Full wwPDB X-ray Structure Validation Report ⓘ

Jan 23, 2024 – 04:09 AM EST

PDB ID : 1N6D
Title : Tricorn protease in complex with tetrapeptide chloromethyl ketone derivative
Authors : Kim, J.-S.; Groll, M.; Huber, R.; Brandstetter, H.
Deposited on : 2002-11-10
Resolution : 2.80 Å(reported)

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

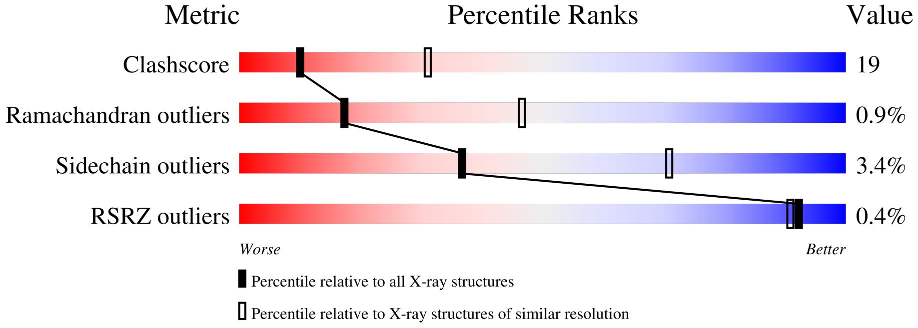
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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

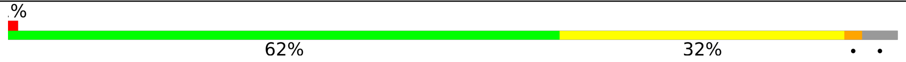
The reported resolution of this entry is 2.80 Å.

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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	
1	B	1071	
1	C	1071	
1	D	1071	
1	E	1071	
1	F	1071	

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Mol	Chain	Length	Quality of chain
2	G	5	
2	H	5	
2	I	5	
2	J	5	
2	K	5	
2	L	5	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 49890 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.

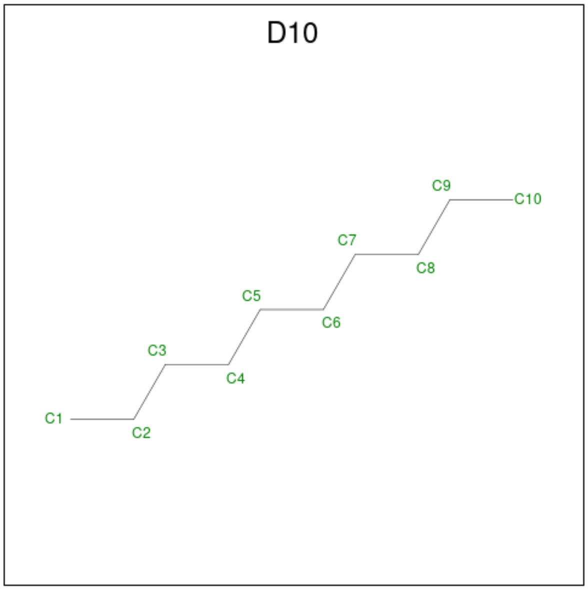
- Molecule 1 is a protein called Tricorn protease.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	A	1023	Total C N O S 8177 5196 1402 1551 28	94	0	0
1	B	1023	Total C N O S 8177 5196 1402 1551 28	94	0	0
1	C	1023	Total C N O S 8177 5196 1402 1551 28	94	0	0
1	D	1023	Total C N O S 8177 5196 1402 1551 28	94	0	0
1	E	1023	Total C N O S 8177 5196 1402 1551 28	94	0	0
1	F	1023	Total C N O S 8177 5196 1402 1551 28	94	0	0

- Molecule 2 is a protein called RVRK.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	G	5	Total C N O 39 24 11 4	0	0	1
2	H	5	Total C N O 39 24 11 4	0	0	1
2	I	5	Total C N O 39 24 11 4	0	0	1
2	J	5	Total C N O 39 24 11 4	0	0	1
2	K	5	Total C N O 39 24 11 4	0	0	1
2	L	5	Total C N O 39 24 11 4	0	0	1

- Molecule 3 is DECANE (three-letter code: D10) (formula: $C_{10}H_{22}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total C 10 10	0	0
3	H	1	Total C 10 10	0	0
3	I	1	Total C 10 10	0	0
3	J	1	Total C 10 10	0	0
3	K	1	Total C 10 10	0	0
3	L	1	Total C 10 10	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	106	Total O 106 106	0	0
4	G	4	Total O 4 4	0	0
4	B	88	Total O 88 88	0	0
4	C	88	Total O 88 88	0	0
4	I	2	Total O 2 2	0	0
4	D	79	Total O 79 79	0	0

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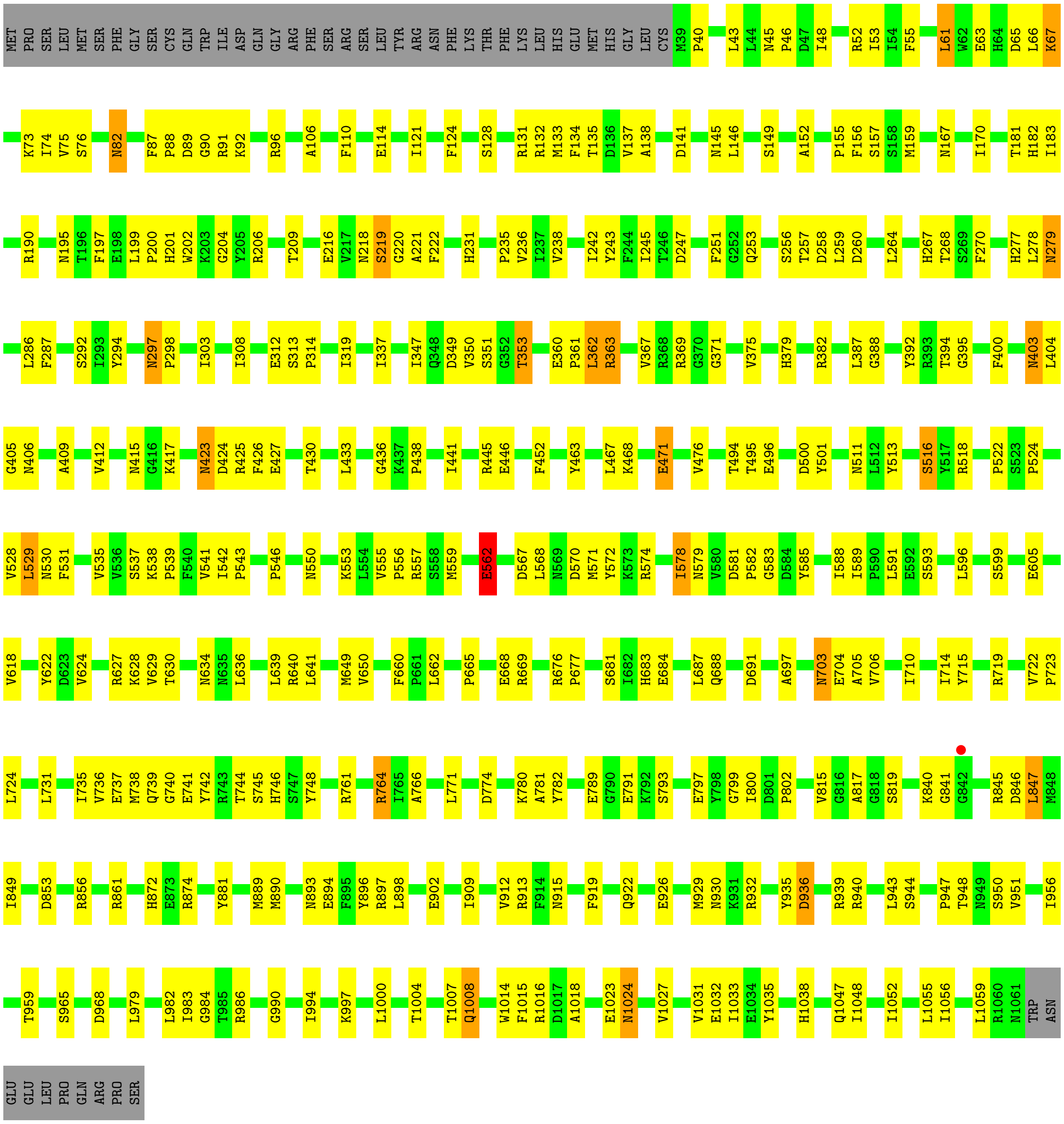
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	J	2	Total O 2 2	0	0
4	E	89	Total O 89 89	0	0
4	F	74	Total O 74 74	0	0
4	L	2	Total O 2 2	0	0

3 Residue-property plots ⓘ

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

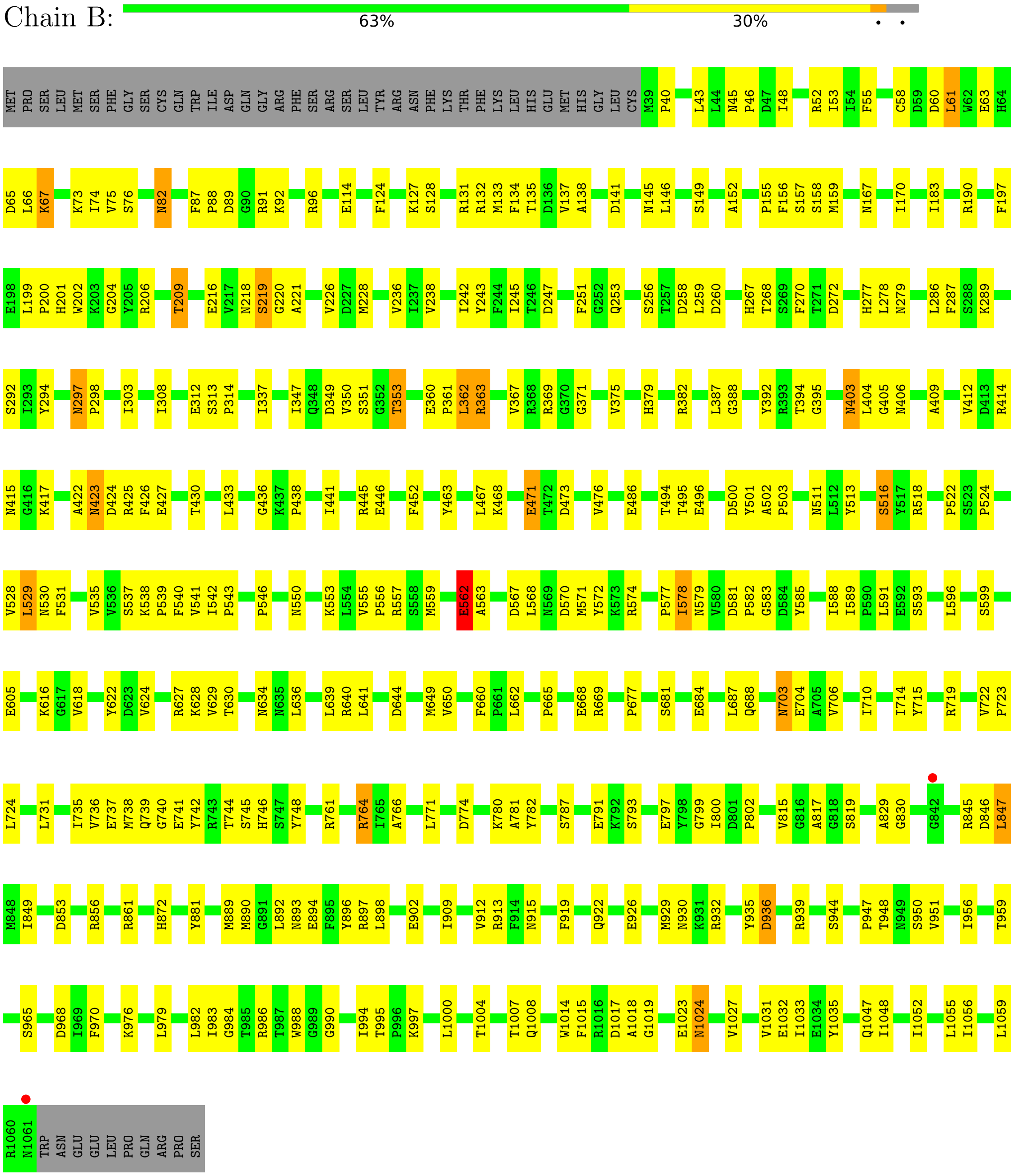
- Molecule 1: Tricorn protease

Chain A:



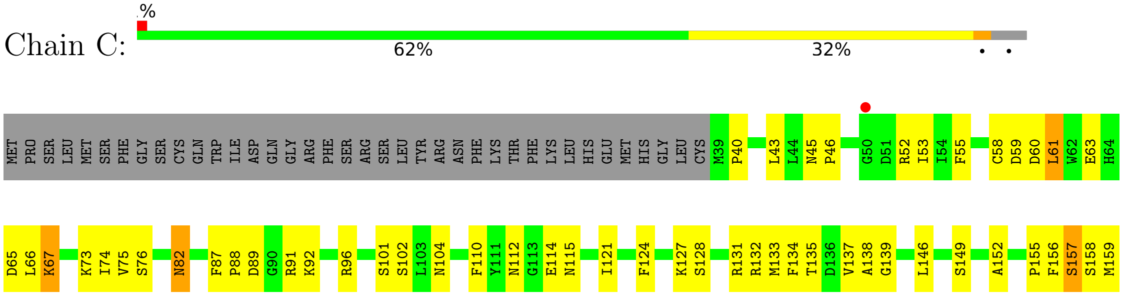
- Molecule 1: Tricorn protease

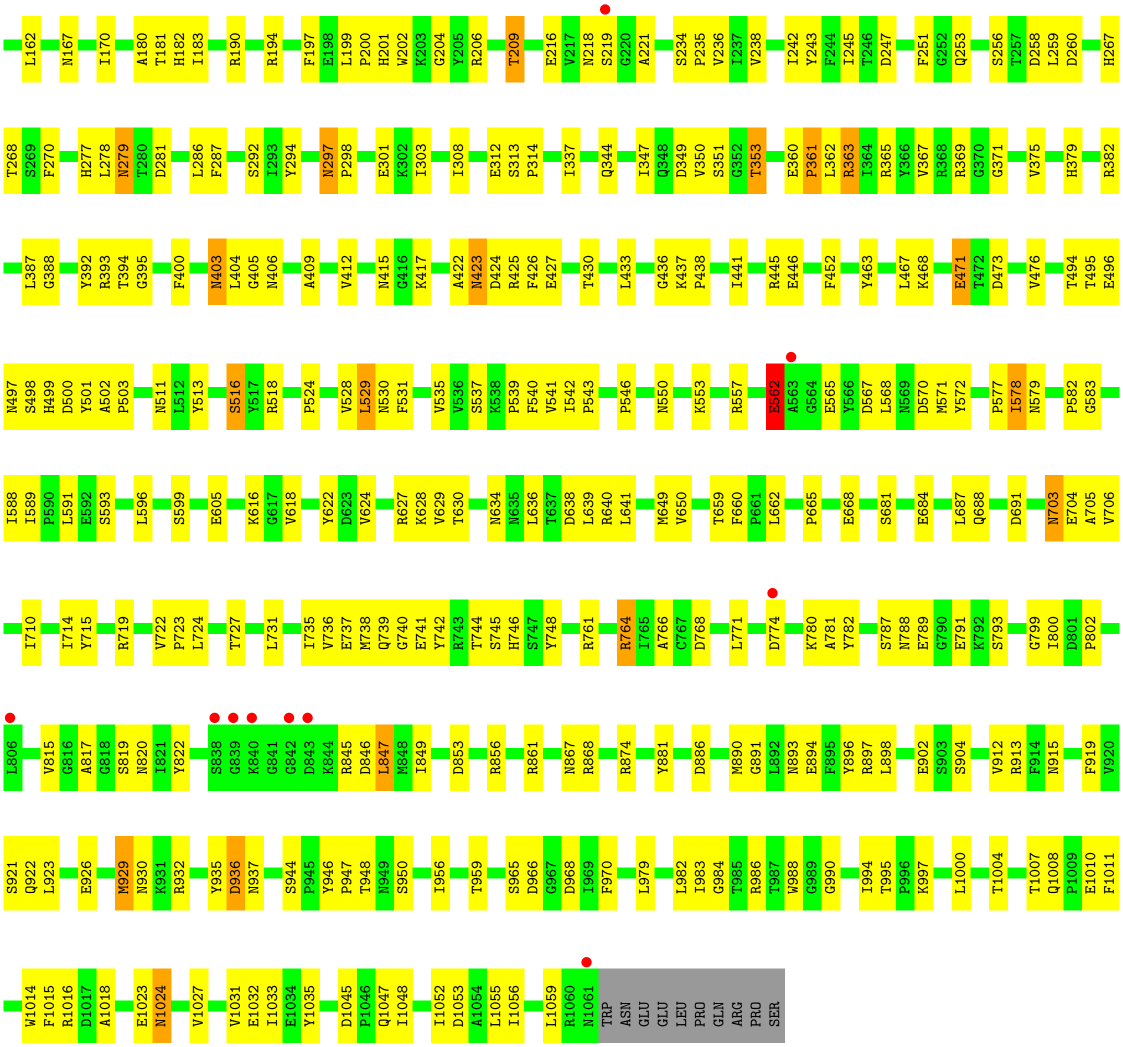
Chain B:



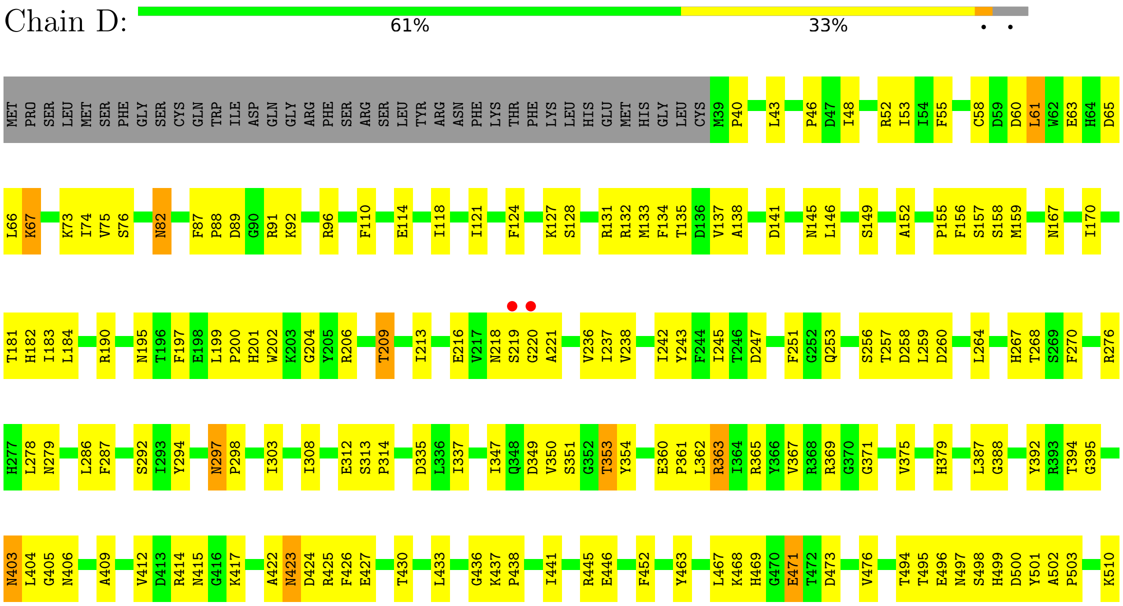
- Molecule 1: Tricorn protease

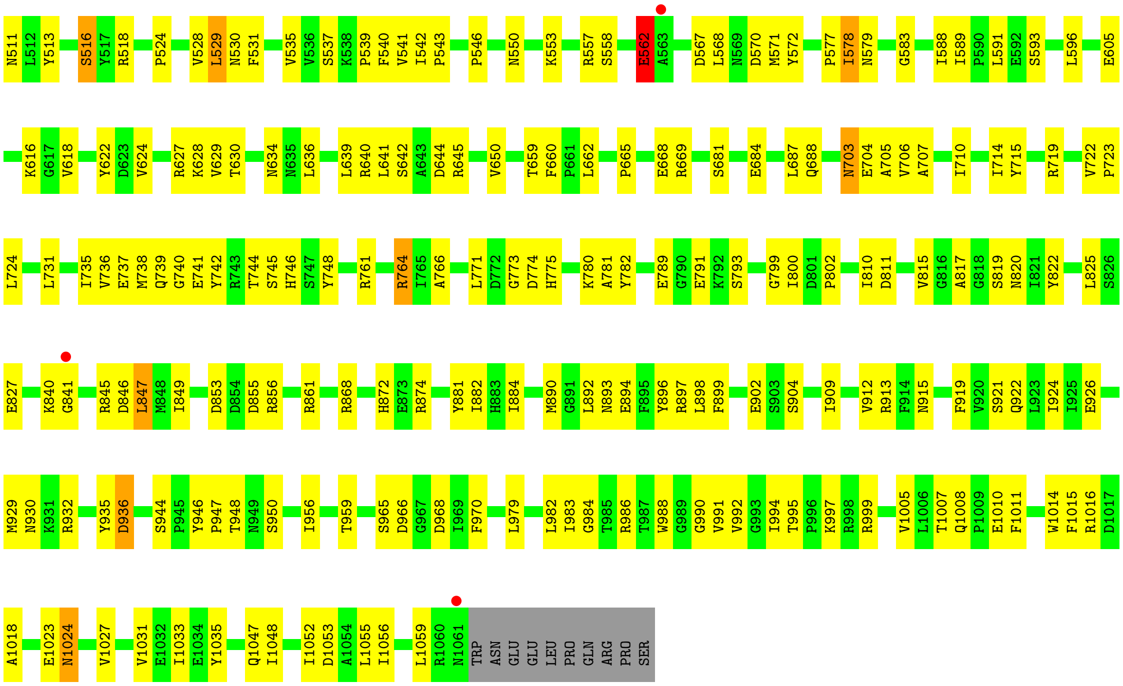
Chain C:



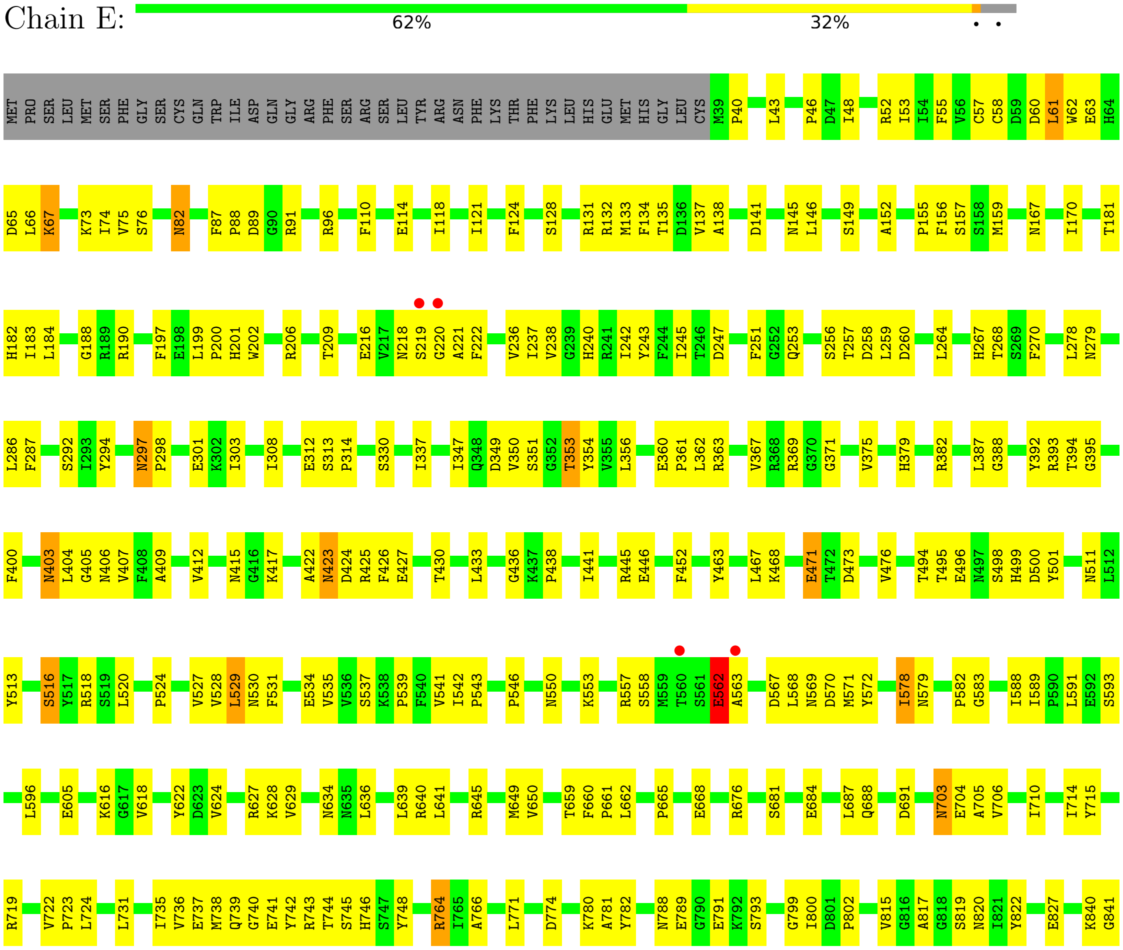


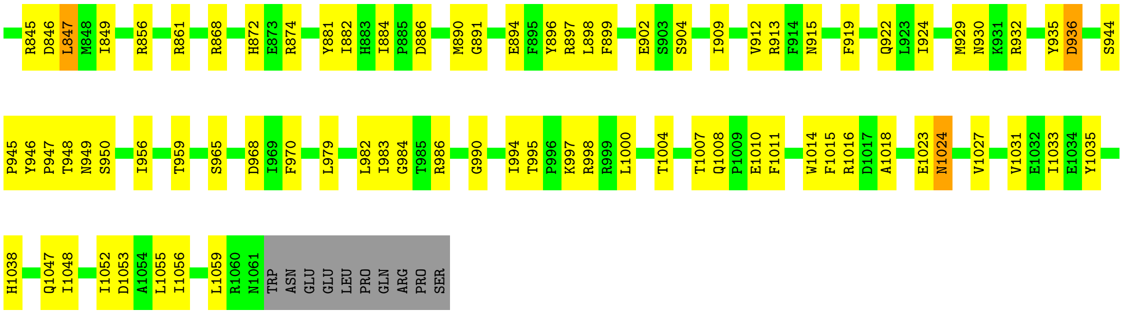
• Molecule 1: Tricorn protease





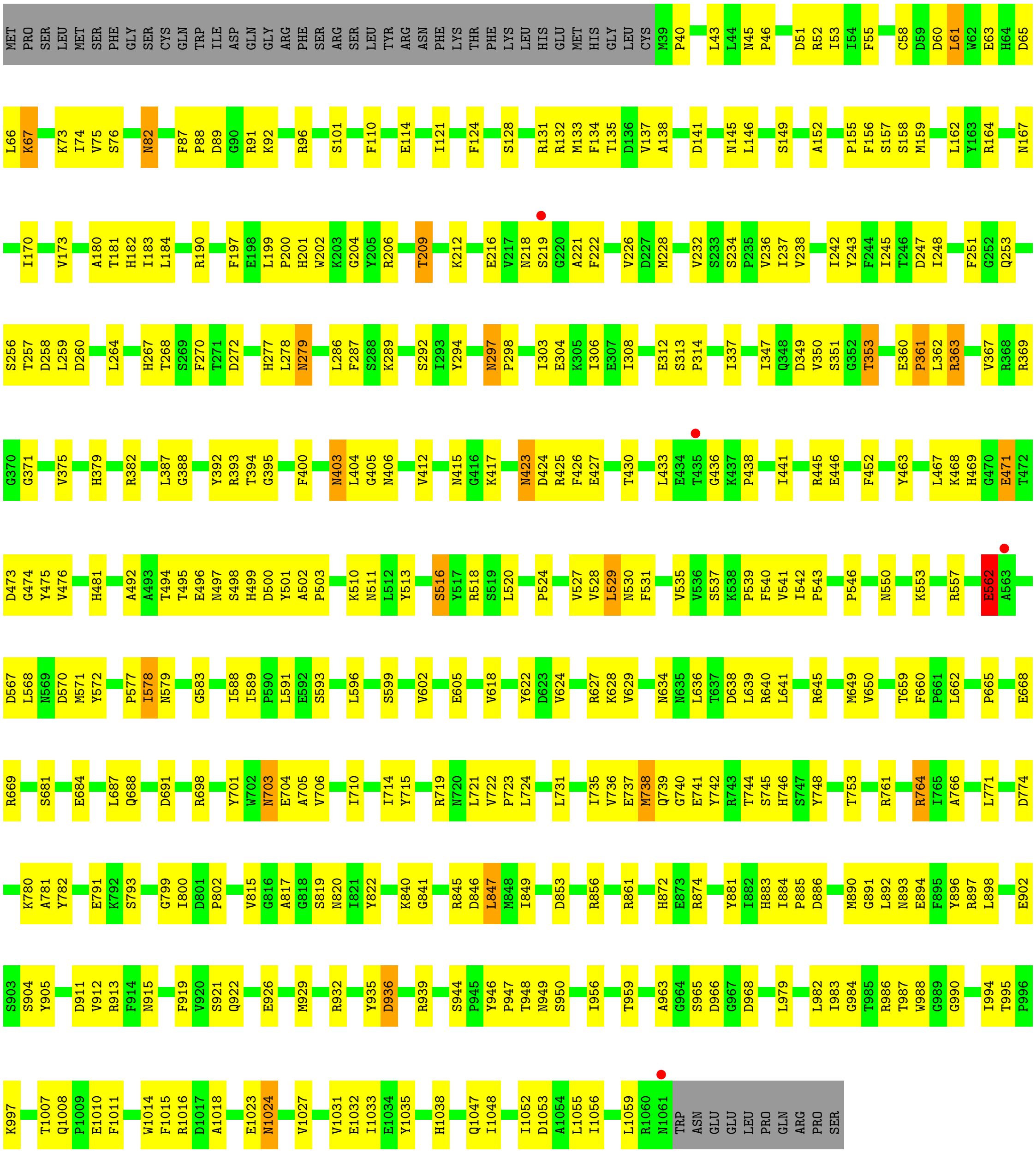
- Molecule 1: Tricorn protease





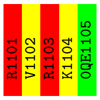
- Molecule 1: Tricorn protease

Chain F:



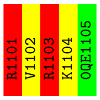
- Molecule 2: RVRK

Chain G:



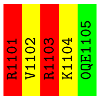
- Molecule 2: RVRK

Chain H:



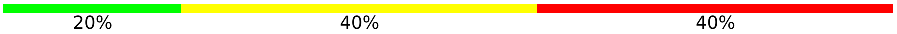
- Molecule 2: RVRK

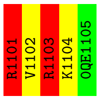
Chain I:



- Molecule 2: RVRK

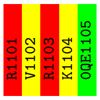
Chain J:





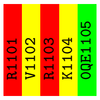
- Molecule 2: RVRK

Chain K:



- Molecule 2: RVRK

Chain L:



4 Data and refinement statistics ⓘ

Property	**Value**	**Source**
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	95.44Å 245.43Å 159.40Å 90.00° 104.79° 90.00°	Depositor
Resolution (Å)	6.00 – 2.80 20.03 – 2.70	Depositor EDS
% Data completeness (in resolution range)	88.7 (6.00-2.80) 75.0 (20.03-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	0.66 (at 2.71Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.285 , 0.315 0.274 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	32.2	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 14.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.079 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	49890	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: D10, 0QE

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	0.50	0/8367	0.64	0/11311
1	B	0.50	0/8367	0.64	0/11311
1	C	0.51	0/8367	0.64	0/11311
1	D	0.50	0/8367	0.64	0/11311
1	E	0.49	0/8367	0.64	0/11311
1	F	0.50	0/8367	0.63	0/11311
2	G	2.21	2/37 (5.4%)	2.86	4/46 (8.7%)
2	H	2.21	2/37 (5.4%)	2.85	4/46 (8.7%)
2	I	2.21	2/37 (5.4%)	2.85	4/46 (8.7%)
2	J	2.21	2/37 (5.4%)	2.85	4/46 (8.7%)
2	K	2.21	2/37 (5.4%)	2.85	4/46 (8.7%)
2	L	2.21	2/37 (5.4%)	2.85	4/46 (8.7%)
All	All	0.52	12/50424 (0.0%)	0.66	24/68142 (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
2	G	0	3
2	H	0	3
2	I	0	3
2	J	0	3
2	K	0	3
2	L	0	3
All	All	0	18

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	1103	ARG	CB-CG	9.19	1.77	1.52
2	H	1103	ARG	CB-CG	9.18	1.77	1.52
2	I	1103	ARG	CB-CG	9.18	1.77	1.52
2	L	1103	ARG	CB-CG	9.18	1.77	1.52
2	G	1103	ARG	CB-CG	9.17	1.77	1.52
2	J	1103	ARG	CB-CG	9.16	1.77	1.52
2	I	1103	ARG	N-CA	-8.09	1.30	1.46
2	L	1103	ARG	N-CA	-8.06	1.30	1.46
2	H	1103	ARG	N-CA	-8.04	1.30	1.46
2	J	1103	ARG	N-CA	-8.04	1.30	1.46
2	K	1103	ARG	N-CA	-8.04	1.30	1.46
2	G	1103	ARG	N-CA	-8.03	1.30	1.46

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	1103	ARG	O-C-N	-9.29	107.83	122.70
2	L	1103	ARG	O-C-N	-9.26	107.89	122.70
2	K	1103	ARG	O-C-N	-9.25	107.90	122.70
2	H	1103	ARG	O-C-N	-9.24	107.92	122.70
2	I	1103	ARG	O-C-N	-9.24	107.92	122.70
2	J	1103	ARG	O-C-N	-9.23	107.93	122.70
2	G	1103	ARG	C-N-CA	8.79	143.67	121.70
2	I	1103	ARG	C-N-CA	8.78	143.65	121.70
2	L	1103	ARG	C-N-CA	8.77	143.64	121.70
2	H	1103	ARG	C-N-CA	8.77	143.63	121.70
2	K	1103	ARG	C-N-CA	8.77	143.62	121.70
2	J	1103	ARG	C-N-CA	8.75	143.59	121.70
2	G	1101	ARG	C-N-CA	7.06	139.36	121.70
2	H	1101	ARG	C-N-CA	7.06	139.35	121.70
2	I	1101	ARG	C-N-CA	7.05	139.34	121.70
2	K	1101	ARG	C-N-CA	7.05	139.32	121.70
2	L	1101	ARG	C-N-CA	7.04	139.31	121.70
2	J	1101	ARG	C-N-CA	7.03	139.28	121.70
2	G	1103	ARG	CA-C-N	6.56	131.62	117.20
2	H	1103	ARG	CA-C-N	6.54	131.59	117.20
2	L	1103	ARG	CA-C-N	6.54	131.59	117.20
2	I	1103	ARG	CA-C-N	6.53	131.58	117.20
2	K	1103	ARG	CA-C-N	6.53	131.57	117.20
2	J	1103	ARG	CA-C-N	6.52	131.55	117.20

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	G	1101	ARG	Sidechain
2	G	1102	VAL	Mainchain
2	G	1103	ARG	Sidechain
2	H	1101	ARG	Sidechain
2	H	1102	VAL	Mainchain
2	H	1103	ARG	Sidechain
2	I	1101	ARG	Sidechain
2	I	1102	VAL	Mainchain
2	I	1103	ARG	Sidechain
2	J	1101	ARG	Sidechain
2	J	1102	VAL	Mainchain
2	J	1103	ARG	Sidechain
2	K	1101	ARG	Sidechain
2	K	1102	VAL	Mainchain
2	K	1103	ARG	Sidechain
2	L	1101	ARG	Sidechain
2	L	1102	VAL	Mainchain
2	L	1103	ARG	Sidechain

5.2 Too-close contacts (i)

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	297	0
1	B	8177	0	8002	300	0
1	C	8177	0	8002	325	0
1	D	8177	0	8002	325	0
1	E	8177	0	8002	318	0
1	F	8177	0	8002	331	0
2	G	39	0	46	8	0
2	H	39	0	46	5	0
2	I	39	0	46	7	0
2	J	39	0	46	7	0
2	K	39	0	46	5	0
2	L	39	0	46	8	0
3	G	10	0	20	2	0
3	H	10	0	20	3	0
3	I	10	0	20	4	0
3	J	10	0	20	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	10	0	20	4	0
3	L	10	0	20	4	0
4	A	106	0	0	15	0
4	B	88	0	0	23	0
4	C	88	0	0	38	0
4	D	79	0	0	32	0
4	E	89	0	0	26	0
4	F	74	0	0	39	0
4	G	4	0	0	3	0
4	I	2	0	0	2	0
4	J	2	0	0	2	0
4	L	2	0	0	3	0
All	All	49890	0	48408	1829	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (1829) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1103:ARG:CB	2:I:1103:ARG:CG	1.77	1.63
2:G:1103:ARG:CB	2:G:1103:ARG:CG	1.77	1.62
2:H:1103:ARG:CG	2:H:1103:ARG:CB	1.77	1.57
2:K:1103:ARG:CB	2:K:1103:ARG:CG	1.77	1.57
2:J:1103:ARG:CB	2:J:1103:ARG:CG	1.77	1.56
2:L:1103:ARG:CB	2:L:1103:ARG:CG	1.77	1.54
2:I:1101:ARG:HD2	4:I:74:HOH:O	1.33	1.22
1:F:51:ASP:HB3	4:F:1143:HOH:O	1.40	1.21
2:L:1101:ARG:HD2	4:L:79:HOH:O	1.42	1.17
2:J:1101:ARG:NH1	4:J:103:HOH:O	1.86	1.01
1:B:486:GLU:HA	4:B:1087:HOH:O	1.61	0.99
1:F:248:ILE:HD12	4:F:1073:HOH:O	1.63	0.99
2:L:1103:ARG:HD2	4:L:246:HOH:O	1.62	0.99
1:E:403:ASN:HD22	1:E:404:LEU:N	1.62	0.95
1:D:403:ASN:HD22	1:D:404:LEU:N	1.64	0.95
1:C:403:ASN:HD22	1:C:404:LEU:N	1.64	0.94
1:F:228:MET:HB3	4:F:1073:HOH:O	1.67	0.94
1:C:206:ARG:H	1:C:1024:ASN:HD21	1.15	0.94
1:A:403:ASN:HD22	1:A:404:LEU:N	1.65	0.94
1:B:403:ASN:HD22	1:B:404:LEU:N	1.65	0.94
2:G:1103:ARG:HD2	4:G:440:HOH:O	1.68	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:206:ARG:H	1:F:1024:ASN:HD21	1.15	0.93
1:A:683:HIS:HB2	4:A:1133:HOH:O	1.70	0.91
1:C:167:ASN:HB2	1:C:170:ILE:HB	1.52	0.91
1:C:351:SER:OG	1:C:353:THR:HG22	1.69	0.91
1:F:403:ASN:HD22	1:F:404:LEU:N	1.67	0.91
1:B:167:ASN:HB2	1:B:170:ILE:HB	1.53	0.90
1:A:167:ASN:HB2	1:A:170:ILE:HB	1.53	0.90
2:G:1103:ARG:CD	4:G:440:HOH:O	2.19	0.90
1:F:167:ASN:HB2	1:F:170:ILE:HB	1.53	0.89
1:F:965:SER:CB	2:L:1104:LYS:O	2.09	0.89
1:E:206:ARG:H	1:E:1024:ASN:HD21	1.20	0.89
1:B:965:SER:CB	2:H:1104:LYS:O	2.07	0.89
1:D:167:ASN:HB2	1:D:170:ILE:HB	1.54	0.89
1:D:351:SER:OG	1:D:353:THR:HG22	1.73	0.89
1:C:965:SER:CB	2:I:1104:LYS:O	2.09	0.89
1:F:173:VAL:HB	4:F:1076:HOH:O	1.72	0.89
1:E:965:SER:CB	2:K:1104:LYS:O	2.09	0.88
1:B:206:ARG:H	1:B:1024:ASN:HD21	1.17	0.88
1:A:403:ASN:ND2	1:A:405:GLY:H	1.71	0.88
1:E:167:ASN:HB2	1:E:170:ILE:HB	1.55	0.88
1:E:351:SER:OG	1:E:353:THR:HG22	1.74	0.88
1:F:403:ASN:ND2	1:F:405:GLY:H	1.72	0.88
1:C:403:ASN:ND2	1:C:405:GLY:H	1.72	0.87
1:E:403:ASN:ND2	1:E:405:GLY:H	1.72	0.87
1:D:825:LEU:HG	4:D:1122:HOH:O	1.72	0.87
1:A:206:ARG:H	1:A:1024:ASN:HD21	1.18	0.87
1:B:403:ASN:ND2	1:B:405:GLY:H	1.72	0.86
1:E:743:ARG:HD3	4:E:1146:HOH:O	1.75	0.86
1:D:206:ARG:H	1:D:1024:ASN:HD21	1.23	0.86
1:F:557:ARG:HH22	1:F:562:GLU:H	1.23	0.86
1:A:382:ARG:HB3	4:A:1135:HOH:O	1.74	0.86
1:D:403:ASN:ND2	1:D:405:GLY:H	1.73	0.85
1:B:494:THR:HG21	1:B:500:ASP:OD1	1.77	0.85
1:B:557:ARG:HH22	1:B:562:GLU:H	1.22	0.85
4:B:1136:HOH:O	1:E:676:ARG:HG3	1.76	0.85
1:D:494:THR:HG21	1:D:500:ASP:OD1	1.77	0.85
1:A:557:ARG:HH22	1:A:562:GLU:H	1.24	0.84
1:D:558:SER:HA	1:F:393:ARG:HD2	1.60	0.84
1:C:102:SER:HB2	4:C:1105:HOH:O	1.77	0.84
1:D:218:ASN:HA	4:D:1103:HOH:O	1.78	0.84
1:E:494:THR:HG21	1:E:500:ASP:OD1	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:965:SER:CB	2:G:1104:LYS:O	2.09	0.83
1:A:167:ASN:HA	4:A:1093:HOH:O	1.77	0.83
1:A:494:THR:HG21	1:A:500:ASP:OD1	1.77	0.83
1:F:350:VAL:HG13	4:F:1100:HOH:O	1.79	0.82
1:C:206:ARG:H	1:C:1024:ASN:ND2	1.76	0.82
1:F:206:ARG:H	1:F:1024:ASN:ND2	1.77	0.82
1:C:557:ARG:HH22	1:C:562:GLU:H	1.25	0.82
1:E:557:ARG:HH22	1:E:562:GLU:H	1.28	0.82
1:D:992:VAL:HG23	4:D:1088:HOH:O	1.78	0.81
1:D:557:ARG:HH22	1:D:562:GLU:H	1.26	0.81
1:B:351:SER:OG	1:B:353:THR:HG22	1.81	0.81
1:F:351:SER:OG	1:F:353:THR:HG22	1.80	0.80
1:B:206:ARG:H	1:B:1024:ASN:ND2	1.78	0.80
2:I:1103:ARG:CG	2:I:1103:ARG:CA	2.60	0.80
1:A:845:ARG:HB3	1:A:847:LEU:HD21	1.63	0.80
1:A:206:ARG:H	1:A:1024:ASN:ND2	1.79	0.80
2:K:1103:ARG:CG	2:K:1103:ARG:CA	2.60	0.80
2:L:1103:ARG:CG	2:L:1103:ARG:CA	2.60	0.79
2:J:1103:ARG:CG	2:J:1103:ARG:CA	2.60	0.79
1:B:40:PRO:HG2	1:B:724:LEU:HD22	1.65	0.79
1:C:159:MET:HB3	4:C:1148:HOH:O	1.81	0.79
1:D:1023:GLU:OE2	4:D:1088:HOH:O	2.01	0.79
1:E:913:ARG:HH21	1:E:1047:GLN:HE21	1.31	0.79
2:G:1103:ARG:CG	2:G:1103:ARG:CA	2.60	0.79
2:H:1103:ARG:CG	2:H:1103:ARG:CA	2.60	0.79
1:E:206:ARG:H	1:E:1024:ASN:ND2	1.80	0.78
1:D:913:ARG:HH21	1:D:1047:GLN:HE21	1.30	0.78
1:C:845:ARG:HB3	1:C:847:LEU:HD21	1.64	0.78
1:F:845:ARG:HB3	1:F:847:LEU:HD21	1.64	0.78
1:C:897:ARG:HD3	4:C:1107:HOH:O	1.82	0.78
1:F:40:PRO:HG2	1:F:724:LEU:HD22	1.65	0.78
1:D:845:ARG:HB3	1:D:847:LEU:HD21	1.65	0.78
1:D:238:VAL:HG11	1:D:298:PRO:HG2	1.65	0.78
1:D:206:ARG:H	1:D:1024:ASN:ND2	1.80	0.78
1:A:351:SER:OG	1:A:353:THR:HG22	1.83	0.78
1:B:845:ARG:HB3	1:B:847:LEU:HD21	1.67	0.77
1:C:238:VAL:HG11	1:C:298:PRO:HG2	1.65	0.77
1:D:539:PRO:HG2	1:D:578:ILE:HG12	1.66	0.77
1:A:73:LYS:HD3	1:A:76:SER:HB3	1.66	0.77
1:F:73:LYS:HD3	1:F:76:SER:HB3	1.65	0.77
1:F:494:THR:HG21	1:F:500:ASP:OD1	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:PRO:HG2	1:D:724:LEU:HD22	1.67	0.77
1:D:965:SER:CB	2:J:1104:LYS:O	2.10	0.77
1:C:539:PRO:HG2	1:C:578:ILE:HG12	1.67	0.77
1:C:494:THR:HG21	1:C:500:ASP:OD1	1.84	0.77
1:B:73:LYS:HD3	1:B:76:SER:HB3	1.65	0.76
1:F:913:ARG:HH21	1:F:1047:GLN:HE21	1.32	0.76
1:C:40:PRO:HG2	1:C:724:LEU:HD22	1.65	0.76
1:E:589:ILE:HD13	1:E:641:LEU:HD22	1.68	0.76
1:A:40:PRO:HG2	1:A:724:LEU:HD22	1.66	0.76
1:C:589:ILE:HD13	1:C:641:LEU:HD22	1.67	0.75
1:B:965:SER:HB3	2:H:1104:LYS:O	1.37	0.75
1:F:238:VAL:HG11	1:F:298:PRO:HG2	1.66	0.75
1:A:913:ARG:HH21	1:A:1047:GLN:HE21	1.32	0.75
1:C:82:ASN:H	1:C:82:ASN:HD22	1.35	0.75
1:E:40:PRO:HG2	1:E:724:LEU:HD22	1.66	0.75
1:A:539:PRO:HG2	1:A:578:ILE:HG12	1.68	0.75
1:B:403:ASN:HD22	1:B:404:LEU:H	1.35	0.75
1:A:589:ILE:HD13	1:A:641:LEU:HD22	1.68	0.75
1:B:539:PRO:HG2	1:B:578:ILE:HG12	1.68	0.74
1:D:589:ILE:HD13	1:D:641:LEU:HD22	1.68	0.74
1:F:557:ARG:NH2	1:F:562:GLU:H	1.85	0.74
4:E:1125:HOH:O	1:F:602:VAL:HA	1.86	0.74
1:A:524:PRO:HD3	1:B:605:GLU:HG3	1.67	0.74
1:D:276:ARG:HD3	4:D:1137:HOH:O	1.87	0.74
1:F:596:LEU:HD11	1:F:662:LEU:HD11	1.69	0.74
1:C:73:LYS:HD3	1:C:76:SER:HB3	1.68	0.74
1:E:845:ARG:HB3	1:E:847:LEU:HD21	1.67	0.74
1:F:721:LEU:HG	4:F:1121:HOH:O	1.86	0.74
1:B:557:ARG:NH2	1:B:562:GLU:H	1.85	0.74
1:E:403:ASN:HD22	1:E:404:LEU:H	1.34	0.74
1:F:589:ILE:HD13	1:F:641:LEU:HD22	1.67	0.74
1:D:349:ASP:OD2	1:D:351:SER:HB3	1.88	0.74
1:E:238:VAL:HG11	1:E:298:PRO:HG2	1.68	0.74
1:E:736:VAL:HG13	4:E:1072:HOH:O	1.88	0.73
1:C:596:LEU:HD11	1:C:662:LEU:HD11	1.70	0.73
1:B:238:VAL:HG11	1:B:298:PRO:HG2	1.69	0.73
1:E:73:LYS:HD3	1:E:76:SER:HB3	1.68	0.73
1:E:539:PRO:HG2	1:E:578:ILE:HG12	1.69	0.73
1:F:539:PRO:HG2	1:F:578:ILE:HG12	1.70	0.73
1:C:393:ARG:HD2	1:E:558:SER:HA	1.71	0.73
1:D:73:LYS:HD3	1:D:76:SER:HB3	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:ARG:HD3	4:C:1093:HOH:O	1.87	0.73
1:A:557:ARG:NH2	1:A:562:GLU:H	1.86	0.73
1:C:913:ARG:HH21	1:C:1047:GLN:HE21	1.36	0.73
1:B:167:ASN:HA	4:B:1098:HOH:O	1.86	0.73
1:B:557:ARG:HH22	1:B:562:GLU:N	1.88	0.72
1:D:557:ARG:NH2	1:D:562:GLU:H	1.88	0.72
1:F:304:GLU:O	4:F:1139:HOH:O	2.07	0.72
1:A:403:ASN:HD22	1:A:404:LEU:H	1.36	0.72
1:A:965:SER:HB3	2:G:1104:LYS:O	1.41	0.72
1:C:403:ASN:HD22	1:C:404:LEU:H	1.37	0.72
1:A:815:VAL:HA	1:A:819:SER:HB3	1.72	0.72
1:B:736:VAL:HA	1:B:739:GLN:HE21	1.55	0.72
1:B:913:ARG:HH21	1:B:1047:GLN:HE21	1.37	0.72
2:I:1103:ARG:CB	2:I:1103:ARG:CD	2.68	0.72
1:D:403:ASN:HD22	1:D:404:LEU:H	1.35	0.72
1:A:297:ASN:HB2	4:A:1074:HOH:O	1.89	0.72
1:E:349:ASP:OD2	1:E:351:SER:HB3	1.90	0.72
1:C:206:ARG:N	1:C:1024:ASN:HD21	1.87	0.71
2:K:1103:ARG:CB	2:K:1103:ARG:CD	2.68	0.71
1:A:736:VAL:HA	1:A:739:GLN:HE21	1.56	0.71
1:B:589:ILE:HD13	1:B:641:LEU:HD22	1.70	0.71
1:A:596:LEU:HD11	1:A:662:LEU:HD11	1.71	0.71
1:E:202:TRP:CH2	1:E:745:SER:HB3	2.24	0.71
2:G:1103:ARG:CB	2:G:1103:ARG:CD	2.68	0.71
1:C:965:SER:HB3	2:I:1104:LYS:O	1.39	0.71
1:F:557:ARG:HH22	1:F:562:GLU:N	1.88	0.71
1:A:409:ALA:HA	4:A:1158:HOH:O	1.91	0.70
1:C:557:ARG:NH2	1:C:562:GLU:H	1.87	0.70
1:F:736:VAL:HA	1:F:739:GLN:HE21	1.55	0.70
1:F:965:SER:HB3	2:L:1104:LYS:O	1.39	0.70
1:C:557:ARG:HH22	1:C:562:GLU:N	1.90	0.70
1:A:605:GLU:HG3	1:B:524:PRO:HD3	1.73	0.70
1:A:238:VAL:HG11	1:A:298:PRO:HG2	1.72	0.70
1:D:82:ASN:HD22	1:D:82:ASN:H	1.39	0.70
1:D:815:VAL:HA	1:D:819:SER:HB3	1.73	0.70
2:L:1103:ARG:CB	2:L:1103:ARG:CD	2.68	0.70
1:B:202:TRP:CH2	1:B:745:SER:HB3	2.27	0.70
1:C:349:ASP:OD2	1:C:351:SER:HB3	1.92	0.70
1:A:557:ARG:HH22	1:A:562:GLU:N	1.89	0.69
1:D:131:ARG:HD2	4:D:1072:HOH:O	1.92	0.69
1:D:775:HIS:HA	4:D:1100:HOH:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:557:ARG:NH2	1:E:562:GLU:H	1.88	0.69
1:E:736:VAL:HA	1:E:739:GLN:HE21	1.56	0.69
1:D:736:VAL:HA	1:D:739:GLN:HE21	1.57	0.69
1:B:735:ILE:O	1:B:739:GLN:HG3	1.92	0.69
1:B:815:VAL:HA	1:B:819:SER:HB3	1.74	0.69
1:F:206:ARG:N	1:F:1024:ASN:HD21	1.88	0.69
1:A:704:GLU:HG3	1:B:939:ARG:NH1	2.06	0.69
1:F:164:ARG:HB3	4:F:1076:HOH:O	1.91	0.69
1:D:557:ARG:HH22	1:D:562:GLU:N	1.91	0.69
2:J:1103:ARG:CB	2:J:1103:ARG:CD	2.68	0.69
1:E:596:LEU:HD11	1:E:662:LEU:HD11	1.73	0.69
1:F:289:LYS:HG2	4:F:1130:HOH:O	1.92	0.69
1:B:585:TYR:HE1	4:B:1084:HOH:O	1.76	0.69
1:D:202:TRP:CH2	1:D:745:SER:HB3	2.28	0.69
1:F:815:VAL:HA	1:F:819:SER:HB3	1.74	0.69
2:H:1103:ARG:CB	2:H:1103:ARG:CD	2.68	0.69
1:C:409:ALA:HA	4:C:1147:HOH:O	1.93	0.68
1:C:815:VAL:HA	1:C:819:SER:HB3	1.73	0.68
1:C:53:ILE:HD12	1:C:66:LEU:HD21	1.75	0.68
1:D:557:ARG:NE	1:F:393:ARG:HH12	1.91	0.68
1:A:82:ASN:HD22	1:A:82:ASN:H	1.40	0.68
1:A:190:ARG:HG3	1:A:216:GLU:OE2	1.93	0.68
1:A:278:LEU:HD23	1:A:287:PHE:HB3	1.76	0.68
1:C:202:TRP:CH2	1:C:745:SER:HB3	2.27	0.68
1:D:190:ARG:HG3	1:D:216:GLU:OE2	1.92	0.68
1:D:596:LEU:HD11	1:D:662:LEU:HD11	1.75	0.68
1:E:557:ARG:HH22	1:E:562:GLU:N	1.91	0.68
1:A:202:TRP:CH2	1:A:745:SER:HB3	2.29	0.68
1:E:82:ASN:H	1:E:82:ASN:HD22	1.39	0.68
1:B:82:ASN:HD22	1:B:82:ASN:H	1.38	0.68
1:F:82:ASN:H	1:F:82:ASN:HD22	1.39	0.68
1:C:736:VAL:HA	1:C:739:GLN:HE21	1.57	0.68
1:E:815:VAL:HA	1:E:819:SER:HB3	1.76	0.68
1:B:660:PHE:HB3	1:B:668:GLU:HB3	1.76	0.68
1:D:494:THR:HG21	1:D:500:ASP:CG	2.14	0.68
1:D:965:SER:HB3	2:J:1104:LYS:O	1.41	0.68
1:F:394:THR:HG21	4:F:1123:HOH:O	1.94	0.67
1:B:596:LEU:HD11	1:B:662:LEU:HD11	1.75	0.67
1:D:53:ILE:HD12	1:D:66:LEU:HD21	1.76	0.67
1:F:190:ARG:HG3	1:F:216:GLU:OE2	1.94	0.67
1:D:735:ILE:O	1:D:739:GLN:HG3	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:53:ILE:HD12	1:E:66:LEU:HD21	1.77	0.67
2:I:1104:LYS:O	4:I:320:HOH:O	2.12	0.67
1:C:278:LEU:HD23	1:C:287:PHE:HB3	1.77	0.67
1:C:735:ILE:O	1:C:739:GLN:HG3	1.94	0.67
1:F:278:LEU:HD23	1:F:287:PHE:HB3	1.76	0.67
1:B:206:ARG:N	1:B:1024:ASN:HD21	1.89	0.67
1:D:494:THR:CG2	1:D:500:ASP:OD1	2.43	0.67
1:E:570:ASP:N	4:E:1104:HOH:O	2.25	0.67
1:A:494:THR:HG21	1:A:500:ASP:CG	2.15	0.66
1:E:206:ARG:N	1:E:1024:ASN:HD21	1.92	0.66
1:E:948:THR:H	1:F:922:GLN:HE22	1.41	0.66
1:F:698:ARG:NH2	4:F:1108:HOH:O	2.29	0.66
1:A:704:GLU:HG3	1:B:939:ARG:HH11	1.59	0.66
1:B:190:ARG:HG3	1:B:216:GLU:OE2	1.95	0.66
1:C:155:PRO:O	1:C:856:ARG:HD2	1.94	0.66
1:C:180:ALA:C	4:C:1080:HOH:O	2.34	0.66
1:F:403:ASN:HD22	1:F:404:LEU:H	1.41	0.66
1:C:922:GLN:HE22	1:D:948:THR:H	1.42	0.66
1:C:948:THR:H	1:D:922:GLN:HE22	1.44	0.66
1:A:948:THR:H	1:B:922:GLN:NE2	1.94	0.66
1:B:127:LYS:HG2	4:B:1129:HOH:O	1.94	0.66
1:D:446:GLU:OE1	1:D:468:LYS:HD2	1.96	0.66
1:E:415:ASN:HB3	1:E:417:LYS:HD3	1.77	0.66
1:D:913:ARG:HH21	1:D:1047:GLN:NE2	1.92	0.66
1:E:190:ARG:HG3	1:E:216:GLU:OE2	1.96	0.66
1:D:268:THR:HG22	1:D:303:ILE:HD11	1.77	0.66
1:E:660:PHE:HB3	1:E:668:GLU:HB3	1.77	0.66
1:E:965:SER:HB3	2:K:1104:LYS:O	1.41	0.66
1:F:53:ILE:HD12	1:F:66:LEU:HD21	1.77	0.66
1:B:349:ASP:OD2	1:B:351:SER:HB3	1.95	0.66
1:A:362:LEU:HD13	1:A:688:GLN:HG3	1.79	0.65
1:D:629:VAL:HB	4:D:1121:HOH:O	1.96	0.65
1:F:660:PHE:HB3	1:F:668:GLU:HB3	1.78	0.65
1:F:735:ILE:O	1:F:739:GLN:HG3	1.96	0.65
1:F:913:ARG:HH21	1:F:1047:GLN:NE2	1.94	0.65
1:C:361:PRO:HG2	1:C:379:HIS:NE2	2.11	0.65
1:D:127:LYS:HE3	4:D:1099:HOH:O	1.96	0.65
1:E:218:ASN:O	4:E:1073:HOH:O	2.14	0.65
1:D:415:ASN:HB3	1:D:417:LYS:HD3	1.77	0.65
1:E:494:THR:HG21	1:E:500:ASP:CG	2.16	0.65
1:F:349:ASP:OD2	1:F:351:SER:HB3	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ARG:N	1:A:1024:ASN:HD21	1.90	0.65
1:B:278:LEU:HD23	1:B:287:PHE:HB3	1.78	0.65
1:C:236:VAL:HG23	1:C:243:TYR:HB2	1.79	0.65
1:C:415:ASN:HB3	1:C:417:LYS:HD3	1.77	0.65
1:F:202:TRP:CH2	1:F:745:SER:HB3	2.31	0.65
1:B:593:SER:O	1:B:624:VAL:HG22	1.95	0.65
1:F:430:THR:HG23	1:F:441:ILE:HD11	1.78	0.65
1:C:43:LEU:HD13	1:C:308:ILE:HD12	1.78	0.65
1:B:268:THR:HG22	1:B:303:ILE:HD11	1.77	0.65
1:B:430:THR:HG23	1:B:441:ILE:HD11	1.78	0.65
1:C:660:PHE:HB3	1:C:668:GLU:HB3	1.78	0.65
1:A:735:ILE:O	1:A:739:GLN:HG3	1.95	0.65
1:A:349:ASP:OD2	1:A:351:SER:HB3	1.96	0.65
1:A:948:THR:H	1:B:922:GLN:HE22	1.45	0.65
1:D:660:PHE:HB3	1:D:668:GLU:HB3	1.78	0.65
1:B:155:PRO:O	1:B:856:ARG:HD2	1.97	0.65
1:D:278:LEU:HD23	1:D:287:PHE:HB3	1.79	0.65
1:F:369:ARG:HD2	1:F:371:GLY:H	1.62	0.64
1:B:494:THR:HG21	1:B:500:ASP:CG	2.17	0.64
1:B:494:THR:CG2	1:B:500:ASP:OD1	2.45	0.64
1:E:913:ARG:HH21	1:E:1047:GLN:NE2	1.95	0.64
1:A:361:PRO:HG2	1:A:379:HIS:NE2	2.12	0.64
1:B:369:ARG:HD2	1:B:371:GLY:H	1.63	0.64
1:D:206:ARG:N	1:D:1024:ASN:HD21	1.95	0.64
1:E:268:THR:HG22	1:E:303:ILE:HD11	1.80	0.64
1:E:278:LEU:HD23	1:E:287:PHE:HB3	1.79	0.64
1:C:351:SER:CB	1:C:353:THR:HG22	2.28	0.64
1:D:213:ILE:HG13	4:D:1110:HOH:O	1.95	0.64
1:F:415:ASN:HB3	1:F:417:LYS:HD3	1.79	0.64
1:A:660:PHE:HB3	1:A:668:GLU:HB3	1.80	0.64
1:E:240:HIS:CD2	4:E:1148:HOH:O	2.51	0.64
1:A:53:ILE:HD12	1:A:66:LEU:HD21	1.80	0.64
1:B:53:ILE:HD12	1:B:66:LEU:HD21	1.78	0.64
1:F:494:THR:HG21	1:F:500:ASP:CG	2.18	0.63
1:A:913:ARG:HH21	1:A:1047:GLN:NE2	1.96	0.63
1:C:494:THR:HG21	1:C:500:ASP:CG	2.19	0.63
1:F:361:PRO:HG2	1:F:379:HIS:NE2	2.12	0.63
1:A:268:THR:HG22	1:A:303:ILE:HD11	1.79	0.63
1:F:510:LYS:O	4:F:1109:HOH:O	2.15	0.63
1:C:766:ALA:HB3	1:C:793:SER:HA	1.79	0.63
1:B:415:ASN:HB3	1:B:417:LYS:HD3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:362:LEU:HD13	1:D:688:GLN:HG3	1.80	0.63
1:D:745:SER:OG	4:D:1088:HOH:O	2.14	0.63
1:E:369:ARG:HD2	1:E:371:GLY:H	1.62	0.63
1:E:766:ALA:HB3	1:E:793:SER:HA	1.80	0.63
1:E:46:PRO:HB2	1:E:286:LEU:CD2	2.29	0.63
1:E:735:ILE:O	1:E:739:GLN:HG3	1.98	0.63
1:A:155:PRO:O	1:A:856:ARG:HD2	1.98	0.63
1:D:43:LEU:HD13	1:D:308:ILE:HD12	1.79	0.63
1:F:498:SER:HB2	4:F:1088:HOH:O	1.98	0.63
1:A:494:THR:CG2	1:A:500:ASP:OD1	2.47	0.63
1:D:369:ARG:HD2	1:D:371:GLY:H	1.62	0.63
1:D:562:GLU:HB2	4:D:1148:HOH:O	1.98	0.63
1:E:362:LEU:HD13	1:E:688:GLN:HG3	1.81	0.63
1:E:494:THR:CG2	1:E:500:ASP:OD1	2.46	0.63
1:C:190:ARG:HG3	1:C:216:GLU:OE2	1.99	0.62
1:C:268:THR:HG22	1:C:303:ILE:HD11	1.80	0.62
1:C:430:THR:HG23	1:C:441:ILE:HD11	1.81	0.62
1:C:913:ARG:HH21	1:C:1047:GLN:NE2	1.97	0.62
1:D:991:VAL:N	4:D:1088:HOH:O	2.31	0.62
1:F:766:ALA:HB3	1:F:793:SER:HA	1.80	0.62
1:B:774:ASP:HA	1:B:817:ALA:HB2	1.80	0.62
1:C:91:ARG:HH11	1:C:114:GLU:HB2	1.64	0.62
1:E:43:LEU:HD13	1:E:308:ILE:HD12	1.82	0.62
1:E:155:PRO:O	1:E:856:ARG:HD2	1.98	0.62
1:A:537:SER:HB3	1:A:583:GLY:O	1.99	0.62
1:C:369:ARG:HD2	1:C:371:GLY:H	1.64	0.62
1:A:430:THR:HG23	1:A:441:ILE:HD11	1.81	0.62
1:C:242:ILE:O	1:C:256:SER:HA	2.00	0.62
1:F:982:LEU:C	1:F:983:ILE:HD12	2.20	0.62
1:B:46:PRO:HB2	1:B:286:LEU:CD2	2.30	0.62
1:B:1055:LEU:O	1:B:1059:LEU:HD13	1.99	0.62
1:A:369:ARG:HD2	1:A:371:GLY:H	1.63	0.62
1:D:155:PRO:O	1:D:856:ARG:HD2	2.00	0.62
1:F:268:THR:HG22	1:F:303:ILE:HD11	1.81	0.62
1:C:393:ARG:HH12	1:E:557:ARG:NE	1.98	0.62
1:C:1055:LEU:HD23	4:C:1137:HOH:O	1.99	0.62
1:E:430:THR:HG23	1:E:441:ILE:HD11	1.81	0.62
1:E:789:GLU:HG3	1:F:577:PRO:HG3	1.81	0.62
1:F:236:VAL:HG23	1:F:243:TYR:HB2	1.81	0.62
1:A:46:PRO:HB2	1:A:286:LEU:CD2	2.30	0.62
1:A:82:ASN:HD21	1:A:96:ARG:HH21	1.48	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:382:ARG:HA	4:B:1126:HOH:O	1.99	0.62
1:F:43:LEU:HD13	1:F:308:ILE:HD12	1.82	0.62
1:A:43:LEU:HD13	1:A:308:ILE:HD12	1.81	0.61
1:C:46:PRO:HB2	1:C:286:LEU:CD2	2.30	0.61
1:D:351:SER:CB	1:D:353:THR:HG22	2.30	0.61
1:E:361:PRO:HG2	1:E:379:HIS:NE2	2.15	0.61
1:D:557:ARG:HG3	1:F:393:ARG:HH22	1.64	0.61
1:B:622:TYR:OH	1:B:627:ARG:HG2	2.01	0.61
1:E:534:GLU:N	4:E:1114:HOH:O	2.32	0.61
1:C:994:ILE:HD12	1:C:1007:THR:HB	1.82	0.61
1:F:593:SER:O	1:F:624:VAL:HG22	2.00	0.61
1:A:91:ARG:HH11	1:A:114:GLU:HB2	1.65	0.61
1:A:235:PRO:O	4:A:1126:HOH:O	2.16	0.61
1:A:253:GLN:HE22	1:A:270:PHE:H	1.48	0.61
1:C:423:ASN:ND2	1:C:427:GLU:H	1.98	0.61
1:B:913:ARG:HH21	1:B:1047:GLN:NE2	1.98	0.61
1:E:43:LEU:HD22	1:E:55:PHE:CE1	2.35	0.61
1:E:188:GLY:HA2	4:E:1119:HOH:O	2.00	0.61
1:B:82:ASN:HD21	1:B:96:ARG:HH21	1.47	0.61
1:B:362:LEU:HD13	1:B:688:GLN:HG3	1.82	0.61
1:C:446:GLU:OE1	1:C:468:LYS:HD2	2.00	0.61
1:F:351:SER:CB	1:F:353:THR:HG22	2.30	0.61
1:B:361:PRO:HG2	1:B:379:HIS:NE2	2.16	0.61
1:C:593:SER:O	1:C:624:VAL:HG22	2.00	0.61
1:A:415:ASN:HB3	1:A:417:LYS:HD3	1.81	0.61
1:C:982:LEU:C	1:C:983:ILE:HD12	2.21	0.61
1:F:242:ILE:O	1:F:256:SER:HA	2.01	0.61
1:B:43:LEU:HD13	1:B:308:ILE:HD12	1.83	0.61
1:F:46:PRO:HB2	1:F:286:LEU:CD2	2.30	0.61
1:A:593:SER:O	1:A:624:VAL:HG22	2.01	0.60
1:E:423:ASN:HD21	1:E:427:GLU:H	1.48	0.60
1:F:423:ASN:ND2	1:F:427:GLU:H	1.99	0.60
1:F:774:ASP:HA	1:F:817:ALA:HB2	1.83	0.60
1:D:423:ASN:ND2	1:D:427:GLU:H	2.00	0.60
1:B:766:ALA:HB3	1:B:793:SER:HA	1.81	0.60
1:D:593:SER:O	1:D:624:VAL:HG22	2.00	0.60
1:E:351:SER:CB	1:E:353:THR:HG22	2.31	0.60
1:F:362:LEU:HD13	1:F:688:GLN:HG3	1.82	0.60
1:C:423:ASN:HD21	1:C:427:GLU:H	1.48	0.60
1:D:91:ARG:HH11	1:D:114:GLU:HB2	1.65	0.60
1:D:766:ALA:HB3	1:D:793:SER:HA	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:774:ASP:HA	1:D:817:ALA:HB2	1.83	0.60
1:E:446:GLU:OE1	1:E:468:LYS:HD2	2.01	0.60
1:F:446:GLU:OE1	1:F:468:LYS:HD2	2.01	0.60
1:A:1055:LEU:O	1:A:1059:LEU:HD13	2.02	0.60
1:C:46:PRO:HB2	1:C:286:LEU:HD21	1.83	0.60
1:C:605:GLU:HG3	1:D:524:PRO:HD3	1.82	0.60
1:E:236:VAL:HG23	1:E:243:TYR:HB2	1.84	0.60
1:E:423:ASN:ND2	1:E:427:GLU:H	1.99	0.60
1:F:306:ILE:HG13	4:F:1139:HOH:O	2.01	0.60
1:A:939:ARG:NH1	1:B:704:GLU:HG3	2.16	0.60
1:C:362:LEU:HD13	1:C:688:GLN:HG3	1.83	0.60
1:E:82:ASN:HD21	1:E:96:ARG:HH21	1.49	0.60
1:F:91:ARG:HH11	1:F:114:GLU:HB2	1.64	0.60
1:F:423:ASN:HD21	1:F:427:GLU:H	1.50	0.60
1:F:537:SER:HB3	1:F:583:GLY:O	2.01	0.60
1:F:721:LEU:N	4:F:1121:HOH:O	2.34	0.60
1:F:994:ILE:HD12	1:F:1007:THR:HB	1.83	0.60
1:A:559:MET:HG2	1:E:356:LEU:HD11	1.84	0.60
1:C:43:LEU:HD22	1:C:55:PHE:CE1	2.37	0.60
1:D:361:PRO:HG2	1:D:379:HIS:NE2	2.16	0.60
1:B:351:SER:CB	1:B:353:THR:HG22	2.31	0.60
1:F:253:GLN:HE22	1:F:270:PHE:H	1.49	0.60
1:C:218:ASN:HB3	1:C:221:ALA:HB3	1.83	0.60
1:D:1055:LEU:O	1:D:1059:LEU:HD13	2.02	0.60
1:E:91:ARG:HH11	1:E:114:GLU:HB2	1.65	0.60
1:F:53:ILE:HG23	1:F:286:LEU:HD21	1.84	0.60
1:A:423:ASN:ND2	1:A:427:GLU:H	2.00	0.59
1:B:556:PRO:HD3	1:D:354:TYR:CD1	2.37	0.59
1:C:774:ASP:HA	1:C:817:ALA:HB2	1.84	0.59
1:D:43:LEU:HD22	1:D:55:PHE:CE1	2.37	0.59
1:D:286:LEU:HD12	1:D:294:TYR:O	2.02	0.59
1:E:253:GLN:HE22	1:E:270:PHE:H	1.50	0.59
1:E:524:PRO:HD3	1:F:605:GLU:HG3	1.83	0.59
1:A:236:VAL:HG23	1:A:243:TYR:HB2	1.84	0.59
1:B:46:PRO:HB2	1:B:286:LEU:HD21	1.84	0.59
1:E:622:TYR:OH	1:E:627:ARG:HG2	2.03	0.59
1:B:582:PRO:HA	4:B:1084:HOH:O	2.01	0.59
1:C:550:ASN:HB3	1:C:553:LYS:HG3	1.84	0.59
1:D:131:ARG:NH1	4:D:1145:HOH:O	2.35	0.59
1:E:286:LEU:HD12	1:E:294:TYR:O	2.03	0.59
1:A:774:ASP:HA	1:A:817:ALA:HB2	1.84	0.59

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:B:242:ILE:O	1:B:256:SER:HA	2.02	0.59
1:B:982:LEU:C	1:B:983:ILE:HD12	2.22	0.59
1:C:104:ASN:ND2	4:C:1126:HOH:O	2.36	0.59
1:D:236:VAL:HG23	1:D:243:TYR:HB2	1.83	0.59
1:B:363:ARG:HB2	4:B:1103:HOH:O	2.03	0.59
1:E:46:PRO:HB2	1:E:286:LEU:HD21	1.84	0.59
1:F:622:TYR:OH	1:F:627:ARG:HG2	2.02	0.59
1:E:242:ILE:O	1:E:256:SER:HA	2.03	0.59
1:E:780:LYS:HD3	1:E:782:TYR:CZ	2.37	0.59
1:A:622:TYR:OH	1:A:627:ARG:HG2	2.03	0.59
1:B:43:LEU:HD22	1:B:55:PHE:CE1	2.38	0.59
1:D:959:THR:O	1:D:984:GLY:HA3	2.03	0.59
1:A:351:SER:CB	1:A:353:THR:HG22	2.33	0.59
1:A:423:ASN:HD21	1:A:427:GLU:H	1.51	0.59
1:A:677:PRO:HD2	1:D:827:GLU:O	2.03	0.59
1:A:930:ASN:HD21	1:B:926:GLU:HG3	1.67	0.59
1:B:236:VAL:HG23	1:B:243:TYR:HB2	1.85	0.59
1:C:703:ASN:HD22	1:C:703:ASN:C	2.06	0.59
1:D:965:SER:O	1:D:968:ASP:HB2	2.03	0.59
1:A:939:ARG:HH11	1:B:704:GLU:HG3	1.68	0.59
1:C:780:LYS:HD3	1:C:782:TYR:CZ	2.38	0.59
1:C:922:GLN:NE2	1:D:948:THR:H	2.00	0.59
1:E:703:ASN:OD1	1:E:706:VAL:HG23	2.03	0.59
1:B:91:ARG:HH11	1:B:114:GLU:HB2	1.67	0.59
1:A:959:THR:O	1:A:984:GLY:HA3	2.03	0.58
1:C:1055:LEU:O	1:C:1059:LEU:HD13	2.03	0.58
1:D:53:ILE:HG23	1:D:286:LEU:HD21	1.85	0.58
1:D:423:ASN:HD21	1:D:427:GLU:H	1.49	0.58
1:F:703:ASN:C	1:F:703:ASN:HD22	2.03	0.58
1:E:537:SER:HB3	1:E:583:GLY:O	2.02	0.58
1:E:593:SER:O	1:E:624:VAL:HG22	2.03	0.58
1:E:739:GLN:NE2	4:E:1072:HOH:O	2.36	0.58
1:C:788:ASN:ND2	4:C:1107:HOH:O	2.35	0.58
1:D:46:PRO:HB2	1:D:286:LEU:CD2	2.32	0.58
1:D:218:ASN:HB3	1:D:221:ALA:HB3	1.86	0.58
1:D:537:SER:HB3	1:D:583:GLY:O	2.03	0.58
1:E:997:LYS:HB2	3:K:2101:D10:H91	1.84	0.58
1:F:218:ASN:HB3	1:F:221:ALA:HB3	1.85	0.58
1:B:423:ASN:HD21	1:B:427:GLU:H	1.52	0.58
1:E:736:VAL:HG22	4:E:1072:HOH:O	2.03	0.58
1:A:719:ARG:HH21	1:A:719:ARG:HG2	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:GLN:HE22	1:C:270:PHE:H	1.50	0.58
1:C:537:SER:HB3	1:C:583:GLY:O	2.03	0.58
1:E:982:LEU:C	1:E:983:ILE:HD12	2.23	0.58
1:F:494:THR:CG2	1:F:500:ASP:OD1	2.50	0.58
1:A:766:ALA:HB3	1:A:793:SER:HA	1.84	0.58
1:C:948:THR:H	1:D:922:GLN:NE2	2.00	0.58
1:F:155:PRO:O	1:F:856:ARG:HD2	2.04	0.58
1:A:46:PRO:HB2	1:A:286:LEU:HD21	1.86	0.58
1:A:242:ILE:O	1:A:256:SER:HA	2.03	0.58
1:B:286:LEU:HD12	1:B:294:TYR:O	2.03	0.58
1:D:82:ASN:HD21	1:D:96:ARG:HH21	1.52	0.58
1:D:703:ASN:C	1:D:703:ASN:HD22	2.06	0.58
1:D:992:VAL:N	4:D:1088:HOH:O	2.36	0.58
1:B:423:ASN:ND2	1:B:427:GLU:H	2.01	0.58
1:D:982:LEU:C	1:D:983:ILE:HD12	2.23	0.58
1:E:415:ASN:HD22	1:E:417:LYS:HD2	1.68	0.58
1:F:43:LEU:HD22	1:F:55:PHE:CE1	2.39	0.58
1:C:524:PRO:HD3	1:D:605:GLU:HG3	1.85	0.58
1:E:53:ILE:HG23	1:E:286:LEU:HD21	1.85	0.58
1:F:890:MET:O	1:F:894:GLU:HG2	2.04	0.58
1:B:218:ASN:HB3	1:B:221:ALA:HB3	1.85	0.58
1:E:774:ASP:HA	1:E:817:ALA:HB2	1.84	0.58
1:F:492:ALA:O	4:F:1110:HOH:O	2.16	0.58
1:F:959:THR:O	1:F:984:GLY:HA3	2.03	0.58
1:A:218:ASN:HB3	1:A:221:ALA:HB3	1.85	0.57
1:E:789:GLU:N	4:E:1112:HOH:O	2.37	0.57
1:E:959:THR:O	1:E:984:GLY:HA3	2.03	0.57
1:F:739:GLN:NE2	4:F:1087:HOH:O	2.37	0.57
1:A:43:LEU:HD22	1:A:55:PHE:CE1	2.38	0.57
1:A:446:GLU:OE1	1:A:468:LYS:HD2	2.04	0.57
1:D:253:GLN:HE22	1:D:270:PHE:H	1.51	0.57
1:D:415:ASN:HD22	1:D:417:LYS:CD	2.18	0.57
1:E:681:SER:O	1:E:684:GLU:HG2	2.04	0.57
1:F:46:PRO:HB2	1:F:286:LEU:HD21	1.85	0.57
1:F:753:THR:HG23	4:F:1106:HOH:O	2.02	0.57
1:B:537:SER:HB3	1:B:583:GLY:O	2.04	0.57
1:C:61:LEU:HB3	1:C:75:VAL:CG1	2.34	0.57
1:F:499:HIS:HD2	4:F:1080:HOH:O	1.87	0.57
1:F:746:HIS:HE1	1:F:990:GLY:O	1.87	0.57
1:A:53:ILE:HG23	1:A:286:LEU:HD21	1.85	0.57
1:C:494:THR:CG2	1:C:500:ASP:OD1	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:558:SER:CA	1:F:393:ARG:HD2	2.33	0.57
1:E:131:ARG:HD2	4:E:1085:HOH:O	2.03	0.57
1:A:943:LEU:HG	4:A:1095:HOH:O	2.04	0.57
1:D:430:THR:HG23	1:D:441:ILE:HD11	1.84	0.57
1:E:703:ASN:HD22	1:E:703:ASN:C	2.08	0.57
1:E:948:THR:H	1:F:922:GLN:NE2	2.02	0.57
1:A:982:LEU:C	1:A:983:ILE:HD12	2.25	0.57
1:B:253:GLN:HE22	1:B:270:PHE:H	1.51	0.57
1:C:286:LEU:HD12	1:C:294:TYR:O	2.04	0.57
1:B:61:LEU:HB3	1:B:75:VAL:CG1	2.34	0.57
1:C:530:ASN:HD21	1:D:530:ASN:HD21	1.52	0.57
1:D:703:ASN:OD1	1:D:706:VAL:HG23	2.04	0.57
1:E:530:ASN:HD21	1:F:530:ASN:HD21	1.53	0.57
1:E:1055:LEU:O	1:E:1059:LEU:HD13	2.04	0.57
1:F:714:ILE:HG21	1:F:741:GLU:HB3	1.87	0.57
1:D:997:LYS:HB2	3:J:2101:D10:H91	1.86	0.57
1:C:622:TYR:OH	1:C:627:ARG:HG2	2.05	0.57
1:D:415:ASN:HD22	1:D:417:LYS:HD2	1.70	0.57
1:E:415:ASN:HD22	1:E:417:LYS:CD	2.18	0.57
1:B:473:ASP:N	4:B:1146:HOH:O	2.38	0.56
1:B:516:SER:HB2	1:B:518:ARG:HG3	1.85	0.56
1:B:719:ARG:HG2	1:B:719:ARG:HH21	1.69	0.56
1:B:959:THR:O	1:B:984:GLY:HA3	2.05	0.56
1:B:559:MET:SD	1:D:354:TYR:HB3	2.45	0.56
1:C:959:THR:O	1:C:984:GLY:HA3	2.05	0.56
1:E:292:SER:HB2	1:E:294:TYR:HE1	1.70	0.56
1:A:415:ASN:HD22	1:A:417:LYS:CD	2.18	0.56
1:C:139:GLY:HA3	4:C:1079:HOH:O	2.06	0.56
1:C:415:ASN:HD22	1:C:417:LYS:HD2	1.71	0.56
1:D:46:PRO:HB2	1:D:286:LEU:HD21	1.87	0.56
1:D:128:SER:HB2	1:D:133:MET:HA	1.87	0.56
1:D:994:ILE:HD12	1:D:1007:THR:HB	1.87	0.56
1:E:990:GLY:HA2	1:E:1023:GLU:OE2	2.06	0.56
1:F:61:LEU:HB3	1:F:75:VAL:CG1	2.35	0.56
1:B:415:ASN:HD22	1:B:417:LYS:HD2	1.71	0.56
1:B:997:LYS:HB2	3:H:2101:D10:H91	1.85	0.56
1:E:61:LEU:HD13	1:E:74:ILE:HD11	1.88	0.56
1:E:347:ILE:HG12	1:E:392:TYR:CD2	2.41	0.56
1:F:286:LEU:HD12	1:F:294:TYR:O	2.04	0.56
1:C:746:HIS:HE1	1:C:990:GLY:O	1.88	0.56
1:D:511:ASN:ND2	1:D:543:PRO:HB3	2.20	0.56

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:A:415:ASN:HD22	1:A:417:LYS:HD2	1.70	0.56
1:A:681:SER:O	1:A:684:GLU:HG2	2.06	0.56
1:B:347:ILE:HG12	1:B:392:TYR:CD2	2.40	0.56
1:C:200:PRO:O	1:C:740:GLY:HA3	2.05	0.56
1:C:997:LYS:HB2	3:I:2101:D10:H91	1.87	0.56
1:E:904:SER:HB2	1:F:473:ASP:OD1	2.04	0.56
1:E:983:ILE:HG23	1:E:1033:ILE:HD13	1.86	0.56
1:C:639:LEU:HG	1:C:650:VAL:HG12	1.87	0.56
1:A:292:SER:HB2	1:A:294:TYR:HE1	1.71	0.56
1:A:997:LYS:HB2	3:G:2101:D10:H91	1.87	0.56
1:C:582:PRO:O	4:C:1131:HOH:O	2.18	0.56
1:F:719:ARG:HG2	1:F:719:ARG:HH21	1.71	0.56
1:B:710:ILE:O	1:B:714:ILE:HG12	2.06	0.56
1:F:350:VAL:N	4:F:1100:HOH:O	2.35	0.56
1:A:87:PHE:HB3	1:A:88:PRO:HD2	1.88	0.56
1:C:182:HIS:CD2	4:C:1133:HOH:O	2.57	0.56
1:E:639:LEU:HG	1:E:650:VAL:HG12	1.88	0.56
1:E:994:ILE:HD12	1:E:1007:THR:HB	1.88	0.56
1:D:681:SER:O	1:D:684:GLU:HG2	2.06	0.55
1:A:61:LEU:HB3	1:A:75:VAL:CG1	2.36	0.55
1:A:780:LYS:HD3	1:A:782:TYR:CZ	2.40	0.55
1:B:297:ASN:HB2	4:B:1124:HOH:O	2.04	0.55
1:B:677:PRO:HD2	1:E:827:GLU:O	2.07	0.55
1:B:53:ILE:HG23	1:B:286:LEU:HD21	1.89	0.55
1:B:681:SER:O	1:B:684:GLU:HG2	2.07	0.55
1:C:473:ASP:OD1	1:D:904:SER:HB2	2.06	0.55
1:C:719:ARG:HG2	1:C:719:ARG:HH21	1.70	0.55
1:D:61:LEU:HD13	1:D:74:ILE:HD11	1.87	0.55
1:E:243:TYR:CD2	1:E:256:SER:HB3	2.41	0.55
1:D:242:ILE:O	1:D:256:SER:HA	2.05	0.55
1:E:516:SER:HB2	1:E:518:ARG:HG3	1.88	0.55
1:E:965:SER:O	1:E:968:ASP:HB2	2.04	0.55
1:B:132:ARG:HD2	1:B:134:PHE:CZ	2.42	0.55
1:D:138:ALA:HB1	1:D:183:ILE:HG22	1.88	0.55
1:E:868:ARG:HH12	1:F:497:ASN:ND2	2.04	0.55
1:F:550:ASN:HB3	1:F:553:LYS:HG3	1.89	0.55
1:F:698:ARG:HD2	4:F:1108:HOH:O	2.06	0.55
1:F:703:ASN:HD22	1:F:704:GLU:N	2.04	0.55
1:A:951:VAL:HG23	4:A:1175:HOH:O	2.07	0.55
1:D:622:TYR:OH	1:D:627:ARG:HG2	2.05	0.55
1:E:128:SER:HB2	1:E:133:MET:HA	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:746:HIS:HE1	1:E:990:GLY:O	1.90	0.55
1:E:91:ARG:HB3	4:E:1147:HOH:O	2.06	0.55
1:E:292:SER:HB2	1:E:294:TYR:CE1	2.42	0.55
1:A:243:TYR:CD2	1:A:256:SER:HB3	2.41	0.55
1:A:994:ILE:HD12	1:A:1007:THR:HB	1.89	0.55
1:C:714:ILE:HG21	1:C:741:GLU:HB3	1.88	0.55
1:D:890:MET:O	1:D:894:GLU:HG2	2.07	0.55
1:E:82:ASN:HD22	1:E:82:ASN:N	2.04	0.55
1:E:403:ASN:HD22	1:E:403:ASN:C	2.10	0.55
1:A:347:ILE:HG12	1:A:392:TYR:CD2	2.42	0.55
1:D:425:ARG:O	1:D:426:PHE:HB2	2.07	0.55
1:E:367:VAL:CG1	1:E:375:VAL:HG21	2.36	0.55
1:F:415:ASN:HD22	1:F:417:LYS:HD2	1.71	0.55
1:F:639:LEU:HG	1:F:650:VAL:HG12	1.89	0.55
1:D:780:LYS:HD3	1:D:782:TYR:CZ	2.42	0.55
1:E:218:ASN:HB3	1:E:221:ALA:HB3	1.89	0.55
1:A:556:PRO:HD3	1:E:354:TYR:CD1	2.42	0.54
1:B:415:ASN:HD22	1:B:417:LYS:CD	2.20	0.54
1:B:511:ASN:ND2	1:B:543:PRO:HB3	2.22	0.54
1:C:528:VAL:HG21	1:C:896:TYR:CD2	2.42	0.54
1:D:91:ARG:CZ	4:D:1132:HOH:O	2.55	0.54
1:A:82:ASN:HD22	1:A:82:ASN:N	2.04	0.54
1:A:511:ASN:ND2	1:A:543:PRO:HB3	2.22	0.54
1:A:714:ILE:HG21	1:A:741:GLU:HB3	1.88	0.54
1:A:889:MET:SD	1:B:522:PRO:HG2	2.48	0.54
1:B:61:LEU:HD13	1:B:74:ILE:HD11	1.88	0.54
1:C:516:SER:HB2	1:C:518:ARG:HG3	1.89	0.54
1:C:703:ASN:OD1	1:C:706:VAL:HG23	2.07	0.54
1:D:82:ASN:HD22	1:D:82:ASN:N	2.05	0.54
1:D:703:ASN:HD22	1:D:704:GLU:N	2.06	0.54
1:F:997:LYS:HB2	3:L:2101:D10:H91	1.87	0.54
1:A:791:GLU:CD	1:A:861:ARG:HE	2.10	0.54
1:B:639:LEU:HG	1:B:650:VAL:HG12	1.89	0.54
1:B:965:SER:O	1:B:968:ASP:HB2	2.07	0.54
1:C:473:ASP:HA	1:D:904:SER:OG	2.06	0.54
1:C:681:SER:O	1:C:684:GLU:HG2	2.06	0.54
1:F:87:PHE:HB3	1:F:88:PRO:HD2	1.89	0.54
1:F:200:PRO:O	1:F:740:GLY:HA3	2.06	0.54
1:B:40:PRO:HG2	1:B:724:LEU:CD2	2.36	0.54
1:B:446:GLU:OE1	1:B:468:LYS:HD2	2.07	0.54
1:B:746:HIS:HE1	1:B:990:GLY:O	1.91	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:200:PRO:O	1:D:740:GLY:HA3	2.07	0.54
1:D:220:GLY:HA2	4:D:1105:HOH:O	2.08	0.54
1:E:511:ASN:ND2	1:E:543:PRO:HB3	2.23	0.54
1:A:200:PRO:O	1:A:740:GLY:HA3	2.08	0.54
1:A:703:ASN:C	1:A:703:ASN:HD22	2.09	0.54
1:C:347:ILE:HG12	1:C:392:TYR:CD2	2.43	0.54
1:C:415:ASN:HD22	1:C:417:LYS:CD	2.21	0.54
1:C:890:MET:O	1:C:894:GLU:HG2	2.07	0.54
1:B:555:VAL:HG22	1:D:354:TYR:OH	2.08	0.54
1:A:292:SER:HB2	1:A:294:TYR:CE1	2.42	0.54
1:A:922:GLN:NE2	1:B:948:THR:H	2.05	0.54
1:C:292:SER:HB2	1:C:294:TYR:HE1	1.73	0.54
1:D:243:TYR:CD2	1:D:256:SER:HB3	2.42	0.54
1:D:810:ILE:HD12	4:D:1122:HOH:O	2.06	0.54
1:E:714:ILE:HG21	1:E:741:GLU:HB3	1.90	0.54
1:F:1055:LEU:O	1:F:1059:LEU:HD13	2.07	0.54
1:C:281:ASP:HA	4:C:1102:HOH:O	2.08	0.54
1:A:403:ASN:HD22	1:A:405:GLY:H	1.56	0.54
1:A:897:ARG:HG2	1:A:898:LEU:HD12	1.89	0.54
1:B:82:ASN:HD22	1:B:82:ASN:N	2.05	0.54
1:B:703:ASN:C	1:B:703:ASN:HD22	2.10	0.54
1:A:106:ALA:HB3	4:A:1170:HOH:O	2.07	0.53
1:B:714:ILE:HG21	1:B:741:GLU:HB3	1.89	0.53
1:C:468:LYS:HE3	1:C:476:VAL:HG22	1.90	0.53
1:C:511:ASN:ND2	1:C:543:PRO:HB3	2.23	0.53
1:D:61:LEU:HB3	1:D:75:VAL:CG1	2.38	0.53
1:D:639:LEU:HG	1:D:650:VAL:HG12	1.90	0.53
1:D:719:ARG:HH21	1:D:719:ARG:HG2	1.73	0.53
1:F:703:ASN:C	1:F:703:ASN:ND2	2.62	0.53
1:A:710:ILE:HD13	1:A:742:TYR:HA	1.90	0.53
1:D:367:VAL:CG1	1:D:375:VAL:HG21	2.39	0.53
1:D:990:GLY:HA2	1:D:1023:GLU:OE2	2.08	0.53
1:A:516:SER:HB2	1:A:518:ARG:HG3	1.91	0.53
1:B:292:SER:HB2	1:B:294:TYR:CE1	2.44	0.53
1:C:565:GLU:HG3	4:C:1157:HOH:O	2.08	0.53
1:F:511:ASN:ND2	1:F:543:PRO:HB3	2.22	0.53
1:F:791:GLU:CD	1:F:861:ARG:HE	2.11	0.53
1:A:152:ALA:HB1	1:A:764:ARG:HH12	1.74	0.53
1:B:951:VAL:HG23	4:B:1141:HOH:O	2.07	0.53
1:E:61:LEU:HB3	1:E:75:VAL:CG1	2.38	0.53
1:F:425:ARG:O	1:F:426:PHE:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:530:ASN:HB3	4:F:1112:HOH:O	2.08	0.53
1:A:286:LEU:HD12	1:A:294:TYR:O	2.07	0.53
2:G:1103:ARG:CG	4:G:440:HOH:O	2.50	0.53
1:B:990:GLY:HA2	1:B:1023:GLU:OE2	2.09	0.53
1:F:780:LYS:HD3	1:F:782:TYR:CZ	2.42	0.53
1:B:200:PRO:O	1:B:740:GLY:HA3	2.08	0.53
1:C:53:ILE:HG23	1:C:286:LEU:HD21	1.89	0.53
1:A:703:ASN:HD22	1:A:704:GLU:N	2.06	0.53
1:B:425:ARG:O	1:B:426:PHE:HB2	2.09	0.53
1:C:727:THR:HB	4:C:1103:HOH:O	2.08	0.53
1:C:904:SER:OG	1:D:473:ASP:HA	2.09	0.53
1:D:714:ILE:HG21	1:D:741:GLU:HB3	1.91	0.53
1:B:292:SER:HB2	1:B:294:TYR:HE1	1.73	0.53
1:C:425:ARG:O	1:C:426:PHE:HB2	2.09	0.53
1:F:173:VAL:CB	4:F:1076:HOH:O	2.41	0.53
1:A:965:SER:O	1:A:968:ASP:HB2	2.09	0.53
1:B:243:TYR:CD2	1:B:256:SER:HB3	2.44	0.53
1:B:550:ASN:HB3	1:B:553:LYS:HG3	1.91	0.53
1:B:791:GLU:CD	1:B:861:ARG:HE	2.11	0.53
1:C:132:ARG:HD2	1:C:134:PHE:CZ	2.43	0.53
1:D:347:ILE:HG12	1:D:392:TYR:CD2	2.44	0.53
1:D:746:HIS:HE1	1:D:990:GLY:O	1.91	0.53
1:F:516:SER:HB2	1:F:518:ARG:HG3	1.90	0.53
1:F:681:SER:O	1:F:684:GLU:HG2	2.08	0.53
1:B:994:ILE:HD12	1:B:1007:THR:HB	1.91	0.53
1:C:128:SER:HB2	1:C:133:MET:HA	1.91	0.53
1:D:91:ARG:NH1	4:D:1132:HOH:O	2.42	0.53
1:A:40:PRO:HG2	1:A:724:LEU:CD2	2.39	0.52
1:A:639:LEU:HG	1:A:650:VAL:HG12	1.90	0.52
1:C:138:ALA:HB1	1:C:183:ILE:HG22	1.92	0.52
1:C:243:TYR:CD2	1:C:256:SER:HB3	2.44	0.52
1:E:529:LEU:O	1:E:529:LEU:HG	2.09	0.52
1:A:132:ARG:HD2	1:A:134:PHE:CZ	2.44	0.52
1:A:425:ARG:O	1:A:426:PHE:HB2	2.08	0.52
1:B:494:THR:HG22	1:B:495:THR:N	2.25	0.52
1:B:513:TYR:HB3	1:B:588:ILE:HD13	1.91	0.52
1:C:87:PHE:HB3	1:C:88:PRO:HD2	1.90	0.52
1:E:152:ALA:HB1	1:E:764:ARG:HH12	1.72	0.52
1:F:557:ARG:HH22	1:F:562:GLU:HB2	1.74	0.52
1:F:703:ASN:OD1	1:F:706:VAL:HG23	2.09	0.52
1:B:997:LYS:HB3	3:H:2101:D10:H71	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1052:ILE:O	1:B:1056:ILE:HG13	2.09	0.52
1:E:425:ARG:O	1:E:426:PHE:HB2	2.09	0.52
1:C:897:ARG:CD	4:C:1107:HOH:O	2.48	0.52
1:D:152:ALA:HB1	1:D:764:ARG:HH12	1.73	0.52
1:E:138:ALA:HB1	1:E:183:ILE:HG22	1.90	0.52
1:E:687:LEU:HD23	1:E:722:VAL:HG11	1.91	0.52
1:E:904:SER:OG	1:F:473:ASP:HA	2.09	0.52
1:A:550:ASN:HB3	1:A:553:LYS:HG3	1.91	0.52
1:E:913:ARG:NH2	1:E:1047:GLN:HE21	2.06	0.52
1:A:990:GLY:HA2	1:A:1023:GLU:OE2	2.10	0.52
1:B:128:SER:HB2	1:B:133:MET:HA	1.91	0.52
1:B:780:LYS:HD3	1:B:782:TYR:CZ	2.43	0.52
1:C:292:SER:HB2	1:C:294:TYR:CE1	2.44	0.52
1:E:890:MET:O	1:E:894:GLU:HG2	2.08	0.52
1:F:415:ASN:HD22	1:F:417:LYS:CD	2.21	0.52
1:A:538:LYS:HD2	4:B:1133:HOH:O	2.08	0.52
1:D:513:TYR:HB3	1:D:588:ILE:HD13	1.92	0.52
1:D:744:THR:HG22	1:D:745:SER:N	2.24	0.52
1:F:128:SER:HB2	1:F:133:MET:HA	1.92	0.52
1:F:197:PHE:HE1	1:F:199:LEU:HD21	1.74	0.52
1:D:557:ARG:NH2	4:D:1148:HOH:O	2.43	0.52
1:A:746:HIS:HE1	1:A:990:GLY:O	1.92	0.52
1:B:367:VAL:CG1	1:B:375:VAL:HG21	2.40	0.52
1:B:897:ARG:HG2	1:B:898:LEU:HD12	1.91	0.52
1:D:710:ILE:HD13	1:D:742:TYR:HA	1.91	0.52
1:E:719:ARG:HG2	1:E:719:ARG:HH21	1.75	0.52
1:F:138:ALA:HB1	1:F:183:ILE:HG22	1.91	0.52
1:A:138:ALA:HB1	1:A:183:ILE:HG22	1.91	0.52
1:A:922:GLN:NE2	1:B:529:LEU:HD23	2.24	0.52
1:B:830:GLY:C	4:B:1081:HOH:O	2.48	0.52
1:C:904:SER:HB2	1:D:473:ASP:OD1	2.10	0.52
1:D:292:SER:HB2	1:D:294:TYR:CE1	2.45	0.52
1:D:703:ASN:C	1:D:703:ASN:ND2	2.63	0.52
1:F:253:GLN:NE2	1:F:268:THR:OG1	2.42	0.52
1:A:513:TYR:HB3	1:A:588:ILE:HD13	1.92	0.51
1:A:710:ILE:O	1:A:714:ILE:HG12	2.10	0.51
1:C:52:ARG:HD2	1:C:63:GLU:OE2	2.09	0.51
1:D:87:PHE:HB3	1:D:88:PRO:HD2	1.92	0.51
1:F:152:ALA:HB1	1:F:764:ARG:HH12	1.74	0.51
1:F:243:TYR:CD2	1:F:256:SER:HB3	2.45	0.51
1:A:61:LEU:HD13	1:A:74:ILE:HD11	1.93	0.51

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:A:258:ASP:C	1:A:260:ASP:H	2.13	0.51
1:A:362:LEU:CD2	1:A:363:ARG:H	2.23	0.51
1:C:703:ASN:C	1:C:703:ASN:ND2	2.63	0.51
1:E:132:ARG:HD2	1:E:134:PHE:CZ	2.45	0.51
1:E:200:PRO:O	1:E:740:GLY:HA3	2.10	0.51
1:F:82:ASN:HD21	1:F:96:ARG:HH21	1.58	0.51
1:A:128:SER:HB2	1:A:133:MET:HA	1.93	0.51
1:C:703:ASN:HD22	1:C:704:GLU:N	2.08	0.51
1:E:568:LEU:HB3	1:E:571:MET:HE2	1.91	0.51
1:E:557:ARG:HH22	1:E:562:GLU:HB2	1.75	0.51
1:E:791:GLU:CD	1:E:861:ARG:HE	2.14	0.51
1:F:557:ARG:NH2	1:F:562:GLU:HB2	2.25	0.51
1:A:494:THR:HG22	1:A:495:THR:N	2.25	0.51
1:B:362:LEU:CD2	1:B:363:ARG:H	2.24	0.51
1:C:180:ALA:CA	4:C:1080:HOH:O	2.58	0.51
1:C:245:ILE:HD11	1:C:278:LEU:HG	1.92	0.51
1:C:393:ARG:HH22	1:E:557:ARG:HG3	1.75	0.51
1:C:990:GLY:HA2	1:C:1023:GLU:OE2	2.10	0.51
1:D:557:ARG:HH22	1:D:562:GLU:HB2	1.75	0.51
1:E:710:ILE:O	1:E:714:ILE:HG12	2.11	0.51
1:F:744:THR:HG22	1:F:745:SER:N	2.24	0.51
1:F:1052:ILE:O	1:F:1056:ILE:HG13	2.10	0.51
1:C:235:PRO:N	4:C:1129:HOH:O	2.42	0.51
1:E:703:ASN:C	1:E:703:ASN:ND2	2.64	0.51
1:F:367:VAL:CG1	1:F:375:VAL:HG21	2.41	0.51
1:F:710:ILE:HD13	1:F:742:TYR:HA	1.92	0.51
1:F:990:GLY:HA2	1:F:1023:GLU:OE2	2.09	0.51
1:B:744:THR:HG22	1:B:745:SER:N	2.26	0.51
1:C:82:ASN:HD21	1:C:96:ARG:HH21	1.57	0.51
1:C:91:ARG:HH11	1:C:114:GLU:CB	2.24	0.51
1:C:719:ARG:HG2	1:C:719:ARG:NH2	2.26	0.51
1:C:744:THR:HG22	1:C:745:SER:N	2.26	0.51
1:D:132:ARG:HD2	1:D:134:PHE:CZ	2.45	0.51
1:D:546:PRO:HG2	1:D:567:ASP:HB3	1.91	0.51
1:E:568:LEU:HB3	1:E:571:MET:CE	2.40	0.51
1:E:781:ALA:HB2	1:E:802:PRO:HG2	1.93	0.51
1:F:897:ARG:HG2	1:F:898:LEU:HD12	1.91	0.51
1:A:522:PRO:HG2	1:B:889:MET:SD	2.51	0.51
1:A:555:VAL:HG22	1:E:354:TYR:CE2	2.45	0.51
1:C:61:LEU:HD13	1:C:74:ILE:HD11	1.93	0.51
1:E:88:PRO:HG2	1:E:89:ASP:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:703:ASN:OD1	1:B:706:VAL:HG23	2.11	0.51
1:C:256:SER:OG	1:C:267:HIS:HE1	1.94	0.51
1:D:258:ASP:C	1:D:260:ASP:H	2.14	0.51
1:D:710:ILE:O	1:D:714:ILE:HG12	2.11	0.51
1:F:52:ARG:HD2	1:F:63:GLU:OE2	2.11	0.51
1:B:703:ASN:HD22	1:B:704:GLU:N	2.09	0.51
1:D:124:PHE:HB3	1:D:152:ALA:CB	2.41	0.51
1:F:528:VAL:HG21	1:F:896:TYR:CD2	2.46	0.51
1:B:1031:VAL:HG12	1:B:1033:ILE:CD1	2.40	0.50
1:C:152:ALA:HB1	1:C:764:ARG:HH12	1.76	0.50
1:C:618:VAL:HG23	1:C:634:ASN:HA	1.92	0.50
1:D:403:ASN:HD22	1:D:405:GLY:H	1.58	0.50
1:D:550:ASN:HB3	1:D:553:LYS:HG3	1.92	0.50
1:D:983:ILE:HG23	1:D:1033:ILE:HD13	1.93	0.50
1:E:930:ASN:HD21	1:F:926:GLU:HG3	1.76	0.50
1:F:687:LEU:HD23	1:F:722:VAL:HG11	1.93	0.50
1:C:403:ASN:HD22	1:C:405:GLY:H	1.56	0.50
1:C:568:LEU:HB3	1:C:571:MET:CE	2.42	0.50
1:D:591:LEU:HD11	1:D:662:LEU:HD21	1.93	0.50
1:E:703:ASN:HD22	1:E:704:GLU:N	2.07	0.50
1:E:946:TYR:CE1	1:F:922:GLN:HB3	2.46	0.50
1:F:132:ARG:HD2	1:F:134:PHE:CZ	2.46	0.50
1:F:247:ASP:HA	1:F:251:PHE:O	2.12	0.50
1:F:719:ARG:HG2	1:F:719:ARG:NH2	2.27	0.50
1:B:710:ILE:HD13	1:B:742:TYR:HA	1.94	0.50
1:C:40:PRO:HG2	1:C:724:LEU:CD2	2.38	0.50
1:C:557:ARG:HH22	1:C:562:GLU:HB2	1.75	0.50
1:D:247:ASP:HA	1:D:251:PHE:O	2.12	0.50
1:A:367:VAL:CG1	1:A:375:VAL:HG21	2.41	0.50
1:A:495:THR:OG1	1:B:787:SER:HB2	2.12	0.50
1:B:245:ILE:HD11	1:B:278:LEU:HG	1.94	0.50
1:B:913:ARG:NH2	1:B:1047:GLN:HE21	2.09	0.50
1:C:687:LEU:HD23	1:C:722:VAL:HG11	1.93	0.50
1:C:897:ARG:HG2	1:C:898:LEU:HD12	1.92	0.50
1:C:1031:VAL:HG12	1:C:1033:ILE:CD1	2.42	0.50
1:D:557:ARG:HE	1:F:393:ARG:HH12	1.56	0.50
1:E:134:PHE:HB2	4:E:1097:HOH:O	2.10	0.50
1:E:557:ARG:NH2	1:E:562:GLU:HB2	2.27	0.50
1:F:997:LYS:HB3	3:L:2101:D10:H71	1.94	0.50
1:A:719:ARG:HG2	1:A:719:ARG:NH2	2.26	0.50
1:A:1031:VAL:HG12	1:A:1033:ILE:CD1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:ASP:OD2	1:B:67:LYS:HB3	2.12	0.50
1:B:258:ASP:C	1:B:260:ASP:H	2.14	0.50
1:B:881:TYR:O	1:B:902:GLU:HG3	2.10	0.50
1:C:494:THR:HG22	1:C:495:THR:N	2.27	0.50
1:C:722:VAL:N	1:C:723:PRO:HD2	2.26	0.50
1:C:868:ARG:HH12	1:D:497:ASN:ND2	2.10	0.50
1:E:618:VAL:HG23	1:E:634:ASN:HA	1.92	0.50
1:F:204:GLY:O	1:F:206:ARG:HG3	2.11	0.50
1:F:347:ILE:HG12	1:F:392:TYR:CD2	2.46	0.50
1:A:744:THR:HG22	1:A:745:SER:N	2.26	0.50
1:A:781:ALA:HB2	1:A:802:PRO:HG2	1.94	0.50
1:B:167:ASN:CA	4:B:1098:HOH:O	2.54	0.50
1:C:181:THR:N	4:C:1080:HOH:O	2.45	0.50
1:C:513:TYR:HB3	1:C:588:ILE:HD13	1.94	0.50
1:C:897:ARG:NE	4:C:1107:HOH:O	2.44	0.50
1:E:124:PHE:HB3	1:E:152:ALA:CB	2.41	0.50
1:E:494:THR:HG22	1:E:495:THR:N	2.27	0.50
1:E:513:TYR:HB3	1:E:588:ILE:HD13	1.93	0.50
1:E:546:PRO:HG2	1:E:567:ASP:HB3	1.93	0.50
1:E:922:GLN:HE22	1:F:948:THR:H	1.59	0.50
1:F:124:PHE:HB3	1:F:152:ALA:CB	2.41	0.50
1:F:781:ALA:HB2	1:F:802:PRO:HG2	1.94	0.50
1:B:256:SER:OG	1:B:267:HIS:HE1	1.94	0.50
1:B:268:THR:HG22	1:B:303:ILE:CD1	2.42	0.50
1:C:791:GLU:CD	1:C:861:ARG:HE	2.15	0.50
1:E:897:ARG:HG2	1:E:898:LEU:HD12	1.94	0.50
1:A:167:ASN:CA	4:A:1093:HOH:O	2.47	0.50
1:A:722:VAL:N	1:A:723:PRO:HD2	2.27	0.50
1:A:881:TYR:O	1:A:902:GLU:HG3	2.11	0.50
1:B:135:THR:HA	1:B:149:SER:O	2.12	0.50
1:C:473:ASP:HA	1:D:904:SER:CB	2.42	0.50
1:C:557:ARG:NH2	1:C:562:GLU:HB2	2.27	0.50
1:D:387:LEU:HD13	1:D:388:GLY:N	2.26	0.50
1:F:403:ASN:HD22	1:F:405:GLY:H	1.54	0.50
1:F:494:THR:HG22	1:F:495:THR:N	2.26	0.50
1:A:312:GLU:HG2	1:A:314:PRO:HD3	1.94	0.50
1:B:88:PRO:HG2	1:B:89:ASP:H	1.76	0.50
1:B:719:ARG:HG2	1:B:719:ARG:NH2	2.26	0.50
1:B:947:PRO:HD2	1:B:950:SER:HB3	1.94	0.50
1:C:162:LEU:HD21	1:C:180:ALA:HB3	1.93	0.50
1:C:197:PHE:HE1	1:C:199:LEU:HD21	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:636:LEU:HD22	1:D:650:VAL:HB	1.94	0.50
1:E:351:SER:OG	1:E:353:THR:CG2	2.56	0.50
1:E:997:LYS:HB3	3:K:2101:D10:H71	1.93	0.50
1:F:91:ARG:HH11	1:F:114:GLU:CB	2.25	0.50
1:F:245:ILE:HD11	1:F:278:LEU:HG	1.93	0.50
1:F:475:TYR:HB2	4:F:1115:HOH:O	2.11	0.50
1:B:61:LEU:HB3	1:B:75:VAL:HG12	1.94	0.49
1:C:639:LEU:HD23	1:C:640:ARG:N	2.27	0.49
1:D:639:LEU:HD23	1:D:640:ARG:N	2.27	0.49
1:E:135:THR:HA	1:E:149:SER:O	2.12	0.49
1:E:247:ASP:HA	1:E:251:PHE:O	2.11	0.49
1:E:387:LEU:HD13	1:E:388:GLY:N	2.27	0.49
1:E:468:LYS:HE3	1:E:476:VAL:HG22	1.94	0.49
1:A:88:PRO:HG2	1:A:89:ASP:H	1.77	0.49
1:A:245:ILE:HD11	1:A:278:LEU:HG	1.95	0.49
1:A:568:LEU:HB3	1:A:571:MET:HE2	1.94	0.49
1:A:639:LEU:HD23	1:A:640:ARG:N	2.27	0.49
1:A:703:ASN:OD1	1:A:706:VAL:HG23	2.12	0.49
1:A:922:GLN:HE22	1:B:948:THR:H	1.60	0.49
1:B:403:ASN:HD22	1:B:403:ASN:C	2.13	0.49
1:D:292:SER:HB2	1:D:294:TYR:HE1	1.77	0.49
1:D:997:LYS:HB3	3:J:2101:D10:H71	1.94	0.49
4:E:1135:HOH:O	1:F:469:HIS:HB2	2.12	0.49
1:F:445:ARG:HH12	1:F:471:GLU:CD	2.16	0.49
1:A:636:LEU:HD22	1:A:650:VAL:HB	1.94	0.49
1:A:687:LEU:HD23	1:A:722:VAL:HG11	1.93	0.49
1:C:1052:ILE:O	1:C:1056:ILE:HG13	2.13	0.49
1:E:197:PHE:HE1	1:E:199:LEU:HD21	1.77	0.49
1:E:550:ASN:HB3	1:E:553:LYS:HG3	1.93	0.49
1:A:387:LEU:HD13	1:A:388:GLY:N	2.28	0.49
1:A:922:GLN:HE22	1:B:948:THR:HB	1.78	0.49
1:B:87:PHE:HB3	1:B:88:PRO:HD2	1.94	0.49
1:C:87:PHE:HD2	1:C:88:PRO:HD2	1.77	0.49
1:C:367:VAL:CG1	1:C:375:VAL:HG21	2.42	0.49
1:F:722:VAL:N	1:F:723:PRO:HD2	2.27	0.49
1:A:256:SER:OG	1:A:267:HIS:HE1	1.95	0.49
1:B:687:LEU:HD12	4:B:1128:HOH:O	2.13	0.49
1:C:710:ILE:O	1:C:714:ILE:HG12	2.13	0.49
1:C:710:ILE:HD13	1:C:742:TYR:HA	1.94	0.49
1:D:557:ARG:NH2	1:D:562:GLU:HB2	2.27	0.49
1:D:568:LEU:HB3	1:D:571:MET:CE	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:452:PHE:HB3	1:F:463:TYR:HB3	1.95	0.49
1:F:965:SER:O	1:F:968:ASP:N	2.45	0.49
1:B:568:LEU:HB3	1:B:571:MET:CE	2.42	0.49
1:B:628:LYS:HE2	4:B:1156:HOH:O	2.11	0.49
1:C:636:LEU:HD22	1:C:650:VAL:HB	1.94	0.49
1:E:569:ASN:HA	4:E:1104:HOH:O	2.13	0.49
1:F:61:LEU:HD13	1:F:74:ILE:HD11	1.94	0.49
1:A:557:ARG:HH22	1:A:562:GLU:HB2	1.78	0.49
1:A:618:VAL:HG23	1:A:634:ASN:HA	1.93	0.49
1:A:997:LYS:HB3	3:G:2101:D10:H71	1.93	0.49
1:B:152:ALA:HB1	1:B:764:ARG:HH12	1.78	0.49
1:B:639:LEU:HD23	1:B:640:ARG:N	2.27	0.49
1:C:135:THR:HA	1:C:149:SER:O	2.13	0.49
1:C:997:LYS:HB3	3:I:2101:D10:H71	1.95	0.49
1:D:88:PRO:HG2	1:D:89:ASP:H	1.78	0.49
1:E:312:GLU:HG2	1:E:314:PRO:HD3	1.94	0.49
1:F:913:ARG:NH2	1:F:1047:GLN:HE21	2.06	0.49
1:B:87:PHE:HD2	1:B:88:PRO:HD2	1.78	0.49
1:B:722:VAL:N	1:B:723:PRO:HD2	2.28	0.49
1:A:703:ASN:C	1:A:703:ASN:ND2	2.66	0.49
1:C:258:ASP:C	1:C:260:ASP:H	2.16	0.49
1:C:936:ASP:HB2	1:C:944:SER:HB2	1.94	0.49
1:D:87:PHE:HD2	1:D:88:PRO:HD2	1.78	0.49
1:D:135:THR:HA	1:D:149:SER:O	2.12	0.49
1:D:897:ARG:HG2	1:D:898:LEU:HD12	1.93	0.49
1:E:91:ARG:HH11	1:E:114:GLU:CB	2.26	0.49
1:E:124:PHE:HB3	1:E:152:ALA:HB2	1.95	0.49
1:E:605:GLU:HG3	1:F:524:PRO:HD3	1.95	0.49
1:F:61:LEU:HB3	1:F:75:VAL:HG12	1.94	0.49
1:A:65:ASP:OD2	1:A:67:LYS:HB3	2.12	0.49
1:A:568:LEU:HB3	1:A:571:MET:CE	2.43	0.49
1:A:574:ARG:HA	1:B:797:GLU:HA	1.95	0.49
1:B:138:ALA:HB1	1:B:183:ILE:HG22	1.94	0.49
1:C:82:ASN:HD22	1:C:82:ASN:N	2.03	0.49
1:C:156:PHE:HB2	1:C:159:MET:HG3	1.95	0.49
1:D:1052:ILE:O	1:D:1056:ILE:HG13	2.13	0.49
1:F:362:LEU:CD2	1:F:363:ARG:H	2.26	0.49
1:F:936:ASP:HB2	1:F:944:SER:HB2	1.94	0.49
1:B:890:MET:O	1:B:894:GLU:HG2	2.13	0.48
1:F:258:ASP:C	1:F:260:ASP:H	2.15	0.48
1:B:247:ASP:HA	1:B:251:PHE:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:555:VAL:HA	1:D:354:TYR:CZ	2.48	0.48
1:C:781:ALA:HB2	1:C:802:PRO:HG2	1.94	0.48
1:D:912:VAL:O	1:D:915:ASN:HB2	2.13	0.48
1:A:91:ARG:HH11	1:A:114:GLU:CB	2.27	0.48
1:A:890:MET:O	1:A:894:GLU:HG2	2.13	0.48
1:B:557:ARG:NH2	1:B:562:GLU:HB2	2.28	0.48
1:B:616:LYS:HB3	4:B:1125:HOH:O	2.12	0.48
1:B:703:ASN:C	1:B:703:ASN:ND2	2.67	0.48
1:C:124:PHE:HB3	1:C:152:ALA:CB	2.44	0.48
1:C:937:ASN:HB3	4:C:1122:HOH:O	2.13	0.48
1:D:468:LYS:HE3	1:D:476:VAL:HG22	1.95	0.48
1:D:913:ARG:NH2	1:D:1047:GLN:HE21	2.03	0.48
1:E:87:PHE:HB3	1:E:88:PRO:HD2	1.94	0.48
1:E:152:ALA:HB1	1:E:764:ARG:NH1	2.28	0.48
1:E:636:LEU:HD22	1:E:650:VAL:HB	1.96	0.48
1:E:881:TYR:O	1:E:902:GLU:HG3	2.13	0.48
1:B:387:LEU:HD13	1:B:388:GLY:N	2.28	0.48
1:B:468:LYS:HE3	1:B:476:VAL:HG22	1.96	0.48
1:B:557:ARG:HH22	1:B:562:GLU:HB2	1.78	0.48
1:D:197:PHE:HE1	1:D:199:LEU:HD21	1.78	0.48
1:D:618:VAL:HG23	1:D:634:ASN:HA	1.95	0.48
1:D:947:PRO:HD2	1:D:950:SER:HB3	1.95	0.48
1:F:570:ASP:HA	1:F:572:TYR:CE1	2.48	0.48
1:F:628:LYS:HG2	1:F:629:VAL:N	2.28	0.48
1:F:636:LEU:HD22	1:F:650:VAL:HB	1.96	0.48
1:A:501:TYR:CD2	1:A:501:TYR:N	2.82	0.48
1:A:913:ARG:NH2	1:A:1047:GLN:HE21	2.06	0.48
1:D:268:THR:HG22	1:D:303:ILE:CD1	2.42	0.48
1:D:502:ALA:HB1	4:D:1125:HOH:O	2.12	0.48
1:D:719:ARG:HG2	1:D:719:ARG:NH2	2.29	0.48
1:E:936:ASP:HB2	1:E:944:SER:HB2	1.94	0.48
1:F:387:LEU:HD13	1:F:388:GLY:N	2.28	0.48
1:A:557:ARG:HH11	1:E:393:ARG:HH12	1.62	0.48
1:D:91:ARG:HH11	1:D:114:GLU:CB	2.26	0.48
1:D:722:VAL:N	1:D:723:PRO:HD2	2.27	0.48
1:E:639:LEU:HD23	1:E:640:ARG:N	2.28	0.48
1:A:135:THR:HA	1:A:149:SER:O	2.14	0.48
1:A:445:ARG:HH12	1:A:471:GLU:CD	2.17	0.48
1:B:52:ARG:HD2	1:B:63:GLU:OE2	2.13	0.48
1:B:528:VAL:HG21	1:B:896:TYR:CD2	2.48	0.48
1:C:127:LYS:HD2	4:C:1118:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:965:SER:O	1:C:968:ASP:HB2	2.14	0.48
1:D:256:SER:OG	1:D:267:HIS:HE1	1.97	0.48
1:D:516:SER:HB2	1:D:518:ARG:HG3	1.95	0.48
1:D:687:LEU:HD23	1:D:722:VAL:HG11	1.94	0.48
1:E:40:PRO:HG2	1:E:724:LEU:CD2	2.41	0.48
1:E:710:ILE:HD13	1:E:742:TYR:HA	1.95	0.48
1:F:88:PRO:HG2	1:F:89:ASP:H	1.79	0.48
1:F:156:PHE:HB2	1:F:159:MET:HG3	1.96	0.48
1:A:350:VAL:HG21	4:A:1155:HOH:O	2.14	0.48
1:C:628:LYS:HG2	1:C:629:VAL:N	2.29	0.48
1:E:258:ASP:C	1:E:260:ASP:H	2.16	0.48
1:E:405:GLY:HA3	4:E:1131:HOH:O	2.12	0.48
1:F:499:HIS:CD2	4:F:1080:HOH:O	2.66	0.48
1:F:997:LYS:NZ	4:F:1142:HOH:O	2.45	0.48
1:A:52:ARG:HD2	1:A:63:GLU:OE2	2.14	0.48
1:B:501:TYR:N	1:B:501:TYR:CD2	2.82	0.48
1:C:268:THR:HG22	1:C:303:ILE:CD1	2.43	0.48
1:C:881:TYR:O	1:C:902:GLU:HG3	2.14	0.48
1:F:292:SER:HB2	1:F:294:TYR:HE1	1.78	0.48
1:F:513:TYR:HB3	1:F:588:ILE:HD13	1.96	0.48
1:B:799:GLY:O	1:B:800:ILE:HG23	2.14	0.48
1:C:183:ILE:HG23	1:C:183:ILE:O	2.13	0.48
1:C:923:LEU:HD22	4:D:1084:HOH:O	2.14	0.48
1:F:234:SER:C	4:F:1074:HOH:O	2.52	0.48
1:A:87:PHE:HD2	1:A:88:PRO:HD2	1.79	0.47
1:A:156:PHE:HB2	1:A:159:MET:HG3	1.96	0.47
1:C:137:VAL:HG22	1:C:146:LEU:HD11	1.95	0.47
1:D:245:ILE:HD11	1:D:278:LEU:HG	1.95	0.47
1:E:403:ASN:HD22	1:E:405:GLY:H	1.59	0.47
1:F:66:LEU:N	4:F:1143:HOH:O	2.47	0.47
1:F:618:VAL:HG23	1:F:634:ASN:HA	1.96	0.47
1:B:570:ASP:HA	1:B:572:TYR:CE1	2.49	0.47
1:C:61:LEU:HB3	1:C:75:VAL:HG12	1.96	0.47
1:C:568:LEU:HB3	1:C:571:MET:HE2	1.95	0.47
1:D:337:ILE:HD12	1:D:350:VAL:HA	1.97	0.47
1:E:43:LEU:HD22	1:E:55:PHE:HE1	1.77	0.47
1:F:292:SER:HB2	1:F:294:TYR:CE1	2.49	0.47
1:F:701:TYR:OH	4:F:1079:HOH:O	2.20	0.47
1:F:949:ASN:HB2	4:F:1136:HOH:O	2.12	0.47
1:F:965:SER:O	1:F:968:ASP:HB2	2.14	0.47
1:F:1031:VAL:HG12	1:F:1033:ILE:CD1	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:ILE:HD11	4:D:1119:HOH:O	2.13	0.47
1:A:799:GLY:O	1:A:800:ILE:HG23	2.15	0.47
1:A:947:PRO:HD2	1:A:950:SER:HB3	1.95	0.47
1:B:618:VAL:HG23	1:B:634:ASN:HA	1.97	0.47
1:B:660:PHE:HB3	1:B:668:GLU:CB	2.44	0.47
1:D:124:PHE:HB3	1:D:152:ALA:HB2	1.96	0.47
1:D:501:TYR:CD2	1:D:501:TYR:N	2.83	0.47
2:L:1101:ARG:CD	4:L:79:HOH:O	2.23	0.47
1:C:131:ARG:HD3	1:C:748:TYR:CD2	2.49	0.47
1:E:570:ASP:HA	1:E:572:TYR:CE1	2.50	0.47
1:E:722:VAL:N	1:E:723:PRO:HD2	2.29	0.47
1:C:337:ILE:HG12	1:C:649:MET:CE	2.45	0.47
1:E:452:PHE:HB3	1:E:463:TYR:HB3	1.97	0.47
1:F:256:SER:OG	1:F:267:HIS:HE1	1.97	0.47
1:F:530:ASN:CG	4:F:1112:HOH:O	2.52	0.47
1:B:530:ASN:OD1	1:B:531:PHE:N	2.47	0.47
1:B:636:LEU:HD22	1:B:650:VAL:HB	1.95	0.47
1:C:87:PHE:CD2	1:C:88:PRO:HD2	2.50	0.47
1:C:929:MET:HB3	4:C:1073:HOH:O	2.15	0.47
1:D:445:ARG:HH12	1:D:471:GLU:CD	2.18	0.47
1:E:947:PRO:HD2	1:E:950:SER:HB3	1.97	0.47
1:F:53:ILE:HG23	1:F:286:LEU:CD2	2.45	0.47
1:F:279:ASN:HD22	1:F:279:ASN:HA	1.55	0.47
1:A:152:ALA:HB1	1:A:764:ARG:NH1	2.29	0.47
1:A:268:THR:HG22	1:A:303:ILE:CD1	2.43	0.47
1:A:467:LEU:HD11	1:A:496:GLU:HB2	1.96	0.47
1:A:874:ARG:HH21	1:A:874:ARG:HG3	1.80	0.47
1:A:947:PRO:HB3	1:B:922:GLN:HB2	1.97	0.47
1:B:156:PHE:HB2	1:B:159:MET:HG3	1.96	0.47
1:B:628:LYS:HG2	1:B:629:VAL:N	2.28	0.47
1:B:687:LEU:HD23	1:B:722:VAL:HG11	1.97	0.47
1:C:204:GLY:O	1:C:206:ARG:HG3	2.14	0.47
1:C:452:PHE:HB3	1:C:463:TYR:HB3	1.97	0.47
1:D:131:ARG:HD3	1:D:748:TYR:CD2	2.50	0.47
1:E:65:ASP:OD2	1:E:67:LYS:HB3	2.15	0.47
1:E:530:ASN:OD1	1:E:531:PHE:N	2.48	0.47
1:E:591:LEU:HD11	1:E:662:LEU:HD21	1.95	0.47
1:E:965:SER:O	1:E:968:ASP:N	2.48	0.47
1:F:468:LYS:HE3	1:F:476:VAL:HG22	1.97	0.47
1:F:639:LEU:HD23	1:F:640:ARG:N	2.30	0.47
1:A:106:ALA:CB	4:A:1170:HOH:O	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:557:ARG:NH2	1:A:562:GLU:HB2	2.28	0.47
1:B:87:PHE:CD2	1:B:88:PRO:HD2	2.50	0.47
1:B:124:PHE:HB3	1:B:152:ALA:CB	2.45	0.47
1:C:74:ILE:HG13	1:C:75:VAL:HG12	1.97	0.47
1:C:351:SER:OG	1:C:353:THR:CG2	2.52	0.47
1:D:152:ALA:HB1	1:D:764:ARG:NH1	2.29	0.47
1:D:494:THR:HG22	1:D:495:THR:N	2.30	0.47
1:D:498:SER:OG	1:D:499:HIS:N	2.47	0.47
1:E:156:PHE:HB2	1:E:159:MET:HG3	1.97	0.47
1:E:719:ARG:HG2	1:E:719:ARG:NH2	2.29	0.47
1:A:1052:ILE:O	1:A:1056:ILE:HG13	2.14	0.47
1:B:137:VAL:HG22	1:B:146:LEU:HD11	1.97	0.47
1:C:155:PRO:HG2	1:C:156:PHE:CD1	2.50	0.47
1:D:53:ILE:HG23	1:D:286:LEU:CD2	2.45	0.47
1:D:350:VAL:HG21	1:D:669:ARG:HH11	1.80	0.47
1:D:568:LEU:HB3	1:D:571:MET:HE2	1.97	0.47
1:D:936:ASP:HB2	1:D:944:SER:HB2	1.97	0.47
1:D:1031:VAL:HG12	1:D:1033:ILE:CD1	2.45	0.47
1:E:704:GLU:HG3	1:F:939:ARG:NH1	2.30	0.47
1:E:744:THR:HG22	1:E:745:SER:N	2.30	0.47
1:C:529:LEU:HG	1:C:529:LEU:O	2.14	0.47
1:D:201:HIS:O	1:D:740:GLY:HA2	2.14	0.47
1:F:197:PHE:CE1	1:F:199:LEU:HD21	2.49	0.47
1:F:337:ILE:HG12	1:F:649:MET:CE	2.45	0.47
1:B:91:ARG:HH11	1:B:114:GLU:CB	2.28	0.46
1:B:204:GLY:O	1:B:206:ARG:HG3	2.16	0.46
1:B:312:GLU:HG2	1:B:314:PRO:HD3	1.97	0.46
1:D:529:LEU:HG	1:D:529:LEU:O	2.14	0.46
1:F:124:PHE:HB3	1:F:152:ALA:HB2	1.97	0.46
1:F:137:VAL:HG22	1:F:146:LEU:HD11	1.96	0.46
1:F:312:GLU:HG2	1:F:314:PRO:HD3	1.96	0.46
1:A:570:ASP:HA	1:A:572:TYR:CE1	2.51	0.46
1:A:628:LYS:HG2	1:A:629:VAL:N	2.29	0.46
1:B:781:ALA:HB2	1:B:802:PRO:HG2	1.95	0.46
1:B:936:ASP:HB2	1:B:944:SER:HB2	1.98	0.46
1:D:541:VAL:HG22	1:D:542:ILE:N	2.30	0.46
1:D:570:ASP:HA	1:D:572:TYR:CE1	2.50	0.46
1:D:781:ALA:HB2	1:D:802:PRO:HG2	1.96	0.46
1:D:799:GLY:O	1:D:800:ILE:HG23	2.15	0.46
1:D:881:TYR:O	1:D:902:GLU:HG3	2.15	0.46
1:D:965:SER:O	1:D:968:ASP:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:268:THR:HG22	1:F:303:ILE:CD1	2.45	0.46
1:F:744:THR:HG22	1:F:745:SER:H	1.79	0.46
1:A:82:ASN:ND2	1:A:96:ARG:HH21	2.12	0.46
1:A:247:ASP:HA	1:A:251:PHE:O	2.14	0.46
1:A:546:PRO:HG2	1:A:567:ASP:HB3	1.97	0.46
1:B:131:ARG:HD3	1:B:748:TYR:CD2	2.51	0.46
1:C:436:GLY:O	1:C:438:PRO:HD3	2.15	0.46
1:D:87:PHE:CD2	1:D:88:PRO:HD2	2.51	0.46
1:D:156:PHE:HB2	1:D:159:MET:HG3	1.97	0.46
1:D:369:ARG:NH2	4:D:1082:HOH:O	2.47	0.46
1:E:1052:ILE:O	1:E:1056:ILE:HG13	2.15	0.46
1:F:87:PHE:HD2	1:F:88:PRO:HD2	1.81	0.46
1:B:983:ILE:HG23	1:B:1033:ILE:HD13	1.97	0.46
1:C:256:SER:OG	1:C:267:HIS:CE1	2.69	0.46
1:D:414:ARG:HA	4:D:1082:HOH:O	2.14	0.46
1:E:87:PHE:HD2	1:E:88:PRO:HD2	1.79	0.46
1:E:245:ILE:HD11	1:E:278:LEU:HG	1.96	0.46
1:E:256:SER:OG	1:E:267:HIS:HE1	1.98	0.46
1:E:799:GLY:O	1:E:800:ILE:HG23	2.16	0.46
1:E:912:VAL:O	1:E:915:ASN:HB2	2.15	0.46
1:F:436:GLY:O	1:F:438:PRO:HD3	2.14	0.46
1:F:710:ILE:O	1:F:714:ILE:HG12	2.15	0.46
1:A:522:PRO:CG	1:B:889:MET:SD	3.04	0.46
1:B:337:ILE:HD12	1:B:350:VAL:HA	1.97	0.46
1:C:387:LEU:HD13	1:C:388:GLY:N	2.29	0.46
1:D:190:ARG:NH2	4:D:1105:HOH:O	2.31	0.46
1:D:528:VAL:HG21	1:D:896:TYR:CD2	2.51	0.46
1:D:628:LYS:HG2	1:D:629:VAL:N	2.31	0.46
1:F:101:SER:HA	4:F:1106:HOH:O	2.15	0.46
1:F:162:LEU:HD21	1:F:180:ALA:HB3	1.98	0.46
1:A:529:LEU:HG	1:A:529:LEU:O	2.16	0.46
1:B:127:LYS:CG	4:B:1129:HOH:O	2.58	0.46
1:C:197:PHE:CE1	1:C:199:LEU:HD21	2.51	0.46
1:C:393:ARG:HH12	1:E:557:ARG:HE	1.62	0.46
1:C:546:PRO:HG2	1:C:567:ASP:HB3	1.96	0.46
1:C:570:ASP:HA	1:C:572:TYR:CE1	2.50	0.46
1:D:406:ASN:HB2	1:D:424:ASP:CG	2.36	0.46
1:E:337:ILE:HD12	1:E:350:VAL:HA	1.98	0.46
1:E:628:LYS:HG2	1:E:629:VAL:N	2.30	0.46
1:F:337:ILE:HD12	1:F:350:VAL:HA	1.98	0.46
1:F:406:ASN:HB2	1:F:424:ASP:CG	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:LEU:HB3	1:A:75:VAL:HG12	1.98	0.46
1:A:541:VAL:HG22	1:A:542:ILE:N	2.31	0.46
1:B:394:THR:OG1	1:B:395:GLY:N	2.49	0.46
1:C:139:GLY:CA	4:C:1079:HOH:O	2.61	0.46
1:C:640:ARG:HD3	4:C:1100:HOH:O	2.14	0.46
1:D:872:HIS:HE1	1:D:902:GLU:OE1	1.99	0.46
1:E:53:ILE:HG23	1:E:286:LEU:CD2	2.45	0.46
1:F:152:ALA:HB1	1:F:764:ARG:NH1	2.30	0.46
1:F:799:GLY:O	1:F:800:ILE:HG23	2.16	0.46
1:A:452:PHE:HB3	1:A:463:TYR:HB3	1.98	0.46
1:B:445:ARG:HH12	1:B:471:GLU:CD	2.18	0.46
1:B:546:PRO:HG2	1:B:567:ASP:HB3	1.98	0.46
1:B:1031:VAL:HG12	1:B:1033:ILE:HD11	1.98	0.46
1:C:88:PRO:HG2	1:C:89:ASP:H	1.80	0.46
1:F:568:LEU:HB3	1:F:571:MET:CE	2.46	0.46
1:A:468:LYS:HE3	1:A:476:VAL:HG22	1.97	0.46
1:A:789:GLU:OE1	1:B:538:LYS:HE2	2.16	0.46
1:B:82:ASN:ND2	1:B:96:ARG:HH21	2.11	0.46
1:C:247:ASP:HA	1:C:251:PHE:O	2.16	0.46
1:C:312:GLU:HG2	1:C:314:PRO:HD3	1.97	0.46
1:C:847:LEU:HD12	1:C:849:ILE:HD11	1.98	0.46
3:I:2101:D10:H42	3:I:2101:D10:H72	1.54	0.46
1:D:530:ASN:OD1	1:D:531:PHE:N	2.49	0.46
2:J:1103:ARG:NH2	4:J:383:HOH:O	2.48	0.46
1:A:131:ARG:HG2	1:A:131:ARG:HH21	1.81	0.46
1:A:394:THR:OG1	1:A:395:GLY:N	2.48	0.46
1:A:1000:LEU:HD12	1:A:1004:THR:HB	1.98	0.46
1:C:201:HIS:O	1:C:740:GLY:HA2	2.16	0.46
1:C:445:ARG:HH12	1:C:471:GLU:CD	2.20	0.46
1:C:956:ILE:HG22	1:C:1055:LEU:HD11	1.98	0.46
1:D:195:ASN:N	4:D:1081:HOH:O	2.32	0.46
1:F:65:ASP:OD2	1:F:67:LYS:HB3	2.16	0.46
1:A:201:HIS:O	1:A:740:GLY:HA2	2.16	0.45
1:C:591:LEU:HD11	1:C:662:LEU:HD21	1.96	0.45
1:C:820:ASN:OD1	1:C:822:TYR:HB2	2.16	0.45
1:D:52:ARG:HD2	1:D:63:GLU:OE2	2.16	0.45
1:D:312:GLU:HG2	1:D:314:PRO:HD3	1.97	0.45
1:E:87:PHE:CD2	1:E:88:PRO:HD2	2.51	0.45
1:F:703:ASN:ND2	1:F:705:ALA:H	2.14	0.45
1:A:363:ARG:HA	1:A:363:ARG:HD3	1.64	0.45
1:B:555:VAL:HG22	1:D:354:TYR:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:362:LEU:CD2	1:E:363:ARG:H	2.30	0.45
1:F:183:ILE:HG23	1:F:183:ILE:O	2.17	0.45
1:F:546:PRO:HG2	1:F:567:ASP:HB3	1.98	0.45
1:F:820:ASN:OD1	1:F:822:TYR:HB2	2.17	0.45
1:A:87:PHE:CD2	1:A:88:PRO:HD2	2.51	0.45
1:A:110:PHE:CD1	1:A:121:ILE:HD11	2.51	0.45
1:B:363:ARG:HA	1:B:363:ARG:HD3	1.66	0.45
1:C:616:LYS:HE3	4:C:1136:HOH:O	2.16	0.45
1:D:703:ASN:ND2	1:D:705:ALA:H	2.14	0.45
1:E:201:HIS:O	1:E:740:GLY:HA2	2.17	0.45
1:E:995:THR:CG2	3:K:2101:D10:H41	2.46	0.45
1:A:87:PHE:CB	1:A:88:PRO:HD2	2.46	0.45
1:B:467:LEU:HD21	1:B:496:GLU:HB3	1.99	0.45
1:C:65:ASP:OD2	1:C:67:LYS:HB3	2.16	0.45
1:C:152:ALA:HB1	1:C:764:ARG:NH1	2.32	0.45
1:C:501:TYR:CD2	1:C:501:TYR:N	2.84	0.45
1:D:791:GLU:CD	1:D:861:ARG:HE	2.20	0.45
1:D:986:ARG:HA	1:D:1027:VAL:O	2.16	0.45
1:E:52:ARG:HD2	1:E:63:GLU:OE2	2.16	0.45
1:E:131:ARG:HD3	1:E:748:TYR:CD2	2.51	0.45
1:F:181:THR:N	4:F:1094:HOH:O	2.50	0.45
1:F:403:ASN:HD22	1:F:403:ASN:C	2.13	0.45
1:F:947:PRO:HD2	1:F:950:SER:HB3	1.99	0.45
1:F:983:ILE:HD12	1:F:983:ILE:N	2.31	0.45
1:C:124:PHE:HB3	1:C:152:ALA:HB2	1.99	0.45
1:C:995:THR:CG2	3:I:2101:D10:H41	2.47	0.45
1:D:82:ASN:ND2	1:D:96:ARG:HH21	2.14	0.45
1:E:202:TRP:CZ3	1:E:745:SER:HB3	2.51	0.45
1:F:131:ARG:HD3	1:F:748:TYR:CD2	2.51	0.45
1:F:983:ILE:HG23	1:F:1033:ILE:HD13	1.99	0.45
1:A:436:GLY:O	1:A:438:PRO:HD3	2.16	0.45
1:B:183:ILE:O	1:B:183:ILE:HG23	2.17	0.45
1:B:201:HIS:O	1:B:740:GLY:HA2	2.16	0.45
1:B:253:GLN:NE2	1:B:268:THR:OG1	2.47	0.45
1:B:555:VAL:HG22	1:D:354:TYR:CZ	2.51	0.45
1:C:58:CYS:C	1:C:60:ASP:H	2.20	0.45
1:C:337:ILE:HD12	1:C:350:VAL:HA	1.97	0.45
1:C:791:GLU:OE2	4:C:1107:HOH:O	2.21	0.45
1:D:360:GLU:OE2	1:D:361:PRO:HD2	2.17	0.45
1:E:330:SER:HB3	4:E:1101:HOH:O	2.17	0.45
1:F:212:LYS:HA	4:F:1122:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:468:LYS:HG2	1:F:473:ASP:HB2	1.99	0.45
1:F:912:VAL:O	1:F:915:ASN:HB2	2.16	0.45
1:B:155:PRO:HG2	1:B:156:PHE:CD1	2.52	0.45
1:B:529:LEU:O	1:B:529:LEU:HG	2.15	0.45
1:C:110:PHE:CD1	1:C:121:ILE:HD11	2.52	0.45
1:C:530:ASN:OD1	1:C:531:PHE:N	2.50	0.45
1:D:65:ASP:OD2	1:D:67:LYS:HB3	2.16	0.45
1:D:137:VAL:HG13	1:D:146:LEU:CD1	2.46	0.45
1:D:253:GLN:NE2	1:D:268:THR:OG1	2.48	0.45
1:E:528:VAL:HG21	1:E:896:TYR:CD2	2.51	0.45
1:F:872:HIS:HE1	1:F:902:GLU:OE1	2.00	0.45
1:A:528:VAL:HG21	1:A:896:TYR:CD2	2.52	0.45
1:A:986:ARG:HA	1:A:1027:VAL:O	2.17	0.45
1:B:152:ALA:HB1	1:B:764:ARG:NH1	2.32	0.45
1:B:314:PRO:HA	1:E:118:ILE:HG22	1.98	0.45
1:C:202:TRP:CZ3	1:C:745:SER:HB3	2.51	0.45
1:C:406:ASN:HB2	1:C:424:ASP:CG	2.37	0.45
1:D:200:PRO:HB3	1:D:737:GLU:OE1	2.16	0.45
1:E:181:THR:HG22	1:E:182:HIS:CE1	2.52	0.45
1:E:500:ASP:OD2	1:E:516:SER:HB3	2.17	0.45
1:F:87:PHE:CB	1:F:88:PRO:HD2	2.47	0.45
1:F:155:PRO:HG2	1:F:156:PHE:CD1	2.51	0.45
1:A:131:ARG:HD3	1:A:748:TYR:CD2	2.52	0.45
1:A:360:GLU:OE2	1:A:361:PRO:HD2	2.16	0.45
1:B:568:LEU:HB3	1:B:571:MET:HE2	1.99	0.45
1:B:847:LEU:N	1:B:847:LEU:HD23	2.32	0.45
1:C:253:GLN:NE2	1:C:268:THR:OG1	2.48	0.45
1:C:540:PHE:HA	1:C:577:PRO:HA	1.99	0.45
1:D:452:PHE:HB3	1:D:463:TYR:HB3	1.98	0.45
1:D:744:THR:HG22	1:D:745:SER:H	1.81	0.45
1:E:82:ASN:ND2	1:E:96:ARG:HH21	2.14	0.45
1:E:137:VAL:HG13	1:E:146:LEU:CD1	2.47	0.45
1:F:591:LEU:HD11	1:F:662:LEU:HD21	1.99	0.45
1:A:297:ASN:CB	4:A:1074:HOH:O	2.57	0.45
1:A:926:GLU:HG3	1:B:930:ASN:HD21	1.81	0.45
1:A:983:ILE:HG23	1:A:1033:ILE:HD13	1.98	0.45
1:C:181:THR:HG22	1:C:182:HIS:CE1	2.51	0.45
1:C:497:ASN:ND2	1:D:868:ARG:HH12	2.15	0.45
1:D:847:LEU:N	1:D:847:LEU:HD23	2.32	0.45
1:E:268:THR:HG22	1:E:303:ILE:CD1	2.44	0.45
1:F:501:TYR:CD2	1:F:501:TYR:N	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:676:ARG:NH2	1:D:811:ASP:OD1	2.45	0.44
1:A:761:ARG:NH2	1:A:853:ASP:OD2	2.50	0.44
1:B:131:ARG:HH21	1:B:131:ARG:HG2	1.82	0.44
1:C:535:VAL:HB	1:C:583:GLY:HA2	1.99	0.44
1:C:913:ARG:NH2	1:C:1047:GLN:HE21	2.09	0.44
1:C:922:GLN:HB3	1:D:946:TYR:CE1	2.52	0.44
1:D:132:ARG:NH2	1:D:158:SER:OG	2.50	0.44
1:E:501:TYR:CD2	1:E:501:TYR:N	2.85	0.44
1:E:872:HIS:HE1	1:E:902:GLU:OE1	2.00	0.44
1:F:360:GLU:OE2	1:F:361:PRO:HD2	2.17	0.44
1:A:314:PRO:HA	1:D:118:ILE:HG22	1.99	0.44
1:A:1031:VAL:HG12	1:A:1033:ILE:HD11	1.98	0.44
1:C:394:THR:OG1	1:C:395:GLY:N	2.50	0.44
1:C:412:VAL:HG13	1:C:433:LEU:HD11	1.98	0.44
1:C:932:ARG:HD3	1:C:935:TYR:OH	2.16	0.44
1:E:409:ALA:HB3	1:E:422:ALA:HB3	1.99	0.44
1:F:82:ASN:HD22	1:F:82:ASN:N	2.04	0.44
1:F:87:PHE:CD2	1:F:88:PRO:HD2	2.52	0.44
1:F:89:ASP:OD1	1:F:91:ARG:HB2	2.16	0.44
1:F:201:HIS:O	1:F:740:GLY:HA2	2.16	0.44
1:A:181:THR:HG22	1:A:182:HIS:CE1	2.53	0.44
1:A:591:LEU:HD11	1:A:662:LEU:HD21	1.98	0.44
1:B:995:THR:CG2	3:H:2101:D10:H41	2.47	0.44
1:C:983:ILE:HG23	1:C:1033:ILE:HD13	1.99	0.44
1:E:467:LEU:HD21	1:E:496:GLU:HB3	1.99	0.44
1:E:527:VAL:HG21	1:F:520:LEU:CD2	2.48	0.44
1:E:922:GLN:NE2	1:F:948:THR:H	2.13	0.44
1:F:350:VAL:HG11	1:F:659:THR:HG21	1.99	0.44
1:F:660:PHE:CD2	1:F:665:PRO:HA	2.52	0.44
1:F:881:TYR:O	1:F:902:GLU:HG3	2.17	0.44
1:B:1048:ILE:O	1:B:1052:ILE:HG13	2.17	0.44
1:C:393:ARG:HD2	1:E:558:SER:CA	2.45	0.44
1:C:660:PHE:HB3	1:C:668:GLU:CB	2.47	0.44
1:E:91:ARG:CZ	4:E:1147:HOH:O	2.66	0.44
1:E:197:PHE:CE1	1:E:199:LEU:HD21	2.53	0.44
1:E:541:VAL:HG22	1:E:542:ILE:N	2.33	0.44
1:E:1031:VAL:HG12	1:E:1033:ILE:CD1	2.47	0.44
1:F:135:THR:HA	1:F:149:SER:O	2.17	0.44
1:A:530:ASN:HD21	1:B:530:ASN:HD21	1.65	0.44
1:B:983:ILE:HD12	1:B:983:ILE:N	2.32	0.44
1:C:437:LYS:HE2	1:C:437:LYS:HB3	1.88	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:904:SER:CB	1:D:473:ASP:HA	2.48	0.44
1:E:220:GLY:HA2	4:E:1126:HOH:O	2.16	0.44
1:E:986:ARG:HA	1:E:1027:VAL:O	2.17	0.44
1:F:535:VAL:HB	1:F:583:GLY:HA2	1.99	0.44
1:A:141:ASP:OD1	1:A:145:ASN:HB2	2.18	0.44
1:C:344:GLN:HA	4:C:1078:HOH:O	2.17	0.44
1:C:393:ARG:HH12	1:E:557:ARG:CZ	2.30	0.44
1:C:904:SER:HB3	4:C:1124:HOH:O	2.17	0.44
1:C:926:GLU:HG3	1:D:930:ASN:HD21	1.82	0.44
1:C:1031:VAL:HG12	1:C:1033:ILE:HD11	1.99	0.44
1:D:43:LEU:HD22	1:D:55:PHE:HE1	1.81	0.44
1:D:856:ARG:HB2	4:D:1099:HOH:O	2.16	0.44
1:E:218:ASN:O	1:E:220:GLY:N	2.51	0.44
1:E:788:ASN:OD1	1:F:518:ARG:HD3	2.17	0.44
1:F:61:LEU:CB	1:F:75:VAL:CG1	2.95	0.44
1:B:351:SER:HB3	1:B:353:THR:HG22	1.99	0.44
1:C:43:LEU:HD22	1:C:55:PHE:HE1	1.82	0.44
1:C:87:PHE:CB	1:C:88:PRO:HD2	2.48	0.44
1:C:234:SER:C	4:C:1129:HOH:O	2.55	0.44
1:C:912:VAL:O	1:C:915:ASN:HB2	2.17	0.44
1:D:995:THR:CG2	3:J:2101:D10:H41	2.48	0.44
1:E:61:LEU:HB3	1:E:75:VAL:HG12	2.00	0.44
1:A:847:LEU:HD12	1:A:849:ILE:HD11	1.99	0.44
1:B:218:ASN:O	1:B:219:SER:C	2.56	0.44
1:B:360:GLU:OE2	1:B:361:PRO:HD2	2.18	0.44
1:C:360:GLU:OE2	1:C:361:PRO:HD2	2.18	0.44
1:C:946:TYR:CE1	1:D:922:GLN:HB3	2.53	0.44
1:D:58:CYS:C	1:D:60:ASP:H	2.20	0.44
1:D:87:PHE:CB	1:D:88:PRO:HD2	2.48	0.44
1:D:204:GLY:O	1:D:206:ARG:HG3	2.18	0.44
1:D:846:ASP:C	1:D:846:ASP:OD2	2.56	0.44
1:E:141:ASP:OD1	1:E:145:ASN:HB2	2.18	0.44
1:E:569:ASN:CA	4:E:1104:HOH:O	2.66	0.44
1:F:181:THR:HG22	1:F:182:HIS:CE1	2.53	0.44
1:F:412:VAL:HG13	1:F:433:LEU:HD11	1.98	0.44
1:A:53:ILE:HG23	1:A:286:LEU:CD2	2.48	0.44
1:A:940:ARG:HD2	4:B:1078:HOH:O	2.18	0.44
1:B:912:VAL:O	1:B:915:ASN:HB2	2.18	0.44
1:C:362:LEU:CD2	1:C:363:ARG:H	2.31	0.44
1:C:1048:ILE:O	1:C:1052:ILE:HG13	2.18	0.44
1:D:546:PRO:CG	1:D:567:ASP:HB3	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:137:VAL:HG22	1:E:146:LEU:HD11	2.00	0.44
1:E:253:GLN:NE2	1:E:268:THR:OG1	2.48	0.44
1:F:40:PRO:HG2	1:F:724:LEU:CD2	2.42	0.44
1:F:132:ARG:NH2	1:F:158:SER:OG	2.51	0.44
1:F:1031:VAL:HG12	1:F:1033:ILE:HD11	1.99	0.44
1:A:124:PHE:HB3	1:A:152:ALA:CB	2.47	0.43
1:A:218:ASN:O	1:A:219:SER:C	2.56	0.43
1:A:337:ILE:HD12	1:A:350:VAL:HA	1.99	0.43
1:C:577:PRO:HG3	1:D:789:GLU:HG3	1.99	0.43
1:C:660:PHE:CD2	1:C:665:PRO:HA	2.53	0.43
1:D:297:ASN:HD22	1:D:298:PRO:HD2	1.83	0.43
1:D:467:LEU:HD11	1:D:496:GLU:HB2	1.99	0.43
1:D:874:ARG:HH21	1:D:874:ARG:HG3	1.83	0.43
1:F:209:THR:OG1	1:F:988:TRP:HD1	2.01	0.43
1:F:660:PHE:HD2	1:F:665:PRO:HA	1.83	0.43
1:F:995:THR:CG2	3:L:2101:D10:H41	2.48	0.43
1:A:279:ASN:HD22	1:A:279:ASN:HA	1.55	0.43
1:A:351:SER:HB3	1:A:353:THR:HG22	2.00	0.43
1:A:847:LEU:HD23	1:A:847:LEU:N	2.33	0.43
1:C:53:ILE:HG23	1:C:286:LEU:CD2	2.48	0.43
1:C:91:ARG:HB2	4:C:1143:HOH:O	2.18	0.43
1:C:132:ARG:NH2	1:C:158:SER:OG	2.51	0.43
1:C:799:GLY:O	1:C:800:ILE:HG23	2.19	0.43
1:D:351:SER:OG	1:D:353:THR:CG2	2.55	0.43
1:D:932:ARG:HD3	1:D:935:TYR:OH	2.18	0.43
1:E:847:LEU:N	1:E:847:LEU:HD23	2.33	0.43
1:A:183:ILE:HG23	1:A:183:ILE:O	2.18	0.43
1:C:209:THR:OG1	1:C:988:TRP:HD1	2.01	0.43
1:C:297:ASN:O	1:C:301:GLU:N	2.49	0.43
1:C:947:PRO:HD2	1:C:950:SER:HB3	2.00	0.43
1:D:409:ALA:HB3	1:D:422:ALA:HB3	1.99	0.43
1:D:847:LEU:HD12	1:D:849:ILE:HD11	2.00	0.43
1:E:360:GLU:OE2	1:E:361:PRO:HD2	2.19	0.43
1:E:423:ASN:C	1:E:423:ASN:HD22	2.22	0.43
1:E:884:ILE:HD13	1:E:924:ILE:HD13	2.01	0.43
1:F:110:PHE:CD1	1:F:121:ILE:HD11	2.53	0.43
1:A:204:GLY:O	1:A:206:ARG:HG3	2.18	0.43
1:A:253:GLN:NE2	1:A:268:THR:OG1	2.49	0.43
1:A:530:ASN:OD1	1:A:531:PHE:N	2.51	0.43
1:A:1048:ILE:O	1:A:1052:ILE:HG13	2.18	0.43
1:B:256:SER:OG	1:B:267:HIS:CE1	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:436:GLY:O	1:B:438:PRO:HD3	2.18	0.43
1:B:846:ASP:C	1:B:847:LEU:HD23	2.39	0.43
1:C:350:VAL:HG11	1:C:659:THR:HG21	2.00	0.43
1:E:131:ARG:HH21	1:E:131:ARG:HG2	1.83	0.43
1:E:337:ILE:HG12	1:E:649:MET:CE	2.48	0.43
1:A:382:ARG:HD2	1:A:691:ASP:CG	2.39	0.43
1:B:362:LEU:HD23	1:B:363:ARG:H	1.82	0.43
1:B:467:LEU:HD11	1:B:496:GLU:HB2	1.99	0.43
1:C:181:THR:HG22	1:C:182:HIS:ND1	2.34	0.43
1:C:541:VAL:HG22	1:C:542:ILE:N	2.34	0.43
1:C:660:PHE:HD2	1:C:665:PRO:HA	1.83	0.43
1:C:703:ASN:ND2	1:C:705:ALA:H	2.16	0.43
1:C:986:ARG:HA	1:C:1027:VAL:O	2.18	0.43
1:D:74:ILE:HG13	1:D:75:VAL:HG12	2.00	0.43
1:D:197:PHE:CE1	1:D:199:LEU:HD21	2.54	0.43
1:D:362:LEU:CD2	1:D:363:ARG:H	2.31	0.43
1:D:365:ARG:HG2	1:D:365:ARG:HH21	1.83	0.43
1:D:436:GLY:O	1:D:438:PRO:HD3	2.19	0.43
1:A:423:ASN:C	1:A:423:ASN:HD22	2.22	0.43
1:A:660:PHE:CD2	1:A:665:PRO:HA	2.54	0.43
1:A:936:ASP:HB2	1:A:944:SER:HB2	2.00	0.43
1:C:61:LEU:CB	1:C:75:VAL:CG1	2.96	0.43
1:C:629:VAL:HG12	1:C:630:THR:N	2.34	0.43
1:C:965:SER:O	1:C:968:ASP:N	2.49	0.43
1:D:40:PRO:HG2	1:D:724:LEU:CD2	2.41	0.43
1:D:467:LEU:HD21	1:D:496:GLU:HB3	2.01	0.43
1:E:535:VAL:N	4:E:1114:HOH:O	2.37	0.43
1:E:904:SER:CB	1:F:473:ASP:HA	2.49	0.43
1:E:956:ILE:HG22	1:E:1055:LEU:HD11	2.00	0.43
1:E:1014:TRP:CH2	1:E:1016:ARG:HA	2.54	0.43
1:F:58:CYS:C	1:F:60:ASP:H	2.22	0.43
1:A:89:ASP:OD1	1:A:91:ARG:HB2	2.19	0.43
1:A:256:SER:OG	1:A:267:HIS:CE1	2.72	0.43
1:B:540:PHE:HA	1:B:577:PRO:HA	2.01	0.43
1:C:137:VAL:HG13	1:C:146:LEU:CD1	2.48	0.43
1:C:789:GLU:HG3	1:D:577:PRO:HG3	2.01	0.43
1:D:61:LEU:HB3	1:D:75:VAL:HG12	2.01	0.43
1:D:890:MET:HA	1:D:893:ASN:HD22	1.83	0.43
1:E:200:PRO:HB3	1:E:737:GLU:OE1	2.19	0.43
1:E:297:ASN:HD22	1:E:298:PRO:HD2	1.83	0.43
1:A:87:PHE:CD1	1:A:92:LYS:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:629:VAL:HG12	1:A:630:THR:N	2.32	0.43
1:A:1032:GLU:C	1:A:1033:ILE:HD12	2.39	0.43
1:B:452:PHE:HB3	1:B:463:TYR:HB3	1.99	0.43
1:C:983:ILE:HD12	1:C:983:ILE:N	2.33	0.43
1:D:510:LYS:NZ	4:D:1115:HOH:O	2.51	0.43
1:E:89:ASP:OD1	1:E:91:ARG:HB2	2.19	0.43
1:E:190:ARG:NH1	4:E:1126:HOH:O	2.46	0.43
1:E:222:PHE:H	1:E:1038:HIS:CD2	2.37	0.43
1:E:394:THR:OG1	1:E:395:GLY:N	2.52	0.43
1:F:530:ASN:CB	4:F:1112:HOH:O	2.65	0.43
1:F:1053:ASP:HA	1:F:1056:ILE:HD12	2.01	0.43
1:A:74:ILE:HG13	1:A:75:VAL:HG12	2.00	0.43
1:A:155:PRO:HG2	1:A:156:PHE:CD1	2.54	0.43
1:B:351:SER:OG	1:B:353:THR:CG2	2.60	0.43
1:B:660:PHE:CD2	1:B:665:PRO:HA	2.53	0.43
1:B:909:ILE:HG12	1:B:956:ILE:CG2	2.48	0.43
1:B:965:SER:O	1:B:968:ASP:N	2.51	0.43
1:B:1032:GLU:C	1:B:1033:ILE:HD12	2.39	0.43
1:C:467:LEU:HD11	1:C:496:GLU:HB2	1.99	0.43
1:D:882:ILE:HD11	1:D:899:PHE:HA	2.00	0.43
1:D:1048:ILE:O	1:D:1052:ILE:HG13	2.18	0.43
1:E:58:CYS:C	1:E:60:ASP:H	2.21	0.43
1:E:714:ILE:HG21	1:E:741:GLU:CB	2.48	0.43
1:E:949:ASN:ND2	1:F:475:TYR:OH	2.52	0.43
1:B:200:PRO:HB3	1:B:737:GLU:OE1	2.19	0.43
1:C:45:ASN:HB3	1:C:277:HIS:CE1	2.54	0.43
1:D:645:ARG:HH21	1:D:645:ARG:HG3	1.84	0.43
1:D:714:ILE:HG21	1:D:741:GLU:CB	2.49	0.43
1:D:820:ASN:OD1	1:D:822:TYR:HB2	2.18	0.43
1:E:909:ILE:HG12	1:E:956:ILE:CG2	2.49	0.43
1:F:498:SER:OG	1:F:499:HIS:N	2.51	0.43
1:F:714:ILE:HG21	1:F:741:GLU:CB	2.49	0.43
1:F:736:VAL:HG21	4:F:1132:HOH:O	2.17	0.43
1:A:406:ASN:HB2	1:A:424:ASP:CG	2.39	0.42
1:B:872:HIS:HE1	1:B:902:GLU:OE1	2.02	0.42
1:B:892:LEU:HD12	1:B:892:LEU:HA	1.90	0.42
1:C:131:ARG:HG2	1:C:131:ARG:HH21	1.83	0.42
1:C:921:SER:HB3	1:C:966:ASP:OD2	2.19	0.42
1:E:412:VAL:HG13	1:E:433:LEU:HD11	2.01	0.42
1:E:660:PHE:HB3	1:E:668:GLU:CB	2.46	0.42
1:E:703:ASN:ND2	1:E:705:ALA:H	2.17	0.42

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:F:847:LEU:HD12	1:F:849:ILE:HD11	2.01	0.42
1:A:137:VAL:HG22	1:A:146:LEU:HD11	2.01	0.42
1:B:581:ASP:HA	1:B:582:PRO:HD3	1.95	0.42
1:C:363:ARG:HD3	1:C:363:ARG:HA	1.65	0.42
1:C:768:ASP:HB2	1:C:780:LYS:HB3	2.01	0.42
1:D:1010:GLU:HB3	1:D:1011:PHE:CE1	2.55	0.42
1:E:57:CYS:HB3	1:E:62:TRP:CD1	2.54	0.42
1:E:846:ASP:OD2	1:E:846:ASP:C	2.57	0.42
1:F:529:LEU:HG	1:F:529:LEU:O	2.18	0.42
1:F:660:PHE:HB3	1:F:668:GLU:CB	2.46	0.42
1:F:986:ARG:HA	1:F:1027:VAL:O	2.19	0.42
1:A:218:ASN:O	1:A:220:GLY:N	2.52	0.42
1:A:912:VAL:O	1:A:915:ASN:HB2	2.19	0.42
1:B:87:PHE:CB	1:B:88:PRO:HD2	2.49	0.42
1:B:403:ASN:HD22	1:B:405:GLY:H	1.56	0.42
1:B:660:PHE:HD2	1:B:665:PRO:HA	1.84	0.42
1:C:167:ASN:CB	1:C:170:ILE:HB	2.37	0.42
1:D:257:THR:HG22	1:D:264:LEU:HA	2.01	0.42
1:D:350:VAL:HG11	1:D:659:THR:HG21	2.01	0.42
1:E:403:ASN:HD21	1:E:405:GLY:H	1.63	0.42
1:E:520:LEU:CD2	1:F:527:VAL:HG21	2.49	0.42
1:F:467:LEU:HD11	1:F:496:GLU:HB2	2.00	0.42
1:F:886:ASP:OD2	1:F:886:ASP:C	2.57	0.42
1:A:222:PHE:H	1:A:1038:HIS:HD2	1.67	0.42
1:A:362:LEU:HD23	1:A:363:ARG:H	1.85	0.42
1:C:297:ASN:HD22	1:C:298:PRO:HD2	1.84	0.42
1:C:912:VAL:HG11	1:C:970:PHE:CE2	2.55	0.42
1:D:912:VAL:HG11	1:D:970:PHE:CE2	2.55	0.42
1:E:445:ARG:HH12	1:E:471:GLU:CD	2.22	0.42
1:E:840:LYS:HD2	1:E:841:GLY:N	2.35	0.42
1:E:846:ASP:C	1:E:847:LEU:HD23	2.40	0.42
1:E:847:LEU:HD12	1:E:849:ILE:HD11	2.01	0.42
1:F:530:ASN:OD1	1:F:531:PHE:N	2.52	0.42
1:A:660:PHE:HB3	1:A:668:GLU:CB	2.47	0.42
1:B:141:ASP:OD1	1:B:145:ASN:HB2	2.19	0.42
1:B:202:TRP:CZ3	1:B:745:SER:HB3	2.53	0.42
1:B:541:VAL:HG22	1:B:542:ILE:N	2.34	0.42
1:C:337:ILE:HG12	1:C:649:MET:HE2	2.01	0.42
1:D:89:ASP:OD1	1:D:91:ARG:HB2	2.19	0.42
1:D:500:ASP:OD2	1:D:516:SER:HB3	2.20	0.42
1:D:557:ARG:HG3	1:F:393:ARG:NH2	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:956:ILE:HG22	1:D:1055:LEU:HD11	2.01	0.42
1:E:167:ASN:O	1:E:170:ILE:HG12	2.19	0.42
1:E:387:LEU:HD12	1:E:400:PHE:CE1	2.54	0.42
1:E:660:PHE:CD2	1:E:665:PRO:HA	2.54	0.42
1:F:890:MET:HA	1:F:893:ASN:HD22	1.84	0.42
1:F:1048:ILE:O	1:F:1052:ILE:HG13	2.20	0.42
1:A:137:VAL:HG13	1:A:146:LEU:CD1	2.50	0.42
1:A:697:ALA:HA	1:A:1008:GLN:HG2	2.02	0.42
1:A:872:HIS:HE1	1:A:902:GLU:OE1	2.02	0.42
1:B:132:ARG:NH1	4:B:1137:HOH:O	2.28	0.42
1:D:141:ASP:OD1	1:D:145:ASN:HB2	2.20	0.42
1:D:350:VAL:HG21	1:D:669:ARG:NH1	2.34	0.42
1:D:469:HIS:CD2	4:D:1124:HOH:O	2.73	0.42
1:D:557:ARG:CZ	1:F:393:ARG:HH12	2.32	0.42
1:E:222:PHE:H	1:E:1038:HIS:HD2	1.68	0.42
1:E:882:ILE:HD11	1:E:899:PHE:HA	2.02	0.42
1:E:886:ASP:O	1:E:891:GLY:HA3	2.20	0.42
1:E:1000:LEU:HB2	1:E:1004:THR:HB	2.02	0.42
1:F:272:ASP:OD1	1:F:289:LYS:NZ	2.53	0.42
1:F:363:ARG:HA	1:F:363:ARG:HD3	1.65	0.42
1:A:197:PHE:HE1	1:A:199:LEU:HD21	1.85	0.42
1:A:997:LYS:HE3	4:A:1143:HOH:O	2.19	0.42
1:B:43:LEU:HD22	1:B:55:PHE:HE1	1.83	0.42
1:B:61:LEU:CB	1:B:75:VAL:CG1	2.97	0.42
1:B:591:LEU:HD11	1:B:662:LEU:HD21	2.01	0.42
1:C:867:ASN:ND2	4:C:1097:HOH:O	2.53	0.42
1:D:87:PHE:CD1	1:D:92:LYS:HB2	2.55	0.42
1:D:629:VAL:HG12	1:D:630:THR:N	2.35	0.42
1:E:820:ASN:OD1	1:E:822:TYR:HB2	2.20	0.42
1:F:297:ASN:HD22	1:F:298:PRO:HD2	1.85	0.42
1:F:541:VAL:HG22	1:F:542:ILE:N	2.34	0.42
1:F:738:MET:SD	1:F:738:MET:C	2.98	0.42
1:A:45:ASN:HB3	1:A:277:HIS:CE1	2.55	0.42
1:A:846:ASP:C	1:A:847:LEU:HD23	2.40	0.42
1:B:87:PHE:CD1	1:B:92:LYS:HB2	2.54	0.42
1:C:714:ILE:HG21	1:C:741:GLU:CB	2.49	0.42
1:D:137:VAL:HG22	1:D:146:LEU:HD11	2.01	0.42
1:E:660:PHE:HD2	1:E:665:PRO:HA	1.84	0.42
1:E:1048:ILE:O	1:E:1052:ILE:HG13	2.19	0.42
1:F:74:ILE:HG13	1:F:75:VAL:HG12	2.01	0.42
1:F:82:ASN:ND2	1:F:96:ARG:HH21	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:PHE:HB3	1:A:152:ALA:HB2	2.01	0.42
1:A:467:LEU:HD21	1:A:496:GLU:HB3	2.01	0.42
1:A:948:THR:HB	1:B:922:GLN:HE22	1.83	0.42
1:D:48:ILE:HB	1:D:286:LEU:HD22	2.01	0.42
1:D:1031:VAL:HG12	1:D:1033:ILE:HD11	2.02	0.42
1:E:184:LEU:HD13	1:E:237:ILE:HG13	2.02	0.42
1:E:286:LEU:HD12	1:E:286:LEU:HA	1.89	0.42
1:E:337:ILE:HG12	1:E:649:MET:HE2	2.01	0.42
1:E:382:ARG:HD2	1:E:691:ASP:CG	2.40	0.42
1:E:436:GLY:O	1:E:438:PRO:HD3	2.20	0.42
1:E:645:ARG:HH21	1:E:645:ARG:HG3	1.84	0.42
1:F:394:THR:OG1	1:F:395:GLY:N	2.53	0.42
1:F:840:LYS:HD2	1:F:841:GLY:N	2.35	0.42
1:F:892:LEU:HD12	1:F:892:LEU:HA	1.90	0.42
1:A:48:ILE:HB	1:A:286:LEU:HD22	2.02	0.42
1:A:403:ASN:HD22	1:A:403:ASN:C	2.13	0.42
1:A:687:LEU:HD23	1:A:687:LEU:HA	1.89	0.42
1:B:535:VAL:HB	1:B:583:GLY:HA2	2.02	0.42
1:C:167:ASN:O	1:C:170:ILE:HG12	2.19	0.42
1:C:502:ALA:N	1:C:503:PRO:CD	2.83	0.42
1:C:638:ASP:OD2	1:C:639:LEU:N	2.53	0.42
1:C:930:ASN:HD21	1:D:926:GLU:HG3	1.85	0.42
1:D:181:THR:HG22	1:D:182:HIS:CE1	2.55	0.42
1:D:535:VAL:HB	1:D:583:GLY:HA2	2.02	0.42
1:D:766:ALA:HA	1:D:855:ASP:OD1	2.19	0.42
1:E:48:ILE:HB	1:E:286:LEU:HD22	2.02	0.42
1:E:256:SER:OG	1:E:267:HIS:CE1	2.73	0.42
1:E:363:ARG:HA	1:E:363:ARG:HD3	1.69	0.42
1:F:87:PHE:CD1	1:F:92:LYS:HB2	2.55	0.42
1:F:257:THR:HG22	1:F:264:LEU:HA	2.02	0.42
1:F:445:ARG:HH22	1:F:471:GLU:HG2	1.85	0.42
1:F:761:ARG:NH2	1:F:853:ASP:OD2	2.52	0.42
1:F:1010:GLU:HB3	1:F:1011:PHE:CE1	2.55	0.42
1:A:660:PHE:HD2	1:A:665:PRO:HA	1.85	0.41
1:A:922:GLN:HE22	1:B:948:THR:CB	2.33	0.41
1:B:74:ILE:HG13	1:B:75:VAL:HG12	2.01	0.41
1:B:132:ARG:NH2	1:B:158:SER:OG	2.53	0.41
1:B:986:ARG:HA	1:B:1027:VAL:O	2.20	0.41
1:C:382:ARG:HD2	1:C:691:ASP:CG	2.41	0.41
1:C:423:ASN:C	1:C:423:ASN:HD22	2.22	0.41
1:C:890:MET:HA	1:C:893:ASN:HD22	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:ARG:HG2	1:D:131:ARG:HH21	1.85	0.41
1:D:394:THR:OG1	1:D:395:GLY:N	2.53	0.41
1:D:846:ASP:C	1:D:847:LEU:HD23	2.40	0.41
1:E:181:THR:HG22	1:E:182:HIS:ND1	2.35	0.41
1:E:423:ASN:HB2	4:E:1131:HOH:O	2.18	0.41
1:E:562:GLU:HB3	1:E:563:ALA:H	1.62	0.41
1:E:1010:GLU:HB3	1:E:1011:PHE:CE1	2.55	0.41
1:F:256:SER:OG	1:F:267:HIS:CE1	2.73	0.41
1:F:351:SER:HB3	1:F:353:THR:HG22	1.99	0.41
1:F:568:LEU:HB3	1:F:571:MET:HE2	2.00	0.41
1:F:905:TYR:N	4:F:1090:HOH:O	2.45	0.41
1:A:350:VAL:HG21	1:A:669:ARG:HH11	1.86	0.41
1:A:500:ASP:OD2	1:A:516:SER:HB3	2.20	0.41
1:A:703:ASN:ND2	1:A:705:ALA:H	2.18	0.41
1:B:414:ARG:NH1	1:B:644:ASP:HA	2.36	0.41
1:C:87:PHE:CD1	1:C:92:LYS:HB2	2.55	0.41
1:C:1014:TRP:CH2	1:C:1016:ARG:HA	2.55	0.41
4:C:1106:HOH:O	1:D:494:THR:HA	2.20	0.41
1:D:921:SER:HB3	1:D:966:ASP:OD2	2.20	0.41
1:D:1014:TRP:CH2	1:D:1016:ARG:HA	2.55	0.41
1:E:945:PRO:CG	1:F:474:GLY:HA2	2.50	0.41
1:F:351:SER:OG	1:F:353:THR:CG2	2.61	0.41
1:F:847:LEU:N	1:F:847:LEU:HD23	2.36	0.41
1:F:921:SER:HB3	1:F:966:ASP:OD2	2.20	0.41
1:F:1014:TRP:CH2	1:F:1016:ARG:HA	2.54	0.41
1:A:61:LEU:CB	1:A:75:VAL:CG1	2.99	0.41
1:A:581:ASP:HA	1:A:582:PRO:HD3	1.90	0.41
1:B:167:ASN:O	1:B:170:ILE:HG12	2.20	0.41
1:B:423:ASN:HD22	1:B:423:ASN:C	2.21	0.41
1:B:714:ILE:HG21	1:B:741:GLU:CB	2.49	0.41
1:B:847:LEU:HD12	1:B:849:ILE:HD11	2.01	0.41
1:C:1032:GLU:C	1:C:1033:ILE:HD12	2.40	0.41
1:D:773:GLY:HA3	4:D:1112:HOH:O	2.20	0.41
1:E:546:PRO:CG	1:E:567:ASP:HB3	2.50	0.41
3:K:2101:D10:H72	3:K:2101:D10:H42	1.54	0.41
1:F:540:PHE:HA	1:F:577:PRO:HA	2.01	0.41
1:A:555:VAL:HG23	4:A:1148:HOH:O	2.20	0.41
1:A:932:ARG:HD3	1:A:935:TYR:OH	2.20	0.41
1:A:1014:TRP:CH2	1:A:1016:ARG:HA	2.56	0.41
1:B:976:LYS:NZ	1:B:1017:ASP:HB2	2.35	0.41
1:C:89:ASP:OD1	1:C:91:ARG:HB2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:209:THR:OG1	1:D:988:TRP:HD1	2.03	0.41
1:D:642:SER:HG	1:D:644:ASP:CG	2.22	0.41
1:E:528:VAL:O	1:E:530:ASN:N	2.53	0.41
1:E:582:PRO:HD2	4:E:1078:HOH:O	2.20	0.41
1:E:639:LEU:HD23	1:E:639:LEU:C	2.41	0.41
1:F:167:ASN:O	1:F:170:ILE:HG12	2.20	0.41
1:F:236:VAL:HG13	4:F:1074:HOH:O	2.18	0.41
3:L:2101:D10:H72	3:L:2101:D10:H42	1.54	0.41
1:B:58:CYS:C	1:B:60:ASP:H	2.24	0.41
1:B:218:ASN:O	1:B:220:GLY:N	2.53	0.41
1:B:297:ASN:HD22	1:B:298:PRO:HD2	1.85	0.41
1:C:498:SER:OG	1:C:499:HIS:N	2.54	0.41
1:E:535:VAL:HB	1:E:583:GLY:HA2	2.03	0.41
1:E:922:GLN:HB3	1:F:946:TYR:CE1	2.56	0.41
1:F:141:ASP:OD1	1:F:145:ASN:HB2	2.20	0.41
1:F:200:PRO:HB3	1:F:737:GLU:OE1	2.20	0.41
1:A:195:ASN:O	1:A:231:HIS:HE1	2.04	0.41
1:B:48:ILE:HB	1:B:286:LEU:HD22	2.01	0.41
1:B:272:ASP:OD1	1:B:289:LYS:NZ	2.53	0.41
1:B:337:ILE:HG12	1:B:649:MET:CE	2.50	0.41
1:B:363:ARG:NH2	4:B:1091:HOH:O	2.52	0.41
1:C:761:ARG:NH2	1:C:853:ASP:OD2	2.53	0.41
1:C:847:LEU:N	1:C:847:LEU:HD23	2.35	0.41
1:C:1045:ASP:HB3	1:C:1048:ILE:HG22	2.01	0.41
1:E:473:ASP:OD1	1:F:904:SER:HB2	2.20	0.41
1:E:498:SER:OG	1:E:499:HIS:N	2.52	0.41
1:F:222:PHE:H	1:F:1038:HIS:HD2	1.67	0.41
1:F:226:VAL:CG1	1:F:228:MET:HE3	2.51	0.41
1:A:744:THR:HG22	1:A:745:SER:H	1.85	0.41
1:A:797:GLU:HA	1:B:574:ARG:HA	2.03	0.41
1:A:840:LYS:HD2	1:A:841:GLY:N	2.36	0.41
1:A:874:ARG:HD3	1:A:1052:ILE:HG21	2.02	0.41
1:B:412:VAL:HG13	1:B:433:LEU:HD11	2.02	0.41
1:B:502:ALA:N	1:B:503:PRO:CD	2.84	0.41
1:B:687:LEU:HD23	1:B:687:LEU:HA	1.92	0.41
1:B:932:ARG:HD3	1:B:935:TYR:OH	2.21	0.41
1:C:58:CYS:O	1:C:60:ASP:N	2.53	0.41
1:C:82:ASN:ND2	1:C:96:ARG:HH21	2.17	0.41
1:C:157:SER:HB2	4:C:1090:HOH:O	2.19	0.41
1:C:180:ALA:HA	4:C:1080:HOH:O	2.20	0.41
1:C:530:ASN:HB3	4:C:1092:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:184:LEU:HD13	1:D:237:ILE:HG13	2.02	0.41
1:D:892:LEU:HD12	1:D:892:LEU:HA	1.94	0.41
1:D:983:ILE:HD12	1:D:983:ILE:N	2.34	0.41
1:F:45:ASN:HB3	1:F:277:HIS:CE1	2.55	0.41
1:F:884:ILE:HA	1:F:885:PRO:HD2	1.94	0.41
1:A:909:ILE:HG12	1:A:956:ILE:CG2	2.51	0.41
1:B:124:PHE:HB3	1:B:152:ALA:HB2	2.01	0.41
1:B:209:THR:OG1	1:B:988:TRP:HD1	2.04	0.41
1:B:681:SER:HB3	1:B:684:GLU:CD	2.41	0.41
1:C:681:SER:HB3	1:C:684:GLU:CD	2.40	0.41
1:C:781:ALA:CB	1:C:802:PRO:HG2	2.51	0.41
1:D:61:LEU:HD13	1:D:74:ILE:CD1	2.51	0.41
1:F:350:VAL:HG21	1:F:669:ARG:HH11	1.85	0.41
1:F:463:TYR:CE1	1:F:481:HIS:HB2	2.56	0.41
1:F:638:ASP:OD2	1:F:639:LEU:N	2.54	0.41
1:A:535:VAL:HB	1:A:583:GLY:HA2	2.02	0.41
1:A:555:VAL:HG22	1:E:354:TYR:CZ	2.56	0.41
1:A:714:ILE:HG21	1:A:741:GLU:CB	2.50	0.41
1:A:983:ILE:HD12	1:A:983:ILE:N	2.35	0.41
1:B:406:ASN:HB2	1:B:424:ASP:CG	2.40	0.41
1:B:744:THR:HG22	1:B:745:SER:H	1.85	0.41
1:B:846:ASP:C	1:B:846:ASP:OD2	2.59	0.41
1:B:1000:LEU:HD12	1:B:1004:THR:HB	2.03	0.41
1:B:1014:TRP:CD1	1:B:1019:GLY:HA2	2.56	0.41
1:C:200:PRO:HB3	1:C:737:GLU:OE1	2.21	0.41
1:C:279:ASN:HD22	1:C:279:ASN:HA	1.56	0.41
1:C:387:LEU:HD12	1:C:400:PHE:CE1	2.56	0.41
1:C:468:LYS:HG2	1:C:473:ASP:HB2	2.02	0.41
1:C:744:THR:HG22	1:C:745:SER:H	1.83	0.41
1:C:787:SER:OG	4:C:1106:HOH:O	2.17	0.41
1:D:155:PRO:HG2	1:D:156:PHE:CD1	2.56	0.41
1:D:202:TRP:CZ3	1:D:745:SER:HB3	2.56	0.41
1:D:412:VAL:HG13	1:D:433:LEU:HD11	2.02	0.41
1:D:502:ALA:N	1:D:503:PRO:CD	2.83	0.41
1:D:660:PHE:HB3	1:D:668:GLU:CB	2.47	0.41
1:D:660:PHE:CD2	1:D:665:PRO:HA	2.56	0.41
1:D:761:ARG:NH2	1:D:853:ASP:OD2	2.54	0.41
1:D:840:LYS:HD2	1:D:841:GLY:N	2.36	0.41
1:D:909:ILE:HG12	1:D:956:ILE:CG2	2.51	0.41
1:D:999:ARG:HH11	1:D:1005:VAL:CG2	2.34	0.41
1:E:221:ALA:N	4:E:1073:HOH:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:257:THR:HG22	1:E:264:LEU:HA	2.02	0.41
1:E:350:VAL:HG11	1:E:659:THR:HG21	2.03	0.41
1:E:468:LYS:HG2	1:E:473:ASP:HB2	2.02	0.41
1:E:912:VAL:HG11	1:E:970:PHE:CE2	2.56	0.41
1:F:387:LEU:HD12	1:F:400:PHE:CE1	2.56	0.41
1:F:932:ARG:HD3	1:F:935:TYR:OH	2.21	0.41
1:F:963:ALA:O	1:F:987:THR:HB	2.20	0.41
1:A:52:ARG:NH1	1:A:90:GLY:O	2.53	0.41
1:A:581:ASP:O	1:A:585:TYR:OH	2.32	0.41
1:B:197:PHE:HE1	1:B:199:LEU:HD21	1.86	0.41
1:B:297:ASN:CB	4:B:1124:HOH:O	2.65	0.41
1:B:629:VAL:HG12	1:B:630:THR:N	2.35	0.41
1:C:874:ARG:HH21	1:C:874:ARG:HG3	1.86	0.41
1:D:110:PHE:CD1	1:D:121:ILE:HD11	2.56	0.41
1:E:74:ILE:HG13	1:E:75:VAL:HG12	2.01	0.41
1:E:406:ASN:HB2	1:E:424:ASP:CG	2.41	0.41
1:E:932:ARG:HD3	1:E:935:TYR:OH	2.20	0.41
1:E:983:ILE:HD12	1:E:983:ILE:N	2.35	0.41
1:F:956:ILE:HG22	1:F:1055:LEU:HD11	2.03	0.41
1:A:257:THR:HG22	1:A:264:LEU:HA	2.02	0.40
1:A:965:SER:O	1:A:968:ASP:N	2.53	0.40
1:B:45:ASN:HB3	1:B:277:HIS:CE1	2.57	0.40
1:B:556:PRO:CD	1:D:354:TYR:CG	3.04	0.40
1:C:112:ASN:HB3	1:C:115:ASN:OD1	2.20	0.40
1:C:365:ARG:HG2	1:C:365:ARG:HH21	1.86	0.40
1:C:409:ALA:HB3	1:C:422:ALA:HB3	2.03	0.40
1:C:639:LEU:HD23	1:C:639:LEU:C	2.42	0.40
1:D:351:SER:HB3	1:D:353:THR:HG22	2.03	0.40
1:D:423:ASN:C	1:D:423:ASN:HD22	2.23	0.40
1:D:616:LYS:HB3	1:D:616:LYS:HE2	1.90	0.40
1:E:87:PHE:CB	1:E:88:PRO:HD2	2.50	0.40
1:E:155:PRO:HG2	1:E:156:PHE:CD1	2.56	0.40
1:F:382:ARG:HD2	1:F:691:ASP:CG	2.41	0.40
1:F:846:ASP:C	1:F:847:LEU:HD23	2.42	0.40
1:F:883:HIS:HA	1:F:911:ASP:O	2.21	0.40
1:F:1032:GLU:C	1:F:1033:ILE:HD12	2.41	0.40
1:A:387:LEU:HD12	1:A:400:PHE:CE1	2.56	0.40
1:B:350:VAL:HG21	1:B:669:ARG:HH11	1.86	0.40
1:B:409:ALA:HB3	1:B:422:ALA:HB3	2.03	0.40
1:C:287:PHE:CZ	1:C:294:TYR:HB2	2.56	0.40
1:C:886:ASP:O	1:C:891:GLY:HA3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:437:LYS:HE2	1:D:437:LYS:HB3	1.85	0.40
1:E:297:ASN:O	1:E:301:GLU:N	2.50	0.40
1:E:467:LEU:HD11	1:E:496:GLU:HB2	2.03	0.40
1:F:92:LYS:HB2	1:F:92:LYS:HE2	1.97	0.40
1:F:137:VAL:HG13	1:F:146:LEU:CD1	2.51	0.40
1:F:184:LEU:HD13	1:F:237:ILE:HG13	2.02	0.40
1:F:645:ARG:HH21	1:F:645:ARG:HG3	1.87	0.40
1:A:167:ASN:O	1:A:170:ILE:HG12	2.22	0.40
1:A:202:TRP:CZ3	1:A:745:SER:HB3	2.56	0.40
1:A:337:ILE:HG12	1:A:649:MET:HE2	2.03	0.40
1:A:412:VAL:HG13	1:A:433:LEU:HD11	2.03	0.40
1:A:890:MET:HA	1:A:893:ASN:HD22	1.86	0.40
1:B:890:MET:HA	1:B:893:ASN:HD22	1.85	0.40
1:C:101:SER:N	4:C:1126:HOH:O	2.54	0.40
1:C:1010:GLU:HB3	1:C:1011:PHE:CE1	2.56	0.40
1:C:1053:ASP:HA	1:C:1056:ILE:HD12	2.02	0.40
1:D:540:PHE:HA	1:D:577:PRO:HA	2.04	0.40
1:E:110:PHE:CD1	1:E:121:ILE:HD11	2.56	0.40
1:E:874:ARG:HG3	1:E:874:ARG:HH21	1.86	0.40
1:F:886:ASP:O	1:F:891:GLY:HA3	2.21	0.40
1:B:562:GLU:HB3	1:B:563:ALA:H	1.62	0.40
1:B:761:ARG:NH2	1:B:853:ASP:OD2	2.54	0.40
1:B:829:ALA:N	4:B:1121:HOH:O	2.54	0.40
1:C:846:ASP:C	1:C:846:ASP:OD2	2.59	0.40
1:C:1000:LEU:HB2	1:C:1004:THR:HB	2.03	0.40
1:D:704:GLU:O	1:D:707:ALA:HB3	2.22	0.40
1:D:1053:ASP:HA	1:D:1056:ILE:HD12	2.03	0.40
1:E:367:VAL:HG12	1:E:375:VAL:HG21	2.03	0.40
1:E:407:VAL:O	1:E:998:ARG:NH1	2.55	0.40
1:E:616:LYS:HE2	1:E:616:LYS:HB3	1.90	0.40
1:E:1053:ASP:HA	1:E:1056:ILE:HD12	2.04	0.40
1:F:232:VAL:HB	4:F:1122:HOH:O	2.20	0.40
1:A:200:PRO:HB3	1:A:737:GLU:OE1	2.21	0.40
1:A:297:ASN:HD22	1:A:298:PRO:HD2	1.85	0.40
1:B:89:ASP:OD1	1:B:91:ARG:HB2	2.22	0.40
1:B:226:VAL:CG1	1:B:228:MET:HE3	2.51	0.40
1:B:912:VAL:HG11	1:B:970:PHE:CE2	2.57	0.40
1:D:335:ASP:HA	4:D:1131:HOH:O	2.21	0.40
1:D:535:VAL:O	1:D:535:VAL:HG23	2.21	0.40
1:D:884:ILE:HD13	1:D:924:ILE:HD13	2.03	0.40
1:E:660:PHE:HA	1:E:661:PRO:HD3	1.96	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:131:ARG:HG2	1:F:131:ARG:HH21	1.86	0.40
1:F:502:ALA:N	1:F:503:PRO:CD	2.85	0.40
1:F:681:SER:HB3	1:F:684:GLU:CD	2.42	0.40
1:F:874:ARG:HG3	1:F:874:ARG:HH21	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1021/1071 (95%)	934 (92%)	78 (8%)	9 (1%)	17	46
1	B	1021/1071 (95%)	934 (92%)	78 (8%)	9 (1%)	17	46
1	C	1021/1071 (95%)	930 (91%)	80 (8%)	11 (1%)	14	41
1	D	1021/1071 (95%)	934 (92%)	78 (8%)	9 (1%)	17	46
1	E	1021/1071 (95%)	934 (92%)	78 (8%)	9 (1%)	17	46
1	F	1021/1071 (95%)	930 (91%)	81 (8%)	10 (1%)	15	44
2	G	2/5 (40%)	1 (50%)	1 (50%)	0	100	100
2	H	2/5 (40%)	1 (50%)	1 (50%)	0	100	100
2	I	2/5 (40%)	1 (50%)	1 (50%)	0	100	100
2	J	2/5 (40%)	1 (50%)	1 (50%)	0	100	100
2	K	2/5 (40%)	1 (50%)	1 (50%)	0	100	100
2	L	2/5 (40%)	1 (50%)	1 (50%)	0	100	100
All	All	6138/6456 (95%)	5602 (91%)	479 (8%)	57 (1%)	17	46

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	219	SER
1	C	219	SER
1	C	562	GLU
1	D	219	SER
1	E	219	SER
1	F	219	SER
1	A	529	LEU
1	A	562	GLU
1	A	579	ASN
1	A	715	TYR
1	B	219	SER
1	B	562	GLU
1	B	579	ASN
1	C	579	ASN
1	C	715	TYR
1	D	529	LEU
1	D	562	GLU
1	D	579	ASN
1	E	529	LEU
1	E	562	GLU
1	E	579	ASN
1	E	715	TYR
1	F	529	LEU
1	F	562	GLU
1	F	579	ASN
1	F	715	TYR
1	A	259	LEU
1	A	919	PHE
1	B	259	LEU
1	B	715	TYR
1	B	919	PHE
1	C	259	LEU
1	C	529	LEU
1	C	919	PHE
1	C	1018	ALA
1	D	259	LEU
1	D	715	TYR
1	D	919	PHE
1	E	259	LEU
1	E	919	PHE
1	F	259	LEU
1	F	919	PHE
1	A	67	LYS

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Mol	Chain	Res	Type
1	A	1018	ALA
1	B	67	LYS
1	B	529	LEU
1	B	1018	ALA
1	C	59	ASP
1	C	67	LYS
1	D	67	LYS
1	D	1018	ALA
1	E	67	LYS
1	E	1018	ALA
1	F	67	LYS
1	F	1018	ALA
1	F	361	PRO
1	C	361	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	883/928 (95%)	853 (97%)	30 (3%)	37	71
1	B	883/928 (95%)	853 (97%)	30 (3%)	37	71
1	C	883/928 (95%)	854 (97%)	29 (3%)	38	72
1	D	883/928 (95%)	855 (97%)	28 (3%)	39	73
1	E	883/928 (95%)	856 (97%)	27 (3%)	40	74
1	F	883/928 (95%)	854 (97%)	29 (3%)	38	72
2	G	4/4 (100%)	3 (75%)	1 (25%)	0	2
2	H	4/4 (100%)	3 (75%)	1 (25%)	0	2
2	I	4/4 (100%)	3 (75%)	1 (25%)	0	2
2	J	4/4 (100%)	3 (75%)	1 (25%)	0	2
2	K	4/4 (100%)	3 (75%)	1 (25%)	0	2
2	L	4/4 (100%)	3 (75%)	1 (25%)	0	2
All	All	5322/5592 (95%)	5143 (97%)	179 (3%)	37	71

All (179) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	LEU
1	A	82	ASN
1	A	157	SER
1	A	209	THR
1	A	279	ASN
1	A	297	ASN
1	A	313	SER
1	A	353	THR
1	A	362	LEU
1	A	363	ARG
1	A	403	ASN
1	A	423	ASN
1	A	471	GLU
1	A	516	SER
1	A	562	GLU
1	A	578	ILE
1	A	599	SER
1	A	703	ASN
1	A	731	LEU
1	A	738	MET
1	A	764	ARG
1	A	771	LEU
1	A	847	LEU
1	A	929	MET
1	A	936	ASP
1	A	979	LEU
1	A	1008	GLN
1	A	1015	PHE
1	A	1024	ASN
1	A	1035	TYR
2	G	1101	ARG
1	B	61	LEU
1	B	82	ASN
1	B	157	SER
1	B	209	THR
1	B	279	ASN
1	B	297	ASN
1	B	313	SER
1	B	353	THR
1	B	362	LEU
1	B	363	ARG
1	B	403	ASN

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Mol	Chain	Res	Type
1	B	423	ASN
1	B	471	GLU
1	B	516	SER
1	B	562	GLU
1	B	578	ILE
1	B	599	SER
1	B	703	ASN
1	B	731	LEU
1	B	738	MET
1	B	764	ARG
1	B	771	LEU
1	B	847	LEU
1	B	929	MET
1	B	936	ASP
1	B	979	LEU
1	B	1008	GLN
1	B	1015	PHE
1	B	1024	ASN
1	B	1035	TYR
2	H	1101	ARG
1	C	61	LEU
1	C	82	ASN
1	C	157	SER
1	C	209	THR
1	C	279	ASN
1	C	297	ASN
1	C	313	SER
1	C	353	THR
1	C	363	ARG
1	C	403	ASN
1	C	423	ASN
1	C	471	GLU
1	C	516	SER
1	C	562	GLU
1	C	578	ILE
1	C	599	SER
1	C	703	ASN
1	C	731	LEU
1	C	738	MET
1	C	764	ARG
1	C	771	LEU
1	C	847	LEU

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Mol	Chain	Res	Type
1	C	929	MET
1	C	936	ASP
1	C	979	LEU
1	C	1008	GLN
1	C	1015	PHE
1	C	1024	ASN
1	C	1035	TYR
2	I	1101	ARG
1	D	61	LEU
1	D	82	ASN
1	D	157	SER
1	D	209	THR
1	D	279	ASN
1	D	297	ASN
1	D	313	SER
1	D	353	THR
1	D	363	ARG
1	D	403	ASN
1	D	423	ASN
1	D	471	GLU
1	D	516	SER
1	D	562	GLU
1	D	578	ILE
1	D	703	ASN
1	D	731	LEU
1	D	738	MET
1	D	764	ARG
1	D	771	LEU
1	D	847	LEU
1	D	929	MET
1	D	936	ASP
1	D	979	LEU
1	D	1008	GLN
1	D	1015	PHE
1	D	1024	ASN
1	D	1035	TYR
2	J	1101	ARG
1	E	61	LEU
1	E	82	ASN
1	E	157	SER
1	E	209	THR
1	E	279	ASN

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Mol	Chain	Res	Type
1	E	297	ASN
1	E	313	SER
1	E	353	THR
1	E	403	ASN
1	E	423	ASN
1	E	471	GLU
1	E	516	SER
1	E	562	GLU
1	E	578	ILE
1	E	703	ASN
1	E	731	LEU
1	E	738	MET
1	E	764	ARG
1	E	771	LEU
1	E	847	LEU
1	E	929	MET
1	E	936	ASP
1	E	979	LEU
1	E	1008	GLN
1	E	1015	PHE
1	E	1024	ASN
1	E	1035	TYR
2	K	1101	ARG
1	F	61	LEU
1	F	82	ASN
1	F	157	SER
1	F	209	THR
1	F	279	ASN
1	F	297	ASN
1	F	313	SER
1	F	353	THR
1	F	363	ARG
1	F	403	ASN
1	F	423	ASN
1	F	471	GLU
1	F	516	SER
1	F	562	GLU
1	F	578	ILE
1	F	599	SER
1	F	703	ASN
1	F	731	LEU
1	F	738	MET

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Mol	Chain	Res	Type
1	F	764	ARG
1	F	771	LEU
1	F	847	LEU
1	F	929	MET
1	F	936	ASP
1	F	979	LEU
1	F	1008	GLN
1	F	1015	PHE
1	F	1024	ASN
1	F	1035	TYR
2	L	1101	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (177) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	64	HIS
1	A	82	ASN
1	A	195	ASN
1	A	253	GLN
1	A	267	HIS
1	A	279	ASN
1	A	297	ASN
1	A	403	ASN
1	A	415	ASN
1	A	423	ASN
1	A	497	ASN
1	A	511	ASN
1	A	611	GLN
1	A	700	ASN
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

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Mol	Chain	Res	Type
1	B	45	ASN
1	B	64	HIS
1	B	82	ASN
1	B	195	ASN
1	B	253	GLN
1	B	267	HIS
1	B	279	ASN
1	B	297	ASN
1	B	403	ASN
1	B	415	ASN
1	B	423	ASN
1	B	481	HIS
1	B	497	ASN
1	B	511	ASN
1	B	530	ASN
1	B	611	GLN
1	B	688	GLN
1	B	700	ASN
1	B	703	ASN
1	B	733	ASN
1	B	739	GLN
1	B	867	ASN
1	B	872	HIS
1	B	922	GLN
1	B	930	ASN
1	B	949	ASN
1	B	1008	GLN
1	B	1024	ASN
1	B	1038	HIS
1	B	1047	GLN
1	C	45	ASN
1	C	64	HIS
1	C	82	ASN
1	C	195	ASN
1	C	218	ASN
1	C	253	GLN
1	C	267	HIS
1	C	277	HIS
1	C	279	ASN
1	C	297	ASN
1	C	403	ASN
1	C	415	ASN

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Mol	Chain	Res	Type
1	C	423	ASN
1	C	481	HIS
1	C	497	ASN
1	C	499	HIS
1	C	511	ASN
1	C	611	GLN
1	C	700	ASN
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	D	45	ASN
1	D	64	HIS
1	D	82	ASN
1	D	195	ASN
1	D	253	GLN
1	D	267	HIS
1	D	277	HIS
1	D	279	ASN
1	D	297	ASN
1	D	403	ASN
1	D	415	ASN
1	D	423	ASN
1	D	481	HIS
1	D	497	ASN
1	D	511	ASN
1	D	530	ASN
1	D	579	ASN
1	D	611	GLN
1	D	700	ASN
1	D	703	ASN
1	D	733	ASN
1	D	739	GLN
1	D	867	ASN

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Mol	Chain	Res	Type
1	D	872	HIS
1	D	922	GLN
1	D	930	ASN
1	D	949	ASN
1	D	1008	GLN
1	D	1024	ASN
1	D	1038	HIS
1	D	1047	GLN
1	E	45	ASN
1	E	82	ASN
1	E	240	HIS
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	415	ASN
1	E	423	ASN
1	E	481	HIS
1	E	497	ASN
1	E	511	ASN
1	E	611	GLN
1	E	700	ASN
1	E	703	ASN
1	E	733	ASN
1	E	739	GLN
1	E	867	ASN
1	E	872	HIS
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	F	45	ASN
1	F	64	HIS
1	F	82	ASN
1	F	195	ASN
1	F	253	GLN
1	F	267	HIS

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Mol	Chain	Res	Type
1	F	279	ASN
1	F	297	ASN
1	F	403	ASN
1	F	415	ASN
1	F	423	ASN
1	F	481	HIS
1	F	497	ASN
1	F	499	HIS
1	F	511	ASN
1	F	530	ASN
1	F	611	GLN
1	F	700	ASN
1	F	703	ASN
1	F	733	ASN
1	F	739	GLN
1	F	867	ASN
1	F	872	HIS
1	F	922	GLN
1	F	930	ASN
1	F	949	ASN
1	F	1008	GLN
1	F	1024	ASN
1	F	1038	HIS
1	F	1047	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	D10	G	2101	2	9,9,9	0.52	0	8,8,8	1.00	0
3	D10	H	2101	2	9,9,9	0.52	0	8,8,8	1.00	0
3	D10	K	2101	2	9,9,9	0.52	0	8,8,8	1.00	0
3	D10	I	2101	2	9,9,9	0.52	0	8,8,8	1.00	0
3	D10	L	2101	2	9,9,9	0.52	0	8,8,8	1.00	0
3	D10	J	2101	2	9,9,9	0.53	0	8,8,8	1.00	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	D10	G	2101	2	-	4/7/7/7	-
3	D10	H	2101	2	-	4/7/7/7	-
3	D10	K	2101	2	-	4/7/7/7	-
3	D10	I	2101	2	-	4/7/7/7	-
3	D10	L	2101	2	-	4/7/7/7	-
3	D10	J	2101	2	-	4/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	2101	D10	C4-C5-C6-C7
3	H	2101	D10	C4-C5-C6-C7
3	I	2101	D10	C4-C5-C6-C7
3	J	2101	D10	C4-C5-C6-C7
3	K	2101	D10	C4-C5-C6-C7
3	L	2101	D10	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
3	G	2101	D10	C5-C6-C7-C8
3	L	2101	D10	C5-C6-C7-C8
3	H	2101	D10	C5-C6-C7-C8
3	I	2101	D10	C5-C6-C7-C8
3	J	2101	D10	C5-C6-C7-C8
3	K	2101	D10	C5-C6-C7-C8
3	I	2101	D10	C1-C2-C3-C4
3	K	2101	D10	C1-C2-C3-C4
3	G	2101	D10	C1-C2-C3-C4
3	H	2101	D10	C1-C2-C3-C4
3	J	2101	D10	C1-C2-C3-C4
3	L	2101	D10	C1-C2-C3-C4
3	J	2101	D10	C2-C3-C4-C5
3	I	2101	D10	C2-C3-C4-C5
3	G	2101	D10	C2-C3-C4-C5
3	K	2101	D10	C2-C3-C4-C5
3	L	2101	D10	C2-C3-C4-C5
3	H	2101	D10	C2-C3-C4-C5

There are no ring outliers.

6 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	2101	D10	2	0
3	H	2101	D10	3	0
3	K	2101	D10	4	0
3	I	2101	D10	4	0
3	L	2101	D10	4	0
3	J	2101	D10	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	1023/1071 (95%)	-0.44	1 (0%)	95	95	15, 35, 57, 80	20 (1%)
1	B	1023/1071 (95%)	-0.45	2 (0%)	95	94	18, 35, 57, 79	20 (1%)
1	C	1023/1071 (95%)	-0.28	11 (1%)	80	75	19, 38, 59, 80	20 (1%)
1	D	1023/1071 (95%)	-0.45	5 (0%)	91	88	19, 36, 57, 79	20 (1%)
1	E	1023/1071 (95%)	-0.44	4 (0%)	92	91	20, 36, 57, 80	20 (1%)
1	F	1023/1071 (95%)	-0.35	4 (0%)	92	91	19, 38, 58, 80	20 (1%)
2	G	4/5 (80%)	-0.55	0	100	100	36, 39, 40, 42	0
2	H	4/5 (80%)	-0.41	0	100	100	36, 39, 40, 42	0
2	I	4/5 (80%)	-0.09	0	100	100	36, 39, 40, 42	0
2	J	4/5 (80%)	-0.25	0	100	100	36, 39, 40, 42	0
2	K	4/5 (80%)	-0.35	0	100	100	36, 39, 40, 42	0
2	L	4/5 (80%)	-0.05	0	100	100	36, 39, 40, 42	0
All	All	6162/6456 (95%)	-0.40	27 (0%)	92	91	15, 36, 58, 80	120 (1%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	219	SER	6.4
1	D	219	SER	5.7
1	C	219	SER	5.6
1	C	839	GLY	5.1
1	B	842	GLY	4.8
1	F	219	SER	4.6
1	C	843	ASP	4.2
1	D	1061	ASN	4.0
1	D	220	GLY	4.0
1	D	563	ALA	3.7
1	C	50	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	838	SER	3.4
1	C	1061	ASN	3.2
1	A	842	GLY	3.2
1	C	563	ALA	3.0
1	E	220	GLY	2.7
1	C	840	LYS	2.6
1	C	806	LEU	2.6
1	C	842	GLY	2.5
1	D	841	GLY	2.5
1	B	1061	ASN	2.2
1	F	1061	ASN	2.2
1	F	563	ALA	2.2
1	F	435	THR	2.1
1	C	774	ASP	2.0
1	E	563	ALA	2.0
1	E	560	THR	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 monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
3	D10	H	2101	10/10	0.90	0.26	0,0,0,0	0
3	D10	L	2101	10/10	0.91	0.33	0,0,0,0	0
3	D10	J	2101	10/10	0.92	0.31	0,0,0,0	0
3	D10	G	2101	10/10	0.93	0.24	0,0,0,0	0
3	D10	I	2101	10/10	0.93	0.35	0,0,0,0	0
3	D10	K	2101	10/10	0.94	0.28	0,0,0,0	0

6.5 Other polymers ⓘ

There are no such residues in this entry.