



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:04 PM GMT

PDB ID : 1N6E
Title : tricorn protease in complex with a tridecapeptide chloromethyl ketone derivative
Authors : Kim, J.-S.; Groll, M.; Huber, R.; Brandstetter, H.
Deposited on : 2002-11-10
Resolution : 2.60 Å(reported)

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

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 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

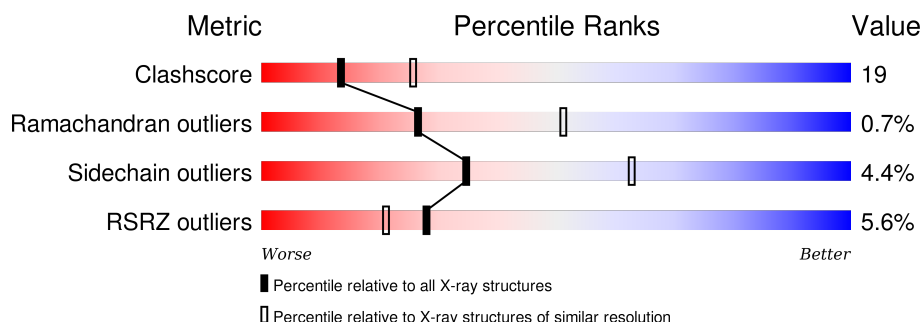
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	1071	<div> <div>3%</div> <div>63% 30% . .</div> </div>
1	C	1071	<div> <div>2%</div> <div>63% 30% . .</div> </div>
1	E	1071	<div> <div>8%</div> <div>58% 35% . .</div> </div>
1	G	1071	<div> <div>3%</div> <div>62% 31% . .</div> </div>
1	I	1071	<div> <div>3%</div> <div>63% 30% . .</div> </div>
1	K	1071	<div> <div>9%</div> <div>60% 33% . .</div> </div>
2	B	13	<div> <div>69%</div> <div>54% 23% 8% 15%</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	13	<div><div><div>54%</div><div></div><div></div><div></div><div></div></div><div><div></div><div>23%</div><div>8%</div><div>15%</div></div></div>
2	F	13	<div><div><div>62%</div><div></div><div></div><div></div><div></div></div><div><div></div><div>31%</div><div>15%</div><div>15%</div></div></div>
2	H	13	<div><div><div>46%</div><div></div><div></div><div></div><div></div></div><div><div></div><div>23%</div><div>8%</div><div>15%</div></div></div>
2	J	13	<div><div><div>46%</div><div></div><div></div><div></div><div></div></div><div><div></div><div>23%</div><div>8%</div><div>15%</div></div></div>
2	L	13	<div><div><div>62%</div><div></div><div></div><div></div><div></div></div><div><div></div><div>23%</div><div>15%</div><div>15%</div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 50544 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.

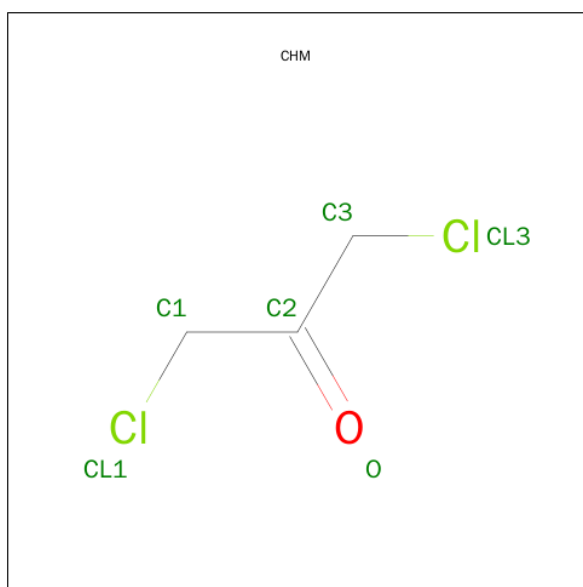
- Molecule 1 is a protein called tricorn protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1023	Total	C	N	O	S	94	0	0
			8177	5196	1402	1551	28			
1	C	1023	Total	C	N	O	S	94	0	0
			8177	5196	1402	1551	28			
1	E	1023	Total	C	N	O	S	94	0	0
			8177	5196	1402	1551	28			
1	G	1023	Total	C	N	O	S	94	0	0
			8177	5196	1402	1551	28			
1	I	1023	Total	C	N	O	S	94	0	0
			8177	5196	1402	1551	28			
1	K	1023	Total	C	N	O	S	94	0	0
			8177	5196	1402	1551	28			

- Molecule 2 is a protein called DQTQKAAAELTFF.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	11	Total	C	N	O	0	0	0
			86	57	13	16			
2	D	11	Total	C	N	O	0	0	0
			86	57	13	16			
2	F	11	Total	C	N	O	0	0	0
			86	57	13	16			
2	H	11	Total	C	N	O	0	0	0
			86	57	13	16			
2	J	11	Total	C	N	O	0	0	0
			86	57	13	16			
2	L	11	Total	C	N	O	0	0	0
			86	57	13	16			

- Molecule 3 is 1,3-DICHLORO-PROPAN-2-ONE (three-letter code: CHM) (formula: C₃H₄Cl₂O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C 1 1	0	0
3	D	1	Total C 1 1	0	0
3	F	1	Total C 1 1	0	0
3	H	1	Total C 1 1	0	0
3	J	1	Total C 1 1	0	0
3	L	1	Total C 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	178	Total O 178 178	0	0
4	B	2	Total O 2 2	0	0
4	C	172	Total O 172 172	0	0
4	D	2	Total O 2 2	0	0
4	E	138	Total O 138 138	0	0
4	F	5	Total O 5 5	0	0

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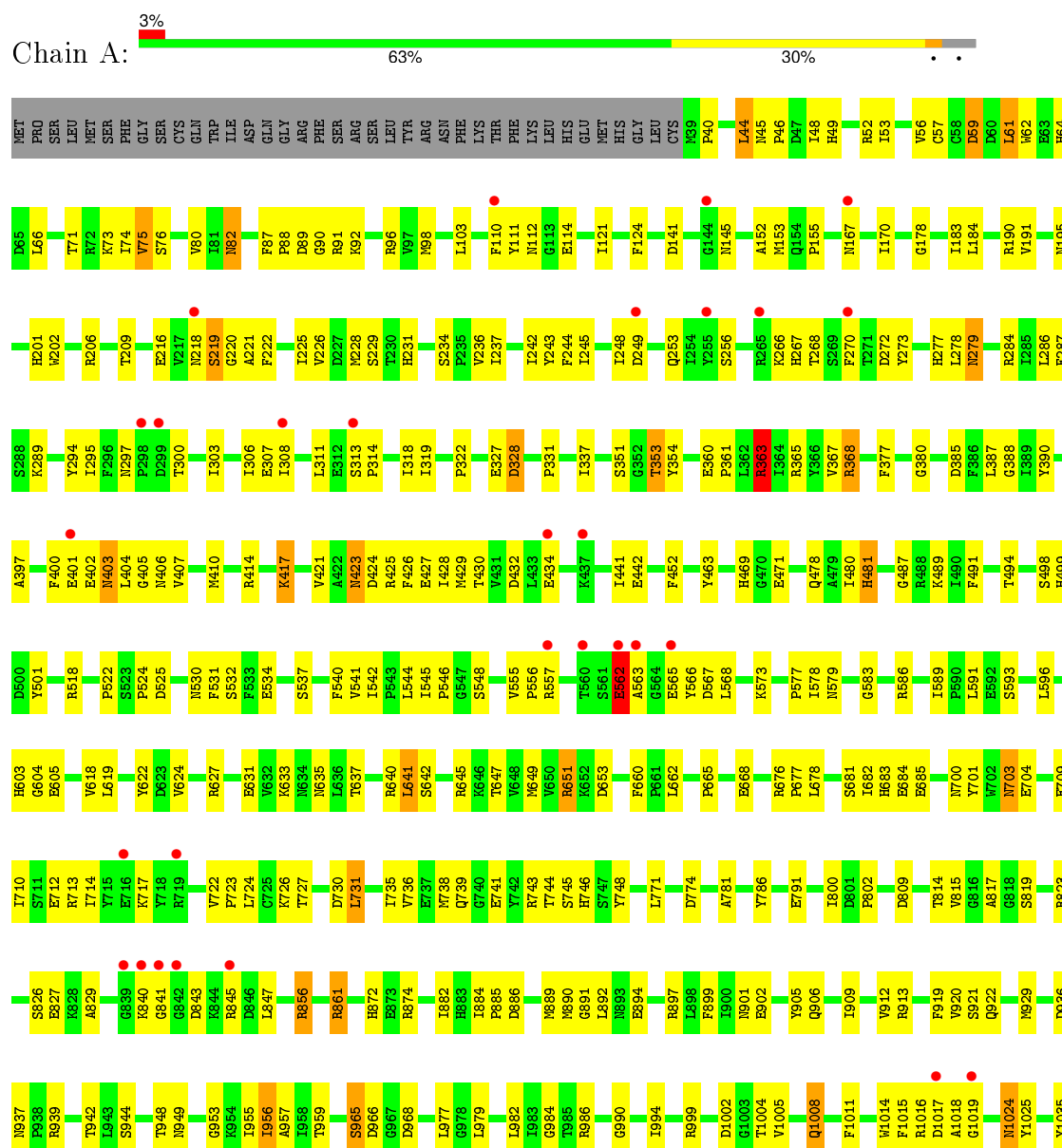
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	154	Total 154	O 154	0	0
4	H	2	Total 2	O 2	0	0
4	I	157	Total 157	O 157	0	0
4	J	2	Total 2	O 2	0	0
4	K	146	Total 146	O 146	0	0
4	L	2	Total 2	O 2	0	0

3 Residue-property plots

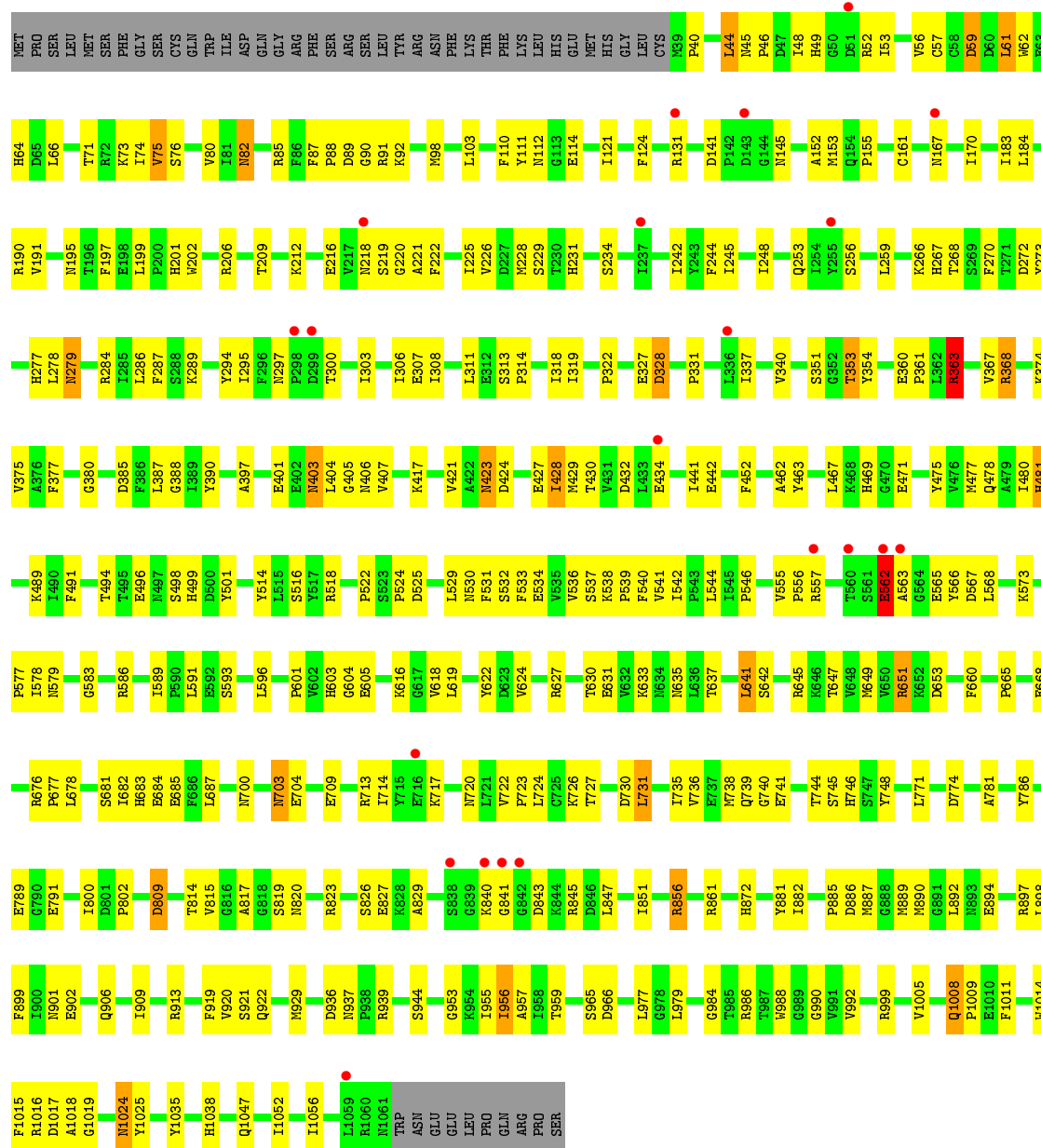
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

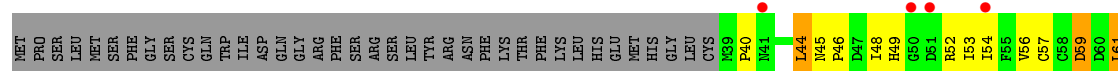


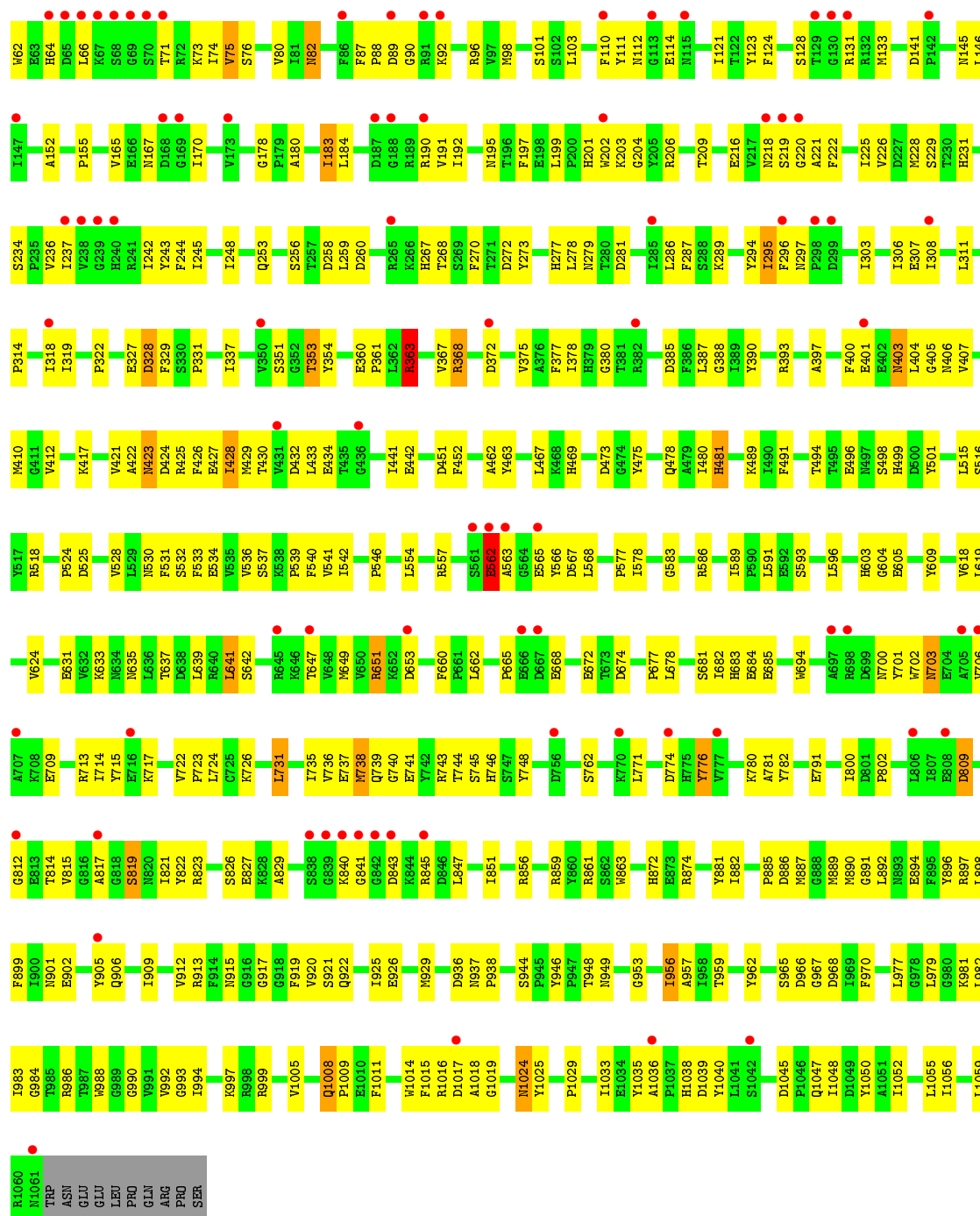


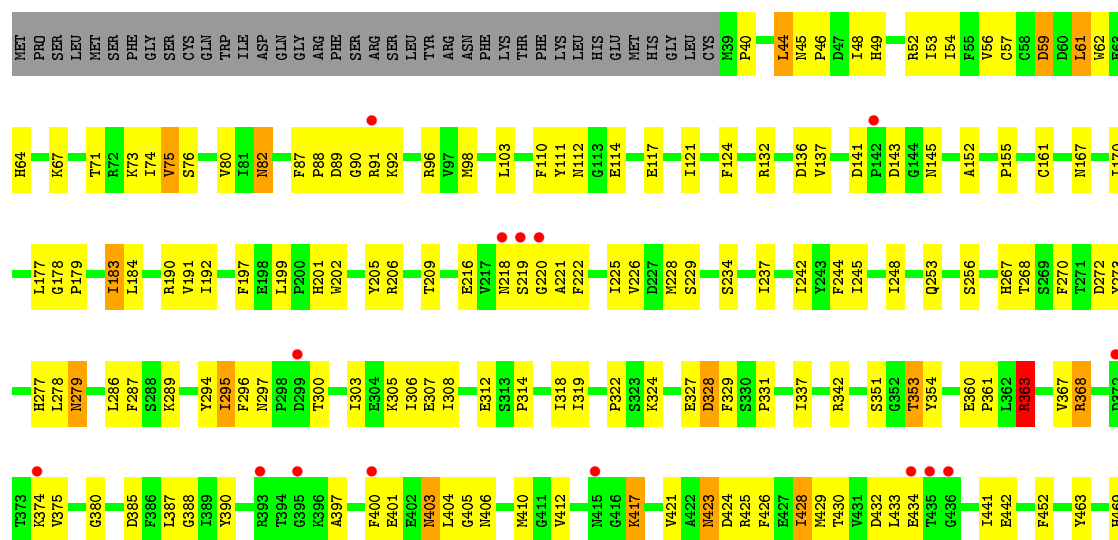
• Molecule 1: tricorn protease

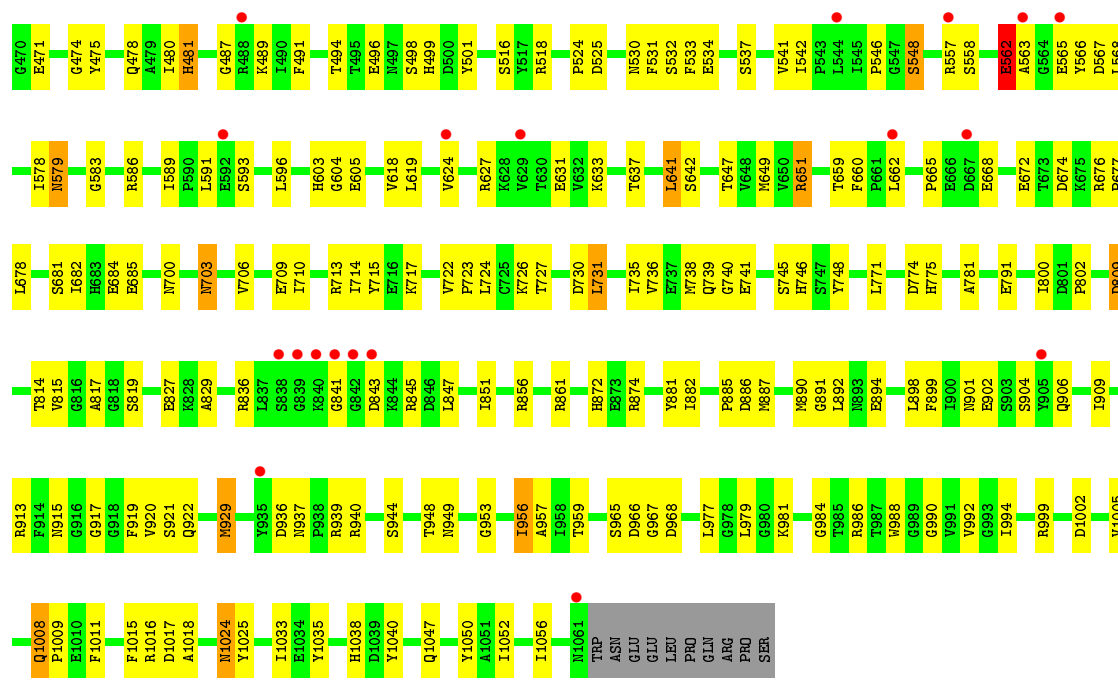


• Molecule 1: tricorn protease



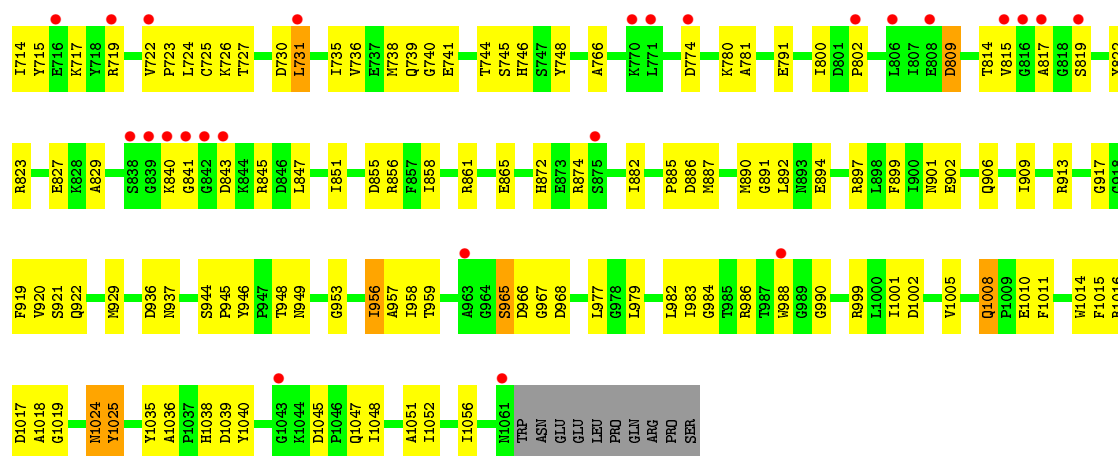




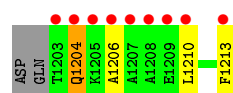


• Molecule 1: tricorn protease

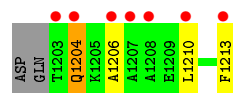




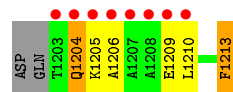
- Molecule 2: DQTQKAAELTFF



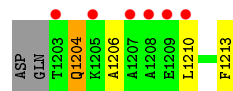
- Molecule 2: DQTQKAAELTFF



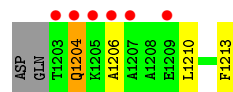
- Molecule 2: DQTQKAAELTFF



- Molecule 2: DQTQKAAAELTFF

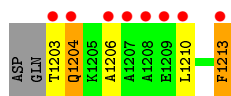


- Molecule 2: DQTQKAAELTFF



● Molecule 2: DQTQKAAAELTFF

Chain L:  62%
46% 23% 15% 15%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.47Å 245.10Å 157.89Å 90.00° 105.19° 90.00°	Depositor
Resolution (Å)	6.00 – 2.60 46.92 – 2.59	Depositor EDS
% Data completeness (in resolution range)	86.6 (6.00-2.60) 85.7 (46.92-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.58Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.254 , 0.288 0.252 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	38.2	Xtriage
Anisotropy	0.499	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 63.0	EDS
Estimated twinning fraction	0.048 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	2 of 208978 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	50544	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 2.74% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.69	0/8367	0.76	1/11311 (0.0%)
1	C	0.69	1/8367 (0.0%)	0.76	1/11311 (0.0%)
1	E	0.68	0/8367	0.75	0/11311
1	G	0.66	0/8367	0.75	0/11311
1	I	0.67	1/8367 (0.0%)	0.75	0/11311
1	K	0.67	0/8367	0.75	0/11311
2	B	1.24	1/87 (1.1%)	0.61	0/116
2	D	1.29	1/87 (1.1%)	0.57	0/116
2	F	1.20	1/87 (1.1%)	0.60	0/116
2	H	1.34	1/87 (1.1%)	0.61	0/116
2	J	1.24	1/87 (1.1%)	0.60	0/116
2	L	1.07	1/87 (1.1%)	0.61	0/116
All	All	0.68	8/50724 (0.0%)	0.75	2/68562 (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	E	0	2
1	K	0	2
All	All	0	4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1213	PHE	C-O	11.24	1.44	1.23
2	D	1213	PHE	C-O	10.99	1.44	1.23
2	B	1213	PHE	C-O	10.43	1.43	1.23
2	J	1213	PHE	C-O	10.35	1.43	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1213	PHE	C-O	9.64	1.41	1.23
2	L	1213	PHE	C-O	8.23	1.39	1.23
1	I	161	CYS	CB-SG	6.32	1.93	1.82
1	C	161	CYS	CB-SG	6.08	1.92	1.82

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	861	ARG	NE-CZ-NH1	-5.53	117.54	120.30
1	C	886	ASP	CB-CG-OD2	5.14	122.92	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	776	TYR	Sidechain
1	E	822	TYR	Sidechain
1	K	1025	TYR	Sidechain
1	K	822	TYR	Sidechain

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	8177	0	8002	300	1
1	C	8177	0	8002	291	1
1	E	8177	0	8002	352	0
1	G	8177	0	8002	317	1
1	I	8177	0	8002	301	1
1	K	8177	0	8002	330	0
2	B	86	0	84	4	0
2	D	86	0	84	4	0
2	F	86	0	84	8	0
2	H	86	0	84	3	0
2	J	86	0	84	4	0
2	L	86	0	84	7	0
3	B	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1	0	0	1	0
3	F	1	0	0	1	0
3	H	1	0	0	1	0
3	J	1	0	0	1	0
3	L	1	0	0	1	0
4	A	178	0	0	29	0
4	B	2	0	0	0	0
4	C	172	0	0	24	0
4	D	2	0	0	0	0
4	E	138	0	0	54	0
4	F	5	0	0	2	0
4	G	154	0	0	32	0
4	H	2	0	0	1	0
4	I	157	0	0	18	0
4	J	2	0	0	0	0
4	K	146	0	0	56	0
4	L	2	0	0	1	0
All	All	50544	0	48516	1807	2

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 19.

All (1807) 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:I:351:SER:OG	1:I:353:THR:HG22	1.41	1.17
1:C:351:SER:OG	1:C:353:THR:HG22	1.46	1.16
1:G:351:SER:OG	1:G:353:THR:HG22	1.47	1.15
1:A:351:SER:OG	1:A:353:THR:HG22	1.45	1.14
1:E:351:SER:OG	1:E:353:THR:HG22	1.46	1.13
1:K:351:SER:OG	1:K:353:THR:HG22	1.52	1.10
4:E:1083:HOH:O	2:F:1213:PHE:HA	1.49	1.09
1:I:342:ARG:HG3	4:I:1095:HOH:O	1.54	1.08
1:K:241:ARG:HB3	4:K:1099:HOH:O	1.54	1.06
2:F:1213:PHE:O	4:F:239:HOH:O	1.73	1.04
1:E:702:TRP:HB3	4:E:1189:HOH:O	1.57	1.03
1:E:128:SER:HB2	4:E:1077:HOH:O	1.63	0.99
1:G:557:ARG:HH22	1:G:562:GLU:HB2	1.25	0.98
1:A:206:ARG:H	1:A:1024:ASN:HD21	1.11	0.98
1:K:557:ARG:HH22	1:K:562:GLU:HB2	1.28	0.97
1:G:276:ARG:HD3	4:G:1079:HOH:O	1.65	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:689:MET:HE3	4:K:1180:HOH:O	1.66	0.95
1:A:557:ARG:HH22	1:A:562:GLU:HB2	1.32	0.95
1:E:982:LEU:HG	4:E:1113:HOH:O	1.67	0.95
1:K:351:SER:HG	1:K:353:THR:HG22	1.26	0.94
1:C:557:ARG:HH22	1:C:562:GLU:HB2	1.32	0.94
1:I:557:ARG:HH22	1:I:562:GLU:HB2	1.29	0.94
1:E:762:SER:HA	4:E:1135:HOH:O	1.66	0.94
1:E:351:SER:HG	1:E:353:THR:HG22	1.25	0.94
1:E:557:ARG:HH22	1:E:562:GLU:HB2	1.30	0.93
1:K:858:ILE:HG13	4:K:1126:HOH:O	1.68	0.93
1:I:351:SER:HG	1:I:353:THR:HG22	1.27	0.92
1:C:471:GLU:HA	4:C:1159:HOH:O	1.70	0.92
1:E:480:ILE:H	1:E:494:THR:CG2	1.83	0.92
1:A:206:ARG:H	1:A:1024:ASN:ND2	1.68	0.91
1:A:351:SER:HG	1:A:353:THR:HG22	1.31	0.91
1:A:480:ILE:H	1:A:494:THR:CG2	1.84	0.90
1:C:351:SER:HG	1:C:353:THR:HG22	1.30	0.90
1:I:206:ARG:H	1:I:1024:ASN:HD21	1.17	0.90
1:C:206:ARG:H	1:C:1024:ASN:HD21	1.16	0.90
1:G:480:ILE:H	1:G:494:THR:CG2	1.83	0.89
1:K:256:SER:HB2	4:K:1099:HOH:O	1.72	0.89
1:G:913:ARG:HH21	1:G:1047:GLN:HE21	1.20	0.89
1:E:74:ILE:HG13	1:E:75:VAL:HG12	1.54	0.88
1:K:480:ILE:H	1:K:494:THR:CG2	1.85	0.88
1:K:206:ARG:H	1:K:1024:ASN:HD21	1.17	0.88
1:K:251:PHE:HB3	4:K:1174:HOH:O	1.73	0.88
1:I:480:ILE:H	1:I:494:THR:CG2	1.87	0.87
1:I:525:ASP:HA	4:K:1090:HOH:O	1.72	0.87
1:I:913:ARG:HH21	1:I:1047:GLN:HE21	1.22	0.87
1:C:480:ILE:H	1:C:494:THR:CG2	1.86	0.87
1:G:736:VAL:HA	1:G:739:GLN:HE21	1.39	0.87
1:K:206:ARG:H	1:K:1024:ASN:ND2	1.72	0.86
1:G:74:ILE:HG13	1:G:75:VAL:HG12	1.58	0.86
1:E:206:ARG:H	1:E:1024:ASN:HD21	1.16	0.86
1:G:351:SER:HG	1:G:353:THR:HG22	1.35	0.86
1:E:206:ARG:H	1:E:1024:ASN:ND2	1.73	0.85
1:I:206:ARG:H	1:I:1024:ASN:ND2	1.73	0.85
1:C:206:ARG:H	1:C:1024:ASN:ND2	1.74	0.85
1:K:736:VAL:HA	1:K:739:GLN:HE21	1.42	0.84
1:E:736:VAL:HA	1:E:739:GLN:HE21	1.40	0.84
1:G:40:PRO:HG2	1:G:724:LEU:HD22	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:73:LYS:HD3	1:K:76:SER:HB3	1.58	0.84
1:A:736:VAL:HA	1:A:739:GLN:HE21	1.41	0.84
1:C:736:VAL:HA	1:C:739:GLN:HE21	1.40	0.84
1:E:889:MET:HG2	4:E:1133:HOH:O	1.78	0.83
1:G:167:ASN:HB2	1:G:170:ILE:HB	1.61	0.83
1:I:736:VAL:HA	1:I:739:GLN:HE21	1.42	0.83
1:K:1001:ILE:HG23	4:K:1086:HOH:O	1.76	0.83
1:A:40:PRO:HG2	1:A:724:LEU:HD22	1.61	0.83
1:E:167:ASN:HB2	1:E:170:ILE:HB	1.58	0.83
1:K:167:ASN:HB2	1:K:170:ILE:HB	1.61	0.83
1:C:40:PRO:HG2	1:C:724:LEU:HD22	1.59	0.83
1:E:533:PHE:N	4:E:1181:HOH:O	2.11	0.83
1:G:206:ARG:H	1:G:1024:ASN:HD21	1.26	0.83
1:A:480:ILE:H	1:A:494:THR:HG22	1.43	0.82
1:C:74:ILE:HG13	1:C:75:VAL:HG12	1.62	0.82
4:E:1181:HOH:O	1:G:525:ASP:HA	1.79	0.82
1:G:206:ARG:H	1:G:1024:ASN:ND2	1.78	0.82
1:K:74:ILE:HG13	1:K:75:VAL:HG12	1.62	0.82
1:I:167:ASN:HB2	1:I:170:ILE:HB	1.60	0.82
1:E:40:PRO:HG2	1:E:724:LEU:HD22	1.62	0.82
1:K:913:ARG:HH21	1:K:1047:GLN:HE21	1.27	0.81
1:K:643:ALA:HA	4:K:1107:HOH:O	1.79	0.81
1:I:40:PRO:HG2	1:I:724:LEU:HD22	1.61	0.81
1:G:681:SER:HB3	1:G:684:GLU:HG2	1.61	0.80
1:K:394:THR:HB	4:K:1150:HOH:O	1.81	0.80
1:E:889:MET:CE	4:E:1133:HOH:O	2.28	0.80
1:G:221:ALA:HB1	4:G:1113:HOH:O	1.80	0.80
1:E:913:ARG:HH21	1:E:1047:GLN:HE21	1.27	0.80
1:E:586:ARG:CZ	2:F:1206:ALA:HB3	2.10	0.80
1:E:1011:PHE:HB3	1:G:936:ASP:OD2	1.82	0.80
1:C:167:ASN:HB2	1:C:170:ILE:HB	1.62	0.80
1:K:709:GLU:OE2	1:K:713:ARG:HD3	1.82	0.80
1:I:74:ILE:HG13	1:I:75:VAL:HG12	1.62	0.79
1:E:480:ILE:H	1:E:494:THR:HG22	1.46	0.79
1:G:480:ILE:H	1:G:494:THR:HG22	1.48	0.79
1:A:206:ARG:N	1:A:1024:ASN:HD21	1.81	0.78
1:A:74:ILE:HG13	1:A:75:VAL:HG12	1.64	0.78
1:G:557:ARG:NH2	1:G:562:GLU:HB2	1.97	0.78
1:I:480:ILE:H	1:I:494:THR:HG22	1.48	0.78
1:E:73:LYS:HD3	1:E:76:SER:HB3	1.64	0.78
1:G:625:LYS:HG3	4:G:1200:HOH:O	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:635:ASN:HA	4:C:1079:HOH:O	1.83	0.78
1:K:40:PRO:HG2	1:K:724:LEU:HD22	1.64	0.77
1:A:167:ASN:HB2	1:A:170:ILE:HB	1.66	0.77
1:K:440:VAL:HG12	4:K:1100:HOH:O	1.82	0.77
1:K:557:ARG:NH2	1:K:562:GLU:HB2	1.99	0.77
1:G:46:PRO:HB2	1:G:286:LEU:HD23	1.65	0.77
1:E:1033:ILE:HB	4:E:1123:HOH:O	1.82	0.77
1:I:709:GLU:OE2	1:I:713:ARG:HD3	1.84	0.77
1:I:46:PRO:HB2	1:I:286:LEU:HD23	1.66	0.77
1:E:46:PRO:HB2	1:E:286:LEU:HD23	1.66	0.77
1:K:203:LYS:HG2	4:K:1166:HOH:O	1.83	0.77
1:C:480:ILE:H	1:C:494:THR:HG22	1.48	0.76
1:E:709:GLU:OE2	1:E:713:ARG:HD3	1.85	0.76
1:I:53:ILE:HG23	1:I:286:LEU:HD21	1.66	0.76
1:I:73:LYS:HD3	1:I:76:SER:HB3	1.66	0.76
1:G:709:GLU:OE2	1:G:713:ARG:HD3	1.84	0.76
1:A:87:PHE:HB3	1:A:88:PRO:HD2	1.67	0.76
1:A:703:ASN:C	1:A:703:ASN:HD22	1.89	0.76
1:K:46:PRO:HB2	1:K:286:LEU:HD23	1.67	0.76
1:K:999:ARG:HG2	1:K:1005:VAL:HG22	1.67	0.76
1:K:586:ARG:CZ	2:L:1206:ALA:HB3	2.15	0.76
1:C:586:ARG:CZ	2:D:1206:ALA:HB3	2.16	0.76
1:E:992:VAL:CG1	4:E:1189:HOH:O	2.33	0.75
1:I:681:SER:HB3	1:I:684:GLU:HG2	1.67	0.75
1:E:703:ASN:C	1:E:703:ASN:HD22	1.89	0.75
1:C:279:ASN:ND2	4:C:1184:HOH:O	2.18	0.75
1:C:284:ARG:HD3	4:C:1092:HOH:O	1.85	0.75
1:A:586:ARG:CZ	2:B:1206:ALA:HB3	2.17	0.75
1:K:533:PHE:N	4:K:1090:HOH:O	2.19	0.75
1:K:681:SER:HB3	1:K:684:GLU:HG2	1.67	0.75
1:K:233:SER:N	4:K:1097:HOH:O	2.20	0.75
1:C:73:LYS:HD3	1:C:76:SER:HB3	1.67	0.75
1:E:557:ARG:NH2	1:E:562:GLU:HB2	2.02	0.74
1:C:913:ARG:HH21	1:C:1047:GLN:HE21	1.33	0.74
1:K:505:PHE:HD1	4:K:1176:HOH:O	1.68	0.74
1:G:53:ILE:HG23	1:G:286:LEU:HD21	1.70	0.74
1:A:73:LYS:HD3	1:A:76:SER:HB3	1.69	0.74
1:K:480:ILE:H	1:K:494:THR:HG22	1.49	0.74
1:E:999:ARG:HG2	1:E:1005:VAL:HG22	1.68	0.74
1:I:557:ARG:NH2	1:I:562:GLU:HB2	2.03	0.74
1:C:936:ASP:HB3	1:C:944:SER:HB2	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:789:GLU:OE1	4:C:1119:HOH:O	2.06	0.74
1:E:681:SER:HB3	1:E:684:GLU:HG2	1.70	0.74
1:K:1010:GLU:OE1	4:K:1079:HOH:O	2.06	0.73
1:A:61:LEU:HB3	1:A:75:VAL:HG13	1.68	0.73
1:A:557:ARG:NH2	1:A:562:GLU:HB2	2.01	0.73
1:I:586:ARG:CZ	2:J:1206:ALA:HB3	2.17	0.73
1:E:498:SER:HB2	4:E:1107:HOH:O	1.86	0.73
1:C:703:ASN:HD22	1:C:703:ASN:C	1.91	0.73
1:A:681:SER:HB3	1:A:684:GLU:HG2	1.71	0.73
1:A:936:ASP:HB3	1:A:944:SER:HB2	1.70	0.73
1:G:586:ARG:CZ	2:H:1206:ALA:HB3	2.19	0.73
1:I:936:ASP:OD2	1:K:1011:PHE:HB3	1.88	0.73
1:I:190:ARG:CZ	4:I:1087:HOH:O	2.36	0.73
1:K:936:ASP:HB3	1:K:944:SER:HB2	1.71	0.73
1:E:46:PRO:HB2	1:E:286:LEU:CD2	2.18	0.72
4:K:1104:HOH:O	2:L:1213:PHE:HA	1.89	0.72
1:G:73:LYS:HD3	1:G:76:SER:HB3	1.70	0.72
1:C:87:PHE:HB3	1:C:88:PRO:HD2	1.71	0.72
1:C:557:ARG:NH2	1:C:562:GLU:HB2	2.04	0.72
1:A:913:ARG:HH21	1:A:1047:GLN:HE21	1.33	0.72
1:K:1008:GLN:NE2	4:K:1182:HOH:O	2.22	0.72
1:A:365:ARG:HA	4:A:1133:HOH:O	1.90	0.72
1:C:709:GLU:OE2	1:C:713:ARG:HD3	1.88	0.72
1:C:351:SER:OG	1:C:353:THR:CG2	2.33	0.72
1:I:403:ASN:HD22	1:I:404:LEU:N	1.87	0.72
1:G:936:ASP:HB3	1:G:944:SER:HB2	1.72	0.72
1:A:253:GLN:HE22	1:A:270:PHE:H	1.38	0.72
1:I:403:ASN:ND2	1:I:405:GLY:H	1.87	0.72
1:I:1011:PHE:HB3	1:K:936:ASP:OD2	1.90	0.71
1:I:351:SER:OG	1:I:353:THR:CG2	2.30	0.71
1:K:61:LEU:HB3	1:K:75:VAL:HG13	1.70	0.71
1:C:593:SER:O	1:C:624:VAL:HG22	1.90	0.71
1:E:206:ARG:N	1:E:1024:ASN:HD21	1.87	0.71
1:C:720:ASN:ND2	4:C:1186:HOH:O	2.12	0.71
1:G:403:ASN:HD22	1:G:404:LEU:N	1.88	0.71
1:E:133:MET:HA	4:E:1077:HOH:O	1.91	0.71
1:A:709:GLU:OE2	1:A:713:ARG:HD3	1.90	0.71
1:E:948:THR:H	1:G:922:GLN:HE22	1.37	0.71
1:C:46:PRO:HB2	1:C:286:LEU:HD23	1.71	0.71
1:E:936:ASP:OD2	1:G:1011:PHE:HB3	1.90	0.71
1:I:703:ASN:C	1:I:703:ASN:HD22	1.94	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:913:ARG:HH21	1:I:1047:GLN:NE2	1.88	0.70
1:E:984:GLY:HA2	4:E:1123:HOH:O	1.90	0.70
1:K:87:PHE:HB3	1:K:88:PRO:HD2	1.73	0.70
1:G:351:SER:OG	1:G:353:THR:CG2	2.35	0.70
1:C:53:ILE:HG23	1:C:286:LEU:HD21	1.74	0.70
1:I:206:ARG:N	1:I:1024:ASN:HD21	1.90	0.70
1:K:53:ILE:HG23	1:K:286:LEU:HD21	1.72	0.70
1:E:936:ASP:HB3	1:E:944:SER:HB2	1.71	0.70
1:C:403:ASN:HD22	1:C:404:LEU:N	1.89	0.70
1:A:593:SER:O	1:A:624:VAL:HG22	1.92	0.70
1:G:1016:ARG:HG3	4:G:1099:HOH:O	1.90	0.70
1:E:557:ARG:NH1	4:E:1152:HOH:O	2.23	0.69
1:I:936:ASP:HB3	1:I:944:SER:HB2	1.72	0.69
1:K:703:ASN:HD22	1:K:703:ASN:C	1.96	0.69
1:I:87:PHE:HB3	1:I:88:PRO:HD2	1.72	0.69
1:G:530:ASN:ND2	1:G:531:PHE:H	1.90	0.69
1:E:403:ASN:HD22	1:E:404:LEU:N	1.90	0.69
1:E:372:ASP:HB2	4:E:1112:HOH:O	1.91	0.69
1:E:812:GLY:HA3	4:E:1150:HOH:O	1.91	0.69
1:G:999:ARG:HG2	1:G:1005:VAL:HG22	1.75	0.69
1:G:61:LEU:HD13	1:G:74:ILE:HD11	1.75	0.69
1:A:403:ASN:HD22	1:A:404:LEU:N	1.90	0.69
1:K:519:SER:OG	4:K:1125:HOH:O	2.10	0.69
1:G:253:GLN:HE22	1:G:270:PHE:H	1.39	0.69
1:C:681:SER:HB3	1:C:684:GLU:HG2	1.73	0.69
1:C:61:LEU:HB3	1:C:75:VAL:HG13	1.75	0.68
1:E:351:SER:OG	1:E:353:THR:CG2	2.35	0.68
1:G:46:PRO:HB2	1:G:286:LEU:CD2	2.23	0.68
1:E:87:PHE:HB3	1:E:88:PRO:HD2	1.76	0.68
1:K:82:ASN:HD22	1:K:82:ASN:H	1.40	0.68
1:A:530:ASN:ND2	1:A:531:PHE:H	1.91	0.68
1:E:61:LEU:HD13	1:E:74:ILE:HD11	1.76	0.68
1:K:206:ARG:N	1:K:1024:ASN:HD21	1.90	0.68
1:K:46:PRO:HB2	1:K:286:LEU:CD2	2.23	0.68
1:K:403:ASN:ND2	1:K:405:GLY:H	1.91	0.68
1:G:87:PHE:HB3	1:G:88:PRO:HD2	1.75	0.68
1:G:557:ARG:HH22	1:G:562:GLU:CB	2.05	0.68
1:G:403:ASN:ND2	1:G:405:GLY:H	1.92	0.68
1:E:61:LEU:HB3	1:E:75:VAL:HG13	1.75	0.67
1:G:703:ASN:C	1:G:703:ASN:HD22	1.97	0.67
1:G:913:ARG:HH21	1:G:1047:GLN:NE2	1.91	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:403:ASN:ND2	1:E:405:GLY:H	1.93	0.67
1:A:403:ASN:ND2	1:A:405:GLY:H	1.92	0.67
1:K:403:ASN:HD22	1:K:404:LEU:N	1.91	0.67
1:K:498:SER:HB2	4:K:1073:HOH:O	1.93	0.67
1:E:253:GLN:HE22	1:E:270:PHE:H	1.42	0.67
1:A:46:PRO:HB2	1:A:286:LEU:HD23	1.76	0.67
1:I:253:GLN:HE22	1:I:270:PHE:H	1.40	0.67
1:I:791:GLU:CD	1:I:861:ARG:HE	1.97	0.67
1:E:949:ASN:ND2	1:G:475:TYR:OH	2.25	0.67
1:I:999:ARG:HG2	1:I:1005:VAL:HG22	1.75	0.67
1:I:530:ASN:ND2	1:I:531:PHE:H	1.94	0.67
1:C:206:ARG:N	1:C:1024:ASN:HD21	1.89	0.66
1:A:53:ILE:HG23	1:A:286:LEU:HD21	1.77	0.66
1:G:218:ASN:HB3	1:G:221:ALA:HB3	1.77	0.66
1:E:82:ASN:HD22	1:E:82:ASN:H	1.44	0.66
1:G:61:LEU:HB3	1:G:75:VAL:HG13	1.76	0.66
1:K:543:PRO:HB3	4:K:1202:HOH:O	1.95	0.66
1:G:82:ASN:HD22	1:G:82:ASN:H	1.43	0.66
1:C:999:ARG:HG2	1:C:1005:VAL:HG22	1.78	0.66
1:C:253:GLN:HE22	1:C:270:PHE:H	1.44	0.66
4:A:1148:HOH:O	1:C:477:MET:HG2	1.95	0.66
1:A:591:LEU:HD12	1:A:596:LEU:HD23	1.78	0.66
2:F:1209:GLU:O	4:F:525:HOH:O	2.14	0.66
1:A:471:GLU:HA	4:A:1170:HOH:O	1.95	0.66
1:A:351:SER:OG	1:A:353:THR:CG2	2.34	0.66
1:E:53:ILE:HG23	1:E:286:LEU:HD21	1.77	0.66
1:C:403:ASN:ND2	1:C:405:GLY:H	1.93	0.66
1:C:591:LEU:HD12	1:C:596:LEU:HD23	1.78	0.66
1:A:999:ARG:HG2	1:A:1005:VAL:HG22	1.77	0.66
1:E:218:ASN:HB3	1:E:221:ALA:HB3	1.78	0.66
1:G:337:ILE:HG13	1:G:649:MET:HE1	1.77	0.65
4:K:1170:HOH:O	2:L:1203:THR:HG23	1.95	0.65
1:A:82:ASN:H	1:A:82:ASN:HD22	1.44	0.65
1:A:284:ARG:HD3	4:A:1095:HOH:O	1.96	0.65
1:E:913:ARG:HH21	1:E:1047:GLN:NE2	1.95	0.65
1:K:746:HIS:CE1	4:K:1104:HOH:O	2.49	0.65
1:C:892:LEU:HD13	1:C:920:VAL:HG21	1.79	0.65
1:I:1002:ASP:HA	4:I:1095:HOH:O	1.96	0.65
1:A:61:LEU:HD13	1:A:74:ILE:HD11	1.78	0.65
1:K:322:PRO:HA	1:K:678:LEU:HD22	1.79	0.65
1:K:256:SER:OG	1:K:267:HIS:HE1	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:909:ILE:HG12	1:G:956:ILE:CG2	2.27	0.65
1:K:301:GLU:HB3	4:K:1195:HOH:O	1.96	0.65
1:E:815:VAL:HA	1:E:819:SER:HB3	1.79	0.65
1:I:46:PRO:HB2	1:I:286:LEU:CD2	2.26	0.65
1:C:82:ASN:H	1:C:82:ASN:HD22	1.43	0.65
1:K:557:ARG:HH22	1:K:562:GLU:CB	2.08	0.65
1:K:591:LEU:HD12	1:K:596:LEU:HD23	1.78	0.65
1:K:319:ILE:HG23	1:K:677:PRO:HB3	1.79	0.64
1:G:322:PRO:HA	1:G:678:LEU:HD22	1.78	0.64
1:K:337:ILE:HG13	1:K:649:MET:HE1	1.76	0.64
1:K:351:SER:OG	1:K:353:THR:CG2	2.39	0.64
1:K:253:GLN:HE22	1:K:270:PHE:H	1.46	0.64
1:A:279:ASN:ND2	4:A:1111:HOH:O	2.30	0.64
1:K:52:ARG:NH1	1:K:90:GLY:O	2.29	0.64
1:G:558:SER:HA	1:K:393:ARG:HE	1.60	0.64
1:I:61:LEU:HB3	1:I:75:VAL:HG13	1.80	0.64
1:C:46:PRO:HB2	1:C:286:LEU:CD2	2.27	0.64
1:C:52:ARG:NH1	1:C:90:GLY:O	2.30	0.64
1:A:815:VAL:HA	1:A:819:SER:HB3	1.80	0.64
1:G:589:ILE:HD13	1:G:641:LEU:HD12	1.80	0.64
1:E:948:THR:HA	4:E:1102:HOH:O	1.97	0.64
1:G:591:LEU:HD12	1:G:596:LEU:HD23	1.78	0.64
1:C:530:ASN:ND2	1:C:531:PHE:H	1.95	0.64
1:I:132:ARG:HA	4:I:1207:HOH:O	1.98	0.64
1:I:913:ARG:NH2	1:I:1047:GLN:HE21	1.94	0.64
1:I:67:LYS:HD2	4:I:1203:HOH:O	1.98	0.64
1:C:700:ASN:HD22	1:C:1008:GLN:NE2	1.96	0.64
1:A:46:PRO:HB2	1:A:286:LEU:CD2	2.28	0.63
1:I:909:ILE:HG12	1:I:956:ILE:CG2	2.28	0.63
1:E:331:PRO:HB3	1:E:649:MET:HE3	1.80	0.63
1:G:593:SER:O	1:G:624:VAL:HG22	1.98	0.63
1:I:322:PRO:HA	1:I:678:LEU:HD22	1.80	0.63
1:C:677:PRO:HD2	1:I:827:GLU:O	1.97	0.63
1:G:660:PHE:HB3	1:G:668:GLU:HB3	1.80	0.63
1:G:206:ARG:N	1:G:1024:ASN:HD21	1.95	0.63
1:C:322:PRO:HA	1:C:678:LEU:HD22	1.79	0.63
1:I:548:SER:O	4:I:1178:HOH:O	2.15	0.63
1:A:676:ARG:CD	4:A:1073:HOH:O	2.47	0.63
1:E:393:ARG:HE	1:I:558:SER:HA	1.63	0.63
1:I:61:LEU:HD13	1:I:74:ILE:HD11	1.79	0.63
1:E:337:ILE:HG13	1:E:649:MET:HE1	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:949:ASN:ND2	1:K:475:TYR:OH	2.24	0.63
1:A:337:ILE:HG13	1:A:649:MET:HE1	1.81	0.62
1:K:537:SER:HB3	1:K:583:GLY:O	1.99	0.62
1:A:322:PRO:HA	1:A:678:LEU:HD22	1.80	0.62
1:G:596:LEU:HD12	1:G:619:LEU:HD11	1.81	0.62
1:K:660:PHE:HB3	1:K:668:GLU:HB3	1.82	0.62
1:I:82:ASN:HD22	1:I:82:ASN:H	1.45	0.62
1:E:52:ARG:NH1	1:E:90:GLY:O	2.33	0.62
1:K:356:LEU:HD23	4:K:1137:HOH:O	1.98	0.62
1:E:983:ILE:HG23	4:E:1123:HOH:O	1.99	0.62
1:K:815:VAL:HA	1:K:819:SER:HB3	1.81	0.62
1:K:892:LEU:HD13	1:K:920:VAL:HG21	1.81	0.62
1:K:913:ARG:HH21	1:K:1047:GLN:NE2	1.96	0.62
1:A:596:LEU:HD12	1:A:619:LEU:HD11	1.82	0.62
1:I:922:GLN:HE22	1:K:948:THR:H	1.48	0.62
1:K:593:SER:O	1:K:624:VAL:HG22	1.99	0.62
1:I:700:ASN:HD22	1:I:1008:GLN:NE2	1.97	0.62
1:G:331:PRO:HB3	1:G:649:MET:HE3	1.81	0.62
1:K:530:ASN:ND2	1:K:531:PHE:H	1.98	0.61
1:C:61:LEU:HD13	1:C:74:ILE:HD11	1.82	0.61
1:A:534:GLU:HG3	1:C:534:GLU:OE2	2.00	0.61
1:K:61:LEU:CB	1:K:75:VAL:HG13	2.30	0.61
1:E:596:LEU:HD12	1:E:619:LEU:HD11	1.83	0.61
1:K:331:PRO:HB3	1:K:649:MET:HE3	1.83	0.61
1:A:676:ARG:HD2	4:A:1073:HOH:O	2.01	0.61
1:E:319:ILE:HG23	1:E:677:PRO:HB3	1.82	0.61
1:K:800:ILE:HG21	1:K:845:ARG:NH2	2.15	0.61
1:C:295:ILE:HG13	1:C:306:ILE:HD11	1.82	0.61
1:I:660:PHE:HB3	1:I:668:GLU:HB3	1.83	0.61
1:A:414:ARG:HD3	4:A:1162:HOH:O	1.99	0.61
1:A:319:ILE:HG23	1:A:677:PRO:HB3	1.82	0.61
1:G:319:ILE:HG23	1:G:677:PRO:HB3	1.82	0.61
1:A:556:PRO:HD3	1:I:354:TYR:CD1	2.36	0.61
1:E:591:LEU:HD12	1:E:596:LEU:HD23	1.81	0.61
1:E:541:VAL:HG22	1:E:542:ILE:N	2.16	0.61
1:E:922:GLN:HE22	1:G:948:THR:H	1.48	0.61
1:K:61:LEU:HD13	1:K:74:ILE:HD11	1.82	0.61
1:A:892:LEU:HD13	1:A:920:VAL:HG21	1.82	0.61
1:G:815:VAL:HA	1:G:819:SER:HB3	1.81	0.61
1:C:40:PRO:HG2	1:C:724:LEU:CD2	2.30	0.61
1:I:218:ASN:HB3	1:I:221:ALA:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:GLN:HB3	1:A:499:HIS:HD2	1.66	0.61
1:A:218:ASN:HB3	1:A:221:ALA:HB3	1.82	0.61
1:K:700:ASN:HD22	1:K:1008:GLN:NE2	1.99	0.61
1:C:791:GLU:CD	1:C:861:ARG:HE	2.03	0.61
1:G:52:ARG:NH1	1:G:90:GLY:O	2.33	0.61
1:E:256:SER:OG	1:E:267:HIS:HE1	1.83	0.60
1:A:534:GLU:OE2	1:C:534:GLU:HG3	2.01	0.60
1:A:52:ARG:NH1	1:A:90:GLY:O	2.34	0.60
1:C:556:PRO:HD3	1:G:354:TYR:CD1	2.35	0.60
1:I:53:ILE:CG2	1:I:286:LEU:HD21	2.31	0.60
1:C:660:PHE:HB3	1:C:668:GLU:HB3	1.84	0.60
1:A:537:SER:HB3	1:A:583:GLY:O	2.02	0.60
1:G:390:TYR:HD1	1:G:397:ALA:HB2	1.67	0.60
1:K:986:ARG:HD2	1:K:1025:TYR:O	2.02	0.60
1:C:603:HIS:HD2	1:C:604:GLY:O	1.85	0.60
1:E:478:GLN:HB3	1:E:499:HIS:HD2	1.66	0.60
1:E:530:ASN:ND2	1:E:531:PHE:H	2.00	0.60
1:K:774:ASP:HA	1:K:817:ALA:HB2	1.84	0.60
1:G:791:GLU:CD	1:G:861:ARG:HE	2.05	0.60
1:K:432:ASP:OD1	1:K:434:GLU:HB3	2.01	0.60
1:K:977:LEU:HB2	1:K:979:LEU:HD13	1.82	0.60
1:G:977:LEU:HB2	1:G:979:LEU:HD13	1.83	0.59
1:A:300:THR:HG21	4:A:1178:HOH:O	2.00	0.59
1:K:909:ILE:HG12	1:K:956:ILE:CG2	2.31	0.59
1:G:537:SER:HB3	1:G:583:GLY:O	2.01	0.59
1:A:480:ILE:N	1:A:494:THR:HG22	2.16	0.59
1:C:815:VAL:HA	1:C:819:SER:HB3	1.84	0.59
1:C:319:ILE:HG23	1:C:677:PRO:HB3	1.83	0.59
1:A:677:PRO:HD2	1:G:827:GLU:O	2.01	0.59
1:E:781:ALA:HB2	1:E:802:PRO:HG2	1.83	0.59
1:K:107:ASP:OD2	4:K:1131:HOH:O	2.16	0.59
1:E:101:SER:N	4:E:1094:HOH:O	2.34	0.59
1:K:390:TYR:HD1	1:K:397:ALA:HB2	1.67	0.59
1:A:791:GLU:CD	1:A:861:ARG:HE	2.05	0.59
1:K:218:ASN:HB3	1:K:221:ALA:HB3	1.84	0.59
1:G:882:ILE:HD11	1:G:899:PHE:HA	1.84	0.59
1:G:753:THR:HB	4:G:1163:HOH:O	2.02	0.59
1:A:557:ARG:HH22	1:A:562:GLU:CB	2.10	0.59
1:I:557:ARG:HH22	1:I:562:GLU:CB	2.10	0.59
1:C:218:ASN:HB3	1:C:221:ALA:HB3	1.84	0.59
1:A:774:ASP:HA	1:A:817:ALA:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:322:PRO:HA	1:E:678:LEU:HD22	1.84	0.59
1:K:791:GLU:CD	1:K:861:ARG:HE	2.06	0.59
1:E:774:ASP:HA	1:E:817:ALA:HB2	1.84	0.59
1:I:537:SER:HB3	1:I:583:GLY:O	2.02	0.59
1:E:229:SER:HB3	1:E:248:ILE:HD11	1.84	0.59
1:E:61:LEU:CB	1:E:75:VAL:HG13	2.33	0.59
1:E:295:ILE:HG13	1:E:306:ILE:HD11	1.85	0.59
1:K:800:ILE:HG21	1:K:845:ARG:HH22	1.68	0.59
1:A:700:ASN:HD22	1:A:1008:GLN:NE2	2.00	0.59
1:G:141:ASP:OD1	1:G:145:ASN:HB2	2.03	0.59
1:G:800:ILE:HG21	1:G:845:ARG:NH2	2.17	0.59
1:E:660:PHE:HB3	1:E:668:GLU:HB3	1.85	0.59
1:A:660:PHE:HB3	1:A:668:GLU:HB3	1.84	0.59
1:K:541:VAL:HG22	1:K:542:ILE:N	2.17	0.59
1:I:319:ILE:HG23	1:I:677:PRO:HB3	1.83	0.59
1:A:256:SER:OG	1:A:267:HIS:HE1	1.86	0.59
1:E:557:ARG:HH22	1:E:562:GLU:CB	2.11	0.59
1:C:809:ASP:HB3	1:C:814:THR:HA	1.85	0.59
1:I:229:SER:HB3	1:I:248:ILE:HD11	1.83	0.59
1:K:229:SER:HB3	1:K:248:ILE:HD11	1.85	0.59
1:I:342:ARG:NH2	4:I:1095:HOH:O	2.34	0.58
1:I:480:ILE:N	1:I:494:THR:HG22	2.18	0.58
1:K:440:VAL:CG1	4:K:1100:HOH:O	2.45	0.58
1:I:800:ILE:HG21	1:I:845:ARG:NH2	2.18	0.58
1:C:746:HIS:NE2	3:D:2213:CHM:C1	2.66	0.58
1:I:478:GLN:HB3	1:I:499:HIS:HD2	1.67	0.58
1:A:603:HIS:HD2	1:A:604:GLY:O	1.86	0.58
1:I:589:ILE:HD13	1:I:641:LEU:HD12	1.85	0.58
1:A:800:ILE:HG21	1:A:845:ARG:HH22	1.67	0.58
1:G:131:ARG:HB2	4:G:1131:HOH:O	2.02	0.58
1:C:557:ARG:HH22	1:C:562:GLU:CB	2.11	0.58
1:G:913:ARG:NH2	1:G:1047:GLN:HE21	1.96	0.58
1:I:286:LEU:HD12	1:I:295:ILE:HG12	1.86	0.58
1:G:800:ILE:HG21	1:G:845:ARG:HH22	1.67	0.58
1:E:800:ILE:HG21	1:E:845:ARG:NH2	2.18	0.58
1:E:593:SER:O	1:E:624:VAL:HG22	2.04	0.58
1:E:909:ILE:HG12	1:E:956:ILE:CG2	2.33	0.58
1:E:430:THR:HG23	1:E:441:ILE:HD11	1.84	0.58
1:G:681:SER:CB	1:G:684:GLU:HG2	2.33	0.58
1:I:403:ASN:C	1:I:403:ASN:HD22	2.07	0.58
1:I:591:LEU:HD12	1:I:596:LEU:HD23	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:909:ILE:HG12	1:A:956:ILE:CG2	2.33	0.58
1:K:307:GLU:HG2	4:K:1177:HOH:O	2.04	0.58
1:I:815:VAL:HA	1:I:819:SER:HB3	1.85	0.58
1:G:478:GLN:HB3	1:G:499:HIS:HD2	1.69	0.58
1:E:222:PHE:HB2	1:E:1038:HIS:HD2	1.69	0.58
1:A:40:PRO:HG2	1:A:724:LEU:CD2	2.31	0.58
1:A:61:LEU:CB	1:A:75:VAL:HG13	2.34	0.58
1:K:286:LEU:HD12	1:K:295:ILE:HG12	1.84	0.58
1:I:593:SER:O	1:I:624:VAL:HG22	2.02	0.58
1:K:480:ILE:N	1:K:494:THR:HG22	2.17	0.58
1:K:73:LYS:HD3	1:K:76:SER:CB	2.32	0.58
1:G:700:ASN:HD22	1:G:1008:GLN:NE2	2.01	0.58
1:C:977:LEU:HB2	1:C:979:LEU:HD13	1.84	0.58
1:C:337:ILE:HG13	1:C:649:MET:HE1	1.84	0.58
1:E:314:PRO:HD2	1:E:726:LYS:HG2	1.86	0.58
1:G:40:PRO:HG2	1:G:724:LEU:CD2	2.32	0.58
1:E:889:MET:HE3	4:E:1133:HOH:O	1.98	0.58
1:I:190:ARG:NH1	4:I:1087:HOH:O	2.34	0.58
1:I:885:PRO:O	1:I:915:ASN:HA	2.04	0.58
1:A:800:ILE:HG21	1:A:845:ARG:NH2	2.17	0.58
1:I:781:ALA:HB2	1:I:802:PRO:HG2	1.85	0.58
1:I:141:ASP:OD1	1:I:145:ASN:HB2	2.04	0.58
1:A:744:THR:HA	4:A:1151:HOH:O	2.02	0.58
1:A:618:VAL:CG2	1:A:631:GLU:HG3	2.34	0.57
1:K:781:ALA:HB2	1:K:802:PRO:HG2	1.86	0.57
1:E:480:ILE:N	1:E:494:THR:HG22	2.18	0.57
1:C:390:TYR:HD1	1:C:397:ALA:HB2	1.69	0.57
1:I:475:TYR:OH	1:K:949:ASN:ND2	2.36	0.57
1:A:913:ARG:HH21	1:A:1047:GLN:NE2	2.01	0.57
1:K:363:ARG:HB3	1:K:380:GLY:O	2.04	0.57
1:A:155:PRO:O	1:A:856:ARG:HD2	2.05	0.57
1:I:337:ILE:HG13	1:I:649:MET:HE1	1.86	0.57
1:E:286:LEU:HD12	1:E:295:ILE:HG12	1.86	0.57
1:C:88:PRO:HG2	1:C:89:ASP:H	1.68	0.57
1:C:596:LEU:HD12	1:C:619:LEU:HD11	1.86	0.57
1:K:337:ILE:HG13	1:K:649:MET:CE	2.35	0.57
1:C:220:GLY:O	1:C:1038:HIS:HB3	2.04	0.57
1:K:406:ASN:HB2	1:K:424:ASP:CG	2.24	0.57
1:C:286:LEU:HD12	1:C:295:ILE:HG12	1.86	0.57
1:A:229:SER:HB3	1:A:248:ILE:HD11	1.87	0.57
1:A:286:LEU:HD12	1:A:295:ILE:HG12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:PRO:HB3	1:A:649:MET:HE3	1.87	0.57
1:C:774:ASP:HA	1:C:817:ALA:HB2	1.86	0.57
1:K:746:HIS:NE2	3:L:2213:CHM:C1	2.67	0.57
1:E:363:ARG:HB3	1:E:380:GLY:O	2.03	0.57
1:C:800:ILE:HG21	1:C:845:ARG:NH2	2.19	0.57
1:I:746:HIS:NE2	3:J:2213:CHM:C1	2.67	0.57
1:E:948:THR:H	1:G:922:GLN:NE2	2.02	0.57
1:C:489:LYS:HG3	1:C:491:PHE:CE1	2.40	0.57
1:K:278:LEU:HD23	1:K:287:PHE:HB3	1.87	0.57
1:G:61:LEU:CB	1:G:75:VAL:HG13	2.35	0.57
1:I:774:ASP:HA	1:I:817:ALA:HB2	1.86	0.57
1:E:475:TYR:OH	1:G:949:ASN:ND2	2.34	0.57
1:C:229:SER:HB3	1:C:248:ILE:HD11	1.85	0.57
1:G:286:LEU:HD12	1:G:295:ILE:HG12	1.87	0.56
1:C:478:GLN:HB3	1:C:499:HIS:HD2	1.70	0.56
1:A:874:ARG:NE	4:A:1176:HOH:O	2.38	0.56
1:I:390:TYR:HD1	1:I:397:ALA:HB2	1.68	0.56
1:K:809:ASP:HB3	1:K:814:THR:HA	1.87	0.56
1:A:727:THR:O	1:A:730:ASP:HB2	2.05	0.56
1:E:1047:GLN:HG2	4:E:1123:HOH:O	2.05	0.56
1:K:735:ILE:O	1:K:739:GLN:HG3	2.05	0.56
1:K:53:ILE:CG2	1:K:286:LEU:HD21	2.35	0.56
1:C:586:ARG:HG3	2:D:1204:GLN:HG3	1.87	0.56
1:G:88:PRO:HG2	1:G:89:ASP:H	1.70	0.56
1:A:218:ASN:O	1:A:220:GLY:N	2.37	0.56
1:A:589:ILE:HD13	1:A:641:LEU:HD12	1.85	0.56
1:E:791:GLU:CD	1:E:861:ARG:HE	2.09	0.56
1:E:737:GLU:HG2	4:E:1197:HOH:O	2.05	0.56
1:A:88:PRO:HG2	1:A:89:ASP:H	1.69	0.56
1:C:676:ARG:HD2	4:C:1072:HOH:O	2.04	0.56
1:A:498:SER:OG	1:A:518:ARG:HG2	2.05	0.56
1:C:314:PRO:HD2	1:C:726:LYS:HG2	1.86	0.56
1:E:537:SER:HB3	1:E:583:GLY:O	2.04	0.56
1:E:913:ARG:NH2	1:E:1047:GLN:HE21	2.01	0.56
1:K:220:GLY:O	1:K:1038:HIS:HB3	2.05	0.56
1:I:977:LEU:HB2	1:I:979:LEU:HD13	1.88	0.56
1:I:546:PRO:HG2	1:I:567:ASP:HB3	1.87	0.56
1:I:909:ILE:HA	1:I:956:ILE:HG22	1.87	0.56
1:K:478:GLN:HB3	1:K:499:HIS:HD2	1.70	0.56
1:E:401:GLU:CD	1:E:401:GLU:H	2.08	0.56
1:K:44:LEU:HD12	1:K:56:VAL:HB	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:882:ILE:HD11	1:E:899:PHE:HA	1.88	0.56
1:G:314:PRO:HD2	1:G:726:LYS:HG2	1.87	0.56
1:C:913:ARG:HH21	1:C:1047:GLN:NE2	1.99	0.56
1:E:390:TYR:HD1	1:E:397:ALA:HB2	1.71	0.56
1:G:674:ASP:HB2	4:G:1150:HOH:O	2.06	0.56
1:E:800:ILE:HG21	1:E:845:ARG:HH22	1.70	0.56
1:A:743:ARG:O	4:A:1151:HOH:O	2.18	0.56
1:A:977:LEU:HB2	1:A:979:LEU:HD13	1.88	0.56
1:K:603:HIS:HD2	1:K:604:GLY:O	1.88	0.56
1:K:882:ILE:HD11	1:K:899:PHE:HA	1.87	0.56
1:G:278:LEU:HD23	1:G:287:PHE:HB3	1.88	0.56
1:I:318:ILE:HG21	1:I:682:ILE:HD11	1.87	0.56
1:E:977:LEU:HB2	1:E:979:LEU:HD13	1.87	0.56
1:I:295:ILE:HG13	1:I:306:ILE:HD11	1.88	0.56
1:K:746:HIS:HA	1:K:748:TYR:CZ	2.41	0.56
1:K:546:PRO:HG2	1:K:567:ASP:HB3	1.88	0.56
1:C:401:GLU:H	1:C:401:GLU:CD	2.08	0.56
1:I:53:ILE:HG23	1:I:286:LEU:CD2	2.36	0.55
1:I:88:PRO:HG2	1:I:89:ASP:H	1.71	0.55
1:C:589:ILE:HD13	1:C:641:LEU:HD12	1.88	0.55
1:E:722:VAL:N	1:E:723:PRO:HD2	2.22	0.55
1:C:253:GLN:NE2	1:C:268:THR:OG1	2.39	0.55
1:G:909:ILE:HA	1:G:956:ILE:HG22	1.88	0.55
1:K:596:LEU:HD12	1:K:619:LEU:HD11	1.88	0.55
1:A:314:PRO:HD2	1:A:726:LYS:HG2	1.86	0.55
1:E:809:ASP:HB3	1:E:814:THR:HA	1.88	0.55
1:C:909:ILE:HG12	1:C:956:ILE:CG2	2.36	0.55
1:G:781:ALA:HB2	1:G:802:PRO:HG2	1.88	0.55
1:G:728:ARG:HD3	4:G:1073:HOH:O	2.04	0.55
1:A:278:LEU:HD23	1:A:287:PHE:HB3	1.88	0.55
1:G:403:ASN:C	1:G:403:ASN:HD22	2.10	0.55
1:I:52:ARG:NH1	1:I:90:GLY:O	2.38	0.55
1:A:417:LYS:NZ	4:A:1164:HOH:O	2.37	0.55
1:C:190:ARG:HG3	1:C:216:GLU:OE2	2.05	0.55
1:A:363:ARG:HB3	1:A:380:GLY:O	2.07	0.55
1:C:155:PRO:O	1:C:856:ARG:HD2	2.06	0.55
1:A:390:TYR:HD1	1:A:397:ALA:HB2	1.71	0.55
1:A:401:GLU:H	1:A:401:GLU:CD	2.08	0.55
1:G:809:ASP:HB3	1:G:814:THR:HA	1.89	0.55
1:G:432:ASP:OD1	1:G:434:GLU:HB3	2.05	0.55
1:G:892:LEU:HD13	1:G:920:VAL:HG21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:278:LEU:HD23	1:I:287:PHE:HB3	1.88	0.55
1:G:401:GLU:CD	1:G:401:GLU:H	2.09	0.55
1:G:703:ASN:ND2	1:G:706:VAL:H	2.04	0.55
1:I:800:ILE:HG21	1:I:845:ARG:HH22	1.70	0.55
1:K:714:ILE:HG21	1:K:741:GLU:HG3	1.89	0.55
1:E:268:THR:HG22	1:E:303:ILE:HD11	1.89	0.55
1:K:62:TRP:HB3	4:K:1152:HOH:O	2.07	0.55
1:C:256:SER:OG	1:C:267:HIS:HE1	1.89	0.55
1:K:295:ILE:HG13	1:K:306:ILE:HD11	1.88	0.55
1:A:253:GLN:NE2	1:A:268:THR:OG1	2.40	0.55
1:A:220:GLY:O	1:A:1038:HIS:HB3	2.06	0.55
1:C:781:ALA:HB2	1:C:802:PRO:HG2	1.88	0.55
1:G:774:ASP:HA	1:G:817:ALA:HB2	1.88	0.55
1:G:184:LEU:HB2	1:G:191:VAL:HB	1.89	0.55
1:G:746:HIS:HA	1:G:748:TYR:CZ	2.42	0.55
1:I:872:HIS:HE1	1:I:902:GLU:OE1	1.89	0.55
1:K:681:SER:CB	1:K:684:GLU:HG2	2.35	0.55
1:I:44:LEU:HD12	1:I:56:VAL:HB	1.88	0.55
1:G:363:ARG:HB3	1:G:380:GLY:O	2.06	0.55
1:G:295:ILE:HG13	1:G:306:ILE:HD11	1.89	0.55
1:E:736:VAL:HB	4:E:1197:HOH:O	2.06	0.55
1:C:387:LEU:HD13	1:C:388:GLY:N	2.22	0.55
1:A:882:ILE:HD11	1:A:899:PHE:HA	1.89	0.55
1:E:546:PRO:HG2	1:E:567:ASP:HB3	1.89	0.55
1:A:541:VAL:HG22	1:A:542:ILE:N	2.22	0.55
1:E:746:HIS:HA	1:E:748:TYR:CZ	2.42	0.54
1:E:993:GLY:HA2	4:E:1083:HOH:O	2.04	0.54
1:E:532:SER:HB2	1:G:525:ASP:OD1	2.06	0.54
1:G:53:ILE:CG2	1:G:286:LEU:HD21	2.36	0.54
1:K:498:SER:CB	4:K:1073:HOH:O	2.48	0.54
1:K:190:ARG:HG3	1:K:216:GLU:OE2	2.07	0.54
1:K:565:GLU:HG2	1:K:566:TYR:N	2.22	0.54
1:I:882:ILE:HD11	1:I:899:PHE:HA	1.89	0.54
1:K:1002:ASP:N	4:K:1180:HOH:O	2.39	0.54
1:E:1016:ARG:O	1:E:1017:ASP:HB2	2.07	0.54
1:G:489:LYS:HG3	1:G:491:PHE:CE1	2.43	0.54
1:E:746:HIS:NE2	3:F:2213:CHM:C1	2.71	0.54
1:E:681:SER:CB	1:E:684:GLU:HG2	2.36	0.54
1:A:809:ASP:HB3	1:A:814:THR:HA	1.88	0.54
1:C:245:ILE:HD11	1:C:278:LEU:HG	1.90	0.54
1:C:541:VAL:HG22	1:C:542:ILE:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:PHE:CB	1:A:88:PRO:HD2	2.35	0.54
1:A:874:ARG:CZ	4:A:1176:HOH:O	2.55	0.54
1:E:700:ASN:HD22	1:E:1008:GLN:NE2	2.05	0.54
1:I:324:LYS:HD2	4:I:1117:HOH:O	2.05	0.54
1:I:892:LEU:HD13	1:I:920:VAL:HG21	1.89	0.54
1:G:190:ARG:HG3	1:G:216:GLU:OE2	2.08	0.54
1:E:256:SER:OG	1:E:267:HIS:CE1	2.60	0.54
1:A:781:ALA:HB2	1:A:802:PRO:HG2	1.89	0.54
1:C:1052:ILE:O	1:C:1056:ILE:HG13	2.07	0.54
1:A:112:ASN:OD1	1:A:114:GLU:HB3	2.08	0.54
1:G:681:SER:HB3	1:G:684:GLU:CG	2.35	0.54
1:E:956:ILE:HD13	1:E:957:ALA:N	2.21	0.54
1:C:800:ILE:HG21	1:C:845:ARG:HH22	1.71	0.54
1:K:565:GLU:HG2	4:K:1178:HOH:O	2.07	0.54
1:C:278:LEU:HD23	1:C:287:PHE:HB3	1.90	0.54
1:C:363:ARG:HB3	1:C:380:GLY:O	2.07	0.54
1:E:44:LEU:HD12	1:E:56:VAL:HB	1.90	0.54
1:G:541:VAL:HG22	1:G:542:ILE:N	2.22	0.54
1:G:480:ILE:N	1:G:494:THR:HG22	2.19	0.54
1:I:681:SER:CB	1:I:684:GLU:HG2	2.34	0.54
1:K:684:GLU:HG3	1:K:685:GLU:N	2.23	0.54
1:E:220:GLY:O	1:E:1038:HIS:HB3	2.08	0.54
1:G:956:ILE:HD13	1:G:957:ALA:N	2.22	0.54
1:E:337:ILE:HG13	1:E:649:MET:CE	2.37	0.54
1:C:746:HIS:HA	1:C:748:TYR:CZ	2.43	0.54
1:A:746:HIS:NE2	3:B:2213:CHM:C1	2.71	0.54
1:E:997:LYS:NZ	4:E:1136:HOH:O	2.41	0.54
1:K:184:LEU:HB2	1:K:191:VAL:HB	1.89	0.54
1:I:525:ASP:OD1	1:K:532:SER:HB2	2.07	0.54
1:E:201:HIS:HE1	4:E:1155:HOH:O	1.90	0.54
1:C:268:THR:HG22	1:C:303:ILE:HD11	1.90	0.54
1:K:1016:ARG:O	1:K:1017:ASP:HB2	2.08	0.54
1:I:901:ASN:HB3	1:K:469:HIS:ND1	2.22	0.54
1:A:430:THR:HG23	1:A:441:ILE:HD11	1.90	0.54
1:E:278:LEU:HD23	1:E:287:PHE:HB3	1.89	0.54
1:C:307:GLU:C	1:C:308:ILE:HD12	2.29	0.54
1:E:565:GLU:HG2	1:E:566:TYR:H	1.73	0.54
1:G:744:THR:HA	4:G:1174:HOH:O	2.08	0.54
1:E:201:HIS:HB3	1:E:736:VAL:HG13	1.91	0.53
1:K:253:GLN:HA	1:K:253:GLN:NE2	2.22	0.53
1:A:295:ILE:HG13	1:A:306:ILE:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:591:LEU:HD13	1:K:662:LEU:HD21	1.90	0.53
1:G:110:PHE:CD2	1:G:121:ILE:HG13	2.43	0.53
1:A:522:PRO:HG2	1:C:889:MET:SD	2.48	0.53
1:C:882:ILE:HD11	1:C:899:PHE:HA	1.90	0.53
1:E:603:HIS:HD2	1:E:604:GLY:O	1.90	0.53
1:E:986:ARG:HD2	1:E:1025:TYR:O	2.06	0.53
1:G:731:LEU:HD22	1:G:735:ILE:CD1	2.38	0.53
1:G:268:THR:HG22	1:G:303:ILE:HD11	1.91	0.53
1:K:343:GLY:HA2	4:K:1095:HOH:O	2.07	0.53
1:A:889:MET:SD	1:C:522:PRO:HG2	2.49	0.53
1:E:701:TYR:O	1:G:939:ARG:HD3	2.08	0.53
1:A:633:LYS:NZ	1:A:665:PRO:O	2.40	0.53
1:I:618:VAL:CG2	1:I:631:GLU:HG3	2.38	0.53
1:I:314:PRO:HD2	1:I:726:LYS:HG2	1.89	0.53
1:C:714:ILE:HG21	1:C:741:GLU:HG3	1.91	0.53
1:A:268:THR:HG22	1:A:303:ILE:HD11	1.91	0.53
1:E:565:GLU:HG2	1:E:566:TYR:N	2.23	0.53
1:A:402:GLU:HB2	4:A:1195:HOH:O	2.08	0.53
1:K:112:ASN:OD1	1:K:114:GLU:HB3	2.08	0.53
1:I:222:PHE:HB2	1:I:1038:HIS:HD2	1.74	0.53
1:C:909:ILE:HA	1:C:956:ILE:HG22	1.90	0.53
1:G:124:PHE:HB3	1:G:152:ALA:CB	2.39	0.53
1:E:432:ASP:OD1	1:E:434:GLU:HB3	2.08	0.53
1:E:1029:PRO:HB3	4:E:1113:HOH:O	2.09	0.53
1:G:681:SER:O	1:G:684:GLU:HG2	2.08	0.53
1:E:909:ILE:HA	1:E:956:ILE:HG22	1.90	0.53
1:G:229:SER:HB3	1:G:248:ILE:HD11	1.90	0.53
1:C:300:THR:HG21	4:C:1154:HOH:O	2.08	0.53
1:G:387:LEU:HD13	1:G:388:GLY:N	2.23	0.53
1:C:403:ASN:C	1:C:403:ASN:HD22	2.12	0.53
1:G:337:ILE:HG13	1:G:649:MET:CE	2.39	0.53
1:K:909:ILE:HA	1:K:956:ILE:HG22	1.91	0.53
1:A:909:ILE:HA	1:A:956:ILE:HG22	1.90	0.53
1:C:840:LYS:HE2	4:C:1213:HOH:O	2.08	0.53
1:I:124:PHE:HB3	1:I:152:ALA:CB	2.39	0.53
1:G:618:VAL:CG2	1:G:631:GLU:HG3	2.38	0.53
1:E:525:ASP:OD1	1:G:532:SER:HB2	2.07	0.53
1:A:555:VAL:HG22	1:I:354:TYR:OH	2.08	0.53
1:G:746:HIS:NE2	3:H:2213:CHM:C1	2.72	0.53
1:I:532:SER:HB2	1:K:525:ASP:OD1	2.08	0.53
1:A:524:PRO:HD3	1:C:605:GLU:CG	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:LEU:HD12	1:C:56:VAL:HB	1.90	0.53
1:A:714:ILE:HG21	1:A:741:GLU:HG3	1.91	0.53
1:C:727:THR:O	1:C:730:ASP:HB2	2.08	0.53
1:G:220:GLY:O	1:G:1038:HIS:HB3	2.08	0.53
1:E:73:LYS:HD3	1:E:76:SER:CB	2.38	0.53
1:A:681:SER:CB	1:A:684:GLU:HG2	2.38	0.53
1:G:307:GLU:C	1:G:308:ILE:HD12	2.29	0.53
1:E:184:LEU:HB2	1:E:191:VAL:HB	1.91	0.53
1:I:307:GLU:C	1:I:308:ILE:HD12	2.29	0.53
1:I:432:ASP:OD1	1:I:434:GLU:HB3	2.08	0.53
1:G:98:MET:HE3	1:G:103:LEU:HD13	1.89	0.53
1:A:1016:ARG:O	1:A:1017:ASP:HB2	2.08	0.53
1:K:480:ILE:H	1:K:494:THR:HG21	1.73	0.53
1:K:403:ASN:C	1:K:403:ASN:HD22	2.11	0.53
1:I:596:LEU:HD12	1:I:619:LEU:HD11	1.90	0.53
1:I:809:ASP:HB3	1:I:814:THR:HA	1.91	0.53
1:G:546:PRO:HG2	1:G:567:ASP:HB3	1.90	0.53
1:G:351:SER:HG	1:G:353:THR:CG2	2.16	0.52
1:G:222:PHE:HB2	1:G:1038:HIS:HD2	1.74	0.52
1:G:1016:ARG:O	1:G:1017:ASP:HB2	2.09	0.52
1:E:218:ASN:O	1:E:220:GLY:N	2.42	0.52
1:G:322:PRO:HB3	1:G:678:LEU:HD13	1.91	0.52
1:K:197:PHE:HE1	1:K:199:LEU:HD21	1.74	0.52
1:I:179:PRO:HG2	4:I:1162:HOH:O	2.09	0.52
1:K:453:THR:HG23	4:K:1176:HOH:O	2.09	0.52
1:I:220:GLY:O	1:I:1038:HIS:HB3	2.09	0.52
1:G:87:PHE:CB	1:G:88:PRO:HD2	2.40	0.52
1:K:222:PHE:HB2	1:K:1038:HIS:HD2	1.73	0.52
1:K:63:GLU:C	4:K:1152:HOH:O	2.47	0.52
1:I:1016:ARG:O	1:I:1017:ASP:HB2	2.08	0.52
1:C:184:LEU:HB2	1:C:191:VAL:HB	1.90	0.52
1:I:155:PRO:O	1:I:856:ARG:HD2	2.09	0.52
1:I:256:SER:OG	1:I:267:HIS:HE1	1.91	0.52
1:E:146:LEU:HD23	1:E:165:VAL:HG21	1.91	0.52
1:E:423:ASN:HD22	1:E:423:ASN:C	2.12	0.52
1:C:61:LEU:CB	1:C:75:VAL:HG13	2.38	0.52
1:I:229:SER:HB3	1:I:248:ILE:CD1	2.39	0.52
1:C:337:ILE:HG13	1:C:649:MET:CE	2.39	0.52
1:A:406:ASN:HB2	1:A:424:ASP:CG	2.30	0.52
1:C:498:SER:OG	1:C:518:ARG:HG2	2.09	0.52
1:I:363:ARG:HB3	1:I:380:GLY:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:618:VAL:CG2	1:C:631:GLU:HG3	2.40	0.52
1:E:892:LEU:HD13	1:E:920:VAL:HG21	1.90	0.52
1:I:61:LEU:CB	1:I:75:VAL:HG13	2.39	0.52
1:E:82:ASN:HD21	1:E:96:ARG:HG2	1.73	0.52
1:E:242:ILE:O	1:E:256:SER:HA	2.09	0.52
1:K:363:ARG:NH2	4:K:1095:HOH:O	2.42	0.52
1:C:1016:ARG:O	1:C:1017:ASP:HB2	2.10	0.52
1:C:110:PHE:CD2	1:C:121:ILE:HG13	2.44	0.52
1:K:242:ILE:O	1:K:256:SER:HA	2.09	0.52
1:K:256:SER:OG	1:K:267:HIS:CE1	2.60	0.52
1:G:53:ILE:HG23	1:G:286:LEU:CD2	2.39	0.52
1:K:681:SER:O	1:K:684:GLU:HG2	2.10	0.52
1:C:703:ASN:ND2	1:C:703:ASN:C	2.62	0.52
1:C:273:TYR:O	1:C:289:LYS:HD2	2.10	0.52
1:I:401:GLU:CD	1:I:401:GLU:H	2.13	0.52
1:I:353:THR:HG23	1:I:354:TYR:CD1	2.45	0.52
1:K:913:ARG:NH2	1:K:1047:GLN:HE21	2.03	0.52
1:G:684:GLU:HG3	1:G:685:GLU:N	2.23	0.52
1:K:82:ASN:HD21	1:K:96:ARG:HG2	1.74	0.52
1:C:218:ASN:O	1:C:220:GLY:N	2.43	0.52
1:I:110:PHE:CD2	1:I:121:ILE:HG13	2.44	0.52
1:C:601:PRO:O	4:C:1096:HOH:O	2.19	0.52
1:K:82:ASN:N	1:K:82:ASN:HD22	2.08	0.52
1:C:64:HIS:HD2	1:C:71:THR:OG1	1.92	0.52
1:C:430:THR:HG23	1:C:441:ILE:HD11	1.91	0.52
1:A:184:LEU:HB2	1:A:191:VAL:HB	1.92	0.52
1:A:489:LYS:HG3	1:A:491:PHE:CE1	2.44	0.52
1:A:684:GLU:HG3	1:A:685:GLU:N	2.25	0.52
1:A:432:ASP:OD1	1:A:434:GLU:HB3	2.09	0.52
1:E:714:ILE:HG21	1:E:741:GLU:HG3	1.91	0.52
1:K:201:HIS:HB3	1:K:736:VAL:HG13	1.91	0.52
1:E:735:ILE:O	1:E:739:GLN:HG3	2.10	0.52
1:G:205:TYR:HA	1:G:1024:ASN:HD21	1.74	0.52
1:I:387:LEU:HD13	1:I:388:GLY:N	2.24	0.52
1:K:234:SER:HB3	1:K:278:LEU:H	1.75	0.52
1:K:633:LYS:NZ	1:K:665:PRO:O	2.42	0.52
1:E:281:ASP:HA	4:E:1162:HOH:O	2.09	0.52
1:E:591:LEU:HD13	1:E:662:LEU:HD21	1.92	0.52
1:K:565:GLU:HG2	1:K:566:TYR:H	1.72	0.52
1:E:273:TYR:O	1:E:289:LYS:HD2	2.10	0.52
1:I:184:LEU:HB2	1:I:191:VAL:HB	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:890:MET:O	1:K:894:GLU:HG2	2.10	0.52
1:A:704:GLU:HG3	1:C:939:ARG:HH11	1.73	0.51
1:K:591:LEU:CD1	1:K:662:LEU:HD21	2.40	0.51
1:I:956:ILE:HD13	1:I:957:ALA:N	2.25	0.51
1:A:605:GLU:CG	1:C:524:PRO:HD3	2.39	0.51
1:C:565:GLU:HG2	1:C:566:TYR:N	2.25	0.51
1:C:616:LYS:HD3	4:C:1079:HOH:O	2.11	0.51
1:A:586:ARG:HG3	2:B:1204:GLN:HG3	1.92	0.51
1:I:337:ILE:HG13	1:I:649:MET:CE	2.40	0.51
1:A:949:ASN:ND2	1:C:475:TYR:OH	2.39	0.51
1:A:327:GLU:O	1:A:328:ASP:O	2.28	0.51
1:C:112:ASN:OD1	1:C:114:GLU:HB3	2.10	0.51
1:I:64:HIS:HD2	1:I:71:THR:OG1	1.93	0.51
1:A:273:TYR:O	1:A:289:LYS:HD2	2.09	0.51
1:K:110:PHE:CD2	1:K:121:ILE:HG13	2.45	0.51
1:E:609:TYR:CE1	4:E:1133:HOH:O	2.54	0.51
1:A:703:ASN:ND2	1:A:703:ASN:C	2.61	0.51
1:K:218:ASN:O	1:K:220:GLY:N	2.43	0.51
1:E:406:ASN:HB2	1:E:424:ASP:CG	2.30	0.51
1:A:318:ILE:HG21	1:A:682:ILE:HD11	1.92	0.51
1:G:965:SER:HA	1:G:990:GLY:O	2.11	0.51
1:I:1052:ILE:O	1:I:1056:ILE:HG13	2.10	0.51
1:K:124:PHE:HB3	1:K:152:ALA:CB	2.40	0.51
1:I:367:VAL:HG12	1:I:375:VAL:HG21	1.92	0.51
1:K:253:GLN:NE2	1:K:268:THR:OG1	2.43	0.51
1:I:87:PHE:CB	1:I:88:PRO:HD2	2.38	0.51
1:G:642:SER:HB2	1:G:647:THR:HB	1.92	0.51
1:I:890:MET:O	1:I:894:GLU:HG2	2.10	0.51
1:I:746:HIS:HA	1:I:748:TYR:CZ	2.45	0.51
1:A:245:ILE:HD11	1:A:278:LEU:HG	1.92	0.51
1:I:197:PHE:HE1	1:I:199:LEU:HD21	1.75	0.51
1:A:64:HIS:HD2	1:A:71:THR:OG1	1.93	0.51
1:A:948:THR:H	1:C:922:GLN:HE22	1.57	0.51
1:C:480:ILE:N	1:C:494:THR:HG22	2.20	0.51
1:K:586:ARG:HG3	2:L:1204:GLN:HG3	1.93	0.51
1:K:681:SER:HB3	1:K:684:GLU:CG	2.40	0.51
1:C:322:PRO:HB3	1:C:678:LEU:HD13	1.91	0.51
1:A:256:SER:OG	1:A:267:HIS:CE1	2.63	0.51
1:I:591:LEU:CD1	1:I:662:LEU:HD21	2.41	0.51
1:A:202:TRP:CH2	1:A:745:SER:HB3	2.46	0.51
1:E:53:ILE:HD12	1:E:66:LEU:HD21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:681:SER:CB	1:C:684:GLU:HG2	2.39	0.51
1:I:546:PRO:CG	1:I:567:ASP:HB3	2.41	0.51
1:I:633:LYS:NZ	1:I:665:PRO:O	2.42	0.51
1:C:423:ASN:HD22	1:C:423:ASN:C	2.14	0.51
1:I:190:ARG:HG3	1:I:216:GLU:OE2	2.10	0.51
1:G:591:LEU:HD13	1:G:662:LEU:HD21	1.92	0.51
1:A:743:ARG:HB3	4:A:1090:HOH:O	2.10	0.51
1:G:284:ARG:HD3	4:G:1179:HOH:O	2.09	0.51
1:I:429:MET:HA	1:I:441:ILE:HD13	1.93	0.51
1:G:44:LEU:HD12	1:G:56:VAL:HB	1.92	0.51
1:I:565:GLU:HG2	1:I:566:TYR:N	2.25	0.51
1:K:401:GLU:CD	1:K:401:GLU:H	2.14	0.51
1:I:218:ASN:O	1:I:220:GLY:N	2.44	0.51
1:K:385:ASP:HB2	1:K:405:GLY:O	2.11	0.51
1:I:940:ARG:HD2	4:K:1098:HOH:O	2.10	0.51
1:A:110:PHE:CD2	1:A:121:ILE:HG13	2.46	0.51
1:G:890:MET:O	1:G:894:GLU:HG2	2.10	0.51
1:K:1052:ILE:O	1:K:1056:ILE:HG13	2.11	0.51
1:G:112:ASN:OD1	1:G:114:GLU:HB3	2.11	0.51
1:I:731:LEU:HD22	1:I:735:ILE:CD1	2.41	0.51
1:K:887:MET:HB2	1:K:917:GLY:C	2.30	0.51
1:A:640:ARG:HD2	4:A:1184:HOH:O	2.10	0.51
1:A:403:ASN:C	1:A:403:ASN:HD22	2.13	0.51
1:G:82:ASN:HD22	1:G:82:ASN:N	2.09	0.51
1:E:591:LEU:CD1	1:E:662:LEU:HD21	2.41	0.51
1:C:429:MET:HA	1:C:441:ILE:HD13	1.93	0.51
1:E:905:TYR:HB2	4:E:1086:HOH:O	2.11	0.51
1:K:533:PHE:C	4:K:1090:HOH:O	2.50	0.50
1:K:87:PHE:CB	1:K:88:PRO:HD2	2.39	0.50
1:G:909:ILE:HG12	1:G:956:ILE:HG21	1.92	0.50
1:I:948:THR:H	1:K:922:GLN:HE22	1.57	0.50
1:E:925:ILE:HG22	4:E:1134:HOH:O	2.11	0.50
1:C:432:ASP:OD1	1:C:434:GLU:HB3	2.11	0.50
1:G:218:ASN:O	1:G:220:GLY:N	2.44	0.50
1:C:222:PHE:HB2	1:C:1038:HIS:HD2	1.76	0.50
1:K:245:ILE:HD11	1:K:278:LEU:HG	1.92	0.50
1:A:986:ARG:HD2	1:A:1025:TYR:O	2.11	0.50
1:A:387:LEU:HD13	1:A:388:GLY:N	2.27	0.50
1:I:541:VAL:HG22	1:I:542:ILE:N	2.26	0.50
1:I:480:ILE:H	1:I:494:THR:HG21	1.75	0.50
1:I:618:VAL:HG21	1:I:631:GLU:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:965:SER:HA	1:A:990:GLY:O	2.11	0.50
1:A:722:VAL:N	1:A:723:PRO:HD2	2.27	0.50
1:G:714:ILE:HG21	1:G:741:GLU:HG3	1.93	0.50
1:I:684:GLU:HG3	1:I:685:GLU:N	2.26	0.50
1:G:591:LEU:CD1	1:G:662:LEU:HD21	2.42	0.50
1:I:82:ASN:HD22	1:I:82:ASN:N	2.09	0.50
1:K:956:ILE:HD13	1:K:957:ALA:N	2.27	0.50
1:I:112:ASN:OD1	1:I:114:GLU:HB3	2.11	0.50
1:K:273:TYR:O	1:K:289:LYS:HD2	2.10	0.50
1:E:110:PHE:CD2	1:E:121:ILE:HG13	2.45	0.50
1:K:872:HIS:HE1	1:K:902:GLU:OE1	1.94	0.50
1:C:331:PRO:HB3	1:C:649:MET:HE3	1.93	0.50
1:I:901:ASN:HB3	1:K:469:HIS:CE1	2.45	0.50
1:G:986:ARG:HD2	1:G:1025:TYR:O	2.12	0.50
1:I:603:HIS:HD2	1:I:604:GLY:O	1.93	0.50
1:K:422:ALA:HB1	4:K:1091:HOH:O	2.12	0.50
1:K:201:HIS:O	1:K:740:GLY:HA2	2.11	0.50
1:K:53:ILE:HG23	1:K:286:LEU:CD2	2.39	0.50
1:C:87:PHE:CB	1:C:88:PRO:HD2	2.37	0.50
1:G:546:PRO:CG	1:G:567:ASP:HB3	2.42	0.50
1:K:372:ASP:HB3	4:K:1197:HOH:O	2.12	0.50
1:G:367:VAL:O	1:G:368:ARG:HD3	2.12	0.50
1:A:939:ARG:HH11	1:C:704:GLU:HG3	1.76	0.50
1:A:637:THR:OG1	1:A:651:ARG:HG2	2.12	0.50
1:E:201:HIS:O	1:E:740:GLY:HA2	2.12	0.50
1:A:61:LEU:HB3	1:A:75:VAL:CG1	2.39	0.50
1:E:703:ASN:C	1:E:703:ASN:ND2	2.59	0.50
1:E:684:GLU:HG3	1:E:685:GLU:N	2.26	0.50
1:E:403:ASN:HD22	1:E:403:ASN:C	2.12	0.50
1:I:565:GLU:HG2	1:I:566:TYR:H	1.76	0.50
1:I:91:ARG:NH2	4:I:1202:HOH:O	2.41	0.50
1:K:64:HIS:HD2	1:K:71:THR:OG1	1.95	0.50
1:A:546:PRO:HG2	1:A:567:ASP:HB3	1.93	0.50
1:A:44:LEU:HD12	1:A:56:VAL:HB	1.94	0.50
1:I:681:SER:O	1:I:684:GLU:HG2	2.11	0.50
1:G:586:ARG:HG3	2:H:1204:GLN:HG3	1.92	0.50
1:A:618:VAL:HG21	1:A:631:GLU:HG3	1.93	0.50
1:K:722:VAL:N	1:K:723:PRO:HD2	2.26	0.50
1:A:565:GLU:HG2	1:A:566:TYR:N	2.26	0.50
1:K:236:VAL:HG23	1:K:243:TYR:HB2	1.94	0.50
1:I:367:VAL:O	1:I:368:ARG:HD3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:314:PRO:HD2	1:K:726:LYS:HG2	1.94	0.50
1:I:714:ILE:HG21	1:I:741:GLU:HG3	1.92	0.50
1:C:319:ILE:HD11	4:I:1179:HOH:O	2.12	0.49
1:I:642:SER:HB2	1:I:647:THR:HB	1.92	0.49
1:I:489:LYS:HG3	1:I:491:PHE:CE1	2.47	0.49
1:C:141:ASP:OD1	1:C:145:ASN:HB2	2.12	0.49
1:G:565:GLU:HG2	1:G:566:TYR:N	2.26	0.49
1:E:1052:ILE:O	1:E:1056:ILE:HG13	2.12	0.49
1:C:544:LEU:N	4:C:1113:HOH:O	2.45	0.49
1:G:480:ILE:H	1:G:494:THR:HG21	1.72	0.49
1:K:124:PHE:HB3	1:K:152:ALA:HB1	1.92	0.49
1:K:887:MET:HG3	1:K:966:ASP:OD2	2.13	0.49
1:E:905:TYR:N	4:E:1086:HOH:O	2.29	0.49
1:E:887:MET:HB2	1:E:917:GLY:C	2.32	0.49
1:G:633:LYS:NZ	1:G:665:PRO:O	2.46	0.49
1:I:703:ASN:C	1:I:703:ASN:ND2	2.64	0.49
1:G:703:ASN:HA	4:G:1097:HOH:O	2.11	0.49
1:I:234:SER:HB3	1:I:278:LEU:H	1.76	0.49
1:I:430:THR:HG23	1:I:441:ILE:HD11	1.94	0.49
1:G:367:VAL:HG12	1:G:375:VAL:HG21	1.93	0.49
1:A:141:ASP:OD1	1:A:145:ASN:HB2	2.11	0.49
1:G:715:TYR:HB3	4:G:1186:HOH:O	2.11	0.49
1:E:64:HIS:HD2	1:E:71:THR:OG1	1.96	0.49
1:K:568:LEU:HD23	1:K:568:LEU:N	2.27	0.49
1:K:703:ASN:ND2	1:K:706:VAL:H	2.10	0.49
1:C:684:GLU:HG3	1:C:685:GLU:N	2.27	0.49
1:E:88:PRO:HG2	1:E:89:ASP:H	1.77	0.49
1:C:242:ILE:O	1:C:256:SER:HA	2.13	0.49
1:G:885:PRO:O	1:G:915:ASN:HA	2.12	0.49
1:C:57:CYS:HB3	1:C:62:TRP:CD1	2.48	0.49
1:K:589:ILE:HD13	1:K:641:LEU:HD12	1.93	0.49
1:G:256:SER:OG	1:G:267:HIS:HE1	1.95	0.49
1:C:327:GLU:O	1:C:328:ASP:O	2.30	0.49
1:I:202:TRP:CH2	1:I:745:SER:HB3	2.47	0.49
1:E:407:VAL:HG13	1:E:421:VAL:HG13	1.95	0.49
1:E:568:LEU:HD23	1:E:568:LEU:N	2.26	0.49
1:I:423:ASN:HD22	1:I:423:ASN:C	2.15	0.49
1:E:190:ARG:HG3	1:E:216:GLU:OE2	2.12	0.49
1:K:546:PRO:CG	1:K:567:ASP:HB3	2.41	0.49
1:G:965:SER:O	1:G:968:ASP:N	2.44	0.49
1:C:374:LYS:HG3	4:C:1144:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:PHE:HB3	1:C:152:ALA:CB	2.42	0.49
1:E:618:VAL:CG2	1:E:631:GLU:HG3	2.42	0.49
1:K:423:ASN:C	1:K:423:ASN:HD22	2.16	0.49
1:K:353:THR:HG23	1:K:354:TYR:CD1	2.47	0.49
1:A:87:PHE:HB3	1:A:88:PRO:CD	2.41	0.49
1:K:703:ASN:C	1:K:703:ASN:ND2	2.65	0.49
1:E:781:ALA:CB	1:E:802:PRO:HG2	2.43	0.49
1:A:242:ILE:O	1:A:256:SER:HA	2.12	0.49
1:G:406:ASN:HB2	1:G:424:ASP:CG	2.32	0.49
1:E:48:ILE:HG12	1:E:49:HIS:N	2.27	0.49
1:E:633:LYS:NZ	1:E:665:PRO:O	2.44	0.49
1:E:124:PHE:HB3	1:E:152:ALA:CB	2.43	0.49
1:E:681:SER:O	1:E:684:GLU:HG2	2.12	0.49
1:I:222:PHE:H	1:I:1038:HIS:CD2	2.29	0.49
1:G:565:GLU:HG2	1:G:566:TYR:H	1.77	0.49
1:E:589:ILE:HD13	1:E:641:LEU:HD12	1.93	0.49
1:E:863:TRP:CD1	4:E:1114:HOH:O	2.55	0.49
1:C:722:VAL:N	1:C:723:PRO:HD2	2.27	0.49
1:C:637:THR:OG1	1:C:651:ARG:HG2	2.13	0.49
1:E:532:SER:HB2	4:E:1181:HOH:O	2.11	0.49
1:K:40:PRO:HG2	1:K:724:LEU:CD2	2.41	0.49
1:I:268:THR:HG22	1:I:303:ILE:HD11	1.95	0.49
1:G:124:PHE:HB3	1:G:152:ALA:HB1	1.94	0.49
1:E:642:SER:HB2	1:E:647:THR:HB	1.94	0.49
1:C:45:ASN:HA	1:C:277:HIS:CD2	2.48	0.49
1:G:353:THR:HG23	1:G:354:TYR:CD1	2.48	0.49
1:I:331:PRO:HB3	1:I:649:MET:HE3	1.93	0.49
1:K:63:GLU:N	4:K:1152:HOH:O	2.45	0.49
1:A:746:HIS:HA	1:A:748:TYR:CZ	2.48	0.49
1:E:245:ILE:HD11	1:E:278:LEU:HG	1.94	0.49
1:A:939:ARG:NH1	1:C:704:GLU:HG3	2.28	0.49
1:G:872:HIS:HE1	1:G:902:GLU:OE1	1.95	0.49
1:I:959:THR:O	1:I:984:GLY:HA3	2.13	0.49
1:E:353:THR:HG23	1:E:354:TYR:CD1	2.48	0.49
1:G:222:PHE:H	1:G:1038:HIS:CD2	2.31	0.49
1:I:322:PRO:HB3	1:I:678:LEU:HD13	1.94	0.49
1:C:840:LYS:CE	4:C:1213:HOH:O	2.59	0.49
1:G:430:THR:HG23	1:G:441:ILE:HD11	1.95	0.49
1:A:190:ARG:HG3	1:A:216:GLU:OE2	2.13	0.48
1:C:229:SER:HB3	1:C:248:ILE:CD1	2.42	0.48
1:A:124:PHE:HB3	1:A:152:ALA:CB	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:959:THR:O	1:A:984:GLY:HA3	2.13	0.48
1:I:965:SER:HA	1:I:990:GLY:O	2.12	0.48
1:C:586:ARG:NE	2:D:1206:ALA:HB3	2.28	0.48
1:G:641:LEU:HD23	1:G:647:THR:O	2.13	0.48
1:I:591:LEU:HD13	1:I:662:LEU:HD21	1.95	0.48
1:A:641:LEU:HD23	1:A:647:THR:O	2.13	0.48
1:C:442:GLU:OE2	1:C:481:HIS:HD2	1.96	0.48
1:K:452:PHE:HB3	1:K:463:TYR:HB3	1.96	0.48
1:E:197:PHE:HE1	1:E:199:LEU:HD21	1.77	0.48
1:E:859:ARG:NH1	4:E:1122:HOH:O	2.46	0.48
1:I:273:TYR:O	1:I:289:LYS:HD2	2.12	0.48
1:C:546:PRO:HG2	1:C:567:ASP:HB3	1.95	0.48
1:E:992:VAL:HG13	4:E:1189:HOH:O	2.06	0.48
1:E:959:THR:HG22	4:E:1113:HOH:O	2.12	0.48
1:A:704:GLU:HG3	1:C:939:ARG:NH1	2.28	0.48
1:I:403:ASN:HD22	1:I:405:GLY:H	1.60	0.48
1:E:827:GLU:O	1:K:677:PRO:HD2	2.13	0.48
1:E:429:MET:HA	1:E:441:ILE:HD13	1.95	0.48
1:A:429:MET:HA	1:A:441:ILE:HD13	1.95	0.48
1:E:641:LEU:HD23	1:E:647:THR:O	2.14	0.48
1:E:885:PRO:HG2	1:E:890:MET:HG2	1.95	0.48
1:K:210:ARG:N	4:K:1083:HOH:O	2.45	0.48
1:K:268:THR:HG22	1:K:303:ILE:HD11	1.95	0.48
1:I:775:HIS:HA	4:I:1188:HOH:O	2.13	0.48
1:E:605:GLU:CG	1:G:524:PRO:HD3	2.42	0.48
1:K:410:MET:HG2	1:K:421:VAL:HG22	1.96	0.48
1:G:735:ILE:O	1:G:739:GLN:HG3	2.13	0.48
1:A:201:HIS:HB3	1:A:736:VAL:HG13	1.94	0.48
1:E:40:PRO:HG2	1:E:724:LEU:CD2	2.37	0.48
1:A:530:ASN:ND2	1:A:531:PHE:N	2.61	0.48
1:I:124:PHE:HB3	1:I:152:ALA:HB1	1.93	0.48
1:I:242:ILE:O	1:I:256:SER:HA	2.13	0.48
1:A:423:ASN:C	1:A:423:ASN:HD22	2.15	0.48
1:C:406:ASN:HB2	1:C:424:ASP:CG	2.32	0.48
1:C:921:SER:HB3	1:C:966:ASP:OD2	2.13	0.48
1:I:516:SER:HB3	1:I:518:ARG:HG3	1.96	0.48
1:K:430:THR:HG23	1:K:441:ILE:HD11	1.95	0.48
1:C:676:ARG:CD	4:C:1072:HOH:O	2.59	0.48
1:A:300:THR:HG22	1:A:300:THR:O	2.13	0.48
1:C:641:LEU:HD23	1:C:647:THR:O	2.14	0.48
1:E:410:MET:HG2	1:E:421:VAL:HG22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:PHE:HA	1:A:577:PRO:HA	1.96	0.48
1:E:425:ARG:O	1:E:426:PHE:HB2	2.14	0.48
1:K:731:LEU:HD22	1:K:735:ILE:CD1	2.43	0.48
1:I:201:HIS:O	1:I:740:GLY:HA2	2.14	0.48
1:K:61:LEU:HB3	1:K:75:VAL:CG1	2.39	0.48
1:A:337:ILE:HG13	1:A:649:MET:CE	2.44	0.48
1:I:649:MET:HE3	1:I:649:MET:HB2	1.74	0.48
1:E:546:PRO:CG	1:E:567:ASP:HB3	2.44	0.48
1:C:124:PHE:HB3	1:C:152:ALA:HB1	1.94	0.48
1:G:429:MET:HA	1:G:441:ILE:HD13	1.95	0.48
1:A:469:HIS:ND1	1:C:901:ASN:HB3	2.27	0.48
1:I:727:THR:O	1:I:730:ASP:HB2	2.14	0.48
1:I:586:ARG:HG3	2:J:1204:GLN:HG3	1.95	0.48
1:I:190:ARG:NH2	1:I:222:PHE:HZ	2.12	0.48
1:I:710:ILE:O	1:I:714:ILE:HG12	2.13	0.48
1:E:124:PHE:HB3	1:E:152:ALA:HB1	1.95	0.48
1:E:637:THR:OG1	1:E:651:ARG:HG2	2.13	0.48
1:K:387:LEU:HD13	1:K:388:GLY:N	2.28	0.48
1:K:141:ASP:OD1	1:K:145:ASN:HB2	2.14	0.48
1:C:633:LYS:NZ	1:C:665:PRO:O	2.45	0.48
1:E:131:ARG:HH21	1:E:131:ARG:HG2	1.79	0.48
1:K:557:ARG:NE	4:K:1164:HOH:O	2.46	0.48
1:E:586:ARG:NE	2:F:1206:ALA:HB3	2.28	0.48
1:K:253:GLN:HA	1:K:253:GLN:HE21	1.78	0.48
1:K:184:LEU:HD13	1:K:237:ILE:HG13	1.96	0.48
1:I:988:TRP:CZ3	1:I:990:GLY:HA3	2.49	0.48
1:K:676:ARG:HD2	4:K:1169:HOH:O	2.14	0.48
1:G:273:TYR:O	1:G:289:LYS:HD2	2.14	0.48
1:G:926:GLU:CD	4:G:1160:HOH:O	2.52	0.48
1:G:766:ALA:HA	1:G:855:ASP:OD1	2.13	0.48
1:A:1011:PHE:HB3	1:C:936:ASP:OD2	2.14	0.47
1:E:498:SER:OG	1:E:518:ARG:HG2	2.14	0.47
1:I:367:VAL:CG1	1:I:375:VAL:HG21	2.43	0.47
1:A:712:GLU:HG3	4:A:1190:HOH:O	2.13	0.47
1:E:965:SER:HA	1:E:990:GLY:O	2.14	0.47
1:G:318:ILE:HG21	1:G:682:ILE:HD11	1.96	0.47
1:A:739:GLN:NE2	4:A:1104:HOH:O	2.45	0.47
1:E:889:MET:HE2	4:E:1133:HOH:O	2.05	0.47
1:I:681:SER:HB3	1:I:684:GLU:CG	2.40	0.47
1:E:703:ASN:ND2	1:E:706:VAL:H	2.11	0.47
1:I:703:ASN:ND2	1:I:706:VAL:H	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:82:ASN:HD21	1:G:96:ARG:HG2	1.78	0.47
1:A:82:ASN:N	1:A:82:ASN:HD22	2.10	0.47
1:K:921:SER:HB3	1:K:966:ASP:OD2	2.14	0.47
1:I:59:ASP:HB3	1:I:80:VAL:HA	1.97	0.47
1:E:554:LEU:N	4:E:1174:HOH:O	2.47	0.47
1:E:452:PHE:HB3	1:E:463:TYR:HB3	1.96	0.47
1:K:425:ARG:O	1:K:426:PHE:HB2	2.14	0.47
1:C:202:TRP:CH2	1:C:745:SER:HB3	2.49	0.47
1:C:353:THR:HG23	1:C:354:TYR:CD1	2.49	0.47
1:C:735:ILE:O	1:C:739:GLN:HG3	2.14	0.47
1:K:88:PRO:HG2	1:K:89:ASP:H	1.79	0.47
1:E:894:GLU:OE1	1:E:897:ARG:NH2	2.47	0.47
1:G:425:ARG:O	1:G:426:PHE:HB2	2.15	0.47
1:K:959:THR:O	1:K:984:GLY:HA3	2.14	0.47
1:C:385:ASP:HB2	1:C:405:GLY:O	2.15	0.47
1:E:385:ASP:HB2	1:E:405:GLY:O	2.14	0.47
1:E:922:GLN:NE2	1:G:948:THR:H	2.11	0.47
1:E:322:PRO:HB3	1:E:678:LEU:HD13	1.96	0.47
1:C:516:SER:HB3	1:C:518:ARG:HG3	1.96	0.47
1:I:363:ARG:HA	1:I:363:ARG:HD3	1.52	0.47
1:G:710:ILE:O	1:G:714:ILE:HG12	2.13	0.47
1:A:307:GLU:C	1:A:308:ILE:HD12	2.34	0.47
1:A:906:GLN:O	1:A:953:GLY:HA3	2.14	0.47
1:I:637:THR:OG1	1:I:651:ARG:HG2	2.13	0.47
1:E:225:ILE:HG13	1:E:226:VAL:HG23	1.97	0.47
1:C:272:ASP:O	1:C:717:LYS:HE2	2.15	0.47
1:G:64:HIS:HD2	1:G:71:THR:OG1	1.98	0.47
1:G:61:LEU:HB3	1:G:75:VAL:CG1	2.43	0.47
1:E:737:GLU:N	4:E:1197:HOH:O	2.46	0.47
1:E:586:ARG:HG3	2:F:1204:GLN:HG3	1.96	0.47
1:I:929:MET:CE	4:I:1166:HOH:O	2.62	0.47
1:E:872:HIS:HE1	1:E:902:GLU:OE1	1.98	0.47
1:I:40:PRO:HG2	1:I:724:LEU:CD2	2.37	0.47
2:L:1206:ALA:HA	4:L:921:HOH:O	2.13	0.47
1:C:73:LYS:HD3	1:C:76:SER:CB	2.40	0.47
1:I:586:ARG:NE	2:J:1206:ALA:HB3	2.30	0.47
1:A:82:ASN:HD21	1:A:96:ARG:HG2	1.79	0.47
1:E:234:SER:HB3	1:E:278:LEU:H	1.79	0.47
1:A:546:PRO:CG	1:A:567:ASP:HB3	2.45	0.47
1:G:151:ASP:OD1	4:G:1094:HOH:O	2.20	0.47
1:C:367:VAL:O	1:C:368:ARG:HD3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:637:THR:OG1	1:K:651:ARG:HG2	2.15	0.47
1:E:387:LEU:HD13	1:E:388:GLY:N	2.30	0.47
1:C:228:MET:HE1	1:C:244:PHE:CE1	2.50	0.47
1:E:57:CYS:HB3	1:E:62:TRP:CD1	2.50	0.47
1:A:57:CYS:HB3	1:A:62:TRP:CD1	2.50	0.47
1:E:61:LEU:HB3	1:E:75:VAL:CG1	2.45	0.47
1:E:681:SER:HB3	1:E:684:GLU:CG	2.43	0.47
1:A:642:SER:HB2	1:A:647:THR:HB	1.97	0.47
1:E:887:MET:HG3	1:E:966:ASP:OD2	2.15	0.47
1:A:360:GLU:HG3	1:A:377:PHE:CZ	2.50	0.47
1:C:890:MET:O	1:C:894:GLU:HG2	2.15	0.47
1:G:637:THR:OG1	1:G:651:ARG:HG2	2.15	0.47
1:A:942:THR:HG21	4:C:1159:HOH:O	2.14	0.47
1:E:533:PHE:C	4:E:1181:HOH:O	2.53	0.47
1:K:322:PRO:HB3	1:K:678:LEU:HD13	1.95	0.47
1:I:887:MET:HB2	1:I:917:GLY:C	2.35	0.47
1:I:178:GLY:HA3	1:I:1040:TYR:CD1	2.50	0.47
1:I:722:VAL:N	1:I:723:PRO:HD2	2.30	0.47
1:C:642:SER:HB2	1:C:647:THR:HB	1.96	0.47
1:C:956:ILE:HD13	1:C:957:ALA:N	2.30	0.47
1:G:229:SER:HB3	1:G:248:ILE:CD1	2.45	0.47
1:E:926:GLU:N	4:E:1134:HOH:O	2.47	0.47
1:E:921:SER:HB3	1:E:966:ASP:OD2	2.15	0.47
1:C:885:PRO:HG2	1:C:890:MET:HG2	1.96	0.47
1:I:534:GLU:N	4:I:1082:HOH:O	2.40	0.47
1:G:423:ASN:C	1:G:423:ASN:HD22	2.17	0.47
1:C:85:ARG:HD3	4:C:1228:HOH:O	2.15	0.47
1:C:555:VAL:HG22	1:G:354:TYR:OH	2.15	0.46
1:E:229:SER:HB3	1:E:248:ILE:CD1	2.45	0.46
1:G:367:VAL:CG1	1:G:375:VAL:HG21	2.45	0.46
1:K:642:SER:HB2	1:K:647:THR:HB	1.97	0.46
1:A:872:HIS:HE1	1:A:902:GLU:OE1	1.97	0.46
1:K:618:VAL:CG2	1:K:631:GLU:HG3	2.44	0.46
1:C:992:VAL:HG11	1:C:1009:PRO:HB2	1.96	0.46
1:E:253:GLN:NE2	1:E:253:GLN:HA	2.30	0.46
1:C:256:SER:OG	1:C:267:HIS:CE1	2.68	0.46
1:C:565:GLU:HG2	1:C:566:TYR:H	1.79	0.46
1:E:605:GLU:HG2	1:G:524:PRO:HD3	1.98	0.46
1:E:829:ALA:HA	1:E:851:ILE:HG22	1.97	0.46
1:E:524:PRO:HD3	1:G:605:GLU:CG	2.44	0.46
1:A:367:VAL:O	1:A:368:ARG:HD3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:452:PHE:HB3	1:I:463:TYR:HB3	1.98	0.46
1:K:501:TYR:CD2	1:K:501:TYR:N	2.83	0.46
1:A:913:ARG:NH2	1:A:1047:GLN:HE21	2.08	0.46
1:G:329:PHE:HD1	1:G:649:MET:SD	2.38	0.46
1:A:322:PRO:HB3	1:A:678:LEU:HD13	1.97	0.46
1:I:887:MET:HG3	1:I:966:ASP:OD2	2.15	0.46
1:G:155:PRO:O	1:G:856:ARG:HD2	2.14	0.46
1:C:48:ILE:HG12	1:C:49:HIS:N	2.30	0.46
1:I:836:ARG:N	4:I:1191:HOH:O	2.48	0.46
1:A:841:GLY:C	1:A:843:ASP:H	2.19	0.46
1:G:57:CYS:HB3	1:G:62:TRP:CD1	2.50	0.46
1:G:471:GLU:HG3	1:G:471:GLU:O	2.15	0.46
1:A:956:ILE:HD13	1:A:957:ALA:N	2.31	0.46
1:K:429:MET:HA	1:K:441:ILE:HD13	1.97	0.46
1:E:387:LEU:HD12	1:E:400:PHE:CE1	2.50	0.46
1:C:540:PHE:HA	1:C:577:PRO:HA	1.97	0.46
1:E:367:VAL:HG12	1:E:375:VAL:HG21	1.97	0.46
1:C:622:TYR:OH	1:C:627:ARG:HG2	2.15	0.46
1:K:1001:ILE:CG1	4:K:1180:HOH:O	2.64	0.46
1:E:946:TYR:CE1	1:G:922:GLN:HB3	2.51	0.46
1:K:319:ILE:CG2	1:K:677:PRO:HB3	2.46	0.46
1:A:994:ILE:HG22	1:A:1008:GLN:O	2.15	0.46
1:E:363:ARG:HD3	1:E:363:ARG:HA	1.50	0.46
1:G:184:LEU:HD13	1:G:237:ILE:HG13	1.98	0.46
1:I:533:PHE:N	1:K:525:ASP:OD1	2.39	0.46
1:G:906:GLN:O	1:G:953:GLY:HA3	2.14	0.46
1:I:906:GLN:O	1:I:953:GLY:HA3	2.15	0.46
1:I:57:CYS:HB3	1:I:62:TRP:CD1	2.50	0.46
1:E:1014:TRP:CD1	1:E:1019:GLY:HA2	2.51	0.46
1:I:471:GLU:HG3	1:I:471:GLU:O	2.15	0.46
1:C:253:GLN:NE2	1:C:253:GLN:HA	2.30	0.46
1:K:322:PRO:HG2	1:K:674:ASP:OD1	2.16	0.46
1:A:524:PRO:HD3	1:C:605:GLU:HG2	1.98	0.46
1:A:605:GLU:HG2	1:C:524:PRO:HD3	1.97	0.46
1:K:367:VAL:O	1:K:368:ARG:HD3	2.16	0.46
1:E:540:PHE:HA	1:E:577:PRO:HA	1.97	0.46
1:E:112:ASN:OD1	1:E:114:GLU:HB3	2.16	0.46
1:K:59:ASP:HB3	1:K:80:VAL:HA	1.97	0.46
1:K:318:ILE:HG21	1:K:682:ILE:HD11	1.98	0.46
1:A:562:GLU:O	1:A:563:ALA:HB3	2.15	0.46
1:K:649:MET:HB2	1:K:649:MET:HE3	1.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:872:HIS:CE1	1:I:902:GLU:OE1	2.67	0.46
1:K:462:ALA:HA	1:K:481:HIS:O	2.16	0.46
1:G:442:GLU:OE2	1:G:481:HIS:HD2	1.98	0.46
1:K:307:GLU:C	1:K:308:ILE:HD12	2.36	0.46
1:G:234:SER:HB3	1:G:278:LEU:H	1.81	0.46
1:I:534:GLU:HG3	1:K:534:GLU:OE2	2.15	0.46
1:C:533:PHE:HB3	1:C:536:VAL:HG11	1.97	0.46
1:E:258:ASP:OD1	1:E:260:ASP:HB2	2.16	0.46
1:A:827:GLU:O	1:G:677:PRO:HD2	2.16	0.46
1:I:256:SER:OG	1:I:267:HIS:CE1	2.69	0.46
1:I:98:MET:HE3	1:I:103:LEU:HD13	1.98	0.46
1:K:48:ILE:HG12	1:K:49:HIS:N	2.31	0.46
1:I:524:PRO:HD3	1:K:605:GLU:CG	2.46	0.46
1:K:146:LEU:HD23	1:K:165:VAL:HG21	1.97	0.46
1:I:45:ASN:HA	1:I:277:HIS:CD2	2.51	0.46
1:E:562:GLU:O	1:E:563:ALA:HB3	2.16	0.45
1:G:295:ILE:O	1:G:303:ILE:HA	2.16	0.45
1:E:541:VAL:CG2	1:E:542:ILE:N	2.78	0.45
1:I:641:LEU:HD23	1:I:647:THR:O	2.17	0.45
1:E:180:ALA:HA	4:E:1072:HOH:O	2.16	0.45
1:G:197:PHE:HE1	1:G:199:LEU:HD21	1.81	0.45
1:A:48:ILE:HG12	1:A:49:HIS:N	2.30	0.45
1:C:360:GLU:HG3	1:C:377:PHE:CZ	2.51	0.45
1:G:190:ARG:NH2	1:G:222:PHE:HZ	2.14	0.45
1:I:387:LEU:HD12	1:I:400:PHE:CE1	2.51	0.45
1:E:190:ARG:NH2	1:E:222:PHE:HZ	2.14	0.45
1:I:184:LEU:HD13	1:I:237:ILE:HG13	1.97	0.45
1:K:885:PRO:HG2	1:K:890:MET:HG2	1.98	0.45
1:G:885:PRO:HG2	1:G:890:MET:HG2	1.98	0.45
1:G:959:THR:O	1:G:984:GLY:HA3	2.15	0.45
1:I:886:ASP:O	1:I:891:GLY:HA3	2.17	0.45
1:G:921:SER:HB3	1:G:966:ASP:OD2	2.16	0.45
1:K:865:GLU:HB3	4:K:1144:HOH:O	2.16	0.45
1:A:45:ASN:HA	1:A:277:HIS:CD2	2.51	0.45
1:C:988:TRP:CZ3	1:C:990:GLY:HA3	2.50	0.45
1:G:59:ASP:HB3	1:G:80:VAL:HA	1.98	0.45
1:I:562:GLU:HB3	1:I:563:ALA:H	1.58	0.45
1:A:731:LEU:HD22	1:A:735:ILE:CD1	2.47	0.45
1:G:1016:ARG:NH1	4:G:1216:HOH:O	2.39	0.45
1:G:530:ASN:ND2	1:G:531:PHE:N	2.62	0.45
1:K:909:ILE:HG12	1:K:956:ILE:HG21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:329:PHE:HD1	1:I:649:MET:SD	2.39	0.45
1:G:894:GLU:OE1	1:G:897:ARG:NH2	2.49	0.45
1:I:965:SER:O	1:I:968:ASP:HB2	2.16	0.45
1:K:387:LEU:HD12	1:K:400:PHE:CE1	2.51	0.45
1:A:249:ASP:HB2	4:A:1208:HOH:O	2.17	0.45
1:A:894:GLU:OE1	1:A:897:ARG:NH2	2.49	0.45
1:C:562:GLU:O	1:C:563:ALA:HB3	2.17	0.45
1:E:731:LEU:HD22	1:E:735:ILE:CD1	2.47	0.45
1:K:586:ARG:NE	2:L:1206:ALA:HB3	2.31	0.45
1:C:462:ALA:HA	1:C:481:HIS:O	2.17	0.45
1:A:360:GLU:OE2	1:A:361:PRO:HD2	2.16	0.45
1:A:840:LYS:O	1:A:843:ASP:HB2	2.17	0.45
1:G:515:LEU:HD23	1:G:539:PRO:HA	1.99	0.45
1:I:385:ASP:HB2	1:I:405:GLY:O	2.17	0.45
1:C:681:SER:O	1:C:684:GLU:HG2	2.16	0.45
1:A:676:ARG:HD3	4:A:1073:HOH:O	2.15	0.45
1:A:222:PHE:H	1:A:1038:HIS:CD2	2.33	0.45
1:C:827:GLU:O	1:I:677:PRO:HD2	2.16	0.45
1:C:300:THR:HG22	1:C:300:THR:O	2.15	0.45
1:K:872:HIS:CE1	1:K:902:GLU:OE1	2.69	0.45
1:C:894:GLU:OE1	1:C:897:ARG:NH2	2.50	0.45
1:E:195:ASN:O	1:E:231:HIS:HE1	1.99	0.45
1:E:318:ILE:HG21	1:E:682:ILE:HD11	1.98	0.45
1:E:92:LYS:HA	1:E:111:TYR:O	2.17	0.45
1:E:141:ASP:OD1	1:E:145:ASN:HB2	2.17	0.45
1:A:353:THR:HG23	1:A:354:TYR:CD1	2.52	0.45
1:I:562:GLU:O	1:I:563:ALA:HB3	2.16	0.45
1:A:936:ASP:OD2	1:C:1011:PHE:HB3	2.16	0.45
1:I:885:PRO:HG2	1:I:890:MET:HG2	1.99	0.45
1:A:228:MET:HE3	1:A:244:PHE:CE1	2.52	0.45
1:I:605:GLU:CG	1:K:524:PRO:HD3	2.47	0.45
1:E:59:ASP:HB3	1:E:80:VAL:HA	1.98	0.45
1:A:452:PHE:HB3	1:A:463:TYR:HB3	1.99	0.45
1:E:155:PRO:O	1:E:856:ARG:HD2	2.17	0.45
1:E:959:THR:O	1:E:984:GLY:HA3	2.17	0.45
1:A:363:ARG:HA	1:A:363:ARG:HD3	1.55	0.45
1:K:894:GLU:OE1	1:K:897:ARG:NH2	2.50	0.45
1:K:228:MET:HE1	1:K:244:PHE:CE1	2.52	0.45
1:G:540:PHE:HA	1:G:577:PRO:HA	1.99	0.45
1:I:360:GLU:OE2	1:I:361:PRO:HD2	2.17	0.45
1:I:300:THR:O	1:I:300:THR:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:984:GLY:CA	4:E:1123:HOH:O	2.58	0.45
1:A:253:GLN:HG3	1:A:266:LYS:HE2	1.98	0.45
1:C:922:GLN:NE2	4:C:1132:HOH:O	2.31	0.45
1:G:243:TYR:CD2	1:G:256:SER:HB3	2.52	0.45
1:C:212:LYS:HE3	4:C:1126:HOH:O	2.17	0.45
1:G:177:LEU:O	4:G:1089:HOH:O	2.21	0.45
1:A:573:LYS:HE2	1:C:786:TYR:CZ	2.52	0.45
1:C:630:THR:HG23	4:C:1225:HOH:O	2.17	0.45
1:G:562:GLU:O	1:G:563:ALA:HB3	2.17	0.45
1:E:826:SER:CB	4:E:1135:HOH:O	2.64	0.45
1:A:480:ILE:H	1:A:494:THR:HG21	1.76	0.45
1:C:913:ARG:NH2	1:C:1047:GLN:HE21	2.07	0.45
1:A:385:ASP:HB2	1:A:405:GLY:O	2.16	0.45
1:E:87:PHE:CB	1:E:88:PRO:HD2	2.41	0.45
1:G:245:ILE:HD11	1:G:278:LEU:HG	1.98	0.45
1:I:57:CYS:HB3	1:I:62:TRP:NE1	2.32	0.45
1:K:906:GLN:O	1:K:953:GLY:HA3	2.17	0.45
1:E:635:ASN:HB3	1:E:653:ASP:OD1	2.17	0.45
1:A:425:ARG:O	1:A:426:PHE:HB2	2.17	0.45
1:G:445:ARG:NH1	4:G:1167:HOH:O	2.49	0.45
1:I:425:ARG:O	1:I:426:PHE:HB2	2.17	0.45
1:I:442:GLU:OE2	1:I:481:HIS:HD2	2.00	0.45
1:I:735:ILE:O	1:I:739:GLN:HG3	2.16	0.45
1:I:82:ASN:HD21	1:I:96:ARG:HG2	1.80	0.45
1:K:360:GLU:OE2	1:K:361:PRO:HD2	2.17	0.45
1:I:136:ASP:OD2	1:I:137:VAL:N	2.44	0.45
1:E:442:GLU:OE2	1:E:481:HIS:HD2	2.00	0.45
1:G:722:VAL:N	1:G:723:PRO:HD2	2.31	0.45
1:A:717:LYS:N	4:A:1229:HOH:O	2.31	0.45
1:G:727:THR:O	1:G:730:ASP:HB2	2.16	0.45
1:K:295:ILE:O	1:K:303:ILE:HA	2.17	0.44
1:K:591:LEU:HD12	1:K:596:LEU:CD2	2.47	0.44
1:I:390:TYR:CD1	1:I:397:ALA:HB2	2.50	0.44
1:G:618:VAL:HG21	1:G:631:GLU:HG3	1.98	0.44
1:E:901:ASN:HB3	1:G:469:HIS:CE1	2.53	0.44
1:E:272:ASP:O	1:E:717:LYS:HE2	2.17	0.44
1:E:840:LYS:O	1:E:843:ASP:HB2	2.17	0.44
1:G:360:GLU:OE2	1:G:361:PRO:HD2	2.16	0.44
1:C:53:ILE:CG2	1:C:286:LEU:HD21	2.46	0.44
1:K:541:VAL:CG2	1:K:542:ILE:N	2.80	0.44
1:E:57:CYS:HB3	1:E:62:TRP:NE1	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:965:SER:HA	1:C:990:GLY:O	2.17	0.44
1:E:307:GLU:C	1:E:308:ILE:HD12	2.37	0.44
1:E:123:TYR:OH	1:E:823:ARG:HD3	2.16	0.44
1:I:295:ILE:O	1:I:303:ILE:HA	2.17	0.44
1:C:87:PHE:HB3	1:C:88:PRO:CD	2.45	0.44
1:I:909:ILE:HG12	1:I:956:ILE:HG21	1.96	0.44
1:G:287:PHE:CE1	1:G:294:TYR:HB2	2.52	0.44
1:C:57:CYS:HB3	1:C:62:TRP:NE1	2.31	0.44
1:E:890:MET:O	1:E:894:GLU:HG2	2.16	0.44
1:E:965:SER:C	1:E:967:GLY:N	2.70	0.44
1:E:228:MET:HE1	1:E:244:PHE:CE1	2.53	0.44
1:C:1014:TRP:CD1	1:C:1019:GLY:HA2	2.52	0.44
1:I:829:ALA:HA	1:I:851:ILE:HG22	1.98	0.44
1:E:473:ASP:HA	1:G:904:SER:OG	2.17	0.44
1:G:45:ASN:HA	1:G:277:HIS:CD2	2.52	0.44
1:K:178:GLY:HA3	1:K:1040:TYR:CD1	2.53	0.44
1:I:568:LEU:N	1:I:568:LEU:HD23	2.31	0.44
1:A:736:VAL:HG22	4:A:1104:HOH:O	2.16	0.44
1:C:586:ARG:HH21	2:D:1204:GLN:HB3	1.81	0.44
1:I:177:LEU:HD21	4:I:1087:HOH:O	2.17	0.44
1:G:1017:ASP:N	4:G:1099:HOH:O	2.49	0.44
1:E:677:PRO:HD3	4:K:1136:HOH:O	2.18	0.44
1:A:243:TYR:CD2	1:A:256:SER:HB3	2.52	0.44
1:E:800:ILE:CG2	1:E:845:ARG:HH22	2.31	0.44
1:E:367:VAL:O	1:E:368:ARG:HD3	2.17	0.44
1:E:534:GLU:OE2	1:G:534:GLU:HG3	2.17	0.44
1:C:201:HIS:O	1:C:740:GLY:HA2	2.17	0.44
1:E:965:SER:O	1:E:968:ASP:N	2.50	0.44
1:I:54:ILE:HA	1:I:62:TRP:O	2.18	0.44
1:I:605:GLU:HG2	1:K:524:PRO:HD3	1.98	0.44
1:C:872:HIS:HE1	1:C:902:GLU:OE1	2.00	0.44
1:E:489:LYS:HG3	1:E:491:PHE:CE1	2.52	0.44
1:I:986:ARG:HD2	1:I:1025:TYR:O	2.17	0.44
1:K:155:PRO:O	1:K:856:ARG:HD2	2.17	0.44
1:G:568:LEU:HD23	1:G:568:LEU:N	2.32	0.44
1:A:253:GLN:HA	1:A:253:GLN:NE2	2.33	0.44
1:K:390:TYR:CD1	1:K:397:ALA:HB2	2.49	0.44
1:C:618:VAL:HG21	1:C:631:GLU:HG3	1.98	0.44
1:G:965:SER:C	1:G:967:GLY:N	2.70	0.44
1:A:565:GLU:HG2	1:A:566:TYR:H	1.81	0.44
1:E:45:ASN:HA	1:E:277:HIS:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:501:TYR:CD2	1:E:501:TYR:N	2.86	0.44
1:I:253:GLN:NE2	1:I:268:THR:OG1	2.49	0.44
1:I:73:LYS:HD3	1:I:76:SER:CB	2.42	0.44
1:G:586:ARG:NE	2:H:1206:ALA:HB3	2.32	0.44
1:G:1016:ARG:HA	4:G:1099:HOH:O	2.17	0.44
1:E:222:PHE:H	1:E:1038:HIS:CD2	2.36	0.44
1:K:337:ILE:HD11	4:K:1165:HOH:O	2.17	0.44
1:C:1008:GLN:NE2	4:C:1190:HOH:O	2.50	0.44
1:K:800:ILE:CG2	1:K:845:ARG:HH22	2.30	0.44
1:I:800:ILE:CG2	1:I:845:ARG:HH22	2.30	0.44
1:K:407:VAL:HG13	1:K:421:VAL:HG13	2.00	0.44
1:G:57:CYS:HB3	1:G:62:TRP:NE1	2.33	0.44
1:A:272:ASP:O	1:A:717:LYS:HE2	2.17	0.44
1:A:525:ASP:OD1	1:C:532:SER:HB2	2.18	0.44
1:I:992:VAL:HG11	1:I:1009:PRO:HB2	2.00	0.44
1:I:205:TYR:HA	1:I:1024:ASN:HD21	1.83	0.44
1:E:295:ILE:O	1:E:303:ILE:HA	2.18	0.44
1:E:268:THR:HG22	1:E:303:ILE:CD1	2.47	0.44
1:A:53:ILE:HD12	1:A:66:LEU:HD21	1.99	0.44
1:E:909:ILE:HG12	1:E:956:ILE:HG21	1.99	0.44
1:E:633:LYS:HE2	1:E:633:LYS:HB2	1.84	0.44
1:I:225:ILE:HG13	1:I:226:VAL:HG23	1.99	0.44
1:I:272:ASP:O	1:I:717:LYS:HE2	2.18	0.44
1:G:202:TRP:CH2	1:G:745:SER:HB3	2.53	0.44
1:C:687:LEU:HA	1:C:687:LEU:HD23	1.86	0.44
1:K:440:VAL:CB	4:K:1100:HOH:O	2.66	0.43
1:E:516:SER:HB3	1:E:518:ARG:HG3	1.99	0.43
1:K:297:ASN:O	1:K:301:GLU:N	2.49	0.43
1:E:591:LEU:HD12	1:E:596:LEU:CD2	2.48	0.43
1:I:781:ALA:CB	1:I:802:PRO:HG2	2.48	0.43
1:C:363:ARG:HD3	1:C:363:ARG:HA	1.55	0.43
1:A:965:SER:O	1:A:968:ASP:N	2.50	0.43
1:C:546:PRO:CG	1:C:567:ASP:HB3	2.48	0.43
1:G:134:PHE:HB2	4:G:1094:HOH:O	2.18	0.43
1:I:534:GLU:OE2	1:K:534:GLU:HG3	2.17	0.43
1:I:524:PRO:HD3	1:K:605:GLU:HG2	1.99	0.43
1:A:897:ARG:NH1	4:A:1146:HOH:O	2.43	0.43
1:A:407:VAL:HG13	1:A:421:VAL:HG13	1.98	0.43
1:E:469:HIS:ND1	1:G:901:ASN:HB3	2.32	0.43
1:C:59:ASP:HB3	1:C:80:VAL:HA	2.00	0.43
1:G:272:ASP:O	1:G:717:LYS:HE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:829:ALA:HA	1:K:851:ILE:HG22	2.00	0.43
1:E:528:VAL:HG21	1:E:896:TYR:CD2	2.53	0.43
1:K:1001:ILE:HG12	4:K:1180:HOH:O	2.18	0.43
1:A:557:ARG:HH22	1:A:562:GLU:H	1.66	0.43
1:E:823:ARG:O	1:E:826:SER:HB3	2.17	0.43
1:C:201:HIS:HB3	1:C:736:VAL:HG13	2.00	0.43
1:A:701:TYR:O	1:C:939:ARG:HD3	2.18	0.43
1:C:428:ILE:HD13	1:C:429:MET:N	2.33	0.43
1:A:487:GLY:HA3	1:A:489:LYS:NZ	2.33	0.43
1:K:622:TYR:OH	1:K:627:ARG:HG2	2.18	0.43
1:G:1053:ASP:OD2	4:G:1223:HOH:O	2.21	0.43
1:E:906:GLN:O	1:E:953:GLY:HA3	2.18	0.43
1:E:183:ILE:HD12	1:E:192:ILE:HD13	1.99	0.43
1:K:195:ASN:O	1:K:231:HIS:HE1	2.02	0.43
1:C:407:VAL:HG13	1:C:421:VAL:HG13	1.99	0.43
1:C:313:SER:O	1:I:117:GLU:HA	2.17	0.43
1:A:921:SER:HB3	1:A:966:ASP:OD2	2.18	0.43
1:E:881:TYR:O	1:E:898:LEU:HD23	2.18	0.43
1:E:992:VAL:HG11	1:E:1009:PRO:HB2	2.00	0.43
1:I:659:THR:O	1:I:668:GLU:HA	2.18	0.43
1:E:922:GLN:HB3	1:G:946:TYR:CE1	2.53	0.43
1:A:222:PHE:HB2	1:A:1038:HIS:HD2	1.82	0.43
1:A:190:ARG:NH2	1:A:222:PHE:HZ	2.16	0.43
1:A:744:THR:HG22	1:A:745:SER:N	2.33	0.43
1:E:184:LEU:HD13	1:E:237:ILE:HG13	2.00	0.43
1:E:921:SER:HB2	1:E:970:PHE:HB2	2.00	0.43
1:I:406:ASN:HB2	1:I:424:ASP:CG	2.39	0.43
1:A:532:SER:HB2	1:C:525:ASP:OD1	2.17	0.43
1:I:579:ASN:HD22	1:I:627:ARG:HH22	1.66	0.43
1:I:474:GLY:HA2	1:K:945:PRO:HD2	2.01	0.43
1:G:297:ASN:C	1:G:297:ASN:HD22	2.21	0.43
1:G:253:GLN:NE2	1:G:268:THR:OG1	2.50	0.43
1:G:558:SER:O	1:K:393:ARG:HG3	2.18	0.43
1:I:922:GLN:NE2	1:K:948:THR:H	2.15	0.43
1:E:322:PRO:HG2	1:E:674:ASP:OD1	2.18	0.43
1:E:423:ASN:ND2	1:E:427:GLU:H	2.16	0.43
1:E:462:ALA:HA	1:E:481:HIS:O	2.17	0.43
1:K:45:ASN:HA	1:K:277:HIS:CD2	2.53	0.43
1:E:962:TYR:HA	4:E:1167:HOH:O	2.17	0.43
1:A:501:TYR:CD2	1:A:501:TYR:N	2.86	0.43
1:A:562:GLU:HB3	1:A:563:ALA:H	1.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:563:ALA:N	4:C:1164:HOH:O	2.50	0.43
1:K:965:SER:HA	1:K:990:GLY:O	2.19	0.43
1:K:307:GLU:N	4:K:1177:HOH:O	2.50	0.43
1:G:499:HIS:HD1	1:G:517:TYR:HD2	1.65	0.43
1:I:245:ILE:HD11	1:I:278:LEU:HG	2.00	0.43
1:E:524:PRO:HD3	1:G:605:GLU:HG2	1.99	0.43
1:K:688:GLN:HA	4:K:1161:HOH:O	2.17	0.43
1:G:1002:ASP:OD1	1:G:1004:THR:OG1	2.31	0.43
1:E:451:ASP:OD1	2:F:1205:LYS:HD2	2.18	0.43
1:G:581:ASP:HB2	4:G:1149:HOH:O	2.18	0.43
1:E:981:LYS:HE2	4:E:1168:HOH:O	2.19	0.43
1:A:229:SER:HB3	1:A:248:ILE:CD1	2.48	0.43
1:A:234:SER:HB3	1:A:278:LEU:H	1.83	0.43
1:G:633:LYS:HE2	1:G:633:LYS:HB2	1.82	0.43
1:G:228:MET:HE1	1:G:244:PHE:CE1	2.54	0.43
1:K:840:LYS:O	1:K:843:ASP:HB2	2.19	0.43
1:G:927:LYS:HD3	4:G:1128:HOH:O	2.18	0.43
1:C:452:PHE:HB3	1:C:463:TYR:HB3	1.99	0.43
1:E:236:VAL:HG23	1:E:243:TYR:HB2	2.00	0.43
1:I:279:ASN:HA	1:I:279:ASN:HD22	1.72	0.43
4:E:1181:HOH:O	1:G:525:ASP:CG	2.57	0.43
1:E:586:ARG:HH21	2:F:1204:GLN:HB3	1.84	0.43
1:E:53:ILE:CG2	1:E:286:LEU:HD21	2.46	0.43
1:E:82:ASN:HD22	1:E:82:ASN:N	2.13	0.43
1:C:82:ASN:HD22	1:C:82:ASN:N	2.12	0.43
1:K:222:PHE:H	1:K:1038:HIS:CD2	2.37	0.43
1:G:363:ARG:HD3	1:G:363:ARG:HA	1.50	0.43
1:K:628:LYS:HA	4:K:1181:HOH:O	2.19	0.43
1:A:313:SER:O	1:G:117:GLU:HA	2.19	0.43
1:E:360:GLU:HG3	1:E:377:PHE:CZ	2.53	0.43
1:K:727:THR:O	1:K:730:ASP:HB2	2.18	0.43
1:K:635:ASN:HB3	1:K:653:ASP:OD1	2.19	0.43
1:A:92:LYS:HA	1:A:111:TYR:O	2.19	0.43
1:E:886:ASP:O	1:E:891:GLY:HA3	2.19	0.43
1:G:800:ILE:CG2	1:G:845:ARG:HH22	2.30	0.43
1:K:428:ILE:HG22	1:K:442:GLU:O	2.18	0.43
1:E:467:LEU:HD11	1:E:496:GLU:HB2	2.00	0.43
1:K:467:LEU:HD11	1:K:496:GLU:HB2	2.01	0.43
1:K:327:GLU:O	1:K:328:ASP:O	2.37	0.43
1:C:501:TYR:N	1:C:501:TYR:CD2	2.86	0.43
1:K:153:MET:HE2	1:K:153:MET:HB2	1.93	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1033:ILE:HD11	1:E:1050:TYR:CD2	2.54	0.43
1:A:735:ILE:O	1:A:739:GLN:HG3	2.18	0.43
1:A:681:SER:O	1:A:684:GLU:HG2	2.18	0.43
1:K:988:TRP:CZ3	1:K:990:GLY:HA3	2.54	0.43
1:A:727:THR:HG22	4:A:1092:HOH:O	2.19	0.43
1:E:390:TYR:CD1	1:E:397:ALA:HB2	2.52	0.43
1:I:498:SER:OG	1:I:518:ARG:HG2	2.18	0.43
1:K:841:GLY:C	1:K:843:ASP:H	2.22	0.43
1:G:884:ILE:HB	1:G:912:VAL:HG12	2.01	0.43
1:G:467:LEU:HD11	1:G:496:GLU:HB2	2.01	0.43
1:A:568:LEU:HD23	1:A:568:LEU:N	2.33	0.43
1:K:562:GLU:O	1:K:563:ALA:HB3	2.18	0.43
1:C:731:LEU:HD22	1:C:735:ILE:CD1	2.49	0.43
1:G:781:ALA:CB	1:G:802:PRO:HG2	2.49	0.43
1:C:841:GLY:C	1:C:843:ASP:H	2.21	0.43
1:K:725:CYS:SG	1:K:730:ASP:HB3	2.59	0.43
1:K:92:LYS:HA	1:K:111:TYR:O	2.19	0.43
1:A:829:ALA:HB3	4:A:1132:HOH:O	2.18	0.43
1:E:780:LYS:HD3	1:E:782:TYR:CZ	2.54	0.43
1:E:1055:LEU:O	1:E:1059:LEU:HD13	2.19	0.43
1:C:562:GLU:HB3	1:C:563:ALA:H	1.59	0.42
1:C:616:LYS:HE2	1:C:653:ASP:CB	2.49	0.42
1:I:183:ILE:HD12	1:I:192:ILE:HD13	2.00	0.42
1:G:390:TYR:CD1	1:G:397:ALA:HB2	2.50	0.42
1:C:649:MET:HE3	1:C:649:MET:HB2	1.75	0.42
1:C:234:SER:HB3	1:C:278:LEU:H	1.84	0.42
1:C:423:ASN:ND2	1:C:427:GLU:H	2.17	0.42
1:E:131:ARG:NH2	1:E:131:ARG:HG2	2.34	0.42
1:G:704:GLU:CD	4:G:1110:HOH:O	2.58	0.42
1:C:514:TYR:HE1	4:C:1106:HOH:O	2.02	0.42
1:A:1002:ASP:OD1	1:A:1004:THR:OG1	2.35	0.42
1:K:1045:ASP:HB3	1:K:1048:ILE:HG22	2.01	0.42
1:C:906:GLN:O	1:C:953:GLY:HA3	2.18	0.42
1:E:123:TYR:HB3	4:E:1135:HOH:O	2.18	0.42
1:C:253:GLN:HG3	1:C:266:LYS:HE2	2.00	0.42
1:K:498:SER:OG	1:K:518:ARG:HG2	2.19	0.42
1:A:471:GLU:HG3	1:A:471:GLU:O	2.19	0.42
1:G:591:LEU:HD12	1:G:596:LEU:CD2	2.46	0.42
1:E:912:VAL:HG11	1:E:970:PHE:CE2	2.54	0.42
1:A:786:TYR:CZ	1:C:573:LYS:HE2	2.53	0.42
1:G:502:ALA:HB1	4:G:1078:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:540:PHE:HA	1:K:577:PRO:HA	2.01	0.42
1:G:886:ASP:O	1:G:891:GLY:HA3	2.18	0.42
1:G:533:PHE:HB3	1:G:536:VAL:HG11	2.01	0.42
1:K:471:GLU:O	1:K:471:GLU:HG3	2.18	0.42
1:G:53:ILE:HD12	1:G:66:LEU:HD21	2.00	0.42
1:A:586:ARG:NE	2:B:1206:ALA:HB3	2.32	0.42
1:I:586:ARG:HH21	2:J:1204:GLN:HB3	1.85	0.42
1:K:956:ILE:O	1:K:956:ILE:CG2	2.68	0.42
1:A:800:ILE:CG2	1:A:845:ARG:HH22	2.31	0.42
1:E:287:PHE:CZ	1:E:294:TYR:HB2	2.54	0.42
1:I:312:GLU:HG2	1:I:314:PRO:HD3	2.01	0.42
1:A:710:ILE:O	1:A:714:ILE:HG12	2.19	0.42
1:G:242:ILE:O	1:G:256:SER:HA	2.19	0.42
1:E:378:ILE:HD11	1:E:410:MET:HG3	2.01	0.42
1:E:308:ILE:CG2	1:E:311:LEU:HD13	2.49	0.42
1:C:318:ILE:HG21	1:C:682:ILE:HD11	1.99	0.42
1:C:195:ASN:O	1:C:231:HIS:HE1	2.03	0.42
1:I:1033:ILE:HD11	1:I:1050:TYR:CD2	2.54	0.42
1:A:544:LEU:N	4:A:1144:HOH:O	2.52	0.42
1:A:884:ILE:HB	1:A:912:VAL:HG12	2.01	0.42
1:I:201:HIS:HB3	1:I:736:VAL:HG13	2.01	0.42
1:C:167:ASN:HB2	1:C:170:ILE:CB	2.42	0.42
1:I:87:PHE:HB3	1:I:88:PRO:CD	2.46	0.42
1:E:87:PHE:HB3	1:E:88:PRO:CD	2.48	0.42
1:K:190:ARG:NH2	1:K:222:PHE:HZ	2.18	0.42
1:K:229:SER:HB3	1:K:248:ILE:CD1	2.48	0.42
1:G:988:TRP:CZ3	1:G:990:GLY:HA3	2.54	0.42
1:K:442:GLU:OE2	1:K:481:HIS:HD2	2.02	0.42
1:C:360:GLU:OE2	1:C:361:PRO:HD2	2.19	0.42
1:C:98:MET:HE3	1:C:103:LEU:HD13	2.02	0.42
1:K:123:TYR:OH	1:K:823:ARG:HD3	2.19	0.42
1:C:959:THR:O	1:C:984:GLY:HA3	2.18	0.42
1:I:412:VAL:HG13	1:I:433:LEU:HD11	2.02	0.42
1:A:922:GLN:NE2	1:C:529:LEU:HD23	2.33	0.42
1:E:412:VAL:HG13	1:E:433:LEU:HD11	2.01	0.42
1:K:982:LEU:C	1:K:983:ILE:HD12	2.40	0.42
1:C:53:ILE:HD12	1:C:66:LEU:HD21	2.01	0.42
1:G:82:ASN:HD21	1:G:96:ARG:HH21	1.66	0.42
1:C:222:PHE:H	1:C:1038:HIS:CD2	2.37	0.42
1:G:131:ARG:HG2	1:G:131:ARG:H	1.61	0.42
1:A:955:ILE:HG22	1:A:956:ILE:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:885:PRO:HG2	1:A:890:MET:HG2	2.00	0.42
1:C:537:SER:HB3	1:C:583:GLY:O	2.19	0.42
1:A:886:ASP:O	1:A:891:GLY:HA3	2.20	0.42
1:K:482:VAL:HG23	1:K:493:ALA:HB2	2.02	0.42
1:E:744:THR:HG22	1:E:745:SER:N	2.34	0.42
1:A:545:ILE:O	1:A:548:SER:HB2	2.19	0.42
1:K:886:ASP:O	1:K:891:GLY:HA3	2.18	0.42
1:I:904:SER:OG	1:K:473:ASP:HA	2.19	0.42
1:K:300:THR:HG22	1:K:300:THR:O	2.19	0.42
1:A:295:ILE:O	1:A:303:ILE:HA	2.19	0.42
1:A:649:MET:HB2	1:A:649:MET:HE3	1.75	0.42
1:C:909:ILE:HG12	1:C:956:ILE:HG21	2.01	0.42
1:A:287:PHE:CZ	1:A:294:TYR:HB2	2.55	0.42
1:I:327:GLU:O	1:I:328:ASP:O	2.36	0.42
1:C:986:ARG:HD2	1:C:1025:TYR:O	2.19	0.42
1:A:823:ARG:O	1:A:826:SER:HB3	2.19	0.42
1:E:422:ALA:HB1	4:E:1087:HOH:O	2.19	0.42
1:E:984:GLY:N	4:E:1123:HOH:O	2.53	0.42
1:C:471:GLU:O	1:C:471:GLU:HG3	2.19	0.42
1:E:393:ARG:HG3	1:I:558:SER:O	2.19	0.42
1:G:499:HIS:CE1	4:H:885:HOH:O	2.73	0.42
1:C:955:ILE:HG22	1:C:956:ILE:N	2.33	0.42
1:C:541:VAL:CG2	1:C:542:ILE:N	2.83	0.42
1:G:423:ASN:ND2	1:G:427:GLU:H	2.17	0.42
1:E:841:GLY:C	1:E:843:ASP:H	2.23	0.42
1:A:98:MET:HE3	1:A:103:LEU:HD13	2.01	0.42
1:E:203:LYS:O	1:E:743:ARG:HG2	2.18	0.42
1:E:1036:ALA:O	1:E:1039:ASP:HB2	2.19	0.42
1:G:535:VAL:HG23	1:G:535:VAL:O	2.19	0.42
1:C:61:LEU:HB3	1:C:75:VAL:CG1	2.46	0.42
1:I:190:ARG:NH2	1:I:222:PHE:CZ	2.88	0.42
1:K:965:SER:O	1:K:968:ASP:N	2.52	0.42
1:E:319:ILE:CG2	1:E:677:PRO:HB3	2.49	0.42
1:G:809:ASP:HA	1:G:815:VAL:HG22	2.02	0.42
1:A:641:LEU:HD22	1:A:645:ARG:HA	2.00	0.42
1:G:487:GLY:HA3	1:G:489:LYS:NZ	2.34	0.42
1:K:641:LEU:HD23	1:K:647:THR:O	2.19	0.42
1:G:236:VAL:HG23	1:G:243:TYR:HB2	2.02	0.42
1:G:54:ILE:HA	1:G:62:TRP:O	2.20	0.42
1:E:428:ILE:HG22	1:E:442:GLU:O	2.20	0.42
1:A:901:ASN:HB3	1:C:469:HIS:ND1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:181:THR:HG22	1:G:182:HIS:CE1	2.55	0.42
1:K:746:HIS:HE1	1:K:990:GLY:O	2.03	0.42
1:I:322:PRO:HG2	1:I:674:ASP:OD1	2.20	0.42
1:G:287:PHE:CZ	1:G:294:TYR:HB2	2.55	0.42
1:C:287:PHE:CZ	1:C:294:TYR:HB2	2.54	0.42
1:C:308:ILE:HD12	1:C:308:ILE:N	2.35	0.42
1:A:406:ASN:O	1:A:423:ASN:HA	2.19	0.42
1:A:124:PHE:HB3	1:A:152:ALA:HB1	2.01	0.42
1:K:676:ARG:CD	4:K:1169:HOH:O	2.68	0.42
1:G:887:MET:HB2	1:G:917:GLY:C	2.40	0.42
1:E:901:ASN:HB3	1:G:469:HIS:ND1	2.35	0.42
1:G:327:GLU:O	1:G:328:ASP:O	2.38	0.42
1:G:867:ASN:HD22	1:G:867:ASN:HA	1.64	0.42
1:G:104:ASN:H	1:G:104:ASN:ND2	2.18	0.42
1:E:533:PHE:HB3	1:E:536:VAL:HG11	2.00	0.42
1:E:329:PHE:HD1	1:E:649:MET:SD	2.43	0.42
1:I:921:SER:HB3	1:I:966:ASP:OD2	2.19	0.42
1:I:579:ASN:HD22	1:I:627:ARG:NH2	2.16	0.42
1:I:939:ARG:HD3	1:K:701:TYR:O	2.19	0.42
1:G:716:GLU:HB3	4:G:1142:HOH:O	2.19	0.42
1:C:197:PHE:HE1	1:C:199:LEU:HD21	1.85	0.42
1:K:489:LYS:HG3	1:K:491:PHE:CE1	2.55	0.42
1:I:881:TYR:O	1:I:898:LEU:HD23	2.20	0.42
1:E:178:GLY:HA3	1:E:1040:TYR:CD1	2.54	0.42
1:C:591:LEU:HD12	1:C:596:LEU:CD2	2.48	0.41
1:E:110:PHE:CE2	1:E:121:ILE:HG13	2.55	0.41
1:C:887:MET:HG3	1:C:966:ASP:OD2	2.20	0.41
1:C:744:THR:HG22	1:C:745:SER:N	2.35	0.41
1:K:687:LEU:HD22	1:K:719:ARG:NH2	2.35	0.41
1:K:780:LYS:CE	4:K:1214:HOH:O	2.67	0.41
1:A:1014:TRP:CD1	1:A:1019:GLY:HA2	2.55	0.41
1:K:480:ILE:N	1:K:494:THR:CG2	2.67	0.41
1:K:586:ARG:HH21	2:L:1204:GLN:HB3	1.84	0.41
1:K:403:ASN:HD22	1:K:405:GLY:H	1.67	0.41
1:I:530:ASN:ND2	1:I:531:PHE:N	2.64	0.41
1:A:591:LEU:HD12	1:A:596:LEU:CD2	2.48	0.41
1:E:677:PRO:HD2	1:K:827:GLU:O	2.21	0.41
1:E:287:PHE:CE1	1:E:294:TYR:HB2	2.55	0.41
1:E:367:VAL:CG1	1:E:375:VAL:HG21	2.50	0.41
1:A:410:MET:HG2	1:A:421:VAL:HG22	2.01	0.41
1:A:91:ARG:HG3	1:A:91:ARG:HH21	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:61:LEU:HB3	1:I:75:VAL:CG1	2.49	0.41
1:A:703:ASN:HD22	1:A:704:GLU:N	2.18	0.41
1:G:929:MET:CE	4:G:1084:HOH:O	2.67	0.41
1:E:401:GLU:CD	1:E:401:GLU:N	2.73	0.41
1:G:387:LEU:HD12	1:G:400:PHE:CE1	2.55	0.41
1:E:406:ASN:O	1:E:423:ASN:HA	2.20	0.41
1:E:618:VAL:HG21	1:E:631:GLU:HG3	2.02	0.41
1:E:988:TRP:CZ3	1:E:990:GLY:HA3	2.55	0.41
1:E:872:HIS:CE1	1:E:902:GLU:OE1	2.72	0.41
1:C:225:ILE:HG13	1:C:226:VAL:HG23	2.02	0.41
1:A:57:CYS:HB3	1:A:62:TRP:NE1	2.35	0.41
1:A:225:ILE:HG13	1:A:226:VAL:HG23	2.02	0.41
1:I:92:LYS:HA	1:I:111:TYR:O	2.21	0.41
1:A:195:ASN:O	1:A:231:HIS:HE1	2.03	0.41
1:G:300:THR:O	1:G:300:THR:HG22	2.19	0.41
1:E:53:ILE:HG23	1:E:286:LEU:CD2	2.45	0.41
1:A:586:ARG:HH21	2:B:1204:GLN:HB3	1.85	0.41
1:K:965:SER:C	1:K:967:GLY:N	2.72	0.41
1:K:781:ALA:CB	1:K:802:PRO:HG2	2.50	0.41
1:K:234:SER:CB	1:K:278:LEU:H	2.33	0.41
1:C:579:ASN:HA	4:C:1171:HOH:O	2.20	0.41
1:G:360:GLU:HG3	1:G:377:PHE:CZ	2.56	0.41
1:K:272:ASP:O	1:K:717:LYS:HE2	2.21	0.41
1:G:498:SER:OG	1:G:518:ARG:HG2	2.21	0.41
1:I:981:LYS:HA	1:I:981:LYS:HD3	1.87	0.41
1:G:178:GLY:HA3	1:G:1040:TYR:CD1	2.56	0.41
1:I:469:HIS:CE1	1:K:901:ASN:HB3	2.55	0.41
1:E:253:GLN:HE21	1:E:253:GLN:HA	1.85	0.41
1:G:73:LYS:HD3	1:G:76:SER:CB	2.45	0.41
1:A:591:LEU:CD1	1:A:662:LEU:HD21	2.50	0.41
1:A:909:ILE:HG12	1:A:956:ILE:HG21	1.99	0.41
1:K:363:ARG:HA	1:K:363:ARG:HD3	1.51	0.41
1:E:994:ILE:HG22	1:E:1008:GLN:O	2.19	0.41
1:A:948:THR:H	1:C:922:GLN:NE2	2.17	0.41
1:C:367:VAL:CG1	1:C:375:VAL:HG21	2.50	0.41
1:G:887:MET:HG3	1:G:966:ASP:OD2	2.21	0.41
1:K:369:ARG:NH2	4:K:1160:HOH:O	2.53	0.41
1:C:829:ALA:HA	1:C:851:ILE:HG22	2.02	0.41
1:C:467:LEU:HD11	1:C:496:GLU:HB2	2.03	0.41
1:K:224:LYS:HD2	1:K:227:ASP:HB2	2.02	0.41
1:E:1045:ASP:HB3	1:E:1048:ILE:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:327:GLU:O	1:E:328:ASP:O	2.38	0.41
1:C:568:LEU:HD23	1:C:568:LEU:N	2.35	0.41
1:I:167:ASN:HB2	1:I:170:ILE:CB	2.43	0.41
1:G:649:MET:HB2	1:G:649:MET:HE3	1.79	0.41
1:A:809:ASP:HA	1:A:815:VAL:HG22	2.03	0.41
1:G:977:LEU:HB3	4:G:1084:HOH:O	2.21	0.41
1:I:809:ASP:HA	1:I:815:VAL:HG22	2.02	0.41
1:C:840:LYS:O	1:C:843:ASP:HB2	2.21	0.41
1:I:633:LYS:HE2	1:I:633:LYS:HB2	1.82	0.41
1:A:965:SER:O	1:A:968:ASP:HB2	2.21	0.41
1:C:327:GLU:HG3	1:C:340:VAL:HG12	2.02	0.41
1:C:579:ASN:HD22	1:C:627:ARG:NH2	2.17	0.41
1:E:469:HIS:CE1	1:G:901:ASN:HB3	2.56	0.41
1:E:360:GLU:OE2	1:E:361:PRO:HD2	2.20	0.41
1:I:48:ILE:HG12	1:I:49:HIS:N	2.36	0.41
1:C:268:THR:HG22	1:C:303:ILE:CD1	2.51	0.41
1:C:53:ILE:HG23	1:C:286:LEU:CD2	2.47	0.41
1:G:703:ASN:C	1:G:703:ASN:ND2	2.67	0.41
1:I:676:ARG:HA	1:I:677:PRO:HD3	1.90	0.41
1:A:541:VAL:CG2	1:A:542:ILE:N	2.84	0.41
1:E:885:PRO:CG	1:E:890:MET:HG2	2.51	0.41
1:E:226:VAL:CG1	1:E:228:MET:HE3	2.51	0.41
1:E:54:ILE:HA	1:E:62:TRP:O	2.21	0.41
1:E:534:GLU:HG3	1:G:534:GLU:OE2	2.21	0.41
1:K:744:THR:HG22	1:K:745:SER:N	2.36	0.41
1:G:344:GLN:OE1	1:G:357:LYS:HE3	2.21	0.41
1:A:622:TYR:OH	1:A:627:ARG:HG2	2.21	0.41
1:G:569:ASN:HA	4:G:1137:HOH:O	2.20	0.41
1:K:99:ARG:NH1	4:K:1135:HOH:O	2.51	0.41
1:E:515:LEU:HD23	1:E:539:PRO:HA	2.02	0.41
1:G:501:TYR:N	1:G:501:TYR:CD2	2.88	0.41
1:I:501:TYR:CD2	1:I:501:TYR:N	2.88	0.41
1:C:153:MET:HB2	1:C:153:MET:HE2	1.93	0.41
1:A:555:VAL:HG13	1:I:354:TYR:CE2	2.56	0.41
1:I:296:PHE:HD1	1:I:303:ILE:HG12	1.85	0.41
1:I:190:ARG:HH21	1:I:222:PHE:HZ	1.68	0.41
1:A:53:ILE:CG2	1:A:286:LEU:HD21	2.49	0.41
1:A:236:VAL:HG23	1:A:243:TYR:HB2	2.02	0.41
1:C:641:LEU:HD22	1:C:645:ARG:HA	2.01	0.41
1:I:234:SER:CB	1:I:278:LEU:H	2.34	0.41
1:A:635:ASN:HB3	1:A:653:ASP:OD1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:823:ARG:O	1:G:826:SER:HB3	2.20	0.41
1:E:351:SER:O	1:E:672:GLU:HB2	2.21	0.41
1:E:746:HIS:CE1	4:E:1083:HOH:O	2.73	0.41
1:E:253:GLN:NE2	1:E:268:THR:OG1	2.51	0.41
1:C:295:ILE:O	1:C:303:ILE:HA	2.20	0.41
1:G:337:ILE:HD13	1:G:350:VAL:HG12	2.03	0.41
1:C:809:ASP:HA	1:C:815:VAL:HG22	2.03	0.41
1:I:319:ILE:CG2	1:I:677:PRO:HB3	2.51	0.41
1:G:312:GLU:HG2	1:G:314:PRO:HD3	2.02	0.41
1:A:423:ASN:ND2	1:A:427:GLU:H	2.19	0.41
1:A:387:LEU:HD12	1:A:400:PHE:CE1	2.56	0.41
1:E:885:PRO:O	1:E:915:ASN:HA	2.21	0.41
1:I:469:HIS:ND1	1:K:901:ASN:HB3	2.36	0.41
1:G:135:THR:HA	1:G:149:SER:O	2.21	0.41
1:A:1048:ILE:O	1:A:1052:ILE:HG13	2.21	0.41
1:G:452:PHE:HB3	1:G:463:TYR:HB3	2.02	0.41
1:K:958:ILE:HD11	1:K:1051:ALA:CB	2.50	0.41
1:I:841:GLY:C	1:I:843:ASP:H	2.25	0.41
1:C:92:LYS:HA	1:C:111:TYR:O	2.21	0.41
1:A:178:GLY:HA3	1:A:1040:TYR:CD1	2.55	0.41
1:G:48:ILE:HG12	1:G:49:HIS:N	2.34	0.41
1:E:639:LEU:C	1:E:639:LEU:HD23	2.41	0.41
1:K:205:TYR:HA	1:K:1024:ASN:HD21	1.85	0.41
1:E:204:GLY:O	1:E:206:ARG:HG3	2.21	0.41
1:C:676:ARG:HA	1:C:677:PRO:HD3	1.94	0.41
1:A:218:ASN:O	1:A:219:SER:C	2.59	0.41
1:C:781:ALA:CB	1:C:802:PRO:HG2	2.50	0.41
1:G:307:GLU:HA	1:G:307:GLU:OE2	2.21	0.41
1:I:367:VAL:HG12	1:I:375:VAL:CG2	2.51	0.41
1:K:618:VAL:HG21	1:K:631:GLU:HG3	2.02	0.41
1:K:367:VAL:CG1	1:K:375:VAL:HG21	2.51	0.41
1:I:294:TYR:CE2	1:I:305:LYS:HB2	2.55	0.41
1:I:410:MET:HG2	1:I:421:VAL:HG22	2.03	0.41
1:E:98:MET:HE3	1:E:103:LEU:HD13	2.03	0.41
1:K:332:LEU:HD11	1:K:338:ALA:HB2	2.03	0.41
1:C:131:ARG:HH21	1:C:131:ARG:HG2	1.86	0.41
1:I:374:LYS:HG3	4:I:1210:HOH:O	2.20	0.41
1:G:190:ARG:HH21	1:G:222:PHE:HZ	1.70	0.40
1:E:296:PHE:HD1	1:E:303:ILE:HG12	1.86	0.40
1:A:73:LYS:HD3	1:A:76:SER:CB	2.43	0.40
1:K:87:PHE:HB3	1:K:88:PRO:CD	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:649:MET:HE3	1:E:649:MET:HB2	1.81	0.40
1:I:994:ILE:HG22	1:I:1008:GLN:O	2.21	0.40
1:K:956:ILE:HG23	1:K:956:ILE:O	2.21	0.40
1:A:957:ALA:HB3	1:A:982:LEU:HD12	2.03	0.40
1:A:401:GLU:N	1:A:401:GLU:CD	2.75	0.40
1:A:184:LEU:HD13	1:A:237:ILE:HG13	2.02	0.40
1:C:141:ASP:C	1:C:141:ASP:OD2	2.60	0.40
1:K:423:ASN:ND2	1:K:427:GLU:H	2.19	0.40
1:I:965:SER:C	1:I:967:GLY:N	2.74	0.40
1:E:780:LYS:CE	4:E:1130:HOH:O	2.69	0.40
1:I:228:MET:HE1	1:I:244:PHE:CE1	2.57	0.40
1:A:59:ASP:HB3	1:A:80:VAL:HA	2.03	0.40
1:K:204:GLY:O	1:K:206:ARG:HG3	2.21	0.40
1:C:480:ILE:H	1:C:494:THR:HG21	1.81	0.40
1:G:525:ASP:HB3	1:G:528:VAL:O	2.21	0.40
1:I:387:LEU:HB2	1:I:404:LEU:HD11	2.03	0.40
1:A:390:TYR:CD1	1:A:397:ALA:HB2	2.53	0.40
1:I:487:GLY:HA3	1:I:489:LYS:NZ	2.36	0.40
1:K:367:VAL:HG12	1:K:375:VAL:HG21	2.03	0.40
1:I:428:ILE:HG22	1:I:442:GLU:O	2.21	0.40
1:A:1055:LEU:O	1:A:1059:LEU:HD13	2.20	0.40
1:K:1014:TRP:CD1	1:K:1019:GLY:HA2	2.56	0.40
1:A:905:TYR:HB2	4:A:1180:HOH:O	2.21	0.40
1:G:635:ASN:HB3	1:G:653:ASP:OD1	2.22	0.40
1:C:823:ARG:O	1:C:826:SER:HB3	2.21	0.40
1:C:538:LYS:HG2	1:C:539:PRO:HD2	2.03	0.40
1:A:442:GLU:OE2	1:A:481:HIS:HD2	2.03	0.40
1:I:417:LYS:HE3	1:I:417:LYS:HB2	1.99	0.40
1:G:201:HIS:HB3	1:G:736:VAL:HG13	2.02	0.40
1:G:956:ILE:CG2	1:G:956:ILE:O	2.70	0.40
1:C:530:ASN:ND2	1:C:531:PHE:N	2.66	0.40
1:C:633:LYS:HB2	1:C:633:LYS:HE2	1.81	0.40
1:E:202:TRP:CH2	1:E:745:SER:HB3	2.56	0.40
1:G:1052:ILE:O	1:G:1056:ILE:HG13	2.21	0.40
1:G:482:VAL:HG23	1:G:493:ALA:HB2	2.02	0.40
1:A:279:ASN:HD22	1:A:279:ASN:HA	1.79	0.40
1:G:319:ILE:CG2	1:G:677:PRO:HB3	2.48	0.40
1:A:190:ARG:HH21	1:A:222:PHE:HZ	1.69	0.40
1:G:401:GLU:CD	1:G:401:GLU:N	2.75	0.40
1:A:633:LYS:HB2	1:A:633:LYS:HE2	1.87	0.40
1:G:566:TYR:O	4:G:1157:HOH:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:424:ASP:OD2	4:G:1076:HOH:O	2.22	0.40
1:A:579:ASN:HD22	1:A:627:ARG:NH2	2.20	0.40
1:C:881:TYR:O	1:C:898:LEU:HD23	2.20	0.40
1:K:766:ALA:HA	1:K:855:ASP:OD1	2.20	0.40
1:K:294:TYR:CE2	1:K:305:LYS:HB2	2.57	0.40
1:K:1036:ALA:O	1:K:1039:ASP:HB2	2.20	0.40
1:G:579:ASN:HD22	1:G:627:ARG:NH2	2.20	0.40
1:G:378:ILE:HA	1:G:378:ILE:HD13	1.91	0.40
1:I:351:SER:O	1:I:672:GLU:HB2	2.22	0.40
1:E:982:LEU:C	1:E:983:ILE:HD12	2.42	0.40
1:G:913:ARG:HD3	1:G:958:ILE:HG22	2.03	0.40
1:K:1024:ASN:HD22	1:K:1024:ASN:HA	1.68	0.40
1:K:253:GLN:HG3	1:K:266:LYS:HE2	2.04	0.40
1:I:177:LEU:HD13	1:I:192:ILE:HD11	2.03	0.40
1:C:319:ILE:CG2	1:C:677:PRO:HB3	2.51	0.40
1:I:922:GLN:HB3	1:K:946:TYR:CE1	2.56	0.40
1:G:131:ARG:NH2	1:G:131:ARG:HG2	2.37	0.40
1:A:645:ARG:HG3	1:A:645:ARG:HH21	1.86	0.40
1:A:417:LYS:HE3	1:A:417:LYS:HB2	1.99	0.40
1:K:54:ILE:HA	1:K:62:TRP:O	2.21	0.40
1:C:226:VAL:CG1	1:C:228:MET:HE3	2.52	0.40
1:G:462:ALA:HA	1:G:481:HIS:O	2.22	0.40
1:G:1055:LEU:O	1:G:1059:LEU:HD13	2.22	0.40
1:E:776:TYR:CZ	1:E:821:ILE:HG22	2.57	0.40
1:A:153:MET:O	4:A:1130:HOH:O	2.21	0.40
1:G:374:LYS:HG3	4:G:1165:HOH:O	2.21	0.40
1:E:694:TRP:HA	1:E:738:MET:HE1	2.04	0.40
1:C:91:ARG:HG3	1:C:91:ARG:HH21	1.86	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ASN:N	1:I:143:ASP:OD2[2_545]	2.06	0.14
1:C:167:ASN:N	1:G:143:ASP:OD2[2_455]	2.12	0.08

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	1021/1071 (95%)	948 (93%)	67 (7%)	6 (1%)	30	56
1	C	1021/1071 (95%)	947 (93%)	66 (6%)	8 (1%)	24	46
1	E	1021/1071 (95%)	950 (93%)	63 (6%)	8 (1%)	24	46
1	G	1021/1071 (95%)	950 (93%)	63 (6%)	8 (1%)	24	46
1	I	1021/1071 (95%)	949 (93%)	64 (6%)	8 (1%)	24	46
1	K	1021/1071 (95%)	947 (93%)	66 (6%)	8 (1%)	24	46
2	B	9/13 (69%)	4 (44%)	5 (56%)	0	100	100
2	D	9/13 (69%)	4 (44%)	5 (56%)	0	100	100
2	F	9/13 (69%)	6 (67%)	3 (33%)	0	100	100
2	H	9/13 (69%)	5 (56%)	4 (44%)	0	100	100
2	J	9/13 (69%)	6 (67%)	3 (33%)	0	100	100
2	L	9/13 (69%)	5 (56%)	4 (44%)	0	100	100
All	All	6180/6504 (95%)	5721 (93%)	413 (7%)	46 (1%)	26	51

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	219	SER
1	C	219	SER
1	E	219	SER
1	E	1018	ALA
1	G	219	SER
1	G	1018	ALA
1	I	219	SER
1	K	219	SER
1	A	328	ASP
1	A	1018	ALA
1	C	328	ASP
1	C	1018	ALA

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Mol	Chain	Res	Type
1	I	1018	ALA
1	K	1018	ALA
1	E	328	ASP
1	E	562	GLU
1	G	328	ASP
1	G	363	ARG
1	I	328	ASP
1	I	363	ARG
1	I	562	GLU
1	I	579	ASN
1	K	328	ASP
1	K	562	GLU
1	A	363	ARG
1	A	562	GLU
1	C	259	LEU
1	C	363	ARG
1	C	562	GLU
1	E	259	LEU
1	E	363	ARG
1	G	562	GLU
1	G	579	ASN
1	G	919	PHE
1	K	259	LEU
1	A	919	PHE
1	C	919	PHE
1	E	715	TYR
1	E	919	PHE
1	G	259	LEU
1	I	715	TYR
1	K	363	ARG
1	K	919	PHE
1	C	820	ASN
1	I	919	PHE
1	K	715	TYR

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	883/928 (95%)	846 (96%)	37 (4%)	36	65
1	C	883/928 (95%)	846 (96%)	37 (4%)	36	65
1	E	883/928 (95%)	844 (96%)	39 (4%)	35	63
1	G	883/928 (95%)	845 (96%)	38 (4%)	35	64
1	I	883/928 (95%)	845 (96%)	38 (4%)	35	64
1	K	883/928 (95%)	848 (96%)	35 (4%)	38	67
2	B	8/10 (80%)	6 (75%)	2 (25%)	1	1
2	D	8/10 (80%)	6 (75%)	2 (25%)	1	1
2	F	8/10 (80%)	6 (75%)	2 (25%)	1	1
2	H	8/10 (80%)	6 (75%)	2 (25%)	1	1
2	J	8/10 (80%)	6 (75%)	2 (25%)	1	1
2	L	8/10 (80%)	6 (75%)	2 (25%)	1	1
All	All	5346/5628 (95%)	5110 (96%)	236 (4%)	35	63

All (236) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LEU
1	A	59	ASP
1	A	61	LEU
1	A	75	VAL
1	A	82	ASN
1	A	183	ILE
1	A	209	THR
1	A	279	ASN
1	A	297	ASN
1	A	311	LEU
1	A	353	THR
1	A	363	ARG
1	A	368	ARG
1	A	403	ASN
1	A	417	LYS
1	A	423	ASN
1	A	428	ILE
1	A	481	HIS
1	A	562	GLU
1	A	578	ILE
1	A	641	LEU
1	A	651	ARG

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Mol	Chain	Res	Type
1	A	683	HIS
1	A	703	ASN
1	A	731	LEU
1	A	738	MET
1	A	771	LEU
1	A	847	LEU
1	A	856	ARG
1	A	929	MET
1	A	937	ASN
1	A	956	ILE
1	A	965	SER
1	A	1008	GLN
1	A	1015	PHE
1	A	1024	ASN
1	A	1035	TYR
2	B	1204	GLN
2	B	1210	LEU
1	C	44	LEU
1	C	59	ASP
1	C	61	LEU
1	C	75	VAL
1	C	82	ASN
1	C	183	ILE
1	C	209	THR
1	C	279	ASN
1	C	297	ASN
1	C	311	LEU
1	C	353	THR
1	C	363	ARG
1	C	368	ARG
1	C	403	ASN
1	C	417	LYS
1	C	423	ASN
1	C	428	ILE
1	C	481	HIS
1	C	562	GLU
1	C	578	ILE
1	C	641	LEU
1	C	651	ARG
1	C	683	HIS
1	C	703	ASN
1	C	731	LEU

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Mol	Chain	Res	Type
1	C	738	MET
1	C	771	LEU
1	C	809	ASP
1	C	847	LEU
1	C	856	ARG
1	C	929	MET
1	C	937	ASN
1	C	956	ILE
1	C	1008	GLN
1	C	1015	PHE
1	C	1024	ASN
1	C	1035	TYR
2	D	1204	GLN
2	D	1210	LEU
1	E	44	LEU
1	E	59	ASP
1	E	61	LEU
1	E	75	VAL
1	E	82	ASN
1	E	183	ILE
1	E	209	THR
1	E	279	ASN
1	E	295	ILE
1	E	297	ASN
1	E	353	THR
1	E	363	ARG
1	E	368	ARG
1	E	403	ASN
1	E	417	LYS
1	E	423	ASN
1	E	428	ILE
1	E	481	HIS
1	E	562	GLU
1	E	578	ILE
1	E	641	LEU
1	E	651	ARG
1	E	683	HIS
1	E	703	ASN
1	E	731	LEU
1	E	738	MET
1	E	771	LEU
1	E	809	ASP

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Mol	Chain	Res	Type
1	E	819	SER
1	E	847	LEU
1	E	874	ARG
1	E	929	MET
1	E	937	ASN
1	E	938	PRO
1	E	956	ILE
1	E	1008	GLN
1	E	1015	PHE
1	E	1024	ASN
1	E	1035	TYR
2	F	1204	GLN
2	F	1210	LEU
1	G	44	LEU
1	G	59	ASP
1	G	61	LEU
1	G	75	VAL
1	G	82	ASN
1	G	104	ASN
1	G	183	ILE
1	G	209	THR
1	G	279	ASN
1	G	295	ILE
1	G	297	ASN
1	G	353	THR
1	G	363	ARG
1	G	368	ARG
1	G	403	ASN
1	G	417	LYS
1	G	423	ASN
1	G	428	ILE
1	G	481	HIS
1	G	496	GLU
1	G	548	SER
1	G	562	GLU
1	G	578	ILE
1	G	641	LEU
1	G	651	ARG
1	G	703	ASN
1	G	731	LEU
1	G	738	MET
1	G	809	ASP

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Mol	Chain	Res	Type
1	G	847	LEU
1	G	929	MET
1	G	937	ASN
1	G	938	PRO
1	G	956	ILE
1	G	1008	GLN
1	G	1015	PHE
1	G	1024	ASN
1	G	1035	TYR
2	H	1204	GLN
2	H	1210	LEU
1	I	44	LEU
1	I	59	ASP
1	I	61	LEU
1	I	75	VAL
1	I	82	ASN
1	I	183	ILE
1	I	209	THR
1	I	279	ASN
1	I	295	ILE
1	I	297	ASN
1	I	353	THR
1	I	363	ARG
1	I	368	ARG
1	I	403	ASN
1	I	417	LYS
1	I	423	ASN
1	I	428	ILE
1	I	481	HIS
1	I	496	GLU
1	I	548	SER
1	I	562	GLU
1	I	578	ILE
1	I	641	LEU
1	I	651	ARG
1	I	703	ASN
1	I	731	LEU
1	I	738	MET
1	I	771	LEU
1	I	809	ASP
1	I	847	LEU
1	I	874	ARG

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Mol	Chain	Res	Type
1	I	929	MET
1	I	937	ASN
1	I	956	ILE
1	I	1008	GLN
1	I	1015	PHE
1	I	1024	ASN
1	I	1035	TYR
2	J	1204	GLN
2	J	1210	LEU
1	K	44	LEU
1	K	59	ASP
1	K	61	LEU
1	K	75	VAL
1	K	82	ASN
1	K	183	ILE
1	K	209	THR
1	K	279	ASN
1	K	297	ASN
1	K	353	THR
1	K	363	ARG
1	K	368	ARG
1	K	403	ASN
1	K	417	LYS
1	K	423	ASN
1	K	428	ILE
1	K	481	HIS
1	K	562	GLU
1	K	578	ILE
1	K	641	LEU
1	K	651	ARG
1	K	703	ASN
1	K	731	LEU
1	K	738	MET
1	K	809	ASP
1	K	847	LEU
1	K	874	ARG
1	K	929	MET
1	K	937	ASN
1	K	956	ILE
1	K	965	SER
1	K	1008	GLN
1	K	1015	PHE

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Mol	Chain	Res	Type
1	K	1024	ASN
1	K	1035	TYR
2	L	1204	GLN
2	L	1210	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (180) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	HIS
1	A	82	ASN
1	A	167	ASN
1	A	176	ASN
1	A	195	ASN
1	A	253	GLN
1	A	267	HIS
1	A	277	HIS
1	A	279	ASN
1	A	297	ASN
1	A	403	ASN
1	A	423	ASN
1	A	481	HIS
1	A	497	ASN
1	A	511	ASN
1	A	530	ASN
1	A	579	ASN
1	A	603	HIS
1	A	611	GLN
1	A	703	ASN
1	A	733	ASN
1	A	739	GLN
1	A	867	ASN
1	A	872	HIS
1	A	922	GLN
1	A	930	ASN
1	A	949	ASN
1	A	1008	GLN
1	A	1024	ASN
1	A	1038	HIS
1	A	1047	GLN
1	C	64	HIS
1	C	82	ASN
1	C	167	ASN

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Mol	Chain	Res	Type
1	C	176	ASN
1	C	253	GLN
1	C	267	HIS
1	C	279	ASN
1	C	297	ASN
1	C	403	ASN
1	C	423	ASN
1	C	481	HIS
1	C	497	ASN
1	C	511	ASN
1	C	530	ASN
1	C	579	ASN
1	C	603	HIS
1	C	611	GLN
1	C	703	ASN
1	C	733	ASN
1	C	739	GLN
1	C	867	ASN
1	C	872	HIS
1	C	922	GLN
1	C	930	ASN
1	C	949	ASN
1	C	1008	GLN
1	C	1024	ASN
1	C	1038	HIS
1	C	1047	GLN
1	E	64	HIS
1	E	77	ASN
1	E	82	ASN
1	E	167	ASN
1	E	176	ASN
1	E	253	GLN
1	E	267	HIS
1	E	277	HIS
1	E	279	ASN
1	E	297	ASN
1	E	403	ASN
1	E	423	ASN
1	E	481	HIS
1	E	497	ASN
1	E	511	ASN
1	E	530	ASN

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Mol	Chain	Res	Type
1	E	579	ASN
1	E	603	HIS
1	E	611	GLN
1	E	635	ASN
1	E	703	ASN
1	E	733	ASN
1	E	739	GLN
1	E	867	ASN
1	E	872	HIS
1	E	901	ASN
1	E	922	GLN
1	E	930	ASN
1	E	949	ASN
1	E	1008	GLN
1	E	1024	ASN
1	E	1038	HIS
1	E	1047	GLN
1	G	64	HIS
1	G	82	ASN
1	G	176	ASN
1	G	253	GLN
1	G	267	HIS
1	G	277	HIS
1	G	279	ASN
1	G	297	ASN
1	G	403	ASN
1	G	423	ASN
1	G	481	HIS
1	G	497	ASN
1	G	499	HIS
1	G	511	ASN
1	G	530	ASN
1	G	603	HIS
1	G	611	GLN
1	G	635	ASN
1	G	703	ASN
1	G	739	GLN
1	G	867	ASN
1	G	872	HIS
1	G	922	GLN
1	G	930	ASN
1	G	949	ASN

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Mol	Chain	Res	Type
1	G	1008	GLN
1	G	1024	ASN
1	G	1038	HIS
1	G	1047	GLN
1	I	64	HIS
1	I	82	ASN
1	I	176	ASN
1	I	253	GLN
1	I	267	HIS
1	I	279	ASN
1	I	297	ASN
1	I	403	ASN
1	I	423	ASN
1	I	481	HIS
1	I	497	ASN
1	I	499	HIS
1	I	511	ASN
1	I	530	ASN
1	I	579	ASN
1	I	603	HIS
1	I	611	GLN
1	I	703	ASN
1	I	739	GLN
1	I	867	ASN
1	I	872	HIS
1	I	922	GLN
1	I	930	ASN
1	I	949	ASN
1	I	1008	GLN
1	I	1024	ASN
1	I	1038	HIS
1	I	1047	GLN
1	K	64	HIS
1	K	82	ASN
1	K	167	ASN
1	K	176	ASN
1	K	253	GLN
1	K	267	HIS
1	K	277	HIS
1	K	279	ASN
1	K	297	ASN
1	K	403	ASN

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Mol	Chain	Res	Type
1	K	423	ASN
1	K	481	HIS
1	K	497	ASN
1	K	511	ASN
1	K	530	ASN
1	K	603	HIS
1	K	611	GLN
1	K	703	ASN
1	K	733	ASN
1	K	739	GLN
1	K	867	ASN
1	K	872	HIS
1	K	901	ASN
1	K	922	GLN
1	K	930	ASN
1	K	949	ASN
1	K	1008	GLN
1	K	1024	ASN
1	K	1038	HIS
1	K	1047	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 ⓘ

Of 6 ligands modelled in this entry, 6 are modelled with single atom - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	1023/1071 (95%)	0.29	30 (2%) 55 48	16, 36, 58, 78	20 (1%)
1	C	1023/1071 (95%)	0.25	21 (2%) 67 61	17, 36, 58, 78	20 (1%)
1	E	1023/1071 (95%)	0.53	86 (8%) 14 9	20, 39, 59, 80	20 (1%)
1	G	1023/1071 (95%)	0.25	36 (3%) 48 40	20, 37, 58, 78	20 (1%)
1	I	1023/1071 (95%)	0.25	34 (3%) 50 43	20, 37, 58, 78	20 (1%)
1	K	1023/1071 (95%)	0.57	96 (9%) 11 6	20, 39, 59, 79	20 (1%)
2	B	11/13 (84%)	3.10	9 (81%) 0 0	52, 84, 96, 99	0
2	D	11/13 (84%)	2.90	7 (63%) 0 0	52, 84, 96, 99	0
2	F	11/13 (84%)	2.84	8 (72%) 0 0	53, 85, 97, 98	0
2	H	11/13 (84%)	2.57	6 (54%) 0 0	52, 84, 96, 99	0
2	J	11/13 (84%)	2.67	6 (54%) 0 0	52, 84, 96, 99	0
2	L	11/13 (84%)	3.98	8 (72%) 0 0	54, 84, 96, 99	0
All	All	6204/6504 (95%)	0.39	347 (5%) 28 21	16, 38, 60, 99	120 (1%)

All (347) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	219	SER	11.6
2	L	1203	THR	11.1
1	G	219	SER	10.6
1	C	842	GLY	9.4
2	H	1203	THR	8.9
2	L	1208	ALA	8.8
1	E	563	ALA	7.4
1	E	1061	ASN	7.2
2	B	1203	THR	7.1
1	E	842	GLY	7.1
1	A	842	GLY	6.7

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Mol	Chain	Res	Type	RSRZ
2	F	1203	THR	6.6
1	K	563	ALA	6.5
1	K	219	SER	6.2
1	E	238	VAL	6.0
1	E	168	ASP	6.0
2	J	1203	THR	5.9
1	E	219	SER	5.8
1	E	841	GLY	5.6
1	I	220	GLY	5.5
2	D	1203	THR	5.5
2	F	1208	ALA	5.4
1	E	838	SER	5.4
1	G	220	GLY	5.3
1	C	434	GLU	5.1
1	E	777	VAL	5.0
1	K	220	GLY	5.0
1	A	434	GLU	5.0
1	K	67	LYS	4.7
1	C	563	ALA	4.7
1	K	65	ASP	4.7
1	E	299	ASP	4.7
1	C	167	ASN	4.6
1	E	50	GLY	4.6
2	L	1206	ALA	4.6
1	E	67	LYS	4.6
1	E	840	LYS	4.6
1	I	1061	ASN	4.6
1	K	168	ASP	4.5
1	I	841	GLY	4.5
1	K	110	PHE	4.5
2	J	1209	GLU	4.5
1	G	1061	ASN	4.5
2	L	1207	ALA	4.5
1	E	220	GLY	4.4
2	D	1207	ALA	4.4
1	E	130	GLY	4.4
2	B	1207	ALA	4.4
1	K	114	GLU	4.4
1	E	110	PHE	4.4
1	K	434	GLU	4.4
1	I	436	GLY	4.3
1	I	563	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
2	D	1208	ALA	4.3
1	E	843	ASP	4.3
1	E	839	GLY	4.3
1	E	562	GLU	4.2
1	A	167	ASN	4.2
1	K	70	SER	4.1
1	K	841	GLY	4.1
1	A	839	GLY	4.1
1	K	806	LEU	4.0
2	D	1204	GLN	4.0
1	A	1061	ASN	4.0
1	E	86	PHE	4.0
1	K	69	GLY	3.9
1	G	563	ALA	3.9
2	J	1206	ALA	3.9
1	E	667	ASP	3.9
1	K	68	SER	3.8
1	K	667	ASP	3.8
1	E	113	GLY	3.8
2	F	1206	ALA	3.8
2	J	1205	LYS	3.7
1	K	66	LEU	3.7
1	K	382	ARG	3.6
1	K	561	SER	3.6
1	G	436	GLY	3.6
1	G	842	GLY	3.6
1	G	435	THR	3.6
1	I	435	THR	3.6
1	I	843	ASP	3.6
1	A	563	ALA	3.5
1	G	434	GLU	3.5
1	E	70	SER	3.5
1	A	557	ARG	3.5
2	L	1204	GLN	3.5
1	K	307	GLU	3.5
1	K	819	SER	3.5
1	K	843	ASP	3.5
1	E	561	SER	3.4
1	E	202	TRP	3.4
1	E	806	LEU	3.4
1	I	842	GLY	3.4
1	K	71	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	653	ASP	3.4
1	E	774	ASP	3.3
1	E	65	ASP	3.3
1	G	557	ARG	3.3
1	K	327	GLU	3.3
1	K	802	PRO	3.3
1	A	841	GLY	3.3
1	G	91	ARG	3.3
1	K	297	ASN	3.3
1	E	68	SER	3.3
1	K	252	GLY	3.2
1	K	238	VAL	3.2
1	C	299	ASP	3.2
1	I	415	ASN	3.2
1	K	91	ARG	3.1
2	B	1206	ALA	3.1
2	F	1209	GLU	3.1
1	I	372	ASP	3.1
1	K	299	ASP	3.1
1	K	305	LYS	3.1
2	B	1213	PHE	3.1
1	C	560	THR	3.1
1	E	64	HIS	3.1
1	K	1061	ASN	3.1
1	C	841	GLY	3.1
1	E	69	GLY	3.1
1	K	842	GLY	3.1
1	G	299	ASP	3.1
1	E	706	VAL	3.1
2	H	1208	ALA	3.0
1	E	237	ILE	3.0
1	K	774	ASP	3.0
1	K	285	ILE	3.0
1	A	298	PRO	3.0
1	K	236	VAL	3.0
1	K	296	PHE	3.0
1	K	126	GLY	3.0
1	K	286	LEU	3.0
1	I	434	GLU	3.0
1	K	653	ASP	3.0
1	I	91	ARG	2.9
1	K	665	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	131	ARG	2.9
1	K	311	LEU	2.9
2	B	1210	LEU	2.9
1	E	66	LEU	2.9
1	A	840	LYS	2.9
1	I	839	GLY	2.9
1	K	295	ILE	2.9
1	I	299	ASP	2.9
1	I	662	LEU	2.9
1	K	250	GLY	2.9
1	I	400	PHE	2.9
1	A	716	GLU	2.8
2	D	1206	ALA	2.8
1	K	817	ALA	2.8
2	J	1204	GLN	2.8
2	B	1204	GLN	2.8
1	E	239	GLY	2.8
1	K	838	SER	2.8
1	C	562	GLU	2.8
1	E	308	ILE	2.8
1	C	298	PRO	2.8
1	E	190	ARG	2.7
1	E	698	ARG	2.7
1	K	255	TYR	2.7
1	A	249	ASP	2.7
1	A	299	ASP	2.7
1	K	372	ASP	2.7
1	E	169	GLY	2.7
1	C	840	LYS	2.7
1	G	625	LYS	2.7
1	E	436	GLY	2.7
1	E	173	VAL	2.7
1	C	716	GLU	2.7
1	K	48	ILE	2.7
1	E	51	ASP	2.7
1	K	272	ASP	2.7
2	H	1207	ALA	2.7
1	C	838	SER	2.7
1	K	770	LYS	2.7
1	A	110	PHE	2.7
1	K	55	PHE	2.7
1	E	71	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	91	ARG	2.7
1	G	667	ASP	2.7
1	K	254	ILE	2.7
2	F	1210	LEU	2.6
2	F	1204	GLN	2.6
1	K	308	ILE	2.6
1	K	52	ARG	2.6
2	H	1210	LEU	2.6
1	K	436	GLY	2.6
1	E	350	VAL	2.6
1	K	704	GLU	2.6
1	E	705	ALA	2.6
1	K	271	THR	2.6
2	L	1209	GLU	2.6
1	G	488	ARG	2.6
1	K	63	GLU	2.6
2	B	1208	ALA	2.6
1	E	812	GLY	2.5
1	G	415	ASN	2.5
1	K	808	GLU	2.5
1	K	815	VAL	2.5
1	K	839	GLY	2.5
1	A	845	ARG	2.5
1	E	845	ARG	2.5
1	K	731	LEU	2.5
2	F	1207	ALA	2.5
2	J	1207	ALA	2.5
2	F	1205	LYS	2.5
1	E	905	TYR	2.5
1	K	705	ALA	2.5
1	K	816	GLY	2.5
1	E	318	ILE	2.5
1	K	1043	GLY	2.5
2	H	1209	GLU	2.5
1	E	298	PRO	2.5
1	K	51	ASP	2.5
1	G	1059	LEU	2.5
1	G	593	SER	2.5
1	K	697	ALA	2.4
1	E	645	ARG	2.4
1	E	1017	ASP	2.4
1	G	218	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	218	ASN	2.4
2	D	1213	PHE	2.4
1	C	557	ARG	2.4
1	E	187	ASP	2.4
1	A	562	GLU	2.4
1	E	817	ALA	2.4
1	K	435	THR	2.4
1	E	1042	SER	2.4
1	E	265	ARG	2.4
1	E	808	GLU	2.4
1	I	565	GLU	2.4
1	I	592	GLU	2.4
1	E	372	ASP	2.4
1	K	265	ARG	2.4
1	K	771	LEU	2.4
2	B	1205	LYS	2.4
1	G	843	ASP	2.4
1	E	41	ASN	2.4
1	K	41	ASN	2.4
1	K	138	ALA	2.3
1	E	218	ASN	2.3
1	G	127	LYS	2.3
1	A	313	SER	2.3
1	I	488	ARG	2.3
1	K	719	ARG	2.3
1	G	458	SER	2.3
1	K	722	VAL	2.3
1	G	373	THR	2.3
1	A	401	GLU	2.3
1	I	557	ARG	2.3
1	I	142	PRO	2.3
2	D	1210	LEU	2.3
1	I	395	GLY	2.3
1	G	627	ARG	2.3
1	K	43	LEU	2.3
1	E	756	ASP	2.3
1	I	840	LYS	2.3
1	E	707	ALA	2.3
1	K	963	ALA	2.3
1	G	624	VAL	2.3
1	E	188	GLY	2.3
2	B	1209	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
2	L	1210	LEU	2.2
1	A	218	ASN	2.2
1	E	115	ASN	2.2
1	E	1036	ALA	2.2
1	G	683	HIS	2.2
1	E	129	THR	2.2
1	E	147	ILE	2.2
1	K	875	SER	2.2
1	E	54	ILE	2.2
1	C	143	ASP	2.2
1	E	240	HIS	2.2
1	K	64	HIS	2.2
1	G	560	THR	2.2
1	G	662	LEU	2.2
1	K	287	PHE	2.2
1	K	706	VAL	2.2
1	A	308	ILE	2.2
1	K	263	ASP	2.2
1	I	838	SER	2.2
1	E	666	GLU	2.2
1	A	565	GLU	2.2
1	E	285	ILE	2.2
1	A	437	LYS	2.2
1	E	92	LYS	2.2
1	I	905	TYR	2.2
1	E	382	ARG	2.2
1	A	560	THR	2.2
1	G	110	PHE	2.1
1	C	255	TYR	2.1
1	K	251	PHE	2.1
1	K	270	PHE	2.1
1	K	488	ARG	2.1
1	A	255	TYR	2.1
1	A	1017	ASP	2.1
1	E	770	LYS	2.1
1	E	431	VAL	2.1
1	G	838	SER	2.1
1	C	131	ARG	2.1
1	K	988	TRP	2.1
1	C	218	ASN	2.1
1	E	716	GLU	2.1
1	I	935	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	1205	LYS	2.1
1	E	697	ALA	2.1
1	K	672	GLU	2.1
1	A	144	GLY	2.1
1	A	719	ARG	2.1
1	A	1019	GLY	2.1
1	G	716	GLU	2.1
1	C	237	ILE	2.1
1	E	142	PRO	2.1
1	E	296	PHE	2.1
1	G	400	PHE	2.1
1	C	51	ASP	2.1
1	I	374	LYS	2.1
1	G	565	GLU	2.1
1	K	643	ALA	2.1
1	C	1059	LEU	2.1
1	G	44	LEU	2.1
1	G	157	SER	2.1
1	K	171	ASN	2.1
1	A	265	ARG	2.1
1	E	89	ASP	2.1
1	K	840	LYS	2.1
1	C	336	LEU	2.0
1	I	629	VAL	2.0
1	K	232	VAL	2.0
1	A	270	PHE	2.0
1	K	202	TRP	2.0
1	G	372	ASP	2.0
1	K	333	ASP	2.0
1	I	544	LEU	2.0
1	K	229	SER	2.0
1	K	167	ASN	2.0
1	E	647	THR	2.0
1	I	393	ARG	2.0
2	L	1213	PHE	2.0
1	E	565	GLU	2.0
1	K	716	GLU	2.0
1	I	624	VAL	2.0
1	K	401	GLU	2.0
1	G	936	ASP	2.0
1	E	401	GLU	2.0
1	I	667	ASP	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(\AA^2)	Q<0.9
3	CHM	B	2213	1/6	0.96	0.27	0.80	52,52,52,52	0
3	CHM	D	2213	1/6	0.87	0.22	0.42	52,52,52,52	0
3	CHM	L	2213	1/6	0.88	0.17	-0.55	59,59,59,59	0
3	CHM	F	2213	1/6	0.86	0.13	-1.05	52,52,52,52	0
3	CHM	J	2213	1/6	0.92	0.12	-1.41	56,56,56,56	0
3	CHM	H	2213	1/6	0.95	0.10	-1.98	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.