



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:10 PM UTC

PDB ID : 1N6D / pdb_00001n6d
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)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

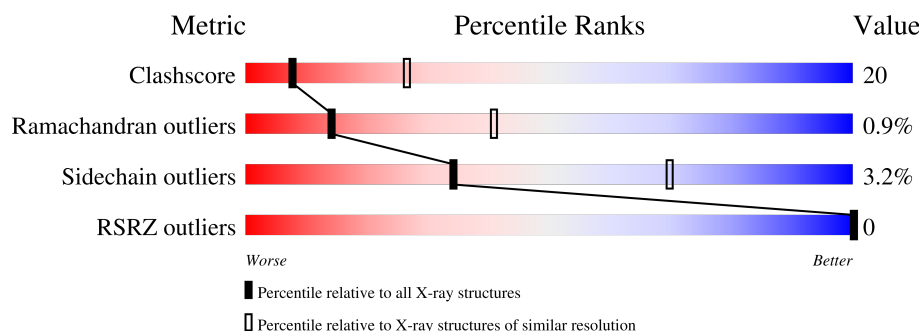
1 Overall quality at a glance

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	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1071	
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	20%20%20%40%
2	H	5	20%20%20%40%
2	I	5	20%20%20%40%
2	J	5	20%20%20%40%
2	K	5	20%20%20%40%
2	L	5	20%20%20%40%

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.

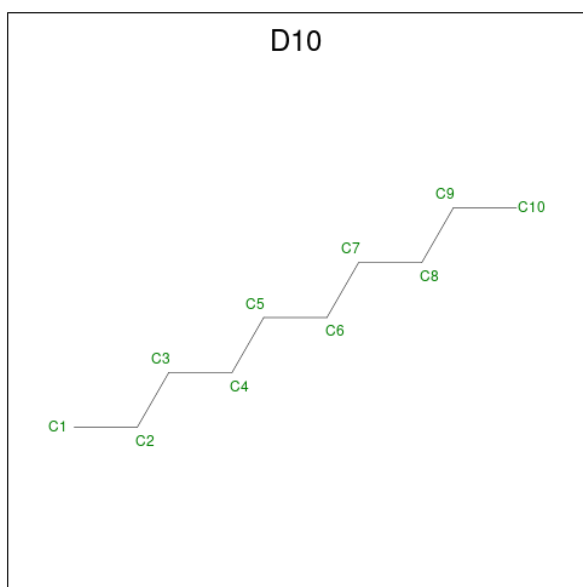
- Molecule 1 is a protein called Tricorn protease.

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

- Molecule 2 is a protein called RVRK.

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

- Molecule 3 is DECANE (CCD ID: D10) (formula: C₁₀H₂₂).



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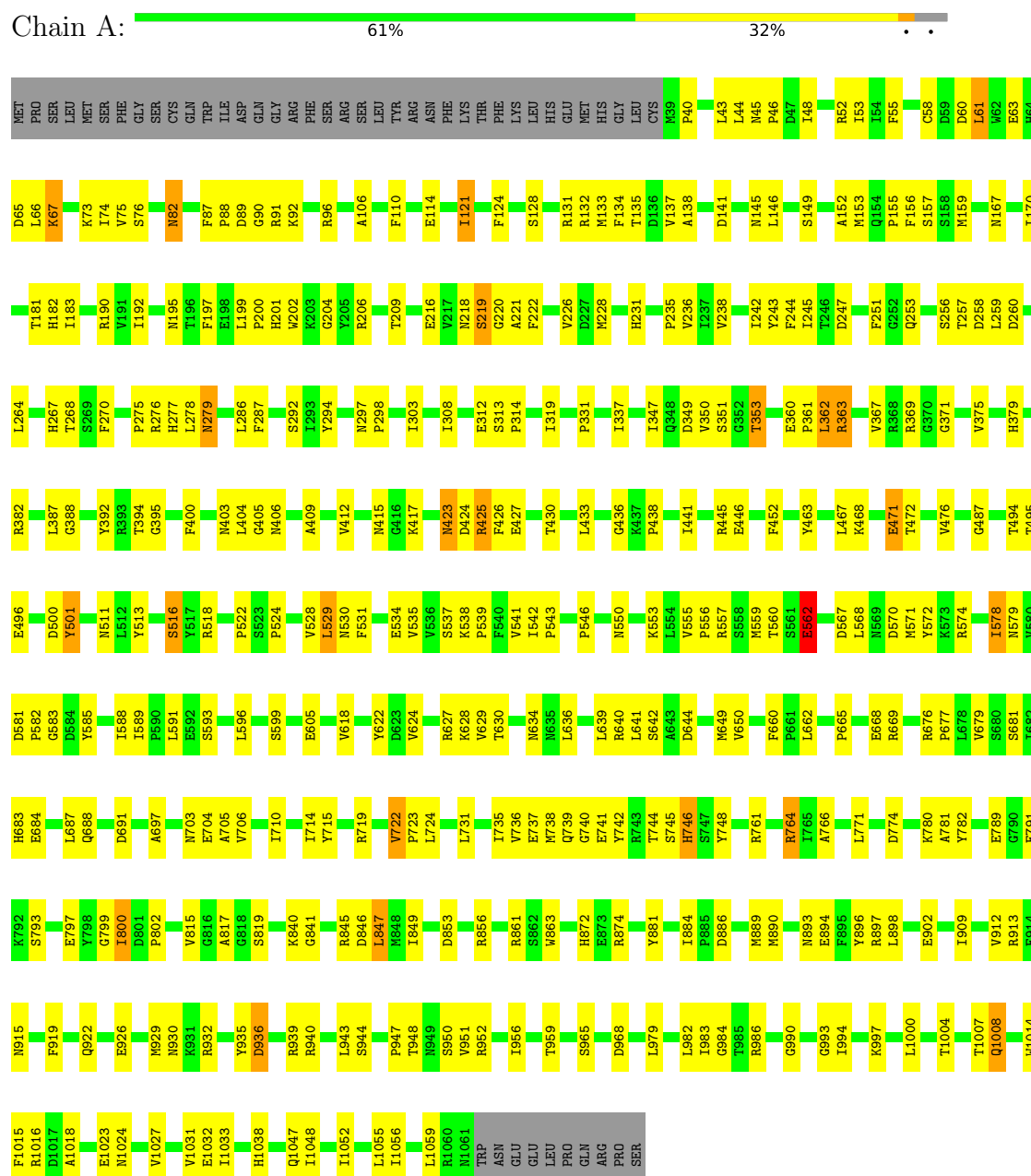
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	J	2	Total 2	O 2	0	0
4	E	89	Total 89	O 89	0	0
4	F	74	Total 74	O 74	0	0
4	L	2	Total 2	O 2	0	0

3 Residue-property plots

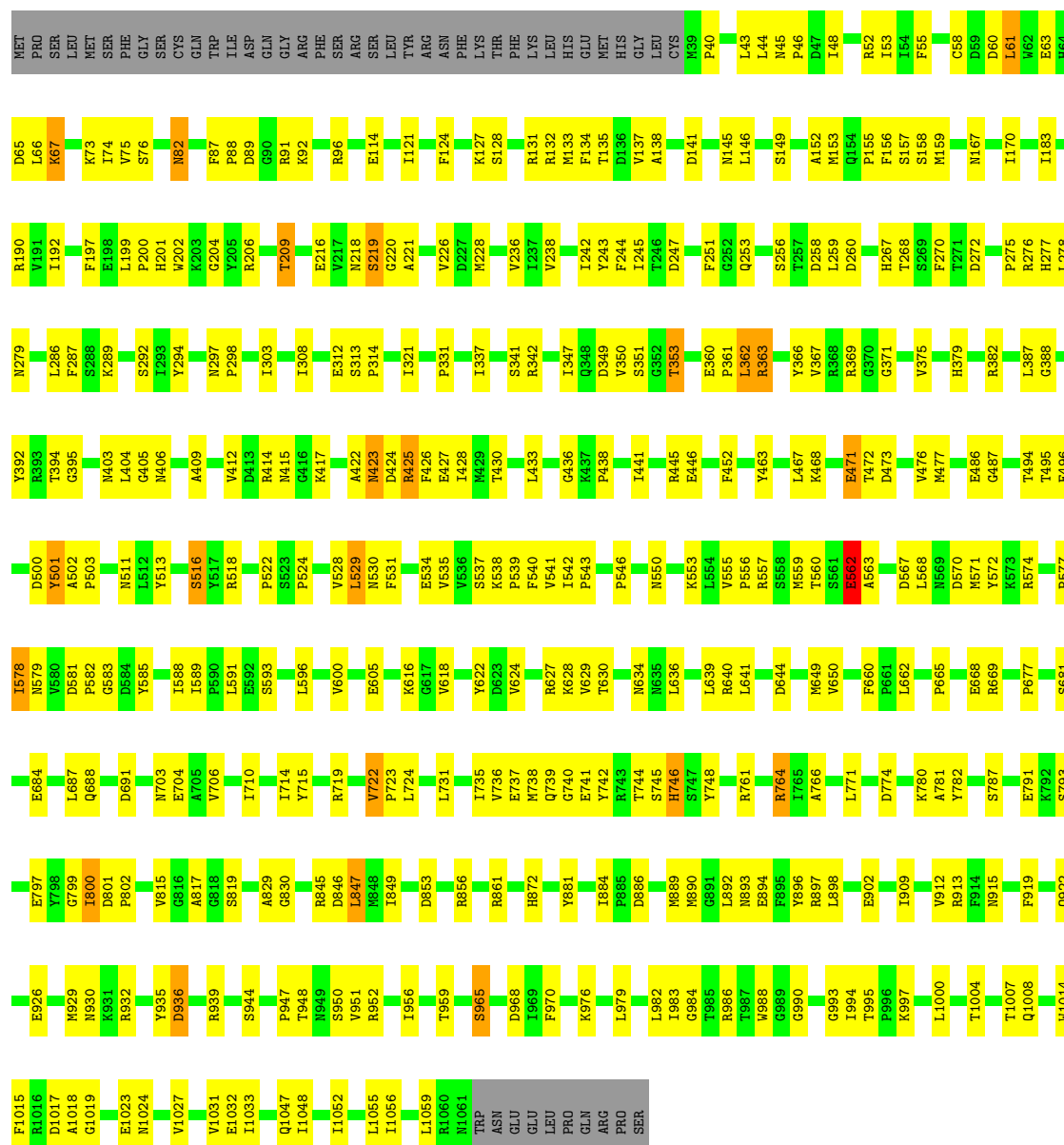
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



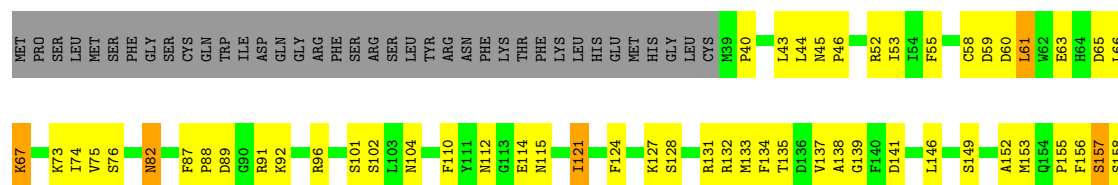
• Molecule 1: Tricorn protease

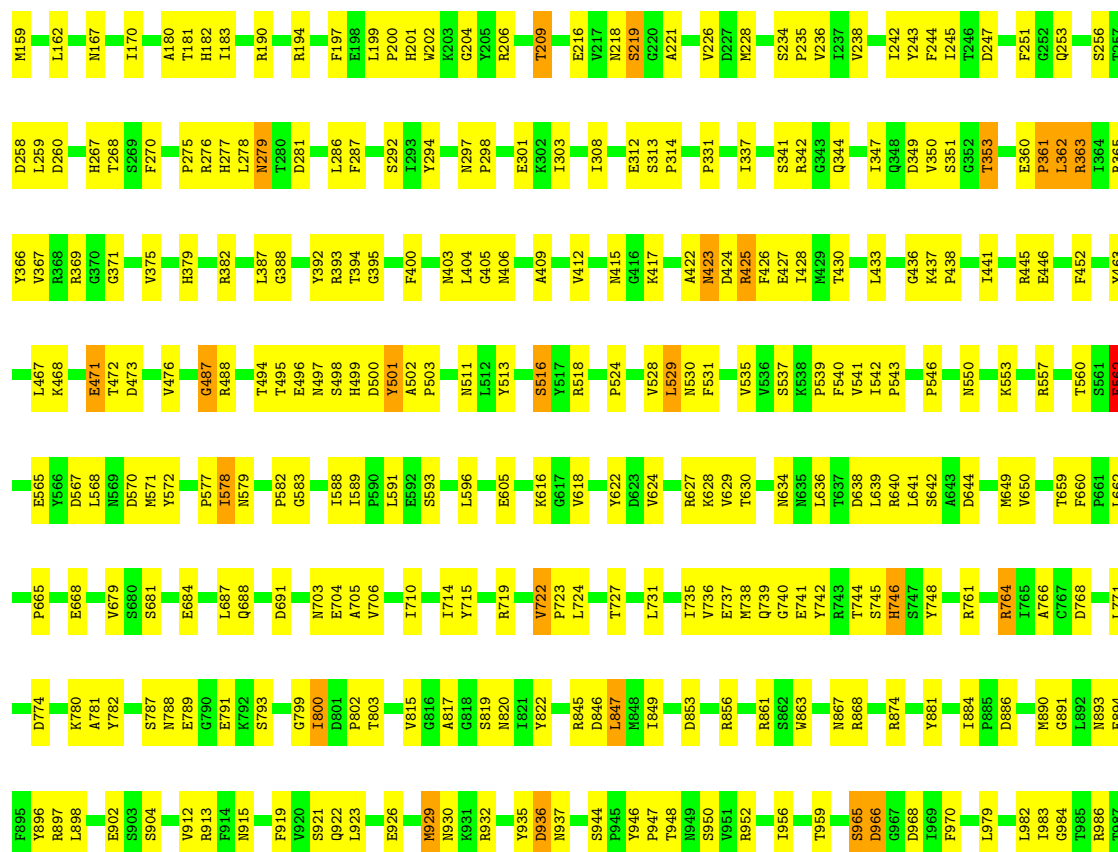
Chain B:  61% 32%



• Molecule 1: Tricorn protease

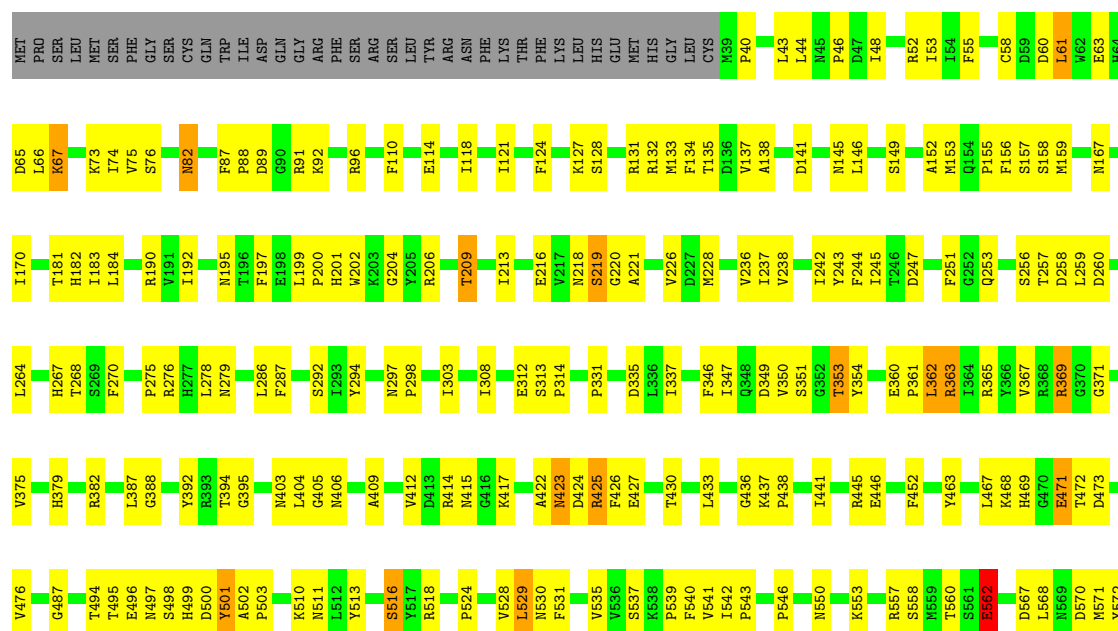
Chain C:  60% 33%

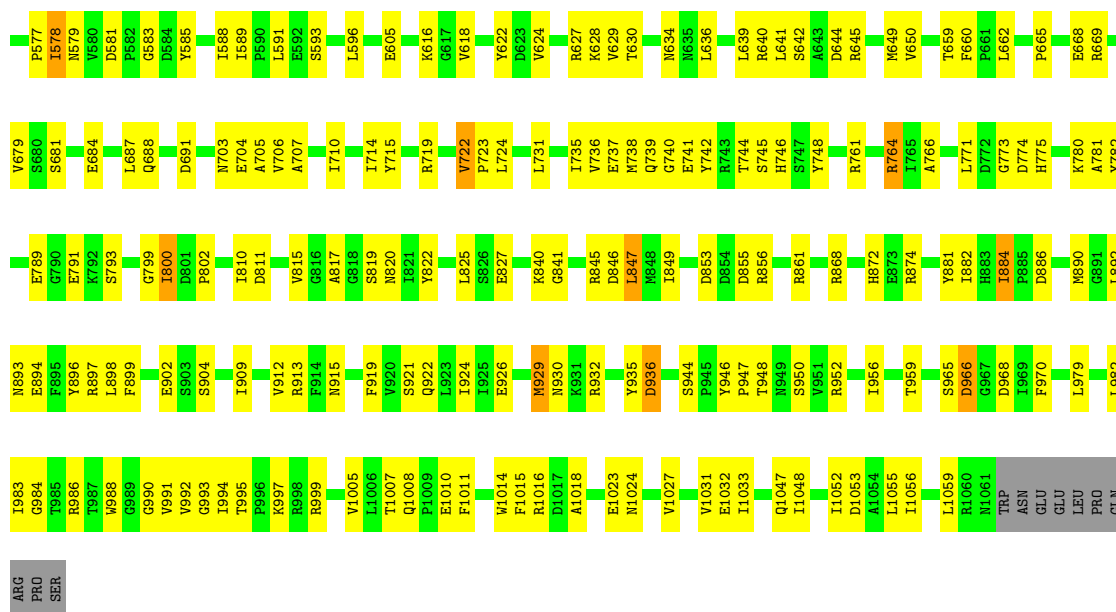




• Molecule 1: Tricorn protease

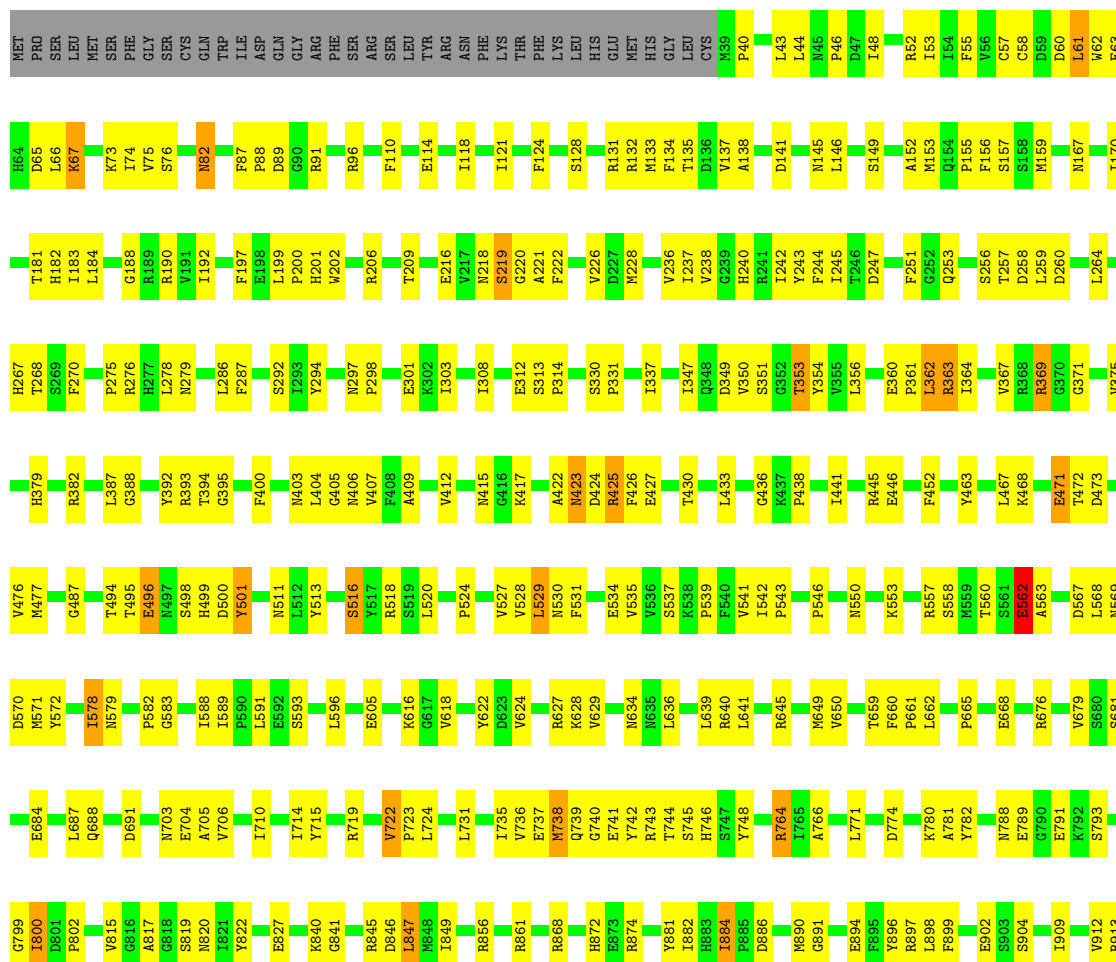
Chain D: 59% 34%





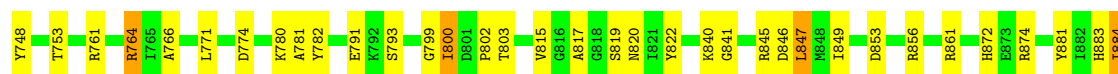
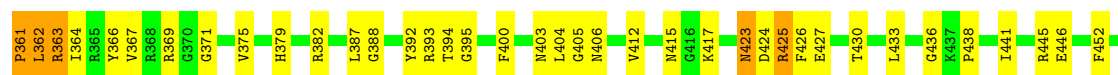
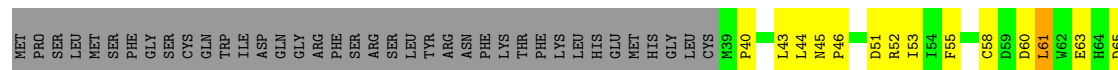
• Molecule 1: Tricorn protease

Chain E: 60% 33%





• Molecule 1: Tricorn protease



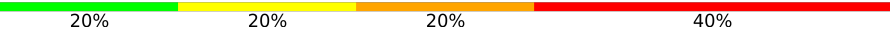
GLN
ARG
PRO
SER

• Molecule 2: RVRK

Chain G: 

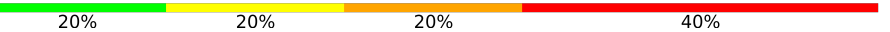


• Molecule 2: RVRK

Chain H: 

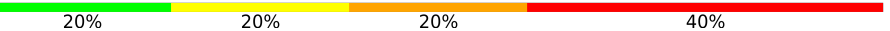


• Molecule 2: RVRK

Chain I: 



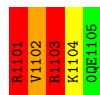
• Molecule 2: RVRK

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 6.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	88.7 (6.00-2.80) 75.4 (6.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.66 (at 2.71Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.285 , 0.315 0.273 , (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 , 12.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.079 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.61	1/8367 (0.0%)	0.92	12/11311 (0.1%)
1	B	0.61	1/8367 (0.0%)	0.93	18/11311 (0.2%)
1	C	0.58	1/8367 (0.0%)	0.92	14/11311 (0.1%)
1	D	0.60	1/8367 (0.0%)	0.92	12/11311 (0.1%)
1	E	0.59	1/8367 (0.0%)	0.92	11/11311 (0.1%)
1	F	0.59	1/8367 (0.0%)	0.91	14/11311 (0.1%)
2	G	2.76	2/37 (5.4%)	5.63	10/46 (21.7%)
2	H	2.76	2/37 (5.4%)	5.63	10/46 (21.7%)
2	I	2.77	2/37 (5.4%)	5.63	10/46 (21.7%)
2	J	2.76	2/37 (5.4%)	5.62	10/46 (21.7%)
2	K	2.76	2/37 (5.4%)	5.63	10/46 (21.7%)
2	L	2.77	2/37 (5.4%)	5.63	10/46 (21.7%)
All	All	0.62	18/50424 (0.0%)	0.99	141/68142 (0.2%)

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 (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	1103	ARG	N-CA	-12.40	1.30	1.45
2	L	1103	ARG	N-CA	-12.36	1.30	1.45
2	H	1103	ARG	N-CA	-12.33	1.30	1.45
2	J	1103	ARG	N-CA	-12.33	1.30	1.45
2	K	1103	ARG	N-CA	-12.33	1.30	1.45
2	G	1103	ARG	N-CA	-12.31	1.30	1.45
2	K	1103	ARG	CB-CG	8.30	1.77	1.52
2	H	1103	ARG	CB-CG	8.30	1.77	1.52
2	I	1103	ARG	CB-CG	8.29	1.77	1.52
2	L	1103	ARG	CB-CG	8.29	1.77	1.52
2	G	1103	ARG	CB-CG	8.28	1.77	1.52
2	J	1103	ARG	CB-CG	8.27	1.77	1.52
1	F	722	VAL	CA-CB	8.16	1.58	1.54
1	E	722	VAL	CA-CB	7.91	1.58	1.54
1	B	722	VAL	CA-CB	7.88	1.58	1.54
1	A	722	VAL	CA-CB	7.58	1.57	1.54
1	D	722	VAL	CA-CB	6.31	1.57	1.54
1	C	722	VAL	CA-CB	5.46	1.56	1.54

All (141) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1101	ARG	CA-C-N	18.84	139.36	121.65
2	G	1101	ARG	C-N-CA	18.84	139.36	121.65
2	H	1101	ARG	CA-C-N	18.83	139.35	121.65
2	H	1101	ARG	C-N-CA	18.83	139.35	121.65
2	I	1101	ARG	CA-C-N	18.81	139.34	121.65
2	I	1101	ARG	C-N-CA	18.81	139.34	121.65
2	K	1101	ARG	CA-C-N	18.80	139.32	121.65
2	K	1101	ARG	C-N-CA	18.80	139.32	121.65
2	L	1101	ARG	CA-C-N	18.79	139.31	121.65
2	L	1101	ARG	C-N-CA	18.79	139.31	121.65
2	J	1101	ARG	CA-C-N	18.76	139.28	121.65
2	J	1101	ARG	C-N-CA	18.76	139.28	121.65
2	G	1103	ARG	O-C-N	-12.73	107.83	122.86
2	L	1103	ARG	O-C-N	-12.69	107.89	122.86
2	K	1103	ARG	O-C-N	-12.68	107.90	122.86
2	H	1103	ARG	O-C-N	-12.66	107.92	122.86
2	I	1103	ARG	O-C-N	-12.66	107.92	122.86
2	J	1103	ARG	O-C-N	-12.65	107.93	122.86
2	G	1103	ARG	CA-C-N	12.21	143.67	121.70
2	G	1103	ARG	C-N-CA	12.21	143.67	121.70
2	I	1103	ARG	CA-C-N	12.19	143.65	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	1103	ARG	C-N-CA	12.19	143.65	121.70
2	L	1103	ARG	CA-C-N	12.19	143.64	121.70
2	L	1103	ARG	C-N-CA	12.19	143.64	121.70
2	H	1103	ARG	CA-C-N	12.18	143.63	121.70
2	H	1103	ARG	C-N-CA	12.18	143.63	121.70
2	K	1103	ARG	CA-C-N	12.18	143.62	121.70
2	K	1103	ARG	C-N-CA	12.18	143.62	121.70
2	J	1103	ARG	CA-C-N	12.16	143.59	121.70
2	J	1103	ARG	C-N-CA	12.16	143.59	121.70
2	J	1102	VAL	N-CA-C	8.12	114.90	106.21
2	G	1102	VAL	N-CA-C	8.10	114.87	106.21
2	K	1102	VAL	N-CA-C	8.08	114.85	106.21
2	I	1102	VAL	N-CA-C	8.05	114.83	106.21
2	L	1102	VAL	N-CA-C	8.05	114.83	106.21
2	H	1102	VAL	N-CA-C	8.05	114.82	106.21
1	B	884	ILE	CA-C-N	7.76	127.82	119.28
1	B	884	ILE	C-N-CA	7.76	127.82	119.28
1	A	884	ILE	CA-C-N	7.07	127.06	119.28
1	A	884	ILE	C-N-CA	7.07	127.06	119.28
1	E	425	ARG	N-CA-C	-7.04	104.30	113.17
1	D	425	ARG	N-CA-C	-6.99	104.36	113.17
1	C	487	GLY	N-CA-C	-6.95	106.81	115.08
1	B	501	TYR	N-CA-C	6.84	117.07	108.45
1	F	425	ARG	N-CA-C	-6.80	104.61	113.17
2	L	1102	VAL	CA-C-N	6.75	131.54	120.94
2	L	1102	VAL	C-N-CA	6.75	131.54	120.94
2	H	1102	VAL	CA-C-N	6.75	131.53	120.94
2	H	1102	VAL	C-N-CA	6.75	131.53	120.94
1	F	884	ILE	CA-C-N	6.75	126.70	119.28
1	F	884	ILE	C-N-CA	6.75	126.70	119.28
2	I	1102	VAL	CA-C-N	6.74	131.53	120.94
2	I	1102	VAL	C-N-CA	6.74	131.53	120.94
2	J	1102	VAL	CA-C-N	6.74	131.52	120.94
2	J	1102	VAL	C-N-CA	6.74	131.52	120.94
2	K	1102	VAL	CA-C-N	6.74	131.52	120.94
2	K	1102	VAL	C-N-CA	6.74	131.52	120.94
1	C	884	ILE	CA-C-N	6.72	126.52	119.05
1	C	884	ILE	C-N-CA	6.72	126.52	119.05
1	D	487	GLY	N-CA-C	-6.70	107.10	115.08
2	G	1102	VAL	CA-C-N	6.69	131.45	120.94
2	G	1102	VAL	C-N-CA	6.69	131.45	120.94
1	F	487	GLY	N-CA-C	-6.64	107.17	115.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	501	TYR	N-CA-C	6.59	116.76	108.45
1	A	425	ARG	N-CA-C	-6.57	105.02	113.16
1	A	501	TYR	N-CA-C	6.56	116.72	108.45
1	C	425	ARG	N-CA-C	-6.55	104.92	113.17
1	B	425	ARG	N-CA-C	-6.49	105.00	113.17
1	F	501	TYR	N-CA-C	6.36	116.46	108.45
1	C	965	SER	CB-CA-C	-6.30	109.29	116.54
1	B	965	SER	CB-CA-C	-6.28	109.32	116.54
1	B	487	GLY	N-CA-C	-6.28	107.61	115.08
1	E	884	ILE	CA-C-N	6.26	126.17	119.28
1	E	884	ILE	C-N-CA	6.26	126.17	119.28
1	A	487	GLY	N-CA-C	-6.22	107.68	115.08
1	E	487	GLY	N-CA-C	-6.19	107.72	115.08
1	C	501	TYR	N-CA-C	6.03	116.05	108.45
1	F	993	GLY	N-CA-C	5.93	118.85	112.33
1	F	965	SER	CB-CA-C	-5.89	109.76	116.54
1	D	362	LEU	N-CA-C	5.89	117.89	110.24
1	B	121	ILE	N-CA-C	5.85	116.84	111.81
1	D	884	ILE	CA-C-N	5.80	125.66	119.28
1	D	884	ILE	C-N-CA	5.80	125.66	119.28
1	C	679	VAL	N-CA-C	5.76	116.23	108.17
1	E	501	TYR	N-CA-C	5.75	115.69	108.45
1	D	952	ARG	N-CA-C	5.66	117.12	111.07
2	H	1103	ARG	N-CA-CB	5.63	118.28	110.17
1	D	679	VAL	N-CA-C	5.63	116.69	108.53
2	L	1103	ARG	N-CA-CB	5.62	118.26	110.17
1	A	952	ARG	N-CA-C	5.61	117.08	111.07
2	I	1103	ARG	N-CA-CB	5.61	118.25	110.17
2	K	1103	ARG	N-CA-CB	5.61	118.25	110.17
1	B	362	LEU	N-CA-C	5.61	117.98	110.35
2	J	1103	ARG	N-CA-CB	5.60	118.24	110.17
1	B	428	ILE	N-CA-C	-5.58	100.45	108.48
1	B	600	VAL	CB-CA-C	-5.58	105.78	111.08
1	B	192	ILE	N-CA-C	5.57	115.97	108.17
2	G	1103	ARG	N-CA-CB	5.57	118.19	110.17
1	A	192	ILE	N-CA-C	5.52	115.89	108.17
1	A	121	ILE	N-CA-C	5.51	116.55	111.81
1	B	993	GLY	N-CA-C	5.47	119.58	112.25
1	A	362	LEU	N-CA-C	5.47	117.79	110.35
1	F	966	ASP	N-CA-C	-5.45	104.77	111.75
1	F	679	VAL	N-CA-C	5.45	115.80	108.17
1	C	966	ASP	N-CA-C	-5.45	105.45	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	966	ASP	N-CA-C	-5.45	105.45	111.71
1	F	952	ARG	N-CA-C	5.45	117.22	111.28
1	D	346	PHE	N-CA-C	5.41	117.62	109.23
1	E	362	LEU	N-CA-C	5.41	117.70	110.35
1	D	993	GLY	N-CA-C	5.38	119.45	112.25
1	B	952	ARG	N-CA-C	5.33	116.78	111.07
1	E	679	VAL	N-CA-C	5.32	116.24	108.53
1	E	993	GLY	N-CA-C	5.32	119.38	112.25
1	A	679	VAL	N-CA-C	5.26	115.53	108.17
1	A	746	HIS	N-CA-C	5.21	119.58	113.23
1	F	362	LEU	N-CA-C	5.20	117.42	110.35
1	F	364	ILE	N-CA-C	-5.19	99.77	107.51
1	B	321	ILE	N-CA-C	5.18	112.27	107.56
1	C	121	ILE	N-CA-C	5.18	116.26	111.81
1	E	364	ILE	N-CA-C	-5.16	100.46	107.99
1	C	362	LEU	N-CA-C	5.13	117.32	110.35
1	B	801	ASP	CA-C-N	5.11	124.77	119.56
1	B	801	ASP	C-N-CA	5.11	124.77	119.56
1	E	192	ILE	N-CA-C	5.11	115.32	108.17
2	K	1103	ARG	CA-CB-CG	-5.09	103.92	114.10
1	C	952	ARG	N-CA-C	5.09	116.83	111.28
2	I	1103	ARG	CA-CB-CG	-5.09	103.92	114.10
2	J	1103	ARG	CA-CB-CG	-5.09	103.92	114.10
2	G	1103	ARG	CA-CB-CG	-5.09	103.92	114.10
2	H	1103	ARG	CA-CB-CG	-5.09	103.93	114.10
1	B	746	HIS	N-CA-C	5.08	119.43	113.23
2	L	1103	ARG	CA-CB-CG	-5.08	103.94	114.10
1	C	428	ILE	N-CA-C	-5.07	101.01	108.11
1	E	966	ASP	N-CA-C	-5.06	105.89	111.71
1	B	366	TYR	N-CA-C	5.06	117.07	109.23
1	F	545	ILE	CB-CA-C	-5.05	106.28	111.08
1	C	746	HIS	N-CA-C	5.05	119.39	113.23
1	D	192	ILE	N-CA-C	5.04	115.23	108.17
1	F	366	TYR	N-CA-C	5.03	117.02	109.23
1	A	993	GLY	N-CA-C	5.01	118.96	112.25
1	C	366	TYR	N-CA-C	5.01	116.99	109.23

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	G	1101	ARG	Sidechain

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Mol	Chain	Res	Type	Group
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

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	311	0
1	B	8177	0	8002	315	0
1	C	8177	0	8002	345	0
1	D	8177	0	8002	345	0
1	E	8177	0	8002	334	0
1	F	8177	0	8002	347	0
2	G	39	0	47	8	0
2	H	39	0	47	5	0
2	I	39	0	47	7	0
2	J	39	0	47	7	0
2	K	39	0	47	5	0
2	L	39	0	47	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	16	0
4	B	88	0	0	23	0
4	C	88	0	0	40	0
4	D	79	0	0	32	0
4	E	89	0	0	26	0
4	F	74	0	0	40	0
4	G	4	0	0	3	0
4	I	2	0	0	2	0
4	J	2	0	0	3	0
4	L	2	0	0	3	0
All	All	49890	0	48414	1929	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 20.

All (1929) 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: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:F:173:VAL:HB	4:F:1076:HOH:O	1.72	0.89
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:965:SER:CB	2:I:1104:LYS:O	2.09	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:965:SER:CB	2:L:1104:LYS:O	2.09	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: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:E:568:LEU:HB3	1:E:571:MET:HE2	1.68	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:A:568:LEU:HB3	1:A:571:MET:HE2	1.68	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:D:568:LEU:HB3	1:D:571:MET:HE2	1.69	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:E:965:SER:CB	2:K:1104:LYS:O	2.09	0.73
1:B:568:LEU:HB3	1:B:571:MET:HE2	1.69	0.72
1:B:557:ARG:HH22	1:B:562:GLU:N	1.88	0.72
1:D:494:THR:HG21	1:D:500:ASP:CG	2.14	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: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
1:C:568:LEU:HB3	1:C:571:MET:HE2	1.70	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:494:THR:HG21	1:A:500:ASP:CG	2.15	0.71
1:B:965:SER:HB3	2:H:1104:LYS:O	1.37	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:180:ALA:C	4:C:1080:HOH:O	2.34	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: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:E:494:THR:HG21	1:E:500:ASP:CG	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:494:THR:HG21	1:B:500:ASP:CG	2.17	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:F:494:THR:HG21	1:F:500:ASP:CG	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:660:PHE:HB3	1:B:668:GLU:HB3	1.76	0.68
1:F:568:LEU:HB3	1:F:571:MET:HE2	1.74	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
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:F:982:LEU:C	1:F:983:ILE:HD12	2.20	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:494:THR:HG21	1:C:500:ASP:CG	2.19	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:F:965:SER:HB3	2:L:1104:LYS:O	1.39	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:982:LEU:C	1:C:983:ILE:HD12	2.21	0.65
1:D:415:ASN:HB3	1:D:417:LYS:HD3	1.77	0.65
1:F:349:ASP:OD2	1:F:351:SER:HB3	1.95	0.65
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:B:982:LEU:C	1:B:983:ILE:HD12	2.22	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: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:228:MET:HE1	1:F:244:PHE:CE1	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:703:ASN:C	1:F:703:ASN:HD22	2.03	0.63
1:A:913:ARG:HH21	1:A:1047:GLN:NE2	1.96	0.63
1:D:982:LEU:C	1:D:983:ILE:HD12	2.23	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:D:228:MET:HE1	1:D:244:PHE:CE1	2.33	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
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:E:982:LEU:C	1:E:983:ILE:HD12	2.23	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:703:ASN:C	1:D:703:ASN:HD22	2.06	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:C:703:ASN:HD22	1:C:703:ASN:C	2.06	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:B:46:PRO:HB2	1:B:286:LEU:CD2	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1055:LEU:O	1:B:1059:LEU:HD13	1.99	0.62
1:A:228:MET:HE1	1:A:244:PHE:CE1	2.35	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:E:703:ASN:HD22	1:E:703:ASN:C	2.08	0.62
1:F:268:THR:HG22	1:F:303:ILE:HD11	1.81	0.62
1:A:982:LEU:C	1:A:983:ILE:HD12	2.25	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
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:E:228:MET:HE1	1:E:244:PHE:CE1	2.36	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:F:242:ILE:O	1:F:256:SER:HA	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:228:MET:HE1	1:C:244:PHE:CE1	2.37	0.60
1:D:331:PRO:HB3	1:D:649:MET:HE3	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:331:PRO:HB3	1:E:649:MET:HE3	1.84	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:A:703:ASN:C	1:A:703:ASN:HD22	2.09	0.59
1:B:228:MET:HE1	1:B:244:PHE:CE1	2.37	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:403:ASN:HD22	1:E:403:ASN:C	2.10	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
1:B:242:ILE:O	1:B:256:SER:HA	2.02	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:C:965:SER:HB3	2:I:1104:LYS:O	1.39	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:A:791:GLU:CD	1:A:861:ARG:HE	2.10	0.59
1:B:43:LEU:HD22	1:B:55:PHE:CE1	2.38	0.59
1:B:703:ASN:C	1:B:703:ASN:HD22	2.10	0.59
1:D:959:THR:O	1:D:984:GLY:HA3	2.03	0.59
1:F:124:PHE:CE2	1:F:153:MET:HE1	2.37	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:D:965:SER:O	1:D:968:ASP:HB2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:939:ARG:HH11	1:B:704:GLU:HG3	1.68	0.59
1:A:965:SER:HB3	2:G:1104:LYS:O	1.41	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:A:124:PHE:CE2	1:A:153:MET:HE1	2.39	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:B:124:PHE:CE2	1:B:153:MET:HE1	2.38	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
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: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:C:403:ASN:HD22	1:C:403:ASN:C	2.11	0.58
1:D:82:ASN:HD21	1:D:96:ARG:HH21	1.52	0.58
1:D:992:VAL:N	4:D:1088:HOH:O	2.36	0.58
1:F:791:GLU:CD	1:F:861:ARG:HE	2.11	0.58
1:B:423:ASN:ND2	1:B:427:GLU:H	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:791:GLU:CD	1:B:861:ARG:HE	2.11	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
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:948:THR:H	1:F:922:GLN:NE2	2.02	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:124:PHE:CE2	1:E:153:MET:HE1	2.39	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:403:ASN:HD22	1:D:403:ASN:C	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:415:ASN:HD22	1:D:417:LYS:HD2	1.70	0.57
1:D:965:SER:HB3	2:J:1104:LYS:O	1.41	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:331:PRO:HB3	1:C:649:MET:HE3	1.87	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:F:703:ASN:C	1:F:703:ASN:ND2	2.62	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:F:403:ASN:HD22	1:F:403:ASN:C	2.13	0.56
1:C:703:ASN:C	1:C:703:ASN:ND2	2.63	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
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:791:GLU:CD	1:E:861:ARG:HE	2.14	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:B:830:GLY:C	4:B:1081:HOH:O	2.48	0.56
1:C:639:LEU:HG	1:C:650:VAL:HG12	1.87	0.56
1:F:337:ILE:HG12	1:F:649:MET:HE1	1.88	0.56
1:A:258:ASP:C	1:A:260:ASP:H	2.13	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:124:PHE:CE2	1:D:153:MET:HE1	2.41	0.56
1:F:331:PRO:HB3	1:F:649:MET:HE3	1.88	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:B:258:ASP:C	1:B:260:ASP:H	2.14	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:C:791:GLU:CD	1:C:861:ARG:HE	2.15	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:E:965:SER:HB3	2:K:1104:LYS:O	1.41	0.55
1:A:331:PRO:HB3	1:A:649:MET:HE3	1.87	0.55
1:D:242:ILE:O	1:D:256:SER:HA	2.05	0.55
1:D:258:ASP:C	1:D:260:ASP:H	2.14	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:B:331:PRO:HB3	1:B:649:MET:HE3	1.88	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:337:ILE:HG12	1:C:649:MET:HE1	1.88	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:F:258:ASP:C	1:F:260:ASP:H	2.15	0.55
1:A:347:ILE:HG12	1:A:392:TYR:CD2	2.42	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: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:403:ASN:HD22	1:B:403:ASN:C	2.13	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:F:445:ARG:HH12	1:F:471:GLU:CD	2.16	0.54
1:A:200:PRO:O	1:A:740:GLY:HA3	2.08	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:D:703:ASN:C	1:D:703:ASN:ND2	2.63	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:A:106:ALA:HB3	4:A:1170:HOH:O	2.07	0.53
1:A:703:ASN:C	1:A:703:ASN:ND2	2.66	0.53
1:B:714:ILE:HG21	1:B:741:GLU:HB3	1.89	0.53
1:C:258:ASP:C	1:C:260:ASP:H	2.16	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: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:E:703:ASN:C	1:E:703:ASN:ND2	2.64	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:425:ARG:O	1:F:426:PHE:HB2	2.08	0.53
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:D:425:ARG:O	1:D:426:PHE:HB2	2.07	0.53
1:F:780:LYS:HD3	1:F:782:TYR:CZ	2.42	0.53
1:A:228:MET:HE1	1:A:244:PHE:CZ	2.44	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: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:E:228:MET:HE1	1:E:244:PHE:CZ	2.44	0.53
1:E:337:ILE:HG12	1:E:649:MET:HE1	1.89	0.53
1:F:173:VAL:CB	4:F:1076:HOH:O	2.41	0.53
1:A:445:ARG:HH12	1:A:471:GLU:CD	2.17	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: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:A:703:ASN:HD22	1:A:704:GLU:N	2.06	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:E:258:ASP:C	1:E:260:ASP:H	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:425:ARG:O	1:B:426:PHE:HB2	2.09	0.52
1:B:997:LYS:HB3	3:H:2101:D10:H71	1.91	0.52
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:F:289:LYS:NZ	4:F:1130:HOH:O	2.42	0.52
1:C:124:PHE:CE2	1:C:153:MET:HE1	2.44	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:445:ARG:HH12	1:D:471:GLU:CD	2.18	0.52
1:D:557:ARG:NH2	4:D:1148:HOH:O	2.43	0.52
1:F:530:ASN:CG	4:F:1112:HOH:O	2.52	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:C:228:MET:HE1	1:C:244:PHE:CZ	2.45	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:F:228:MET:HE1	1:F:244:PHE:CZ	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:362:LEU:CD2	1:A:363:ARG:H	2.23	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:F:234:SER:C	4:F:1074:HOH:O	2.52	0.51
1:E:557:ARG:HH22	1:E:562:GLU:HB2	1.75	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: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:781:ALA:HB2	1:E:802:PRO:HG2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:406:ASN:HB2	1:D:424:ASP:CG	2.36	0.51
1:E:88:PRO:HG2	1:E:89:ASP:H	1.76	0.51
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: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:F:406:ASN:HB2	1:F:424:ASP:CG	2.36	0.51
1:B:228:MET:HE1	1:B:244:PHE:CZ	2.46	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:445:ARG:HH12	1:B:471:GLU:CD	2.18	0.50
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:D:228:MET:HE1	1:D:244:PHE:CZ	2.45	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:445:ARG:HH12	1:C:471:GLU:CD	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:65:ASP:OD2	1:B:67:LYS:HB3	2.12	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: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: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:D:791:GLU:CD	1:D:861:ARG:HE	2.20	0.50
1:F:403:ASN:HD22	1:F:405:GLY:H	1.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:58:CYS:C	1:C:60:ASP:H	2.20	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
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: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:337:ILE:HG12	1:B:649:MET:HE1	1.94	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:628:LYS:HE2	4:B:1156:HOH:O	2.11	0.49
1:C:234:SER:C	4:C:1129:HOH:O	2.55	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:B:703:ASN:C	1:B:703:ASN:ND2	2.67	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: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: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:C:406:ASN:HB2	1:C:424:ASP:CG	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:218:ASN:O	1:B:219:SER:C	2.56	0.48
1:B:247:ASP:HA	1:B:251:PHE:O	2.13	0.48
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:58:CYS:C	1:D:60:ASP:H	2.20	0.48
1:D:846:ASP:C	1:D:846:ASP:OD2	2.56	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: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:A:337:ILE:HG12	1:A:649:MET:HE1	1.94	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:E:423:ASN:HD22	1:E:423:ASN:C	2.22	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:A:1032:GLU:C	1:A:1033:ILE:HD12	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:846:ASP:C	1:B:847:LEU:HD23	2.39	0.48
1:C:127:LYS:HD2	4:C:1118:HOH:O	2.13	0.48
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: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:A:218:ASN:O	1:A:219:SER:C	2.56	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: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:D:337:ILE:HG12	1:D:649:MET:HE1	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:A:423:ASN:C	1:A:423:ASN:HD22	2.22	0.47
1:B:570:ASP:HA	1:B:572:TYR:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1032:GLU:C	1:B:1033:ILE:HD12	2.39	0.47
1:C:61:LEU:HB3	1:C:75:VAL:HG12	1.96	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
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:C:423:ASN:C	1:C:423:ASN:HD22	2.22	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
1:E:58:CYS:C	1:E:60:ASP:H	2.21	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:A:406:ASN:HB2	1:A:424:ASP:CG	2.39	0.47
1:C:181:THR:N	4:C:1080:HOH:O	2.45	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:E:846:ASP:OD2	1:E:846:ASP:C	2.57	0.47
1:F:256:SER:OG	1:F:267:HIS:HE1	1.97	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: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:F:886:ASP:OD2	1:F:886:ASP:C	2.57	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:382:ARG:HD2	1:A:691:ASP:CG	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:445:ARG:HH12	1:E:471:GLU:CD	2.22	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:846:ASP:C	1:E:847:LEU:HD23	2.40	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
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:F:738:MET:SD	1:F:738:MET:C	2.98	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: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:A:846:ASP:C	1:A:847:LEU:HD23	2.40	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:58:CYS:C	1:F:60:ASP:H	2.22	0.47
1:F:197:PHE:CE1	1:F:199:LEU:HD21	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:568:LEU:HB3	1:E:571:MET:CE	2.40	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:403:ASN:HD22	1:A:403:ASN:C	2.13	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:C:863:TRP:CD1	4:C:1097:HOH:O	2.68	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
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:D:846:ASP:C	1:D:847:LEU:HD23	2.40	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:423:ASN:HD22	1:B:423:ASN:C	2.21	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:C:568:LEU:HB3	1:C:571:MET:CE	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:1032:GLU:C	1:C:1033:ILE:HD12	2.40	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: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:E:639:LEU:HD23	1:E:639:LEU:C	2.41	0.46
1:F:337:ILE:HD12	1:F:350:VAL:HA	1.98	0.46
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:58:CYS:C	1:B:60:ASP:H	2.24	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:406:ASN:HB2	1:B:424:ASP:CG	2.40	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:C:226:VAL:HG13	1:C:228:MET:HE2	1.98	0.46
1:A:468:LYS:HE3	1:A:476:VAL:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:681:SER:HB3	1:B:684:GLU:CD	2.41	0.46
1:C:201:HIS:O	1:C:740:GLY:HA2	2.16	0.46
1:C:382:ARG:HD2	1:C:691:ASP:CG	2.41	0.46
1:C:642:SER:HG	1:C:644:ASP:CG	2.22	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:B:846:ASP:C	1:B:846:ASP:OD2	2.59	0.45
1:C:591:LEU:HD11	1:C:662:LEU:HD21	1.96	0.45
1:C:681:SER:HB3	1:C:684:GLU:CD	2.40	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
1:D:423:ASN:C	1:D:423:ASN:HD22	2.23	0.45
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:226:VAL:HG13	1:B:228:MET:HE2	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:406:ASN:HB2	1:E:424:ASP:CG	2.41	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:B:568:LEU:HB3	1:B:571:MET:CE	2.42	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:C:639:LEU:HD23	1:C:639:LEU:C	2.42	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:E:382:ARG:HD2	1:E:691:ASP:CG	2.40	0.45
1:F:181:THR:N	4:F:1094:HOH:O	2.50	0.45
1:F:382:ARG:HD2	1:F:691:ASP:CG	2.41	0.45
1:F:846:ASP:C	1:F:847:LEU:HD23	2.42	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:F:1032:GLU:C	1:F:1033:ILE:HD12	2.41	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:681:SER:HB3	1:F:684:GLU:CD	2.42	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: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:847:LEU:HD23	1:B:847:LEU:N	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:C:802:PRO:O	1:C:803:THR:C	2.58	0.45
1:C:886:ASP:C	1:C:886:ASP:OD2	2.60	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:141:ASP:C	1:C:141:ASP:OD2	2.60	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:C:846:ASP:C	1:C:847:LEU:HD23	2.41	0.45
1:D:847:LEU:HD23	1:D:847:LEU:N	2.32	0.45
1:D:1032:GLU:C	1:D:1033:ILE:HD12	2.42	0.45
1:E:268:THR:HG22	1:E:303:ILE:CD1	2.44	0.45
1:E:886:ASP:C	1:E:886:ASP:OD2	2.60	0.45
1:F:501:TYR:CD2	1:F:501:TYR:N	2.84	0.45
1:A:676:ARG:NH2	1:D:811:ASP:OD1	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:639:LEU:HD23	1:B:639:LEU:C	2.42	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:D:382:ARG:HD2	1:D:691:ASP:CG	2.41	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:226:VAL:HG13	1:A:228:MET:HE2	2.00	0.44
1:A:275:PRO:C	1:A:276:ARG:HG2	2.42	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:226:VAL:HG13	1:E:228:MET:HE2	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:A:190:ARG:NH2	1:A:216:GLU:CD	2.74	0.44
1:A:846:ASP:C	1:A:846:ASP:OD2	2.59	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:C:846:ASP:C	1:C:846:ASP:OD2	2.59	0.44
1:E:91:ARG:CZ	4:E:1147:HOH:O	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:382:ARG:HD2	1:B:691:ASP:CG	2.42	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
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:349:ASP:O	1:D:350:VAL:C	2.61	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:F:423:ASN:C	1:F:423:ASN:HD22	2.26	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:218:ASN:O	1:C:219:SER:C	2.61	0.44
1:C:530:ASN:CG	4:C:1092:HOH:O	2.61	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:181:THR:HG22	1:F:182:HIS:CE1	2.53	0.44
1:F:275:PRO:C	1:F:276:ARG:HG2	2.43	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
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: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:226:VAL:HG13	1:D:228:MET:HE2	1.99	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:58:CYS:C	1:A:60:ASP:H	2.26	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:639:LEU:HD23	1:D:639:LEU:C	2.42	0.43
1:D:932:ARG:HD3	1:D:935:TYR:OH	2.18	0.43
1:E:847:LEU:HD23	1:E:847:LEU:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:F:341:SER:O	1:F:342:ARG:C	2.61	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
1:B:436:GLY:O	1:B:438:PRO:HD3	2.18	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: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: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: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:A:639:LEU:HD23	1:A:639:LEU:C	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:605:GLU:CD	4:J:103:HOH:O	2.62	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:E:1032:GLU:C	1:E:1033:ILE:HD12	2.44	0.43
1:F:846:ASP:C	1:F:846:ASP:OD2	2.61	0.43
1:A:87:PHE:CD1	1:A:92:LYS:HB2	2.54	0.43
1:A:629:VAL:HG12	1:A:630:THR:N	2.32	0.43
1:B:452:PHE:HB3	1:B:463:TYR:HB3	1.99	0.43
1:C:341:SER:O	1:C:342:ARG:C	2.62	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:349:ASP:O	1:F:350:VAL:C	2.62	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:681:SER:HB3	1:E:684:GLU:CD	2.44	0.42
1:E:703:ASN:ND2	1:E:705:ALA:H	2.17	0.42
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:190:ARG:NH2	1:D:216:GLU:CD	2.77	0.42
1:D:568:LEU:HB3	1:D:571:MET:CE	2.43	0.42
1:D:886:ASP:OD2	1:D:886:ASP:C	2.62	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:F:529:LEU:O	1:F:529:LEU:HG	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:D:681:SER:HB3	1:D:684:GLU:CD	2.44	0.42
1:E:190:ARG:NH2	1:E:216:GLU:CD	2.77	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:218:ASN:O	1:F:219:SER:C	2.61	0.42
1:F:467:LEU:HD11	1:F:496:GLU:HB2	2.00	0.42
1:F:639:LEU:HD23	1:F:639:LEU:C	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:349:ASP:O	1:C:350:VAL:C	2.59	0.42
1:C:912:VAL:HG11	1:C:970:PHE:CE2	2.55	0.42
1:D:275:PRO:C	1:D:276:ARG:HG2	2.45	0.42
1:D:912:VAL:HG11	1:D:970:PHE:CE2	2.55	0.42
1:E:840:LYS:HD2	1:E:841:GLY:N	2.35	0.42
1:E:847:LEU:HD12	1:E:849:ILE:HD11	2.01	0.42
1:F:182:HIS:ND1	1:F:196:THR:OG1	2.52	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: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
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:141:ASP:C	1:F:141:ASP:OD2	2.62	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:681:SER:HB3	1:A:684:GLU:CD	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:45:ASN:HB3	1:A:277:HIS:CE1	2.55	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:218:ASN:O	1:E:219:SER:C	2.62	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
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:275:PRO:C	1:E:276:ARG:HG2	2.43	0.42
1:E:286:LEU:HD12	1:E:286:LEU:HA	1.89	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:687:LEU:HD23	1:A:687:LEU:HA	1.89	0.42
1:B:190:ARG:NH2	1:B:216:GLU:CD	2.77	0.42
1:B:476:VAL:C	1:B:477:MET:HE2	2.45	0.42
1:B:535:VAL:HB	1:B:583:GLY:HA2	2.02	0.42
1:B:886:ASP:C	1:B:886:ASP:OD2	2.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:802:PRO:O	1:F:803:THR:C	2.61	0.42
1:F:1010:GLU:HB3	1:F:1011:PHE:CE1	2.55	0.42
1:A:568:LEU:HB3	1:A:571:MET:CE	2.43	0.41
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:890:MET:HA	1:C:893:ASN:HD22	1.84	0.41
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:642:SER:HG	1:D:644:ASP:CG	2.27	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:476:VAL:C	1:E:477:MET:HE2	2.45	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: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:A:863:TRP:CD1	4:A:1105:HOH:O	2.72	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:349:ASP:O	1:E:350:VAL:C	2.63	0.41
1:E:406:ASN:HD22	1:E:424:ASP:CG	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:847:LEU:HD23	1:F:847:LEU:N	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:275:PRO:C	1:B:276:ARG:HG2	2.45	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: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:476:VAL:C	1:F:477:MET:HE2	2.45	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:541:VAL:HG22	1:B:542:ILE:N	2.34	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
1:D:209:THR:OG1	1:D:988:TRP:HD1	2.03	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: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: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:F:568:LEU:HB3	1:F:571:MET:CE	2.46	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:HD23	1:C:847:LEU:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:341:SER:O	1:B:342:ARG:C	2.63	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:534:GLU:CD	1:B:534:GLU:HG3	2.46	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:886:ASP:OD2	1:A:886:ASP:C	2.64	0.41
1:B:141:ASP:C	1:B:141:ASP:OD2	2.64	0.41
1:B:744:THR:HG22	1:B:745:SER:H	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:275:PRO:C	1:C:276:ARG:HG2	2.46	0.41
1:C:874:ARG:HH21	1:C:874:ARG:HG3	1.86	0.41
1:C:929:MET:HE2	1:C:929:MET:HA	2.02	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:929:MET:HA	1:E:929:MET:HE2	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:ASN:HB3	1:C:115:ASN:OD1	2.20	0.40
1:C:190:ARG:NH2	1:C:216:GLU:CD	2.79	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:D:218:ASN:O	1:D:219:SER:C	2.64	0.40
1:D:258:ASP:C	1:D:260:ASP:N	2.79	0.40
1:D:351:SER:HB3	1:D:353:THR:HG22	2.03	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:883:HIS:HA	1:F:911:ASP:O	2.21	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
1:D:437:LYS:HE2	1:D:437:LYS:HB3	1.85	0.40
1:D:929:MET:HE2	1:D:929:MET:HA	2.02	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: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:258:ASP:C	1:B:260:ASP:N	2.79	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:D:581:ASP:O	1:D:585:TYR:OH	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:487:GLY:O	1:C:488:ARG:C	2.65	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:A:642:SER:HG	1:A:644:ASP:CG	2.28	0.40
1:B:89:ASP:OD1	1:B:91:ARG:HB2	2.22	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
1:E:738:MET:C	1:E:738:MET:SD	3.04	0.40
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:874:ARG:HG3	1:F:874:ARG:HH21	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1021/1071 (95%)	934 (92%)	78 (8%)	9 (1%)	14	41
1	B	1021/1071 (95%)	934 (92%)	78 (8%)	9 (1%)	14	41
1	C	1021/1071 (95%)	930 (91%)	80 (8%)	11 (1%)	11	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	1021/1071 (95%)	934 (92%)	78 (8%)	9 (1%)	14	41
1	E	1021/1071 (95%)	934 (92%)	78 (8%)	9 (1%)	14	41
1	F	1021/1071 (95%)	930 (91%)	81 (8%)	10 (1%)	12	38
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%)	14	41

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

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Mol	Chain	Res	Type
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
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%)	855 (97%)	28 (3%)	34	70
1	B	883/928 (95%)	856 (97%)	27 (3%)	35	70
1	C	883/928 (95%)	857 (97%)	26 (3%)	37	73
1	D	883/928 (95%)	855 (97%)	28 (3%)	34	70
1	E	883/928 (95%)	854 (97%)	29 (3%)	33	69
1	F	883/928 (95%)	856 (97%)	27 (3%)	35	70
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%)	5151 (97%)	171 (3%)	34	70

All (171) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LEU
1	A	61	LEU
1	A	82	ASN
1	A	157	SER
1	A	209	THR
1	A	279	ASN
1	A	313	SER
1	A	353	THR
1	A	363	ARG
1	A	423	ASN
1	A	471	GLU
1	A	472	THR
1	A	516	SER
1	A	560	THR
1	A	562	GLU
1	A	578	ILE
1	A	599	SER
1	A	731	LEU
1	A	738	MET
1	A	764	ARG
1	A	771	LEU
1	A	800	ILE

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Mol	Chain	Res	Type
1	A	847	LEU
1	A	929	MET
1	A	936	ASP
1	A	979	LEU
1	A	1008	GLN
1	A	1015	PHE
2	G	1101	ARG
1	B	44	LEU
1	B	61	LEU
1	B	82	ASN
1	B	157	SER
1	B	209	THR
1	B	279	ASN
1	B	313	SER
1	B	353	THR
1	B	363	ARG
1	B	423	ASN
1	B	471	GLU
1	B	472	THR
1	B	516	SER
1	B	560	THR
1	B	562	GLU
1	B	578	ILE
1	B	731	LEU
1	B	738	MET
1	B	764	ARG
1	B	771	LEU
1	B	800	ILE
1	B	847	LEU
1	B	929	MET
1	B	936	ASP
1	B	979	LEU
1	B	1008	GLN
1	B	1015	PHE
2	H	1101	ARG
1	C	44	LEU
1	C	61	LEU
1	C	82	ASN
1	C	157	SER
1	C	209	THR
1	C	279	ASN
1	C	313	SER

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Mol	Chain	Res	Type
1	C	353	THR
1	C	363	ARG
1	C	423	ASN
1	C	471	GLU
1	C	472	THR
1	C	516	SER
1	C	560	THR
1	C	562	GLU
1	C	578	ILE
1	C	731	LEU
1	C	738	MET
1	C	764	ARG
1	C	771	LEU
1	C	800	ILE
1	C	847	LEU
1	C	929	MET
1	C	936	ASP
1	C	979	LEU
1	C	1008	GLN
2	I	1101	ARG
1	D	44	LEU
1	D	61	LEU
1	D	82	ASN
1	D	157	SER
1	D	209	THR
1	D	279	ASN
1	D	313	SER
1	D	353	THR
1	D	363	ARG
1	D	369	ARG
1	D	423	ASN
1	D	471	GLU
1	D	472	THR
1	D	516	SER
1	D	560	THR
1	D	562	GLU
1	D	578	ILE
1	D	731	LEU
1	D	738	MET
1	D	764	ARG
1	D	771	LEU
1	D	800	ILE

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Mol	Chain	Res	Type
1	D	847	LEU
1	D	929	MET
1	D	936	ASP
1	D	979	LEU
1	D	1008	GLN
1	D	1015	PHE
2	J	1101	ARG
1	E	44	LEU
1	E	61	LEU
1	E	82	ASN
1	E	157	SER
1	E	209	THR
1	E	279	ASN
1	E	313	SER
1	E	353	THR
1	E	363	ARG
1	E	369	ARG
1	E	423	ASN
1	E	471	GLU
1	E	472	THR
1	E	496	GLU
1	E	516	SER
1	E	560	THR
1	E	562	GLU
1	E	578	ILE
1	E	731	LEU
1	E	738	MET
1	E	764	ARG
1	E	771	LEU
1	E	800	ILE
1	E	847	LEU
1	E	929	MET
1	E	936	ASP
1	E	979	LEU
1	E	1008	GLN
1	E	1015	PHE
2	K	1101	ARG
1	F	44	LEU
1	F	61	LEU
1	F	82	ASN
1	F	157	SER
1	F	209	THR

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Mol	Chain	Res	Type
1	F	279	ASN
1	F	313	SER
1	F	353	THR
1	F	363	ARG
1	F	423	ASN
1	F	471	GLU
1	F	472	THR
1	F	516	SER
1	F	562	GLU
1	F	578	ILE
1	F	599	SER
1	F	731	LEU
1	F	738	MET
1	F	764	ARG
1	F	771	LEU
1	F	800	ILE
1	F	847	LEU
1	F	929	MET
1	F	936	ASP
1	F	979	LEU
1	F	1008	GLN
1	F	1015	PHE
2	L	1101	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (189) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	64	HIS
1	A	82	ASN
1	A	145	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	511	ASN
1	A	611	GLN
1	A	688	GLN

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Mol	Chain	Res	Type
1	A	703	ASN
1	A	733	ASN
1	A	739	GLN
1	A	867	ASN
1	A	872	HIS
1	A	901	ASN
1	A	922	GLN
1	A	930	ASN
1	A	949	ASN
1	A	1008	GLN
1	A	1024	ASN
1	A	1038	HIS
1	A	1047	GLN
1	B	41	ASN
1	B	64	HIS
1	B	82	ASN
1	B	145	ASN
1	B	195	ASN
1	B	253	GLN
1	B	267	HIS
1	B	277	HIS
1	B	279	ASN
1	B	297	ASN
1	B	403	ASN
1	B	415	ASN
1	B	423	ASN
1	B	469	HIS
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	703	ASN
1	B	733	ASN
1	B	739	GLN
1	B	867	ASN
1	B	872	HIS
1	B	893	ASN
1	B	901	ASN
1	B	922	GLN
1	B	930	ASN

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Mol	Chain	Res	Type
1	B	937	ASN
1	B	949	ASN
1	B	1008	GLN
1	B	1024	ASN
1	B	1038	HIS
1	B	1047	GLN
1	C	41	ASN
1	C	64	HIS
1	C	82	ASN
1	C	145	ASN
1	C	195	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
1	C	423	ASN
1	C	469	HIS
1	C	497	ASN
1	C	499	HIS
1	C	511	ASN
1	C	530	ASN
1	C	611	GLN
1	C	688	GLN
1	C	703	ASN
1	C	733	ASN
1	C	739	GLN
1	C	867	ASN
1	C	872	HIS
1	C	893	ASN
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	41	ASN
1	D	64	HIS
1	D	82	ASN

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Mol	Chain	Res	Type
1	D	145	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	469	HIS
1	D	481	HIS
1	D	497	ASN
1	D	511	ASN
1	D	611	GLN
1	D	688	GLN
1	D	703	ASN
1	D	739	GLN
1	D	867	ASN
1	D	872	HIS
1	D	893	ASN
1	D	922	GLN
1	D	930	ASN
1	D	949	ASN
1	D	1008	GLN
1	D	1024	ASN
1	D	1047	GLN
1	E	41	ASN
1	E	45	ASN
1	E	64	HIS
1	E	82	ASN
1	E	145	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	469	HIS

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Mol	Chain	Res	Type
1	E	497	ASN
1	E	511	ASN
1	E	611	GLN
1	E	688	GLN
1	E	703	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	41	ASN
1	F	64	HIS
1	F	82	ASN
1	F	145	ASN
1	F	195	ASN
1	F	253	GLN
1	F	267	HIS
1	F	279	ASN
1	F	297	ASN
1	F	403	ASN
1	F	415	ASN
1	F	423	ASN
1	F	469	HIS
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	688	GLN
1	F	703	ASN
1	F	739	GLN
1	F	867	ASN
1	F	872	HIS
1	F	893	ASN
1	F	901	ASN
1	F	922	GLN

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Mol	Chain	Res	Type
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 ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	-	9,9,9	0.56	0	8,8,8	1.06	1 (12%)
3	D10	J	2101	-	9,9,9	0.56	0	8,8,8	1.06	1 (12%)
3	D10	I	2101	-	9,9,9	0.56	0	8,8,8	1.06	1 (12%)
3	D10	K	2101	-	9,9,9	0.56	0	8,8,8	1.06	1 (12%)
3	D10	H	2101	-	9,9,9	0.56	0	8,8,8	1.06	1 (12%)
3	D10	L	2101	-	9,9,9	0.56	0	8,8,8	1.06	1 (12%)

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	-	-	3/7/7/7	-
3	D10	J	2101	-	-	3/7/7/7	-
3	D10	I	2101	-	-	3/7/7/7	-
3	D10	K	2101	-	-	3/7/7/7	-
3	D10	H	2101	-	-	3/7/7/7	-
3	D10	L	2101	-	-	3/7/7/7	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	2101	D10	C1-C2-C3	-2.13	98.96	113.36
3	L	2101	D10	C1-C2-C3	-2.13	98.98	113.36
3	H	2101	D10	C1-C2-C3	-2.13	98.98	113.36
3	K	2101	D10	C1-C2-C3	-2.13	98.99	113.36
3	I	2101	D10	C1-C2-C3	-2.12	99.01	113.36
3	J	2101	D10	C1-C2-C3	-2.12	99.02	113.36

There are no chirality outliers.

All (18) 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
3	G	2101	D10	C5-C6-C7-C8
3	H	2101	D10	C5-C6-C7-C8
3	I	2101	D10	C5-C6-C7-C8
3	K	2101	D10	C5-C6-C7-C8
3	L	2101	D10	C5-C6-C7-C8
3	J	2101	D10	C5-C6-C7-C8
3	I	2101	D10	C1-C2-C3-C4
3	K	2101	D10	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
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

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	J	2101	D10	3	0
3	I	2101	D10	4	0
3	K	2101	D10	4	0
3	H	2101	D10	3	0
3	L	2101	D10	4	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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1023/1071 (95%)	-1.44	0 100 100	8, 35, 56, 80	20 (1%)
1	B	1023/1071 (95%)	-1.46	0 100 100	8, 35, 56, 79	20 (1%)
1	C	1023/1071 (95%)	-1.33	0 100 100	8, 38, 57, 80	20 (1%)
1	D	1023/1071 (95%)	-1.42	0 100 100	8, 36, 56, 79	20 (1%)
1	E	1023/1071 (95%)	-1.43	0 100 100	8, 35, 56, 80	20 (1%)
1	F	1023/1071 (95%)	-1.37	0 100 100	8, 38, 57, 80	20 (1%)
2	G	4/5 (80%)	-1.36	0 100 100	36, 39, 40, 42	0
2	H	4/5 (80%)	-1.58	0 100 100	36, 39, 40, 42	0
2	I	4/5 (80%)	-1.44	0 100 100	36, 39, 40, 42	0
2	J	4/5 (80%)	-1.34	0 100 100	36, 39, 40, 42	0
2	K	4/5 (80%)	-1.44	0 100 100	36, 39, 40, 42	0
2	L	4/5 (80%)	-1.61	0 100 100	36, 39, 40, 42	0
All	All	6162/6456 (95%)	-1.41	0 100 100	8, 36, 56, 80	120 (1%)

There are no RSRZ outliers to report.

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	D10	L	2101	10/10	0.91	0.12	0,0,0,0	0
3	D10	J	2101	10/10	0.94	0.11	0,0,0,0	0
3	D10	I	2101	10/10	0.94	0.11	0,0,0,0	0
3	D10	H	2101	10/10	0.95	0.10	0,0,0,0	0
3	D10	G	2101	10/10	0.95	0.09	0,0,0,0	0
3	D10	K	2101	10/10	0.96	0.11	0,0,0,0	0

6.5 Other polymers [i](#)

There are no such residues in this entry.