



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 09:51 AM UTC

PDB ID : 6IWQ / pdb_00006iwq
Title : Crystal structure of GalNAc-T7 with Mn2+
Authors : Yu, C.; Yin, Y.X.
Deposited on : 2018-12-06
Resolution : 2.95 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
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

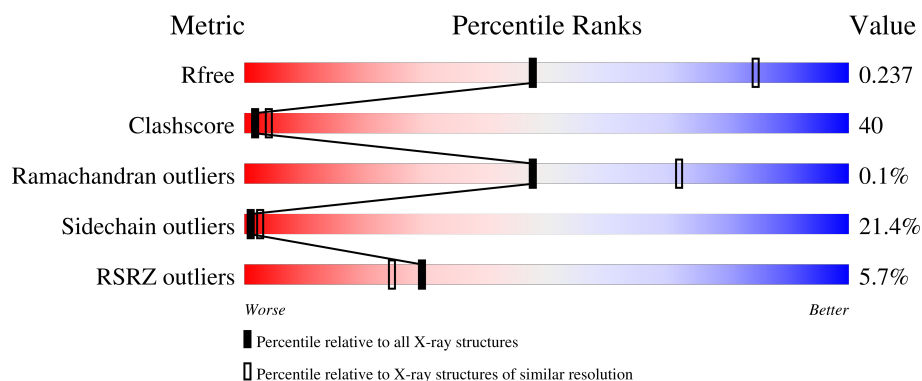
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	597	4% 42% 35% 14% • 9%
1	B	597	6% 37% 39% 14% • 9%
1	C	597	5% 46% 34% 11% • 9%
1	D	597	5% 39% 39% 14% • 9%
1	E	597	5% 39% 39% 13% • 9%

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Mol	Chain	Length	Quality of chain
1	F	597	8% 38% 40% 12% • 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26834 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 N-acetylgalactosaminyltransferase 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	546	Total	C	N	O	S	0	0	0
			4440	2855	757	805	23			
1	B	546	Total	C	N	O	S	0	0	0
			4440	2855	757	805	23			
1	C	546	Total	C	N	O	S	0	0	0
			4440	2855	757	805	23			
1	D	546	Total	C	N	O	S	0	0	0
			4440	2855	757	805	23			
1	E	546	Total	C	N	O	S	0	0	0
			4440	2855	757	805	23			
1	F	546	Total	C	N	O	S	0	0	0
			4440	2855	757	805	23			

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		
2	D	1	Total	Mn	0	0
			1	1		
2	E	1	Total	Mn	0	0
			1	1		
2	F	1	Total	Mn	0	0
			1	1		

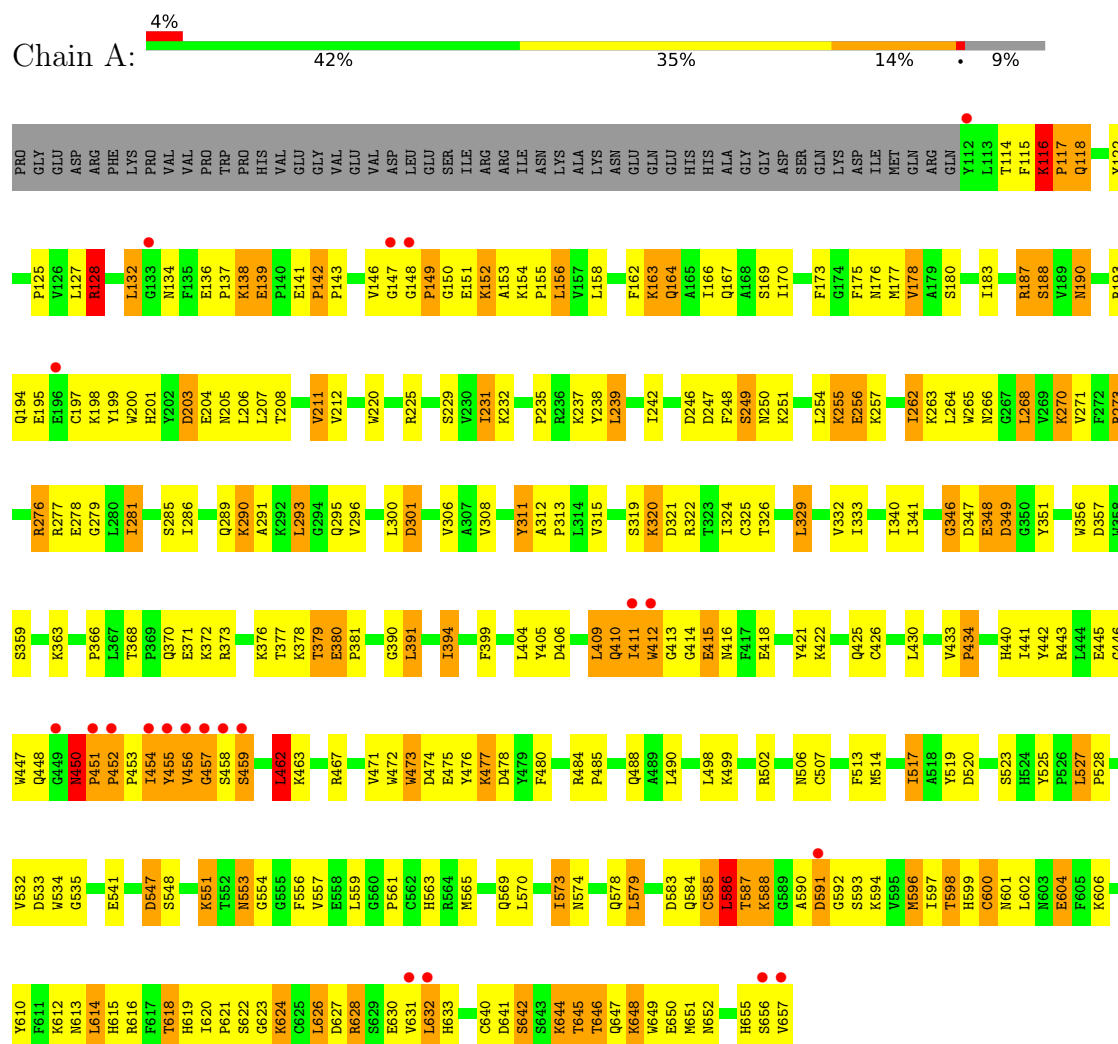
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	42	Total 42	O 42	0	0
3	B	31	Total 31	O 31	0	0
3	C	42	Total 42	O 42	0	0
3	D	25	Total 25	O 25	0	0
3	E	30	Total 30	O 30	0	0
3	F	18	Total 18	O 18	0	0

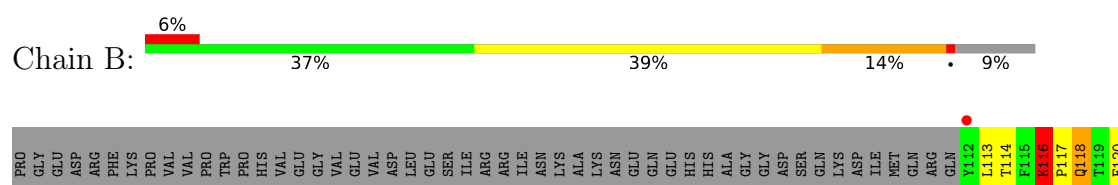
3 Residue-property plots

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.

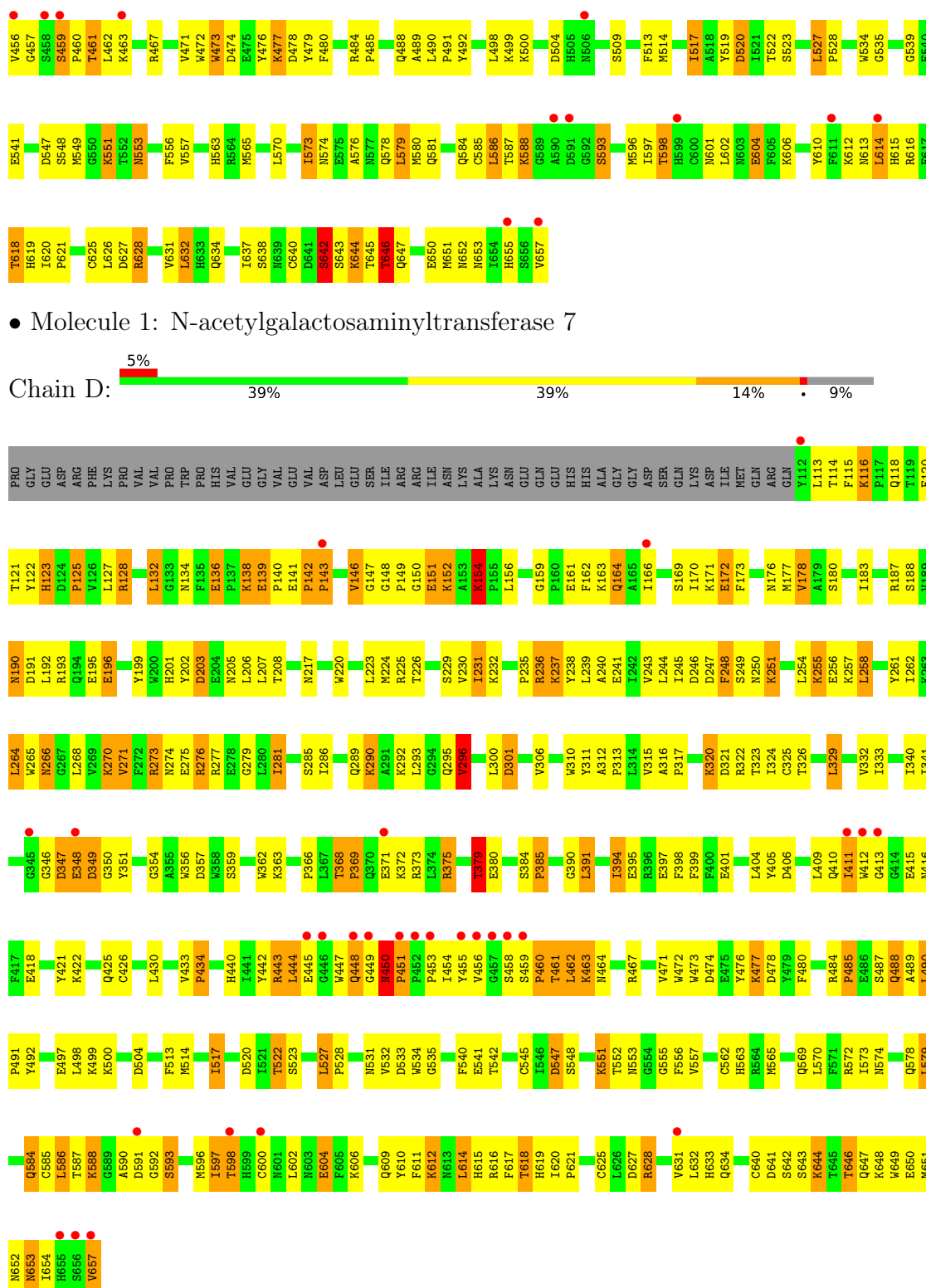
• Molecule 1: N-acetylgalactosaminyltransferase 7



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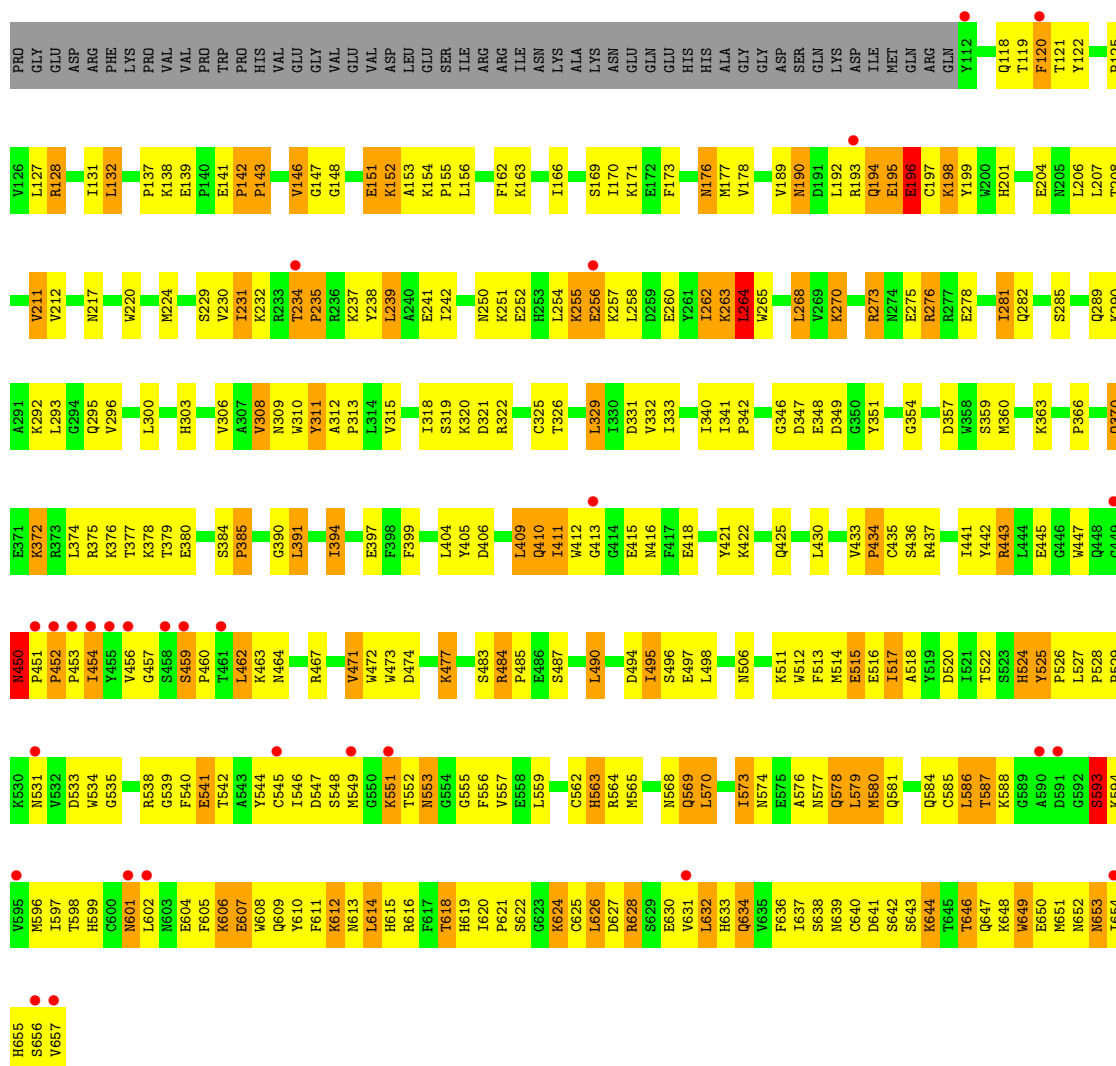




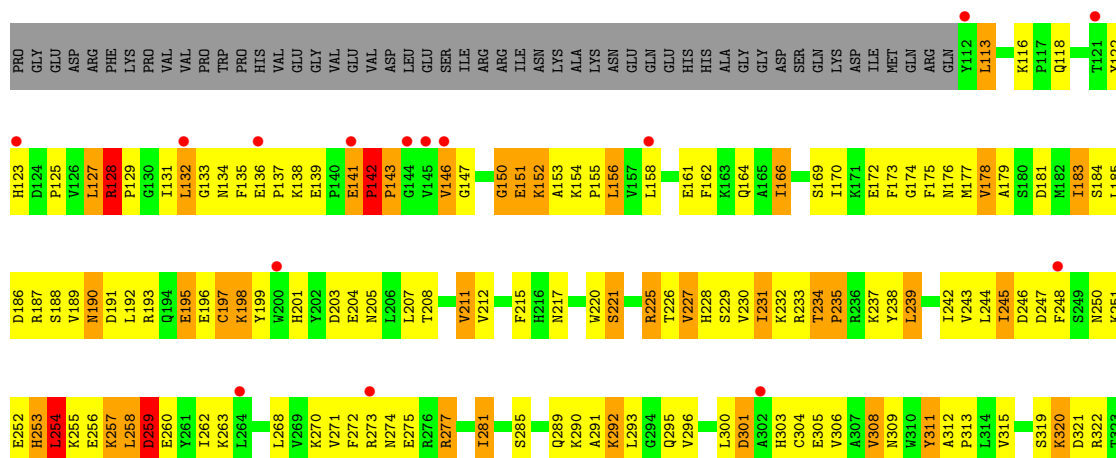


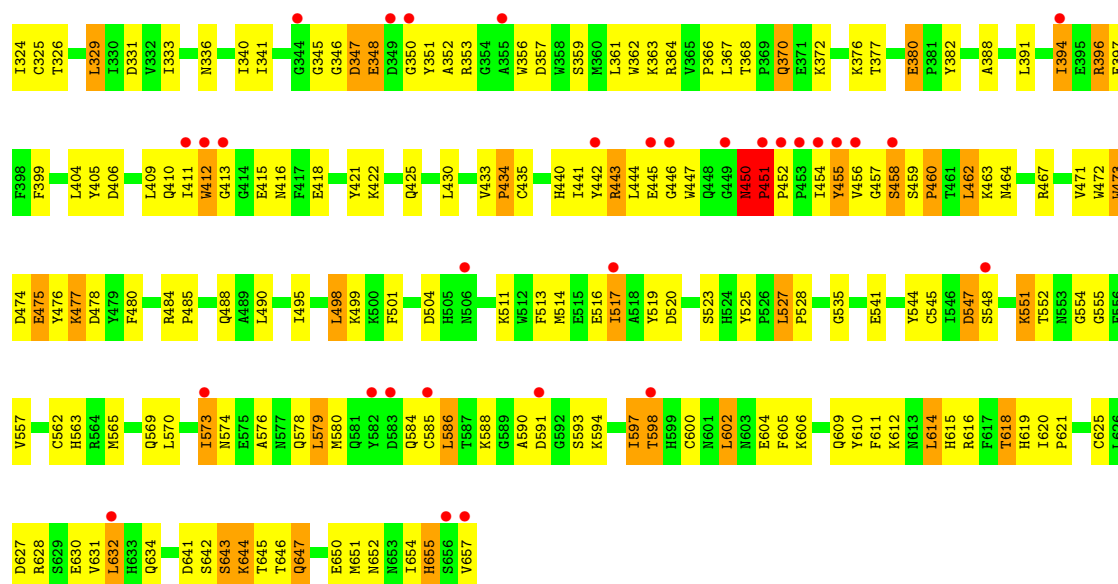
• Molecule 1: N-acetylgalactosaminyltransferase 7





• Molecule 1: N-acetylgalactosaminyltransferase 7





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	137.69Å 158.23Å 251.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.25 – 2.95 49.25 – 2.95	Depositor EDS
% Data completeness (in resolution range)	88.9 (49.25-2.95) 88.9 (49.25-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 2.96Å)	Xtriage
Refinement program	PHENIX (dev_2400: ???)	Depositor
R, R_{free}	0.225 , 0.239 0.223 , 0.237	Depositor DCC
R_{free} test set	5179 reflections (4.46%)	wwPDB-VP
Wilson B-factor (Å ²)	55.2	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 32.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	26834	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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: MN

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	1.13	27/4569 (0.6%)	1.14	47/6192 (0.8%)
1	B	1.00	25/4569 (0.5%)	1.18	48/6192 (0.8%)
1	C	1.02	22/4569 (0.5%)	1.15	45/6192 (0.7%)
1	D	0.94	16/4569 (0.4%)	1.10	35/6192 (0.6%)
1	E	0.92	16/4569 (0.4%)	1.14	44/6192 (0.7%)
1	F	0.85	13/4569 (0.3%)	1.11	29/6192 (0.5%)
All	All	0.98	119/27414 (0.4%)	1.14	248/37152 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	C	0	2
All	All	0	4

All (119) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	137	PRO	N-CD	9.50	1.61	1.47
1	F	451	PRO	C-N	8.42	1.41	1.33
1	E	137	PRO	N-CD	8.36	1.59	1.47
1	C	156	LEU	C-O	-7.34	1.15	1.24
1	A	271	VAL	C-O	-6.96	1.17	1.24
1	A	450	ASN	C-N	6.62	1.41	1.33
1	C	450	ASN	C-N	6.61	1.41	1.33
1	E	451	PRO	C-N	6.42	1.41	1.33
1	A	270	LYS	C-O	-6.33	1.16	1.23
1	B	319	SER	C-O	-6.32	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	527	LEU	C-N	6.31	1.40	1.33
1	E	450	ASN	C-N	6.30	1.40	1.33
1	B	451	PRO	C-N	6.27	1.40	1.33
1	D	451	PRO	C-N	6.26	1.40	1.33
1	C	158	LEU	C-O	-6.18	1.16	1.24
1	B	116	LYS	C-N	6.18	1.40	1.33
1	F	450	ASN	C-N	6.17	1.40	1.33
1	E	528	PRO	C-N	6.14	1.40	1.33
1	A	291	ALA	C-O	-6.14	1.17	1.24
1	C	451	PRO	C-N	6.05	1.40	1.33
1	B	527	LEU	C-N	6.05	1.40	1.33
1	D	527	LEU	C-N	6.04	1.40	1.33
1	A	527	LEU	C-N	6.04	1.40	1.33
1	C	527	LEU	C-N	6.04	1.40	1.33
1	D	154	LYS	C-N	6.01	1.40	1.33
1	C	124	ASP	C-N	6.00	1.40	1.33
1	B	141	GLU	C-N	5.99	1.40	1.33
1	A	116	LYS	C-N	5.95	1.40	1.33
1	B	452	PRO	C-N	5.89	1.40	1.33
1	C	151	GLU	CA-C	-5.82	1.45	1.52
1	F	528	PRO	C-N	5.76	1.40	1.33
1	B	460	PRO	N-CD	5.76	1.55	1.47
1	A	380	GLU	C-N	5.71	1.40	1.33
1	A	596	MET	C-O	-5.68	1.16	1.23
1	B	139	GLU	C-N	5.67	1.41	1.33
1	D	206	LEU	CA-C	-5.67	1.45	1.53
1	A	291	ALA	CA-C	-5.66	1.45	1.53
1	C	155	PRO	C-O	-5.66	1.17	1.23
1	E	525	TYR	C-N	5.64	1.40	1.33
1	E	154	LYS	C-N	5.64	1.41	1.33
1	C	179	ALA	C-O	-5.62	1.17	1.24
1	E	139	GLU	C-N	5.61	1.41	1.33
1	B	317	PRO	C-O	-5.57	1.17	1.24
1	D	139	GLU	C-N	5.57	1.40	1.33
1	B	341	ILE	C-N	5.56	1.40	1.33
1	B	136	GLU	C-N	5.55	1.40	1.33
1	B	154	LYS	C-N	5.55	1.41	1.33
1	E	451	PRO	N-CD	5.54	1.55	1.47
1	C	451	PRO	N-CD	5.50	1.55	1.47
1	F	128	ARG	C-N	5.50	1.40	1.33
1	C	116	LYS	CA-C	-5.50	1.47	1.53
1	A	587	THR	C-O	-5.48	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	234	THR	C-N	5.48	1.40	1.33
1	D	136	GLU	C-N	5.47	1.40	1.33
1	E	452	PRO	N-CD	5.47	1.55	1.47
1	B	321	ASP	C-O	-5.43	1.17	1.23
1	A	528	PRO	C-N	5.42	1.40	1.33
1	A	586	LEU	CA-C	-5.41	1.46	1.52
1	A	247	ASP	C-O	-5.41	1.17	1.23
1	C	459	SER	C-N	5.41	1.41	1.34
1	C	154	LYS	CA-C	-5.41	1.46	1.53
1	D	296	VAL	C-O	-5.39	1.18	1.24
1	A	459	SER	C-N	5.39	1.40	1.33
1	B	528	PRO	C-N	5.38	1.40	1.33
1	B	149	PRO	N-CD	5.37	1.55	1.47
1	A	128	ARG	C-N	5.36	1.40	1.33
1	C	163	LYS	C-O	-5.35	1.18	1.24
1	C	528	PRO	C-N	5.35	1.40	1.33
1	D	528	PRO	C-N	5.35	1.40	1.33
1	C	142	PRO	C-N	5.35	1.40	1.33
1	F	452	PRO	N-CD	5.34	1.55	1.47
1	C	452	PRO	N-CD	5.32	1.55	1.47
1	D	142	PRO	C-N	5.32	1.40	1.33
1	D	368	THR	C-N	5.32	1.40	1.33
1	B	128	ARG	C-N	5.32	1.40	1.33
1	C	127	LEU	CA-C	-5.32	1.46	1.52
1	E	142	PRO	C-N	5.31	1.40	1.33
1	B	117	PRO	N-CD	5.31	1.55	1.47
1	C	154	LYS	C-N	5.30	1.40	1.33
1	A	142	PRO	C-N	5.28	1.40	1.33
1	A	125	PRO	N-CD	5.26	1.55	1.47
1	E	385	PRO	N-CD	5.26	1.55	1.47
1	E	125	PRO	N-CD	5.25	1.55	1.47
1	F	125	PRO	N-CD	5.24	1.55	1.47
1	B	125	PRO	N-CD	5.24	1.55	1.47
1	A	187	ARG	C-O	-5.24	1.16	1.23
1	A	117	PRO	N-CD	5.23	1.55	1.47
1	A	139	GLU	C-N	5.23	1.40	1.33
1	C	125	PRO	N-CD	5.22	1.55	1.47
1	D	125	PRO	N-CD	5.19	1.55	1.47
1	B	129	PRO	N-CD	5.19	1.55	1.47
1	D	460	PRO	N-CD	5.18	1.55	1.47
1	B	143	PRO	N-CD	5.17	1.54	1.47
1	A	446	GLY	C-O	-5.12	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	155	PRO	N-CD	5.11	1.54	1.47
1	D	485	PRO	N-CD	5.11	1.54	1.47
1	F	143	PRO	N-CD	5.11	1.54	1.47
1	A	188	SER	CA-C	-5.10	1.46	1.52
1	C	179	ALA	CA-C	-5.10	1.46	1.52
1	B	381	PRO	N-CD	5.10	1.54	1.47
1	B	137	PRO	N-CD	5.10	1.54	1.47
1	F	235	PRO	N-CD	5.09	1.54	1.47
1	A	453	PRO	N-CD	5.08	1.54	1.47
1	E	155	PRO	N-CD	5.08	1.54	1.47
1	D	385	PRO	N-CD	5.08	1.54	1.47
1	B	155	PRO	N-CD	5.07	1.54	1.47
1	B	385	PRO	N-CD	5.06	1.54	1.47
1	D	143	PRO	N-CD	5.06	1.54	1.47
1	F	129	PRO	N-CD	5.06	1.54	1.47
1	A	143	PRO	N-CD	5.05	1.54	1.47
1	D	369	PRO	N-CD	5.05	1.54	1.47
1	F	155	PRO	N-CD	5.05	1.54	1.47
1	C	140	PRO	N-CD	5.05	1.54	1.47
1	E	143	PRO	N-CD	5.04	1.54	1.47
1	F	460	PRO	N-CD	5.03	1.54	1.47
1	E	235	PRO	N-CD	5.01	1.54	1.47
1	F	142	PRO	N-CD	5.01	1.54	1.47
1	B	142	PRO	N-CD	5.01	1.54	1.47
1	A	381	PRO	N-CD	5.00	1.54	1.47

All (248) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	133	GLY	N-CA-C	-13.27	91.23	110.60
1	B	654	ILE	N-CA-C	12.80	123.65	110.72
1	F	247	ASP	N-CA-C	-10.67	97.28	110.41
1	E	119	THR	CA-C-N	-9.95	109.11	123.05
1	E	119	THR	C-N-CA	-9.95	109.11	123.05
1	F	451	PRO	CA-C-N	-9.21	112.94	119.66
1	F	451	PRO	C-N-CA	-9.21	112.94	119.66
1	B	135	PHE	N-CA-C	9.15	121.33	111.36
1	C	451	PRO	CA-C-N	-9.08	113.12	119.66
1	C	451	PRO	C-N-CA	-9.08	113.12	119.66
1	A	452	PRO	O-C-N	9.02	125.39	121.15
1	A	553	ASN	CA-C-N	-9.01	112.99	123.08
1	A	553	ASN	C-N-CA	-9.01	112.99	123.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	293	LEU	N-CA-C	8.99	121.08	111.28
1	C	553	ASN	CA-C-N	-8.94	113.06	123.08
1	C	553	ASN	C-N-CA	-8.94	113.06	123.08
1	B	141	GLU	CA-C-N	-8.79	113.33	119.66
1	B	141	GLU	C-N-CA	-8.79	113.33	119.66
1	E	516	GLU	N-CA-C	8.75	120.59	111.14
1	A	148	GLY	C-N-CD	8.54	139.38	120.60
1	D	159	GLY	C-N-CD	8.49	139.28	120.60
1	D	293	LEU	N-CA-C	8.49	120.61	111.36
1	A	293	LEU	N-CA-C	8.19	120.29	111.36
1	D	593	SER	N-CA-C	-8.16	102.89	112.92
1	B	148	GLY	C-N-CD	8.01	138.23	120.60
1	B	459	SER	C-N-CD	7.86	137.88	120.60
1	C	644	LYS	N-CA-C	7.80	119.57	111.14
1	E	580	MET	N-CA-C	7.78	122.08	109.40
1	E	593	SER	N-CA-C	-7.72	104.29	112.93
1	E	524	HIS	N-CA-C	7.68	119.73	111.36
1	A	646	THR	N-CA-C	-7.66	99.70	110.50
1	F	257	LYS	N-CA-C	-7.64	103.80	113.43
1	D	450	ASN	N-CA-C	7.50	120.24	108.55
1	F	150	GLY	N-CA-C	7.49	122.35	112.77
1	E	471	VAL	N-CA-C	7.43	119.10	111.00
1	C	593	SER	N-CA-C	-7.38	104.31	112.72
1	C	293	LEU	N-CA-C	7.32	119.26	111.28
1	C	646	THR	N-CA-C	-7.21	101.01	110.53
1	F	311	TYR	N-CA-C	7.20	118.91	111.14
1	A	311	TYR	N-CA-C	7.19	118.91	111.14
1	B	311	TYR	N-CA-C	7.19	118.90	111.14
1	E	311	TYR	N-CA-C	7.18	118.90	111.14
1	B	292	LYS	N-CA-C	7.17	119.17	111.36
1	C	642	SER	N-CA-C	-7.14	101.11	110.53
1	C	311	TYR	N-CA-C	7.14	118.85	111.14
1	C	459	SER	CA-C-N	-7.14	111.55	118.97
1	C	459	SER	C-N-CA	-7.14	111.55	118.97
1	E	292	LYS	N-CA-C	7.14	119.14	111.36
1	A	450	ASN	N-CA-C	7.09	123.11	107.95
1	C	133	GLY	CA-C-O	-7.05	114.39	121.30
1	E	528	PRO	CA-C-N	-6.99	113.46	120.31
1	E	528	PRO	C-N-CA	-6.99	113.46	120.31
1	B	154	LYS	CA-C-N	-6.97	112.79	119.76
1	B	154	LYS	C-N-CA	-6.97	112.79	119.76
1	B	116	LYS	CA-C-N	-6.97	113.48	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	116	LYS	C-N-CA	-6.97	113.48	120.31
1	A	116	LYS	CA-C-N	-6.92	113.67	120.52
1	A	116	LYS	C-N-CA	-6.92	113.67	120.52
1	A	346	GLY	N-CA-C	6.92	121.03	112.73
1	E	451	PRO	CA-C-N	-6.91	113.27	120.38
1	E	451	PRO	C-N-CA	-6.91	113.27	120.38
1	B	451	PRO	CA-C-N	-6.88	113.29	120.38
1	B	451	PRO	C-N-CA	-6.88	113.29	120.38
1	D	451	PRO	CA-C-N	-6.87	113.30	120.38
1	D	451	PRO	C-N-CA	-6.87	113.30	120.38
1	E	139	GLU	CA-C-N	-6.78	112.77	119.76
1	E	139	GLU	C-N-CA	-6.78	112.77	119.76
1	F	128	ARG	CA-C-N	-6.77	113.01	119.85
1	F	128	ARG	C-N-CA	-6.77	113.01	119.85
1	C	142	PRO	CA-C-N	-6.76	113.03	119.85
1	C	142	PRO	C-N-CA	-6.76	113.03	119.85
1	E	142	PRO	CA-C-N	-6.75	113.04	119.85
1	E	142	PRO	C-N-CA	-6.75	113.04	119.85
1	E	570	LEU	N-CA-C	6.75	119.66	110.55
1	D	142	PRO	CA-C-N	-6.70	113.08	119.85
1	D	142	PRO	C-N-CA	-6.70	113.08	119.85
1	B	452	PRO	CA-C-N	-6.69	112.60	119.83
1	B	452	PRO	C-N-CA	-6.69	112.60	119.83
1	F	528	PRO	CA-C-N	-6.69	113.41	120.03
1	F	528	PRO	C-N-CA	-6.69	113.41	120.03
1	A	142	PRO	CA-C-N	-6.67	113.11	119.85
1	A	142	PRO	C-N-CA	-6.67	113.11	119.85
1	A	451	PRO	CA-C-N	6.66	124.46	119.66
1	A	451	PRO	C-N-CA	6.66	124.46	119.66
1	A	128	ARG	CA-C-N	-6.65	112.91	119.76
1	A	128	ARG	C-N-CA	-6.65	112.91	119.76
1	E	646	THR	N-CA-C	-6.65	101.12	110.50
1	D	139	GLU	CA-C-N	-6.63	112.93	119.76
1	D	139	GLU	C-N-CA	-6.63	112.93	119.76
1	D	136	GLU	CA-C-N	-6.61	113.17	119.85
1	D	136	GLU	C-N-CA	-6.61	113.17	119.85
1	C	124	ASP	CA-C-N	-6.59	113.50	120.03
1	C	124	ASP	C-N-CA	-6.59	113.50	120.03
1	D	527	LEU	CA-C-N	-6.58	113.61	120.38
1	D	527	LEU	C-N-CA	-6.58	113.61	120.38
1	C	450	ASN	CA-C-N	-6.58	113.61	120.38
1	C	450	ASN	C-N-CA	-6.58	113.61	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	154	LYS	CA-C-N	-6.57	112.73	119.83
1	D	154	LYS	C-N-CA	-6.57	112.73	119.83
1	E	119	THR	N-CA-C	6.56	118.23	111.14
1	E	450	ASN	CA-C-N	-6.56	113.62	120.38
1	E	450	ASN	C-N-CA	-6.56	113.62	120.38
1	C	527	LEU	CA-C-N	-6.56	113.62	120.38
1	C	527	LEU	C-N-CA	-6.56	113.62	120.38
1	F	450	ASN	CA-C-N	-6.56	113.63	120.38
1	F	450	ASN	C-N-CA	-6.56	113.63	120.38
1	A	139	GLU	CA-C-N	-6.55	113.03	119.78
1	A	139	GLU	C-N-CA	-6.55	113.03	119.78
1	A	527	LEU	CA-C-N	-6.55	113.63	120.38
1	A	527	LEU	C-N-CA	-6.55	113.63	120.38
1	C	347	ASP	N-CA-C	6.55	118.42	111.28
1	B	128	ARG	CA-C-N	-6.55	113.02	119.76
1	B	128	ARG	C-N-CA	-6.55	113.02	119.76
1	B	527	LEU	CA-C-N	-6.54	113.64	120.38
1	B	527	LEU	C-N-CA	-6.54	113.64	120.38
1	F	293	LEU	N-CA-C	6.53	118.39	111.28
1	F	527	LEU	CA-C-N	-6.52	113.67	120.38
1	F	527	LEU	C-N-CA	-6.52	113.67	120.38
1	E	525	TYR	CA-C-N	-6.51	113.23	120.14
1	E	525	TYR	C-N-CA	-6.51	113.23	120.14
1	D	276	ARG	N-CA-C	6.49	122.28	113.97
1	B	293	LEU	N-CA-C	6.47	118.33	111.28
1	A	137	PRO	CA-N-CD	-6.46	102.96	112.00
1	B	450	ASN	N-CA-C	6.45	120.32	109.09
1	B	139	GLU	CA-C-N	-6.44	113.35	119.85
1	B	139	GLU	C-N-CA	-6.44	113.35	119.85
1	B	528	PRO	CA-C-N	-6.41	113.38	119.85
1	B	528	PRO	C-N-CA	-6.41	113.38	119.85
1	E	264	LEU	N-CA-C	-6.40	101.48	110.50
1	B	136	GLU	CA-C-N	-6.39	113.17	119.76
1	B	136	GLU	C-N-CA	-6.39	113.17	119.76
1	E	154	LYS	CA-C-N	-6.39	113.17	119.76
1	E	154	LYS	C-N-CA	-6.39	113.17	119.76
1	B	341	ILE	CA-C-N	-6.38	113.40	119.85
1	B	341	ILE	C-N-CA	-6.38	113.40	119.85
1	A	528	PRO	CA-C-N	-6.37	113.42	119.85
1	A	528	PRO	C-N-CA	-6.37	113.42	119.85
1	A	450	ASN	CA-C-N	-6.36	113.83	120.38
1	A	450	ASN	C-N-CA	-6.36	113.83	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	528	PRO	CA-C-N	-6.34	113.44	119.85
1	C	528	PRO	C-N-CA	-6.34	113.44	119.85
1	D	528	PRO	CA-C-N	-6.34	113.44	119.85
1	D	528	PRO	C-N-CA	-6.34	113.44	119.85
1	E	234	THR	CA-C-N	-6.34	113.23	119.76
1	E	234	THR	C-N-CA	-6.34	113.23	119.76
1	E	137	PRO	CA-N-CD	-6.28	103.20	112.00
1	B	148	GLY	N-CA-C	-6.27	99.56	112.34
1	C	450	ASN	N-CA-C	6.27	119.99	109.09
1	C	154	LYS	N-CA-C	-6.25	102.17	109.93
1	D	311	TYR	N-CA-C	6.23	118.08	111.28
1	C	410	GLN	N-CA-C	6.17	117.88	111.03
1	F	153	ALA	N-CA-C	-6.17	103.23	112.54
1	A	452	PRO	CA-C-N	-6.11	112.20	119.84
1	A	452	PRO	C-N-CA	-6.11	112.20	119.84
1	C	520	ASP	N-CA-C	6.11	117.94	111.28
1	E	459	SER	CA-C-N	-6.10	112.28	119.05
1	E	459	SER	C-N-CA	-6.10	112.28	119.05
1	E	262	ILE	CA-C-N	6.08	128.43	120.28
1	E	262	ILE	C-N-CA	6.08	128.43	120.28
1	B	150	GLY	N-CA-C	6.07	120.53	112.77
1	C	292	LYS	N-CA-C	6.02	117.92	111.36
1	B	346	GLY	N-CA-C	5.98	119.91	112.73
1	F	259	ASP	N-CA-C	-5.98	104.84	111.36
1	B	490	LEU	N-CA-C	-5.96	101.31	110.32
1	A	263	LYS	CA-C-N	5.94	128.84	120.28
1	A	263	LYS	C-N-CA	5.94	128.84	120.28
1	E	196	GLU	N-CA-C	-5.90	105.18	112.38
1	D	488	GLN	N-CA-C	5.90	117.38	111.07
1	A	459	SER	CA-C-N	-5.90	112.79	119.28
1	A	459	SER	C-N-CA	-5.90	112.79	119.28
1	A	457	GLY	N-CA-C	-5.88	105.67	112.50
1	F	250	ASN	N-CA-C	5.87	120.61	112.45
1	E	490	LEU	N-CA-C	-5.86	101.30	110.14
1	D	148	GLY	N-CA-C	-5.83	100.45	112.34
1	A	380	GLU	CA-C-N	-5.82	113.70	119.92
1	A	380	GLU	C-N-CA	-5.82	113.70	119.92
1	E	148	GLY	N-CA-C	-5.80	100.50	112.34
1	C	154	LYS	CA-C-N	-5.79	113.81	119.78
1	C	154	LYS	C-N-CA	-5.79	113.81	119.78
1	C	148	GLY	N-CA-C	-5.78	100.54	112.34
1	B	402	LEU	N-CA-C	-5.72	106.14	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	462	LEU	N-CA-C	-5.71	105.57	112.54
1	D	250	ASN	N-CA-C	5.70	118.70	111.69
1	B	264	LEU	N-CA-C	-5.69	102.61	110.35
1	B	463	LYS	N-CA-C	-5.69	105.83	112.89
1	C	346	GLY	N-CA-C	5.59	121.42	111.02
1	A	149	PRO	CA-N-CD	-5.59	103.68	111.50
1	C	179	ALA	N-CA-C	-5.57	104.85	111.03
1	F	254	LEU	N-CA-C	-5.55	105.38	111.82
1	A	473	TRP	N-CA-C	5.55	118.26	111.82
1	C	473	TRP	N-CA-C	5.55	118.26	111.82
1	A	203	ASP	N-CA-C	5.54	117.32	111.28
1	A	248	PHE	N-CA-C	5.54	119.23	111.74
1	F	473	TRP	N-CA-C	5.52	118.22	111.82
1	B	281	ILE	CB-CA-C	-5.50	104.81	112.02
1	F	281	ILE	CB-CA-C	-5.50	104.81	112.02
1	A	281	ILE	CB-CA-C	-5.49	104.83	112.02
1	E	281	ILE	CB-CA-C	-5.48	104.84	112.02
1	D	281	ILE	CB-CA-C	-5.47	104.86	112.02
1	C	281	ILE	CB-CA-C	-5.46	104.86	112.02
1	F	227	VAL	N-CA-C	-5.42	105.09	110.62
1	B	553	ASN	N-CA-C	5.41	119.05	111.74
1	B	554	GLY	N-CA-C	-5.39	97.67	113.30
1	A	490	LEU	N-CA-C	-5.36	101.28	109.64
1	D	654	ILE	N-CA-C	5.36	116.84	111.00
1	C	490	LEU	N-CA-C	-5.36	101.28	109.64
1	F	490	LEU	N-CA-C	-5.34	101.31	109.64
1	F	484	ARG	CA-C-N	-5.33	113.17	119.84
1	F	484	ARG	C-N-CA	-5.33	113.17	119.84
1	C	484	ARG	CA-C-N	-5.30	113.21	119.84
1	C	484	ARG	C-N-CA	-5.30	113.21	119.84
1	A	484	ARG	CA-C-N	-5.30	113.22	119.84
1	A	484	ARG	C-N-CA	-5.30	113.22	119.84
1	B	203	ASP	N-CA-C	5.28	117.03	111.28
1	B	484	ARG	CA-C-N	-5.28	113.25	119.84
1	B	484	ARG	C-N-CA	-5.28	113.25	119.84
1	B	257	LYS	N-CA-C	-5.26	105.55	111.28
1	F	382	TYR	N-CA-C	-5.20	101.17	109.07
1	D	172	GLU	N-CA-C	5.19	117.02	111.36
1	D	368	THR	CA-C-N	-5.18	113.58	119.28
1	D	368	THR	C-N-CA	-5.18	113.58	119.28
1	A	594	LYS	N-CA-C	-5.17	102.81	110.46
1	D	347	ASP	N-CA-C	5.15	116.14	108.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	629	SER	N-CA-C	5.15	115.81	107.32
1	F	292	LYS	N-CA-C	5.15	116.97	111.36
1	B	552	THR	N-CA-C	5.12	116.62	108.79
1	A	434	PRO	CA-N-CD	-5.12	104.83	112.00
1	C	434	PRO	CA-N-CD	-5.11	104.84	112.00
1	C	203	ASP	N-CA-C	5.11	116.85	111.28
1	B	434	PRO	CA-N-CD	-5.10	104.86	112.00
1	D	490	LEU	N-CA-C	-5.09	101.70	109.64
1	C	346	GLY	CA-C-N	5.09	127.10	120.28
1	C	346	GLY	C-N-CA	5.09	127.10	120.28
1	E	434	PRO	CA-N-CD	-5.09	104.88	112.00
1	F	434	PRO	CA-N-CD	-5.09	104.88	112.00
1	A	528	PRO	CA-N-CD	-5.08	104.88	112.00
1	C	155	PRO	N-CA-C	5.08	119.29	111.21
1	E	384	SER	CA-C-N	-5.08	113.41	119.05
1	E	384	SER	C-N-CA	-5.08	113.41	119.05
1	D	434	PRO	CA-N-CD	-5.07	104.90	112.00
1	D	379	THR	N-CA-C	5.04	119.12	112.92
1	E	462	LEU	CA-C-N	-5.04	112.33	121.14
1	E	462	LEU	C-N-CA	-5.04	112.33	121.14
1	B	404	LEU	CB-CA-C	-5.03	109.29	116.34
1	F	388	ALA	N-CA-C	-5.02	105.81	111.28
1	D	203	ASP	N-CA-C	-5.02	102.44	109.96
1	D	384	SER	CA-C-N	-5.01	113.48	119.05
1	D	384	SER	C-N-CA	-5.01	113.48	119.05

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	553	ASN	Peptide
1	B	645	THR	Peptide
1	C	346	GLY	Peptide
1	C	348	GLU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4440	0	4329	284	0
1	B	4440	0	4329	449	0
1	C	4440	0	4327	277	0
1	D	4440	0	4331	388	0
1	E	4440	0	4329	395	0
1	F	4440	0	4331	367	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	42	0	0	9	0
3	B	31	0	0	10	0
3	C	42	0	0	7	0
3	D	25	0	0	4	0
3	E	30	0	0	6	0
3	F	18	0	0	8	0
All	All	26834	0	25976	2123	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 40.

All (2123) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:545:CYS:HB3	1:E:562:CYS:SG	1.57	1.43
1:B:614:LEU:CD1	1:B:616:ARG:HD3	1.55	1.36
1:F:128:ARG:HG3	1:F:201:HIS:CD2	1.62	1.32
1:A:332:VAL:HG13	1:A:442:TYR:CD2	1.65	1.30
1:D:456:VAL:HG13	1:D:657:VAL:C	1.56	1.30
1:E:513:PHE:CE1	1:E:517:ILE:HD11	1.67	1.30
1:E:545:CYS:CB	1:E:562:CYS:HG	1.44	1.29
1:B:616:ARG:CG	1:B:648:LYS:HE3	1.61	1.29
1:D:585:CYS:SG	1:D:600:CYS:HB3	1.71	1.28
1:E:363:LYS:HD2	1:E:525:TYR:CE2	1.68	1.28
1:B:554:GLY:HA3	1:B:597:ILE:O	1.28	1.28
1:B:608:TRP:CZ3	1:B:626:LEU:HD21	1.68	1.27
1:B:614:LEU:HD13	1:B:616:ARG:CD	1.63	1.27
1:E:545:CYS:CB	1:E:562:CYS:SG	2.23	1.26
1:F:141:GLU:OE2	1:F:142:PRO:HD3	1.35	1.25
1:F:226:THR:HG22	1:F:304:CYS:O	1.31	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:625:CYS:SG	1:C:640:CYS:HB2	1.76	1.24
1:D:625:CYS:CB	1:D:640:CYS:SG	2.27	1.23
1:F:585:CYS:CB	1:F:600:CYS:SG	2.26	1.23
1:B:625:CYS:SG	1:B:640:CYS:HA	1.77	1.22
1:C:627:ASP:OD1	1:C:646:THR:HB	1.41	1.20
1:D:443:ARG:HD2	1:D:447:TRP:CE3	1.76	1.20
1:F:258:LEU:CD2	1:F:262:ILE:HD11	1.71	1.19
1:F:141:GLU:OE2	1:F:142:PRO:CD	1.92	1.18
1:D:643:SER:HB3	1:D:648:LYS:NZ	1.60	1.17
1:F:166:ILE:HG23	1:F:176:ASN:ND2	1.60	1.17
1:B:495:ILE:HD12	1:B:498:LEU:CD1	1.75	1.16
1:F:226:THR:HG21	1:F:304:CYS:H	1.07	1.16
1:D:522:THR:CG2	1:D:527:LEU:HD11	1.76	1.16
1:E:625:CYS:SG	1:E:640:CYS:HB2	1.85	1.16
1:F:545:CYS:SG	1:F:562:CYS:SG	1.44	1.16
1:D:590:ALA:HA	1:D:592:GLY:H	1.11	1.15
1:B:495:ILE:CD1	1:B:498:LEU:HD12	1.76	1.15
1:B:601:ASN:CB	1:B:604:GLU:HG3	1.77	1.14
1:F:226:THR:CG2	1:F:304:CYS:H	1.59	1.14
1:A:132:LEU:HD23	1:A:199:TYR:CE1	1.82	1.14
1:A:153:ALA:HB3	1:A:190:ASN:HD22	1.12	1.14
1:B:625:CYS:HB3	1:B:640:CYS:SG	1.88	1.13
1:F:258:LEU:HD22	1:F:262:ILE:HD11	1.30	1.13
1:F:585:CYS:SG	1:F:600:CYS:SG	1.14	1.13
1:D:545:CYS:SG	1:D:562:CYS:CB	2.38	1.12
1:A:414:GLY:HA2	1:A:415:GLU:HB3	1.26	1.11
1:B:333:ILE:CG2	1:B:441:ILE:HD13	1.81	1.11
1:D:522:THR:HG22	1:D:527:LEU:CD1	1.82	1.10
1:D:258:LEU:O	1:D:262:ILE:HG12	1.50	1.10
1:B:585:CYS:HB2	1:B:600:CYS:HB2	1.28	1.10
1:A:132:LEU:CD2	1:A:199:TYR:HE1	1.63	1.10
1:D:348:GLU:HA	1:D:350:GLY:H	1.14	1.10
1:F:133:GLY:H	1:F:136:GLU:HG2	0.99	1.10
1:B:304:CYS:HB3	1:B:439:GLY:O	1.52	1.09
1:E:193:ARG:HH22	1:E:310:TRP:HA	1.05	1.09
1:E:627:ASP:HB2	1:E:647:GLN:HG3	1.22	1.09
1:A:455:TYR:HB2	1:A:456:VAL:HG23	1.35	1.09
1:C:457:GLY:HA2	1:C:459:SER:H	1.10	1.09
1:D:132:LEU:HD23	1:D:199:TYR:HE1	1.10	1.09
1:F:136:GLU:OE2	1:F:138:LYS:HG3	1.53	1.09
1:F:197:CYS:SG	1:F:435:CYS:SG	1.21	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:LEU:CD2	1:A:199:TYR:CE1	2.36	1.08
1:B:616:ARG:CD	1:B:648:LYS:HE3	1.84	1.08
1:E:627:ASP:HB2	1:E:647:GLN:CG	1.83	1.08
1:B:608:TRP:HZ3	1:B:626:LEU:HD21	0.92	1.08
1:D:347:ASP:HB2	1:D:351:TYR:H	1.19	1.08
1:B:626:LEU:HB2	1:B:649:TRP:CH2	1.88	1.08
1:F:116:LYS:HD3	1:F:397:GLU:OE1	1.52	1.08
1:F:348:GLU:HA	1:F:350:GLY:H	1.13	1.08
1:B:538:ARG:O	1:B:649:TRP:HB3	1.52	1.07
1:D:443:ARG:CD	1:D:447:TRP:CE3	2.36	1.07
1:D:545:CYS:SG	1:D:562:CYS:SG	1.09	1.07
1:B:495:ILE:CD1	1:B:498:LEU:CD1	2.31	1.06
1:E:625:CYS:SG	1:E:640:CYS:CB	2.43	1.06
1:C:162:PHE:O	1:C:166:ILE:HG13	1.55	1.05
1:D:208:THR:CG2	1:D:240:ALA:HB2	1.85	1.05
1:A:153:ALA:HB3	1:A:190:ASN:ND2	1.70	1.05
1:B:616:ARG:HG2	1:B:648:LYS:HE3	1.38	1.05
1:F:133:GLY:HA2	1:F:136:GLU:HG3	1.30	1.05
1:F:348:GLU:N	1:F:348:GLU:OE1	1.89	1.05
1:B:552:THR:HB	1:B:584:GLN:HE22	1.20	1.05
1:B:333:ILE:CG2	1:B:441:ILE:CD1	2.34	1.05
1:B:625:CYS:CB	1:B:640:CYS:SG	2.45	1.05
1:A:153:ALA:CB	1:A:190:ASN:ND2	2.21	1.04
1:B:574:ASN:HD22	1:B:578:GLN:HG3	1.18	1.04
1:C:203:ASP:O	1:C:204:GLU:HB2	1.55	1.04
1:C:574:ASN:HD22	1:C:578:GLN:HG3	1.18	1.04
1:D:584:GLN:HG2	1:D:597:ILE:HG23	1.40	1.04
1:E:627:ASP:HB3	3:E:808:HOH:O	1.58	1.03
1:F:574:ASN:HD22	1:F:578:GLN:HG3	1.18	1.03
1:E:332:VAL:HG13	1:E:442:TYR:CD2	1.94	1.03
1:C:116:LYS:HE2	1:C:397:GLU:OE1	1.59	1.03
1:A:132:LEU:HD23	1:A:199:TYR:HE1	0.91	1.02
1:D:585:CYS:SG	1:D:600:CYS:CB	2.46	1.02
1:D:139:GLU:HG3	1:D:140:PRO:HD2	1.35	1.02
1:D:236:ARG:HG3	1:D:236:ARG:HH11	1.22	1.02
1:A:276:ARG:HD2	1:A:278:GLU:OE2	1.59	1.02
1:C:632:LEU:H	1:C:632:LEU:HD12	1.21	1.02
1:B:301:ASP:OD2	1:B:440:HIS:HE1	1.40	1.01
1:E:193:ARG:HH22	1:E:310:TRP:CA	1.72	1.01
1:B:596:MET:HE3	1:B:598:THR:CG2	1.90	1.01
1:C:155:PRO:HD3	1:C:339:GLU:HG3	1.39	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:485:PRO:O	1:D:488:GLN:HG3	1.60	1.01
1:E:627:ASP:CB	1:E:647:GLN:HG3	1.89	1.01
1:B:333:ILE:HG21	1:B:441:ILE:CD1	1.90	1.01
1:F:133:GLY:N	1:F:136:GLU:HG2	1.74	1.01
1:F:243:VAL:HG12	1:F:245:ILE:CD1	1.90	1.01
1:B:506:ASN:HB3	3:B:804:HOH:O	1.59	1.01
1:D:625:CYS:SG	1:D:640:CYS:SG	1.11	1.00
1:A:574:ASN:HD22	1:A:578:GLN:HG3	1.26	1.00
1:C:372:LYS:HE3	1:C:378:LYS:HZ1	1.25	1.00
1:E:457:GLY:HA2	1:E:459:SER:H	1.23	1.00
1:F:136:GLU:CD	1:F:138:LYS:HG3	1.87	1.00
1:B:583:ASP:OD1	1:B:584:GLN:HG3	1.61	1.00
1:E:413:GLY:CA	1:E:464:ASN:HD22	1.74	0.99
1:A:332:VAL:HG13	1:A:442:TYR:HD2	1.00	0.99
1:D:348:GLU:OE1	1:D:348:GLU:N	1.96	0.98
1:A:456:VAL:HG13	1:A:458:SER:HB3	1.44	0.98
1:E:370:GLN:OE1	1:E:370:GLN:N	1.96	0.98
1:C:625:CYS:SG	1:C:640:CYS:CB	2.51	0.98
1:D:132:LEU:HD23	1:D:199:TYR:CE1	1.98	0.98
1:E:632:LEU:HD12	1:E:632:LEU:H	1.26	0.97
1:E:625:CYS:HG	1:E:640:CYS:CB	1.77	0.97
1:F:172:GLU:HG2	1:F:173:PHE:CE2	1.98	0.97
1:B:150:GLY:HA3	1:B:183:ILE:HG23	1.45	0.97
1:B:333:ILE:HG21	1:B:441:ILE:HD11	1.46	0.97
1:E:363:LYS:CD	1:E:525:TYR:CE2	2.48	0.97
1:A:454:ILE:HD12	1:A:455:TYR:N	1.79	0.96
1:E:193:ARG:NH2	1:E:310:TRP:HA	1.78	0.96
1:E:624:LYS:HG3	1:E:638:SER:C	1.90	0.96
1:D:443:ARG:HD2	1:D:447:TRP:CZ3	1.99	0.96
1:A:456:VAL:HG13	1:A:458:SER:CB	1.95	0.96
1:B:534:TRP:HA	1:B:651:MET:CE	1.96	0.96
1:B:603:ASN:HB3	1:B:606:LYS:HE2	1.48	0.96
1:C:207:LEU:HD21	1:C:319:SER:HA	1.46	0.96
1:D:456:VAL:CG1	1:D:657:VAL:C	2.38	0.95
1:F:363:LYS:HD2	1:F:525:TYR:CZ	2.01	0.95
1:E:627:ASP:OD1	1:E:646:THR:HB	1.67	0.95
1:F:545:CYS:CB	1:F:562:CYS:SG	2.53	0.95
1:F:197:CYS:SG	1:F:435:CYS:CB	2.54	0.95
1:E:166:ILE:HG12	1:E:178:VAL:HG21	1.48	0.95
1:B:458:SER:O	1:B:462:LEU:HB3	1.65	0.95
1:B:626:LEU:HD23	1:B:637:ILE:HG22	1.46	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:601:ASN:O	1:B:604:GLU:HB2	1.66	0.94
1:E:556:PHE:CD2	1:E:594:LYS:HD3	2.02	0.94
1:E:363:LYS:HD2	1:E:525:TYR:CZ	2.02	0.94
1:A:332:VAL:CG1	1:A:442:TYR:HD2	1.80	0.94
1:F:128:ARG:HG3	1:F:201:HIS:HD2	1.26	0.94
1:D:522:THR:HG22	1:D:527:LEU:HD11	1.38	0.94
1:B:625:CYS:SG	1:B:640:CYS:CA	2.55	0.94
1:B:246:ASP:OD1	1:B:249:SER:HB2	1.68	0.94
1:D:171:LYS:HD3	1:D:448:GLN:HE22	1.32	0.94
1:D:456:VAL:HG13	1:D:657:VAL:O	1.67	0.94
1:B:626:LEU:C	1:B:649:TRP:HH2	1.76	0.94
1:A:347:ASP:HB2	1:A:351:TYR:O	1.68	0.94
1:B:587:THR:HG21	1:B:605:PHE:CG	2.04	0.93
1:B:301:ASP:OD2	1:B:440:HIS:CE1	2.21	0.93
1:D:590:ALA:HA	1:D:592:GLY:N	1.83	0.93
1:D:132:LEU:CD2	1:D:199:TYR:HE1	1.81	0.93
1:D:348:GLU:HB2	1:D:349:ASP:HA	1.47	0.93
1:B:391:LEU:HD13	1:B:438:VAL:HG21	1.50	0.93
1:F:641:ASP:H	1:F:647:GLN:HE22	1.12	0.92
1:A:147:GLY:O	1:D:489:ALA:HB1	1.70	0.92
1:D:132:LEU:CD2	1:D:199:TYR:CE1	2.52	0.92
1:D:161:GLU:OE1	1:D:161:GLU:N	2.03	0.92
1:F:243:VAL:HG12	1:F:245:ILE:HD11	1.49	0.92
1:B:534:TRP:N	1:B:651:MET:HE2	1.83	0.92
1:B:588:LYS:NZ	1:B:588:LYS:HB3	1.84	0.91
1:B:616:ARG:HD2	1:B:648:LYS:HE3	1.52	0.91
1:B:626:LEU:CB	1:B:649:TRP:CH2	2.52	0.91
1:D:522:THR:HG21	1:D:527:LEU:HD11	1.51	0.91
1:F:226:THR:CG2	1:F:304:CYS:N	2.32	0.91
1:D:237:LYS:HG3	1:D:238:TYR:CD2	2.06	0.91
1:D:443:ARG:NE	1:D:447:TRP:CZ3	2.38	0.91
1:A:414:GLY:HA2	1:A:415:GLU:CB	1.96	0.91
1:C:474:ASP:O	1:C:477:LYS:HG2	1.71	0.91
1:F:396:ARG:HG2	1:F:396:ARG:HH11	1.36	0.91
1:B:495:ILE:HD12	1:B:498:LEU:HD12	0.93	0.91
1:F:226:THR:HG21	1:F:304:CYS:N	1.86	0.91
1:B:333:ILE:CB	1:B:441:ILE:HD13	2.01	0.91
1:E:514:MET:HE2	1:E:518:ALA:HB3	1.50	0.90
1:A:153:ALA:CB	1:A:190:ASN:HD22	1.78	0.90
1:B:552:THR:HB	1:B:584:GLN:NE2	1.85	0.90
1:E:281:ILE:HD11	1:E:413:GLY:H	1.37	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:619:HIS:NE2	1:B:621:PRO:HG2	1.86	0.90
1:A:147:GLY:C	1:D:489:ALA:HB1	1.97	0.90
1:F:456:VAL:C	1:F:458:SER:HA	1.96	0.89
1:D:248:PHE:CE1	1:D:275:GLU:O	2.24	0.89
1:D:273:ARG:HG2	1:D:273:ARG:HH11	1.34	0.89
1:B:533:ASP:C	1:B:651:MET:HE2	1.96	0.89
1:D:643:SER:HB3	1:D:648:LYS:HZ1	1.22	0.89
1:E:462:LEU:HD11	1:E:487:SER:OG	1.72	0.89
1:B:266:ASN:HD21	1:C:500:LYS:HZ1	1.14	0.89
1:B:616:ARG:CG	1:B:648:LYS:CE	2.50	0.89
1:C:457:GLY:HA2	1:C:459:SER:N	1.88	0.89
1:F:348:GLU:HA	1:F:350:GLY:N	1.87	0.89
1:D:347:ASP:HB3	1:D:348:GLU:CA	2.01	0.89
1:F:258:LEU:O	1:F:262:ILE:HG12	1.71	0.89
1:A:147:GLY:O	1:D:489:ALA:CB	2.21	0.89
1:C:208:THR:CG2	1:C:240:ALA:HB2	2.01	0.89
1:F:641:ASP:H	1:F:647:GLN:NE2	1.70	0.89
1:B:534:TRP:CA	1:B:651:MET:CE	2.52	0.88
1:B:458:SER:HB3	1:B:459:SER:OG	1.71	0.88
1:B:644:LYS:HA	1:B:645:THR:C	1.98	0.88
1:B:626:LEU:O	1:B:649:TRP:CH2	2.26	0.88
1:B:534:TRP:HA	1:B:651:MET:HE3	1.55	0.88
1:F:133:GLY:H	1:F:136:GLU:CG	1.85	0.88
1:F:475:GLU:OE1	1:F:511:LYS:HE2	1.74	0.88
1:A:474:ASP:O	1:A:477:LYS:HG2	1.74	0.88
1:E:474:ASP:O	1:E:477:LYS:HG2	1.74	0.88
1:D:122:TYR:CE1	1:D:203:ASP:HB3	2.08	0.87
1:D:584:GLN:HG3	1:D:598:THR:O	1.73	0.87
1:F:116:LYS:CD	1:F:397:GLU:OE1	2.22	0.87
1:C:485:PRO:O	1:C:488:GLN:HG3	1.74	0.87
1:F:474:ASP:O	1:F:477:LYS:HG2	1.74	0.87
1:B:485:PRO:O	1:B:488:GLN:HG3	1.74	0.87
1:F:215:PHE:CE1	1:F:254:LEU:HD13	2.10	0.87
1:B:608:TRP:HZ3	1:B:626:LEU:CD2	1.82	0.87
1:B:626:LEU:CB	1:B:649:TRP:HH2	1.84	0.87
1:E:624:LYS:HG3	1:E:638:SER:O	1.75	0.87
1:B:474:ASP:O	1:B:477:LYS:HG2	1.75	0.86
1:D:237:LYS:HD2	1:D:238:TYR:CE2	2.10	0.86
1:E:548:SER:O	1:E:551:LYS:HG3	1.74	0.86
1:F:346:GLY:HA2	1:F:366:PRO:HB3	1.56	0.86
1:A:590:ALA:HB1	1:A:591:ASP:HA	1.55	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:485:PRO:O	1:F:488:GLN:HG3	1.74	0.86
1:A:485:PRO:O	1:A:488:GLN:HG3	1.74	0.86
1:F:186:ASP:OD1	1:F:228:HIS:HD2	1.57	0.86
1:A:533:ASP:OD2	1:A:612:LYS:HE2	1.76	0.86
1:C:346:GLY:HA2	1:C:366:PRO:HB3	1.55	0.86
1:D:208:THR:HB	1:D:295:GLN:HG3	1.58	0.86
1:E:556:PHE:CE2	1:E:594:LYS:HD3	2.10	0.86
1:B:495:ILE:HD11	1:B:498:LEU:HD13	1.57	0.86
1:B:616:ARG:HD2	1:B:648:LYS:CE	2.05	0.86
1:D:348:GLU:HA	1:D:350:GLY:N	1.89	0.86
1:D:450:ASN:HB2	1:D:451:PRO:HD2	1.57	0.86
1:F:454:ILE:HD12	1:F:460:PRO:CD	2.04	0.86
1:C:207:LEU:HD23	1:C:319:SER:OG	1.76	0.86
1:F:128:ARG:CG	1:F:201:HIS:CD2	2.56	0.86
1:B:596:MET:HE3	1:B:598:THR:HG23	1.57	0.85
1:F:655:HIS:CA	3:F:809:HOH:O	2.23	0.85
1:B:304:CYS:CB	1:B:439:GLY:O	2.24	0.85
1:B:333:ILE:HB	1:B:441:ILE:HD13	1.58	0.85
1:B:587:THR:HG21	1:B:605:PHE:CD2	2.11	0.85
1:D:258:LEU:CD1	1:D:262:ILE:HD11	2.06	0.85
1:D:443:ARG:CD	1:D:447:TRP:CZ3	2.56	0.85
1:F:454:ILE:HD12	1:F:460:PRO:HD3	1.55	0.85
1:D:166:ILE:HG12	1:D:178:VAL:HG21	1.58	0.85
1:E:143:PRO:HG2	1:E:146:VAL:HG12	1.59	0.85
1:E:276:ARG:HD2	1:E:278:GLU:OE2	1.76	0.85
1:B:626:LEU:C	1:B:649:TRP:CH2	2.54	0.85
1:A:641:ASP:H	1:A:647:GLN:HE22	1.21	0.85
1:C:207:LEU:CD2	1:C:319:SER:OG	2.24	0.85
1:D:208:THR:HG21	1:D:240:ALA:HB2	1.55	0.85
1:E:628:ARG:HG2	1:E:628:ARG:HH11	1.38	0.85
1:B:346:GLY:HA3	1:B:366:PRO:HB3	1.58	0.85
1:D:122:TYR:HE1	1:D:203:ASP:HB3	1.41	0.85
1:D:347:ASP:HB3	1:D:348:GLU:C	2.01	0.85
1:E:513:PHE:CE1	1:E:517:ILE:CD1	2.58	0.84
1:B:601:ASN:HB2	1:B:604:GLU:HG3	1.59	0.84
1:D:600:CYS:SG	1:D:604:GLU:O	2.36	0.84
1:F:632:LEU:H	1:F:632:LEU:HD12	1.42	0.84
1:D:347:ASP:OD2	1:D:351:TYR:HB2	1.76	0.84
1:B:450:ASN:HB2	1:B:451:PRO:HD2	1.57	0.84
1:F:457:GLY:N	1:F:458:SER:HA	1.90	0.84
1:B:122:TYR:CE1	1:B:203:ASP:HB2	2.13	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:253:HIS:CE1	1:F:254:LEU:HD21	2.13	0.84
1:D:332:VAL:HG13	1:D:442:TYR:CD1	2.13	0.84
1:E:413:GLY:HA3	1:E:464:ASN:HD22	1.40	0.84
1:D:625:CYS:SG	1:D:640:CYS:CB	2.66	0.84
1:C:281:ILE:HG12	1:C:415:GLU:HG2	1.60	0.83
1:B:281:ILE:HD11	1:B:413:GLY:H	1.41	0.83
1:F:413:GLY:HA3	1:F:464:ASN:HD22	1.41	0.83
1:B:495:ILE:CD1	1:B:498:LEU:HD13	2.08	0.83
1:F:133:GLY:CA	1:F:136:GLU:HG3	2.08	0.83
1:A:346:GLY:HA3	1:A:366:PRO:HB3	1.60	0.83
1:D:574:ASN:HD22	1:D:578:GLN:HG3	1.43	0.83
1:F:150:GLY:HA3	1:F:183:ILE:HG23	1.60	0.83
1:D:143:PRO:HG2	1:D:146:VAL:HG12	1.59	0.83
1:C:628:ARG:O	1:C:646:THR:HG21	1.78	0.82
1:B:147:GLY:O	1:C:489:ALA:HB1	1.78	0.82
1:B:342:PRO:O	1:D:632:LEU:HD12	1.79	0.82
1:E:457:GLY:HA2	1:E:459:SER:N	1.95	0.82
1:D:173:PHE:CD2	1:D:177:MET:HG3	2.15	0.82
1:E:346:GLY:HA2	1:E:366:PRO:HA	1.59	0.82
1:C:628:ARG:CD	1:C:646:THR:HG22	2.09	0.82
1:D:236:ARG:HG3	1:D:236:ARG:NH1	1.93	0.82
1:B:588:LYS:HD3	1:B:637:ILE:HD11	1.61	0.82
1:B:601:ASN:HB3	1:B:604:GLU:HG3	1.60	0.82
1:F:226:THR:CG2	1:F:304:CYS:O	2.24	0.81
1:E:162:PHE:O	1:E:166:ILE:HG13	1.80	0.81
1:E:545:CYS:SG	1:E:562:CYS:HA	2.19	0.81
1:E:627:ASP:OD1	1:E:646:THR:CB	2.27	0.81
1:F:655:HIS:HA	3:F:809:HOH:O	1.79	0.81
1:B:645:THR:OG1	1:B:646:THR:HA	1.79	0.81
1:B:628:ARG:HG2	1:B:629:SER:N	1.96	0.81
1:E:132:LEU:HD23	1:E:199:TYR:HE1	1.43	0.81
1:B:563:HIS:ND1	1:B:565:MET:HB2	1.96	0.81
1:C:153:ALA:O	1:C:339:GLU:HG2	1.80	0.81
1:F:368:THR:O	1:F:372:LYS:HG3	1.80	0.81
1:F:547:ASP:HB2	1:F:569:GLN:HG2	1.63	0.81
1:C:563:HIS:ND1	1:C:565:MET:HB2	1.96	0.81
1:F:574:ASN:HD22	1:F:578:GLN:CG	1.94	0.81
1:D:563:HIS:ND1	1:D:565:MET:HB2	1.96	0.81
1:B:391:LEU:CD1	1:B:438:VAL:CG2	2.59	0.80
1:B:447:TRP:C	1:B:448:GLN:HE21	1.89	0.80
1:A:347:ASP:HB3	1:A:351:TYR:H	1.47	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:166:ILE:HG23	1:F:176:ASN:HD21	1.42	0.80
1:F:442:TYR:HD1	1:F:443:ARG:H	1.28	0.80
1:B:547:ASP:HB2	1:B:569:GLN:HG2	1.63	0.80
1:E:332:VAL:HG13	1:E:442:TYR:HD2	1.39	0.80
1:E:545:CYS:N	1:E:562:CYS:SG	2.54	0.80
1:A:136:GLU:HG2	3:A:829:HOH:O	1.79	0.80
1:D:443:ARG:HH11	1:D:443:ARG:HG3	1.46	0.80
1:D:611:PHE:CD1	1:E:204:GLU:HB2	2.16	0.80
1:F:133:GLY:HA2	1:F:136:GLU:CG	2.12	0.80
1:F:243:VAL:CG1	1:F:245:ILE:HD11	2.11	0.80
1:C:454:ILE:HD13	1:C:460:PRO:HD3	1.62	0.80
1:F:614:LEU:O	1:F:615:HIS:HB2	1.82	0.80
1:D:584:GLN:HG2	1:D:597:ILE:CG2	2.11	0.80
1:D:547:ASP:HB2	1:D:569:GLN:HG2	1.63	0.80
1:B:614:LEU:O	1:B:615:HIS:HB2	1.79	0.79
1:D:122:TYR:CE1	1:D:203:ASP:CB	2.65	0.79
1:A:547:ASP:HB2	1:A:569:GLN:HG2	1.63	0.79
1:A:563:HIS:ND1	1:A:565:MET:HB2	1.96	0.79
1:A:585:CYS:HB2	1:A:600:CYS:SG	2.22	0.79
1:A:628:ARG:HG2	1:A:649:TRP:CH2	2.17	0.79
1:F:136:GLU:OE1	1:F:138:LYS:HG3	1.82	0.79
1:F:363:LYS:HD2	1:F:525:TYR:CE1	2.17	0.79
1:B:162:PHE:O	1:B:166:ILE:HG13	1.82	0.79
1:B:413:GLY:HA3	1:B:464:ASN:HD22	1.48	0.79
1:E:545:CYS:SG	3:E:806:HOH:O	2.41	0.79
1:A:368:THR:HB	1:A:370:GLN:OE1	1.83	0.78
1:D:522:THR:HG22	1:D:527:LEU:HD12	1.64	0.78
1:F:166:ILE:CG2	1:F:176:ASN:ND2	2.43	0.78
1:F:580:MET:HG2	1:F:585:CYS:SG	2.23	0.78
1:B:538:ARG:O	1:B:649:TRP:CB	2.30	0.78
1:F:655:HIS:CG	3:F:809:HOH:O	2.34	0.78
3:A:813:HOH:O	1:C:631:VAL:CG1	2.30	0.78
1:C:456:VAL:HG22	3:C:810:HOH:O	1.83	0.78
1:E:574:ASN:ND2	1:E:578:GLN:HG3	1.98	0.78
1:E:196:GLU:HG3	3:E:813:HOH:O	1.84	0.78
1:F:226:THR:HG22	1:F:304:CYS:C	2.08	0.78
1:C:207:LEU:HD21	1:C:319:SER:CA	2.14	0.78
1:E:193:ARG:CZ	1:E:435:CYS:O	2.32	0.78
1:B:554:GLY:N	1:B:598:THR:HG22	1.99	0.78
1:B:453:PRO:HB3	1:D:164:GLN:OE1	1.83	0.78
1:B:626:LEU:HD23	1:B:637:ILE:CG2	2.14	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:459:SER:H	1:B:462:LEU:H	1.30	0.78
1:C:574:ASN:HD22	1:C:578:GLN:CG	1.94	0.78
1:C:155:PRO:HB3	1:C:337:THR:CG2	2.14	0.78
1:A:332:VAL:CG1	1:A:442:TYR:CD2	2.58	0.77
1:B:625:CYS:SG	1:B:640:CYS:CB	2.72	0.77
1:B:443:ARG:HH11	1:B:443:ARG:HG3	1.49	0.77
1:C:443:ARG:HG3	1:C:443:ARG:HH11	1.50	0.77
1:E:514:MET:HE2	1:E:518:ALA:CB	2.13	0.77
1:F:444:LEU:N	1:F:444:LEU:HD12	1.99	0.77
1:B:574:ASN:HD22	1:B:578:GLN:CG	1.94	0.77
1:E:513:PHE:CZ	1:E:517:ILE:HD11	2.20	0.77
1:A:628:ARG:HH11	1:A:628:ARG:HG3	1.49	0.77
1:B:474:ASP:O	1:B:477:LYS:CG	2.31	0.77
1:B:348:GLU:N	1:B:349:ASP:O	2.17	0.77
1:F:177:MET:HE1	1:F:221:SER:OG	1.84	0.77
1:B:625:CYS:SG	1:B:647:GLN:NE2	2.58	0.77
1:D:347:ASP:HB3	1:D:348:GLU:HA	1.64	0.77
1:D:258:LEU:HD12	1:D:262:ILE:HD11	1.65	0.77
1:B:191:ASP:OD1	1:B:193:ARG:HG3	1.83	0.77
1:B:596:MET:HE3	1:B:598:THR:HG21	1.67	0.77
1:B:347:ASP:HB3	1:B:351:TYR:H	1.49	0.77
1:D:139:GLU:HG3	1:D:140:PRO:CD	2.14	0.77
1:D:116:LYS:HD2	1:D:401:GLU:OE2	1.85	0.76
1:E:415:GLU:HG2	1:E:416:ASN:N	1.99	0.76
1:D:143:PRO:CG	1:D:146:VAL:HG12	2.15	0.76
1:E:189:VAL:CG1	1:E:340:ILE:HD12	2.15	0.76
1:D:474:ASP:O	1:D:477:LYS:HG2	1.86	0.76
1:E:625:CYS:HG	1:E:640:CYS:HG	0.81	0.76
1:B:321:ASP:HB3	1:B:324:ILE:HG13	1.67	0.76
1:A:128:ARG:HG3	1:A:201:HIS:CD2	2.21	0.76
1:B:586:LEU:N	1:B:586:LEU:HD23	2.01	0.76
1:F:545:CYS:SG	1:F:562:CYS:CB	2.74	0.76
1:C:155:PRO:CB	1:C:337:THR:HG23	2.16	0.76
1:C:113:LEU:N	1:C:113:LEU:HD23	2.01	0.75
1:E:143:PRO:CG	1:E:146:VAL:HG12	2.15	0.75
1:A:332:VAL:HG13	1:A:442:TYR:CE2	2.21	0.75
1:E:189:VAL:HG11	1:E:340:ILE:HD12	1.69	0.75
1:B:585:CYS:HB2	1:B:600:CYS:CB	2.12	0.75
1:B:615:HIS:O	1:B:648:LYS:HB3	1.87	0.75
1:E:624:LYS:CG	1:E:638:SER:C	2.59	0.75
1:D:632:LEU:HD23	1:D:633:HIS:N	2.02	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:132:LEU:HD23	1:E:199:TYR:CE1	2.22	0.75
1:C:132:LEU:HB3	1:C:199:TYR:CE1	2.22	0.75
1:F:143:PRO:HG2	1:F:146:VAL:HG12	1.69	0.75
1:A:166:ILE:HG23	1:A:176:ASN:ND2	2.02	0.75
1:B:534:TRP:CA	1:B:651:MET:HE3	2.13	0.75
1:E:614:LEU:O	1:E:615:HIS:HB2	1.85	0.75
1:F:226:THR:HG22	1:F:304:CYS:H	1.52	0.75
1:D:180:SER:OG	1:D:225:ARG:NH1	2.20	0.74
1:D:208:THR:H	1:D:295:GLN:HE21	1.33	0.74
1:E:176:ASN:HD21	1:E:178:VAL:HG22	1.52	0.74
1:F:348:GLU:CA	1:F:350:GLY:H	1.95	0.74
1:F:175:PHE:CE1	1:F:441:ILE:HG22	2.22	0.74
1:F:563:HIS:ND1	1:F:565:MET:HB2	2.02	0.74
1:A:147:GLY:C	1:D:489:ALA:CB	2.61	0.74
1:A:447:TRP:CD1	1:A:448:GLN:H	2.05	0.74
1:E:454:ILE:HB	1:E:457:GLY:H	1.52	0.74
1:F:172:GLU:HG2	1:F:173:PHE:CD2	2.22	0.74
1:B:601:ASN:CA	1:B:604:GLU:HG3	2.17	0.74
1:D:443:ARG:HD2	1:D:447:TRP:HE3	1.48	0.74
1:F:197:CYS:CB	1:F:435:CYS:SG	2.71	0.74
1:A:281:ILE:HD12	1:A:410:GLN:O	1.88	0.74
1:D:348:GLU:CA	1:D:350:GLY:H	1.99	0.74
1:F:133:GLY:N	1:F:136:GLU:CG	2.44	0.74
1:A:559:LEU:HB3	1:A:633:HIS:HB3	1.70	0.74
1:E:176:ASN:HD21	1:E:178:VAL:CG2	2.00	0.74
1:F:258:LEU:O	1:F:262:ILE:CG1	2.35	0.74
1:F:442:TYR:HD1	1:F:443:ARG:N	1.84	0.74
1:F:228:HIS:O	1:F:231:ILE:HG22	1.87	0.74
1:F:254:LEU:HD23	1:F:254:LEU:N	2.03	0.74
1:D:497:GLU:HG3	3:D:821:HOH:O	1.87	0.73
1:F:195:GLU:OE1	1:F:195:GLU:HA	1.87	0.73
1:A:632:LEU:HD23	3:A:817:HOH:O	1.89	0.73
1:E:628:ARG:HG2	1:E:628:ARG:NH1	1.98	0.73
1:A:147:GLY:HA3	1:D:489:ALA:HB2	1.70	0.73
1:B:266:ASN:HD21	1:C:500:LYS:NZ	1.87	0.73
1:C:456:VAL:O	1:C:459:SER:HB3	1.87	0.73
1:F:268:LEU:O	1:F:268:LEU:HD13	1.88	0.73
1:F:351:TYR:O	1:F:367:LEU:HB2	1.87	0.73
1:B:632:LEU:HD12	1:B:632:LEU:N	2.04	0.73
1:D:456:VAL:CG1	1:D:657:VAL:O	2.36	0.73
1:E:207:LEU:CD1	1:E:319:SER:OG	2.36	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:413:GLY:HA3	1:E:464:ASN:ND2	2.02	0.73
1:E:471:VAL:HB	1:E:495:ILE:HD11	1.70	0.73
1:F:192:LEU:HD12	1:F:331:ASP:OD2	1.88	0.73
1:F:226:THR:HG22	1:F:304:CYS:N	2.03	0.73
1:B:554:GLY:CA	1:B:597:ILE:O	2.23	0.73
1:B:585:CYS:CB	1:B:600:CYS:HB2	2.14	0.73
1:E:363:LYS:CD	1:E:525:TYR:CZ	2.68	0.73
1:A:190:ASN:ND2	1:A:190:ASN:H	1.86	0.73
1:D:347:ASP:HB2	1:D:351:TYR:N	1.99	0.73
1:D:584:GLN:HG3	1:D:598:THR:C	2.13	0.73
1:E:580:MET:HG2	1:E:585:CYS:SG	2.28	0.73
1:A:301:ASP:OD2	1:A:440:HIS:NE2	2.22	0.73
1:A:377:THR:HG22	1:A:379:THR:H	1.54	0.73
1:D:346:GLY:HA2	1:D:366:PRO:HB3	1.69	0.73
1:E:569:GLN:HB2	3:E:806:HOH:O	1.87	0.73
1:B:623:GLY:C	3:B:802:HOH:O	2.32	0.72
1:C:132:LEU:C	1:C:132:LEU:HD12	2.14	0.72
1:E:545:CYS:CA	1:E:562:CYS:HG	2.00	0.72
1:E:556:PHE:HD2	1:E:594:LYS:HD3	1.53	0.72
1:B:391:LEU:CD1	1:B:438:VAL:HG21	2.18	0.72
1:D:176:ASN:HD21	1:D:178:VAL:HG22	1.54	0.72
1:D:611:PHE:CD1	1:E:204:GLU:CB	2.71	0.72
1:E:413:GLY:HA2	1:E:464:ASN:HD22	1.54	0.72
1:D:281:ILE:HD11	1:D:413:GLY:H	1.53	0.72
1:B:628:ARG:HG2	1:B:629:SER:H	1.52	0.72
1:D:231:ILE:HD12	1:D:265:TRP:CD1	2.25	0.72
1:E:176:ASN:ND2	1:E:178:VAL:HG22	2.04	0.72
1:E:614:LEU:CD1	1:E:616:ARG:CZ	2.67	0.72
1:C:627:ASP:CG	1:C:647:GLN:HG2	2.14	0.72
1:D:641:ASP:HB3	1:D:644:LYS:HG2	1.70	0.72
1:E:552:THR:HB	1:E:584:GLN:OE1	1.89	0.72
1:F:454:ILE:N	1:F:455:TYR:HA	2.04	0.72
1:C:371:GLU:HG2	1:C:519:TYR:OH	1.89	0.72
1:E:196:GLU:OE2	1:E:196:GLU:HA	1.87	0.72
1:E:551:LYS:HB3	1:E:551:LYS:NZ	2.05	0.72
1:B:551:LYS:O	1:B:552:THR:CG2	2.37	0.72
1:F:231:ILE:HD13	1:F:231:ILE:C	2.15	0.72
1:F:346:GLY:HA2	1:F:366:PRO:CB	2.20	0.72
1:A:628:ARG:NH1	1:A:646:THR:HA	2.05	0.72
1:E:627:ASP:CG	1:E:647:GLN:HG3	2.14	0.72
1:F:141:GLU:OE2	1:F:142:PRO:HD2	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:ASN:HD22	1:A:578:GLN:CG	2.02	0.72
1:B:333:ILE:HG22	1:B:441:ILE:CD1	2.19	0.72
1:C:264:LEU:O	1:C:265:TRP:HB2	1.90	0.72
1:F:268:LEU:HD13	1:F:268:LEU:C	2.14	0.72
1:B:413:GLY:CA	1:B:464:ASN:HD22	2.02	0.72
1:D:643:SER:HB3	1:D:648:LYS:HZ2	1.50	0.71
1:E:462:LEU:HG	1:E:490:LEU:CD2	2.20	0.71
1:F:215:PHE:HE1	1:F:254:LEU:HD13	1.55	0.71
1:F:627:ASP:OD1	1:F:646:THR:HB	1.89	0.71
1:F:632:LEU:HD12	1:F:632:LEU:N	2.04	0.71
1:B:459:SER:N	1:B:462:LEU:H	1.87	0.71
1:E:193:ARG:HH21	1:E:437:ARG:H	1.36	0.71
1:D:456:VAL:HB	1:D:459:SER:OG	1.89	0.71
1:F:234:THR:HG21	1:F:239:LEU:HG	1.71	0.71
1:A:162:PHE:O	1:A:166:ILE:HG13	1.91	0.71
1:B:122:TYR:CE1	1:B:203:ASP:CB	2.73	0.71
1:B:333:ILE:HG22	1:B:441:ILE:HD13	1.73	0.71
1:B:127:LEU:HD12	1:B:377:THR:HG21	1.73	0.71
1:B:587:THR:CG2	1:B:605:PHE:CD2	2.72	0.71
1:E:456:VAL:HG23	1:E:459:SER:CB	2.21	0.71
1:E:545:CYS:CA	1:E:562:CYS:SG	2.79	0.71
1:F:184:SER:O	1:F:225:ARG:NH2	2.24	0.71
1:A:279:GLY:HA2	1:A:411:ILE:HD12	1.73	0.71
1:A:450:ASN:HD22	1:A:450:ASN:N	1.88	0.71
1:B:266:ASN:ND2	1:C:500:LYS:HZ1	1.89	0.71
1:B:645:THR:N	1:B:646:THR:OG1	2.24	0.71
1:F:166:ILE:O	1:F:170:ILE:HG13	1.91	0.70
1:F:345:GLY:O	1:F:350:GLY:CA	2.39	0.70
1:B:554:GLY:CA	1:B:598:THR:HG22	2.21	0.70
1:E:456:VAL:HG23	1:E:459:SER:HB3	1.73	0.70
1:A:162:PHE:CD1	1:D:455:TYR:HD2	2.09	0.70
1:D:485:PRO:O	1:D:488:GLN:CG	2.39	0.70
1:F:454:ILE:HG21	1:F:458:SER:O	1.92	0.70
1:D:166:ILE:HG23	1:D:176:ASN:ND2	2.06	0.70
1:E:224:MET:HE1	1:E:258:LEU:HD11	1.72	0.70
1:F:255:LYS:HB2	1:F:256:GLU:OE2	1.92	0.70
1:A:346:GLY:HA2	3:A:822:HOH:O	1.92	0.70
1:D:614:LEU:O	1:D:615:HIS:HB2	1.89	0.70
1:D:161:GLU:H	1:D:161:GLU:CD	1.97	0.70
1:A:136:GLU:OE2	1:A:193:ARG:NH2	2.24	0.70
1:F:655:HIS:CB	3:F:809:HOH:O	2.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:628:ARG:HH11	1:C:646:THR:HG22	1.56	0.70
1:F:413:GLY:CA	1:F:464:ASN:HD22	2.05	0.70
1:E:120:PHE:CZ	1:E:207:LEU:HD11	2.27	0.69
1:F:215:PHE:HE1	1:F:254:LEU:CD1	2.04	0.69
1:C:372:LYS:HE3	1:C:378:LYS:NZ	2.04	0.69
1:E:632:LEU:HD12	1:E:632:LEU:N	2.04	0.69
1:C:628:ARG:NH1	1:C:646:THR:HA	2.07	0.69
1:E:540:PHE:O	1:E:542:THR:HG23	1.92	0.69
1:F:258:LEU:HD22	1:F:262:ILE:CD1	2.18	0.69
1:A:455:TYR:CB	1:A:456:VAL:HG23	2.20	0.69
1:F:228:HIS:O	1:F:231:ILE:CG2	2.40	0.69
1:C:422:LYS:HG2	1:C:472:TRP:CZ2	2.28	0.69
1:E:120:PHE:HZ	1:E:207:LEU:CD1	2.06	0.69
1:A:162:PHE:CE1	1:D:455:TYR:HD2	2.11	0.69
1:A:190:ASN:HD22	1:A:190:ASN:H	1.41	0.69
1:A:422:LYS:HG2	1:A:472:TRP:CZ2	2.28	0.69
1:A:456:VAL:HG13	1:A:458:SER:HB2	1.73	0.69
1:B:527:LEU:N	1:B:527:LEU:HD12	2.08	0.69
1:C:207:LEU:CD2	1:C:207:LEU:H	2.05	0.69
1:E:193:ARG:NH2	1:E:436:SER:HA	2.07	0.69
1:F:377:THR:OG1	1:F:380:GLU:HG2	1.91	0.69
1:B:422:LYS:HG2	1:B:472:TRP:CZ2	2.28	0.69
1:B:585:CYS:C	1:B:586:LEU:HD23	2.18	0.69
1:E:411:ILE:HD13	1:E:411:ILE:N	2.08	0.69
1:A:347:ASP:HB3	1:A:351:TYR:N	2.08	0.69
1:C:196:GLU:CB	3:C:801:HOH:O	2.40	0.68
1:D:237:LYS:HG3	1:D:238:TYR:CE2	2.27	0.68
1:B:548:SER:HB2	1:B:581:GLN:HE22	1.58	0.68
1:B:625:CYS:N	1:B:640:CYS:SG	2.66	0.68
1:A:584:GLN:HG2	1:A:598:THR:O	1.92	0.68
1:C:632:LEU:H	1:C:632:LEU:CD1	1.93	0.68
1:E:372:LYS:C	1:E:372:LYS:HD3	2.19	0.68
1:F:422:LYS:HG2	1:F:472:TRP:CZ2	2.28	0.68
1:E:166:ILE:O	1:E:170:ILE:HG13	1.93	0.68
1:E:454:ILE:HD13	1:E:457:GLY:HA3	1.75	0.68
1:D:171:LYS:HG2	1:D:448:GLN:NE2	2.09	0.68
1:D:271:VAL:CG2	1:D:273:ARG:HH12	2.06	0.68
1:D:422:LYS:HG2	1:D:472:TRP:CZ2	2.28	0.68
1:E:646:THR:O	1:E:647:GLN:HB2	1.94	0.68
1:C:527:LEU:HD12	1:C:527:LEU:N	2.08	0.68
1:E:224:MET:CE	1:E:258:LEU:CD1	2.71	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:136:GLU:OE1	1:F:138:LYS:N	2.27	0.68
1:F:164:GLN:OE1	1:F:164:GLN:HA	1.93	0.68
1:B:574:ASN:ND2	1:B:578:GLN:HG3	2.03	0.68
1:B:601:ASN:CB	1:B:604:GLU:CG	2.65	0.68
1:D:128:ARG:HG3	1:D:201:HIS:CD2	2.29	0.68
1:F:253:HIS:ND1	1:F:254:LEU:CD2	2.57	0.68
1:A:414:GLY:CA	1:A:415:GLU:HB3	2.12	0.68
1:F:627:ASP:OD1	1:F:628:ARG:N	2.26	0.68
1:C:628:ARG:HD3	1:C:646:THR:HG22	1.76	0.68
1:D:273:ARG:HG2	1:D:273:ARG:NH1	2.05	0.68
1:F:255:LYS:O	1:F:256:GLU:HB2	1.94	0.68
1:A:646:THR:O	1:A:647:GLN:HB2	1.92	0.67
1:C:122:TYR:CE1	1:C:203:ASP:HB3	2.29	0.67
1:C:474:ASP:O	1:C:477:LYS:CG	2.40	0.67
1:F:133:GLY:CA	1:F:136:GLU:CG	2.68	0.67
1:A:474:ASP:O	1:A:477:LYS:CG	2.42	0.67
1:D:586:LEU:HD22	1:D:597:ILE:HG12	1.76	0.67
1:F:122:TYR:CZ	1:F:203:ASP:HB3	2.30	0.67
1:B:535:GLY:HA3	1:B:652:ASN:O	1.94	0.67
1:C:116:LYS:CE	1:C:397:GLU:OE1	2.37	0.67
1:D:208:THR:HB	1:D:295:GLN:CG	2.25	0.67
1:D:258:LEU:HD11	1:D:262:ILE:HD11	1.75	0.67
1:B:620:ILE:HG22	1:B:621:PRO:HD3	1.75	0.67
1:D:527:LEU:HD12	1:D:527:LEU:N	2.08	0.67
1:E:422:LYS:HG2	1:E:472:TRP:CZ2	2.29	0.67
1:D:138:LYS:H	1:D:138:LYS:CD	2.07	0.67
1:E:527:LEU:CD1	1:E:527:LEU:H	2.07	0.67
1:F:301:ASP:OD2	1:F:440:HIS:NE2	2.27	0.67
1:A:414:GLY:HA2	1:A:415:GLU:OE2	1.94	0.67
1:D:347:ASP:CB	1:D:351:TYR:H	2.04	0.67
1:A:348:GLU:HA	1:A:348:GLU:OE1	1.94	0.67
1:B:230:VAL:O	1:B:231:ILE:HG23	1.95	0.67
1:E:545:CYS:N	1:E:562:CYS:HG	1.91	0.67
1:C:509:SER:HB2	3:C:839:HOH:O	1.95	0.67
1:E:527:LEU:N	1:E:527:LEU:HD12	2.08	0.67
1:B:230:VAL:C	1:B:231:ILE:HG23	2.20	0.67
1:B:454:ILE:HG13	1:B:454:ILE:O	1.92	0.67
1:B:626:LEU:CA	1:B:649:TRP:HH2	2.07	0.67
1:C:628:ARG:HD2	1:C:646:THR:HG22	1.75	0.67
1:E:406:ASP:CG	1:E:498:LEU:HD21	2.20	0.67
1:D:235:PRO:HB2	1:D:238:TYR:CD2	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:585:CYS:HB2	1:F:600:CYS:SG	2.28	0.67
1:A:447:TRP:O	1:A:448:GLN:HG2	1.95	0.66
1:A:454:ILE:HD12	1:A:454:ILE:C	2.19	0.66
1:B:391:LEU:HD13	1:B:438:VAL:CG2	2.20	0.66
1:E:120:PHE:HZ	1:E:207:LEU:HD11	1.58	0.66
1:D:279:GLY:HA2	1:D:411:ILE:HD12	1.77	0.66
1:E:166:ILE:HG12	1:E:178:VAL:CG2	2.25	0.66
1:E:484:ARG:CG	1:E:484:ARG:HH11	2.08	0.66
1:F:573:ILE:HD11	1:F:610:TYR:CD2	2.30	0.66
1:B:619:HIS:HE2	1:B:621:PRO:HG2	1.58	0.66
1:B:627:ASP:OD1	1:B:628:ARG:N	2.28	0.66
1:B:347:ASP:HB3	1:B:349:ASP:O	1.95	0.66
1:B:580:MET:HG2	1:B:585:CYS:SG	2.35	0.66
1:B:616:ARG:HG3	1:B:648:LYS:HE3	1.72	0.66
1:C:196:GLU:HB3	3:C:801:HOH:O	1.94	0.66
1:D:643:SER:CB	1:D:648:LYS:NZ	2.50	0.66
1:C:573:ILE:HD11	1:C:610:TYR:CD2	2.30	0.66
1:D:443:ARG:CZ	1:D:447:TRP:CZ3	2.78	0.66
1:A:203:ASP:C	1:A:204:GLU:HG3	2.19	0.66
1:D:241:GLU:HG3	1:D:243:VAL:HG23	1.77	0.66
1:D:413:GLY:HA3	1:D:464:ASN:HD22	1.61	0.66
1:E:576:ALA:O	1:E:606:LYS:HB2	1.96	0.66
1:F:396:ARG:HG2	1:F:396:ARG:NH1	2.04	0.66
1:F:474:ASP:O	1:F:477:LYS:CG	2.42	0.66
1:C:195:GLU:OE2	1:C:198:LYS:HE2	1.96	0.66
1:C:642:SER:O	1:C:643:SER:OG	2.08	0.66
1:D:563:HIS:CE1	1:D:565:MET:HB2	2.31	0.66
1:B:533:ASP:C	1:B:651:MET:CE	2.68	0.66
1:D:190:ASN:HD22	1:D:190:ASN:N	1.94	0.66
1:A:457:GLY:HA2	1:A:463:LYS:NZ	2.11	0.65
1:A:563:HIS:CE1	1:A:565:MET:HB2	2.31	0.65
1:A:583:ASP:OD2	1:A:599:HIS:HD2	1.78	0.65
1:C:563:HIS:CE1	1:C:565:MET:HB2	2.31	0.65
1:D:241:GLU:HB2	1:D:270:LYS:NZ	2.12	0.65
1:E:529:PRO:HG2	1:E:574:ASN:ND2	2.10	0.65
1:E:609:GLN:CD	1:E:611:PHE:CZ	2.74	0.65
1:B:534:TRP:O	1:B:653:ASN:ND2	2.29	0.65
1:B:603:ASN:CB	1:B:606:LYS:HE2	2.26	0.65
1:B:617:PHE:CB	1:B:626:LEU:HD12	2.26	0.65
1:F:258:LEU:HD22	1:F:258:LEU:O	1.97	0.65
1:B:563:HIS:CE1	1:B:565:MET:HB2	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:139:GLU:OE1	1:F:139:GLU:HA	1.96	0.65
1:A:363:LYS:HD2	1:A:525:TYR:CZ	2.32	0.65
1:C:632:LEU:HD12	1:C:632:LEU:N	2.04	0.65
1:E:241:GLU:OE1	1:E:270:LYS:HE3	1.96	0.65
1:B:534:TRP:CA	1:B:651:MET:HE2	2.24	0.65
1:E:132:LEU:CD2	1:E:199:TYR:CE1	2.79	0.65
1:D:237:LYS:CD	1:D:238:TYR:CE2	2.80	0.65
1:D:220:TRP:HZ2	1:D:261:TYR:CD2	2.15	0.64
1:B:347:ASP:HB2	1:B:351:TYR:O	1.97	0.64
1:B:472:TRP:CZ3	1:B:502:ARG:HG3	2.31	0.64
1:B:620:ILE:HB	1:B:621:PRO:CD	2.27	0.64
1:F:231:ILE:HD13	1:F:231:ILE:O	1.96	0.64
1:B:279:GLY:HA2	1:B:411:ILE:HD12	1.79	0.64
1:D:349:ASP:OD1	1:D:349:ASP:N	2.23	0.64
1:E:377:THR:OG1	1:E:380:GLU:HG2	1.97	0.64
1:C:281:ILE:HD11	1:C:413:GLY:H	1.60	0.64
1:C:467:ARG:O	1:C:471:VAL:HG12	1.98	0.64
1:D:454:ILE:CG2	1:D:459:SER:OG	2.46	0.64
1:E:190:ASN:HD22	1:E:190:ASN:C	2.05	0.64
1:E:346:GLY:HA2	1:E:366:PRO:CA	2.26	0.64
1:F:641:ASP:N	1:F:647:GLN:HE22	1.89	0.64
1:B:588:LYS:HB3	1:B:588:LYS:HZ1	1.60	0.64
1:D:136:GLU:CD	1:D:193:ARG:HH22	2.04	0.64
1:E:224:MET:HE1	1:E:258:LEU:CD1	2.28	0.64
1:A:561:PRO:HG3	1:C:337:THR:HG21	1.77	0.64
1:B:259:ASP:OD2	1:B:273:ARG:NH2	2.30	0.64
1:D:241:GLU:HB2	1:D:270:LYS:HZ3	1.63	0.64
1:D:574:ASN:HD22	1:D:578:GLN:CG	2.10	0.64
1:E:641:ASP:O	1:E:642:SER:HB3	1.96	0.64
1:B:620:ILE:CB	1:B:621:PRO:CD	2.76	0.64
1:D:467:ARG:O	1:D:471:VAL:HG12	1.98	0.64
1:F:454:ILE:CG2	1:F:460:PRO:HD3	2.28	0.64
1:B:189:VAL:HG13	1:B:340:ILE:HD12	1.79	0.64
1:B:601:ASN:HB3	1:B:604:GLU:CG	2.26	0.64
1:B:641:ASP:O	1:B:642:SER:HB3	1.96	0.64
1:F:187:ARG:NE	1:F:225:ARG:HH12	1.96	0.64
1:F:444:LEU:N	1:F:444:LEU:CD1	2.61	0.64
1:B:616:ARG:HG2	1:B:648:LYS:HG2	1.80	0.64
1:E:467:ARG:O	1:E:471:VAL:HG12	1.98	0.64
1:F:207:LEU:HD11	1:F:319:SER:HA	1.80	0.64
1:C:371:GLU:OE2	1:C:383:ARG:NH2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:276:ARG:CD	1:E:278:GLU:OE2	2.46	0.64
1:C:454:ILE:HD13	1:C:460:PRO:CD	2.28	0.63
1:D:371:GLU:O	1:D:375:ARG:HG2	1.97	0.63
1:F:345:GLY:O	1:F:350:GLY:HA2	1.98	0.63
1:A:132:LEU:HD22	1:A:199:TYR:CE1	2.31	0.63
1:C:155:PRO:CD	1:C:339:GLU:HG3	2.21	0.63
1:B:132:LEU:HG	1:B:136:GLU:OE1	1.98	0.63
1:E:563:HIS:ND1	1:E:565:MET:HB2	2.14	0.63
1:F:574:ASN:HB2	1:F:578:GLN:H	1.64	0.63
1:A:414:GLY:HA3	1:A:416:ASN:H	1.63	0.63
1:A:467:ARG:O	1:A:471:VAL:HG12	1.98	0.63
1:B:587:THR:CG2	1:B:605:PHE:CG	2.80	0.63
1:F:467:ARG:O	1:F:471:VAL:HG12	1.98	0.63
1:B:467:ARG:O	1:B:471:VAL:HG12	1.98	0.63
1:A:632:LEU:HA	1:C:341:ILE:HG23	1.78	0.63
1:B:609:GLN:NE2	1:B:611:PHE:HZ	1.96	0.63
1:B:624:LYS:N	3:B:802:HOH:O	2.31	0.63
1:C:173:PHE:CD2	1:C:177:MET:HG3	2.34	0.63
1:C:255:LYS:O	1:C:256:GLU:HB2	1.99	0.63
1:D:237:LYS:HD2	1:D:238:TYR:CZ	2.33	0.63
1:D:456:VAL:HG12	1:D:458:SER:H	1.62	0.63
1:E:494:ASP:CG	1:E:496:SER:HG	2.07	0.63
1:B:626:LEU:HB2	1:B:649:TRP:HH2	1.39	0.63
1:C:136:GLU:CD	1:C:193:ARG:HH12	2.06	0.63
1:C:231:ILE:HD12	1:C:265:TRP:NE1	2.14	0.63
1:A:207:LEU:HD11	1:A:319:SER:HA	1.80	0.62
1:C:208:THR:HB	1:C:295:GLN:HG3	1.80	0.62
1:E:255:LYS:O	1:E:256:GLU:HB2	1.99	0.62
1:E:370:GLN:H	1:E:370:GLN:CD	2.05	0.62
1:F:272:PHE:CD2	1:F:290:LYS:HB3	2.33	0.62
1:A:641:ASP:O	1:A:647:GLN:NE2	2.32	0.62
1:D:522:THR:CG2	1:D:527:LEU:CD1	2.51	0.62
1:B:551:LYS:C	1:B:552:THR:HG23	2.24	0.62
1:D:166:ILE:HG12	1:D:178:VAL:CG2	2.28	0.62
1:A:116:LYS:O	1:A:322:ARG:NH2	2.33	0.62
1:B:395:GLU:OE1	1:B:397:GLU:HG3	2.00	0.62
1:C:412:TRP:O	1:C:461:THR:HG23	2.00	0.62
1:D:235:PRO:HB2	1:D:238:TYR:HD2	1.63	0.62
1:D:333:ILE:HG12	1:D:340:ILE:HG12	1.81	0.62
1:E:276:ARG:HH11	1:E:276:ARG:CG	2.13	0.62
1:F:227:VAL:O	1:F:230:VAL:HG22	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:346:GLY:HA2	1:F:366:PRO:CA	2.29	0.62
1:F:353:ARG:NH2	1:F:520:ASP:OD2	2.30	0.62
1:B:602:LEU:HD22	1:B:603:ASN:HA	1.82	0.62
1:D:171:LYS:HD3	1:D:448:GLN:NE2	2.09	0.62
1:D:271:VAL:HG22	1:D:273:ARG:HH12	1.64	0.62
1:E:128:ARG:HG3	1:E:201:HIS:CD2	2.34	0.62
1:E:193:ARG:HH12	1:E:309:ASN:C	2.06	0.62
1:F:183:ILE:HG21	1:F:225:ARG:NH1	2.14	0.62
1:F:258:LEU:O	1:F:262:ILE:CD1	2.47	0.62
1:F:574:ASN:ND2	1:F:578:GLN:HG3	2.03	0.62
1:E:193:ARG:HG2	1:E:437:ARG:HD2	1.80	0.62
1:E:483:SER:C	1:E:485:PRO:HD3	2.24	0.62
1:F:190:ASN:C	1:F:190:ASN:HD22	2.05	0.62
1:A:455:TYR:O	1:A:455:TYR:HD1	1.82	0.62
1:B:333:ILE:HG12	1:B:340:ILE:HG12	1.81	0.62
1:E:540:PHE:CD2	1:E:541:GLU:HG3	2.35	0.62
1:C:206:LEU:HD13	1:C:206:LEU:N	2.14	0.62
1:C:627:ASP:CB	1:C:647:GLN:HG2	2.30	0.62
1:A:122:TYR:OH	1:A:206:LEU:CD2	2.48	0.62
1:E:454:ILE:HB	1:E:457:GLY:N	2.13	0.62
1:C:527:LEU:CD1	1:C:527:LEU:H	2.13	0.61
1:C:574:ASN:HB2	1:C:578:GLN:H	1.64	0.61
1:E:333:ILE:HG12	1:E:340:ILE:HG12	1.81	0.61
1:F:347:ASP:HB3	3:F:804:HOH:O	2.00	0.61
1:A:255:LYS:O	1:A:256:GLU:HB2	1.99	0.61
1:B:574:ASN:HB2	1:B:578:GLN:H	1.64	0.61
1:E:551:LYS:HB3	1:E:551:LYS:HZ2	1.65	0.61
1:F:220:TRP:CZ3	1:F:257:LYS:HG2	2.34	0.61
1:B:547:ASP:CB	1:B:569:GLN:HG2	2.31	0.61
1:E:363:LYS:HD3	1:E:525:TYR:OH	2.00	0.61
1:C:347:ASP:HB3	1:C:351:TYR:H	1.65	0.61
1:D:354:GLY:HA3	1:D:362:TRP:CH2	2.35	0.61
1:E:252:GLU:OE1	1:E:255:LYS:HE3	2.00	0.61
1:A:333:ILE:HG12	1:A:340:ILE:HG12	1.81	0.61
1:A:627:ASP:OD1	1:A:646:THR:HB	2.01	0.61
1:F:333:ILE:HG12	1:F:340:ILE:HG12	1.81	0.61
1:A:628:ARG:HD2	1:A:646:THR:HG22	1.83	0.61
1:F:211:VAL:HG22	1:F:242:ILE:HG12	1.83	0.61
1:B:255:LYS:O	1:B:256:GLU:HB2	2.00	0.61
1:C:118:GLN:OE1	1:C:120:PHE:HB3	1.99	0.61
1:C:241:GLU:HB2	1:C:270:LYS:NZ	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:456:VAL:O	1:C:459:SER:CB	2.47	0.61
1:D:527:LEU:CD1	1:D:527:LEU:H	2.13	0.61
1:D:547:ASP:CB	1:D:569:GLN:HG2	2.30	0.61
1:E:552:THR:HB	1:E:553:ASN:OD1	1.99	0.61
1:F:258:LEU:HD23	1:F:262:ILE:HD11	1.77	0.61
1:A:162:PHE:CD1	1:D:455:TYR:CD2	2.88	0.61
1:C:190:ASN:HD22	1:C:190:ASN:C	2.05	0.61
1:C:203:ASP:O	1:C:204:GLU:CB	2.34	0.61
1:D:136:GLU:OE1	1:D:193:ARG:NH2	2.29	0.61
1:E:413:GLY:CA	1:E:464:ASN:ND2	2.55	0.61
1:E:619:HIS:CE1	1:E:621:PRO:HG2	2.36	0.61
1:A:619:HIS:CE1	1:A:621:PRO:HG2	2.36	0.61
1:B:629:SER:N	1:B:634:GLN:O	2.33	0.61
1:C:132:LEU:HB3	1:C:199:TYR:HE1	1.63	0.61
1:C:207:LEU:HD21	1:C:319:SER:CB	2.31	0.61
1:E:281:ILE:HD11	1:E:413:GLY:N	2.11	0.61
1:A:211:VAL:HG22	1:A:242:ILE:HG12	1.83	0.61
1:D:610:TYR:OH	1:D:612:LYS:HD2	2.01	0.61
1:F:253:HIS:H	1:F:253:HIS:CD2	2.19	0.61
1:A:122:TYR:CZ	1:A:206:LEU:HD23	2.36	0.60
1:A:451:PRO:HB2	1:A:452:PRO:HD2	1.81	0.60
1:B:551:LYS:O	1:B:552:THR:HG22	2.01	0.60
1:E:264:LEU:O	1:E:265:TRP:HB2	2.00	0.60
1:F:253:HIS:ND1	1:F:254:LEU:HD23	2.15	0.60
1:F:619:HIS:CE1	1:F:621:PRO:HG2	2.36	0.60
1:F:657:VAL:O	1:F:657:VAL:HG12	2.00	0.60
1:A:207:LEU:HD12	1:A:207:LEU:N	2.16	0.60
1:A:592:GLY:HA3	3:A:820:HOH:O	2.00	0.60
1:A:614:LEU:O	1:A:615:HIS:HB2	2.01	0.60
1:E:207:LEU:N	1:E:207:LEU:HD12	2.16	0.60
1:E:495:ILE:O	1:E:495:ILE:HG13	2.01	0.60
1:E:627:ASP:HB2	1:E:647:GLN:HG2	1.78	0.60
1:F:175:PHE:CE1	1:F:441:ILE:CG2	2.84	0.60
1:A:118:GLN:NE2	1:A:322:ARG:H	1.99	0.60
1:B:211:VAL:HG22	1:B:242:ILE:HG12	1.83	0.60
1:D:172:GLU:HG2	1:D:251:LYS:NZ	2.17	0.60
1:E:207:LEU:HD11	1:E:319:SER:HA	1.82	0.60
1:E:551:LYS:HE3	1:E:555:GLY:CA	2.32	0.60
1:A:208:THR:OG1	1:A:295:GLN:HG3	2.02	0.60
1:C:179:ALA:O	1:C:180:SER:C	2.43	0.60
1:C:619:HIS:CE1	1:C:621:PRO:HG2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:161:GLU:HG2	1:F:162:PHE:N	2.16	0.60
1:B:175:PHE:CE1	1:B:441:ILE:HG22	2.37	0.60
1:C:628:ARG:HD3	1:C:646:THR:CG2	2.31	0.60
1:E:605:PHE:C	1:E:607:GLU:HG3	2.26	0.60
1:E:605:PHE:HA	1:E:607:GLU:OE2	2.02	0.60
1:F:547:ASP:CB	1:F:569:GLN:HG2	2.30	0.60
1:B:458:SER:C	1:B:462:LEU:HB3	2.26	0.60
1:C:573:ILE:CD1	1:C:610:TYR:CD2	2.84	0.60
1:E:211:VAL:HG22	1:E:242:ILE:HG12	1.83	0.60
1:C:211:VAL:HG22	1:C:242:ILE:HG12	1.83	0.60
1:C:372:LYS:CE	1:C:378:LYS:HZ1	2.09	0.60
1:D:208:THR:HG22	1:D:240:ALA:HB2	1.81	0.60
1:E:456:VAL:O	1:E:459:SER:HB3	2.01	0.60
1:E:641:ASP:HB3	1:E:644:LYS:HD2	1.82	0.60
1:B:527:LEU:H	1:B:527:LEU:CD1	2.13	0.60
1:C:122:TYR:HE1	1:C:203:ASP:HB3	1.66	0.60
1:C:631:VAL:O	1:C:631:VAL:HG23	2.02	0.60
1:E:173:PHE:CD2	1:E:177:MET:HG3	2.36	0.60
1:F:253:HIS:CE1	1:F:254:LEU:CD2	2.84	0.60
1:A:547:ASP:CB	1:A:569:GLN:HG2	2.31	0.60
1:A:554:GLY:N	1:A:597:ILE:O	2.24	0.60
1:B:150:GLY:CA	1:B:183:ILE:HG23	2.28	0.60
1:B:459:SER:H	1:B:462:LEU:N	1.99	0.60
1:B:649:TRP:HE3	1:B:649:TRP:H	1.50	0.60
1:C:347:ASP:HB2	1:C:351:TYR:O	2.02	0.60
1:D:619:HIS:CE1	1:D:621:PRO:HG2	2.36	0.60
1:F:611:PHE:HE1	1:F:618:THR:CG2	2.14	0.60
1:A:574:ASN:HB2	1:A:578:GLN:H	1.65	0.60
1:B:264:LEU:HD22	1:B:265:TRP:N	2.17	0.60
1:E:208:THR:OG1	1:E:295:GLN:HG3	2.02	0.60
1:F:573:ILE:CD1	1:F:610:TYR:CD2	2.84	0.60
1:B:538:ARG:C	1:B:649:TRP:HB3	2.25	0.59
1:D:346:GLY:HA2	1:D:366:PRO:CB	2.30	0.59
1:E:207:LEU:HD13	1:E:319:SER:OG	2.02	0.59
1:A:246:ASP:OD1	1:A:249:SER:OG	2.20	0.59
1:B:459:SER:H	1:B:461:THR:N	1.99	0.59
1:B:577:ASN:HB2	1:B:606:LYS:HB3	1.83	0.59
1:C:614:LEU:O	1:C:615:HIS:HB2	2.01	0.59
1:D:138:LYS:N	1:D:138:LYS:HD2	2.16	0.59
1:F:193:ARG:NH2	1:F:308:VAL:CG2	2.66	0.59
1:B:450:ASN:CB	1:B:451:PRO:HD2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:ASP:OD2	1:D:205:ASN:HB2	2.02	0.59
1:E:540:PHE:CD2	1:E:541:GLU:CG	2.85	0.59
1:C:449:GLY:C	3:C:806:HOH:O	2.45	0.59
1:D:412:TRP:O	1:D:461:THR:HG23	2.02	0.59
1:F:590:ALA:HB1	1:F:591:ASP:HA	1.83	0.59
1:F:641:ASP:O	1:F:642:SER:HB3	2.01	0.59
1:A:118:GLN:HE22	1:A:322:ARG:N	1.99	0.59
1:A:349:ASP:OD2	1:A:378:LYS:HE3	2.02	0.59
1:C:347:ASP:CB	1:C:351:TYR:H	2.15	0.59
1:D:395:GLU:OE1	1:D:397:GLU:HB3	2.03	0.59
1:F:351:TYR:O	1:F:367:LEU:CB	2.49	0.59
1:B:588:LYS:HB3	1:B:588:LYS:HZ2	1.66	0.59
1:B:641:ASP:HB3	1:B:643:SER:HB3	1.84	0.59
1:C:443:ARG:HH11	1:C:443:ARG:CG	2.14	0.59
1:D:191:ASP:OD1	1:D:193:ARG:HD3	2.03	0.59
1:F:136:GLU:OE2	1:F:138:LYS:CG	2.41	0.59
1:F:187:ARG:NE	1:F:225:ARG:NH1	2.51	0.59
1:B:552:THR:HB	1:B:584:GLN:CD	2.28	0.59
1:B:588:LYS:CD	1:B:637:ILE:HD11	2.33	0.59
1:D:346:GLY:HA2	1:D:366:PRO:CA	2.32	0.59
1:E:276:ARG:HH11	1:E:276:ARG:HG3	1.67	0.59
1:E:564:ARG:H	1:E:569:GLN:HE22	1.49	0.59
1:A:262:ILE:HD13	1:A:265:TRP:HZ3	1.66	0.59
1:C:143:PRO:HG3	1:C:146:VAL:HB	1.85	0.59
1:C:625:CYS:HG	1:C:640:CYS:CB	2.06	0.59
1:D:255:LYS:O	1:D:256:GLU:HB2	2.01	0.59
1:A:118:GLN:NE2	1:A:321:ASP:HA	2.17	0.59
1:A:574:ASN:ND2	1:A:578:GLN:HG3	2.09	0.59
1:B:527:LEU:N	1:B:527:LEU:CD1	2.66	0.59
1:C:281:ILE:HD11	1:C:413:GLY:N	2.18	0.59
1:C:527:LEU:N	1:C:527:LEU:CD1	2.66	0.59
1:C:574:ASN:ND2	1:C:578:GLN:HG3	2.03	0.59
1:D:150:GLY:HA3	1:D:183:ILE:HG23	1.85	0.59
1:A:584:GLN:HB3	1:A:597:ILE:CG2	2.32	0.58
1:C:155:PRO:HB3	1:C:337:THR:HG23	1.79	0.58
1:C:231:ILE:HD12	1:C:265:TRP:CD1	2.38	0.58
1:C:335:GLY:HA3	1:C:444:LEU:HD21	1.85	0.58
1:A:169:SER:HB2	1:A:177:MET:HB2	1.84	0.58
1:A:231:ILE:HD12	1:A:265:TRP:NE1	2.18	0.58
1:B:116:LYS:O	1:B:322:ARG:NH2	2.36	0.58
1:C:410:GLN:O	1:C:411:ILE:CG2	2.50	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:LEU:HD12	1:D:504:ASP:HB3	1.85	0.58
1:F:208:THR:OG1	1:F:295:GLN:HG3	2.02	0.58
1:F:243:VAL:CG1	1:F:245:ILE:CD1	2.73	0.58
1:F:410:GLN:O	1:F:464:ASN:ND2	2.34	0.58
1:B:156:LEU:HD22	1:B:158:LEU:HD21	1.85	0.58
1:B:412:TRP:HE3	1:B:461:THR:HG21	1.68	0.58
1:B:632:LEU:HD12	1:B:632:LEU:H	1.68	0.58
1:D:208:THR:CB	1:D:295:GLN:HG3	2.33	0.58
1:D:450:ASN:HB2	1:D:451:PRO:CD	2.32	0.58
1:A:590:ALA:HB1	1:A:591:ASP:CA	2.30	0.58
1:D:548:SER:O	1:D:551:LYS:HB2	2.04	0.58
1:E:544:TYR:C	1:E:562:CYS:SG	2.87	0.58
1:F:641:ASP:O	1:F:643:SER:N	2.34	0.58
1:D:246:ASP:O	1:D:274:ASN:HB2	2.03	0.58
1:E:192:LEU:HD12	1:E:331:ASP:OD2	2.03	0.58
1:E:260:GLU:O	1:E:263:LYS:HB2	2.03	0.58
1:E:527:LEU:H	1:E:527:LEU:HD12	1.66	0.58
1:B:322:ARG:HD2	1:B:395:GLU:OE2	2.03	0.58
1:C:207:LEU:CD2	1:C:319:SER:CB	2.80	0.58
1:E:533:ASP:OD2	1:E:612:LYS:NZ	2.35	0.58
1:D:162:PHE:O	1:D:166:ILE:HG13	2.03	0.58
1:D:271:VAL:HG22	1:D:273:ARG:NH1	2.19	0.58
1:B:616:ARG:HG3	1:B:648:LYS:CE	2.32	0.58
1:C:539:GLY:HA3	1:C:628:ARG:HH21	1.69	0.58
1:D:125:PRO:HB3	1:D:202:TYR:HD1	1.69	0.58
1:B:166:ILE:HG23	1:B:176:ASN:OD1	2.03	0.58
1:C:192:LEU:HD12	1:C:331:ASP:OD2	2.04	0.58
1:D:231:ILE:HD12	1:D:265:TRP:NE1	2.19	0.58
1:E:231:ILE:HD12	1:E:265:TRP:NE1	2.19	0.58
1:A:456:VAL:CG1	1:A:458:SER:HB3	2.27	0.58
1:D:450:ASN:CB	1:D:451:PRO:HD2	2.32	0.58
1:E:235:PRO:HB2	1:E:238:TYR:HD2	1.68	0.58
1:F:137:PRO:O	1:F:138:LYS:HB2	2.04	0.58
1:A:457:GLY:HA2	1:A:463:LYS:HZ3	1.69	0.57
3:A:813:HOH:O	1:C:631:VAL:HG11	2.01	0.57
1:F:187:ARG:CD	1:F:225:ARG:HH12	2.17	0.57
1:A:153:ALA:CB	1:A:190:ASN:HD21	2.14	0.57
1:D:169:SER:HB2	1:D:177:MET:HB2	1.86	0.57
1:E:471:VAL:HG13	1:E:472:TRP:CD1	2.38	0.57
1:E:498:LEU:HD12	1:E:498:LEU:H	1.69	0.57
1:A:255:LYS:NZ	3:A:801:HOH:O	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:SER:O	1:A:551:LYS:HB2	2.04	0.57
1:B:377:THR:OG1	1:B:380:GLU:HG2	2.03	0.57
1:D:315:VAL:O	1:D:315:VAL:HG12	2.04	0.57
1:D:527:LEU:CD1	1:D:527:LEU:N	2.66	0.57
1:D:574:ASN:HB2	1:D:578:GLN:H	1.70	0.57
1:E:527:LEU:CD1	1:E:527:LEU:N	2.66	0.57
1:E:538:ARG:NH1	1:E:564:ARG:HE	2.01	0.57
1:F:166:ILE:CG2	1:F:176:ASN:CG	2.77	0.57
1:F:600:CYS:HB3	1:F:605:PHE:HD2	1.69	0.57
1:C:194:GLN:O	1:C:197:CYS:HB2	2.04	0.57
1:C:220:TRP:CZ3	1:C:257:LYS:HG2	2.39	0.57
1:D:474:ASP:O	1:D:477:LYS:CG	2.52	0.57
1:E:564:ARG:CA	1:E:569:GLN:OE1	2.52	0.57
1:A:553:ASN:HA	1:A:598:THR:HA	1.85	0.57
1:B:450:ASN:HB2	1:B:451:PRO:CD	2.32	0.57
1:B:649:TRP:N	1:B:649:TRP:CE3	2.73	0.57
1:D:264:LEU:HD22	1:D:265:TRP:N	2.20	0.57
1:D:320:LYS:NZ	3:D:803:HOH:O	2.35	0.57
1:E:176:ASN:C	1:E:176:ASN:HD22	2.11	0.57
1:F:127:LEU:HD23	1:F:199:TYR:O	2.04	0.57
1:B:614:LEU:O	1:B:648:LYS:HD3	2.04	0.57
1:D:443:ARG:C	1:D:444:LEU:HD12	2.29	0.57
1:F:172:GLU:HG2	1:F:173:PHE:CZ	2.39	0.57
1:F:225:ARG:HH21	1:F:225:ARG:CG	2.17	0.57
1:C:410:GLN:C	1:C:411:ILE:HG23	2.30	0.57
1:D:122:TYR:CE1	1:D:203:ASP:HB2	2.38	0.57
1:E:220:TRP:CZ3	1:E:257:LYS:HG2	2.39	0.57
1:E:614:LEU:HD11	1:E:616:ARG:CZ	2.33	0.57
1:E:649:TRP:CD1	1:E:649:TRP:N	2.73	0.57
1:A:150:GLY:O	1:A:187:ARG:NH2	2.38	0.57
1:B:620:ILE:HB	1:B:621:PRO:HD2	1.86	0.57
1:C:627:ASP:HB2	1:C:647:GLN:HG2	1.87	0.57
1:D:631:VAL:HG23	1:D:631:VAL:O	2.03	0.57
1:E:471:VAL:CB	1:E:495:ILE:HD11	2.35	0.57
1:F:455:TYR:N	1:F:455:TYR:CD1	2.73	0.57
1:B:116:LYS:NZ	1:B:397:GLU:OE1	2.35	0.57
1:B:551:LYS:O	1:B:552:THR:HG23	2.05	0.57
1:B:553:ASN:HA	1:B:598:THR:HA	1.87	0.57
1:B:554:GLY:HA3	1:B:598:THR:HG22	1.86	0.57
1:D:171:LYS:HG2	1:D:448:GLN:CD	2.30	0.57
1:D:346:GLY:HA2	1:D:366:PRO:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:513:PHE:HE1	1:E:517:ILE:HD11	1.52	0.57
1:F:136:GLU:OE1	1:F:138:LYS:CG	2.53	0.57
1:A:220:TRP:CZ3	1:A:257:LYS:HG2	2.39	0.56
1:B:301:ASP:H	1:B:391:LEU:HD22	1.70	0.56
1:C:264:LEU:CD2	1:C:265:TRP:N	2.67	0.56
1:C:301:ASP:OD2	1:C:440:HIS:NE2	2.36	0.56
1:E:609:GLN:NE2	1:E:611:PHE:HZ	2.03	0.56
1:A:207:LEU:CD1	1:A:319:SER:OG	2.53	0.56
1:B:647:GLN:HG3	1:B:647:GLN:O	2.04	0.56
1:D:447:TRP:CD1	1:D:448:GLN:N	2.73	0.56
1:E:189:VAL:HG11	1:E:340:ILE:CD1	2.36	0.56
1:F:346:GLY:CA	1:F:366:PRO:HB3	2.33	0.56
1:A:194:GLN:HG3	1:A:351:TYR:OH	2.05	0.56
1:A:585:CYS:CB	1:A:600:CYS:SG	2.92	0.56
1:B:626:LEU:HB2	1:B:649:TRP:CZ3	2.39	0.56
1:B:653:ASN:HD22	1:B:653:ASN:N	2.02	0.56
1:D:236:ARG:HH11	1:D:236:ARG:CG	2.07	0.56
1:E:152:LYS:H	1:E:152:LYS:HD3	1.70	0.56
1:E:484:ARG:N	1:E:485:PRO:HD3	2.21	0.56
1:C:180:SER:HB2	1:C:338:TYR:CZ	2.39	0.56
1:E:332:VAL:HG13	1:E:442:TYR:CE2	2.41	0.56
1:A:412:TRP:CD1	1:A:413:GLY:N	2.73	0.56
1:C:264:LEU:O	1:C:265:TRP:CB	2.50	0.56
1:E:151:GLU:HA	1:E:153:ALA:H	1.70	0.56
1:E:194:GLN:HG3	1:E:351:TYR:OH	2.05	0.56
1:A:122:TYR:OH	1:A:206:LEU:HD21	2.05	0.56
1:E:574:ASN:HB2	1:E:578:GLN:H	1.70	0.56
1:A:628:ARG:HH11	1:A:628:ARG:CG	2.13	0.56
1:C:548:SER:O	1:C:549:MET:HB2	2.05	0.56
1:D:643:SER:CB	1:D:648:LYS:HZ2	2.16	0.56
1:E:576:ALA:O	1:E:577:ASN:HB2	2.04	0.56
1:F:207:LEU:CD1	1:F:319:SER:OG	2.53	0.56
1:B:506:ASN:CB	3:B:804:HOH:O	2.32	0.56
1:B:536:GLU:HA	1:B:569:GLN:O	2.06	0.56
1:E:193:ARG:HG2	1:E:437:ARG:CD	2.34	0.56
1:F:609:GLN:HG3	1:F:611:PHE:CE1	2.41	0.56
1:A:414:GLY:HA3	1:A:416:ASN:OD1	2.04	0.56
1:C:264:LEU:HD22	1:C:265:TRP:N	2.21	0.56
1:D:412:TRP:O	1:D:461:THR:CG2	2.53	0.56
1:E:494:ASP:OD1	1:E:496:SER:OG	2.24	0.56
1:F:162:PHE:O	1:F:166:ILE:HG13	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:ARG:NH2	1:B:306:VAL:O	2.35	0.56
1:C:348:GLU:O	1:C:348:GLU:HG2	2.05	0.56
1:D:164:GLN:HA	1:D:164:GLN:HE21	1.71	0.56
1:E:234:THR:HG22	1:E:310:TRP:HE1	1.71	0.56
1:E:443:ARG:HD3	1:E:447:TRP:CZ3	2.41	0.56
1:F:641:ASP:C	1:F:643:SER:H	2.14	0.56
1:B:585:CYS:SG	1:B:600:CYS:CB	2.94	0.55
1:B:645:THR:OG1	1:B:646:THR:CA	2.52	0.55
1:F:352:ALA:HB3	1:F:364:ARG:NH2	2.22	0.55
1:A:587:THR:OG1	1:A:588:LYS:N	2.32	0.55
1:B:458:SER:O	1:B:462:LEU:CB	2.48	0.55
1:B:591:ASP:N	1:B:591:ASP:OD1	2.39	0.55
1:C:155:PRO:CB	1:C:337:THR:CG2	2.80	0.55
1:C:457:GLY:CA	1:C:459:SER:H	2.02	0.55
1:D:411:ILE:HG23	1:D:411:ILE:O	2.06	0.55
1:E:644:LYS:O	1:E:646:THR:O	2.24	0.55
1:B:197:CYS:SG	1:B:379:THR:CG2	2.94	0.55
1:B:297:LEU:HG	1:B:396:ARG:HG2	1.86	0.55
1:B:362:TRP:C	1:B:363:LYS:HG2	2.32	0.55
1:E:120:PHE:CZ	1:E:207:LEU:CD1	2.86	0.55
1:A:346:GLY:CA	1:A:366:PRO:HB3	2.33	0.55
1:C:239:LEU:HD13	1:C:268:LEU:HD11	1.89	0.55
1:C:573:ILE:HD13	1:C:610:TYR:CB	2.37	0.55
1:C:122:TYR:CE1	1:C:203:ASP:CB	2.89	0.55
1:E:189:VAL:HG12	1:E:190:ASN:N	2.21	0.55
1:F:573:ILE:HD13	1:F:610:TYR:CB	2.36	0.55
1:F:351:TYR:O	1:F:367:LEU:N	2.40	0.55
1:B:620:ILE:CG2	1:B:621:PRO:HD3	2.37	0.55
1:C:132:LEU:HB3	1:C:199:TYR:CD1	2.41	0.55
1:E:627:ASP:OD1	1:E:646:THR:OG1	2.24	0.55
1:F:454:ILE:HG23	1:F:460:PRO:HD3	1.89	0.55
1:B:354:GLY:O	1:B:385:PRO:HD2	2.07	0.55
1:B:444:LEU:HD12	1:B:444:LEU:N	2.22	0.55
1:F:177:MET:HE3	1:F:181:ASP:OD1	2.07	0.55
1:A:262:ILE:CD1	1:A:265:TRP:HZ3	2.19	0.55
1:E:239:LEU:HD13	1:E:268:LEU:HD11	1.89	0.55
1:F:122:TYR:CD1	1:F:123:HIS:N	2.75	0.55
1:E:169:SER:HB2	1:E:177:MET:HB2	1.89	0.55
1:B:415:GLU:HG2	1:B:416:ASN:N	2.21	0.54
1:B:616:ARG:HG2	1:B:648:LYS:CE	2.22	0.54
1:E:552:THR:HB	1:E:584:GLN:HE22	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:415:GLU:HG2	1:F:416:ASN:N	2.21	0.54
1:B:611:PHE:HE2	1:B:618:THR:CG2	2.20	0.54
1:B:617:PHE:HB3	1:B:626:LEU:HD12	1.89	0.54
1:C:166:ILE:O	1:C:170:ILE:HG13	2.08	0.54
1:D:176:ASN:HD22	1:D:176:ASN:C	2.14	0.54
1:D:533:ASP:OD2	1:D:612:LYS:CE	2.55	0.54
1:E:194:GLN:O	1:E:197:CYS:HB2	2.07	0.54
1:A:166:ILE:O	1:A:170:ILE:HG13	2.07	0.54
1:B:231:ILE:HG13	1:B:232:LYS:N	2.22	0.54
1:B:548:SER:HB2	1:B:581:GLN:NE2	2.22	0.54
1:C:241:GLU:HB2	1:C:270:LYS:HZ3	1.71	0.54
1:C:584:GLN:HG2	1:C:598:THR:C	2.32	0.54
1:D:286:ILE:CG2	1:D:290:LYS:HD2	2.38	0.54
1:E:207:LEU:HD12	1:E:207:LEU:H	1.72	0.54
1:E:224:MET:CE	1:E:258:LEU:HD13	2.36	0.54
1:E:471:VAL:CG1	1:E:495:ILE:HD11	2.37	0.54
1:A:231:ILE:HD12	1:A:265:TRP:CD1	2.42	0.54
1:F:244:LEU:C	1:F:245:ILE:HD12	2.32	0.54
1:A:176:ASN:C	1:A:176:ASN:HD22	2.15	0.54
1:A:279:GLY:CA	1:A:411:ILE:HD12	2.38	0.54
1:A:373:ARG:HD2	1:A:373:ARG:O	2.07	0.54
1:B:360:MET:HE1	1:B:468:VAL:HG11	1.89	0.54
1:B:611:PHE:HE2	1:B:618:THR:HG23	1.72	0.54
1:E:118:GLN:NE2	1:E:120:PHE:O	2.41	0.54
1:A:626:LEU:O	1:A:647:GLN:HA	2.07	0.54
1:B:371:GLU:HG2	1:B:519:TYR:OH	2.08	0.54
1:C:372:LYS:HG3	3:C:823:HOH:O	2.08	0.54
1:D:625:CYS:HB2	1:D:640:CYS:SG	2.40	0.54
1:E:193:ARG:NH2	1:E:310:TRP:CA	2.54	0.54
1:E:443:ARG:HD3	1:E:447:TRP:CE3	2.43	0.54
1:A:346:GLY:HA3	1:A:366:PRO:CB	2.35	0.54
1:A:641:ASP:OD1	1:A:642:SER:N	2.41	0.54
1:D:551:LYS:HG2	1:D:555:GLY:HA3	1.88	0.54
1:E:512:TRP:HE1	1:F:516:GLU:HB2	1.73	0.54
1:E:598:THR:HG22	1:E:599:HIS:N	2.23	0.54
1:A:286:ILE:CG2	1:A:290:LYS:HD2	2.37	0.54
1:B:474:ASP:O	1:B:477:LYS:HG3	2.06	0.54
1:D:585:CYS:HG	1:D:600:CYS:CB	2.07	0.54
1:E:192:LEU:HD22	1:E:342:PRO:HD3	1.89	0.54
1:E:552:THR:CB	1:E:584:GLN:OE1	2.54	0.54
1:E:593:SER:O	1:E:636:PHE:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:128:ARG:CG	1:F:201:HIS:HD2	2.11	0.54
1:F:548:SER:O	1:F:551:LYS:HB2	2.08	0.54
1:B:166:ILE:O	1:B:170:ILE:HG13	2.08	0.54
1:B:534:TRP:C	1:B:651:MET:HE3	2.33	0.54
1:B:601:ASN:C	1:B:604:GLU:HG3	2.32	0.54
1:C:194:GLN:HG3	1:C:351:TYR:OH	2.08	0.54
1:C:450:ASN:H	1:C:450:ASN:ND2	2.05	0.54
1:B:551:LYS:C	1:B:552:THR:CG2	2.80	0.54
1:B:614:LEU:HD13	1:B:616:ARG:HD3	0.68	0.54
1:B:624:LYS:HG3	1:B:638:SER:C	2.32	0.54
1:C:463:LYS:HE3	1:C:491:PRO:O	2.08	0.54
1:D:286:ILE:HG22	1:D:290:LYS:HD2	1.90	0.54
1:E:587:THR:HB	1:E:605:PHE:CD1	2.42	0.54
1:F:353:ARG:NH2	1:F:520:ASP:CG	2.66	0.54
1:A:207:LEU:HD12	1:A:207:LEU:H	1.72	0.53
1:A:485:PRO:O	1:A:488:GLN:CG	2.54	0.53
1:B:299:TYR:O	1:B:391:LEU:HA	2.07	0.53
1:B:388:ALA:CB	3:B:803:HOH:O	2.55	0.53
1:B:411:ILE:HG23	1:B:411:ILE:O	2.07	0.53
1:D:191:ASP:OD2	1:D:193:ARG:NH1	2.41	0.53
1:D:224:MET:HE1	1:D:258:LEU:HD11	1.89	0.53
1:D:443:ARG:NE	1:D:447:TRP:CE3	2.71	0.53
1:F:197:CYS:SG	1:F:435:CYS:CA	2.95	0.53
1:A:583:ASP:OD2	1:A:599:HIS:CD2	2.61	0.53
1:A:632:LEU:HB2	1:C:341:ILE:CG2	2.38	0.53
1:B:626:LEU:CD2	1:B:637:ILE:HG22	2.29	0.53
1:D:203:ASP:C	1:D:205:ASN:H	2.15	0.53
1:D:224:MET:HE3	1:D:258:LEU:HD13	1.90	0.53
1:E:557:VAL:HG21	1:E:586:LEU:HD13	1.90	0.53
1:E:622:SER:OG	1:E:624:LYS:HB2	2.08	0.53
1:A:122:TYR:O	1:A:320:LYS:HG2	2.08	0.53
1:E:552:THR:HB	1:E:584:GLN:NE2	2.24	0.53
1:A:276:ARG:CD	1:A:278:GLU:OE2	2.46	0.53
1:B:212:VAL:HG21	1:B:299:TYR:CE1	2.43	0.53
1:C:349:ASP:N	1:C:349:ASP:OD1	2.40	0.53
1:C:646:THR:O	1:C:647:GLN:HG3	2.09	0.53
1:D:125:PRO:HB3	1:D:202:TYR:CD1	2.43	0.53
1:E:332:VAL:CG1	1:E:442:TYR:HD2	2.18	0.53
1:E:485:PRO:HG3	1:E:531:ASN:ND2	2.23	0.53
1:E:627:ASP:OD1	1:E:628:ARG:N	2.36	0.53
1:A:286:ILE:HG22	1:A:290:LYS:HD2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:166:ILE:O	1:D:170:ILE:HG13	2.08	0.53
1:D:611:PHE:CD1	1:E:204:GLU:HB3	2.42	0.53
1:E:552:THR:HB	1:E:584:GLN:CD	2.33	0.53
1:F:346:GLY:HA2	1:F:366:PRO:HA	1.89	0.53
1:F:454:ILE:CD1	1:F:460:PRO:HD3	2.33	0.53
1:A:412:TRP:CD1	1:A:412:TRP:C	2.86	0.53
1:B:197:CYS:SG	1:B:379:THR:HG21	2.49	0.53
1:B:552:THR:CB	1:B:584:GLN:HE22	2.07	0.53
1:D:258:LEU:HD12	1:D:262:ILE:CD1	2.36	0.53
1:F:215:PHE:CE1	1:F:254:LEU:CD1	2.81	0.53
1:B:231:ILE:HD13	1:B:265:TRP:NE1	2.24	0.53
1:D:220:TRP:CZ3	1:D:257:LYS:HG2	2.43	0.53
1:F:197:CYS:SG	1:F:435:CYS:HA	2.49	0.53
1:F:413:GLY:O	1:F:415:GLU:OE2	2.26	0.53
1:F:551:LYS:HG2	1:F:555:GLY:HA3	1.91	0.53
1:A:447:TRP:CD1	1:A:448:GLN:N	2.75	0.53
1:F:272:PHE:CE2	1:F:290:LYS:HB3	2.44	0.53
1:A:239:LEU:HD13	1:A:268:LEU:HD11	1.89	0.53
1:A:532:VAL:HB	1:A:573:ILE:HG23	1.90	0.53
1:B:132:LEU:CD2	1:B:136:GLU:OE1	2.57	0.53
1:E:452:PRO:HB2	1:E:453:PRO:HD2	1.91	0.53
1:E:553:ASN:OD1	1:E:553:ASN:N	2.42	0.53
1:A:136:GLU:OE2	1:A:193:ARG:NH1	2.42	0.52
1:B:458:SER:C	1:B:460:PRO:HA	2.34	0.52
1:B:459:SER:N	1:B:460:PRO:CA	2.72	0.52
1:C:346:GLY:HA2	1:C:366:PRO:CB	2.32	0.52
1:C:476:TYR:O	1:C:477:LYS:C	2.51	0.52
1:C:626:LEU:O	1:C:647:GLN:HA	2.08	0.52
1:F:141:GLU:OE2	1:F:141:GLU:HA	2.08	0.52
1:B:127:LEU:HD12	1:B:377:THR:CG2	2.38	0.52
1:E:217:ASN:HD21	1:E:250:ASN:HB2	1.75	0.52
1:A:586:LEU:N	1:A:586:LEU:CD2	2.73	0.52
1:B:264:LEU:O	1:B:265:TRP:HB2	2.09	0.52
1:D:136:GLU:CD	1:D:193:ARG:NH2	2.67	0.52
1:D:410:GLN:HB2	1:D:460:PRO:HB2	1.91	0.52
1:F:136:GLU:OE1	1:F:138:LYS:CA	2.57	0.52
1:A:414:GLY:CA	1:A:415:GLU:CB	2.79	0.52
1:B:189:VAL:CG1	1:B:340:ILE:HD12	2.38	0.52
1:B:264:LEU:CD2	1:B:265:TRP:N	2.73	0.52
1:C:155:PRO:HB3	1:C:337:THR:HG21	1.89	0.52
1:D:329:LEU:HG	1:D:434:PRO:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:551:LYS:HE3	1:E:555:GLY:HA3	1.92	0.52
1:F:176:ASN:C	1:F:176:ASN:HD22	2.15	0.52
1:A:590:ALA:HA	1:A:591:ASP:C	2.34	0.52
1:C:193:ARG:NH2	1:C:308:VAL:CG2	2.73	0.52
1:D:271:VAL:CG2	1:D:273:ARG:NH1	2.73	0.52
1:A:183:ILE:CG2	1:A:187:ARG:HD2	2.40	0.52
1:B:150:GLY:HA3	1:B:183:ILE:CG2	2.29	0.52
1:B:573:ILE:HD11	1:B:610:TYR:CD2	2.45	0.52
1:E:454:ILE:HD13	1:E:457:GLY:CA	2.40	0.52
1:F:195:GLU:OE1	1:F:198:LYS:HE3	2.08	0.52
1:F:230:VAL:O	1:F:234:THR:HG22	2.09	0.52
1:A:533:ASP:OD2	1:A:612:LYS:CE	2.52	0.52
1:B:360:MET:HE1	1:B:468:VAL:CG1	2.40	0.52
1:E:626:LEU:O	1:E:647:GLN:HA	2.10	0.52
1:A:329:LEU:HG	1:A:434:PRO:HA	1.92	0.52
1:B:147:GLY:O	1:C:489:ALA:CB	2.53	0.52
1:B:388:ALA:HB3	3:B:803:HOH:O	2.08	0.52
1:B:444:LEU:N	1:B:444:LEU:CD1	2.73	0.52
1:B:450:ASN:ND2	1:B:450:ASN:H	2.08	0.52
1:C:628:ARG:HB2	1:C:634:GLN:O	2.10	0.52
1:D:223:LEU:HD12	1:D:223:LEU:O	2.10	0.52
1:D:262:ILE:O	1:D:264:LEU:O	2.27	0.52
1:D:456:VAL:HG11	1:D:463:LYS:HZ2	1.74	0.52
1:F:281:ILE:HD11	1:F:413:GLY:H	1.75	0.52
1:C:207:LEU:CD2	1:C:207:LEU:N	2.73	0.52
1:C:217:ASN:HD21	1:C:250:ASN:HB2	1.74	0.52
1:C:329:LEU:HG	1:C:434:PRO:HA	1.92	0.52
1:D:264:LEU:CD2	1:D:265:TRP:N	2.73	0.52
1:E:574:ASN:HD22	1:E:578:GLN:CG	2.23	0.52
1:F:258:LEU:O	1:F:262:ILE:HD11	2.09	0.52
1:B:576:ALA:O	1:B:606:LYS:HB3	2.10	0.52
1:E:207:LEU:CD1	1:E:319:SER:CB	2.88	0.52
1:E:556:PHE:HE2	1:E:594:LYS:HD3	1.70	0.52
1:F:225:ARG:NH2	1:F:225:ARG:CG	2.73	0.52
1:A:266:ASN:HD21	1:D:500:LYS:NZ	2.08	0.51
1:C:286:ILE:HG22	1:C:290:LYS:HD2	1.91	0.51
1:D:444:LEU:N	1:D:444:LEU:CD1	2.73	0.51
1:E:329:LEU:HG	1:E:434:PRO:HA	1.92	0.51
1:E:354:GLY:O	1:E:385:PRO:HD2	2.09	0.51
1:E:452:PRO:HB2	1:E:453:PRO:CD	2.41	0.51
1:F:520:ASP:OD1	1:F:520:ASP:N	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:588:LYS:HD2	1:A:588:LYS:O	2.10	0.51
1:E:411:ILE:HD13	1:E:411:ILE:H	1.74	0.51
1:E:494:ASP:CG	1:E:496:SER:OG	2.52	0.51
1:E:514:MET:CE	1:E:518:ALA:CB	2.86	0.51
1:E:653:ASN:HD22	1:E:653:ASN:N	2.07	0.51
1:F:363:LYS:HD2	1:F:525:TYR:OH	2.10	0.51
1:B:443:ARG:HD2	1:B:447:TRP:CE3	2.45	0.51
1:B:574:ASN:ND2	1:B:578:GLN:CG	2.69	0.51
1:C:627:ASP:CG	1:C:647:GLN:CG	2.82	0.51
1:D:138:LYS:CD	1:D:138:LYS:N	2.73	0.51
1:E:193:ARG:NE	1:E:435:CYS:O	2.43	0.51
1:E:234:THR:HG22	1:E:310:TRP:NE1	2.25	0.51
1:E:535:GLY:HA3	1:E:652:ASN:O	2.10	0.51
1:F:329:LEU:HG	1:F:434:PRO:HA	1.92	0.51
1:B:586:LEU:HA	1:B:596:MET:O	2.09	0.51
1:C:574:ASN:ND2	1:C:578:GLN:CG	2.69	0.51
1:D:485:PRO:HG3	1:D:531:ASN:ND2	2.25	0.51
1:E:534:TRP:CH2	1:E:653:ASN:HB3	2.45	0.51
1:F:232:LYS:NZ	3:F:802:HOH:O	2.43	0.51
1:B:149:PRO:HG2	1:C:491:PRO:HG3	1.92	0.51
1:B:443:ARG:HH11	1:B:443:ARG:CG	2.16	0.51
1:B:459:SER:N	1:B:460:PRO:HA	2.25	0.51
1:B:329:LEU:HG	1:B:434:PRO:HA	1.92	0.51
1:B:576:ALA:O	1:B:606:LYS:HD2	2.10	0.51
1:C:207:LEU:N	1:C:207:LEU:HD22	2.25	0.51
1:D:136:GLU:OE2	1:D:193:ARG:NH2	2.43	0.51
1:D:413:GLY:CA	1:D:464:ASN:HD22	2.22	0.51
1:E:360:MET:HE3	1:E:473:TRP:CZ2	2.45	0.51
1:E:511:LYS:O	1:E:515:GLU:HG3	2.10	0.51
1:E:605:PHE:HD1	1:E:607:GLU:OE2	1.92	0.51
1:E:624:LYS:HD2	1:E:639:ASN:OD1	2.11	0.51
1:F:258:LEU:HD22	1:F:258:LEU:C	2.36	0.51
1:B:134:ASN:OD1	1:B:134:ASN:N	2.32	0.51
1:B:362:TRP:O	1:B:363:LYS:HG2	2.10	0.51
1:B:522:THR:CG2	1:B:527:LEU:HD11	2.41	0.51
1:D:453:PRO:C	1:D:454:ILE:HD13	2.36	0.51
1:E:608:TRP:CZ3	1:E:626:LEU:HD13	2.46	0.51
1:F:345:GLY:O	1:F:350:GLY:HA3	2.09	0.51
1:A:628:ARG:NH1	1:A:628:ARG:CG	2.73	0.51
1:B:342:PRO:O	1:D:632:LEU:CD1	2.56	0.51
1:B:462:LEU:O	1:B:462:LEU:HG	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:552:THR:CG2	1:B:584:GLN:OE1	2.58	0.51
1:C:207:LEU:H	1:C:207:LEU:HD22	1.73	0.51
1:D:208:THR:H	1:D:295:GLN:NE2	2.06	0.51
1:D:237:LYS:CG	1:D:238:TYR:CE2	2.93	0.51
1:F:232:LYS:NZ	1:F:233:ARG:HH11	2.08	0.51
1:F:454:ILE:CG2	1:F:458:SER:O	2.58	0.51
1:A:371:GLU:HG2	1:A:519:TYR:OH	2.10	0.51
1:B:203:ASP:OD2	1:B:205:ASN:HB2	2.11	0.51
1:B:585:CYS:HG	1:B:600:CYS:CB	2.23	0.51
1:B:629:SER:HB3	1:B:634:GLN:CB	2.41	0.51
1:C:522:THR:CG2	1:C:527:LEU:HD11	2.41	0.51
1:D:632:LEU:HD23	1:D:633:HIS:H	1.76	0.51
1:E:563:HIS:CD2	1:E:563:HIS:N	2.78	0.51
1:B:459:SER:N	1:B:461:THR:N	2.59	0.51
1:B:616:ARG:CD	1:B:648:LYS:CE	2.65	0.51
1:A:476:TYR:O	1:A:477:LYS:C	2.53	0.50
1:A:641:ASP:HB3	1:A:644:LYS:HG3	1.93	0.50
1:D:138:LYS:H	1:D:138:LYS:HD2	1.71	0.50
1:D:264:LEU:CD2	1:D:265:TRP:H	2.25	0.50
1:D:533:ASP:OD2	1:D:612:LYS:HE2	2.11	0.50
1:E:564:ARG:HA	1:E:569:GLN:OE1	2.12	0.50
1:F:362:TRP:O	1:F:363:LYS:HG2	2.11	0.50
1:A:502:ARG:HG3	1:A:507:CYS:HB2	1.93	0.50
1:C:443:ARG:CG	1:C:443:ARG:NH1	2.73	0.50
1:C:534:TRP:CH2	1:C:653:ASN:HB3	2.47	0.50
1:D:220:TRP:CZ2	1:D:261:TYR:CD2	2.97	0.50
1:D:264:LEU:O	1:D:265:TRP:HB2	2.11	0.50
1:D:454:ILE:HG21	1:D:459:SER:OG	2.11	0.50
1:E:574:ASN:ND2	1:E:578:GLN:CG	2.73	0.50
1:F:152:LYS:O	1:F:189:VAL:HA	2.12	0.50
1:B:443:ARG:CG	1:B:443:ARG:NH1	2.73	0.50
1:C:456:VAL:O	1:C:456:VAL:HG23	2.12	0.50
1:D:143:PRO:HG3	1:D:146:VAL:HG12	1.94	0.50
1:D:348:GLU:CB	1:D:349:ASP:HA	2.22	0.50
1:D:415:GLU:HG2	1:D:416:ASN:N	2.25	0.50
1:E:152:LYS:N	1:E:152:LYS:CD	2.73	0.50
1:A:628:ARG:HG2	1:A:649:TRP:CZ2	2.46	0.50
1:E:143:PRO:HG3	1:E:146:VAL:HG12	1.94	0.50
1:E:285:SER:O	1:E:289:GLN:HG3	2.12	0.50
1:E:526:PRO:HG2	1:E:602:LEU:HD13	1.91	0.50
1:E:573:ILE:HD13	1:E:610:TYR:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:186:ASP:OD1	1:F:228:HIS:CD2	2.49	0.50
1:F:232:LYS:HZ3	1:F:233:ARG:HH11	1.59	0.50
1:A:457:GLY:N	1:A:458:SER:CA	2.74	0.50
1:B:192:LEU:HG	1:B:342:PRO:HG3	1.93	0.50
1:D:354:GLY:HA3	1:D:362:TRP:HH2	1.75	0.50
1:D:553:ASN:N	1:D:584:GLN:OE1	2.43	0.50
1:E:462:LEU:HG	1:E:490:LEU:HD21	1.93	0.50
1:E:525:TYR:N	1:E:525:TYR:CD1	2.79	0.50
1:E:573:ILE:CD1	1:E:610:TYR:CD2	2.94	0.50
1:A:118:GLN:NE2	1:A:322:ARG:N	2.58	0.50
1:B:405:TYR:O	1:B:406:ASP:C	2.55	0.50
1:B:614:LEU:HD22	1:B:648:LYS:HE2	1.94	0.50
1:C:347:ASP:HB3	1:C:350:GLY:H	1.76	0.50
1:D:443:ARG:CZ	1:D:447:TRP:CH2	2.95	0.50
1:D:611:PHE:HD1	1:E:204:GLU:CB	2.23	0.50
1:E:363:LYS:CD	1:E:525:TYR:HE2	2.20	0.50
1:C:628:ARG:NH1	1:C:646:THR:HG22	2.25	0.50
1:D:196:GLU:OE2	1:D:379:THR:OG1	2.28	0.50
1:D:248:PHE:CZ	1:D:275:GLU:O	2.63	0.50
1:E:405:TYR:O	1:E:406:ASP:C	2.55	0.50
1:E:609:GLN:CD	1:E:611:PHE:HZ	2.18	0.50
1:F:230:VAL:HG21	1:F:242:ILE:HD13	1.94	0.50
1:A:600:CYS:O	1:A:601:ASN:OD1	2.29	0.50
1:C:447:TRP:CD1	1:C:448:GLN:H	2.30	0.50
1:E:630:GLU:O	1:E:633:HIS:ND1	2.45	0.50
1:F:156:LEU:HD22	1:F:158:LEU:CD2	2.42	0.50
1:F:254:LEU:N	1:F:254:LEU:CD2	2.73	0.50
1:F:443:ARG:NH1	1:F:447:TRP:CH2	2.79	0.50
1:A:122:TYR:OH	1:A:206:LEU:HD23	2.11	0.50
1:C:405:TYR:O	1:C:406:ASP:C	2.55	0.50
1:E:462:LEU:HG	1:E:490:LEU:HD22	1.94	0.50
1:E:540:PHE:CE2	1:E:541:GLU:CD	2.90	0.50
1:F:405:TYR:O	1:F:406:ASP:C	2.55	0.50
1:A:579:LEU:O	1:A:586:LEU:HD23	2.11	0.49
1:A:632:LEU:CB	1:C:341:ILE:CG2	2.90	0.49
1:B:260:GLU:OE1	1:B:263:LYS:NZ	2.44	0.49
1:D:273:ARG:NH1	1:D:273:ARG:CG	2.73	0.49
1:E:231:ILE:HD12	1:E:265:TRP:CD1	2.47	0.49
1:F:203:ASP:OD1	1:F:205:ASN:HB2	2.12	0.49
1:A:281:ILE:HD13	1:A:409:LEU:HB3	1.93	0.49
1:A:414:GLY:CA	1:A:416:ASN:H	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:PRO:HD3	1:C:339:GLU:CG	2.28	0.49
1:C:348:GLU:N	1:C:350:GLY:N	2.60	0.49
1:C:447:TRP:CD1	1:C:448:GLN:N	2.80	0.49
1:C:459:SER:O	1:C:463:LYS:CB	2.60	0.49
1:D:552:THR:CA	1:D:584:GLN:OE1	2.60	0.49
1:F:655:HIS:CD2	3:F:809:HOH:O	2.62	0.49
1:A:162:PHE:CE1	1:D:455:TYR:CD2	2.98	0.49
1:A:447:TRP:C	1:A:448:GLN:CG	2.85	0.49
1:A:532:VAL:HB	1:A:573:ILE:CG2	2.42	0.49
1:C:373:ARG:O	1:C:373:ARG:HD3	2.12	0.49
1:D:171:LYS:CD	1:D:448:GLN:HE22	2.15	0.49
1:D:405:TYR:O	1:D:406:ASP:C	2.55	0.49
1:D:450:ASN:N	1:D:450:ASN:ND2	2.60	0.49
1:E:282:GLN:NE2	1:E:409:LEU:O	2.41	0.49
1:E:410:GLN:HB3	1:E:411:ILE:HG12	1.93	0.49
1:F:406:ASP:HB2	1:F:498:LEU:HD21	1.95	0.49
1:C:180:SER:OG	1:C:225:ARG:NH1	2.46	0.49
1:C:235:PRO:HB2	1:C:238:TYR:HD2	1.78	0.49
1:D:447:TRP:HD1	1:D:448:GLN:H	1.59	0.49
1:F:231:ILE:C	1:F:231:ILE:CD1	2.86	0.49
1:F:271:VAL:O	1:F:272:PHE:HD1	1.95	0.49
1:F:272:PHE:HD2	1:F:290:LYS:HB3	1.76	0.49
1:F:585:CYS:HB2	1:F:600:CYS:HB3	1.94	0.49
1:A:173:PHE:CD2	1:A:177:MET:HG3	2.47	0.49
1:A:601:ASN:HB2	1:A:604:GLU:OE1	2.13	0.49
1:C:485:PRO:O	1:C:488:GLN:CG	2.54	0.49
1:C:547:ASP:OD2	1:C:549:MET:HE2	2.12	0.49
1:D:312:ALA:N	1:D:313:PRO:CD	2.75	0.49
1:E:460:PRO:O	1:E:464:ASN:CG	2.56	0.49
1:E:484:ARG:HH11	1:E:484:ARG:HG3	1.77	0.49
1:A:128:ARG:HG3	1:A:201:HIS:HD2	1.72	0.49
1:B:122:TYR:CE1	1:B:203:ASP:HB3	2.46	0.49
1:B:570:LEU:O	1:B:581:GLN:HG3	2.12	0.49
1:C:476:TYR:C	1:C:478:ASP:N	2.68	0.49
1:E:514:MET:HE2	1:E:514:MET:HA	1.94	0.49
1:A:156:LEU:HD22	1:A:158:LEU:CD2	2.42	0.49
1:B:461:THR:O	1:B:464:ASN:N	2.45	0.49
1:B:615:HIS:O	1:B:648:LYS:CB	2.56	0.49
1:D:281:ILE:HD12	1:D:410:GLN:O	2.13	0.49
1:F:268:LEU:C	1:F:268:LEU:CD1	2.86	0.49
1:F:631:VAL:HA	1:F:632:LEU:C	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:GLY:HA2	1:A:415:GLU:CD	2.37	0.49
1:D:115:PHE:HE2	1:D:426:CYS:O	1.96	0.49
1:E:552:THR:CA	1:E:584:GLN:OE1	2.61	0.49
1:E:627:ASP:CB	3:E:808:HOH:O	2.37	0.49
1:F:450:ASN:N	1:F:450:ASN:ND2	2.60	0.49
1:A:152:LYS:CD	1:A:152:LYS:N	2.76	0.49
1:B:149:PRO:CG	1:C:491:PRO:HG3	2.43	0.49
1:B:614:LEU:O	1:B:615:HIS:CB	2.51	0.49
1:C:584:GLN:HG2	1:C:598:THR:O	2.13	0.49
1:E:473:TRP:O	1:E:474:ASP:HB2	2.13	0.49
1:F:230:VAL:HG23	1:F:231:ILE:N	2.28	0.49
1:A:116:LYS:NZ	3:A:806:HOH:O	2.46	0.49
1:A:405:TYR:O	1:A:406:ASP:C	2.55	0.49
1:B:450:ASN:ND2	1:B:450:ASN:N	2.60	0.49
1:B:485:PRO:O	1:B:488:GLN:CG	2.54	0.49
1:C:601:ASN:HB2	1:C:604:GLU:OE1	2.13	0.49
1:E:598:THR:HG22	1:E:599:HIS:H	1.77	0.49
1:F:220:TRP:CD1	1:F:220:TRP:C	2.91	0.49
1:F:442:TYR:CD1	1:F:443:ARG:N	2.73	0.49
1:F:544:TYR:CE2	3:F:812:HOH:O	2.55	0.49
1:A:641:ASP:H	1:A:647:GLN:NE2	1.99	0.48
1:B:169:SER:HB2	1:B:177:MET:HB2	1.95	0.48
1:B:180:SER:OG	1:B:225:ARG:NH1	2.46	0.48
1:D:180:SER:CB	1:D:225:ARG:HH12	2.26	0.48
1:E:230:VAL:O	1:E:234:THR:HG23	2.12	0.48
1:E:264:LEU:O	1:E:265:TRP:CB	2.61	0.48
1:E:454:ILE:HB	1:E:457:GLY:CA	2.43	0.48
1:F:183:ILE:CG2	1:F:225:ARG:NH1	2.75	0.48
1:B:281:ILE:HD12	1:B:410:GLN:O	2.13	0.48
1:B:318:ILE:O	1:B:321:ASP:O	2.30	0.48
1:B:624:LYS:CG	1:B:638:SER:C	2.86	0.48
1:C:132:LEU:C	1:C:132:LEU:CD1	2.85	0.48
1:E:262:ILE:O	1:E:262:ILE:CG2	2.60	0.48
1:E:637:ILE:O	1:E:637:ILE:HG13	2.13	0.48
1:D:362:TRP:C	1:D:363:LYS:HG2	2.37	0.48
1:D:485:PRO:HB2	1:D:534:TRP:CD2	2.48	0.48
1:D:600:CYS:SG	1:D:604:GLU:HB3	2.53	0.48
1:E:193:ARG:NH1	1:E:308:VAL:O	2.45	0.48
1:E:614:LEU:HD12	1:E:616:ARG:CZ	2.43	0.48
1:E:632:LEU:H	1:E:632:LEU:CD1	1.96	0.48
1:A:363:LYS:HD2	1:A:525:TYR:OH	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:ASP:HB3	1:B:273:ARG:HA	1.95	0.48
1:B:347:ASP:CB	1:B:349:ASP:O	2.61	0.48
1:C:141:GLU:HG2	1:C:142:PRO:HD2	1.96	0.48
1:D:586:LEU:N	1:D:586:LEU:HD23	2.29	0.48
1:E:548:SER:O	1:E:549:MET:HB3	2.13	0.48
1:E:573:ILE:HD13	1:E:610:TYR:CB	2.44	0.48
1:C:166:ILE:HG23	1:C:176:ASN:ND2	2.28	0.48
1:C:208:THR:HG21	1:C:240:ALA:HB2	1.89	0.48
1:C:410:GLN:O	1:C:411:ILE:HG23	2.13	0.48
1:D:166:ILE:HG23	1:D:176:ASN:CG	2.38	0.48
1:E:262:ILE:O	1:E:262:ILE:HG22	2.13	0.48
1:E:276:ARG:CG	1:E:276:ARG:NH1	2.73	0.48
1:E:454:ILE:CB	1:E:457:GLY:HA3	2.43	0.48
1:F:476:TYR:O	1:F:477:LYS:C	2.53	0.48
1:D:116:LYS:O	1:D:322:ARG:NH2	2.45	0.48
1:D:476:TYR:C	1:D:478:ASP:N	2.70	0.48
1:F:177:MET:CE	1:F:221:SER:OG	2.59	0.48
1:F:217:ASN:CG	1:F:251:LYS:HG2	2.39	0.48
1:F:574:ASN:ND2	1:F:578:GLN:CG	2.69	0.48
1:A:584:GLN:HG2	1:A:598:THR:C	2.39	0.48
1:B:620:ILE:HG22	1:B:621:PRO:CD	2.42	0.48
1:B:624:LYS:HG3	1:B:638:SER:O	2.13	0.48
1:C:264:LEU:HD23	1:C:265:TRP:H	1.79	0.48
1:C:348:GLU:H	1:C:350:GLY:N	2.12	0.48
1:D:476:TYR:O	1:D:477:LYS:C	2.54	0.48
1:D:586:LEU:N	1:D:586:LEU:CD2	2.76	0.48
1:D:614:LEU:HD13	1:D:616:ARG:HB3	1.96	0.48
1:F:143:PRO:CB	1:F:151:GLU:OE2	2.62	0.48
1:F:475:GLU:OE1	1:F:511:LYS:CE	2.56	0.48
1:B:347:ASP:O	1:B:348:GLU:C	2.54	0.48
1:C:154:LYS:NZ	3:C:805:HOH:O	2.46	0.48
1:C:209:SER:OG	1:C:296:VAL:HG22	2.14	0.48
1:C:410:GLN:C	1:C:411:ILE:CG2	2.87	0.48
1:C:551:LYS:HE3	1:C:556:PHE:O	2.14	0.48
1:D:375:ARG:NH1	1:D:380:GLU:O	2.38	0.48
1:F:207:LEU:H	1:F:207:LEU:HD12	1.78	0.48
1:F:228:HIS:C	1:F:231:ILE:HG22	2.38	0.48
1:A:312:ALA:N	1:A:313:PRO:CD	2.77	0.48
1:B:601:ASN:HB2	1:B:604:GLU:CG	2.36	0.48
1:B:632:LEU:HD22	1:B:634:GLN:HE22	1.78	0.48
1:C:113:LEU:HG	1:C:504:ASP:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:152:LYS:H	1:E:152:LYS:CD	2.24	0.48
1:A:180:SER:OG	1:A:225:ARG:NH1	2.46	0.48
1:A:195:GLU:OE2	1:A:198:LYS:HE3	2.14	0.48
1:C:208:THR:HG22	1:C:240:ALA:HB2	1.90	0.48
1:D:301:ASP:OD2	1:D:440:HIS:NE2	2.47	0.48
1:D:642:SER:HA	1:D:643:SER:HA	1.69	0.48
1:E:152:LYS:HD3	1:E:152:LYS:N	2.28	0.48
1:E:539:GLY:O	1:E:542:THR:OG1	2.29	0.48
1:F:113:LEU:HD12	1:F:504:ASP:HB3	1.96	0.48
1:F:312:ALA:N	1:F:313:PRO:CD	2.77	0.48
1:A:220:TRP:CE3	1:A:257:LYS:HE3	2.49	0.47
1:A:551:LYS:HE3	1:A:556:PHE:O	2.14	0.47
1:B:312:ALA:N	1:B:313:PRO:CD	2.77	0.47
1:B:348:GLU:N	1:B:349:ASP:C	2.72	0.47
1:B:597:ILE:C	1:B:598:THR:HG23	2.39	0.47
1:D:190:ASN:HD22	1:D:190:ASN:H	1.61	0.47
1:D:321:ASP:HB3	1:D:324:ILE:HD12	1.96	0.47
1:D:609:GLN:CD	1:D:611:PHE:CZ	2.92	0.47
1:E:141:GLU:HG2	1:E:142:PRO:HD2	1.96	0.47
1:E:552:THR:CB	1:E:553:ASN:OD1	2.62	0.47
1:E:563:HIS:CD2	1:E:563:HIS:H	2.31	0.47
1:F:146:VAL:HA	1:F:147:GLY:HA2	1.64	0.47
1:A:122:TYR:CD2	1:A:205:ASN:HB3	2.49	0.47
1:B:266:ASN:ND2	1:C:500:LYS:NZ	2.54	0.47
1:C:220:TRP:CE3	1:C:257:LYS:HE3	2.49	0.47
1:C:312:ALA:N	1:C:313:PRO:CD	2.77	0.47
1:C:587:THR:OG1	1:C:588:LYS:N	2.47	0.47
1:D:323:THR:HG22	1:D:398:PHE:CE1	2.49	0.47
1:F:134:ASN:ND2	1:F:204:GLU:OE2	2.47	0.47
1:F:454:ILE:CB	1:F:458:SER:O	2.62	0.47
1:A:370:GLN:CD	1:A:370:GLN:H	2.22	0.47
1:B:208:THR:OG1	1:B:295:GLN:HG3	2.14	0.47
1:B:254:LEU:O	1:B:273:ARG:NH1	2.39	0.47
1:B:463:LYS:HE3	1:B:491:PRO:O	2.15	0.47
1:D:120:PHE:CE2	1:D:207:LEU:HD21	2.49	0.47
1:D:141:GLU:HG2	1:D:142:PRO:HD2	1.96	0.47
1:D:346:GLY:CA	1:D:366:PRO:HA	2.44	0.47
1:E:189:VAL:HG13	1:E:340:ILE:HD12	1.95	0.47
1:E:220:TRP:CE3	1:E:257:LYS:HE3	2.49	0.47
1:E:564:ARG:H	1:E:569:GLN:NE2	2.12	0.47
1:F:444:LEU:CD1	1:F:444:LEU:H	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:485:PRO:O	1:F:488:GLN:CG	2.54	0.47
1:B:626:LEU:CD2	1:B:637:ILE:CG2	2.88	0.47
1:B:653:ASN:ND2	1:B:653:ASN:N	2.60	0.47
1:C:415:GLU:H	1:C:415:GLU:HG3	1.50	0.47
1:D:552:THR:HA	1:D:584:GLN:OE1	2.13	0.47
1:E:347:ASP:N	1:E:347:ASP:OD1	2.45	0.47
1:F:187:ARG:HG2	1:F:225:ARG:HH22	1.79	0.47
1:B:363:LYS:HD2	1:B:525:TYR:CE1	2.49	0.47
1:B:412:TRP:O	1:B:461:THR:HG22	2.14	0.47
1:D:173:PHE:HD2	1:D:177:MET:HG3	1.75	0.47
1:D:264:LEU:HD23	1:D:265:TRP:H	1.80	0.47
1:D:627:ASP:OD1	1:D:646:THR:HB	2.14	0.47
1:E:193:ARG:HH22	1:E:310:TRP:N	2.11	0.47
1:F:190:ASN:C	1:F:190:ASN:ND2	2.73	0.47
1:A:147:GLY:CA	1:D:489:ALA:HB2	2.42	0.47
1:A:152:LYS:CD	1:A:152:LYS:H	2.27	0.47
1:B:552:THR:HG22	1:B:584:GLN:OE1	2.15	0.47
1:C:141:GLU:OE1	1:C:232:LYS:NZ	2.46	0.47
1:D:262:ILE:O	1:D:262:ILE:HG22	2.14	0.47
1:D:266:ASN:N	1:D:266:ASN:ND2	2.60	0.47
1:D:653:ASN:N	1:D:653:ASN:ND2	2.63	0.47
1:F:573:ILE:HD13	1:F:610:TYR:HB3	1.96	0.47
1:A:138:LYS:HB2	1:A:138:LYS:HE3	1.55	0.47
1:A:235:PRO:HB2	1:A:238:TYR:HD2	1.78	0.47
1:A:377:THR:HB	1:A:380:GLU:HG2	1.95	0.47
1:A:622:SER:OG	1:A:624:LYS:CG	2.63	0.47
1:A:622:SER:OG	1:A:624:LYS:HG3	2.14	0.47
1:B:227:VAL:O	1:B:231:ILE:HG23	2.14	0.47
1:B:260:GLU:CD	1:B:263:LYS:NZ	2.73	0.47
1:B:502:ARG:HG2	1:B:507:CYS:HB2	1.96	0.47
1:B:506:ASN:ND2	3:B:804:HOH:O	2.46	0.47
1:B:601:ASN:O	1:B:604:GLU:CB	2.52	0.47
1:C:254:LEU:O	1:C:273:ARG:NH2	2.48	0.47
1:C:264:LEU:CD2	1:C:264:LEU:C	2.87	0.47
1:C:450:ASN:ND2	1:C:450:ASN:N	2.60	0.47
1:C:596:MET:HB3	1:C:596:MET:HE2	1.73	0.47
1:D:176:ASN:ND2	1:D:176:ASN:C	2.73	0.47
1:D:316:ALA:N	1:D:317:PRO:HD2	2.29	0.47
1:D:551:LYS:HE3	1:D:556:PHE:O	2.14	0.47
1:D:642:SER:HA	1:D:644:LYS:HB2	1.97	0.47
1:E:190:ASN:C	1:E:190:ASN:ND2	2.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:312:ALA:N	1:E:313:PRO:CD	2.77	0.47
1:E:556:PHE:CD2	1:E:594:LYS:CD	2.89	0.47
1:F:203:ASP:O	1:F:204:GLU:HB2	2.15	0.47
1:F:362:TRP:C	1:F:363:LYS:HG2	2.40	0.47
1:F:611:PHE:HB2	1:F:614:LEU:HB2	1.96	0.47
1:A:632:LEU:HA	1:C:341:ILE:CG2	2.45	0.47
1:B:459:SER:N	1:B:460:PRO:C	2.72	0.47
1:D:141:GLU:OE1	1:D:232:LYS:NZ	2.46	0.47
1:E:325:CYS:HB2	1:E:394:ILE:HG23	1.97	0.47
1:E:606:LYS:HG3	1:E:606:LYS:O	2.15	0.47
1:F:132:LEU:CD2	1:F:199:TYR:HE1	2.28	0.47
1:F:246:ASP:O	1:F:274:ASN:HB2	2.15	0.47
1:A:457:GLY:N	1:A:458:SER:HA	2.29	0.47
1:B:588:LYS:CG	1:B:637:ILE:HD11	2.45	0.47
1:D:164:GLN:HA	1:D:164:GLN:NE2	2.30	0.47
1:D:520:ASP:O	1:D:523:SER:HB3	2.15	0.47
1:E:189:VAL:CG1	1:E:190:ASN:N	2.78	0.47
1:E:318:ILE:O	1:E:321:ASP:O	2.32	0.47
1:A:200:TRP:HZ2	1:A:377:THR:HG21	1.79	0.47
1:B:113:LEU:N	1:B:113:LEU:HD23	2.30	0.47
1:B:325:CYS:HB2	1:B:394:ILE:HG23	1.97	0.47
1:B:346:GLY:N	3:B:806:HOH:O	2.48	0.47
1:E:141:GLU:OE1	1:E:232:LYS:NZ	2.46	0.47
1:E:556:PHE:HD2	1:E:594:LYS:CD	2.23	0.47
1:F:132:LEU:HD23	1:F:199:TYR:HE1	1.80	0.47
1:F:217:ASN:OD1	1:F:251:LYS:HG2	2.15	0.47
1:F:579:LEU:O	1:F:586:LEU:HD23	2.15	0.47
1:B:230:VAL:C	1:B:231:ILE:CG2	2.85	0.46
1:C:206:LEU:N	1:C:206:LEU:CD1	2.78	0.46
1:C:579:LEU:O	1:C:586:LEU:HD23	2.15	0.46
1:D:217:ASN:HA	1:D:254:LEU:CD1	2.45	0.46
1:E:454:ILE:HB	1:E:457:GLY:HA3	1.97	0.46
1:A:262:ILE:HD13	1:A:262:ILE:HA	1.73	0.46
1:A:321:ASP:HB3	1:A:324:ILE:HD12	1.96	0.46
1:A:347:ASP:OD1	1:A:372:LYS:NZ	2.33	0.46
1:C:321:ASP:HB3	1:C:324:ILE:HD12	1.96	0.46
1:D:492:TYR:HE2	3:D:825:HOH:O	1.98	0.46
1:E:624:LYS:CG	1:E:638:SER:O	2.54	0.46
1:F:325:CYS:HB2	1:F:394:ILE:HG23	1.97	0.46
1:A:141:GLU:HG2	1:A:142:PRO:HD2	1.96	0.46
1:A:346:GLY:C	1:A:366:PRO:HB3	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:GLU:OE1	1:B:303:HIS:HD2	1.97	0.46
1:B:348:GLU:CA	1:B:349:ASP:C	2.88	0.46
1:B:552:THR:C	1:B:554:GLY:HA2	2.40	0.46
1:C:580:MET:HG2	1:C:585:CYS:SG	2.56	0.46
1:D:190:ASN:H	1:D:190:ASN:ND2	2.13	0.46
1:D:316:ALA:HB3	1:D:317:PRO:HD3	1.96	0.46
1:D:587:THR:OG1	1:D:588:LYS:N	2.47	0.46
1:E:609:GLN:NE2	1:E:611:PHE:CZ	2.83	0.46
1:F:253:HIS:CG	1:F:254:LEU:HD23	2.50	0.46
1:F:321:ASP:HB3	1:F:324:ILE:HD12	1.96	0.46
1:F:554:GLY:N	1:F:597:ILE:O	2.22	0.46
1:F:641:ASP:C	1:F:643:SER:N	2.73	0.46
1:A:156:LEU:HD22	1:A:158:LEU:HD21	1.96	0.46
1:B:380:GLU:O	1:B:381:PRO:C	2.56	0.46
1:B:590:ALA:HA	1:B:591:ASP:HA	1.66	0.46
1:D:266:ASN:N	1:D:266:ASN:HD22	2.12	0.46
1:D:271:VAL:HG21	1:D:273:ARG:HH12	1.76	0.46
1:E:207:LEU:HD12	1:E:319:SER:OG	2.14	0.46
1:B:276:ARG:HB3	1:B:276:ARG:NH1	2.30	0.46
1:D:443:ARG:HG3	1:D:443:ARG:NH1	2.20	0.46
1:A:325:CYS:HB2	1:A:394:ILE:HG23	1.97	0.46
1:D:226:THR:O	1:D:230:VAL:HG23	2.16	0.46
1:D:443:ARG:HD3	1:D:447:TRP:CE3	2.44	0.46
1:D:456:VAL:HG11	1:D:463:LYS:NZ	2.31	0.46
1:D:640:CYS:HA	1:D:647:GLN:HE22	1.81	0.46
1:E:303:HIS:O	1:E:441:ILE:HG13	2.15	0.46
1:E:490:LEU:CD1	1:E:656:SER:O	2.63	0.46
1:A:266:ASN:HD21	1:D:500:LYS:HZ3	1.62	0.46
1:B:616:ARG:HD2	1:B:648:LYS:HE2	1.96	0.46
1:B:655:HIS:N	1:B:655:HIS:CD2	2.83	0.46
1:C:534:TRP:CZ2	1:C:653:ASN:HB3	2.51	0.46
1:D:584:GLN:CG	1:D:597:ILE:HG23	2.29	0.46
1:F:151:GLU:H	1:F:151:GLU:HG2	1.45	0.46
1:F:156:LEU:HD22	1:F:158:LEU:HD21	1.96	0.46
1:F:501:PHE:CD1	1:F:501:PHE:C	2.93	0.46
1:A:195:GLU:O	1:A:198:LYS:HG3	2.16	0.46
1:B:212:VAL:CG2	1:B:299:TYR:CE1	2.99	0.46
1:C:463:LYS:HG3	1:C:492:TYR:HA	1.98	0.46
1:D:191:ASP:CG	1:D:193:ARG:HH11	2.24	0.46
1:E:548:SER:O	1:E:549:MET:CB	2.63	0.46
1:E:593:SER:O	1:E:636:PHE:CB	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:LEU:O	1:A:273:ARG:NH2	2.48	0.46
1:A:473:TRP:CZ3	1:A:480:PHE:HB2	2.51	0.46
1:C:573:ILE:HD13	1:C:610:TYR:HB3	1.97	0.46
1:D:203:ASP:C	1:D:205:ASN:N	2.73	0.46
1:D:443:ARG:NH1	1:D:443:ARG:CG	2.73	0.46
1:D:447:TRP:CD1	1:D:448:GLN:H	2.32	0.46
1:D:520:ASP:OD1	1:D:520:ASP:N	2.41	0.46
1:E:584:GLN:HG2	1:E:598:THR:C	2.41	0.46
1:F:136:GLU:OE1	1:F:138:LYS:CB	2.64	0.46
1:F:413:GLY:HA3	1:F:464:ASN:ND2	2.22	0.46
1:B:473:TRP:CZ3	1:B:480:PHE:HB2	2.51	0.46
1:C:241:GLU:CB	1:C:270:LYS:NZ	2.78	0.46
1:D:151:GLU:HA	1:D:152:LYS:HA	1.71	0.46
1:D:348:GLU:N	1:D:348:GLU:CD	2.73	0.46
1:D:473:TRP:O	1:D:474:ASP:HB2	2.17	0.46
1:E:122:TYR:HB3	1:E:320:LYS:HA	1.98	0.46
1:E:556:PHE:CE2	1:E:594:LYS:HB3	2.51	0.46
1:F:177:MET:O	1:F:181:ASP:OD1	2.34	0.46
1:F:225:ARG:NH2	1:F:225:ARG:HG2	2.30	0.46
1:A:262:ILE:HD13	1:A:265:TRP:CZ3	2.50	0.45
1:B:559:LEU:HD22	1:B:628:ARG:HG3	1.98	0.45
1:C:473:TRP:CZ3	1:C:480:PHE:HB2	2.51	0.45
1:E:608:TRP:HZ3	1:E:626:LEU:HD13	1.80	0.45
1:F:336:ASN:HB2	1:F:444:LEU:HD21	1.98	0.45
1:F:590:ALA:HA	1:F:591:ASP:C	2.41	0.45
1:A:377:THR:HG22	1:A:378:LYS:N	2.32	0.45
1:A:590:ALA:HA	1:A:592:GLY:N	2.30	0.45
1:A:632:LEU:CB	1:C:341:ILE:HG22	2.46	0.45
1:B:212:VAL:CG2	1:B:299:TYR:CD1	2.99	0.45
1:B:552:THR:HB	1:B:584:GLN:OE1	2.16	0.45
1:B:585:CYS:CB	1:B:600:CYS:CB	2.85	0.45
1:C:573:ILE:CD1	1:C:610:TYR:HD2	2.29	0.45
1:E:574:ASN:CG	1:E:578:GLN:HG3	2.41	0.45
1:F:191:ASP:OD1	1:F:193:ARG:HB2	2.16	0.45
1:A:574:ASN:ND2	1:A:578:GLN:CG	2.76	0.45
1:B:122:TYR:O	1:B:320:LYS:HE2	2.16	0.45
1:B:156:LEU:CD2	1:B:158:LEU:HD21	2.47	0.45
1:B:326:THR:HG23	1:B:433:VAL:HG23	1.99	0.45
1:C:646:THR:C	1:C:647:GLN:HG3	2.40	0.45
1:E:193:ARG:NH1	1:E:435:CYS:O	2.50	0.45
1:E:454:ILE:CD1	1:E:457:GLY:HA3	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:522:THR:HG22	1:E:527:LEU:HD11	1.97	0.45
1:A:463:LYS:HB2	1:A:463:LYS:HE3	1.59	0.45
1:C:276:ARG:HG3	1:C:276:ARG:NH1	2.31	0.45
1:C:326:THR:HG23	1:C:433:VAL:HG23	1.99	0.45
1:E:375:ARG:NH2	1:E:380:GLU:O	2.30	0.45
1:E:412:TRP:O	1:E:412:TRP:CE3	2.70	0.45
1:E:540:PHE:CE2	1:E:541:GLU:CG	3.00	0.45
1:F:230:VAL:HG23	1:F:242:ILE:HD11	1.99	0.45
1:B:262:ILE:O	1:B:262:ILE:HG22	2.16	0.45
1:C:325:CYS:HB2	1:C:394:ILE:HG23	1.97	0.45
1:E:494:ASP:OD2	1:E:496:SER:OG	2.33	0.45
1:F:230:VAL:CG2	1:F:242:ILE:CD1	2.95	0.45
1:F:473:TRP:CZ3	1:F:480:PHE:HB2	2.51	0.45
1:B:391:LEU:HD12	1:B:438:VAL:CG2	2.43	0.45
1:C:206:LEU:HD13	1:C:206:LEU:H	1.82	0.45
1:C:412:TRP:O	1:C:412:TRP:CG	2.70	0.45
1:D:609:GLN:HG2	1:D:618:THR:HG23	1.98	0.45
1:F:179:ALA:O	1:F:183:ILE:HG13	2.16	0.45
1:B:171:LYS:HG2	1:B:448:GLN:CD	2.42	0.45
1:B:412:TRP:O	1:B:412:TRP:CE3	2.70	0.45
1:C:357:ASP:C	1:C:357:ASP:OD1	2.60	0.45
1:C:627:ASP:OD1	1:C:647:GLN:N	2.49	0.45
1:D:118:GLN:NE2	1:D:120:PHE:HB3	2.32	0.45
1:D:325:CYS:HB2	1:D:394:ILE:HG23	1.97	0.45
1:D:326:THR:HG23	1:D:433:VAL:HG23	1.99	0.45
1:F:346:GLY:CA	1:F:366:PRO:HA	2.47	0.45
1:F:495:ILE:HD12	1:F:495:ILE:HA	1.85	0.45
1:A:586:LEU:N	1:A:586:LEU:HD23	2.32	0.45
1:B:152:LYS:O	1:B:153:ALA:HB3	2.16	0.45
1:B:336:ASN:HB2	1:B:444:LEU:HD21	1.99	0.45
1:B:383:ARG:HA	1:B:431:LEU:HD23	1.99	0.45
1:D:644:LYS:HA	1:D:644:LYS:HD3	1.61	0.45
1:E:120:PHE:O	1:E:120:PHE:CD1	2.70	0.45
1:E:569:GLN:CB	3:E:806:HOH:O	2.56	0.45
1:A:357:ASP:OD1	1:A:357:ASP:C	2.60	0.45
1:A:363:LYS:HD2	1:A:525:TYR:CE1	2.51	0.45
1:C:241:GLU:CB	1:C:270:LYS:HZ3	2.29	0.45
1:D:357:ASP:C	1:D:357:ASP:OD1	2.60	0.45
1:D:443:ARG:HH11	1:D:443:ARG:CG	2.15	0.45
1:D:450:ASN:CB	1:D:451:PRO:CD	2.93	0.45
1:D:585:CYS:HB2	1:D:600:CYS:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:459:SER:O	1:E:463:LYS:N	2.45	0.45
1:E:463:LYS:O	1:E:463:LYS:HG2	2.17	0.45
1:E:498:LEU:HD12	1:E:498:LEU:N	2.32	0.45
1:E:553:ASN:N	1:E:584:GLN:OE1	2.49	0.45
1:E:653:ASN:N	1:E:653:ASN:ND2	2.60	0.45
1:B:173:PHE:CD2	1:B:177:MET:HG3	2.52	0.45
1:B:443:ARG:CD	1:B:447:TRP:CE3	2.99	0.45
1:D:368:THR:O	1:D:372:LYS:HG3	2.17	0.45
1:E:176:ASN:HD21	1:E:178:VAL:HG23	1.80	0.45
1:E:565:MET:N	1:E:569:GLN:OE1	2.50	0.45
1:F:245:ILE:CD1	1:F:245:ILE:N	2.79	0.45
1:A:326:THR:HG23	1:A:433:VAL:HG23	1.99	0.44
1:E:326:THR:HG23	1:E:433:VAL:HG23	1.99	0.44
1:E:615:HIS:O	1:E:648:LYS:HA	2.16	0.44
1:E:628:ARG:HH11	1:E:628:ARG:CG	2.15	0.44
1:B:301:ASP:H	1:B:391:LEU:CD2	2.29	0.44
1:B:559:LEU:HD22	1:B:628:ARG:CG	2.46	0.44
1:C:463:LYS:HE3	1:C:492:TYR:HA	1.99	0.44
1:D:532:VAL:HB	1:D:573:ILE:HG23	1.98	0.44
1:D:653:ASN:N	1:D:653:ASN:HD22	2.13	0.44
1:F:471:VAL:HG13	1:F:472:TRP:CD1	2.53	0.44
1:B:231:ILE:CD1	1:B:265:TRP:NE1	2.80	0.44
1:B:357:ASP:C	1:B:357:ASP:OD1	2.60	0.44
1:D:412:TRP:O	1:D:412:TRP:CE3	2.70	0.44
1:E:281:ILE:CD1	1:E:413:GLY:H	2.20	0.44
1:E:372:LYS:C	1:E:372:LYS:CD	2.86	0.44
1:E:522:THR:CG2	1:E:527:LEU:HD11	2.47	0.44
1:A:118:GLN:HE21	1:A:321:ASP:HA	1.80	0.44
1:A:200:TRP:CZ2	1:A:377:THR:HG21	2.52	0.44
1:A:368:THR:CB	1:A:370:GLN:OE1	2.61	0.44
1:A:645:THR:O	1:A:648:LYS:HB2	2.17	0.44
1:B:332:VAL:HG13	1:B:442:TYR:CD1	2.53	0.44
1:B:611:PHE:CE2	1:B:618:THR:HG23	2.51	0.44
1:D:473:TRP:CZ3	1:D:480:PHE:HB2	2.51	0.44
1:E:303:HIS:HB2	1:E:441:ILE:HD12	1.98	0.44
1:E:357:ASP:C	1:E:357:ASP:OD1	2.60	0.44
1:E:579:LEU:O	1:E:586:LEU:HD23	2.17	0.44
1:E:605:PHE:CD1	1:E:607:GLU:OE2	2.70	0.44
1:F:221:SER:O	1:F:225:ARG:HB2	2.18	0.44
1:F:454:ILE:HD12	1:F:460:PRO:CG	2.46	0.44
1:F:545:CYS:N	1:F:562:CYS:SG	2.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:627:ASP:OD1	1:F:646:THR:CB	2.61	0.44
1:A:141:GLU:OE1	1:A:232:LYS:NZ	2.46	0.44
1:A:152:LYS:H	1:A:152:LYS:HD3	1.83	0.44
1:B:132:LEU:CG	1:B:136:GLU:OE1	2.63	0.44
1:B:347:ASP:C	1:B:349:ASP:O	2.61	0.44
1:B:495:ILE:HD12	1:B:495:ILE:HA	1.79	0.44
1:B:609:GLN:NE2	1:B:611:PHE:CZ	2.81	0.44
1:C:471:VAL:HG13	1:C:472:TRP:CD1	2.53	0.44
1:C:616:ARG:HG2	1:C:618:THR:HG22	2.00	0.44
1:D:208:THR:O	1:D:296:VAL:HG13	2.17	0.44
1:F:226:THR:HG22	1:F:304:CYS:CA	2.47	0.44
1:F:254:LEU:O	1:F:258:LEU:HB3	2.17	0.44
1:F:326:THR:HG23	1:F:433:VAL:HG23	1.99	0.44
1:F:412:TRP:CE3	1:F:412:TRP:O	2.70	0.44
1:F:609:GLN:NE2	1:F:611:PHE:HZ	2.15	0.44
1:B:450:ASN:CB	1:B:451:PRO:CD	2.93	0.44
1:B:587:THR:HB	1:B:607:GLU:OE2	2.17	0.44
1:B:617:PHE:HB3	1:B:626:LEU:CD1	2.47	0.44
1:C:191:ASP:OD1	1:C:193:ARG:HB2	2.18	0.44
1:C:303:HIS:HB2	1:C:441:ILE:HD12	2.00	0.44
1:C:346:GLY:HA3	1:C:366:PRO:HA	2.00	0.44
1:D:573:ILE:HD12	1:D:579:LEU:HG	1.98	0.44
1:F:143:PRO:CG	1:F:146:VAL:HG12	2.44	0.44
1:F:454:ILE:HG21	1:F:460:PRO:HD3	1.99	0.44
1:B:471:VAL:HG13	1:B:472:TRP:CD1	2.52	0.44
1:B:520:ASP:OD1	1:B:520:ASP:N	2.41	0.44
1:C:655:HIS:CD2	1:C:655:HIS:O	2.70	0.44
1:D:614:LEU:O	1:D:615:HIS:CB	2.60	0.44
1:E:193:ARG:CG	1:E:437:ARG:CD	2.95	0.44
1:F:235:PRO:HB2	1:F:238:TYR:HD2	1.83	0.44
1:F:584:GLN:HG2	1:F:598:THR:C	2.43	0.44
1:A:456:VAL:O	1:A:657:VAL:O	2.35	0.44
1:A:471:VAL:HG13	1:A:472:TRP:CD1	2.53	0.44
1:B:236:ARG:HA	1:B:236:ARG:HD2	1.55	0.44
1:B:495:ILE:HD11	1:B:498:LEU:CD1	2.16	0.44
1:D:513:PHE:CE1	1:D:517:ILE:HD11	2.53	0.44
1:E:450:ASN:ND2	1:E:450:ASN:N	2.65	0.44
1:F:513:PHE:CE1	1:F:517:ILE:HD11	2.53	0.44
1:F:609:GLN:CD	1:F:611:PHE:CZ	2.95	0.44
1:B:175:PHE:CE1	1:B:441:ILE:CG2	3.01	0.44
1:B:625:CYS:CA	1:B:640:CYS:SG	3.05	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:476:TYR:O	1:C:479:TYR:N	2.51	0.44
1:C:527:LEU:HD12	1:C:527:LEU:H	1.74	0.44
1:D:190:ASN:N	1:D:190:ASN:ND2	2.60	0.44
1:D:443:ARG:NE	1:D:447:TRP:CH2	2.82	0.44
1:E:195:GLU:O	1:E:198:LYS:CG	2.66	0.44
1:E:654:ILE:HD13	1:E:654:ILE:HA	1.71	0.44
1:F:357:ASP:OD1	1:F:357:ASP:C	2.60	0.44
1:B:161:GLU:HG2	1:B:162:PHE:N	2.32	0.43
1:B:629:SER:O	1:B:630:GLU:C	2.61	0.43
1:E:551:LYS:NZ	1:E:551:LYS:CB	2.73	0.43
1:F:152:LYS:O	1:F:188:SER:O	2.36	0.43
1:F:230:VAL:HG21	1:F:242:ILE:CD1	2.48	0.43
1:A:447:TRP:C	1:A:448:GLN:HG2	2.44	0.43
1:B:143:PRO:HG2	1:B:146:VAL:HG22	1.98	0.43
1:B:447:TRP:CD1	1:B:448:GLN:H	2.36	0.43
1:B:628:ARG:HE	1:B:628:ARG:HB3	1.67	0.43
1:C:264:LEU:HD23	1:C:265:TRP:N	2.32	0.43
1:C:513:PHE:CE1	1:C:517:ILE:HD11	2.53	0.43
1:D:123:HIS:CD2	3:D:803:HOH:O	2.71	0.43
1:D:243:VAL:HG12	1:D:245:ILE:HD11	2.00	0.43
1:D:347:ASP:CB	1:D:348:GLU:C	2.85	0.43
1:D:471:VAL:HG13	1:D:472:TRP:CD1	2.52	0.43
1:A:122:TYR:CE2	1:A:206:LEU:HD23	2.53	0.43
1:A:596:MET:HE2	1:A:596:MET:HB3	1.78	0.43
1:B:122:TYR:HE1	1:B:203:ASP:CB	2.28	0.43
1:B:631:VAL:HA	1:B:632:LEU:C	2.43	0.43
1:E:122:TYR:CE1	1:E:206:LEU:HD23	2.53	0.43
1:E:254:LEU:O	1:E:273:ARG:NH2	2.51	0.43
1:E:462:LEU:HD12	1:E:462:LEU:HA	1.81	0.43
1:E:484:ARG:O	1:E:487:SER:HB2	2.18	0.43
1:E:614:LEU:HD12	1:E:616:ARG:NE	2.33	0.43
1:F:580:MET:HE3	1:F:585:CYS:SG	2.58	0.43
1:A:455:TYR:HB2	1:A:456:VAL:CG2	2.27	0.43
1:B:596:MET:HG2	1:B:597:ILE:N	2.33	0.43
1:B:613:ASN:ND2	3:B:807:HOH:O	2.51	0.43
1:B:626:LEU:HB3	1:B:649:TRP:CH2	2.47	0.43
1:C:476:TYR:O	1:C:478:ASP:N	2.51	0.43
1:C:520:ASP:OD1	1:C:520:ASP:N	2.51	0.43
1:D:390:GLY:C	1:D:391:LEU:HD23	2.44	0.43
1:E:311:TYR:CE1	1:E:315:VAL:HG21	2.54	0.43
1:E:520:ASP:OD1	1:E:520:ASP:N	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:573:ILE:CD1	1:F:610:TYR:HD2	2.30	0.43
1:A:513:PHE:CE1	1:A:517:ILE:HD11	2.53	0.43
1:B:218:GLU:O	1:B:253:HIS:HE1	2.01	0.43
1:B:447:TRP:CD1	1:B:448:GLN:N	2.87	0.43
1:B:450:ASN:H	1:B:450:ASN:HD22	1.66	0.43
1:C:390:GLY:C	1:C:391:LEU:HD23	2.44	0.43
1:D:224:MET:HE3	1:D:258:LEU:CD1	2.49	0.43
1:D:310:TRP:O	1:D:313:PRO:HD2	2.18	0.43
1:D:540:PHE:O	1:D:542:THR:HG23	2.18	0.43
1:D:616:ARG:HG2	1:D:618:THR:HG22	2.00	0.43
1:E:390:GLY:C	1:E:391:LEU:HD23	2.44	0.43
1:F:641:ASP:HB3	1:F:644:LYS:HD3	2.01	0.43
1:A:220:TRP:CZ3	1:A:257:LYS:HE3	2.53	0.43
1:A:311:TYR:CE1	1:A:315:VAL:HG21	2.54	0.43
1:A:450:ASN:N	1:A:450:ASN:ND2	2.60	0.43
1:A:616:ARG:HG2	1:A:618:THR:HG22	2.00	0.43
1:C:284:ARG:NH1	1:C:415:GLU:OE1	2.48	0.43
1:D:224:MET:CE	1:D:258:LEU:CD1	2.96	0.43
1:E:360:MET:O	1:E:360:MET:HG2	2.18	0.43
1:B:156:LEU:HD22	1:B:158:LEU:CD2	2.47	0.43
1:B:412:TRP:O	1:B:461:THR:CG2	2.67	0.43
1:C:166:ILE:CG2	1:C:176:ASN:ND2	2.81	0.43
1:E:363:LYS:CD	1:E:525:TYR:OH	2.65	0.43
1:E:552:THR:C	1:E:553:ASN:OD1	2.61	0.43
1:E:553:ASN:HA	1:E:598:THR:HA	2.01	0.43
1:A:590:ALA:CA	1:A:591:ASP:C	2.91	0.43
1:B:603:ASN:HB3	1:B:606:LYS:CE	2.33	0.43
1:D:244:LEU:C	1:D:245:ILE:HD13	2.43	0.43
1:E:556:PHE:CE1	1:E:596:MET:HB2	2.54	0.43
1:F:215:PHE:HE1	1:F:254:LEU:HD12	1.81	0.43
1:B:166:ILE:HG12	1:B:178:VAL:HG21	2.01	0.43
1:B:644:LYS:HA	1:B:646:THR:N	2.31	0.43
1:C:146:VAL:HA	1:C:147:GLY:HA2	1.80	0.43
1:C:194:GLN:H	1:C:194:GLN:HG2	1.68	0.43
1:D:171:LYS:CG	1:D:448:GLN:NE2	2.80	0.43
1:D:332:VAL:HG13	1:D:442:TYR:HD1	1.79	0.43
1:D:369:PRO:HA	1:D:372:LYS:HG3	2.01	0.43
1:A:138:LYS:H	1:A:138:LYS:HG3	1.59	0.43
1:A:166:ILE:HG12	1:A:178:VAL:HG21	2.01	0.43
1:A:412:TRP:CG	1:A:413:GLY:N	2.87	0.43
1:A:610:TYR:OH	1:A:612:LYS:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:623:GLY:O	1:A:640:CYS:SG	2.77	0.43
1:B:533:ASP:O	1:B:651:MET:HE1	2.19	0.43
1:C:118:GLN:NE2	1:C:322:ARG:H	2.17	0.43
1:D:484:ARG:O	1:D:487:SER:HB3	2.19	0.43
1:D:534:TRP:CH2	1:D:653:ASN:HB3	2.54	0.43
1:F:281:ILE:HD13	1:F:409:LEU:HB3	2.00	0.43
1:F:370:GLN:HG3	1:F:519:TYR:CE1	2.54	0.43
1:A:535:GLY:HA3	1:A:652:ASN:O	2.19	0.42
1:B:118:GLN:NE2	1:B:120:PHE:O	2.52	0.42
1:C:220:TRP:CZ3	1:C:257:LYS:HE3	2.53	0.42
1:C:264:LEU:HD22	1:C:264:LEU:C	2.43	0.42
1:C:311:TYR:CE1	1:C:315:VAL:HG21	2.54	0.42
1:D:166:ILE:HA	1:D:178:VAL:CG1	2.49	0.42
1:E:220:TRP:CZ3	1:E:257:LYS:HE3	2.53	0.42
1:E:224:MET:HE3	1:E:258:LEU:CD1	2.49	0.42
1:E:545:CYS:SG	1:E:562:CYS:CA	2.98	0.42
1:E:614:LEU:CD1	1:E:616:ARG:NE	2.82	0.42
1:F:207:LEU:HD12	1:F:207:LEU:N	2.34	0.42
1:A:136:GLU:CD	1:A:193:ARG:HH22	2.21	0.42
1:A:421:TYR:HB3	1:A:425:GLN:NE2	2.35	0.42
1:C:553:ASN:HA	1:C:598:THR:HA	2.01	0.42
1:D:132:LEU:HD22	1:D:199:TYR:CE1	2.47	0.42
1:D:217:ASN:HA	1:D:254:LEU:HD11	2.01	0.42
1:E:122:TYR:O	1:E:320:LYS:HG3	2.19	0.42
1:E:276:ARG:NE	1:E:278:GLU:OE2	2.51	0.42
1:E:484:ARG:CG	1:E:484:ARG:NH1	2.73	0.42
1:F:311:TYR:CE1	1:F:315:VAL:HG21	2.54	0.42
1:A:390:GLY:C	1:A:391:LEU:HD23	2.44	0.42
1:B:122:TYR:HE1	1:B:203:ASP:HB3	1.84	0.42
1:C:410:GLN:O	1:C:411:ILE:HG22	2.17	0.42
1:C:421:TYR:HB3	1:C:425:GLN:NE2	2.34	0.42
1:D:281:ILE:HD13	1:D:409:LEU:HB3	2.01	0.42
1:A:455:TYR:HA	1:A:456:VAL:HA	1.64	0.42
1:B:301:ASP:O	1:B:304:CYS:SG	2.75	0.42
1:B:311:TYR:CE1	1:B:315:VAL:HG21	2.54	0.42
1:D:146:VAL:HA	1:D:147:GLY:HA2	1.70	0.42
1:F:421:TYR:HB3	1:F:425:GLN:NE2	2.35	0.42
1:A:149:PRO:O	1:A:149:PRO:HD2	2.19	0.42
1:A:285:SER:O	1:A:289:GLN:HG3	2.19	0.42
1:B:276:ARG:HG3	1:B:278:GLU:OE2	2.19	0.42
1:B:347:ASP:HB3	1:B:351:TYR:N	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:GLY:C	1:B:391:LEU:HD23	2.44	0.42
1:B:533:ASP:O	1:B:651:MET:CE	2.67	0.42
1:B:587:THR:HG22	1:B:605:PHE:HB3	2.02	0.42
1:B:619:HIS:CD2	1:B:621:PRO:HG2	2.54	0.42
1:B:646:THR:O	1:B:647:GLN:HG2	2.18	0.42
1:D:208:THR:H	1:D:295:GLN:HG3	1.85	0.42
1:D:375:ARG:HH21	1:D:375:ARG:HG3	1.84	0.42
1:D:610:TYR:HB2	1:D:617:PHE:CE1	2.55	0.42
1:E:192:LEU:HD11	1:E:340:ILE:HG22	2.02	0.42
1:E:235:PRO:HB2	1:E:238:TYR:CD2	2.51	0.42
1:E:578:GLN:HE21	1:E:578:GLN:HB3	1.68	0.42
1:E:632:LEU:HD22	1:E:634:GLN:NE2	2.34	0.42
1:B:237:LYS:H	1:B:237:LYS:HG2	1.62	0.42
1:B:513:PHE:CE1	1:B:517:ILE:HD11	2.53	0.42
1:C:151:GLU:HA	1:C:152:LYS:HA	1.81	0.42
1:C:356:TRP:CZ2	1:C:514:MET:HE1	2.55	0.42
1:D:285:SER:O	1:D:289:GLN:HG3	2.19	0.42
1:D:354:GLY:CA	1:D:362:TRP:CH2	3.02	0.42
1:D:356:TRP:CZ2	1:D:514:MET:HE1	2.55	0.42
1:D:450:ASN:ND2	1:D:450:ASN:H	2.17	0.42
1:D:462:LEU:HD11	1:D:487:SER:HB2	2.01	0.42
1:D:641:ASP:O	1:D:644:LYS:HB2	2.18	0.42
1:E:411:ILE:N	1:E:411:ILE:CD1	2.76	0.42
1:E:616:ARG:HG2	1:E:618:THR:HG22	2.00	0.42
1:F:135:PHE:HB3	1:F:309:ASN:OD1	2.19	0.42
1:F:151:GLU:HA	1:F:152:LYS:C	2.44	0.42
1:F:285:SER:O	1:F:289:GLN:HG3	2.19	0.42
1:F:445:GLU:HG2	1:F:446:GLY:N	2.33	0.42
1:F:473:TRP:O	1:F:474:ASP:HB2	2.19	0.42
1:B:443:ARG:HD2	1:B:447:TRP:CZ3	2.54	0.42
1:B:627:ASP:HA	1:B:647:GLN:HB2	2.02	0.42
1:D:154:LYS:HB3	1:D:154:LYS:HE3	1.74	0.42
1:E:544:TYR:HD2	1:E:630:GLU:OE1	2.03	0.42
1:F:176:ASN:HD21	1:F:178:VAL:HG22	1.84	0.42
1:F:356:TRP:CZ2	1:F:514:MET:HE1	2.55	0.42
1:F:399:PHE:CE1	1:F:404:LEU:HA	2.55	0.42
1:A:118:GLN:NE2	1:A:321:ASP:CA	2.83	0.42
1:A:134:ASN:OD1	1:A:134:ASN:N	2.47	0.42
1:A:588:LYS:CD	1:A:588:LYS:C	2.93	0.42
1:B:321:ASP:CB	1:B:324:ILE:HG13	2.43	0.42
1:B:344:GLY:O	1:B:364:ARG:NH1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:620:ILE:CB	1:B:621:PRO:HD3	2.48	0.42
1:C:399:PHE:CE1	1:C:404:LEU:HA	2.55	0.42
1:D:553:ASN:HA	1:D:598:THR:HA	2.01	0.42
1:E:421:TYR:HB3	1:E:425:GLN:NE2	2.35	0.42
1:E:580:MET:CG	1:E:585:CYS:SG	3.04	0.42
1:F:185:LEU:HA	1:F:225:ARG:HG3	2.01	0.42
1:F:585:CYS:HB2	1:F:600:CYS:CB	2.50	0.42
1:B:276:ARG:HB3	1:B:276:ARG:CZ	2.50	0.42
1:C:262:ILE:HD13	1:C:262:ILE:HA	1.76	0.42
1:D:399:PHE:CE1	1:D:404:LEU:HA	2.55	0.42
1:D:421:TYR:HB3	1:D:425:GLN:NE2	2.35	0.42
1:D:443:ARG:C	1:D:444:LEU:CD1	2.90	0.42
1:F:459:SER:OG	1:F:462:LEU:HB2	2.19	0.42
1:A:175:PHE:CE1	1:A:441:ILE:HG22	2.54	0.42
1:A:276:ARG:HD2	1:A:278:GLU:CD	2.40	0.42
1:A:414:GLY:CA	1:A:415:GLU:OE2	2.65	0.42
1:B:281:ILE:HD13	1:B:409:LEU:HB3	2.01	0.42
1:B:614:LEU:HD11	1:B:616:ARG:HH11	1.85	0.42
1:C:285:SER:O	1:C:289:GLN:HG3	2.19	0.42
1:D:348:GLU:C	1:D:348:GLU:CD	2.87	0.42
1:E:399:PHE:CE1	1:E:404:LEU:HA	2.55	0.42
1:E:512:TRP:NE1	1:F:516:GLU:HB2	2.33	0.42
1:E:568:ASN:O	1:E:581:GLN:NE2	2.53	0.42
1:E:573:ILE:CD1	1:E:610:TYR:CB	2.97	0.42
1:E:601:ASN:O	1:E:604:GLU:HB2	2.20	0.42
1:F:172:GLU:CG	1:F:173:PHE:CE2	2.86	0.42
1:F:189:VAL:HG13	1:F:340:ILE:HD12	2.02	0.42
1:F:230:VAL:CG2	1:F:242:ILE:HD13	2.49	0.42
1:A:153:ALA:HB1	1:A:190:ASN:HD21	1.85	0.41
1:B:259:ASP:CG	1:B:273:ARG:HH21	2.26	0.41
1:B:399:PHE:HE1	1:B:419:ILE:HD13	1.85	0.41
1:B:574:ASN:HB3	1:B:576:ALA:N	2.35	0.41
1:B:628:ARG:HA	1:B:635:VAL:HA	2.01	0.41
1:B:646:THR:HG22	1:B:647:GLN:N	2.35	0.41
1:C:190:ASN:C	1:C:190:ASN:ND2	2.73	0.41
1:C:627:ASP:OD1	1:C:646:THR:C	2.63	0.41
1:F:457:GLY:N	1:F:458:SER:CA	2.72	0.41
1:F:476:TYR:O	1:F:478:ASP:N	2.53	0.41
1:F:602:LEU:HD23	1:F:602:LEU:HA	1.95	0.41
1:A:207:LEU:HD13	1:A:319:SER:OG	2.19	0.41
1:A:476:TYR:O	1:A:478:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:576:ALA:O	1:B:606:LYS:CD	2.68	0.41
1:C:539:GLY:CA	1:C:628:ARG:HH21	2.31	0.41
1:E:262:ILE:O	1:E:264:LEU:O	2.38	0.41
1:E:546:ILE:CG2	1:E:557:VAL:HG11	2.50	0.41
1:F:228:HIS:O	1:F:231:ILE:HG23	2.16	0.41
1:A:356:TRP:CZ2	1:A:514:MET:HE1	2.55	0.41
1:A:520:ASP:OD1	1:A:520:ASP:N	2.41	0.41
1:B:195:GLU:OE1	1:B:198:LYS:NZ	2.47	0.41
1:B:622:SER:O	1:B:624:LYS:HB2	2.20	0.41
1:D:163:LYS:HG3	1:D:164:GLN:N	2.33	0.41
1:E:374:LEU:HD23	1:E:374:LEU:HA	1.89	0.41
1:F:303:HIS:HB2	1:F:441:ILE:HD12	2.02	0.41
1:A:115:PHE:HE2	1:A:426:CYS:O	2.03	0.41
1:A:311:TYR:CZ	1:A:315:VAL:HG21	2.56	0.41
1:B:245:ILE:HD13	1:B:245:ILE:HA	1.90	0.41
1:B:573:ILE:CD1	1:B:610:TYR:CD2	3.03	0.41
1:C:547:ASP:OD2	1:C:549:MET:SD	2.79	0.41
1:D:191:ASP:CG	1:D:193:ARG:NH1	2.79	0.41
1:D:354:GLY:O	1:D:385:PRO:HD2	2.20	0.41
1:D:535:GLY:HA3	1:D:652:ASN:O	2.19	0.41
1:D:628:ARG:HD2	1:D:649:TRP:CH2	2.55	0.41
1:E:146:VAL:HA	1:E:147:GLY:HA2	1.70	0.41
1:F:258:LEU:CD2	1:F:262:ILE:CD1	2.66	0.41
1:F:535:GLY:HA3	1:F:652:ASN:O	2.19	0.41
1:F:574:ASN:HB3	1:F:576:ALA:N	2.35	0.41
1:F:641:ASP:CB	1:F:644:LYS:HD3	2.51	0.41
1:A:176:ASN:HD21	1:A:178:VAL:HG22	1.84	0.41
1:A:462:LEU:HD23	1:A:462:LEU:HA	1.92	0.41
1:B:388:ALA:N	3:B:803:HOH:O	2.40	0.41
1:B:421:TYR:HB3	1:B:425:GLN:NE2	2.35	0.41
1:B:573:ILE:HD13	1:B:610:TYR:HB3	2.03	0.41
1:B:620:ILE:HB	1:B:621:PRO:HD3	2.01	0.41
1:C:644:LYS:N	1:C:645:THR:HA	2.35	0.41
1:F:128:ARG:O	1:F:199:TYR:HB3	2.21	0.41
1:F:170:ILE:O	1:F:174:GLY:N	2.45	0.41
1:F:611:PHE:HE1	1:F:618:THR:HG21	1.85	0.41
1:A:122:TYR:CE2	1:A:205:ASN:HB3	2.55	0.41
1:A:356:TRP:HZ2	1:A:514:MET:HE1	1.86	0.41
1:A:399:PHE:CE1	1:A:404:LEU:HA	2.55	0.41
1:A:473:TRP:O	1:A:474:ASP:HB2	2.19	0.41
1:B:356:TRP:CZ2	1:B:514:MET:HE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:632:LEU:H	1:B:632:LEU:CD1	2.27	0.41
1:C:454:ILE:CD1	1:C:460:PRO:HD3	2.42	0.41
1:C:574:ASN:HB3	1:C:576:ALA:N	2.35	0.41
1:C:653:ASN:N	1:C:653:ASN:HD22	2.19	0.41
1:D:190:ASN:HD21	1:D:340:ILE:HB	1.86	0.41
1:E:406:ASP:CB	1:E:498:LEU:HD21	2.50	0.41
1:E:454:ILE:CG1	1:E:457:GLY:HA3	2.51	0.41
1:F:156:LEU:HD12	1:F:183:ILE:HD11	2.01	0.41
1:F:192:LEU:HD11	1:F:340:ILE:HG22	2.01	0.41
1:F:207:LEU:HD13	1:F:319:SER:OG	2.19	0.41
1:F:256:GLU:CA	1:F:259:ASP:OD1	2.68	0.41
1:F:311:TYR:CZ	1:F:315:VAL:HG21	2.56	0.41
1:F:411:ILE:O	1:F:411:ILE:HG23	2.19	0.41
1:B:619:HIS:O	1:B:623:GLY:HA2	2.21	0.41
1:C:152:LYS:O	1:C:153:ALA:HB3	2.20	0.41
1:C:463:LYS:HE3	1:C:492:TYR:C	2.45	0.41
1:D:208:THR:N	1:D:295:GLN:HG3	2.35	0.41
1:A:153:ALA:HB1	1:A:190:ASN:ND2	2.23	0.41
1:B:356:TRP:HZ2	1:B:514:MET:HE1	1.86	0.41
1:B:642:SER:O	1:B:642:SER:OG	2.30	0.41
1:C:548:SER:HB2	1:C:581:GLN:HE22	1.85	0.41
1:E:194:GLN:HE21	1:E:194:GLN:HB3	1.65	0.41
1:F:116:LYS:O	1:F:322:ARG:NH2	2.51	0.41
1:A:451:PRO:HB2	1:A:452:PRO:CD	2.50	0.41
1:A:590:ALA:CB	1:A:591:ASP:CA	2.95	0.41
1:B:136:GLU:CD	1:B:136:GLU:C	2.88	0.41
1:B:311:TYR:CZ	1:B:315:VAL:HG21	2.56	0.41
1:B:347:ASP:CB	1:B:351:TYR:O	2.65	0.41
1:B:443:ARG:HG3	1:B:443:ARG:NH1	2.23	0.41
1:B:627:ASP:CB	1:B:647:GLN:HB2	2.51	0.41
1:C:124:ASP:OD2	1:C:320:LYS:HD2	2.21	0.41
1:C:128:ARG:O	1:C:129:PRO:C	2.61	0.41
1:C:143:PRO:CG	1:C:146:VAL:HB	2.50	0.41
1:C:262:ILE:HD13	1:C:265:TRP:HZ3	1.86	0.41
1:C:262:ILE:O	1:C:262:ILE:HG22	2.21	0.41
1:C:443:ARG:HD2	1:C:447:TRP:CE3	2.56	0.41
1:C:535:GLY:HA3	1:C:652:ASN:O	2.19	0.41
1:D:243:VAL:HG22	1:D:270:LYS:HD2	2.01	0.41
1:D:596:MET:HE2	1:D:596:MET:HB3	1.73	0.41
1:E:311:TYR:CZ	1:E:315:VAL:HG21	2.56	0.41
1:E:322:ARG:HH11	1:E:397:GLU:HB3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:573:ILE:HD12	1:E:610:TYR:CD2	2.55	0.41
1:F:174:GLY:CA	1:F:447:TRP:HB2	2.51	0.41
1:F:193:ARG:NH2	1:F:308:VAL:HG22	2.36	0.41
1:F:248:PHE:HB3	1:F:277:ARG:HB2	2.03	0.41
1:F:356:TRP:HZ2	1:F:514:MET:HE1	1.86	0.41
1:F:394:ILE:HG21	1:F:394:ILE:HD13	1.73	0.41
1:F:614:LEU:HD13	1:F:616:ARG:HH21	1.85	0.41
1:B:410:GLN:O	1:B:411:ILE:C	2.63	0.41
1:B:553:ASN:O	1:B:553:ASN:CG	2.64	0.41
1:C:311:TYR:CZ	1:C:315:VAL:HG21	2.56	0.41
1:D:217:ASN:OD1	1:D:249:SER:HB3	2.19	0.41
1:D:447:TRP:CD1	1:D:449:GLY:H	2.39	0.41
1:D:632:LEU:HD22	1:D:634:GLN:HG3	2.02	0.41
1:E:551:LYS:HD3	1:E:556:PHE:O	2.21	0.41
1:F:258:LEU:CD2	1:F:258:LEU:C	2.93	0.41
1:A:163:LYS:HG3	1:A:164:GLN:N	2.36	0.40
1:B:207:LEU:HB3	1:B:295:GLN:HB2	2.02	0.40
1:B:629:SER:O	1:B:632:LEU:O	2.40	0.40
1:C:286:ILE:CG2	1:C:290:LYS:HD2	2.52	0.40
1:D:134:ASN:OD1	1:D:134:ASN:N	2.37	0.40
1:D:187:ARG:O	1:D:187:ARG:HG3	2.20	0.40
1:D:476:TYR:O	1:D:478:ASP:N	2.54	0.40
1:D:534:TRP:CZ2	1:D:653:ASN:HB3	2.56	0.40
1:E:141:GLU:HA	1:E:142:PRO:HD3	1.84	0.40
1:E:454:ILE:H	1:E:454:ILE:HG13	1.70	0.40
1:F:118:GLN:NE2	1:F:320:LYS:O	2.54	0.40
1:F:243:VAL:HG21	1:F:291:ALA:HB2	2.02	0.40
1:F:450:ASN:HD22	1:F:450:ASN:H	1.69	0.40
1:F:552:THR:HB	1:F:584:GLN:OE1	2.21	0.40
1:F:616:ARG:HD3	1:F:625:CYS:SG	2.61	0.40
1:A:183:ILE:HG21	1:A:187:ARG:HD2	2.02	0.40
1:B:113:LEU:HG	1:B:504:ASP:HB3	2.03	0.40
1:B:147:GLY:H	1:C:489:ALA:HB2	1.87	0.40
1:B:453:PRO:CB	1:D:164:GLN:OE1	2.62	0.40
1:C:263:LYS:HE3	1:C:263:LYS:HB3	1.58	0.40
1:C:332:VAL:HG13	1:C:442:TYR:CD1	2.56	0.40
1:D:183:ILE:CG2	1:D:187:ARG:HD3	2.51	0.40
1:D:356:TRP:HZ2	1:D:514:MET:HE1	1.86	0.40
1:E:176:ASN:ND2	1:E:176:ASN:C	2.73	0.40
1:F:356:TRP:HA	1:F:361:LEU:O	2.21	0.40
1:A:167:GLN:NE2	3:A:810:HOH:O	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:PRO:HB2	1:A:534:TRP:CD2	2.57	0.40
1:B:230:VAL:CG2	1:B:231:ILE:N	2.85	0.40
1:D:394:ILE:HG21	1:D:394:ILE:HD13	1.73	0.40
1:D:453:PRO:O	1:D:454:ILE:HD13	2.21	0.40
1:D:456:VAL:C	1:D:458:SER:H	2.29	0.40
1:E:415:GLU:CG	1:E:416:ASN:N	2.79	0.40
1:E:626:LEU:HD12	1:E:637:ILE:HG22	2.04	0.40
1:D:173:PHE:CD2	1:D:177:MET:CG	2.94	0.40
1:D:371:GLU:O	1:D:375:ARG:CG	2.68	0.40
1:E:326:THR:HG23	1:E:433:VAL:CG2	2.52	0.40
1:E:524:HIS:C	1:E:525:TYR:CD1	3.00	0.40
1:F:176:ASN:ND2	1:F:176:ASN:C	2.80	0.40
1:A:590:ALA:C	1:A:592:GLY:N	2.79	0.40
1:C:356:TRP:HZ2	1:C:514:MET:HE1	1.86	0.40
1:D:264:LEU:O	1:D:265:TRP:CB	2.70	0.40
1:F:143:PRO:HB2	1:F:151:GLU:CD	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	544/597 (91%)	515 (95%)	29 (5%)	0	100	100
1	B	544/597 (91%)	518 (95%)	25 (5%)	1 (0%)	43	66
1	C	544/597 (91%)	517 (95%)	27 (5%)	0	100	100
1	D	544/597 (91%)	521 (96%)	22 (4%)	1 (0%)	43	66
1	E	544/597 (91%)	520 (96%)	24 (4%)	0	100	100
1	F	544/597 (91%)	518 (95%)	25 (5%)	1 (0%)	43	66
All	All	3264/3582 (91%)	3109 (95%)	152 (5%)	3 (0%)	48	72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	459	SER
1	F	451	PRO
1	D	491	PRO

5.3.2 Protein sidechains [i](#)

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	480/525 (91%)	367 (76%)	113 (24%)	1	1
1	B	480/525 (91%)	380 (79%)	100 (21%)	1	3
1	C	480/525 (91%)	393 (82%)	87 (18%)	2	4
1	D	480/525 (91%)	379 (79%)	101 (21%)	1	2
1	E	480/525 (91%)	374 (78%)	106 (22%)	1	2
1	F	480/525 (91%)	371 (77%)	109 (23%)	1	2
All	All	2880/3150 (91%)	2264 (79%)	616 (21%)	1	2

All (616) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	THR
1	A	116	LYS
1	A	117	PRO
1	A	118	GLN
1	A	127	LEU
1	A	128	ARG
1	A	132	LEU
1	A	138	LYS
1	A	139	GLU
1	A	146	VAL
1	A	151	GLU
1	A	152	LYS
1	A	154	LYS
1	A	156	LEU

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Mol	Chain	Res	Type
1	A	163	LYS
1	A	164	GLN
1	A	178	VAL
1	A	188	SER
1	A	190	ASN
1	A	197	CYS
1	A	211	VAL
1	A	212	VAL
1	A	229	SER
1	A	231	ILE
1	A	237	LYS
1	A	239	LEU
1	A	249	SER
1	A	250	ASN
1	A	251	LYS
1	A	255	LYS
1	A	256	GLU
1	A	262	ILE
1	A	264	LEU
1	A	268	LEU
1	A	270	LYS
1	A	273	ARG
1	A	276	ARG
1	A	277	ARG
1	A	290	LYS
1	A	293	LEU
1	A	296	VAL
1	A	300	LEU
1	A	301	ASP
1	A	306	VAL
1	A	308	VAL
1	A	320	LYS
1	A	329	LEU
1	A	341	ILE
1	A	348	GLU
1	A	349	ASP
1	A	359	SER
1	A	376	LYS
1	A	379	THR
1	A	391	LEU
1	A	394	ILE
1	A	409	LEU

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Mol	Chain	Res	Type
1	A	410	GLN
1	A	411	ILE
1	A	412	TRP
1	A	415	GLU
1	A	418	GLU
1	A	430	LEU
1	A	443	ARG
1	A	445	GLU
1	A	450	ASN
1	A	454	ILE
1	A	455	TYR
1	A	456	VAL
1	A	459	SER
1	A	462	LEU
1	A	475	GLU
1	A	477	LYS
1	A	498	LEU
1	A	499	LYS
1	A	506	ASN
1	A	517	ILE
1	A	523	SER
1	A	527	LEU
1	A	541	GLU
1	A	547	ASP
1	A	551	LYS
1	A	557	VAL
1	A	570	LEU
1	A	573	ILE
1	A	579	LEU
1	A	585	CYS
1	A	586	LEU
1	A	588	LYS
1	A	591	ASP
1	A	593	SER
1	A	598	THR
1	A	600	CYS
1	A	602	LEU
1	A	604	GLU
1	A	606	LYS
1	A	613	ASN
1	A	614	LEU
1	A	618	THR

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Mol	Chain	Res	Type
1	A	620	ILE
1	A	624	LYS
1	A	626	LEU
1	A	628	ARG
1	A	630	GLU
1	A	631	VAL
1	A	632	LEU
1	A	642	SER
1	A	644	LYS
1	A	645	THR
1	A	648	LYS
1	A	650	GLU
1	A	651	MET
1	A	655	HIS
1	A	656	SER
1	B	114	THR
1	B	116	LYS
1	B	118	GLN
1	B	127	LEU
1	B	132	LEU
1	B	134	ASN
1	B	136	GLU
1	B	139	GLU
1	B	141	GLU
1	B	151	GLU
1	B	152	LYS
1	B	154	LYS
1	B	156	LEU
1	B	164	GLN
1	B	178	VAL
1	B	192	LEU
1	B	193	ARG
1	B	205	ASN
1	B	211	VAL
1	B	212	VAL
1	B	229	SER
1	B	230	VAL
1	B	231	ILE
1	B	234	THR
1	B	236	ARG
1	B	239	LEU
1	B	248	PHE

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Mol	Chain	Res	Type
1	B	249	SER
1	B	251	LYS
1	B	254	LEU
1	B	255	LYS
1	B	264	LEU
1	B	268	LEU
1	B	270	LYS
1	B	275	GLU
1	B	276	ARG
1	B	277	ARG
1	B	290	LYS
1	B	296	VAL
1	B	301	ASP
1	B	304	CYS
1	B	306	VAL
1	B	308	VAL
1	B	329	LEU
1	B	341	ILE
1	B	349	ASP
1	B	359	SER
1	B	376	LYS
1	B	379	THR
1	B	383	ARG
1	B	391	LEU
1	B	394	ILE
1	B	395	GLU
1	B	396	ARG
1	B	397	GLU
1	B	411	ILE
1	B	418	GLU
1	B	430	LEU
1	B	438	VAL
1	B	443	ARG
1	B	445	GLU
1	B	448	GLN
1	B	450	ASN
1	B	454	ILE
1	B	460	PRO
1	B	463	LYS
1	B	477	LYS
1	B	495	ILE
1	B	496	SER

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Mol	Chain	Res	Type
1	B	497	GLU
1	B	499	LYS
1	B	502	ARG
1	B	517	ILE
1	B	523	SER
1	B	541	GLU
1	B	547	ASP
1	B	557	VAL
1	B	570	LEU
1	B	573	ILE
1	B	579	LEU
1	B	586	LEU
1	B	587	THR
1	B	588	LYS
1	B	591	ASP
1	B	601	ASN
1	B	602	LEU
1	B	612	LYS
1	B	614	LEU
1	B	618	THR
1	B	622	SER
1	B	624	LYS
1	B	628	ARG
1	B	631	VAL
1	B	632	LEU
1	B	634	GLN
1	B	647	GLN
1	B	649	TRP
1	B	653	ASN
1	B	655	HIS
1	B	656	SER
1	C	113	LEU
1	C	114	THR
1	C	116	LYS
1	C	121	THR
1	C	138	LYS
1	C	146	VAL
1	C	149	PRO
1	C	151	GLU
1	C	190	ASN
1	C	197	CYS
1	C	205	ASN

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Mol	Chain	Res	Type
1	C	206	LEU
1	C	207	LEU
1	C	209	SER
1	C	211	VAL
1	C	212	VAL
1	C	229	SER
1	C	231	ILE
1	C	237	LYS
1	C	239	LEU
1	C	251	LYS
1	C	255	LYS
1	C	256	GLU
1	C	264	LEU
1	C	268	LEU
1	C	270	LYS
1	C	273	ARG
1	C	275	GLU
1	C	276	ARG
1	C	296	VAL
1	C	300	LEU
1	C	301	ASP
1	C	306	VAL
1	C	308	VAL
1	C	320	LYS
1	C	329	LEU
1	C	337	THR
1	C	339	GLU
1	C	341	ILE
1	C	349	ASP
1	C	359	SER
1	C	376	LYS
1	C	378	LYS
1	C	379	THR
1	C	391	LEU
1	C	394	ILE
1	C	415	GLU
1	C	418	GLU
1	C	430	LEU
1	C	443	ARG
1	C	444	LEU
1	C	450	ASN
1	C	461	THR

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Mol	Chain	Res	Type
1	C	462	LEU
1	C	477	LYS
1	C	498	LEU
1	C	499	LYS
1	C	517	ILE
1	C	523	SER
1	C	541	GLU
1	C	551	LYS
1	C	557	VAL
1	C	570	LEU
1	C	573	ILE
1	C	579	LEU
1	C	586	LEU
1	C	588	LYS
1	C	593	SER
1	C	597	ILE
1	C	598	THR
1	C	602	LEU
1	C	604	GLU
1	C	606	LYS
1	C	612	LYS
1	C	613	ASN
1	C	614	LEU
1	C	618	THR
1	C	620	ILE
1	C	628	ARG
1	C	632	LEU
1	C	637	ILE
1	C	638	SER
1	C	642	SER
1	C	646	THR
1	C	650	GLU
1	C	651	MET
1	C	657	VAL
1	D	114	THR
1	D	116	LYS
1	D	121	THR
1	D	123	HIS
1	D	127	LEU
1	D	128	ARG
1	D	132	LEU
1	D	138	LYS

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Mol	Chain	Res	Type
1	D	146	VAL
1	D	149	PRO
1	D	151	GLU
1	D	152	LYS
1	D	154	LYS
1	D	156	LEU
1	D	164	GLN
1	D	178	VAL
1	D	188	SER
1	D	190	ASN
1	D	192	LEU
1	D	195	GLU
1	D	196	GLU
1	D	229	SER
1	D	231	ILE
1	D	236	ARG
1	D	237	LYS
1	D	239	LEU
1	D	247	ASP
1	D	248	PHE
1	D	251	LYS
1	D	255	LYS
1	D	258	LEU
1	D	264	LEU
1	D	266	ASN
1	D	268	LEU
1	D	270	LYS
1	D	271	VAL
1	D	273	ARG
1	D	276	ARG
1	D	277	ARG
1	D	290	LYS
1	D	292	LYS
1	D	296	VAL
1	D	300	LEU
1	D	301	ASP
1	D	306	VAL
1	D	320	LYS
1	D	329	LEU
1	D	341	ILE
1	D	348	GLU
1	D	349	ASP

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Mol	Chain	Res	Type
1	D	359	SER
1	D	373	ARG
1	D	375	ARG
1	D	379	THR
1	D	391	LEU
1	D	394	ILE
1	D	411	ILE
1	D	418	GLU
1	D	430	LEU
1	D	443	ARG
1	D	444	LEU
1	D	445	GLU
1	D	448	GLN
1	D	450	ASN
1	D	461	THR
1	D	462	LEU
1	D	463	LYS
1	D	477	LYS
1	D	490	LEU
1	D	498	LEU
1	D	499	LYS
1	D	517	ILE
1	D	522	THR
1	D	541	GLU
1	D	547	ASP
1	D	551	LYS
1	D	557	VAL
1	D	570	LEU
1	D	572	ARG
1	D	579	LEU
1	D	584	GLN
1	D	586	LEU
1	D	588	LYS
1	D	591	ASP
1	D	593	SER
1	D	597	ILE
1	D	598	THR
1	D	602	LEU
1	D	604	GLU
1	D	606	LYS
1	D	612	LYS
1	D	614	LEU

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Mol	Chain	Res	Type
1	D	618	THR
1	D	620	ILE
1	D	628	ARG
1	D	644	LYS
1	D	646	THR
1	D	650	GLU
1	D	651	MET
1	D	653	ASN
1	D	657	VAL
1	E	120	PHE
1	E	121	THR
1	E	127	LEU
1	E	128	ARG
1	E	131	ILE
1	E	132	LEU
1	E	138	LYS
1	E	146	VAL
1	E	151	GLU
1	E	152	LYS
1	E	156	LEU
1	E	163	LYS
1	E	171	LYS
1	E	176	ASN
1	E	190	ASN
1	E	194	GLN
1	E	195	GLU
1	E	196	GLU
1	E	198	LYS
1	E	211	VAL
1	E	212	VAL
1	E	229	SER
1	E	231	ILE
1	E	237	LYS
1	E	239	LEU
1	E	251	LYS
1	E	255	LYS
1	E	256	GLU
1	E	263	LYS
1	E	264	LEU
1	E	268	LEU
1	E	270	LYS
1	E	273	ARG

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Mol	Chain	Res	Type
1	E	275	GLU
1	E	276	ARG
1	E	290	LYS
1	E	296	VAL
1	E	300	LEU
1	E	306	VAL
1	E	308	VAL
1	E	329	LEU
1	E	341	ILE
1	E	348	GLU
1	E	349	ASP
1	E	359	SER
1	E	370	GLN
1	E	372	LYS
1	E	376	LYS
1	E	378	LYS
1	E	379	THR
1	E	391	LEU
1	E	394	ILE
1	E	409	LEU
1	E	410	GLN
1	E	411	ILE
1	E	418	GLU
1	E	430	LEU
1	E	443	ARG
1	E	445	GLU
1	E	450	ASN
1	E	454	ILE
1	E	477	LYS
1	E	484	ARG
1	E	495	ILE
1	E	497	GLU
1	E	506	ASN
1	E	515	GLU
1	E	517	ILE
1	E	541	GLU
1	E	547	ASP
1	E	551	LYS
1	E	553	ASN
1	E	559	LEU
1	E	563	HIS
1	E	569	GLN

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Mol	Chain	Res	Type
1	E	570	LEU
1	E	573	ILE
1	E	578	GLN
1	E	579	LEU
1	E	586	LEU
1	E	587	THR
1	E	588	LYS
1	E	593	SER
1	E	597	ILE
1	E	601	ASN
1	E	606	LYS
1	E	607	GLU
1	E	612	LYS
1	E	613	ASN
1	E	614	LEU
1	E	618	THR
1	E	620	ILE
1	E	624	LYS
1	E	626	LEU
1	E	628	ARG
1	E	631	VAL
1	E	632	LEU
1	E	634	GLN
1	E	643	SER
1	E	644	LYS
1	E	649	TRP
1	E	650	GLU
1	E	651	MET
1	E	653	ASN
1	E	655	HIS
1	E	657	VAL
1	F	113	LEU
1	F	127	LEU
1	F	128	ARG
1	F	131	ILE
1	F	132	LEU
1	F	141	GLU
1	F	142	PRO
1	F	146	VAL
1	F	151	GLU
1	F	152	LYS
1	F	154	LYS

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Mol	Chain	Res	Type
1	F	156	LEU
1	F	166	ILE
1	F	169	SER
1	F	178	VAL
1	F	183	ILE
1	F	190	ASN
1	F	195	GLU
1	F	196	GLU
1	F	197	CYS
1	F	198	LYS
1	F	211	VAL
1	F	212	VAL
1	F	221	SER
1	F	225	ARG
1	F	229	SER
1	F	231	ILE
1	F	234	THR
1	F	237	LYS
1	F	239	LEU
1	F	245	ILE
1	F	252	GLU
1	F	253	HIS
1	F	254	LEU
1	F	258	LEU
1	F	259	ASP
1	F	260	GLU
1	F	263	LYS
1	F	270	LYS
1	F	273	ARG
1	F	275	GLU
1	F	277	ARG
1	F	292	LYS
1	F	296	VAL
1	F	300	LEU
1	F	301	ASP
1	F	305	GLU
1	F	306	VAL
1	F	308	VAL
1	F	320	LYS
1	F	329	LEU
1	F	341	ILE
1	F	347	ASP

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Mol	Chain	Res	Type
1	F	348	GLU
1	F	359	SER
1	F	370	GLN
1	F	376	LYS
1	F	380	GLU
1	F	391	LEU
1	F	394	ILE
1	F	396	ARG
1	F	412	TRP
1	F	418	GLU
1	F	430	LEU
1	F	443	ARG
1	F	450	ASN
1	F	451	PRO
1	F	455	TYR
1	F	458	SER
1	F	462	LEU
1	F	463	LYS
1	F	475	GLU
1	F	477	LYS
1	F	498	LEU
1	F	499	LYS
1	F	517	ILE
1	F	523	SER
1	F	527	LEU
1	F	541	GLU
1	F	547	ASP
1	F	551	LYS
1	F	557	VAL
1	F	570	LEU
1	F	573	ILE
1	F	579	LEU
1	F	586	LEU
1	F	588	LYS
1	F	593	SER
1	F	594	LYS
1	F	597	ILE
1	F	598	THR
1	F	602	LEU
1	F	604	GLU
1	F	606	LYS
1	F	612	LYS

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Mol	Chain	Res	Type
1	F	614	LEU
1	F	618	THR
1	F	620	ILE
1	F	630	GLU
1	F	632	LEU
1	F	634	GLN
1	F	643	SER
1	F	644	LYS
1	F	645	THR
1	F	647	GLN
1	F	650	GLU
1	F	651	MET
1	F	654	ILE
1	F	655	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (118) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	GLN
1	A	167	GLN
1	A	176	ASN
1	A	190	ASN
1	A	201	HIS
1	A	266	ASN
1	A	289	GLN
1	A	343	GLN
1	A	425	GLN
1	A	450	ASN
1	A	568	ASN
1	A	574	ASN
1	A	577	ASN
1	A	578	GLN
1	A	599	HIS
1	A	603	ASN
1	A	634	GLN
1	A	647	GLN
1	A	653	ASN
1	B	118	GLN
1	B	123	HIS
1	B	253	HIS
1	B	266	ASN
1	B	289	GLN

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Mol	Chain	Res	Type
1	B	303	HIS
1	B	370	GLN
1	B	425	GLN
1	B	440	HIS
1	B	448	GLN
1	B	450	ASN
1	B	464	ASN
1	B	568	ASN
1	B	574	ASN
1	B	577	ASN
1	B	578	GLN
1	B	581	GLN
1	B	601	ASN
1	B	603	ASN
1	B	609	GLN
1	B	634	GLN
1	B	647	GLN
1	B	653	ASN
1	B	655	HIS
1	C	118	GLN
1	C	190	ASN
1	C	266	ASN
1	C	289	GLN
1	C	343	GLN
1	C	370	GLN
1	C	425	GLN
1	C	450	ASN
1	C	568	ASN
1	C	574	ASN
1	C	578	GLN
1	C	603	ASN
1	C	652	ASN
1	C	653	ASN
1	C	655	HIS
1	D	176	ASN
1	D	190	ASN
1	D	201	HIS
1	D	266	ASN
1	D	289	GLN
1	D	295	GLN
1	D	343	GLN
1	D	410	GLN

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Mol	Chain	Res	Type
1	D	425	GLN
1	D	448	GLN
1	D	450	ASN
1	D	464	ASN
1	D	568	ASN
1	D	574	ASN
1	D	577	ASN
1	D	578	GLN
1	D	603	ASN
1	D	613	ASN
1	D	647	GLN
1	D	653	ASN
1	E	176	ASN
1	E	190	ASN
1	E	194	GLN
1	E	201	HIS
1	E	266	ASN
1	E	343	GLN
1	E	425	GLN
1	E	450	ASN
1	E	464	ASN
1	E	506	ASN
1	E	568	ASN
1	E	574	ASN
1	E	577	ASN
1	E	578	GLN
1	E	581	GLN
1	E	603	ASN
1	E	634	GLN
1	E	647	GLN
1	E	653	ASN
1	F	134	ASN
1	F	176	ASN
1	F	190	ASN
1	F	194	GLN
1	F	201	HIS
1	F	228	HIS
1	F	250	ASN
1	F	274	ASN
1	F	289	GLN
1	F	343	GLN
1	F	425	GLN

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Mol	Chain	Res	Type
1	F	450	ASN
1	F	464	ASN
1	F	568	ASN
1	F	574	ASN
1	F	577	ASN
1	F	578	GLN
1	F	603	ASN
1	F	615	HIS
1	F	647	GLN
1	F	653	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	546/597 (91%)	-0.12	21 (3%)	44	36	19, 33, 61, 95	0
1	B	546/597 (91%)	0.38	36 (6%)	24	21	21, 42, 89, 153	0
1	C	546/597 (91%)	0.20	27 (4%)	35	29	26, 38, 70, 109	0
1	D	546/597 (91%)	0.48	28 (5%)	33	28	27, 52, 81, 121	0
1	E	546/597 (91%)	0.34	29 (5%)	32	27	27, 48, 86, 142	0
1	F	546/597 (91%)	0.76	46 (8%)	17	15	37, 65, 91, 129	0
All	All	3276/3582 (91%)	0.34	187 (5%)	29	24	19, 46, 85, 153	0

All (187) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	657	VAL	6.7
1	B	452	PRO	6.0
1	F	452	PRO	5.7
1	D	657	VAL	5.6
1	A	147	GLY	5.6
1	F	657	VAL	5.2
1	B	456	VAL	5.1
1	B	645	THR	4.9
1	E	456	VAL	4.8
1	A	458	SER	4.7
1	F	458	SER	4.6
1	F	456	VAL	4.4
1	E	549	MET	4.3
1	B	626	LEU	4.2
1	A	455	TYR	4.2
1	B	457	GLY	4.2
1	B	451	PRO	4.1
1	A	148	GLY	4.1
1	A	449	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	E	657	VAL	4.0
1	D	452	PRO	4.0
1	F	598	THR	4.0
1	F	591	ASP	4.0
1	F	442	TYR	3.9
1	C	458	SER	3.8
1	A	457	GLY	3.8
1	E	452	PRO	3.8
1	C	112	TYR	3.8
1	C	455	TYR	3.8
1	E	453	PRO	3.7
1	F	455	TYR	3.7
1	A	456	VAL	3.7
1	B	454	ILE	3.6
1	C	159	GLY	3.6
1	E	413	GLY	3.6
1	B	656	SER	3.5
1	F	451	PRO	3.5
1	D	600	CYS	3.5
1	F	454	ILE	3.5
1	B	458	SER	3.5
1	E	451	PRO	3.5
1	A	454	ILE	3.5
1	E	590	ALA	3.4
1	B	122	TYR	3.4
1	B	655	HIS	3.4
1	C	459	SER	3.4
1	D	451	PRO	3.3
1	C	411	ILE	3.3
1	E	454	ILE	3.2
1	F	248	PHE	3.2
1	D	446	GLY	3.2
1	B	112	TYR	3.2
1	B	646	THR	3.1
1	F	136	GLU	3.1
1	E	193	ARG	3.1
1	D	458	SER	3.1
1	A	452	PRO	3.1
1	E	631	VAL	3.1
1	B	592	GLY	3.1
1	B	401	GLU	3.1
1	B	494	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	631	VAL	3.0
1	F	112	TYR	3.0
1	F	411	ILE	3.0
1	B	455	TYR	2.9
1	B	448	GLN	2.9
1	D	591	ASP	2.9
1	B	654	ILE	2.9
1	D	413	GLY	2.9
1	A	591	ASP	2.9
1	A	657	VAL	2.9
1	B	141	GLU	2.9
1	F	656	SER	2.9
1	B	450	ASN	2.8
1	B	411	ILE	2.8
1	D	411	ILE	2.8
1	D	631	VAL	2.8
1	F	146	VAL	2.8
1	C	456	VAL	2.8
1	E	656	SER	2.8
1	C	452	PRO	2.8
1	C	657	VAL	2.8
1	F	583	ASP	2.8
1	A	656	SER	2.8
1	B	159	GLY	2.8
1	E	461	THR	2.7
1	F	446	GLY	2.7
1	B	453	PRO	2.7
1	A	451	PRO	2.7
1	E	120	PHE	2.7
1	F	302	ALA	2.7
1	A	112	TYR	2.7
1	D	655	HIS	2.7
1	E	551	LYS	2.6
1	D	112	TYR	2.6
1	E	112	TYR	2.6
1	F	144	GLY	2.6
1	F	449	GLY	2.6
1	D	459	SER	2.6
1	D	598	THR	2.6
1	C	339	GLU	2.6
1	E	654	ILE	2.6
1	F	123	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	133	GLY	2.6
1	C	122	TYR	2.6
1	E	545	CYS	2.6
1	F	585	CYS	2.6
1	D	448	GLN	2.6
1	E	595	VAL	2.5
1	C	448	GLN	2.5
1	C	590	ALA	2.5
1	C	655	HIS	2.5
1	E	591	ASP	2.5
1	E	459	SER	2.5
1	B	539	GLY	2.5
1	F	132	LEU	2.5
1	D	455	TYR	2.5
1	C	349	ASP	2.5
1	C	591	ASP	2.5
1	C	614	LEU	2.5
1	A	631	VAL	2.4
1	F	413	GLY	2.4
1	F	145	VAL	2.4
1	C	611	PHE	2.4
1	A	411	ILE	2.4
1	F	350	GLY	2.4
1	C	412	TRP	2.4
1	F	573	ILE	2.4
1	C	451	PRO	2.4
1	D	143	PRO	2.4
1	C	449	GLY	2.4
1	B	590	ALA	2.4
1	F	506	ASN	2.3
1	C	414	GLY	2.3
1	B	591	ASP	2.3
1	E	458	SER	2.3
1	F	141	GLU	2.3
1	B	412	TRP	2.3
1	D	449	GLY	2.3
1	A	412	TRP	2.3
1	F	412	TRP	2.3
1	D	457	GLY	2.3
1	E	256	GLU	2.2
1	B	642	SER	2.2
1	E	449	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	344	GLY	2.2
1	C	506	ASN	2.2
1	E	602	LEU	2.2
1	A	459	SER	2.2
1	F	548	SER	2.2
1	F	632	LEU	2.2
1	D	456	VAL	2.2
1	F	158	LEU	2.2
1	F	445	GLU	2.2
1	B	460	PRO	2.2
1	B	644	LYS	2.2
1	F	582	TYR	2.2
1	C	463	LYS	2.1
1	D	345	GLY	2.1
1	D	166	ILE	2.1
1	A	632	LEU	2.1
1	F	264	LEU	2.1
1	A	196	GLU	2.1
1	B	136	GLU	2.1
1	D	371	GLU	2.1
1	D	445	GLU	2.1
1	F	394	ILE	2.1
1	C	599	HIS	2.1
1	F	453	PRO	2.1
1	E	234	THR	2.1
1	F	273	ARG	2.1
1	B	348	GLU	2.1
1	F	517	ILE	2.1
1	E	531	ASN	2.1
1	D	412	TRP	2.1
1	C	413	GLY	2.0
1	C	196	GLU	2.0
1	D	348	GLU	2.0
1	D	656	SER	2.0
1	D	453	PRO	2.0
1	B	602	LEU	2.0
1	E	601	ASN	2.0
1	F	121	THR	2.0
1	F	355	ALA	2.0
1	F	349	ASP	2.0
1	F	200	TRP	2.0
1	E	455	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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
2	MN	D	701	1/1	0.69	0.15	74,74,74,74	0
2	MN	A	701	1/1	0.75	0.17	87,87,87,87	0
2	MN	B	701	1/1	0.77	0.12	80,80,80,80	0
2	MN	E	701	1/1	0.79	0.10	90,90,90,90	0
2	MN	F	701	1/1	0.85	0.12	82,82,82,82	0
2	MN	C	701	1/1	0.90	0.15	73,73,73,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.