70	0.72
1:H:240:SER:HB2	1:H:377:MET:HA	1.70	0.72
1:G:370:THR:HG23	1:G:388:ASN:HA	1.71	0.72
1:J:276:LYS:HD2	1:J:317:ASP:O	1.89	0.72
1:E:154:ARG:HG2	1:E:159:PRO:HA	1.70	0.72
1:B:154:ARG:HG2	1:B:159:PRO:HA	1.69	0.72
1:D:121:TYR:CZ	1:D:208:ILE:HD13	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:248:SER:OG	1:E:373:ILE:HD11	1.88	0.72
1:K:254:LYS:HG2	1:K:311:LEU:HD11	1.72	0.72
1:L:401:ASP:HB2	1:L:403:LYS:H	1.53	0.72
1:A:401:ASP:HB2	1:A:402:GLY:HA2	1.72	0.72
1:L:417:ALA:HB2	1:L:473:PRO:HD3	1.72	0.71
1:J:74:SER:OG	1:J:178:GLN:NE2	2.23	0.71
1:K:25:THR:HG23	1:K:25:THR:O	1.88	0.71
1:A:372:ASN:ND2	1:A:388:ASN:H	1.89	0.71
1:E:447:THR:HG22	1:E:450:ASN:H	1.54	0.71
1:E:126:MET:HG3	1:E:170:GLY:HA3	1.72	0.71
1:D:372:ASN:HD22	1:D:372:ASN:N	1.86	0.70
1:C:202:ASP:OD1	1:C:204:THR:OG1	2.09	0.70
1:D:371:TYR:C	1:D:372:ASN:HD22	1.93	0.70
1:J:372:ASN:ND2	1:J:388:ASN:H	1.89	0.70
1:B:247:VAL:O	1:B:248:SER:CB	2.39	0.70
1:A:126:MET:HE2	1:A:170:GLY:HA3	1.73	0.70
1:E:73:VAL:HG21	1:E:123:SER:O	1.91	0.70
1:J:81:GLY:HA2	1:J:88:ARG:HD3	1.74	0.70
1:C:45:ASP:HB3	1:C:51:LYS:HE3	1.73	0.70
1:E:403:LYS:O	1:E:403:LYS:HG2	1.91	0.70
1:F:60:ILE:HD12	1:F:350:PHE:HB3	1.74	0.70
1:A:427:LEU:O	1:A:465:THR:HG22	1.91	0.69
1:F:217:TRP:O	1:F:221:VAL:HG23	1.91	0.69
1:L:122:ILE:HG22	1:L:164:VAL:HG21	1.73	0.69
1:G:130:THR:HG22	1:G:133:GLU:H	1.57	0.69
1:I:131:LEU:HD22	1:I:135:LEU:CD2	2.22	0.69
1:H:401:ASP:OD1	1:H:402:GLY:HA2	1.92	0.69
1:G:381:LYS:HE2	2:G:490:HOH:O	1.93	0.69
1:L:32:ILE:HA	1:L:36:ILE:HG12	1.73	0.69
1:K:54:LEU:HD22	1:K:58:LYS:HE2	1.75	0.69
1:J:234:TYR:OH	1:J:256:ARG:HD2	1.92	0.69
1:I:450:ASN:N	1:I:451:PRO:HD3	2.08	0.68
1:D:359:GLU:HG3	1:D:400:GLU:HG2	1.76	0.68
1:G:273:ARG:HG3	1:G:273:ARG:HH11	1.59	0.68
1:E:247:VAL:O	1:E:248:SER:CB	2.41	0.68
1:L:81:GLY:O	1:L:105:GLY:HA3	1.93	0.68
1:D:126:MET:HE3	1:D:187:TYR:HE1	1.56	0.68
1:A:186:GLU:OE1	1:D:189:ARG:NH2	2.26	0.68
1:F:42:PRO:HD3	1:G:429:GLN:HE22	1.57	0.68
1:C:403:LYS:HB2	1:C:484:GLU:HG3	1.76	0.68
1:G:280:ASP:HA	1:G:323:ASN:HD22	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:231:PHE:HE1	1:L:320:PRO:HG2	1.58	0.68
1:K:329:ASN:HD21	1:K:336:THR:H	1.42	0.68
1:H:348:LYS:HB3	1:H:437:LEU:HD11	1.76	0.68
1:H:428:GLY:CA	1:H:464:ASP:HA	2.24	0.67
1:G:265:ASP:HA	1:G:271:ARG:HG3	1.75	0.67
1:L:298:ASP:OD1	1:L:300:LYS:HG2	1.92	0.67
1:A:248:SER:OG	1:A:373:ILE:HD11	1.94	0.67
1:D:160:GLU:H	1:D:160:GLU:CD	1.97	0.67
1:G:186:GLU:OE1	1:K:189:ARG:NH2	2.27	0.67
1:B:47:ARG:CB	1:B:47:ARG:HH11	2.07	0.67
1:K:372:ASN:ND2	1:K:388:ASN:H	1.93	0.67
1:D:126:MET:HE1	1:D:187:TYR:CE1	2.30	0.67
1:E:374:GLU:HG2	1:E:385:SER:HB3	1.77	0.67
1:G:4:ARG:NH1	1:G:4:ARG:HG3	2.00	0.66
1:L:401:ASP:HB3	1:L:403:LYS:HG2	1.77	0.66
1:A:126:MET:CE	1:A:187:TYR:HE1	2.09	0.66
1:D:38:GLU:HG2	1:D:41:SER:HB2	1.77	0.66
1:G:451:PRO:O	1:G:453:VAL:N	2.27	0.66
1:G:67:TRP:CD1	1:G:68:PRO:HA	2.31	0.66
1:H:122:ILE:HD11	1:H:137:TRP:CE2	2.31	0.66
1:B:189:ARG:NH1	1:B:189:ARG:HG3	2.10	0.66
1:H:14:LYS:NZ	1:H:314:LYS:O	2.19	0.66
1:H:141:CYS:C	1:H:142:ASN:HD22	1.99	0.66
1:L:19:HIS:HD2	1:L:64:ASN:HB2	1.60	0.66
1:G:372:ASN:ND2	1:G:388:ASN:H	1.93	0.66
1:G:235:HIS:CE1	1:G:280:ASP:OD1	2.49	0.66
1:D:189:ARG:HG3	1:D:189:ARG:NH1	2.11	0.66
1:K:262:LYS:CG	1:L:259:GLY:HA2	2.26	0.65
1:B:141:CYS:C	1:B:142:ASN:HD22	2.00	0.65
1:G:454:VAL:O	1:G:455:ASP:HB3	1.95	0.65
1:B:366:VAL:HG12	1:B:367:GLU:H	1.61	0.65
1:A:292:LYS:HG3	1:A:294:GLU:HG3	1.77	0.65
1:B:183:THR:OG1	1:B:186:GLU:HG2	1.97	0.65
1:I:126:MET:HE2	1:I:170:GLY:HA3	1.79	0.65
1:G:315:MET:HB2	1:G:318:ILE:HD12	1.77	0.65
1:L:25:THR:HG23	1:L:25:THR:O	1.96	0.65
1:L:122:ILE:CG2	1:L:164:VAL:HG21	2.27	0.65
1:L:142:ASN:HD21	1:L:164:VAL:H	1.43	0.65
1:K:348:LYS:HB3	1:K:437:LEU:CD2	2.27	0.65
1:D:126:MET:CE	1:D:187:TYR:CE1	2.76	0.65
1:I:141:CYS:C	1:I:142:ASN:HD22	1.99	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:189:ARG:NH1	1:L:189:ARG:HG3	2.03	0.65
1:H:239:GLY:HA3	1:H:240:SER:OG	1.97	0.65
1:A:242:ASP:HB3	1:A:245:GLU:HB2	1.79	0.65
1:H:151:GLN:HE21	1:H:151:GLN:HA	1.61	0.65
1:D:464:ASP:C	1:D:466:GLU:H	2.01	0.64
1:D:360:LYS:HB2	1:D:398:ILE:HG22	1.78	0.64
1:K:239:GLY:HA3	1:K:240:SER:OG	1.97	0.64
1:D:126:MET:HE1	1:D:187:TYR:HE1	1.59	0.64
1:H:428:GLY:HA3	1:H:464:ASP:HA	1.79	0.64
1:H:169:ILE:O	1:H:169:ILE:HG22	1.97	0.64
1:E:447:THR:HG22	1:E:449:GLU:H	1.62	0.64
1:G:273:ARG:CG	1:G:273:ARG:HH11	2.10	0.64
1:D:449:GLU:O	1:D:450:ASN:CB	2.44	0.64
1:D:130:THR:HG23	2:D:576:HOH:O	1.96	0.64
1:I:363:LYS:NZ	1:J:367:GLU:OE1	2.30	0.64
1:H:279:LEU:HD22	1:H:282:TRP:HB3	1.80	0.64
1:G:4:ARG:HH11	1:G:4:ARG:CG	2.06	0.64
1:B:110:ILE:HG21	1:B:162:TYR:CD2	2.33	0.64
1:C:171:ASN:HD22	1:C:178:GLN:HE22	1.46	0.63
1:C:13:VAL:HG12	1:C:14:LYS:HG2	1.79	0.63
1:B:125:ASN:HD21	1:B:128:THR:HG23	1.64	0.63
1:C:4:ARG:HB3	1:C:367:GLU:HB2	1.80	0.63
1:A:223:GLN:NE2	1:B:216:ILE:HD11	2.11	0.63
1:E:126:MET:HG3	1:E:170:GLY:CA	2.28	0.63
1:L:220:ARG:NH1	1:L:220:ARG:HG3	2.05	0.63
1:H:299:LEU:O	1:H:303:ILE:HG12	1.98	0.63
1:F:295:GLU:HG2	1:F:297:TYR:CE1	2.34	0.63
1:J:244:TYR:O	1:J:247:VAL:O	2.17	0.63
1:I:183:THR:OG1	1:I:186:GLU:HG3	1.99	0.63
1:G:220[A]:ARG:HH11	1:G:220[A]:ARG:HA	1.64	0.63
1:H:110:ILE:O	1:H:114:ARG:HD2	1.99	0.63
1:L:447:THR:HG23	1:L:450:ASN:H	1.64	0.63
1:C:235:HIS:CE1	1:C:280:ASP:OD1	2.52	0.62
1:K:276:LYS:HD2	1:K:317:ASP:O	1.99	0.62
1:B:428:GLY:HA3	1:B:464:ASP:OD2	1.99	0.62
1:C:427:LEU:O	1:C:465:THR:HG22	1.98	0.62
1:K:401:ASP:HB2	1:K:402:GLY:CA	2.29	0.62
1:D:343:LEU:HD13	1:D:347:TYR:CE2	2.34	0.62
1:L:369:GLU:HB3	1:L:391:PHE:HD2	1.64	0.62
1:C:461:ILE:HD13	1:C:469:HIS:HD2	1.64	0.62
1:E:45:ASP:HB3	1:E:51:LYS:HD3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ASP:O	1:A:205:ILE:HG12	1.99	0.62
1:H:235:HIS:CD2	1:H:281:GLU:HB2	2.33	0.62
1:C:154:ARG:HG2	1:C:159:PRO:HA	1.81	0.62
1:K:141:CYS:C	1:K:142:ASN:HD22	2.03	0.62
1:L:248:SER:HB2	1:L:371:TYR:OH	2.00	0.62
1:B:142:ASN:HD21	1:B:164:VAL:H	1.48	0.61
1:H:283:ASN:ND2	1:H:324:LEU:CD1	2.63	0.61
1:G:235:HIS:HE1	1:G:280:ASP:OD1	1.83	0.61
1:I:73:VAL:HG21	1:I:123:SER:O	2.00	0.61
1:H:370:THR:HG23	1:H:388:ASN:HA	1.81	0.61
1:K:25:THR:O	1:K:25:THR:CG2	2.48	0.61
1:L:377:MET:O	1:L:378:PHE:HB3	2.00	0.61
1:H:344:THR:HG22	1:H:345:PRO:HD2	1.82	0.61
1:J:374:GLU:HG3	1:J:385:SER:HB3	1.82	0.61
1:H:88:ARG:NH1	1:H:102:ASN:O	2.33	0.61
1:G:53:VAL:O	1:G:57:VAL:HG23	1.99	0.61
1:H:70:GLY:O	1:H:73:VAL:HG12	2.00	0.61
1:F:111:GLU:HG3	2:F:494:HOH:O	2.01	0.61
1:B:239:GLY:H	1:B:378:PHE:H	1.49	0.60
1:C:73:VAL:O	1:C:125:ASN:HB2	2.01	0.60
1:I:450:ASN:H	1:I:451:PRO:CD	2.10	0.60
1:H:66:ARG:HA	1:H:121:TYR:O	2.00	0.60
1:C:131:LEU:HD22	1:C:135:LEU:HD23	1.83	0.60
1:F:29:GLY:H	1:F:98:GLN:HE22	1.50	0.60
1:E:401:ASP:N	1:E:401:ASP:OD1	2.29	0.60
1:I:271:ARG:O	1:I:272:LYS:HB2	2.01	0.60
1:G:122:ILE:HD11	1:G:137:TRP:CE2	2.36	0.60
1:G:70:GLY:O	1:G:73:VAL:HG12	2.01	0.60
1:J:32:ILE:HG23	1:J:33:TYR:N	2.12	0.60
1:A:126:MET:HE1	1:A:187:TYR:HE1	1.66	0.60
1:L:483:LEU:O	1:L:484:GLU:HB2	2.01	0.60
1:A:450:ASN:HB3	1:A:453:VAL:HG23	1.83	0.59
1:L:337:GLU:HA	1:L:337:GLU:OE2	2.01	0.59
1:J:49:PHE:N	1:J:49:PHE:HD1	2.00	0.59
1:F:360:LYS:HB2	1:F:398:ILE:HG22	1.83	0.59
1:A:99:GLU:OE1	1:D:146:ASN:HB2	2.02	0.59
1:B:370:THR:HG23	1:B:388:ASN:HA	1.83	0.59
1:D:429:GLN:HA	1:D:464:ASP:HB2	1.85	0.59
1:G:71:ASN:ND2	1:G:178:GLN:HE22	1.99	0.59
1:A:63:PRO:HG2	1:A:64:ASN:HB2	1.84	0.59
1:J:248:SER:OG	1:J:373:ILE:HD13	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:GLU:O	1:A:450:ASN:CB	2.48	0.59
1:A:450:ASN:H	1:A:451:PRO:HD3	1.67	0.59
1:D:14:LYS:NZ	1:D:314:LYS:O	2.32	0.59
1:F:147:THR:CG2	2:F:486:HOH:O	2.51	0.59
1:K:430:LYS:HG2	1:K:482:GLU:O	2.03	0.59
1:D:280:ASP:HA	1:D:323:ASN:HD22	1.68	0.59
1:K:229:ILE:O	1:K:273:ARG:NH1	2.35	0.59
1:K:301:ASP:O	1:K:304:PHE:HB3	2.03	0.59
1:D:439:GLY:HA3	1:D:454:VAL:HG12	1.85	0.59
1:A:282:TRP:O	1:A:283:ASN:HB2	2.02	0.58
1:B:285:TRP:NE1	1:B:379:ILE:HD11	2.18	0.58
1:B:287:ARG:HG2	1:B:295:GLU:OE1	2.03	0.58
1:A:359:GLU:CG	1:A:400:GLU:HG2	2.29	0.58
1:E:25:THR:HG22	1:E:25:THR:O	2.03	0.58
1:D:126:MET:HE2	1:D:170:GLY:HA3	1.85	0.58
1:A:171:ASN:HD22	1:A:178:GLN:HE22	1.50	0.58
1:A:423:ARG:HG2	1:A:466:GLU:OE1	2.03	0.58
1:E:359:GLU:HG3	1:E:400:GLU:HG2	1.84	0.58
1:L:447:THR:O	1:L:449:GLU:N	2.30	0.58
1:E:5:ILE:HG12	1:E:366:VAL:HG22	1.85	0.58
1:E:125:ASN:HD21	1:E:128:THR:CG2	1.97	0.58
1:G:373:ILE:CD1	1:G:386:VAL:HB	2.34	0.58
1:D:126:MET:HE3	1:D:187:TYR:CE1	2.39	0.58
1:A:171:ASN:HD22	1:A:178:GLN:NE2	2.02	0.58
1:I:299:LEU:HB3	1:I:442:VAL:O	2.04	0.58
1:I:60:ILE:CD1	1:I:350:PHE:HB3	2.33	0.58
1:E:403:LYS:HB2	1:E:484:GLU:HA	1.85	0.58
1:G:130:THR:CG2	1:G:133:GLU:H	2.16	0.58
1:J:49:PHE:N	1:J:49:PHE:CD1	2.71	0.58
1:C:9:PRO:HA	1:C:362:VAL:HG21	1.85	0.58
1:J:32:ILE:CG2	1:J:33:TYR:H	2.15	0.58
1:K:259:GLY:HA2	1:L:262:LYS:HD3	1.86	0.58
1:J:73:VAL:C	1:J:75:ASN:H	2.07	0.58
1:H:448:MET:HG2	1:H:449:GLU:N	2.18	0.58
1:L:24:PHE:HD1	1:L:66:ARG:HB3	1.69	0.58
1:L:9:PRO:O	1:L:398:ILE:HD11	2.03	0.57
1:H:54:LEU:O	1:H:58:LYS:HD3	2.04	0.57
1:C:247:VAL:CG2	1:C:247:VAL:O	2.51	0.57
1:E:220:ARG:HD3	2:E:899:HOH:O	2.03	0.57
1:I:229:ILE:O	1:I:273:ARG:NH1	2.38	0.57
1:G:19:HIS:O	1:G:321:LEU:HA	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:GLY:O	1:B:154:ARG:NH2	2.36	0.57
1:E:401:ASP:CB	1:E:402:GLY:HA2	2.34	0.57
1:I:401:ASP:H	1:I:402:GLY:HA2	1.70	0.57
1:D:110:ILE:HG21	1:D:162:TYR:CD2	2.40	0.57
1:B:254:LYS:HG3	1:B:311:LEU:HD11	1.84	0.57
1:K:77:HIS:CE1	1:K:128:THR:HG22	2.40	0.57
1:D:438:THR:OG1	1:D:439:GLY:N	2.37	0.57
1:H:144:LYS:HD3	1:H:161:PRO:HG3	1.86	0.57
1:L:189:ARG:CG	1:L:189:ARG:HH11	2.15	0.57
1:L:126:MET:HE1	1:L:169:ILE:O	2.05	0.57
1:K:314:LYS:HE2	1:K:395:ALA:HB2	1.87	0.57
1:D:370:THR:HG23	1:D:388:ASN:HA	1.86	0.57
1:E:235:HIS:CD2	1:E:281:GLU:HB2	2.40	0.57
1:A:296:PRO:HB2	1:A:445:ARG:HE	1.68	0.57
1:F:327:LEU:HG	1:F:328:VAL:HG23	1.86	0.57
1:D:147:THR:HG22	1:D:149:TYR:H	1.70	0.57
1:D:452:ASN:HA	1:D:455:ASP:HB2	1.85	0.57
1:A:22:GLY:CA	1:A:64:ASN:HB3	2.34	0.57
1:J:472:LYS:O	1:J:475:SER:HB3	2.05	0.57
1:B:220:ARG:HD3	2:B:502:HOH:O	2.04	0.57
1:L:7:VAL:HG13	1:L:362:VAL:HG11	1.87	0.57
1:J:208:ILE:HG13	1:J:231:PHE:HB2	1.85	0.57
1:C:147:THR:HG22	1:C:150:ALA:H	1.69	0.57
1:B:366:VAL:HG12	1:B:367:GLU:N	2.20	0.57
1:H:71:ASN:HA	1:H:178:GLN:HE22	1.69	0.57
1:J:373:ILE:CD1	1:J:386:VAL:HG13	2.31	0.56
1:A:32:ILE:HG23	1:A:33:TYR:N	2.16	0.56
1:I:145:GLY:O	1:I:154:ARG:NH2	2.37	0.56
1:F:110:ILE:HG21	1:F:162:TYR:CD2	2.40	0.56
1:H:319:VAL:O	1:H:319:VAL:HG22	2.05	0.56
1:H:239:GLY:H	1:H:377:MET:HB2	1.69	0.56
1:H:67:TRP:CD1	1:H:68:PRO:HA	2.40	0.56
1:G:24:PHE:CD1	1:G:66:ARG:HB3	2.40	0.56
1:A:262:LYS:CG	1:B:259:GLY:HA2	2.35	0.56
1:B:428:GLY:HA2	1:B:464:ASP:HA	1.87	0.56
1:K:448:MET:O	1:K:449:GLU:HB2	2.05	0.56
1:H:254:LYS:HB2	1:H:311:LEU:HD11	1.86	0.56
1:B:277:ILE:HB	1:B:319:VAL:HB	1.88	0.56
1:K:73:VAL:C	1:K:75:ASN:H	2.09	0.56
1:H:151:GLN:NE2	1:H:154:ARG:HE	2.04	0.56
1:F:163:ASN:ND2	1:F:165:LYS:HE2	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:130:THR:CG2	1:F:132:ASP:HB2	2.35	0.56
1:I:160:GLU:H	1:I:160:GLU:CD	2.09	0.56
1:F:208:ILE:HG13	1:F:231:PHE:HB2	1.88	0.56
1:I:442:VAL:HG23	1:I:443:ASN:OD1	2.05	0.56
1:I:227:ASP:HB3	1:I:228:VAL:HG13	1.87	0.56
1:B:47:ARG:CG	1:B:47:ARG:HH11	2.19	0.56
1:I:401:ASP:N	1:I:402:GLY:HA2	2.20	0.56
1:F:282:TRP:O	1:F:283:ASN:HB2	2.06	0.56
1:D:418:LEU:HD12	1:D:420:VAL:CG2	2.35	0.56
1:A:125:ASN:O	1:A:129:GLY:HA3	2.06	0.56
1:F:254:LYS:HG3	1:F:311:LEU:HD11	1.88	0.56
1:H:142:ASN:HD22	1:H:142:ASN:N	2.04	0.56
1:K:233:SER:HB2	1:K:280:ASP:OD1	2.06	0.56
1:G:49:PHE:N	1:G:49:PHE:CD1	2.74	0.56
1:G:67:TRP:CG	1:G:68:PRO:HA	2.41	0.56
1:A:22:GLY:HA2	1:A:64:ASN:HB3	1.87	0.56
1:D:4:ARG:NH2	1:D:423:ARG:HG3	2.20	0.56
1:F:240:SER:HB3	1:F:286:TYR:CD2	2.40	0.56
1:E:67:TRP:HE3	1:E:122:ILE:HG22	1.71	0.56
1:E:74:SER:OG	1:E:178:GLN:NE2	2.27	0.55
1:D:418:LEU:HD12	1:D:420:VAL:HG23	1.89	0.55
1:F:27:HIS:CD2	1:F:32:ILE:HG13	2.41	0.55
1:L:145:GLY:O	1:L:154:ARG:NH2	2.39	0.55
1:A:401:ASP:HB2	1:A:402:GLY:CA	2.35	0.55
1:K:125:ASN:HD21	1:K:128:THR:HB	1.71	0.55
1:G:344:THR:HB	1:G:345:PRO:HD2	1.88	0.55
1:E:294:GLU:OE2	1:E:335:HIS:HE1	1.90	0.55
1:G:32:ILE:HD11	1:G:104:PHE:CB	2.36	0.55
1:I:71:ASN:HA	1:I:178:GLN:HE22	1.71	0.55
1:I:142:ASN:HD21	1:I:164:VAL:H	1.55	0.55
1:I:75:ASN:HD21	1:I:94:LEU:H	1.53	0.55
1:C:370:THR:OG1	1:C:388:ASN:HA	2.05	0.55
1:D:163:ASN:C	1:D:163:ASN:HD22	2.10	0.55
1:G:326:GLN:HB2	1:G:330:ALA:O	2.06	0.55
1:B:329:ASN:HD21	1:B:336:THR:H	1.54	0.55
1:E:405:LEU:HB3	1:E:481:VAL:HG22	1.88	0.55
1:C:28:LEU:HD11	1:C:293:LEU:HD23	1.88	0.55
1:K:291:ASN:H	1:K:291:ASN:HD22	1.51	0.55
1:B:403:LYS:HG2	1:B:403:LYS:O	2.07	0.55
1:H:405:LEU:HB3	1:H:481:VAL:HG13	1.86	0.55
1:A:298:ASP:OD1	1:A:300:LYS:HG2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:369:GLU:O	1:I:370:THR:HB	2.06	0.55
1:A:401:ASP:HB2	1:A:403:LYS:H	1.72	0.55
1:K:202:ASP:OD1	1:K:204:THR:OG1	2.23	0.55
1:H:26:GLU:HG2	1:H:27:HIS:H	1.71	0.55
1:A:122:ILE:HD11	1:A:137:TRP:CE2	2.42	0.55
1:J:247:VAL:O	1:J:248:SER:CB	2.54	0.55
1:F:398:ILE:HD11	1:F:483:LEU:HD11	1.89	0.55
1:I:298:ASP:OD1	1:I:300:LYS:HG2	2.06	0.55
1:G:67:TRP:O	1:G:122:ILE:HA	2.07	0.55
1:I:126:MET:CE	1:I:187:TYR:HE1	2.19	0.55
1:D:77:HIS:O	1:D:80:ASP:HB2	2.07	0.55
1:H:239:GLY:HA3	1:H:378:PHE:H	1.72	0.55
1:H:77:HIS:O	1:H:80:ASP:HB2	2.07	0.55
1:L:442:VAL:HG23	1:L:443:ASN:HD22	1.72	0.55
1:F:172:GLU:OE2	1:F:235:HIS:CD2	2.60	0.55
1:D:229:ILE:O	1:D:273:ARG:NH1	2.40	0.55
1:G:220[A]:ARG:HH11	1:G:220[A]:ARG:CA	2.20	0.54
1:I:300:LYS:HG3	1:I:301:ASP:N	2.21	0.54
1:C:215:PRO:HG3	1:D:266:MET:HB3	1.88	0.54
1:E:329:ASN:HD21	1:E:336:THR:H	1.54	0.54
1:J:50:ARG:O	1:J:53:VAL:HG12	2.06	0.54
1:F:280:ASP:HA	1:F:323:ASN:HD22	1.71	0.54
1:L:279:LEU:O	1:L:322:ALA:HA	2.08	0.54
1:C:225:ALA:HB1	1:C:229:ILE:HG23	1.89	0.54
1:A:356:HIS:HB3	1:A:478:VAL:HG21	1.88	0.54
1:H:61:LYS:HE2	1:H:355:ASN:OD1	2.06	0.54
1:B:282:TRP:O	1:B:283:ASN:HB2	2.07	0.54
1:L:372:ASN:ND2	1:L:388:ASN:H	2.05	0.54
1:D:434:VAL:HG22	1:D:479:ILE:HG12	1.89	0.54
1:H:283:ASN:HD22	1:H:324:LEU:CD1	2.21	0.54
1:H:239:GLY:HA3	1:H:240:SER:CB	2.38	0.54
1:A:403:LYS:O	1:A:403:LYS:HG2	2.08	0.54
1:H:370:THR:CG2	1:H:388:ASN:HA	2.38	0.54
1:C:122:ILE:HG23	1:C:164:VAL:HG21	1.87	0.54
1:L:26:GLU:CG	1:L:326:GLN:HE22	2.08	0.54
1:B:239:GLY:N	1:B:378:PHE:H	2.05	0.54
1:J:171:ASN:ND2	1:J:178:GLN:HE22	2.06	0.54
1:F:130:THR:HG22	1:F:132:ASP:N	2.22	0.54
1:G:436:THR:HB	1:G:457:THR:HG22	1.90	0.54
1:D:427:LEU:HB3	1:D:465:THR:H	1.72	0.54
1:D:71:ASN:HA	1:D:178:GLN:HE22	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:261:LYS:NZ	1:E:265:ASP:OD2	2.40	0.54
1:C:140:TYR:O	1:C:153:ARG:HD3	2.08	0.54
1:I:420:VAL:CG2	1:I:471:PHE:HE2	2.21	0.54
1:A:292:LYS:CG	1:A:294:GLU:HG3	2.38	0.54
1:H:120:PRO:HD2	2:H:1007:HOH:O	2.07	0.54
1:A:343:LEU:HD13	1:A:347:TYR:CE2	2.42	0.54
1:B:32:ILE:HD11	1:B:104:PHE:CB	2.38	0.54
1:L:126:MET:HE1	1:L:187:TYR:HE1	1.74	0.53
1:K:372:ASN:HD22	1:K:388:ASN:H	1.56	0.53
1:F:411:ASN:OD1	1:F:413:ARG:HG3	2.08	0.53
1:G:6:VAL:HG22	1:G:423:ARG:HB2	1.90	0.53
1:I:434:VAL:HG22	1:I:479:ILE:HG13	1.90	0.53
1:H:428:GLY:HA2	1:H:464:ASP:HA	1.89	0.53
1:K:268:ASP:O	1:K:272:LYS:HG3	2.08	0.53
1:E:465:THR:O	1:E:466:GLU:HB2	2.08	0.53
1:B:419:LYS:HG2	1:B:470:THR:OG1	2.08	0.53
1:L:329:ASN:HD21	1:L:336:THR:N	1.91	0.53
1:B:239:GLY:H	1:B:378:PHE:N	2.06	0.53
1:H:122:ILE:HD11	1:H:137:TRP:CZ2	2.43	0.53
1:J:434:VAL:HG22	1:J:479:ILE:HG12	1.90	0.53
1:I:272:LYS:H	1:I:274:GLY:H	1.57	0.53
1:B:329:ASN:HD21	1:B:336:THR:N	2.07	0.53
1:K:24:PHE:CE1	1:K:26:GLU:HB3	2.42	0.53
1:I:353:ILE:O	1:I:357:SER:HB3	2.09	0.53
1:H:434:VAL:HG22	1:H:479:ILE:HG12	1.89	0.53
1:K:329:ASN:ND2	1:K:336:THR:H	2.05	0.53
1:J:125:ASN:HD21	1:J:128:THR:HB	1.73	0.53
1:I:238:THR:HG21	1:I:304:PHE:CZ	2.44	0.53
1:B:20:ILE:HB	1:B:312:LEU:HD13	1.90	0.53
1:L:280:ASP:HA	1:L:323:ASN:HD22	1.74	0.53
1:A:32:ILE:CG2	1:A:33:TYR:H	2.19	0.53
1:I:398:ILE:HG22	1:I:399:SER:O	2.09	0.53
1:F:461:ILE:HG22	1:F:463:VAL:HG13	1.90	0.53
1:I:57:VAL:O	1:I:60:ILE:HG22	2.09	0.53
1:E:248:SER:OG	1:E:373:ILE:CD1	2.55	0.53
1:H:392:LEU:HD13	1:H:418:LEU:HD11	1.90	0.53
1:A:126:MET:HE2	1:A:170:GLY:CA	2.39	0.53
1:L:378:PHE:CE2	1:L:379:ILE:HG22	2.44	0.53
1:J:268:ASP:N	2:J:495:HOH:O	2.41	0.53
1:D:37:TYR:CE2	1:D:39:GLU:HG3	2.44	0.53
1:L:298:ASP:HB3	1:L:445:ARG:HH21	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:401:ASP:HB2	1:B:403:LYS:N	2.24	0.53
1:K:447:THR:O	1:K:451:PRO:HA	2.09	0.53
1:B:276:LYS:HE3	1:B:317:ASP:O	2.09	0.53
1:I:296:PRO:HB2	1:I:445:ARG:HH12	1.74	0.53
1:G:141:CYS:C	1:G:142:ASN:HD22	2.12	0.53
1:E:370:THR:HB	2:E:956:HOH:O	2.08	0.53
1:L:131:LEU:HD22	1:L:135:LEU:CD2	2.39	0.53
1:K:154:ARG:HG2	1:K:159:PRO:HA	1.91	0.53
1:G:130:THR:HG22	1:G:133:GLU:HB2	1.91	0.52
1:E:32:ILE:HD11	1:E:104:PHE:CB	2.39	0.52
1:C:427:LEU:HD22	1:C:428:GLY:H	1.75	0.52
1:F:122:ILE:HD13	1:F:137:TRP:CH2	2.44	0.52
1:J:370:THR:HG23	1:J:388:ASN:HA	1.92	0.52
1:F:73:VAL:HA	1:F:76:TYR:HB3	1.91	0.52
1:H:32:ILE:HD11	1:H:104:PHE:CG	2.45	0.52
1:L:362:VAL:CG2	1:L:398:ILE:HG13	2.40	0.52
1:I:247:VAL:O	1:I:247:VAL:HG23	2.08	0.52
1:K:401:ASP:CG	1:K:403:LYS:HD3	2.29	0.52
1:L:24:PHE:CD1	1:L:66:ARG:HB3	2.44	0.52
1:G:262:LYS:HE3	1:G:265:ASP:OD2	2.10	0.52
1:K:427:LEU:O	1:K:428:GLY:O	2.28	0.52
1:L:24:PHE:CD1	1:L:66:ARG:HD3	2.45	0.52
1:I:279:LEU:HD22	1:I:282:TRP:HB3	1.91	0.52
1:J:84:PRO:HB2	1:J:87:GLN:OE1	2.09	0.52
1:L:374:GLU:HG3	1:L:385:SER:HB3	1.92	0.52
1:K:348:LYS:HD2	1:K:455:ASP:HA	1.91	0.52
1:A:262:LYS:HE3	1:A:265:ASP:OD2	2.09	0.52
1:B:67:TRP:CD1	1:B:68:PRO:HA	2.45	0.52
1:G:309:LEU:O	1:G:313:GLN:HG3	2.09	0.52
1:J:67:TRP:O	1:J:122:ILE:HA	2.10	0.52
1:L:14:LYS:HE3	1:L:314:LYS:O	2.10	0.52
1:G:145:GLY:O	1:G:154:ARG:NH2	2.42	0.52
1:G:60:ILE:O	1:G:354:VAL:HG11	2.10	0.52
1:C:11:LYS:O	1:C:362:VAL:HG23	2.09	0.52
1:I:91:ARG:HG3	2:I:507:HOH:O	2.09	0.52
1:I:231:PHE:HE1	1:I:320:PRO:HG2	1.73	0.52
1:C:260:VAL:O	1:C:264:ILE:HD12	2.10	0.52
1:C:125:ASN:ND2	1:C:128:THR:H	2.00	0.52
1:K:142:ASN:HD21	1:K:164:VAL:H	1.58	0.52
1:I:219:LEU:HD11	1:J:215:PRO:HB2	1.91	0.52
1:H:121:TYR:CE1	1:H:208:ILE:HD12	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ILE:HD12	1:A:137:TRP:CZ2	2.45	0.51
1:F:66:ARG:HA	1:F:121:TYR:O	2.10	0.51
1:L:236:PHE:O	1:L:282:TRP:HA	2.11	0.51
1:E:244:TYR:O	1:E:247:VAL:O	2.28	0.51
1:B:286:TYR:HA	1:B:379:ILE:HD13	1.92	0.51
1:G:49:PHE:N	1:G:49:PHE:HD1	2.09	0.51
1:L:265:ASP:O	1:L:271:ARG:NH1	2.44	0.51
1:J:248:SER:OG	1:J:373:ILE:CD1	2.59	0.51
1:C:182:MET:HB3	1:C:186:GLU:HG3	1.92	0.51
1:D:189:ARG:HH11	1:D:189:ARG:CG	2.21	0.51
1:H:13:VAL:HG12	1:H:14:LYS:HD3	1.93	0.51
1:B:32:ILE:HD11	1:B:104:PHE:CG	2.46	0.51
1:F:242:ASP:HB3	1:F:245:GLU:HB2	1.91	0.51
1:A:252:LEU:O	1:A:256:ARG:HG2	2.11	0.51
1:I:408:ALA:HA	1:I:478:VAL:HB	1.92	0.51
1:G:286:TYR:OH	1:G:300:LYS:NZ	2.36	0.51
1:F:234:TYR:OH	1:F:256:ARG:HD3	2.09	0.51
1:A:110:ILE:HG21	1:A:162:TYR:CD2	2.45	0.51
1:C:4:ARG:NH1	1:C:421:PRO:HB2	2.26	0.51
1:J:278:ALA:O	1:J:280:ASP:N	2.44	0.51
1:E:262:LYS:HD3	1:F:259:GLY:HA2	1.92	0.51
1:F:407:ILE:O	1:F:478:VAL:HA	2.10	0.51
1:I:348:LYS:HB3	1:I:437:LEU:HD11	1.93	0.51
1:J:289:SER:HB3	1:J:379:ILE:HG13	1.92	0.51
1:D:436:THR:OG1	1:D:477:SER:HB3	2.11	0.51
1:J:428:GLY:HA3	1:J:429:GLN:C	2.30	0.51
1:D:458:SER:O	1:D:459:GLU:HB3	2.10	0.51
1:C:291:ASN:ND2	1:C:291:ASN:H	2.04	0.51
1:A:352:LEU:O	1:A:355:ASN:O	2.28	0.51
1:H:306:CYS:HB3	1:H:353:ILE:HD11	1.91	0.51
1:E:71:ASN:ND2	1:E:178:GLN:OE1	2.43	0.51
1:I:126:MET:HE1	1:I:187:TYR:CE1	2.46	0.51
1:B:231:PHE:HA	1:B:276:LYS:O	2.10	0.51
1:H:306:CYS:HB3	1:H:353:ILE:CD1	2.41	0.51
1:A:325:ALA:HA	1:A:326:GLN:HG3	1.93	0.51
1:L:243:TYR:CD2	1:L:414:LYS:HG2	2.46	0.51
1:H:326:GLN:HB2	1:H:330:ALA:O	2.11	0.51
1:D:464:ASP:OD2	1:D:465:THR:HG22	2.11	0.51
1:K:401:ASP:N	1:K:402:GLY:HA2	2.26	0.51
1:K:428:GLY:N	1:K:465:THR:HG22	2.26	0.51
1:F:73:VAL:HG21	1:F:123:SER:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:105:GLY:N	1:H:108:GLU:OE1	2.42	0.51
1:C:266:MET:HB3	1:D:215:PRO:HG3	1.93	0.51
1:I:247:VAL:O	1:I:248:SER:CB	2.58	0.51
1:I:126:MET:HE1	1:I:187:TYR:HE1	1.76	0.51
1:H:147:THR:HB	2:H:485:HOH:O	2.10	0.51
1:C:262:LYS:CD	1:D:259:GLY:HA2	2.41	0.51
1:A:208:ILE:HG13	1:A:231:PHE:HB2	1.92	0.51
1:I:378:PHE:CG	1:I:379:ILE:N	2.79	0.50
1:G:164:VAL:HG22	1:G:167:TRP:CZ2	2.46	0.50
1:J:372:ASN:HD22	1:J:388:ASN:H	1.58	0.50
1:D:6:VAL:HG23	1:D:423:ARG:HB2	1.93	0.50
1:C:247:VAL:HG23	1:C:247:VAL:O	2.11	0.50
1:L:262:LYS:O	1:L:266:MET:HG3	2.11	0.50
1:A:154:ARG:HG2	1:A:159:PRO:HA	1.93	0.50
1:E:280:ASP:HA	1:E:323:ASN:HD22	1.75	0.50
1:D:67:TRP:CE2	1:D:68:PRO:HB3	2.47	0.50
1:K:70:GLY:HA2	2:K:485:HOH:O	2.11	0.50
1:L:378:PHE:CG	1:L:379:ILE:N	2.80	0.50
1:D:243:TYR:CD2	1:D:414:LYS:HG3	2.46	0.50
1:D:154:ARG:HG2	1:D:159:PRO:HA	1.93	0.50
1:F:314:LYS:HD2	1:F:395:ALA:HB2	1.93	0.50
1:B:189:ARG:CG	1:B:189:ARG:HH11	2.21	0.50
1:C:122:ILE:HD13	1:C:137:TRP:CH2	2.47	0.50
1:K:286:TYR:OH	1:K:300:LYS:NZ	2.39	0.50
1:E:240:SER:HB3	1:E:286:TYR:CG	2.46	0.50
1:F:8:ASP:O	1:F:362:VAL:HG12	2.11	0.50
1:J:66:ARG:HA	1:J:121:TYR:O	2.12	0.50
1:D:32:ILE:O	1:D:37:TYR:HB3	2.11	0.50
1:A:236:PHE:O	1:A:282:TRP:HA	2.11	0.50
1:F:235:HIS:CE1	1:F:280:ASP:OD1	2.65	0.50
1:A:288:VAL:O	1:A:379:ILE:HD11	2.11	0.50
1:G:397:SER:O	1:G:405:LEU:HD12	2.11	0.50
1:C:142:ASN:ND2	1:C:164:VAL:H	2.06	0.50
1:L:447:THR:H	1:L:451:PRO:HD3	1.75	0.50
1:K:401:ASP:HB2	1:K:402:GLY:HA2	1.94	0.50
1:I:70:GLY:O	1:I:73:VAL:HG12	2.12	0.50
1:H:225:ALA:HB1	1:H:229:ILE:HG23	1.93	0.50
1:H:280:ASP:HA	1:H:323:ASN:HB2	1.94	0.50
1:E:370:THR:CG2	1:E:388:ASN:HA	2.41	0.50
1:B:451:PRO:HG2	1:B:452:ASN:ND2	2.25	0.50
1:H:131:LEU:HD23	1:H:194:TYR:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:427:LEU:HB3	1:I:465:THR:H	1.76	0.50
1:K:372:ASN:O	1:K:373:ILE:HG23	2.11	0.49
1:D:140:TYR:O	1:D:153:ARG:HD3	2.11	0.49
1:A:347:TYR:HD2	1:A:348:LYS:HD3	1.77	0.49
1:H:353:ILE:O	1:H:357:SER:HB3	2.11	0.49
1:E:206:LYS:HA	1:E:230:ASP:OD1	2.13	0.49
1:I:239:GLY:HA3	1:I:240:SER:OG	2.12	0.49
1:D:24:PHE:O	1:D:326:GLN:HB3	2.12	0.49
1:C:189:ARG:NH2	1:E:186:GLU:OE1	2.45	0.49
1:J:452:ASN:ND2	1:J:455:ASP:OD1	2.45	0.49
1:J:447:THR:O	1:J:448:MET:HB3	2.12	0.49
1:L:126:MET:CE	1:L:187:TYR:HE1	2.25	0.49
1:A:147:THR:HG22	1:A:149:TYR:H	1.77	0.49
1:L:214:ASP:O	1:L:217:TRP:HB3	2.12	0.49
1:H:380:ASN:HD22	1:H:381:LYS:N	2.10	0.49
1:H:135:LEU:HD21	1:L:94:LEU:HD11	1.94	0.49
1:K:217:TRP:C	1:K:217:TRP:CD1	2.86	0.49
1:K:259:GLY:CA	1:L:262:LYS:HD3	2.42	0.49
1:L:442:VAL:HG23	1:L:443:ASN:ND2	2.27	0.49
1:K:113:CYS:HA	1:K:116:ILE:CD1	2.43	0.49
1:I:61:LYS:HE2	1:I:355:ASN:OD1	2.11	0.49
1:J:251:TYR:HD1	1:J:254:LYS:HE3	1.77	0.49
1:L:241:GLU:HB2	2:L:486:HOH:O	2.12	0.49
1:D:273:ARG:HH11	1:D:273:ARG:HG3	1.77	0.49
1:D:164:VAL:HG22	1:D:167:TRP:NE1	2.27	0.49
1:J:394:ALA:HB2	1:J:409:VAL:HB	1.94	0.49
1:E:341:LEU:C	1:E:341:LEU:HD12	2.33	0.49
1:I:4:ARG:NH2	1:I:423:ARG:HB2	2.28	0.49
1:G:88:ARG:NH1	1:G:102:ASN:O	2.44	0.49
1:I:26:GLU:HG2	1:I:69:GLY:HA2	1.95	0.49
1:B:32:ILE:C	1:B:32:ILE:HD13	2.33	0.49
1:A:238:THR:HG23	1:A:239:GLY:N	2.27	0.49
1:A:336:THR:HA	1:A:341:LEU:HA	1.95	0.49
1:H:234:TYR:OH	1:H:256:ARG:HD2	2.13	0.49
1:L:299:LEU:O	1:L:303:ILE:HG12	2.13	0.49
1:K:255:GLU:HA	1:K:255:GLU:OE2	2.13	0.49
1:H:427:LEU:HD13	1:H:428:GLY:H	1.78	0.49
1:K:448:MET:O	1:K:449:GLU:CB	2.61	0.49
1:K:116:ILE:HD11	1:K:118:ALA:HB3	1.93	0.49
1:D:31:CYS:HA	1:D:328:VAL:O	2.13	0.49
1:H:6:VAL:HG22	1:H:423:ARG:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:LYS:HE2	1:B:394:ALA:O	2.13	0.48
1:H:60:ILE:O	1:H:354:VAL:HG11	2.13	0.48
1:K:236:PHE:CG	1:K:253:LEU:HD13	2.48	0.48
1:E:120:PRO:HG2	1:E:164:VAL:HB	1.95	0.48
1:L:154:ARG:CG	1:L:159:PRO:HA	2.26	0.48
1:L:32:ILE:HG22	1:L:36:ILE:HD11	1.95	0.48
1:B:285:TRP:CD1	1:B:379:ILE:HD11	2.48	0.48
1:A:325:ALA:CA	1:A:326:GLN:HG3	2.43	0.48
1:K:183:THR:OG1	1:K:186:GLU:HG2	2.12	0.48
1:H:399:SER:HB3	1:H:406:PHE:HE2	1.78	0.48
1:G:378:PHE:CG	1:G:379:ILE:N	2.81	0.48
1:I:17:SER:O	1:I:20:ILE:HG12	2.13	0.48
1:E:122:ILE:HG13	1:E:167:TRP:CZ3	2.49	0.48
1:G:463:VAL:HG12	1:G:464:ASP:N	2.28	0.48
1:I:173:MET:CE	1:I:182:MET:HG3	2.43	0.48
1:F:126:MET:HE2	1:F:169:ILE:C	2.33	0.48
1:A:4:ARG:NH1	1:A:423:ARG:HG3	2.27	0.48
1:A:122:ILE:CD1	1:A:137:TRP:CE2	2.97	0.48
1:H:77:HIS:CE1	1:H:128:THR:HG22	2.48	0.48
1:D:145:GLY:O	1:D:154:ARG:NH2	2.36	0.48
1:E:174:TYR:CD1	1:E:175:GLY:N	2.81	0.48
1:G:23:HIS:CE1	1:G:350:PHE:CE1	3.01	0.48
1:K:220:ARG:HA	1:K:220:ARG:HH11	1.77	0.48
1:G:428:GLY:CA	1:G:429:GLN:C	2.82	0.48
1:C:403:LYS:CB	1:C:484:GLU:HG3	2.43	0.48
1:L:262:LYS:HE3	1:L:262:LYS:HA	1.95	0.48
1:H:233:SER:HB2	1:H:280:ASP:OD1	2.13	0.48
1:L:447:THR:C	1:L:449:GLU:H	2.14	0.48
1:F:9:PRO:HA	1:F:362:VAL:HG11	1.94	0.48
1:F:251:TYR:OH	1:F:393:ASP:OD2	2.28	0.48
1:G:32:ILE:HG23	1:G:33:TYR:H	1.78	0.48
1:G:340:GLY:HA3	2:G:496:HOH:O	2.14	0.48
1:F:427:LEU:HD22	1:F:428:GLY:H	1.78	0.48
1:K:394:ALA:HA	1:K:408:ALA:O	2.13	0.48
1:B:240:SER:OG	1:B:377:MET:HA	2.14	0.48
1:J:329:ASN:ND2	1:J:335:HIS:HA	2.29	0.48
1:K:450:ASN:N	1:K:451:PRO:HD3	2.29	0.48
1:A:110:ILE:HG22	1:A:114:ARG:HD2	1.96	0.48
1:E:131:LEU:HD22	1:E:135:LEU:HD22	1.95	0.48
1:A:184:ALA:HA	1:A:217:TRP:CE3	2.48	0.48
1:C:125:ASN:ND2	1:C:125:ASN:C	2.66	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:CYS:C	1:C:142:ASN:HD22	2.18	0.48
1:A:126:MET:HE3	1:A:187:TYR:HE1	1.77	0.48
1:H:110:ILE:HG13	1:H:162:TYR:CD1	2.49	0.48
1:K:226:GLY:O	1:K:273:ARG:HD3	2.14	0.48
1:B:329:ASN:ND2	1:B:336:THR:H	2.11	0.48
1:F:370:THR:HG23	1:F:388:ASN:HA	1.96	0.48
1:I:60:ILE:CD1	1:I:350:PHE:CB	2.80	0.48
1:C:122:ILE:HD13	1:C:137:TRP:CZ2	2.49	0.48
1:E:286:TYR:C	1:E:286:TYR:CD2	2.87	0.48
1:F:428:GLY:HA3	1:F:464:ASP:HA	1.96	0.48
1:L:350:PHE:O	1:L:354:VAL:HG23	2.14	0.48
1:E:60:ILE:HD13	1:E:347:TYR:CZ	2.49	0.48
1:A:126:MET:HE1	1:A:187:TYR:CE1	2.46	0.47
1:I:90:VAL:HG22	1:I:101:THR:HA	1.95	0.47
1:J:5:ILE:HD11	1:J:392:LEU:HD21	1.97	0.47
1:E:295:GLU:HG2	1:E:297:TYR:CE1	2.49	0.47
1:A:60:ILE:HG22	1:A:60:ILE:O	2.14	0.47
1:J:61:LYS:HB2	1:J:354:VAL:HG11	1.95	0.47
1:F:56:ALA:O	1:F:347:TYR:OH	2.29	0.47
1:G:110:ILE:HG21	1:G:162:TYR:CD2	2.48	0.47
1:H:363:LYS:NZ	1:H:363:LYS:HB3	2.29	0.47
1:H:345:PRO:HA	1:H:348:LYS:HB2	1.96	0.47
1:C:219:LEU:CD1	1:D:215:PRO:HB2	2.44	0.47
1:C:276:LYS:HE3	1:C:317:ASP:O	2.14	0.47
1:L:238:THR:O	1:L:284:VAL:HA	2.15	0.47
1:F:145:GLY:O	1:F:154:ARG:NH2	2.47	0.47
1:G:428:GLY:HA2	1:G:429:GLN:C	2.35	0.47
1:F:130:THR:HG21	1:F:132:ASP:HB2	1.96	0.47
1:L:327:LEU:HG	1:L:328:VAL:HG23	1.97	0.47
1:C:428:GLY:HA3	1:C:464:ASP:HA	1.97	0.47
1:E:287:ARG:HD3	1:E:295:GLU:OE2	2.14	0.47
1:G:147:THR:HB	2:G:485:HOH:O	2.14	0.47
1:J:112:TYR:O	1:J:116:ILE:HG12	2.14	0.47
1:J:347:TYR:CD2	1:J:347:TYR:C	2.88	0.47
1:C:434:VAL:HG22	1:C:479:ILE:HG12	1.96	0.47
1:B:239:GLY:HA3	1:B:240:SER:HG	1.78	0.47
1:J:248:SER:H	1:J:250:VAL:HG23	1.79	0.47
1:K:208:ILE:N	1:K:208:ILE:HD12	2.30	0.47
1:L:380:ASN:OD1	1:L:382:MET:HG3	2.14	0.47
1:E:212:CYS:SG	1:E:213:ASP:N	2.86	0.47
1:E:46:GLU:H	1:E:46:GLU:CD	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:319:VAL:O	1:C:319:VAL:HG22	2.15	0.47
1:E:74:SER:O	1:E:128:THR:HB	2.14	0.47
1:C:291:ASN:HD22	1:C:291:ASN:N	2.05	0.47
1:I:464:ASP:C	1:I:466:GLU:H	2.16	0.47
1:L:22:GLY:HA3	1:L:64:ASN:HD22	1.80	0.47
1:L:25:THR:CG2	1:L:25:THR:O	2.62	0.47
1:F:130:THR:HG22	1:F:133:GLU:H	1.80	0.47
1:H:26:GLU:CG	1:H:27:HIS:H	2.28	0.47
1:I:420:VAL:HG22	1:I:471:PHE:HE2	1.80	0.47
1:I:348:LYS:CB	1:I:437:LEU:HD11	2.45	0.47
1:E:238:THR:HG21	1:E:304:PHE:CE1	2.50	0.47
1:B:435:TYR:HA	1:B:457:THR:O	2.15	0.47
1:F:441:ASP:N	1:F:441:ASP:OD1	2.48	0.47
1:A:160:GLU:HB3	2:A:506:HOH:O	2.14	0.47
1:L:45:ASP:OD1	1:L:47:ARG:NH1	2.48	0.47
1:D:50:ARG:NH2	1:D:340:GLY:O	2.47	0.47
1:B:45:ASP:OD1	1:B:47:ARG:NH1	2.46	0.47
1:B:427:LEU:O	1:B:428:GLY:O	2.32	0.47
1:I:4:ARG:NH2	1:I:423:ARG:HD2	2.29	0.47
1:F:18:ARG:HG3	2:F:659:HOH:O	2.13	0.47
1:E:41:SER:HA	1:E:42:PRO:HD2	1.70	0.47
1:B:280:ASP:HA	1:B:323:ASN:HD22	1.80	0.47
1:H:285:TRP:NE1	1:H:379:ILE:HD11	2.30	0.47
1:B:52:ASP:O	1:B:55:GLU:HB3	2.14	0.47
1:C:183:THR:OG1	1:C:186:GLU:HG2	2.15	0.47
1:F:141:CYS:C	1:F:142:ASN:HD22	2.18	0.47
1:I:479:ILE:HG22	1:I:481:VAL:HG13	1.97	0.47
1:A:318:ILE:HG22	1:A:319:VAL:HG12	1.96	0.47
1:K:309:LEU:O	1:K:313:GLN:HG3	2.15	0.47
1:H:407:ILE:O	1:H:478:VAL:HA	2.15	0.47
1:A:163:ASN:HD22	1:A:163:ASN:C	2.17	0.47
1:I:3:TYR:CD1	1:I:418:LEU:HD21	2.50	0.47
1:L:19:HIS:CD2	1:L:64:ASN:HB2	2.46	0.47
1:L:268:ASP:O	1:L:269:THR:C	2.54	0.47
1:F:447:THR:O	1:F:448:MET:CB	2.63	0.47
1:I:24:PHE:CD1	1:I:25:THR:N	2.83	0.47
1:A:206:LYS:HA	1:A:230:ASP:OD1	2.15	0.47
1:C:372:ASN:ND2	1:C:388:ASN:H	2.13	0.46
1:I:24:PHE:HD1	1:I:25:THR:H	1.62	0.46
1:I:18:ARG:HG2	1:I:63:PRO:HB3	1.96	0.46
1:L:375:GLY:O	1:L:383:PRO:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:427:LEU:HD22	1:D:428:GLY:H	1.79	0.46
1:K:22:GLY:O	1:K:323:ASN:HA	2.15	0.46
1:K:24:PHE:CZ	1:K:26:GLU:HB3	2.50	0.46
1:G:147:THR:HG22	1:G:150:ALA:H	1.80	0.46
1:G:410:VAL:HG22	1:G:476:CYS:HB2	1.97	0.46
1:G:244:TYR:O	1:G:248:SER:HB3	2.14	0.46
1:G:130:THR:HG22	1:G:133:GLU:CB	2.45	0.46
1:K:401:ASP:CB	1:K:402:GLY:HA2	2.46	0.46
1:K:80:ASP:CG	1:K:91:ARG:HH21	2.17	0.46
1:K:121:TYR:C	1:K:121:TYR:CD1	2.89	0.46
1:J:144:LYS:HE3	1:J:161:PRO:HG3	1.97	0.46
1:K:16:ILE:HG22	1:K:16:ILE:O	2.16	0.46
1:L:74:SER:OG	1:L:178:GLN:NE2	2.36	0.46
1:L:32:ILE:HG12	1:L:33:TYR:N	2.31	0.46
1:H:142:ASN:HD21	1:H:164:VAL:H	1.63	0.46
1:A:286:TYR:HA	1:A:379:ILE:HD12	1.98	0.46
1:A:238:THR:HG23	1:A:239:GLY:H	1.80	0.46
1:D:13:VAL:HB	1:D:361:LEU:HD23	1.97	0.46
1:J:32:ILE:HD11	1:J:104:PHE:CD2	2.50	0.46
1:A:401:ASP:HB2	1:A:403:LYS:N	2.30	0.46
1:G:428:GLY:HA2	1:G:429:GLN:O	2.16	0.46
1:F:172:GLU:OE2	1:F:235:HIS:HD2	1.98	0.46
1:D:172:GLU:OE2	1:D:235:HIS:CD2	2.68	0.46
1:D:26:GLU:HG2	1:D:27:HIS:H	1.80	0.46
1:D:401:ASP:N	1:D:402:GLY:HA2	2.31	0.46
1:H:295:GLU:HG2	1:H:297:TYR:CE1	2.51	0.46
1:K:345:PRO:HA	1:K:348:LYS:HB2	1.98	0.46
1:K:345:PRO:HG3	1:K:454:VAL:HG21	1.98	0.46
1:D:372:ASN:ND2	1:D:388:ASN:H	2.13	0.46
1:D:67:TRP:O	1:D:122:ILE:HA	2.15	0.46
1:I:242:ASP:OD2	1:I:243:TYR:N	2.48	0.46
1:B:9:PRO:HB3	1:B:483:LEU:HD11	1.97	0.46
1:F:300:LYS:HG3	1:F:301:ASP:N	2.31	0.46
1:I:32:ILE:HD11	1:I:104:PHE:CB	2.46	0.46
1:J:400:GLU:HA	1:J:400:GLU:OE1	2.16	0.46
1:D:341:LEU:HD12	1:D:341:LEU:C	2.35	0.46
1:E:74:SER:HB3	1:E:179:VAL:HG13	1.98	0.46
1:F:287:ARG:HD2	1:F:296:PRO:HD2	1.98	0.46
1:E:348:LYS:HD3	1:E:456:ILE:HD12	1.98	0.46
1:B:126:MET:HG3	1:B:170:GLY:HA2	1.98	0.46
1:F:260:VAL:HA	1:F:263:LEU:HD12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:45:ASP:OD1	1:K:46:GLU:N	2.49	0.45
1:D:238:THR:O	1:D:284:VAL:HA	2.16	0.45
1:A:90:VAL:HB	1:D:146:ASN:O	2.16	0.45
1:C:290:ASP:OD1	1:C:293:LEU:N	2.46	0.45
1:F:122:ILE:HD12	1:F:123:SER:N	2.32	0.45
1:C:22:GLY:HA2	1:C:64:ASN:HB2	1.97	0.45
1:H:239:GLY:CA	1:H:378:PHE:H	2.29	0.45
1:H:106:THR:O	1:H:110:ILE:HG12	2.16	0.45
1:A:434:VAL:HG22	1:A:479:ILE:HG12	1.98	0.45
1:F:421:PRO:HA	1:F:468:GLU:HG3	1.99	0.45
1:B:189:ARG:NH2	1:C:186:GLU:OE1	2.50	0.45
1:L:126:MET:CE	1:L:170:GLY:HA3	2.42	0.45
1:C:4:ARG:NH2	1:C:466:GLU:OE2	2.41	0.45
1:I:358:GLY:HA3	1:I:398:ILE:O	2.17	0.45
1:B:126:MET:HG3	1:B:170:GLY:CA	2.47	0.45
1:B:196:LYS:HG2	1:B:197:TRP:N	2.31	0.45
1:L:4:ARG:NH2	1:L:423:ARG:HB2	2.31	0.45
1:E:372:ASN:HD21	1:E:388:ASN:H	1.62	0.45
1:B:325:ALA:HA	1:B:326:GLN:HA	1.71	0.45
1:A:37:TYR:OH	1:A:85:LYS:NZ	2.48	0.45
1:J:353:ILE:O	1:J:357:SER:HB3	2.17	0.45
1:E:74:SER:HG	1:E:178:GLN:HE21	1.58	0.45
1:H:67:TRP:O	1:H:122:ILE:HA	2.16	0.45
1:L:448:MET:N	1:L:451:PRO:HD3	2.31	0.45
1:K:235:HIS:HE1	1:K:280:ASP:OD1	1.98	0.45
1:H:128:THR:O	1:H:128:THR:HG22	2.16	0.45
1:I:304:PHE:O	1:I:308:VAL:HG23	2.17	0.45
1:I:24:PHE:CD1	1:I:66:ARG:HB3	2.52	0.45
1:L:147:THR:HG22	1:L:150:ALA:H	1.80	0.45
1:L:136:HIS:CG	1:L:149:TYR:CE2	3.04	0.45
1:I:255:GLU:HG3	1:J:262:LYS:NZ	2.31	0.45
1:H:75:ASN:O	1:H:75:ASN:ND2	2.49	0.45
1:G:341:LEU:HD12	1:G:341:LEU:C	2.37	0.45
1:D:183:THR:OG1	1:D:186:GLU:HG2	2.17	0.45
1:H:325:ALA:HA	1:H:326:GLN:HA	1.67	0.45
1:F:314:LYS:HE3	1:F:394:ALA:O	2.17	0.45
1:D:339:ASP:OD2	1:D:340:GLY:N	2.46	0.45
1:I:307:GLY:HA3	1:I:412:TYR:OH	2.17	0.45
1:G:70:GLY:H	1:G:171:ASN:ND2	2.15	0.45
1:E:32:ILE:HD11	1:E:104:PHE:CG	2.52	0.45
1:A:240:SER:HB3	1:A:286:TYR:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:TRP:CE3	1:A:378:PHE:HE1	2.34	0.45
1:A:139:GLU:HG2	1:A:201:PHE:CZ	2.51	0.45
1:J:29:GLY:H	1:J:98:GLN:HE22	1.64	0.45
1:F:88:ARG:NH1	1:F:102:ASN:O	2.46	0.45
1:C:121:TYR:C	1:C:121:TYR:CD1	2.89	0.45
1:J:122:ILE:HD11	1:J:167:TRP:CH2	2.52	0.45
1:C:259:GLY:CA	1:D:262:LYS:HD3	2.46	0.45
1:C:401:ASP:OD1	1:C:402:GLY:HA2	2.17	0.45
1:L:292:LYS:HE2	1:L:292:LYS:HB3	1.59	0.45
1:H:268:ASP:HB3	1:H:271:ARG:HH12	1.80	0.45
1:H:449:GLU:O	1:H:450:ASN:HB2	2.17	0.45
1:F:75:ASN:HD21	1:F:94:LEU:H	1.65	0.45
1:I:26:GLU:HB3	1:I:28:LEU:HB2	1.99	0.45
1:J:51:LYS:HA	1:J:54:LEU:HB2	1.98	0.45
1:F:449:GLU:OE2	1:F:449:GLU:HA	2.17	0.45
1:I:126:MET:CE	1:I:187:TYR:CE1	2.99	0.44
1:F:73:VAL:C	1:F:75:ASN:H	2.20	0.44
1:C:295:GLU:HG2	1:C:297:TYR:CE1	2.52	0.44
1:H:283:ASN:HD21	1:H:324:LEU:HD11	1.82	0.44
1:D:122:ILE:HD11	1:D:167:TRP:CH2	2.52	0.44
1:A:131:LEU:HD13	1:A:135:LEU:HD11	1.99	0.44
1:J:20:ILE:HD11	1:J:21:TYR:CZ	2.52	0.44
1:A:436:THR:O	1:A:456:ILE:HA	2.17	0.44
1:C:423:ARG:HH12	1:C:425:GLU:CD	2.20	0.44
1:H:30:ARG:O	1:H:329:ASN:ND2	2.33	0.44
1:C:24:PHE:CD1	1:C:25:THR:N	2.85	0.44
1:K:401:ASP:H	1:K:402:GLY:HA2	1.82	0.44
1:I:286:TYR:HA	1:I:379:ILE:HD12	1.99	0.44
1:B:435:TYR:O	1:B:477:SER:HA	2.17	0.44
1:G:75:ASN:HB3	1:G:179:VAL:HG11	1.98	0.44
1:F:26:GLU:HG3	1:F:69:GLY:HA2	1.99	0.44
1:C:122:ILE:HD12	1:C:123:SER:N	2.32	0.44
1:A:243:TYR:O	1:A:247:VAL:HG22	2.17	0.44
1:B:424:VAL:HG11	1:B:427:LEU:HD12	2.00	0.44
1:F:281:GLU:HG2	1:F:325:ALA:HB2	2.00	0.44
1:K:295:GLU:HG2	1:K:297:TYR:CE1	2.53	0.44
1:H:438:THR:HG21	1:H:472:LYS:HE3	1.98	0.44
1:A:9:PRO:HA	1:A:362:VAL:HG21	1.99	0.44
1:H:174:TYR:CE2	1:H:212:CYS:HB3	2.52	0.44
1:E:209:ALA:HB2	1:E:229:ILE:HG21	2.00	0.44
1:A:219:LEU:HD21	1:A:263:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:80:ASP:N	1:G:80:ASP:OD1	2.51	0.44
1:E:447:THR:CG2	1:E:449:GLU:H	2.30	0.44
1:C:131:LEU:HD22	1:C:135:LEU:CD2	2.46	0.44
1:C:11:LYS:O	1:C:362:VAL:CG2	2.65	0.44
1:K:253:LEU:HD21	1:K:279:LEU:HD11	1.99	0.44
1:D:238:THR:HG21	1:D:304:PHE:CE1	2.53	0.44
1:K:423:ARG:HG2	1:K:466:GLU:OE1	2.17	0.44
1:C:127:GLY:HA3	1:C:179:VAL:O	2.16	0.44
1:H:333:ALA:O	1:H:347:TYR:HB2	2.18	0.44
1:G:139:GLU:HG2	1:G:201:PHE:CZ	2.53	0.44
1:H:220:ARG:HA	1:H:220:ARG:HD2	1.59	0.44
1:I:73:VAL:O	1:I:125:ASN:HB2	2.17	0.44
1:G:245:GLU:HG3	1:G:375:GLY:HA3	1.98	0.44
1:G:45:ASP:C	1:G:47:ARG:H	2.21	0.44
1:A:58:LYS:HE3	1:A:115:GLU:O	2.18	0.44
1:D:25:THR:O	1:D:25:THR:HG23	2.17	0.44
1:I:49:PHE:HB2	1:I:54:LEU:HD11	2.00	0.44
1:C:284:VAL:O	1:C:297:TYR:HE1	2.00	0.44
1:K:401:ASP:HB2	1:K:403:LYS:N	2.32	0.44
1:I:325:ALA:HA	1:I:326:GLN:HA	1.73	0.44
1:J:80:ASP:O	1:J:89:PRO:HD2	2.18	0.44
1:G:122:ILE:HD11	1:G:137:TRP:CZ2	2.52	0.44
1:A:242:ASP:OD2	1:A:243:TYR:N	2.50	0.44
1:C:171:ASN:HD22	1:C:178:GLN:NE2	2.15	0.44
1:F:235:HIS:CD2	1:F:281:GLU:HB2	2.52	0.44
1:F:447:THR:O	1:F:448:MET:HB3	2.18	0.44
1:I:254:LYS:HG2	1:I:311:LEU:HD11	2.00	0.44
1:I:405:LEU:HB3	1:I:481:VAL:HG22	1.99	0.44
1:B:188:ALA:HB1	1:B:224:GLU:HB2	1.99	0.44
1:F:450:ASN:C	1:F:452:ASN:H	2.22	0.44
1:E:219:LEU:HD13	1:F:216:ILE:HD12	1.99	0.44
1:A:182:MET:HB3	1:A:186:GLU:HG3	2.00	0.43
1:H:240:SER:CB	1:H:377:MET:HA	2.42	0.43
1:K:401:ASP:HB2	1:K:402:GLY:C	2.38	0.43
1:F:314:LYS:HA	1:F:361:LEU:HD11	2.00	0.43
1:C:401:ASP:OD1	1:C:401:ASP:N	2.37	0.43
1:D:192:LYS:HE3	1:D:224:GLU:O	2.17	0.43
1:B:238:THR:O	1:B:284:VAL:HA	2.18	0.43
1:L:5:ILE:HD12	1:L:420:VAL:HG11	1.99	0.43
1:L:398:ILE:CG2	1:L:399:SER:O	2.61	0.43
1:D:226:GLY:O	1:D:273:ARG:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:71:ASN:HA	1:L:178:GLN:HE22	1.83	0.43
1:K:173:MET:HE3	1:K:181:HIS:HA	1.99	0.43
1:I:206:LYS:HA	1:I:230:ASP:OD1	2.17	0.43
1:D:30:ARG:HH21	1:D:294:GLU:CD	2.20	0.43
1:H:248:SER:OG	1:H:373:ILE:HD11	2.16	0.43
1:H:251:TYR:CZ	1:H:390:PRO:HD2	2.53	0.43
1:B:261:LYS:HD3	1:B:318:ILE:HG23	1.99	0.43
1:A:66:ARG:HA	1:A:121:TYR:O	2.18	0.43
1:L:192:LYS:HD3	1:L:224:GLU:O	2.17	0.43
1:H:382:MET:HA	1:H:383:PRO:HD3	1.88	0.43
1:H:425:GLU:HA	1:H:425:GLU:OE2	2.18	0.43
1:C:298:ASP:OD1	1:C:300:LYS:HG2	2.18	0.43
1:G:142:ASN:HD21	1:G:164:VAL:N	2.05	0.43
1:G:142:ASN:ND2	1:G:163:ASN:HA	2.33	0.43
1:J:380:ASN:ND2	1:J:382:MET:HB2	2.34	0.43
1:D:73:VAL:C	1:D:75:ASN:H	2.22	0.43
1:A:132:ASP:OD2	1:F:77:HIS:NE2	2.48	0.43
1:D:32:ILE:HD11	1:D:104:PHE:CG	2.53	0.43
1:K:311:LEU:HA	1:K:314:LYS:HD2	2.01	0.43
1:G:321:LEU:HD11	1:G:323:ASN:HD21	1.83	0.43
1:B:243:TYR:HD1	1:B:300:LYS:HB2	1.82	0.43
1:E:9:PRO:HA	1:E:362:VAL:HG21	2.01	0.43
1:B:84:PRO:HA	2:B:509:HOH:O	2.18	0.43
1:J:239:GLY:HA3	1:J:240:SER:OG	2.18	0.43
1:A:45:ASP:OD1	1:A:47:ARG:HD3	2.19	0.43
1:A:50:ARG:NH2	1:A:52:ASP:OD2	2.44	0.43
1:I:324:LEU:HD13	1:I:350:PHE:HE2	1.83	0.43
1:C:287:ARG:HD2	1:C:295:GLU:CD	2.38	0.43
1:D:32:ILE:HD11	1:D:104:PHE:CB	2.49	0.43
1:F:450:ASN:O	1:F:453:VAL:HG12	2.19	0.43
1:F:243:TYR:CE1	1:F:247:VAL:HG11	2.53	0.43
1:K:436:THR:O	1:K:456:ILE:HA	2.18	0.43
1:I:365:HIS:HE1	1:I:367:GLU:HG2	1.83	0.43
1:C:235:HIS:HE1	1:C:280:ASP:OD1	2.01	0.43
1:G:27:HIS:HA	1:G:32:ILE:HG21	2.00	0.43
1:B:401:ASP:HB2	1:B:403:LYS:H	1.83	0.43
1:E:32:ILE:HG23	1:E:33:TYR:H	1.82	0.43
1:I:32:ILE:C	1:I:32:ILE:HD13	2.39	0.43
1:C:20:ILE:HD12	1:C:312:LEU:HB3	2.00	0.43
1:E:411:ASN:OD1	1:E:413:ARG:HB2	2.19	0.43
1:A:88:ARG:HA	1:A:89:PRO:HD3	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:427:LEU:HD22	1:L:428:GLY:N	2.33	0.43
1:H:298:ASP:HA	1:H:345:PRO:HG3	2.01	0.43
1:H:169:ILE:HA	1:H:169:ILE:HD12	1.93	0.43
1:I:75:ASN:HA	1:I:128:THR:OG1	2.18	0.43
1:I:407:ILE:O	1:I:478:VAL:HA	2.18	0.43
1:A:145:GLY:O	1:A:154:ARG:NH2	2.45	0.43
1:A:285:TRP:CD1	1:A:379:ILE:HD13	2.54	0.43
1:K:214:ASP:HB3	1:K:217:TRP:HB3	1.99	0.43
1:E:348:LYS:HD2	1:E:455:ASP:HA	2.01	0.43
1:L:4:ARG:HG2	1:L:421:PRO:HG2	2.01	0.43
1:I:233:SER:HA	1:I:278:ALA:O	2.19	0.43
1:C:352:LEU:HD11	1:C:478:VAL:HG12	2.01	0.43
1:B:68:PRO:CG	1:B:73:VAL:HG23	2.44	0.43
1:J:188:ALA:HB1	1:J:220:ARG:O	2.19	0.43
1:E:370:THR:HG21	1:E:388:ASN:OD1	2.19	0.43
1:L:141:CYS:C	1:L:142:ASN:HD22	2.22	0.43
1:D:4:ARG:HH22	1:D:423:ARG:HG3	1.84	0.43
1:E:167:TRP:O	1:E:207:ALA:HA	2.18	0.43
1:H:32:ILE:HD11	1:H:104:PHE:CB	2.49	0.43
1:E:223:GLN:HE22	1:F:216:ILE:HD13	1.84	0.43
1:K:436:THR:OG1	1:K:477:SER:HB3	2.18	0.43
1:J:8:ASP:HA	1:J:9:PRO:HD2	1.77	0.43
1:F:71:ASN:O	1:F:95:ALA:HB2	2.19	0.43
1:F:174:TYR:CE2	1:F:212:CYS:HB3	2.54	0.43
1:C:309:LEU:O	1:C:313:GLN:HG3	2.18	0.43
1:K:404:LYS:HE2	1:K:480:GLU:OE2	2.18	0.43
1:D:81:GLY:O	1:D:105:GLY:HA3	2.19	0.43
1:H:206:LYS:HA	1:H:230:ASP:OD1	2.19	0.43
1:C:125:ASN:OD1	1:C:128:THR:HG22	2.19	0.43
1:E:298:ASP:OD1	1:E:300:LYS:HG2	2.19	0.43
1:B:441:ASP:C	1:B:443:ASN:H	2.21	0.43
1:G:282:TRP:O	1:G:283:ASN:HB2	2.19	0.43
1:G:202:ASP:OD1	1:G:204:THR:HB	2.19	0.43
1:E:150:ALA:O	1:E:151:GLN:C	2.56	0.43
1:D:32:ILE:HD11	1:D:104:PHE:HB3	2.01	0.43
1:L:120:PRO:HG2	1:L:164:VAL:HB	2.01	0.43
1:K:428:GLY:HA2	1:K:429:GLN:HA	1.68	0.43
1:G:464:ASP:C	1:G:466:GLU:N	2.72	0.43
1:G:247:VAL:O	1:G:248:SER:HB3	2.18	0.43
1:I:255:GLU:HG3	1:J:262:LYS:HZ1	1.84	0.43
1:A:233:SER:HA	1:A:278:ALA:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:67:TRP:CE2	1:F:68:PRO:HB3	2.54	0.43
1:D:60:ILE:HA	1:D:60:ILE:HD13	1.63	0.43
1:D:52:ASP:N	1:D:52:ASP:OD1	2.52	0.43
1:L:325:ALA:HA	1:L:326:GLN:HA	1.56	0.42
1:D:464:ASP:C	1:D:466:GLU:N	2.66	0.42
1:D:27:HIS:HA	1:D:32:ILE:HG21	2.01	0.42
1:B:73:VAL:HG21	1:B:123:SER:O	2.19	0.42
1:D:372:ASN:N	1:D:372:ASN:ND2	2.58	0.42
1:G:262:LYS:NZ	1:H:255:GLU:HG3	2.33	0.42
1:H:169:ILE:O	1:H:169:ILE:CG2	2.66	0.42
1:K:154:ARG:CG	1:K:159:PRO:HA	2.49	0.42
1:F:8:ASP:O	1:F:362:VAL:CG1	2.67	0.42
1:B:298:ASP:OD1	1:B:300:LYS:HG3	2.19	0.42
1:B:353:ILE:O	1:B:357:SER:HB3	2.18	0.42
1:E:313:GLN:HE22	1:E:357:SER:HB2	1.84	0.42
1:D:319:VAL:HG22	1:D:319:VAL:O	2.19	0.42
1:J:247:VAL:O	1:J:248:SER:HB3	2.19	0.42
1:A:262:LYS:O	1:A:266:MET:HG3	2.19	0.42
1:H:240:SER:HA	1:H:286:TYR:CD1	2.54	0.42
1:E:70:GLY:O	1:E:73:VAL:HG12	2.19	0.42
1:K:158:HIS:HA	1:K:159:PRO:HD2	1.88	0.42
1:E:284:VAL:O	1:E:297:TYR:HE1	2.02	0.42
1:F:380:ASN:O	1:F:381:LYS:HB2	2.19	0.42
1:F:135:LEU:O	1:F:139:GLU:HG3	2.18	0.42
1:E:217:TRP:C	1:E:217:TRP:CD1	2.92	0.42
1:D:26:GLU:HG2	1:D:27:HIS:N	2.33	0.42
1:A:22:GLY:HA3	1:A:64:ASN:HB3	2.00	0.42
1:B:126:MET:HB3	1:B:126:MET:HE3	1.74	0.42
1:D:238:THR:HG21	1:D:304:PHE:CZ	2.53	0.42
1:A:234:TYR:O	1:A:279:LEU:HD23	2.19	0.42
1:L:110:ILE:O	1:L:114:ARG:HG2	2.19	0.42
1:G:32:ILE:HD11	1:G:104:PHE:HB3	2.00	0.42
1:I:4:ARG:HG3	1:I:5:ILE:N	2.34	0.42
1:I:47:ARG:HH21	1:I:111:GLU:CD	2.21	0.42
1:A:328:VAL:O	1:A:330:ALA:N	2.51	0.42
1:B:299:LEU:HD13	1:B:454:VAL:HG21	2.01	0.42
1:E:403:LYS:HB2	1:E:484:GLU:CA	2.48	0.42
1:J:4:ARG:HB3	1:J:367:GLU:HB2	2.01	0.42
1:B:220:ARG:HA	1:B:220:ARG:HD2	1.78	0.42
1:B:105:GLY:H	1:B:108:GLU:HB2	1.85	0.42
1:C:282:TRP:O	1:C:283:ASN:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:VAL:HA	1:B:63:PRO:HD3	1.90	0.42
1:G:220[A]:ARG:HA	1:G:220[A]:ARG:HD2	1.88	0.42
1:L:450:ASN:N	1:L:451:PRO:HD2	2.35	0.42
1:C:288:VAL:HG12	1:C:290:ASP:H	1.84	0.42
1:G:463:VAL:CG1	1:G:464:ASP:N	2.83	0.42
1:I:174:TYR:CE2	1:I:212:CYS:HB3	2.55	0.42
1:E:279:LEU:HD13	1:E:282:TRP:CD1	2.54	0.42
1:L:88:ARG:HA	1:L:89:PRO:HD3	1.84	0.42
1:C:235:HIS:CD2	1:C:281:GLU:HB2	2.55	0.42
1:L:135:LEU:O	1:L:139:GLU:HG3	2.20	0.42
1:E:437:LEU:HB2	1:E:456:ILE:HG13	2.01	0.42
1:J:101:THR:O	1:J:102:ASN:HB2	2.20	0.42
1:C:88:ARG:HA	1:C:89:PRO:HD3	1.91	0.42
1:B:60:ILE:HD12	1:B:350:PHE:HB3	2.02	0.42
1:G:434:VAL:HG22	1:G:479:ILE:HG12	2.02	0.42
1:I:446:ASN:OD1	1:I:454:VAL:HG22	2.19	0.42
1:I:9:PRO:HA	1:I:362:VAL:HG21	2.01	0.42
1:D:428:GLY:HA3	1:D:464:ASP:HA	2.01	0.42
1:C:125:ASN:HD22	1:C:126:MET:N	2.18	0.42
1:K:235:HIS:CE1	1:K:280:ASP:OD1	2.73	0.42
1:D:273:ARG:NH1	1:D:273:ARG:HG3	2.34	0.42
1:E:239:GLY:HA3	1:E:240:SER:OG	2.20	0.42
1:E:309:LEU:O	1:E:313:GLN:HG3	2.20	0.42
1:A:36:ILE:HG23	1:A:328:VAL:HG21	2.02	0.42
1:J:174:TYR:CE2	1:J:212:CYS:HB3	2.55	0.42
1:D:217:TRP:O	1:D:221:VAL:HG23	2.20	0.42
1:A:430:LYS:NZ	1:A:484:GLU:OE1	2.53	0.42
1:G:22:GLY:HA3	1:G:64:ASN:HB3	2.02	0.42
1:I:380:ASN:OD1	1:I:382:MET:HG3	2.20	0.42
1:J:4:ARG:NH2	1:J:423:ARG:HG3	2.35	0.42
1:E:401:ASP:HB2	1:E:402:GLY:HA2	2.01	0.42
1:C:219:LEU:HD13	1:D:215:PRO:HB2	2.01	0.42
1:I:255:GLU:HG3	1:J:262:LYS:CE	2.50	0.42
1:D:81:GLY:HA2	1:D:88:ARG:HD3	2.02	0.42
1:L:467:PHE:CD1	1:L:468:GLU:N	2.88	0.42
1:B:239:GLY:CA	1:B:378:PHE:H	2.33	0.42
1:J:373:ILE:H	1:J:373:ILE:HG13	1.66	0.42
1:G:262:LYS:HG3	1:H:259:GLY:HA2	2.02	0.42
1:E:374:GLU:HG2	1:E:385:SER:CB	2.48	0.42
1:L:311:LEU:O	1:L:314:LYS:HB2	2.20	0.42
1:I:3:TYR:CD2	1:I:3:TYR:N	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:TYR:HD1	1:B:300:LYS:CB	2.33	0.42
1:D:60:ILE:HD11	1:D:351:GLU:CA	2.50	0.42
1:G:9:PRO:HA	1:G:362:VAL:HG11	2.02	0.42
1:K:325:ALA:HA	1:K:326:GLN:HA	1.75	0.42
1:L:235:HIS:CE1	1:L:280:ASP:OD1	2.73	0.41
1:L:281:GLU:HG2	1:L:325:ALA:HB2	2.02	0.41
1:H:154:ARG:HG2	1:H:159:PRO:HA	2.03	0.41
1:E:238:THR:OG1	1:E:239:GLY:N	2.53	0.41
1:E:130:THR:HB	1:E:133:GLU:H	1.84	0.41
1:L:6:VAL:HG22	1:L:423:ARG:HB3	2.02	0.41
1:A:209:ALA:HB2	1:A:229:ILE:HG21	2.02	0.41
1:E:372:ASN:HD22	1:E:388:ASN:H	1.65	0.41
1:K:317:ASP:OD1	1:K:317:ASP:N	2.52	0.41
1:H:77:HIS:NE2	1:J:132:ASP:OD2	2.51	0.41
1:H:105:GLY:O	1:H:107:ASP:N	2.53	0.41
1:A:378:PHE:CG	1:A:379:ILE:N	2.88	0.41
1:E:141:CYS:HB3	1:E:164:VAL:CG1	2.49	0.41
1:E:130:THR:HG22	1:E:131:LEU:N	2.35	0.41
1:L:328:VAL:HG22	1:L:334:ILE:HB	2.02	0.41
1:I:326:GLN:HB2	1:I:330:ALA:O	2.21	0.41
1:E:192:LYS:O	1:E:196:LYS:HB2	2.20	0.41
1:J:398:ILE:HA	1:J:398:ILE:HD13	1.94	0.41
1:J:182:MET:HB3	1:J:186:GLU:HG2	2.02	0.41
1:G:403:LYS:HB2	1:G:484:GLU:HA	2.01	0.41
1:B:157:GLY:O	1:B:159:PRO:HD3	2.20	0.41
1:G:451:PRO:HB2	1:G:452:ASN:H	1.59	0.41
1:K:427:LEU:HD22	1:K:430:LYS:HD3	2.01	0.41
1:F:460:THR:O	1:F:461:ILE:HD12	2.20	0.41
1:I:284:VAL:CG1	1:I:286:TYR:HE2	2.33	0.41
1:D:122:ILE:HD11	1:D:167:TRP:CZ3	2.55	0.41
1:D:24:PHE:HB3	1:D:324:LEU:O	2.21	0.41
1:E:60:ILE:O	1:E:354:VAL:HG11	2.21	0.41
1:E:348:LYS:HB3	1:E:437:LEU:HD13	2.01	0.41
1:D:85:LYS:HE2	1:D:108:GLU:OE2	2.20	0.41
1:L:34:GLY:O	1:L:336:THR:OG1	2.35	0.41
1:K:262:LYS:O	1:K:266:MET:HG3	2.20	0.41
1:H:239:GLY:HA2	1:H:286:TYR:HB3	2.01	0.41
1:E:225:ALA:O	1:E:229:ILE:HG12	2.21	0.41
1:L:171:ASN:ND2	1:L:172:GLU:HG3	2.36	0.41
1:C:238:THR:O	1:C:285:TRP:N	2.44	0.41
1:H:359:GLU:O	1:H:360:LYS:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:465:THR:O	1:D:466:GLU:HB2	2.19	0.41
1:D:26:GLU:HG3	1:D:69:GLY:CA	2.45	0.41
1:L:282:TRP:CZ3	1:L:308:VAL:HG11	2.55	0.41
1:D:359:GLU:HG3	1:D:400:GLU:CG	2.48	0.41
1:H:4:ARG:NH1	1:H:4:ARG:HG3	2.17	0.41
1:C:122:ILE:CG1	1:C:167:TRP:CZ3	3.03	0.41
1:D:359:GLU:CG	1:D:400:GLU:HG2	2.47	0.41
1:E:348:LYS:HB3	1:E:437:LEU:CD1	2.51	0.41
1:E:391:PHE:CD1	1:E:413:ARG:HG2	2.56	0.41
1:C:285:TRP:O	1:C:378:PHE:HA	2.21	0.41
1:A:335:HIS:O	1:A:342:ILE:N	2.50	0.41
1:G:254:LYS:HG3	1:G:311:LEU:HD11	2.03	0.41
1:I:41:SER:HA	1:I:42:PRO:HD2	1.83	0.41
1:C:47:ARG:HB2	1:C:47:ARG:HE	1.65	0.41
1:A:291:ASN:N	1:A:291:ASN:OD1	2.51	0.41
1:G:163:ASN:O	1:G:165:LYS:HD2	2.20	0.41
1:C:202:ASP:HA	1:C:203:PRO:HD3	1.89	0.41
1:A:122:ILE:CD1	1:A:137:TRP:CZ2	3.04	0.41
1:K:450:ASN:HB3	1:K:453:VAL:HG23	2.02	0.41
1:B:451:PRO:HG2	1:B:452:ASN:HD21	1.86	0.41
1:G:246:THR:C	1:G:247:VAL:O	2.59	0.41
1:I:283:ASN:HB2	1:I:325:ALA:O	2.20	0.41
1:L:192:LYS:O	1:L:196:LYS:HB3	2.20	0.41
1:C:407:ILE:O	1:C:478:VAL:HA	2.20	0.41
1:K:32:ILE:HG22	1:K:33:TYR:N	2.35	0.41
1:G:214:ASP:HA	1:G:215:PRO:HD2	1.88	0.41
1:D:74:SER:HA	1:D:125:ASN:OD1	2.21	0.41
1:G:398:ILE:HG13	1:G:404:LYS:O	2.21	0.41
1:C:49:PHE:O	1:C:50:ARG:C	2.58	0.41
1:A:262:LYS:CB	1:A:262:LYS:NZ	2.71	0.41
1:C:24:PHE:HD1	1:C:25:THR:H	1.68	0.41
1:C:314:LYS:HE2	1:C:394:ALA:O	2.21	0.41
1:B:434:VAL:HG23	1:B:461:ILE:HG12	2.02	0.41
1:C:406:PHE:N	1:C:406:PHE:CD2	2.88	0.41
1:G:472:LYS:HE3	1:G:472:LYS:HB2	1.94	0.41
1:L:26:GLU:HG3	1:L:28:LEU:HB2	2.02	0.41
1:C:74:SER:HA	1:C:125:ASN:ND2	2.36	0.41
1:E:25:THR:CG2	1:E:25:THR:O	2.69	0.41
1:I:401:ASP:HB2	1:I:403:LYS:H	1.86	0.41
1:K:280:ASP:HA	1:K:323:ASN:HD22	1.86	0.41
1:I:173:MET:HE3	1:I:182:MET:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:GLU:HA	1:A:161:PRO:HD3	1.96	0.41
1:A:319:VAL:O	1:A:319:VAL:HG22	2.20	0.41
1:F:24:PHE:CD2	1:F:326:GLN:HG2	2.55	0.41
1:E:422:ILE:HB	1:E:467:PHE:CE2	2.56	0.41
1:A:28:LEU:HD23	1:A:29:GLY:N	2.36	0.41
1:E:208:ILE:HG13	1:E:231:PHE:CD2	2.56	0.41
1:D:219:LEU:HA	1:D:219:LEU:HD23	1.90	0.41
1:H:176:GLU:H	1:H:176:GLU:HG3	1.52	0.41
1:E:28:LEU:HD13	1:E:330:ALA:HB1	2.03	0.41
1:C:163:ASN:C	1:C:163:ASN:HD22	2.24	0.41
1:G:401:ASP:N	1:G:402:GLY:HA2	2.35	0.41
1:I:131:LEU:CD2	1:I:135:LEU:CD2	2.95	0.41
1:K:239:GLY:CA	1:K:240:SER:OG	2.66	0.41
1:L:447:THR:C	1:L:449:GLU:N	2.74	0.41
1:H:318:ILE:HG22	1:H:319:VAL:HG12	2.03	0.41
1:F:163:ASN:HD22	1:F:165:LYS:HE2	1.86	0.41
1:D:325:ALA:HA	1:D:326:GLN:HA	1.78	0.41
1:L:362:VAL:HG23	1:L:398:ILE:HG13	2.03	0.40
1:E:235:HIS:HD2	1:E:281:GLU:OE1	2.05	0.40
1:K:208:ILE:HA	1:K:231:PHE:HB2	2.03	0.40
1:K:16:ILE:HD12	1:K:361:LEU:HB2	2.03	0.40
1:C:25:THR:O	1:C:25:THR:HG23	2.20	0.40
1:I:254:LYS:O	1:I:258:ILE:HG13	2.21	0.40
1:L:352:LEU:O	1:L:356:HIS:HB2	2.21	0.40
1:D:246:THR:OG1	1:D:300:LYS:HE2	2.21	0.40
1:H:236:PHE:CG	1:H:253:LEU:HD13	2.56	0.40
1:G:422:ILE:HB	1:G:467:PHE:CE2	2.56	0.40
1:B:45:ASP:HB3	1:B:51:LYS:HD3	2.04	0.40
1:L:66:ARG:HA	1:L:121:TYR:O	2.21	0.40
1:D:88:ARG:HA	1:D:89:PRO:HD3	1.91	0.40
1:J:282:TRP:O	1:J:283:ASN:HB2	2.21	0.40
1:I:19:HIS:HD2	1:I:64:ASN:OD1	2.04	0.40
1:L:199:LYS:HE2	1:L:205:ILE:O	2.20	0.40
1:L:295:GLU:HG2	1:L:297:TYR:CE1	2.56	0.40
1:K:256:ARG:O	1:K:260:VAL:HG23	2.21	0.40
1:J:171:ASN:HD22	1:J:178:GLN:HE22	1.69	0.40
1:A:243:TYR:CZ	1:A:247:VAL:HG21	2.56	0.40
1:G:171:ASN:O	1:G:172:GLU:C	2.59	0.40
1:K:73:VAL:C	1:K:75:ASN:N	2.74	0.40
1:E:32:ILE:HD13	1:E:32:ILE:C	2.42	0.40
1:A:219:LEU:HD11	1:B:215:PRO:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:298:ASP:C	1:C:345:PRO:HG2	2.42	0.40
1:D:231:PHE:HA	1:D:276:LYS:O	2.21	0.40
1:L:235:HIS:CD2	1:L:281:GLU:HB2	2.57	0.40
1:D:121:TYR:CD1	1:D:121:TYR:C	2.95	0.40
1:E:141:CYS:HB3	1:E:164:VAL:HG13	2.02	0.40
1:I:32:ILE:HD11	1:I:104:PHE:CG	2.57	0.40
1:L:23:HIS:O	1:L:65:LEU:HA	2.22	0.40
1:I:217:TRP:C	1:I:217:TRP:CD1	2.94	0.40
1:J:32:ILE:CG2	1:J:33:TYR:N	2.81	0.40
1:J:141:CYS:C	1:J:142:ASN:HD22	2.24	0.40
1:A:126:MET:CE	1:A:170:GLY:HA3	2.45	0.40
1:G:67:TRP:CB	1:G:109:PHE:CE1	3.05	0.40
1:F:295:GLU:HG2	1:F:297:TYR:CZ	2.56	0.40
1:F:295:GLU:HA	1:F:296:PRO:HD3	1.89	0.40
1:K:424:VAL:HG22	1:K:427:LEU:HB2	2.03	0.40
1:C:262:LYS:HD2	1:D:259:GLY:CA	2.51	0.40
1:G:464:ASP:C	1:G:466:GLU:H	2.24	0.40
1:F:77:HIS:NE2	1:F:128:THR:CG2	2.84	0.40
1:K:326:GLN:O	1:K:332:GLY:HA2	2.22	0.40
1:F:140:TYR:O	1:F:153:ARG:HD3	2.21	0.40
1:L:218:ASN:HB2	1:L:263:LEU:HD23	2.03	0.40
1:A:428:GLY:HA2	1:A:429:GLN:HA	1.88	0.40
1:H:148:TYR:CD2	1:H:148:TYR:C	2.94	0.40
1:F:403:LYS:HB2	1:F:403:LYS:HZ2	1.86	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	481/484 (99%)	434 (90%)	42 (9%)	5 (1%)	19 61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	481/484 (99%)	435 (90%)	39 (8%)	7 (2%)	13	50
1	C	481/484 (99%)	433 (90%)	42 (9%)	6 (1%)	16	56
1	D	481/484 (99%)	434 (90%)	38 (8%)	9 (2%)	10	43
1	E	481/484 (99%)	431 (90%)	41 (8%)	9 (2%)	10	43
1	F	481/484 (99%)	433 (90%)	39 (8%)	9 (2%)	10	43
1	G	482/484 (100%)	424 (88%)	47 (10%)	11 (2%)	8	36
1	H	481/484 (99%)	418 (87%)	53 (11%)	10 (2%)	9	40
1	I	481/484 (99%)	426 (89%)	42 (9%)	13 (3%)	6	32
1	J	479/484 (99%)	416 (87%)	50 (10%)	13 (3%)	6	32
1	K	481/484 (99%)	433 (90%)	42 (9%)	6 (1%)	16	56
1	L	482/484 (100%)	420 (87%)	54 (11%)	8 (2%)	11	46
All	All	5772/5808 (99%)	5137 (89%)	529 (9%)	106 (2%)	11	45

All (106) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	450	ASN
1	B	227	ASP
1	B	428	GLY
1	D	450	ASN
1	D	465	THR
1	E	428	GLY
1	E	466	GLU
1	F	286	TYR
1	G	451	PRO
1	G	452	ASN
1	I	272	LYS
1	I	450	ASN
1	I	465	THR
1	J	279	LEU
1	J	374	GLU
1	K	428	GLY
1	L	283	ASN
1	A	247	VAL
1	A	283	ASN
1	C	248	SER
1	D	363	LYS
1	E	248	SER

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Mol	Chain	Res	Type
1	E	329	ASN
1	F	247	VAL
1	G	474	PHE
1	H	29	GLY
1	H	106	THR
1	H	339	ASP
1	H	401	ASP
1	H	428	GLY
1	I	61	LYS
1	I	172	GLU
1	I	248	SER
1	K	449	GLU
1	L	172	GLU
1	L	356	HIS
1	A	172	GLU
1	B	27	HIS
1	B	248	SER
1	B	286	TYR
1	C	283	ASN
1	C	286	TYR
1	D	466	GLU
1	E	196	LYS
1	F	74	SER
1	F	440	PRO
1	F	465	THR
1	G	172	GLU
1	G	247	VAL
1	H	400	GLU
1	I	247	VAL
1	I	286	TYR
1	I	329	ASN
1	I	466	GLU
1	J	32	ILE
1	J	305	ALA
1	J	440	PRO
1	J	450	ASN
1	L	47	ARG
1	A	329	ASN
1	C	4	ARG
1	C	50	ARG
1	D	227	ASP
1	D	459	GLU

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Mol	Chain	Res	Type
1	F	283	ASN
1	F	329	ASN
1	F	448	MET
1	G	286	TYR
1	H	329	ASN
1	H	450	ASN
1	I	399	SER
1	J	74	SER
1	J	286	TYR
1	J	329	ASN
1	J	356	HIS
1	K	74	SER
1	K	286	TYR
1	L	248	SER
1	L	378	PHE
1	B	50	ARG
1	B	290	ASP
1	C	241	GLU
1	D	18	ARG
1	D	464	ASP
1	E	18	ARG
1	E	331	LEU
1	F	449	GLU
1	G	329	ASN
1	I	85	LYS
1	I	451	PRO
1	J	248	SER
1	L	279	LEU
1	D	286	TYR
1	G	46	GLU
1	G	453	VAL
1	G	455	ASP
1	H	440	PRO
1	J	401	ASP
1	H	340	GLY
1	E	379	ILE
1	G	424	VAL
1	J	63	PRO
1	K	14	LYS
1	L	463	VAL
1	E	145	GLY
1	K	450	ASN

### 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	419/420 (100%)	371 (88%)	48 (12%)	7	28
1	B	419/420 (100%)	366 (87%)	53 (13%)	5	24
1	C	419/420 (100%)	371 (88%)	48 (12%)	7	28
1	D	419/420 (100%)	370 (88%)	49 (12%)	7	27
1	E	419/420 (100%)	374 (89%)	45 (11%)	8	31
1	F	419/420 (100%)	371 (88%)	48 (12%)	7	28
1	G	420/420 (100%)	359 (86%)	61 (14%)	4	18
1	H	419/420 (100%)	362 (86%)	57 (14%)	5	20
1	I	419/420 (100%)	374 (89%)	45 (11%)	8	31
1	J	417/420 (99%)	366 (88%)	51 (12%)	6	25
1	K	419/420 (100%)	367 (88%)	52 (12%)	6	24
1	L	420/420 (100%)	374 (89%)	46 (11%)	8	30
All	All	5028/5040 (100%)	4425 (88%)	603 (12%)	6	26

All (603) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LEU
1	A	32	ILE
1	A	46	GLU
1	A	47	ARG
1	A	51	LYS
1	A	61	LYS
1	A	64	ASN
1	A	97	GLN
1	A	121	TYR
1	A	122	ILE
1	A	123	SER
1	A	131	LEU
1	A	144	LYS
1	A	160	GLU

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Mol	Chain	Res	Type
1	A	163	ASN
1	A	164	VAL
1	A	176	GLU
1	A	179	VAL
1	A	199	LYS
1	A	206	LYS
1	A	216	ILE
1	A	261	LYS
1	A	262	LYS
1	A	263	LEU
1	A	279	LEU
1	A	287	ARG
1	A	291	ASN
1	A	292	LYS
1	A	319	VAL
1	A	328	VAL
1	A	348	LYS
1	A	353	ILE
1	A	359	GLU
1	A	362	VAL
1	A	382	MET
1	A	403	LYS
1	A	409	VAL
1	A	415	GLU
1	A	418	LEU
1	A	425	GLU
1	A	427	LEU
1	A	430	LYS
1	A	454	VAL
1	A	460	THR
1	A	465	THR
1	A	478	VAL
1	A	481	VAL
1	A	484	GLU
1	B	25	THR
1	B	32	ILE
1	B	41	SER
1	B	46	GLU
1	B	47	ARG
1	B	73	VAL
1	B	97	GLN
1	B	111	GLU

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Mol	Chain	Res	Type
1	B	114	ARG
1	B	121	TYR
1	B	126	MET
1	B	128	THR
1	B	131	LEU
1	B	135	LEU
1	B	144	LYS
1	B	146	ASN
1	B	147	THR
1	B	164	VAL
1	B	165	LYS
1	B	179	VAL
1	B	189	ARG
1	B	196	LYS
1	B	241	GLU
1	B	248	SER
1	B	262	LYS
1	B	277	ILE
1	B	279	LEU
1	B	287	ARG
1	B	288	VAL
1	B	291	ASN
1	B	292	LYS
1	B	293	LEU
1	B	295	GLU
1	B	319	VAL
1	B	355	ASN
1	B	359	GLU
1	B	362	VAL
1	B	364	THR
1	B	370	THR
1	B	403	LYS
1	B	409	VAL
1	B	415	GLU
1	B	419	LYS
1	B	422	ILE
1	B	427	LEU
1	B	430	LYS
1	B	431	LYS
1	B	445	ARG
1	B	452	ASN
1	B	454	VAL

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Mol	Chain	Res	Type
1	B	462	THR
1	B	465	THR
1	B	478	VAL
1	C	7	VAL
1	C	30	ARG
1	C	47	ARG
1	C	60	ILE
1	C	64	ASN
1	C	86	ASP
1	C	87	GLN
1	C	121	TYR
1	C	122	ILE
1	C	128	THR
1	C	131	LEU
1	C	132	ASP
1	C	142	ASN
1	C	144	LYS
1	C	163	ASN
1	C	164	VAL
1	C	179	VAL
1	C	185	ASP
1	C	189	ARG
1	C	206	LYS
1	C	224	GLU
1	C	241	GLU
1	C	242	ASP
1	C	247	VAL
1	C	261	LYS
1	C	262	LYS
1	C	263	LEU
1	C	279	LEU
1	C	287	ARG
1	C	291	ASN
1	C	293	LEU
1	C	314	LYS
1	C	359	GLU
1	C	370	THR
1	C	373	ILE
1	C	397	SER
1	C	400	GLU
1	C	401	ASP
1	C	404	LYS

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Mol	Chain	Res	Type
1	C	409	VAL
1	C	415	GLU
1	C	418	LEU
1	C	424	VAL
1	C	427	LEU
1	C	450	ASN
1	C	452	ASN
1	C	465	THR
1	C	481	VAL
1	D	10	LYS
1	D	18	ARG
1	D	32	ILE
1	D	43	LEU
1	D	46	GLU
1	D	55	GLU
1	D	60	ILE
1	D	75	ASN
1	D	79	GLU
1	D	87	GLN
1	D	97	GLN
1	D	111	GLU
1	D	121	TYR
1	D	122	ILE
1	D	131	LEU
1	D	132	ASP
1	D	135	LEU
1	D	151	GLN
1	D	160	GLU
1	D	163	ASN
1	D	179	VAL
1	D	186	GLU
1	D	189	ARG
1	D	192	LYS
1	D	223	GLN
1	D	241	GLU
1	D	261	LYS
1	D	262	LYS
1	D	268	ASP
1	D	279	LEU
1	D	287	ARG
1	D	319	VAL
1	D	359	GLU

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Mol	Chain	Res	Type
1	D	367	GLU
1	D	370	THR
1	D	372	ASN
1	D	379	ILE
1	D	401	ASP
1	D	403	LYS
1	D	404	LYS
1	D	415	GLU
1	D	424	VAL
1	D	427	LEU
1	D	433	THR
1	D	458	SER
1	D	465	THR
1	D	478	VAL
1	D	481	VAL
1	D	484	GLU
1	E	6	VAL
1	E	25	THR
1	E	28	LEU
1	E	32	ILE
1	E	54	LEU
1	E	55	GLU
1	E	60	ILE
1	E	79	GLU
1	E	86	ASP
1	E	87	GLN
1	E	97	GLN
1	E	114	ARG
1	E	121	TYR
1	E	122	ILE
1	E	128	THR
1	E	130	THR
1	E	131	LEU
1	E	135	LEU
1	E	164	VAL
1	E	165	LYS
1	E	179	VAL
1	E	254	LYS
1	E	262	LYS
1	E	279	LEU
1	E	286	TYR
1	E	287	ARG

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Mol	Chain	Res	Type
1	E	291	ASN
1	E	292	LYS
1	E	293	LEU
1	E	319	VAL
1	E	355	ASN
1	E	356	HIS
1	E	359	GLU
1	E	370	THR
1	E	386	VAL
1	E	400	GLU
1	E	401	ASP
1	E	403	LYS
1	E	409	VAL
1	E	422	ILE
1	E	427	LEU
1	E	433	THR
1	E	447	THR
1	E	454	VAL
1	E	459	GLU
1	F	51	LYS
1	F	55	GLU
1	F	86	ASP
1	F	103	ARG
1	F	121	TYR
1	F	122	ILE
1	F	128	THR
1	F	130	THR
1	F	131	LEU
1	F	135	LEU
1	F	142	ASN
1	F	144	LYS
1	F	147	THR
1	F	155	LYS
1	F	160	GLU
1	F	164	VAL
1	F	179	VAL
1	F	196	LYS
1	F	198	MET
1	F	199	LYS
1	F	254	LYS
1	F	272	LYS
1	F	276	LYS

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Mol	Chain	Res	Type
1	F	279	LEU
1	F	291	ASN
1	F	293	LEU
1	F	314	LYS
1	F	316	SER
1	F	319	VAL
1	F	353	ILE
1	F	359	GLU
1	F	362	VAL
1	F	367	GLU
1	F	370	THR
1	F	373	ILE
1	F	387	GLU
1	F	403	LYS
1	F	415	GLU
1	F	422	ILE
1	F	424	VAL
1	F	441	ASP
1	F	443	ASN
1	F	450	ASN
1	F	453	VAL
1	F	457	THR
1	F	461	ILE
1	F	481	VAL
1	F	484	GLU
1	G	4	ARG
1	G	32	ILE
1	G	46	GLU
1	G	47	ARG
1	G	49	PHE
1	G	64	ASN
1	G	75	ASN
1	G	80	ASP
1	G	86	ASP
1	G	97	GLN
1	G	114	ARG
1	G	121	TYR
1	G	122	ILE
1	G	123	SER
1	G	128	THR
1	G	130	THR
1	G	131	LEU

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Mol	Chain	Res	Type
1	G	135	LEU
1	G	147	THR
1	G	151	GLN
1	G	160	GLU
1	G	165	LYS
1	G	179	VAL
1	G	192	LYS
1	G	204	THR
1	G	241	GLU
1	G	248	SER
1	G	249	THR
1	G	258	ILE
1	G	262	LYS
1	G	263	LEU
1	G	271	ARG
1	G	272	LYS
1	G	273	ARG
1	G	279	LEU
1	G	287	ARG
1	G	293	LEU
1	G	314	LYS
1	G	319	VAL
1	G	321	LEU
1	G	339	ASP
1	G	341	LEU
1	G	359	GLU
1	G	360	LYS
1	G	373	ILE
1	G	381	LYS
1	G	398	ILE
1	G	403	LYS
1	G	409	VAL
1	G	415	GLU
1	G	423	ARG
1	G	424	VAL
1	G	427	LEU
1	G	429	GLN
1	G	457	THR
1	G	462	THR
1	G	466	GLU
1	G	472	LYS
1	G	476	CYS

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Mol	Chain	Res	Type
1	G	478	VAL
1	G	483	LEU
1	H	4	ARG
1	H	8	ASP
1	H	32	ILE
1	H	114	ARG
1	H	123	SER
1	H	130	THR
1	H	131	LEU
1	H	135	LEU
1	H	151	GLN
1	H	160	GLU
1	H	164	VAL
1	H	169	ILE
1	H	179	VAL
1	H	186	GLU
1	H	189	ARG
1	H	192	LYS
1	H	199	LYS
1	H	216	ILE
1	H	220	ARG
1	H	229	ILE
1	H	240	SER
1	H	241	GLU
1	H	252	LEU
1	H	263	LEU
1	H	279	LEU
1	H	293	LEU
1	H	294	GLU
1	H	300	LYS
1	H	306	CYS
1	H	314	LYS
1	H	319	VAL
1	H	338	LYS
1	H	339	ASP
1	H	344	THR
1	H	355	ASN
1	H	359	GLU
1	H	362	VAL
1	H	373	ILE
1	H	380	ASN
1	H	397	SER

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Mol	Chain	Res	Type
1	H	398	ILE
1	H	400	GLU
1	H	401	ASP
1	H	403	LYS
1	H	409	VAL
1	H	418	LEU
1	H	424	VAL
1	H	427	LEU
1	H	430	LYS
1	H	433	THR
1	H	448	MET
1	H	458	SER
1	H	459	GLU
1	H	460	THR
1	H	464	ASP
1	H	466	GLU
1	H	481	VAL
1	I	3	TYR
1	I	4	ARG
1	I	32	ILE
1	I	79	GLU
1	I	91	ARG
1	I	121	TYR
1	I	128	THR
1	I	131	LEU
1	I	132	ASP
1	I	144	LYS
1	I	147	THR
1	I	160	GLU
1	I	164	VAL
1	I	165	LYS
1	I	179	VAL
1	I	189	ARG
1	I	192	LYS
1	I	199	LYS
1	I	206	LYS
1	I	213	ASP
1	I	216	ILE
1	I	227	ASP
1	I	261	LYS
1	I	262	LYS
1	I	273	ARG

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Mol	Chain	Res	Type
1	I	279	LEU
1	I	287	ARG
1	I	293	LEU
1	I	319	VAL
1	I	324	LEU
1	I	338	LYS
1	I	362	VAL
1	I	370	THR
1	I	386	VAL
1	I	401	ASP
1	I	424	VAL
1	I	427	LEU
1	I	445	ARG
1	I	448	MET
1	I	450	ASN
1	I	455	ASP
1	I	460	THR
1	I	463	VAL
1	I	477	SER
1	I	481	VAL
1	J	7	VAL
1	J	47	ARG
1	J	49	PHE
1	J	51	LYS
1	J	53	VAL
1	J	59	ARG
1	J	60	ILE
1	J	79	GLU
1	J	121	TYR
1	J	122	ILE
1	J	126	MET
1	J	131	LEU
1	J	135	LEU
1	J	147	THR
1	J	151	GLN
1	J	160	GLU
1	J	164	VAL
1	J	171	ASN
1	J	179	VAL
1	J	189	ARG
1	J	196	LYS
1	J	206	LYS

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Mol	Chain	Res	Type
1	J	220	ARG
1	J	227	ASP
1	J	261	LYS
1	J	262	LYS
1	J	272	LYS
1	J	279	LEU
1	J	287	ARG
1	J	290	ASP
1	J	291	ASN
1	J	292	LYS
1	J	338	LYS
1	J	359	GLU
1	J	363	LYS
1	J	370	THR
1	J	373	ILE
1	J	379	ILE
1	J	380	ASN
1	J	386	VAL
1	J	409	VAL
1	J	413	ARG
1	J	427	LEU
1	J	445	ARG
1	J	447	THR
1	J	449	GLU
1	J	454	VAL
1	J	457	THR
1	J	472	LYS
1	J	477	SER
1	J	481	VAL
1	K	2	SER
1	K	4	ARG
1	K	5	ILE
1	K	25	THR
1	K	32	ILE
1	K	45	ASP
1	K	50	ARG
1	K	54	LEU
1	K	59	ARG
1	K	64	ASN
1	K	87	GLN
1	K	116	ILE
1	K	121	TYR

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Mol	Chain	Res	Type
1	K	131	LEU
1	K	135	LEU
1	K	151	GLN
1	K	163	ASN
1	K	164	VAL
1	K	179	VAL
1	K	185	ASP
1	K	186	GLU
1	K	189	ARG
1	K	235	HIS
1	K	254	LYS
1	K	255	GLU
1	K	261	LYS
1	K	279	LEU
1	K	287	ARG
1	K	290	ASP
1	K	291	ASN
1	K	353	ILE
1	K	355	ASN
1	K	359	GLU
1	K	362	VAL
1	K	369	GLU
1	K	382	MET
1	K	392	LEU
1	K	400	GLU
1	K	401	ASP
1	K	403	LYS
1	K	404	LYS
1	K	409	VAL
1	K	415	GLU
1	K	424	VAL
1	K	447	THR
1	K	448	MET
1	K	462	THR
1	K	465	THR
1	K	472	LYS
1	K	477	SER
1	K	478	VAL
1	K	481	VAL
1	L	11	LYS
1	L	18	ARG
1	L	32	ILE

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Mol	Chain	Res	Type
1	L	46	GLU
1	L	51	LYS
1	L	79	GLU
1	L	97	GLN
1	L	101	THR
1	L	121	TYR
1	L	131	LEU
1	L	135	LEU
1	L	147	THR
1	L	163	ASN
1	L	164	VAL
1	L	179	VAL
1	L	185	ASP
1	L	189	ARG
1	L	196	LYS
1	L	206	LYS
1	L	214	ASP
1	L	220	ARG
1	L	241	GLU
1	L	250	VAL
1	L	254	LYS
1	L	262	LYS
1	L	287	ARG
1	L	289	SER
1	L	293	LEU
1	L	355	ASN
1	L	359	GLU
1	L	364	THR
1	L	373	ILE
1	L	381	LYS
1	L	386	VAL
1	L	400	GLU
1	L	415	GLU
1	L	424	VAL
1	L	425	GLU
1	L	427	LEU
1	L	430	LYS
1	L	441	ASP
1	L	449	GLU
1	L	452	ASN
1	L	481	VAL
1	L	482	GLU

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Mol	Chain	Res	Type
1	L	484	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (126) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	163	ASN
1	A	178	GLN
1	A	223	GLN
1	A	235	HIS
1	A	372	ASN
1	A	469	HIS
1	B	19	HIS
1	B	64	ASN
1	B	142	ASN
1	B	163	ASN
1	B	323	ASN
1	B	329	ASN
1	B	335	HIS
1	B	372	ASN
1	B	452	ASN
1	C	87	GLN
1	C	125	ASN
1	C	142	ASN
1	C	163	ASN
1	C	178	GLN
1	C	235	HIS
1	C	291	ASN
1	C	323	ASN
1	C	372	ASN
1	D	19	HIS
1	D	64	ASN
1	D	97	GLN
1	D	163	ASN
1	D	178	GLN
1	D	235	HIS
1	D	291	ASN
1	D	323	ASN
1	D	372	ASN
1	D	443	ASN
1	D	450	ASN
1	D	452	ASN

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Mol	Chain	Res	Type
1	D	469	HIS
1	E	19	HIS
1	E	23	HIS
1	E	64	ASN
1	E	71	ASN
1	E	97	GLN
1	E	178	GLN
1	E	223	GLN
1	E	235	HIS
1	E	291	ASN
1	E	323	ASN
1	E	329	ASN
1	E	335	HIS
1	E	372	ASN
1	E	452	ASN
1	F	19	HIS
1	F	64	ASN
1	F	71	ASN
1	F	75	ASN
1	F	98	GLN
1	F	142	ASN
1	F	163	ASN
1	F	178	GLN
1	F	235	HIS
1	F	323	ASN
1	F	429	GLN
1	G	23	HIS
1	G	71	ASN
1	G	97	GLN
1	G	142	ASN
1	G	163	ASN
1	G	171	ASN
1	G	235	HIS
1	G	291	ASN
1	G	323	ASN
1	G	329	ASN
1	G	372	ASN
1	G	429	GLN
1	G	452	ASN
1	H	19	HIS
1	H	142	ASN
1	H	151	GLN

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Mol	Chain	Res	Type
1	H	178	GLN
1	H	235	HIS
1	H	283	ASN
1	H	365	HIS
1	H	372	ASN
1	H	380	ASN
1	I	19	HIS
1	I	64	ASN
1	I	71	ASN
1	I	75	ASN
1	I	87	GLN
1	I	142	ASN
1	I	146	ASN
1	I	178	GLN
1	I	313	GLN
1	I	365	HIS
1	I	452	ASN
1	J	64	ASN
1	J	75	ASN
1	J	98	GLN
1	J	142	ASN
1	J	171	ASN
1	J	178	GLN
1	J	291	ASN
1	J	329	ASN
1	J	372	ASN
1	J	380	ASN
1	K	19	HIS
1	K	142	ASN
1	K	163	ASN
1	K	178	GLN
1	K	291	ASN
1	K	329	ASN
1	K	372	ASN
1	K	443	ASN
1	L	19	HIS
1	L	64	ASN
1	L	97	GLN
1	L	142	ASN
1	L	163	ASN
1	L	178	GLN
1	L	223	GLN

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Mol	Chain	Res	Type
1	L	291	ASN
1	L	323	ASN
1	L	329	ASN
1	L	372	ASN
1	L	443	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	483/484 (99%)	-0.56	1 (0%) 95 87	26, 38, 55, 63	6 (1%)
1	B	483/484 (99%)	-0.62	1 (0%) 95 87	23, 36, 51, 68	5 (1%)
1	C	483/484 (99%)	-0.59	1 (0%) 95 87	21, 37, 57, 71	8 (1%)
1	D	483/484 (99%)	-0.57	0 100 100	23, 37, 55, 68	11 (2%)
1	E	483/484 (99%)	-0.53	1 (0%) 95 87	21, 37, 60, 72	8 (1%)
1	F	483/484 (99%)	-0.55	0 100 100	19, 39, 60, 69	14 (2%)
1	G	483/484 (99%)	-0.47	2 (0%) 93 80	30, 46, 60, 72	11 (2%)
1	H	483/484 (99%)	-0.31	3 (0%) 90 73	34, 56, 68, 81	8 (1%)
1	I	483/484 (99%)	-0.36	3 (0%) 90 73	31, 50, 76, 86	22 (4%)
1	J	481/484 (99%)	-0.36	2 (0%) 93 80	30, 55, 78, 87	22 (4%)
1	K	483/484 (99%)	-0.48	1 (0%) 95 87	25, 46, 60, 79	13 (2%)
1	L	483/484 (99%)	-0.29	7 (1%) 78 51	29, 50, 77, 86	12 (2%)
All	All	5794/5808 (99%)	-0.47	22 (0%) 93 80	19, 44, 68, 87	140 (2%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	484	GLU	3.5
1	I	462	THR	3.0
1	I	2	SER	2.9
1	G	484	GLU	2.8
1	L	463	VAL	2.8
1	H	429	GLN	2.8
1	E	484	GLU	2.6
1	B	484	GLU	2.6
1	G	449	GLU	2.6
1	L	462	THR	2.6
1	L	484	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	484	GLU	2.4
1	H	482	GLU	2.3
1	L	428	GLY	2.3
1	J	440	PRO	2.3
1	L	416	ASP	2.2
1	A	428	GLY	2.2
1	L	7	VAL	2.1
1	H	339	ASP	2.0
1	J	428	GLY	2.0
1	L	8	ASP	2.0
1	I	431	LYS	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.