



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 30, 2026 – 03:19 PM UTC

PDB ID : 4ZKT / pdb_00004zkt
Title : Crystal structure of the progenitor M complex of Clostridium botulinum type E neurotoxin
Authors : Eswaramoorthy, S.; Swaminathan, S.
Deposited on : 2015-04-30
Resolution : 3.05 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

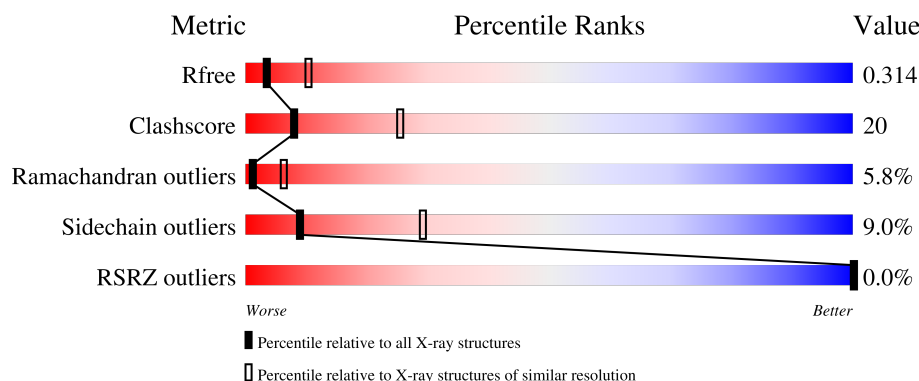
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

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	1252	57% 33% 8% .
1	C	1252	58% 34% 7% .
1	E	1252	57% 34% 8% .
2	B	1163	52% 36% 7% .
2	D	1163	52% 36% 7% .

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Mol	Chain	Length	Quality of chain
2	F	1163	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: green (52%), yellow (35%), and orange (8%). The orange segment is further divided into two sub-segments, each marked with a dot (••).

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 56952 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 Bontoxilysin A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1235	Total	C	N	O	S	0	0	0
			9978	6351	1665	1940	22			
1	C	1235	Total	C	N	O	S	0	0	0
			9978	6351	1665	1940	22			
1	E	1235	Total	C	N	O	S	0	0	0
			9978	6351	1665	1940	22			

- Molecule 2 is a protein called Botulinum neurotoxin type E, nontoxic-nonhemagglutinin component, NTNH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1114	Total	C	N	O	S	0	0	0
			9005	5804	1451	1726	24			
2	D	1114	Total	C	N	O	S	0	0	0
			9005	5804	1451	1726	24			
2	F	1114	Total	C	N	O	S	0	0	0
			9005	5804	1451	1726	24			

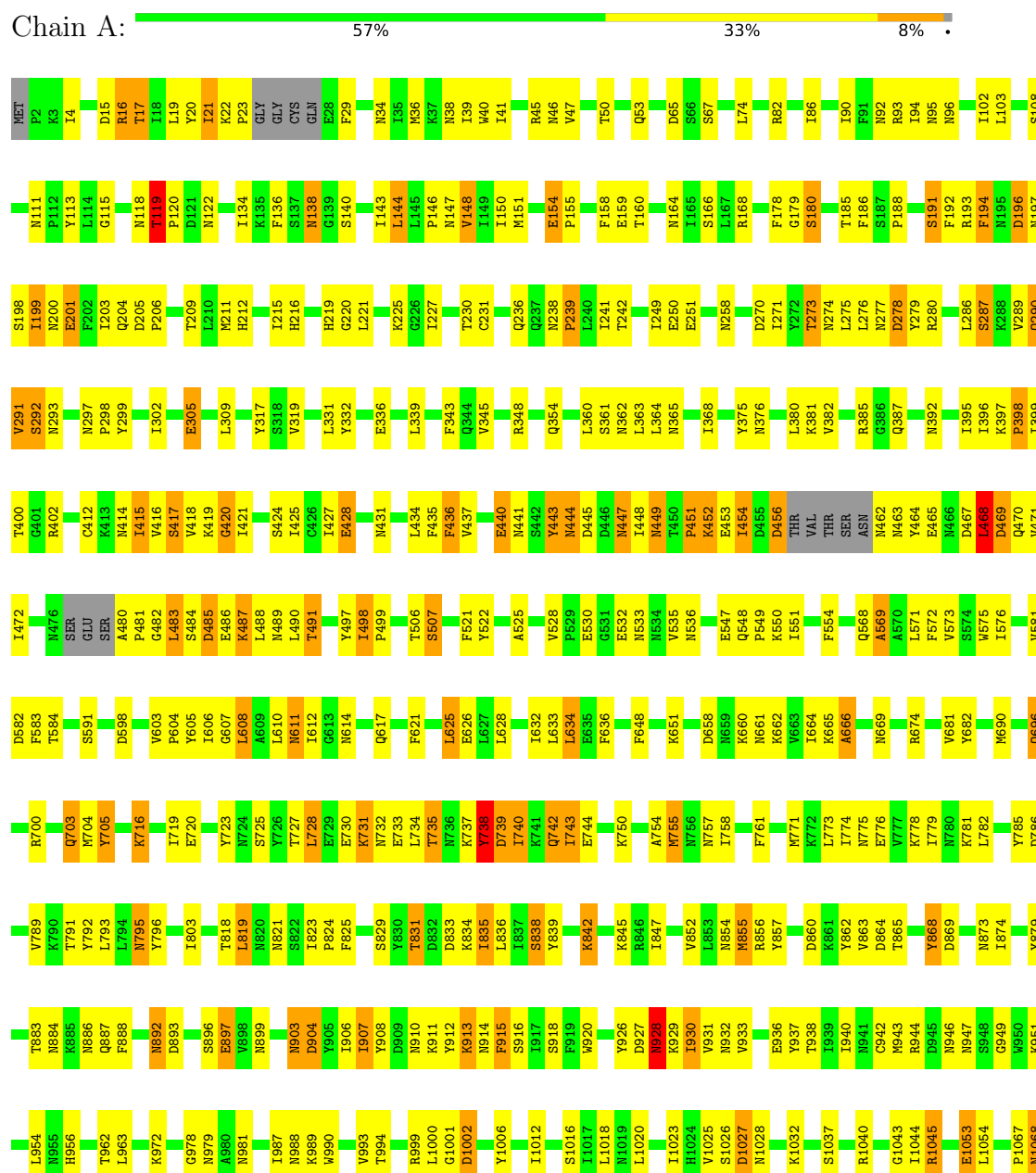
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

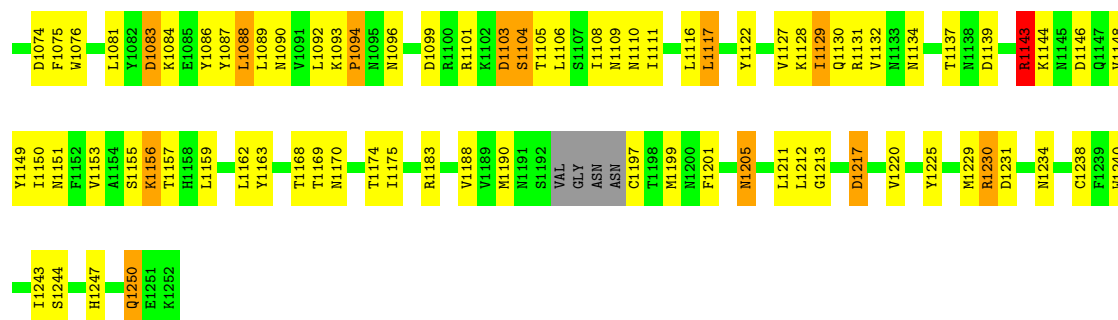
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	E	1	Total	Zn	0	0
			1	1		

3 Residue-property plots [i](#)

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.

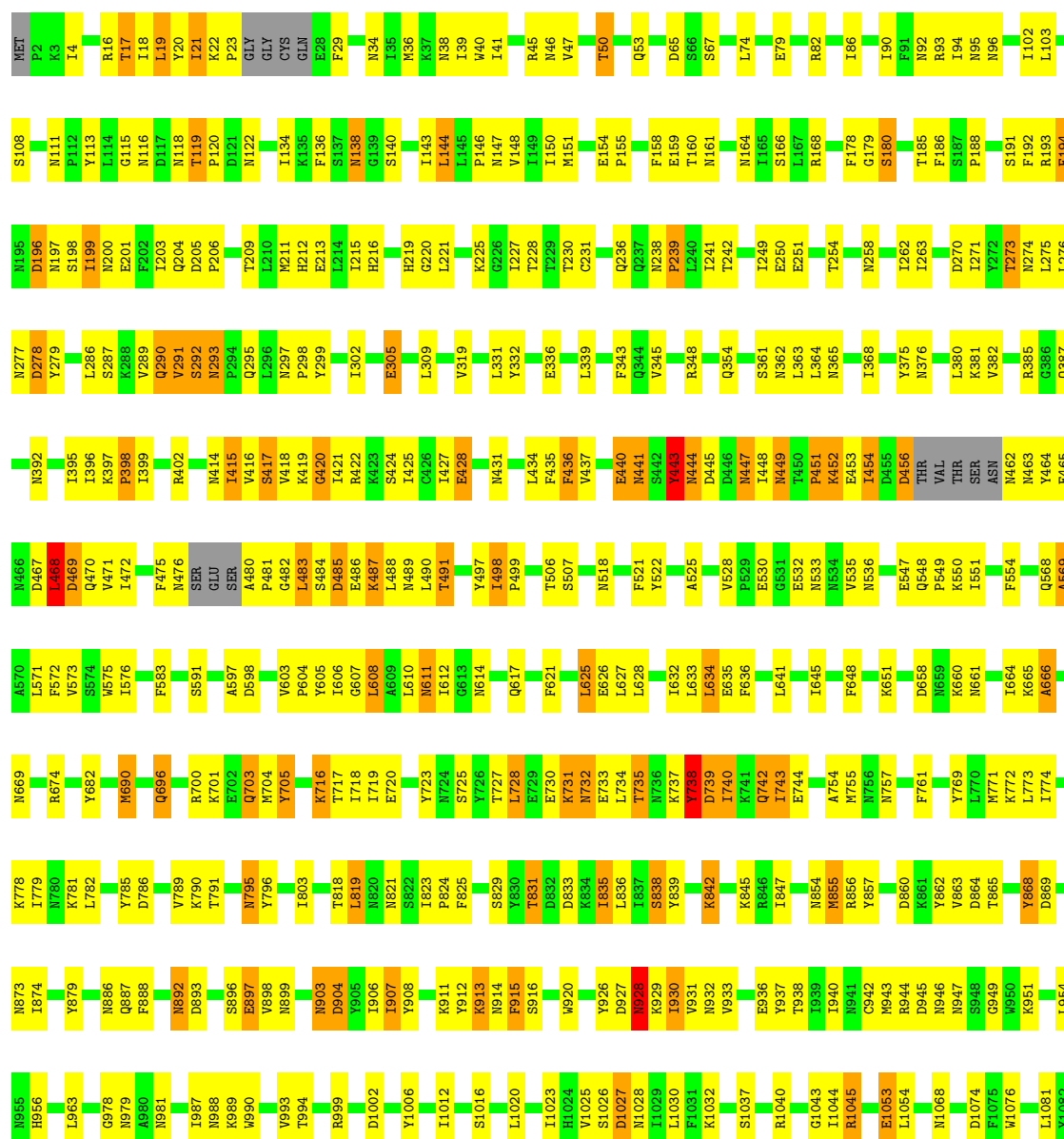
• Molecule 1: Bontoxilysin A

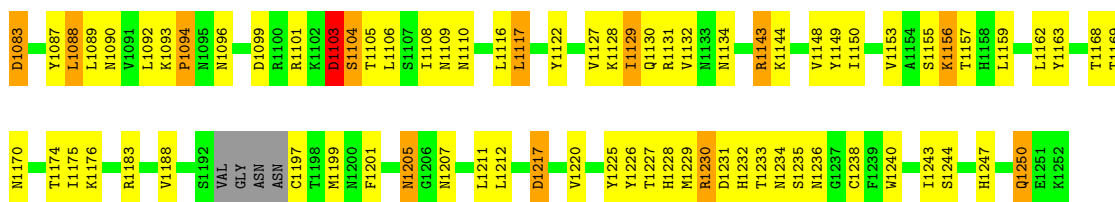




● Molecule 1: Bontoxilysin A

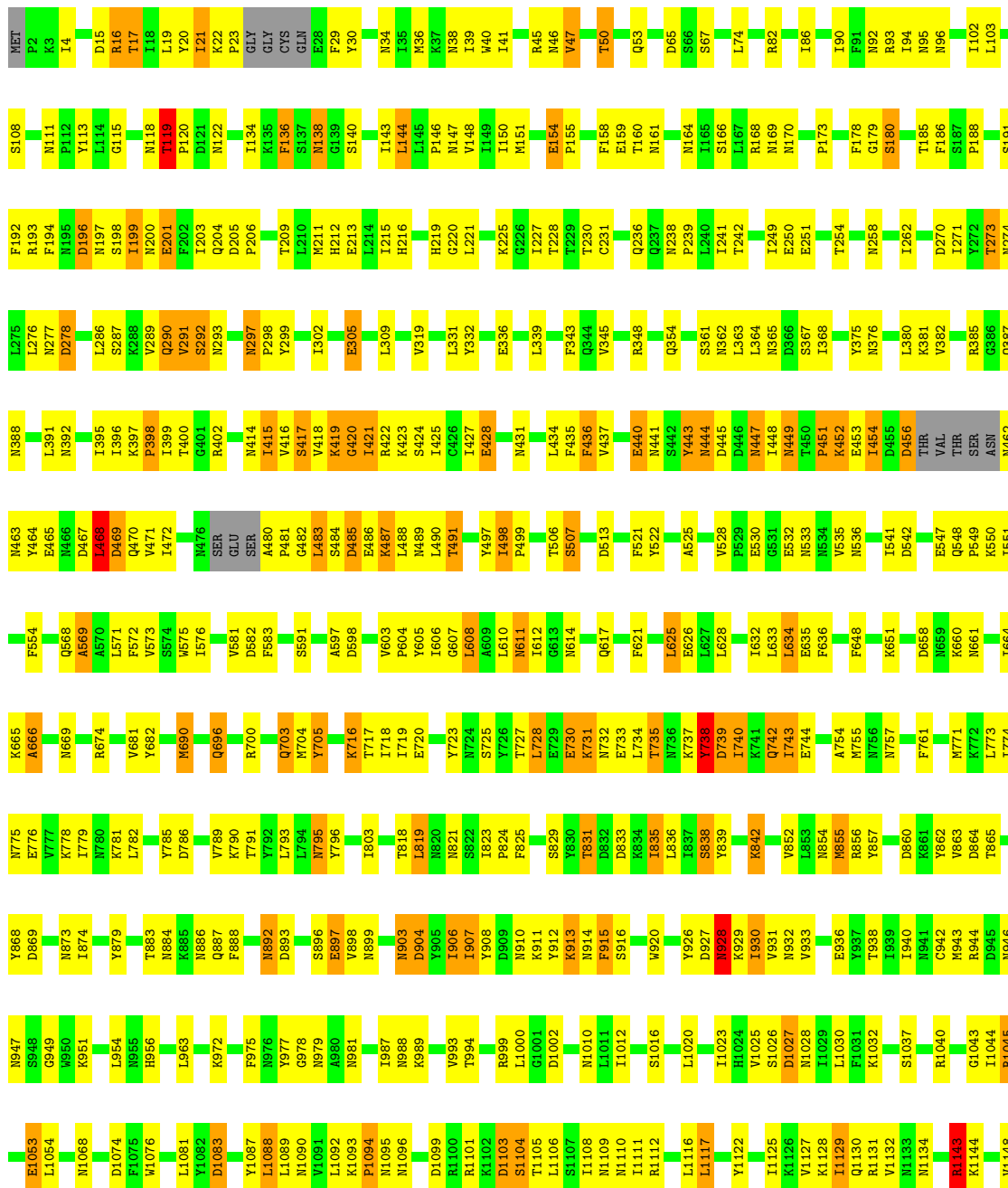
Chain C: 58% 34% 7%



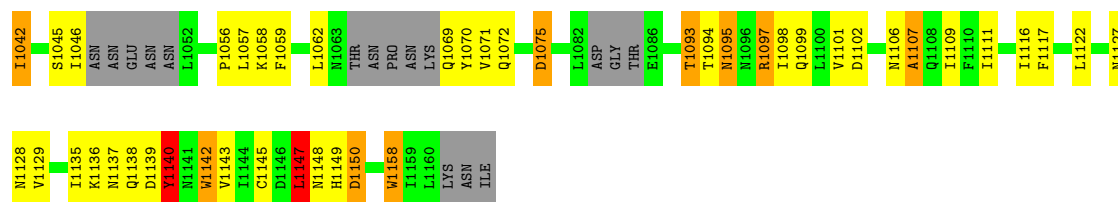


• Molecule 1: Bontoxilysin A

Chain E: 57% 34% 8%

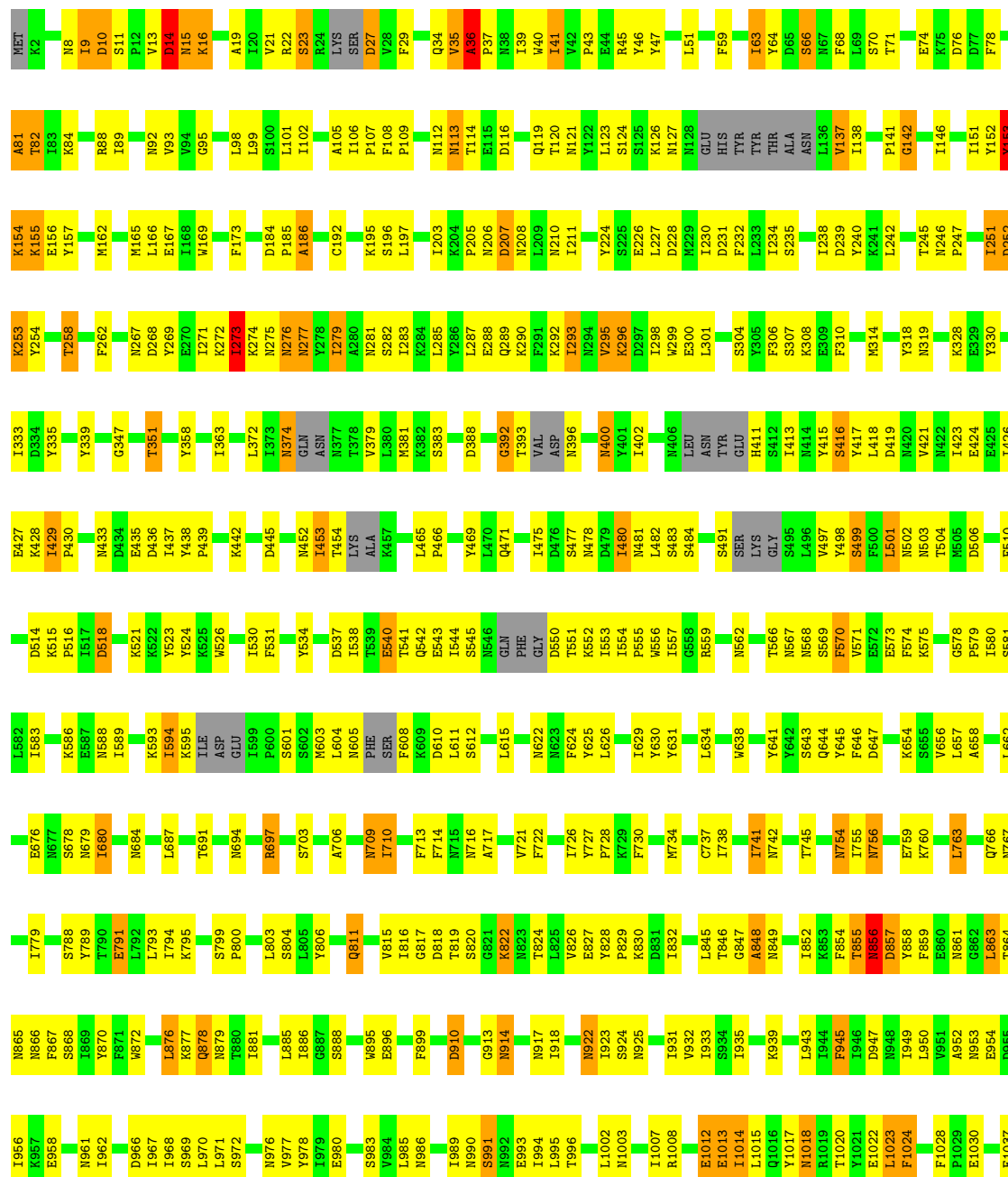






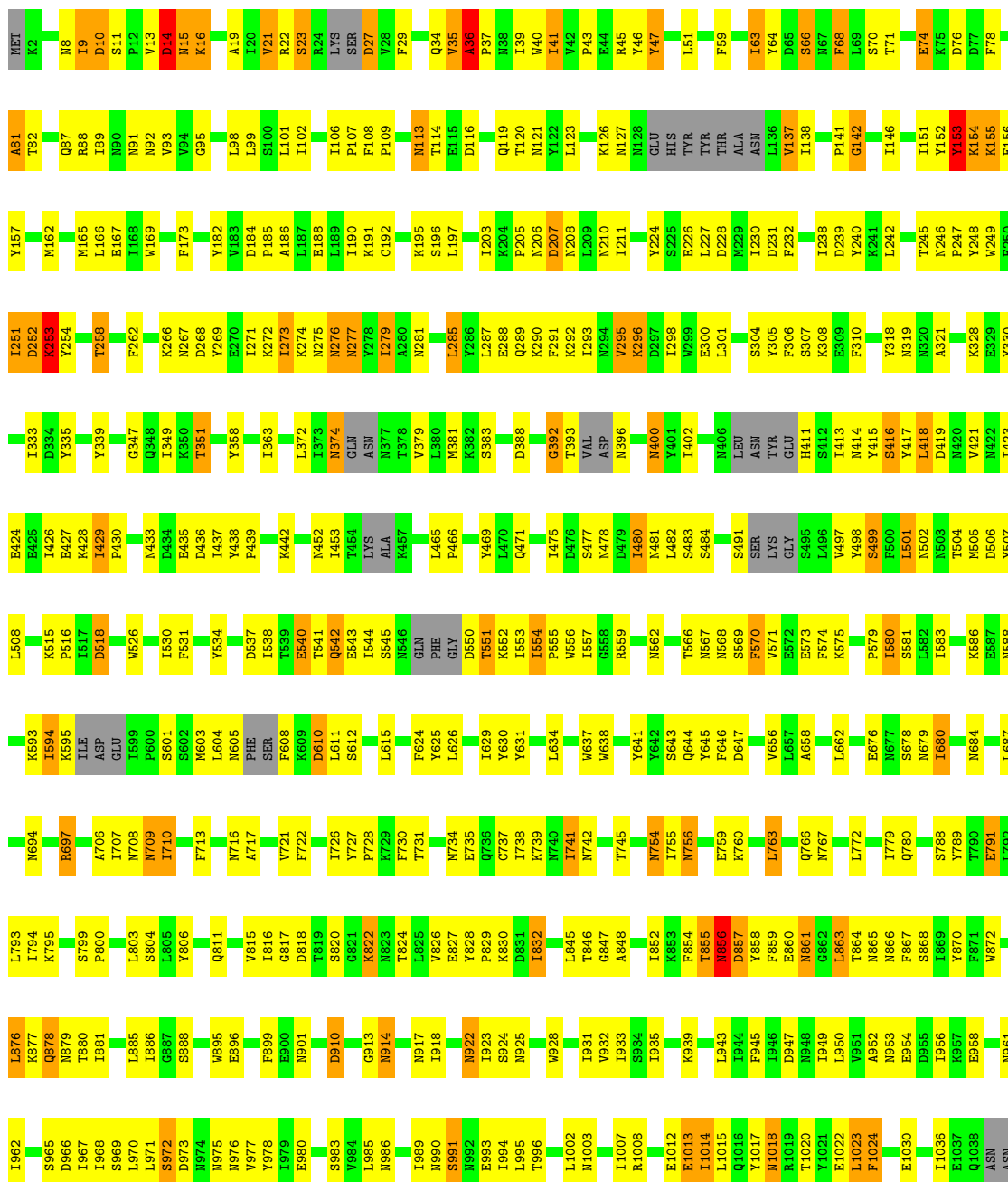
- Molecule 2: Botulinum neurotoxin type E, nontoxic-nonhemagglutinin component, NTNH

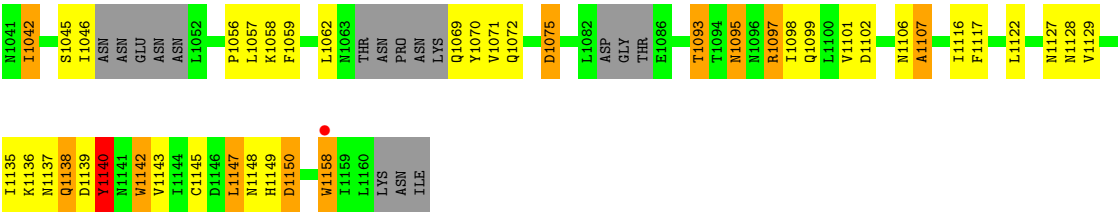
Chain D: 52% 36% 7% . .



- Molecule 2: Botulinum neurotoxin type E, nontoxic-nonhemagglutinin component, NTNH

Chain F:





4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	192.60Å 192.60Å 286.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.30 – 3.05 49.30 – 3.05	Depositor EDS
% Data completeness (in resolution range)	59.7 (49.30-3.05) 59.8 (49.30-3.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 3.07Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.243 , 0.321 0.247 , 0.314	Depositor DCC
R_{free} test set	1630 reflections (0.69%)	wwPDB-VP
Wilson B-factor (Å ²)	110.6	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 189.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	0.135 for -h,-k,l 0.196 for h,-h-k,-l 0.137 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	56952	wwPDB-VP
Average B, all atoms (Å ²)	134.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.18% 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 [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.75	0/10176	1.00	14/13800 (0.1%)
1	C	0.73	0/10176	1.00	11/13800 (0.1%)
1	E	0.70	0/10176	0.98	13/13800 (0.1%)
2	B	0.85	9/9182 (0.1%)	1.04	19/12454 (0.2%)
2	D	0.80	12/9182 (0.1%)	1.02	20/12454 (0.2%)
2	F	0.77	8/9182 (0.1%)	1.01	17/12454 (0.1%)
All	All	0.77	29/58074 (0.0%)	1.01	94/78762 (0.1%)

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

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

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	116	ASP	C-O	8.53	1.33	1.24
2	D	116	ASP	C-O	7.35	1.32	1.24
2	B	116	ASP	N-CA	7.05	1.54	1.46
2	F	116	ASP	N-CA	6.67	1.54	1.46
2	B	392	GLY	N-CA	6.50	1.51	1.45
2	B	551	THR	N-CA	6.44	1.54	1.45
2	B	116	ASP	CA-C	6.42	1.60	1.52
2	D	116	ASP	N-CA	6.26	1.53	1.46
2	D	945	PHE	CA-C	-5.90	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	35	VAL	CA-C	5.83	1.60	1.52
2	B	35	VAL	CA-CB	5.75	1.62	1.54
2	D	392	GLY	N-CA	5.73	1.50	1.45
2	D	119	GLN	C-O	5.66	1.30	1.23
2	F	116	ASP	C-O	5.56	1.30	1.24
2	D	120	THR	CA-C	5.48	1.59	1.52
2	D	282	SER	C-O	5.43	1.28	1.24
2	F	35	VAL	CA-C	5.41	1.59	1.52
2	D	116	ASP	CA-C	5.40	1.59	1.52
2	F	123	LEU	C-O	5.39	1.30	1.24
2	B	283	ILE	CA-C	5.38	1.58	1.53
2	F	35	VAL	CA-CB	5.34	1.61	1.54
2	F	551	THR	N-CA	5.31	1.52	1.45
2	D	283	ILE	CA-C	5.30	1.58	1.53
2	F	392	GLY	N-CA	5.26	1.50	1.45
2	D	124	SER	C-O	5.22	1.30	1.23
2	F	120	THR	CA-C	5.19	1.59	1.52
2	D	35	VAL	CA-CB	5.19	1.61	1.54
2	B	282	SER	C-O	5.12	1.28	1.24
2	D	123	LEU	CA-C	5.10	1.59	1.52

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	36	ALA	CA-C-N	11.14	133.77	119.84
2	B	36	ALA	C-N-CA	11.14	133.77	119.84
2	D	36	ALA	CA-C-N	10.87	133.42	119.84
2	D	36	ALA	C-N-CA	10.87	133.42	119.84
2	F	36	ALA	CA-C-N	10.82	133.36	119.84
2	F	36	ALA	C-N-CA	10.82	133.36	119.84
1	A	489	ASN	N-CA-C	8.21	121.89	107.61
1	E	464	TYR	N-CA-C	8.08	121.44	109.24
1	C	489	ASN	N-CA-C	8.05	121.62	107.61
1	C	1023	ILE	N-CA-C	7.83	119.08	108.11
1	E	489	ASN	N-CA-C	7.64	121.28	108.13
1	A	464	TYR	N-CA-C	7.36	120.10	109.14
1	A	1023	ILE	N-CA-C	7.32	118.36	108.11
1	E	1023	ILE	N-CA-C	7.28	118.30	108.11
1	C	464	TYR	N-CA-C	7.14	120.03	109.24
2	B	116	ASP	N-CA-C	6.92	118.71	111.03
2	D	1023	LEU	N-CA-C	6.86	120.64	109.59
2	B	137	VAL	N-CA-C	6.85	117.70	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1062	LEU	N-CA-C	6.62	116.79	108.45
2	F	137	VAL	N-CA-C	6.61	117.36	108.11
2	B	1023	LEU	N-CA-C	6.50	120.05	109.59
2	F	1023	LEU	N-CA-C	6.45	119.97	109.59
2	F	1042	ILE	N-CA-C	6.36	116.55	106.88
2	D	116	ASP	N-CA-C	6.36	118.08	111.03
1	C	115	GLY	N-CA-C	-6.34	104.25	111.85
2	D	137	VAL	N-CA-C	6.33	116.98	108.11
1	E	115	GLY	N-CA-C	-6.29	104.30	111.85
2	F	116	ASP	N-CA-C	6.25	117.96	111.03
1	A	115	GLY	N-CA-C	-6.21	104.39	111.85
2	F	594	ILE	N-CA-C	6.12	117.92	108.44
2	D	594	ILE	N-CA-C	6.05	117.81	108.44
2	D	1042	ILE	N-CA-C	6.04	116.06	106.88
2	B	1042	ILE	N-CA-C	5.99	115.99	106.88
2	B	594	ILE	N-CA-C	5.93	117.63	108.44
2	B	392	GLY	N-CA-C	5.92	119.75	111.10
2	F	47	TYR	N-CA-C	5.87	118.43	111.33
2	B	1111	ILE	N-CA-C	-5.79	102.06	109.30
1	A	21	ILE	N-CA-C	5.76	116.98	108.45
1	A	662	LYS	N-CA-C	-5.75	105.93	113.12
2	B	1062	LEU	N-CA-C	5.72	116.64	108.74
2	D	741	ILE	CB-CA-C	-5.69	104.46	112.14
2	B	741	ILE	CB-CA-C	-5.66	104.49	112.14
2	F	34	GLN	N-CA-C	5.66	117.21	110.19
2	F	477	SER	N-CA-C	5.64	117.58	110.24
2	F	1150	ASP	N-CA-C	5.63	118.23	110.35
1	C	1023	ILE	CB-CA-C	-5.54	102.43	110.63
1	A	868	TYR	N-CA-C	-5.53	101.86	110.10
1	C	868	TYR	N-CA-C	-5.53	101.86	110.10
2	D	1062	LEU	N-CA-C	5.53	116.36	108.74
2	B	1150	ASP	N-CA-C	5.51	118.07	110.35
1	E	906	ILE	CB-CA-C	-5.47	106.25	111.44
2	D	1150	ASP	N-CA-C	5.47	118.00	110.35
1	A	412	CYS	N-CA-C	5.46	117.25	107.80
2	B	47	TYR	N-CA-C	5.46	117.94	111.33
2	B	477	SER	N-CA-C	5.46	117.34	110.24
1	E	21	ILE	N-CA-C	5.44	116.50	108.45
2	D	392	GLY	N-CA-C	5.39	118.96	111.10
1	C	928	ASN	N-CA-C	5.38	122.25	110.80
1	C	906	ILE	CB-CA-C	-5.37	106.33	111.44
1	A	148	VAL	N-CA-C	5.36	116.39	108.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	554	ILE	CB-CA-C	-5.34	104.64	110.78
2	D	119	GLN	N-CA-C	5.34	116.25	108.14
2	F	119	GLN	N-CA-C	5.34	116.25	108.14
2	D	477	SER	N-CA-C	5.30	117.14	110.24
1	A	1143	ARG	NE-CZ-NH2	5.30	123.97	119.20
1	C	415	ILE	N-CA-C	5.29	116.10	108.48
1	C	21	ILE	N-CA-C	5.29	116.28	108.45
2	B	996	THR	N-CA-C	-5.27	104.59	111.02
2	F	741	ILE	CB-CA-C	-5.27	105.03	112.14
2	B	938	LEU	N-CA-C	-5.26	105.63	111.36
2	D	445	ASP	N-CA-C	-5.23	103.01	110.59
1	E	1143	ARG	NE-CZ-NH2	5.23	123.90	119.20
1	A	119	THR	CA-C-N	-5.22	114.58	119.85
1	A	119	THR	C-N-CA	-5.22	114.58	119.85
1	E	415	ILE	N-CA-C	5.20	115.97	108.48
2	D	293	ILE	N-CA-C	5.20	115.71	108.84
2	F	392	GLY	N-CA-C	5.20	118.69	111.10
2	B	1037	GLU	N-CA-C	5.18	117.06	109.24
1	C	443	TYR	N-CA-C	5.17	117.91	111.24
2	D	1116	ILE	N-CA-C	5.13	115.35	110.42
1	A	928	ASN	N-CA-C	5.12	121.71	110.80
1	E	119	THR	CA-C-N	-5.12	114.68	119.85
1	E	119	THR	C-N-CA	-5.12	114.68	119.85
1	A	415	ILE	N-CA-C	5.10	115.83	108.48
1	E	47	VAL	CB-CA-C	-5.10	104.89	111.88
2	D	34	GLN	N-CA-C	5.09	116.50	110.19
1	E	730	GLU	N-CA-C	-5.07	105.44	110.97
1	E	928	ASN	N-CA-C	5.06	121.58	110.80
2	F	21	VAL	N-CA-C	5.03	117.26	108.95
2	B	119	GLN	N-CA-C	5.03	116.16	108.42
2	B	413	ILE	N-CA-C	5.02	115.19	108.17
2	D	578	GLY	CA-C-N	5.02	126.11	119.84
2	D	578	GLY	C-N-CA	5.02	126.11	119.84
2	D	1037	GLU	N-CA-C	5.00	116.80	109.24

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	36	ALA	Peptide
2	D	36	ALA	Peptide
2	F	1138	GLN	Peptide

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Mol	Chain	Res	Type	Group
2	F	36	ALA	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	9978	0	9735	358	1
1	C	9978	0	9735	377	1
1	E	9978	0	9735	378	0
2	B	9005	0	8666	391	0
2	D	9005	0	8666	375	0
2	F	9005	0	8666	388	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
All	All	56952	0	55203	2202	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (2202) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:885:LEU:HG	2:D:886:ILE:HD12	1.33	1.09
2:F:885:LEU:HG	2:F:886:ILE:HD12	1.32	1.09
2:B:436:ASP:HA	2:B:437:ILE:HB	1.34	1.08
2:B:885:LEU:HG	2:B:886:ILE:HD12	1.29	1.08
2:D:436:ASP:HA	2:D:437:ILE:HB	1.35	1.05
2:F:436:ASP:HA	2:F:437:ILE:HB	1.37	1.03
2:B:818:ASP:OD2	2:B:820:SER:OG	1.79	0.99
2:F:818:ASP:OD2	2:F:820:SER:OG	1.80	0.98
2:D:818:ASP:OD2	2:D:820:SER:OG	1.80	0.98
1:C:1130:GLN:O	1:C:1148:VAL:HG23	1.63	0.98
1:A:1130:GLN:O	1:A:1148:VAL:HG23	1.66	0.96
1:E:1130:GLN:O	1:E:1148:VAL:HG23	1.66	0.95
1:C:628:LEU:HB2	1:E:419:LYS:HE3	1.48	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:VAL:HB	1:A:290:GLN:HA	1.49	0.91
1:E:238:ASN:CG	1:E:239:PRO:HD2	1.96	0.89
2:B:879:ASN:HB3	2:B:881:ILE:HG22	1.54	0.89
1:C:289:VAL:HB	1:C:290:GLN:HA	1.53	0.89
1:A:238:ASN:CG	1:A:239:PRO:HD2	1.98	0.89
2:D:879:ASN:HB3	2:D:881:ILE:HG22	1.55	0.89
1:E:289:VAL:HB	1:E:290:GLN:HA	1.53	0.88
1:C:227:ILE:HD11	1:C:274:ASN:HB2	1.57	0.86
1:A:289:VAL:HB	1:A:290:GLN:CA	2.06	0.86
2:D:1045:SER:OG	2:D:1046:ILE:N	2.09	0.86
1:C:855:MET:O	1:C:856:ARG:HD3	1.76	0.85
2:F:879:ASN:HB3	2:F:881:ILE:HG22	1.58	0.85
1:A:227:ILE:HD11	1:A:274:ASN:HB2	1.59	0.84
1:A:855:MET:O	1:A:856:ARG:HD3	1.77	0.84
1:C:238:ASN:CG	1:C:239:PRO:HD2	2.03	0.84
1:E:227:ILE:HD11	1:E:274:ASN:HB2	1.58	0.84
2:F:1045:SER:OG	2:F:1046:ILE:N	2.07	0.84
1:C:289:VAL:HB	1:C:290:GLN:CA	2.09	0.83
1:E:855:MET:O	1:E:856:ARG:HD3	1.79	0.83
1:E:289:VAL:HB	1:E:290:GLN:CA	2.09	0.83
2:D:1137:ASN:HB3	2:D:1142:TRP:HE1	1.46	0.81
1:A:1155:SER:O	1:A:1157:THR:N	2.13	0.81
1:A:522:TYR:CE2	1:A:611:ASN:HB2	2.16	0.81
2:B:1045:SER:OG	2:B:1046:ILE:N	2.12	0.81
1:A:897:GLU:HG2	1:A:1032:LYS:HB2	1.61	0.81
1:E:1155:SER:O	1:E:1157:THR:N	2.13	0.81
1:E:522:TYR:CE2	1:E:611:ASN:HB2	2.17	0.80
1:C:1155:SER:O	1:C:1157:THR:N	2.14	0.80
2:B:1137:ASN:HB3	2:B:1142:TRP:HE1	1.47	0.79
1:E:421:ILE:HD11	2:D:510:PHE:CD1	2.17	0.79
1:E:513:ASP:OD1	2:D:521:LYS:NZ	2.16	0.79
1:C:627:LEU:HB3	1:E:419:LYS:HE2	1.65	0.79
1:C:522:TYR:CE2	1:C:611:ASN:HB2	2.17	0.78
1:E:897:GLU:HG2	1:E:1032:LYS:HB2	1.65	0.77
2:F:1137:ASN:HB3	2:F:1142:TRP:HE1	1.48	0.77
2:F:603:MET:O	2:F:605:ASN:N	2.17	0.76
1:A:199:ILE:HA	1:A:705:TYR:HE2	1.50	0.76
1:C:897:GLU:HG2	1:C:1032:LYS:HB2	1.67	0.76
2:B:815:VAL:O	2:B:816:ILE:HG13	1.87	0.74
2:D:526:TRP:CE2	2:D:530:ILE:HD11	2.23	0.74
1:E:728:LEU:HA	1:E:731:LYS:HB2	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:436:PHE:C	1:C:436:PHE:HD1	1.96	0.74
1:A:610:LEU:HD11	1:A:704:MET:HE2	1.69	0.74
2:F:108:PHE:HB3	2:F:162:MET:HG3	1.70	0.73
2:B:108:PHE:HB3	2:B:162:MET:HG3	1.69	0.73
1:A:836:LEU:HD11	2:B:945:PHE:CD1	2.24	0.73
2:B:603:MET:O	2:B:605:ASN:N	2.22	0.73
2:B:526:TRP:CE2	2:B:530:ILE:HD11	2.24	0.73
2:D:381:MET:HE1	2:D:471:GLN:HB3	1.69	0.73
1:C:836:LEU:HB2	2:D:995:LEU:HD11	1.69	0.73
1:E:436:PHE:HD1	1:E:436:PHE:C	1.96	0.73
1:A:728:LEU:HA	1:A:731:LYS:HB2	1.70	0.73
1:C:728:LEU:HA	1:C:731:LYS:HB2	1.69	0.73
2:D:603:MET:O	2:D:605:ASN:N	2.21	0.73
2:B:1127:ASN:O	2:B:1129:VAL:N	2.22	0.72
2:F:556:TRP:HA	2:F:559:ARG:HD3	1.71	0.72
1:A:227:ILE:HD12	1:A:271:ILE:HA	1.72	0.72
1:E:436:PHE:C	1:E:436:PHE:CD1	2.67	0.72
2:F:381:MET:HE1	2:F:471:GLN:HB3	1.70	0.72
1:C:436:PHE:C	1:C:436:PHE:CD1	2.66	0.72
2:D:815:VAL:O	2:D:816:ILE:HG13	1.89	0.72
2:F:436:ASP:HA	2:F:437:ILE:CB	2.16	0.72
2:B:381:MET:HE1	2:B:471:GLN:HB3	1.71	0.72
2:D:108:PHE:HB3	2:D:162:MET:HG3	1.72	0.72
2:F:815:VAL:O	2:F:816:ILE:HG13	1.90	0.71
1:A:436:PHE:C	1:A:436:PHE:HD1	1.97	0.71
1:A:436:PHE:C	1:A:436:PHE:CD1	2.68	0.71
1:C:199:ILE:HA	1:C:705:TYR:HE2	1.53	0.71
2:D:469:TYR:CZ	2:D:562:ASN:HB2	2.25	0.71
2:B:59:PHE:HB2	2:B:452:ASN:ND2	2.06	0.71
1:C:610:LEU:HD11	1:C:704:MET:HE2	1.71	0.71
2:D:63:ILE:HD12	2:D:358:TYR:HB3	1.72	0.71
2:F:469:TYR:CZ	2:F:562:ASN:HB2	2.26	0.71
1:C:118:ASN:HA	1:C:119:THR:HB	1.74	0.70
1:E:738:TYR:HA	1:E:743:ILE:HG13	1.73	0.70
2:F:626:LEU:HA	2:F:629:ILE:HD12	1.74	0.70
2:B:876:LEU:O	2:B:877:LYS:HB2	1.92	0.70
2:B:63:ILE:HD12	2:B:358:TYR:HB3	1.73	0.70
1:E:199:ILE:HA	1:E:705:TYR:HE2	1.56	0.70
2:F:21:VAL:HG13	2:F:121:ASN:HA	1.72	0.70
1:E:610:LEU:HD11	1:E:704:MET:HE2	1.71	0.69
2:F:526:TRP:CE2	2:F:530:ILE:HD11	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ASN:ND2	1:A:239:PRO:HD2	2.06	0.69
2:B:556:TRP:HA	2:B:559:ARG:HD3	1.75	0.69
2:D:121:ASN:CB	2:D:127:ASN:HA	2.22	0.69
2:F:59:PHE:HB2	2:F:452:ASN:ND2	2.08	0.69
1:A:118:ASN:HA	1:A:119:THR:HB	1.74	0.69
1:C:944:ARG:HG2	1:C:1026:SER:HA	1.72	0.69
2:F:224:TYR:O	2:F:392:GLY:HA2	1.93	0.69
2:D:867:PHE:HB2	2:D:985:LEU:O	1.93	0.68
1:C:227:ILE:HD12	1:C:271:ILE:HA	1.75	0.68
2:D:224:TYR:O	2:D:392:GLY:HA2	1.93	0.68
2:F:876:LEU:O	2:F:877:LYS:HB2	1.93	0.68
2:B:21:VAL:HG13	2:B:121:ASN:HA	1.75	0.68
1:A:705:TYR:CD1	1:A:705:TYR:C	2.72	0.68
2:D:626:LEU:HA	2:D:629:ILE:HD12	1.76	0.68
1:E:238:ASN:ND2	1:E:239:PRO:HD2	2.07	0.68
2:B:626:LEU:HA	2:B:629:ILE:HD12	1.74	0.68
2:F:63:ILE:HD12	2:F:358:TYR:HB3	1.76	0.68
1:C:449:ASN:O	1:C:451:PRO:HD3	1.94	0.68
2:D:556:TRP:HA	2:D:559:ARG:HD3	1.76	0.68
2:B:469:TYR:CZ	2:B:562:ASN:HB2	2.28	0.68
1:E:944:ARG:HG2	1:E:1026:SER:HA	1.75	0.67
2:D:1149:HIS:CG	2:D:1150:ASP:N	2.62	0.67
1:E:449:ASN:O	1:E:451:PRO:HD3	1.94	0.67
1:E:836:LEU:HB2	2:F:995:LEU:HD11	1.75	0.67
1:E:227:ILE:HD12	1:E:271:ILE:HA	1.76	0.67
1:A:738:TYR:HA	1:A:743:ILE:HG13	1.76	0.67
1:C:1207:ASN:OD1	2:D:811:GLN:N	2.28	0.67
2:D:876:LEU:O	2:D:877:LYS:HB2	1.94	0.67
2:D:59:PHE:HB2	2:D:452:ASN:ND2	2.08	0.67
2:D:423:ILE:HG23	2:D:423:ILE:O	1.94	0.67
2:B:1149:HIS:CG	2:B:1150:ASP:N	2.62	0.67
1:C:738:TYR:HA	1:C:743:ILE:HG13	1.76	0.67
1:A:449:ASN:O	1:A:451:PRO:HD3	1.94	0.67
2:D:1127:ASN:O	2:D:1129:VAL:N	2.27	0.66
1:A:20:TYR:HB3	1:A:29:PHE:HB3	1.77	0.66
1:E:904:ASP:HA	1:E:907:ILE:HD11	1.75	0.66
2:B:393:THR:HG1	2:B:396:ASN:N	1.92	0.66
2:F:1127:ASN:O	2:F:1129:VAL:N	2.27	0.66
2:B:295:VAL:O	2:B:298:ILE:N	2.29	0.66
2:B:436:ASP:HA	2:B:437:ILE:CB	2.12	0.66
2:F:423:ILE:O	2:F:423:ILE:HG23	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:867:PHE:HB2	2:F:985:LEU:O	1.95	0.66
2:B:423:ILE:HG23	2:B:423:ILE:O	1.93	0.66
1:A:944:ARG:HG2	1:A:1026:SER:HA	1.76	0.66
2:F:1149:HIS:CG	2:F:1150:ASP:N	2.64	0.66
2:B:877:LYS:HB3	2:B:878:GLN:HB3	1.78	0.66
1:E:154:GLU:HB2	1:E:155:PRO:HD2	1.78	0.66
1:C:154:GLU:HB2	1:C:155:PRO:HD2	1.77	0.65
1:C:705:TYR:CD1	1:C:705:TYR:C	2.74	0.65
2:D:21:VAL:HG13	2:D:121:ASN:HA	1.77	0.65
2:F:877:LYS:HB3	2:F:878:GLN:HB3	1.78	0.65
1:C:628:LEU:CB	1:E:419:LYS:HE3	2.25	0.65
2:D:877:LYS:HB3	2:D:878:GLN:HB3	1.78	0.65
1:E:118:ASN:HA	1:E:119:THR:HB	1.77	0.65
1:E:928:ASN:HB3	1:E:930:ILE:HG22	1.77	0.65
2:B:867:PHE:HB2	2:B:985:LEU:O	1.97	0.65
2:D:1013:GLU:O	2:D:1014:ILE:HB	1.97	0.65
2:F:121:ASN:CB	2:F:127:ASN:HA	2.27	0.65
1:C:238:ASN:ND2	1:C:239:PRO:HD2	2.11	0.65
2:B:121:ASN:CB	2:B:127:ASN:HA	2.26	0.65
1:E:771:MET:HA	1:E:774:ILE:HG22	1.79	0.64
1:A:928:ASN:HB3	1:A:930:ILE:HG22	1.79	0.64
1:C:415:ILE:HD12	1:C:425:ILE:HD12	1.78	0.64
1:C:836:LEU:HD11	2:D:945:PHE:CD1	2.32	0.64
1:E:236:GLN:HB3	1:E:241:ILE:HD13	1.79	0.64
1:E:926:TYR:HB3	1:E:1250:GLN:CG	2.28	0.64
1:A:216:HIS:NE2	1:A:251:GLU:OE1	2.30	0.64
1:A:289:VAL:CB	1:A:290:GLN:HA	2.23	0.64
1:A:771:MET:HA	1:A:774:ILE:HG22	1.79	0.64
1:A:987:ILE:C	1:A:989:LYS:H	2.06	0.64
1:A:926:TYR:HB3	1:A:1250:GLN:CG	2.28	0.64
1:E:216:HIS:NE2	1:E:251:GLU:OE1	2.31	0.64
2:B:1013:GLU:O	2:B:1014:ILE:HB	1.97	0.64
1:A:415:ILE:HD12	1:A:425:ILE:HD12	1.79	0.64
1:A:468:LEU:O	1:A:470:GLN:N	2.31	0.64
1:E:705:TYR:C	1:E:705:TYR:CD1	2.75	0.64
1:E:836:LEU:HD11	2:F:945:PHE:CD1	2.33	0.64
2:B:1137:ASN:HB3	2:B:1142:TRP:NE1	2.13	0.64
2:D:552:LYS:O	2:D:713:PHE:HD1	1.81	0.64
2:B:35:VAL:HG12	2:B:36:ALA:H	1.63	0.64
2:D:35:VAL:HG12	2:D:36:ALA:H	1.63	0.64
2:F:1013:GLU:O	2:F:1014:ILE:HB	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:415:ILE:HD12	1:E:425:ILE:HD12	1.79	0.64
1:E:468:LEU:O	1:E:470:GLN:N	2.30	0.63
1:A:904:ASP:HA	1:A:907:ILE:HD11	1.79	0.63
2:B:13:VAL:HG12	2:B:14:ASP:N	2.14	0.63
2:B:579:PRO:C	2:B:581:SER:H	2.06	0.63
2:B:1122:LEU:HD21	2:B:1158:TRP:CZ2	2.33	0.63
1:C:365:ASN:O	1:C:368:ILE:HG22	1.97	0.63
2:B:224:TYR:O	2:B:392:GLY:HA2	1.97	0.63
1:E:454:ILE:HD13	1:E:666:ALA:HA	1.79	0.63
2:B:990:ASN:HB3	2:B:993:GLU:CD	2.23	0.63
2:B:608:PHE:O	2:B:612:SER:N	2.31	0.63
2:D:1122:LEU:HD21	2:D:1158:TRP:CZ2	2.33	0.63
2:D:1137:ASN:HB3	2:D:1142:TRP:NE1	2.12	0.63
2:F:269:TYR:OH	2:F:288:GLU:HB2	1.98	0.63
1:A:154:GLU:HB2	1:A:155:PRO:HD2	1.79	0.63
1:C:926:TYR:HB3	1:C:1250:GLN:CG	2.29	0.63
2:B:856:ASN:HB3	2:B:859:PHE:CE2	2.34	0.63
2:D:245:THR:O	2:D:247:PRO:C	2.42	0.63
2:D:990:ASN:HB3	2:D:993:GLU:CD	2.23	0.63
1:C:857:TYR:CZ	1:C:860:ASP:HA	2.33	0.63
2:D:608:PHE:O	2:D:612:SER:N	2.32	0.63
2:F:1122:LEU:HD21	2:F:1158:TRP:CZ2	2.33	0.63
2:B:427:GLU:C	2:B:430:PRO:HD3	2.24	0.63
1:A:926:TYR:HB3	1:A:1250:GLN:HG3	1.80	0.63
2:F:990:ASN:HB3	2:F:993:GLU:CD	2.24	0.62
1:C:444:ASN:OD1	1:C:445:ASP:N	2.33	0.62
1:C:928:ASN:HB3	1:C:930:ILE:HG22	1.80	0.62
2:F:961:ASN:OD1	2:F:962:ILE:N	2.33	0.62
1:C:754:ALA:O	1:C:757:ASN:HB2	1.99	0.62
2:B:910:ASP:HB3	2:B:914:ASN:HB2	1.81	0.62
2:B:962:ILE:O	2:B:962:ILE:HG22	1.99	0.62
2:D:295:VAL:O	2:D:298:ILE:N	2.31	0.62
2:F:429:ILE:N	2:F:430:PRO:CD	2.63	0.62
1:C:216:HIS:NE2	1:C:251:GLU:OE1	2.33	0.62
1:C:771:MET:HA	1:C:774:ILE:HG22	1.82	0.62
1:C:1205:ASN:C	1:C:1205:ASN:OD1	2.42	0.62
1:E:219:HIS:ND1	1:E:250:GLU:OE2	2.27	0.62
2:B:552:LYS:O	2:B:713:PHE:HD1	1.83	0.62
2:D:269:TYR:OH	2:D:288:GLU:HB2	1.98	0.62
2:F:295:VAL:O	2:F:298:ILE:N	2.32	0.62
1:A:914:ASN:O	1:A:915:PHE:HB3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:926:TYR:HB3	1:C:1250:GLN:HG3	1.81	0.62
2:B:268:ASP:HA	2:B:271:ILE:HG22	1.80	0.62
2:B:429:ILE:N	2:B:430:PRO:CD	2.63	0.62
2:D:268:ASP:HA	2:D:271:ILE:HG22	1.81	0.62
2:F:962:ILE:O	2:F:962:ILE:HG22	2.00	0.62
1:E:926:TYR:HB3	1:E:1250:GLN:HG3	1.80	0.62
2:D:910:ASP:HB3	2:D:914:ASN:HB2	1.82	0.62
2:D:962:ILE:O	2:D:962:ILE:HG22	2.00	0.62
2:F:35:VAL:HG12	2:F:36:ALA:H	1.65	0.62
2:F:608:PHE:O	2:F:612:SER:N	2.32	0.62
1:A:365:ASN:O	1:A:368:ILE:HG22	2.00	0.62
1:E:414:ASN:HA	1:E:424:SER:HA	1.81	0.62
1:A:236:GLN:HB3	1:A:241:ILE:HD13	1.82	0.61
1:C:20:TYR:HB3	1:C:29:PHE:HB3	1.81	0.61
2:D:427:GLU:C	2:D:430:PRO:HD3	2.24	0.61
1:C:454:ILE:HD13	1:C:666:ALA:HA	1.81	0.61
1:E:119:THR:H	1:E:120:PRO:CD	2.14	0.61
1:E:1205:ASN:C	1:E:1205:ASN:OD1	2.43	0.61
2:D:1093:THR:HG23	2:D:1095:ASN:H	1.65	0.61
2:F:268:ASP:HA	2:F:271:ILE:HG22	1.82	0.61
1:A:380:LEU:HA	1:A:385:ARG:HB3	1.82	0.61
1:E:857:TYR:CZ	1:E:860:ASP:HA	2.36	0.61
2:B:1149:HIS:CE1	2:B:1150:ASP:HB3	2.35	0.61
2:D:961:ASN:OD1	2:D:962:ILE:N	2.33	0.61
2:F:1023:LEU:HD13	2:F:1158:TRP:HZ3	1.66	0.61
2:F:1137:ASN:HB3	2:F:1142:TRP:NE1	2.14	0.61
1:C:414:ASN:HA	1:C:424:SER:HA	1.82	0.61
2:F:184:ASP:OD1	2:F:185:PRO:HD2	2.01	0.61
2:F:245:THR:O	2:F:247:PRO:C	2.42	0.61
2:F:910:ASP:HB3	2:F:914:ASN:HB2	1.83	0.61
1:C:1131:ARG:HD2	1:C:1132:VAL:N	2.16	0.61
1:A:1205:ASN:C	1:A:1205:ASN:OD1	2.43	0.61
1:C:236:GLN:HB3	1:C:241:ILE:HD13	1.83	0.61
1:A:454:ILE:HD13	1:A:666:ALA:HA	1.82	0.61
1:C:468:LEU:O	1:C:470:GLN:N	2.33	0.61
2:D:552:LYS:HB2	2:D:713:PHE:HE1	1.65	0.61
2:D:956:ILE:HG22	2:D:956:ILE:O	2.00	0.61
1:E:981:ASN:HD21	2:F:414:ASN:HB3	1.64	0.61
2:D:856:ASN:HB3	2:D:859:PHE:CE2	2.36	0.61
1:C:289:VAL:CB	1:C:290:GLN:HA	2.27	0.60
2:B:184:ASP:OD1	2:B:185:PRO:HD2	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:427:GLU:C	2:F:430:PRO:HD3	2.26	0.60
1:A:754:ALA:O	1:A:757:ASN:HB2	1.99	0.60
1:A:854:ASN:HB2	1:A:865:THR:HG22	1.82	0.60
1:A:1131:ARG:HD2	1:A:1132:VAL:N	2.15	0.60
1:C:427:ILE:CD1	1:C:521:PHE:HA	2.31	0.60
2:F:956:ILE:HG22	2:F:956:ILE:O	2.00	0.60
1:C:914:ASN:O	1:C:915:PHE:HB3	2.00	0.60
1:C:448:ILE:O	1:C:449:ASN:C	2.44	0.60
1:C:904:ASP:HA	1:C:907:ILE:HD11	1.82	0.60
1:E:365:ASN:O	1:E:368:ILE:HG22	2.00	0.60
2:F:856:ASN:HB3	2:F:859:PHE:CE2	2.36	0.60
1:C:219:HIS:ND1	1:C:250:GLU:OE2	2.28	0.60
1:E:380:LEU:HA	1:E:385:ARG:HB3	1.84	0.60
2:D:184:ASP:OD1	2:D:185:PRO:HD2	2.02	0.60
1:E:211:MET:HE2	1:E:339:LEU:HD21	1.84	0.60
1:E:427:ILE:CD1	1:E:521:PHE:HA	2.31	0.60
1:E:914:ASN:O	1:E:915:PHE:HB3	2.01	0.60
2:B:269:TYR:OH	2:B:288:GLU:HB2	2.01	0.60
2:B:552:LYS:HB2	2:B:713:PHE:HE1	1.65	0.60
2:D:13:VAL:HG12	2:D:14:ASP:N	2.16	0.60
2:D:246:ASN:ND2	2:D:413:ILE:O	2.34	0.60
2:D:429:ILE:N	2:D:430:PRO:CD	2.65	0.60
2:D:1023:LEU:HD13	2:D:1158:TRP:HZ3	1.67	0.60
2:F:246:ASN:ND2	2:F:413:ILE:O	2.34	0.60
2:F:465:LEU:HB3	2:F:466:PRO:HD2	1.84	0.60
2:F:465:LEU:HB3	2:F:466:PRO:CD	2.32	0.60
2:F:552:LYS:O	2:F:713:PHE:HD1	1.83	0.60
2:B:605:ASN:HA	2:B:754:ASN:HB2	1.83	0.60
2:F:989:ILE:HG22	2:F:994:ILE:HG13	1.82	0.60
1:C:738:TYR:O	1:C:739:ASP:C	2.45	0.60
1:C:1211:LEU:HD12	1:C:1225:TYR:HB3	1.83	0.60
1:E:754:ALA:O	1:E:757:ASN:HB2	2.01	0.60
1:A:414:ASN:HA	1:A:424:SER:HA	1.84	0.60
1:A:705:TYR:C	1:A:705:TYR:HD1	2.09	0.60
1:C:143:ILE:HD13	1:C:491:THR:HG23	1.83	0.59
1:C:779:ILE:O	1:C:779:ILE:HG22	2.02	0.59
2:B:544:ILE:HD12	2:B:553:ILE:HD12	1.83	0.59
2:D:544:ILE:HD12	2:D:553:ILE:HD12	1.82	0.59
1:C:417:SER:OG	1:C:418:VAL:N	2.33	0.59
2:B:411:HIS:HA	2:B:624:PHE:HE1	1.66	0.59
1:A:857:TYR:CZ	1:A:860:ASP:HA	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:836:LEU:CB	2:D:995:LEU:HD11	2.31	0.59
2:B:498:TYR:OH	2:B:559:ARG:O	2.21	0.59
2:D:989:ILE:HG22	2:D:994:ILE:HG13	1.84	0.59
2:F:544:ILE:HD12	2:F:553:ILE:HD12	1.83	0.59
1:A:417:SER:OG	1:A:418:VAL:N	2.34	0.59
2:D:605:ASN:HA	2:D:754:ASN:HB2	1.84	0.59
2:F:579:PRO:C	2:F:581:SER:H	2.08	0.59
1:A:219:HIS:ND1	1:A:250:GLU:OE2	2.28	0.59
2:B:961:ASN:OD1	2:B:962:ILE:N	2.35	0.59
2:D:552:LYS:O	2:D:713:PHE:CD1	2.55	0.59
1:A:427:ILE:CD1	1:A:521:PHE:HA	2.33	0.59
1:A:448:ILE:O	1:A:449:ASN:C	2.45	0.59
1:E:854:ASN:HB2	1:E:865:THR:HG22	1.85	0.59
2:D:579:PRO:C	2:D:581:SER:H	2.10	0.59
1:C:1131:ARG:HD2	1:C:1131:ARG:C	2.28	0.59
1:E:448:ILE:O	1:E:449:ASN:C	2.45	0.59
2:B:543:GLU:HA	2:B:552:LYS:HA	1.83	0.59
2:B:552:LYS:O	2:B:713:PHE:CD1	2.56	0.59
2:B:956:ILE:O	2:B:956:ILE:HG22	2.03	0.59
2:B:1142:TRP:N	2:B:1142:TRP:CD1	2.70	0.59
1:A:368:ILE:HD11	1:A:395:ILE:HA	1.84	0.59
1:A:462:ASN:HB3	1:A:463:ASN:HA	1.85	0.59
2:B:1093:THR:HG23	2:B:1095:ASN:H	1.66	0.59
2:F:9:ILE:HG23	2:F:10:ASP:H	1.67	0.59
1:A:143:ILE:HD13	1:A:491:THR:HG23	1.83	0.59
1:E:987:ILE:C	1:E:989:LYS:H	2.10	0.59
2:F:543:GLU:HA	2:F:552:LYS:HA	1.85	0.59
1:A:454:ILE:HD11	1:A:456:ASP:OD1	2.03	0.58
1:E:198:SER:O	1:E:200:ASN:N	2.36	0.58
1:E:444:ASN:OD1	1:E:445:ASP:N	2.36	0.58
2:B:1023:LEU:HD12	2:B:1024:PHE:N	2.17	0.58
2:D:1149:HIS:CE1	2:D:1150:ASP:HB3	2.38	0.58
1:A:1155:SER:O	1:A:1156:LYS:C	2.47	0.58
1:C:854:ASN:HB2	1:C:865:THR:HG22	1.84	0.58
1:E:628:LEU:HD23	1:E:632:ILE:HB	1.85	0.58
2:B:574:PHE:C	2:B:574:PHE:CD2	2.81	0.58
2:D:469:TYR:CE2	2:D:562:ASN:HB2	2.38	0.58
2:D:526:TRP:CZ2	2:D:530:ILE:HD11	2.38	0.58
1:A:453:GLU:O	1:A:454:ILE:HG22	2.03	0.58
1:E:453:GLU:O	1:E:454:ILE:HG22	2.04	0.58
1:E:943:MET:HB3	1:E:947:ASN:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:246:ASN:ND2	2:B:413:ILE:O	2.35	0.58
1:E:454:ILE:HD11	1:E:456:ASP:OD1	2.03	0.58
1:E:779:ILE:O	1:E:779:ILE:HG22	2.03	0.58
2:D:465:LEU:HB3	2:D:466:PRO:HD2	1.86	0.58
2:F:804:SER:O	2:F:818:ASP:HA	2.03	0.58
1:A:836:LEU:HB2	2:B:995:LEU:HD11	1.85	0.58
1:A:1211:LEU:HD12	1:A:1225:TYR:HB3	1.84	0.58
1:C:436:PHE:HD1	1:C:437:VAL:N	2.01	0.58
1:E:143:ILE:HD13	1:E:491:THR:HG23	1.83	0.58
1:E:417:SER:OG	1:E:418:VAL:N	2.32	0.58
2:D:436:ASP:HA	2:D:437:ILE:CB	2.14	0.58
2:F:13:VAL:HG12	2:F:14:ASP:N	2.18	0.58
1:A:738:TYR:O	1:A:739:ASP:C	2.44	0.58
1:A:454:ILE:CD1	1:A:456:ASP:OD1	2.51	0.58
1:A:779:ILE:HG22	1:A:779:ILE:O	2.03	0.58
1:C:164:ASN:HB3	1:C:180:SER:OG	2.04	0.58
1:C:211:MET:HE2	1:C:339:LEU:HD21	1.86	0.58
1:E:1131:ARG:HD2	1:E:1132:VAL:N	2.18	0.58
2:B:245:THR:O	2:B:247:PRO:C	2.46	0.58
1:A:164:ASN:HB3	1:A:180:SER:OG	2.03	0.58
1:C:168:ARG:HA	1:C:497:TYR:HB2	1.86	0.58
2:D:574:PHE:C	2:D:574:PHE:CD2	2.81	0.58
2:F:469:TYR:CE2	2:F:562:ASN:HB2	2.39	0.58
1:A:444:ASN:OD1	1:A:445:ASP:N	2.37	0.58
1:C:154:GLU:HB2	1:C:155:PRO:CD	2.34	0.58
2:D:113:ASN:HB3	2:D:279:ILE:CB	2.33	0.58
2:D:465:LEU:HB3	2:D:466:PRO:CD	2.34	0.58
2:F:788:SER:O	2:F:791:GLU:HB3	2.04	0.58
1:A:1044:ILE:HG22	1:A:1045:ARG:N	2.19	0.57
1:A:1131:ARG:HD2	1:A:1131:ARG:C	2.27	0.57
1:C:824:PRO:HB3	2:D:952:ALA:HB2	1.86	0.57
2:D:788:SER:O	2:D:791:GLU:HB3	2.04	0.57
2:D:804:SER:O	2:D:818:ASP:HA	2.04	0.57
2:F:227:LEU:HD11	2:F:231:ASP:HB2	1.86	0.57
2:F:411:HIS:HA	2:F:624:PHE:HE1	1.69	0.57
1:A:605:TYR:CD1	1:A:605:TYR:O	2.57	0.57
2:B:856:ASN:HB3	2:B:859:PHE:HE2	1.69	0.57
2:B:989:ILE:HG22	2:B:994:ILE:HG13	1.86	0.57
2:D:1023:LEU:HD12	2:D:1024:PHE:N	2.19	0.57
1:E:738:TYR:O	1:E:739:ASP:C	2.47	0.57
2:B:428:LYS:C	2:B:430:PRO:HD2	2.29	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:498:TYR:OH	2:D:559:ARG:O	2.21	0.57
2:D:756:ASN:OD1	2:D:756:ASN:N	2.37	0.57
2:D:990:ASN:O	2:D:991:SER:C	2.47	0.57
2:F:552:LYS:O	2:F:713:PHE:CD1	2.57	0.57
2:F:1142:TRP:CD1	2:F:1142:TRP:N	2.72	0.57
1:E:20:TYR:HB3	1:E:29:PHE:HB3	1.84	0.57
1:E:236:GLN:HB3	1:E:241:ILE:CD1	2.33	0.57
2:B:554:ILE:HG21	2:B:556:TRP:CE2	2.39	0.57
2:B:1023:LEU:HD13	2:B:1158:TRP:HZ3	1.68	0.57
2:D:543:GLU:HA	2:D:552:LYS:HA	1.87	0.57
1:A:168:ARG:HA	1:A:497:TYR:HB2	1.87	0.57
1:C:628:LEU:HD23	1:C:632:ILE:HB	1.86	0.57
1:E:168:ARG:HA	1:E:497:TYR:HB2	1.87	0.57
1:E:368:ILE:HD11	1:E:395:ILE:HA	1.85	0.57
1:E:824:PRO:CB	2:F:952:ALA:HB2	2.35	0.57
2:F:1093:THR:HG23	2:F:1095:ASN:H	1.69	0.57
1:A:211:MET:HE2	1:A:339:LEU:HD21	1.86	0.57
1:C:416:VAL:HG13	1:C:420:GLY:N	2.20	0.57
1:E:154:GLU:HB2	1:E:155:PRO:CD	2.35	0.57
1:E:164:ASN:HB3	1:E:180:SER:OG	2.04	0.57
1:E:454:ILE:CD1	1:E:456:ASP:OD1	2.52	0.57
1:C:380:LEU:HA	1:C:385:ARG:HB3	1.86	0.57
1:C:857:TYR:OH	1:C:860:ASP:HA	2.05	0.57
2:B:81:ALA:O	2:B:82:THR:C	2.47	0.57
2:D:552:LYS:HB2	2:D:713:PHE:CE1	2.40	0.57
1:A:309:LEU:CD2	1:A:319:VAL:HG12	2.35	0.57
1:C:453:GLU:O	1:C:454:ILE:HG22	2.04	0.57
2:B:166:LEU:HD12	2:B:196:SER:HB2	1.86	0.57
2:D:742:ASN:HA	2:D:745:THR:HG22	1.87	0.57
2:F:552:LYS:HB2	2:F:713:PHE:HE1	1.69	0.57
2:F:574:PHE:C	2:F:574:PHE:CD2	2.82	0.57
1:A:289:VAL:HB	1:A:290:GLN:CB	2.35	0.57
1:C:368:ILE:HD11	1:C:395:ILE:HA	1.86	0.57
1:E:436:PHE:HD1	1:E:437:VAL:N	2.01	0.57
1:E:836:LEU:HD13	2:F:991:SER:HA	1.87	0.57
1:C:943:MET:HB3	1:C:947:ASN:HA	1.86	0.57
2:D:9:ILE:HG23	2:D:10:ASP:H	1.69	0.57
2:F:870:TYR:CE2	2:F:983:SER:OG	2.57	0.57
1:A:198:SER:O	1:A:200:ASN:N	2.38	0.56
1:E:705:TYR:C	1:E:705:TYR:HD1	2.13	0.56
1:E:742:GLN:O	1:E:744:GLU:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:605:ASN:HA	2:F:754:ASN:HB2	1.87	0.56
2:B:895:TRP:O	2:B:896:GLU:HG2	2.05	0.56
2:F:40:TRP:O	2:F:137:VAL:HA	2.05	0.56
2:F:113:ASN:HB3	2:F:279:ILE:CB	2.34	0.56
2:F:756:ASN:N	2:F:756:ASN:OD1	2.37	0.56
2:F:1023:LEU:HD13	2:F:1158:TRP:CZ3	2.40	0.56
2:F:1149:HIS:CE1	2:F:1150:ASP:HB3	2.40	0.56
1:A:427:ILE:HG22	1:A:428:GLU:N	2.19	0.56
1:C:987:ILE:C	1:C:989:LYS:H	2.13	0.56
1:E:452:LYS:HB2	1:E:651:LYS:HE2	1.88	0.56
1:E:1149:TYR:CD1	1:E:1183:ARG:HD2	2.40	0.56
2:B:756:ASN:OD1	2:B:756:ASN:N	2.39	0.56
2:B:804:SER:O	2:B:818:ASP:HA	2.04	0.56
2:B:943:LEU:HD23	2:B:953:ASN:HA	1.88	0.56
1:A:452:LYS:HB2	1:A:651:LYS:HE2	1.87	0.56
1:A:628:LEU:HD23	1:A:632:ILE:HB	1.86	0.56
1:C:481:PRO:HG2	1:C:483:LEU:HD21	1.88	0.56
1:C:1155:SER:O	1:C:1156:LYS:C	2.49	0.56
2:B:526:TRP:CZ2	2:B:530:ILE:HD11	2.40	0.56
1:C:454:ILE:HD11	1:C:456:ASP:OD1	2.05	0.56
1:C:824:PRO:CB	2:D:952:ALA:HB2	2.36	0.56
2:B:465:LEU:HB3	2:B:466:PRO:CD	2.36	0.56
2:B:788:SER:O	2:B:791:GLU:HB3	2.04	0.56
2:D:227:LEU:HD11	2:D:231:ASP:HB2	1.88	0.56
2:D:393:THR:HG1	2:D:396:ASN:N	2.03	0.56
1:A:289:VAL:HB	1:A:290:GLN:HB3	1.88	0.56
1:A:436:PHE:HD1	1:A:437:VAL:N	2.03	0.56
1:A:1150:ILE:HG22	1:A:1162:LEU:HD12	1.86	0.56
1:C:1163:TYR:O	1:C:1175:ILE:HG23	2.05	0.56
1:E:1155:SER:O	1:E:1156:LYS:C	2.48	0.56
2:B:113:ASN:HB3	2:B:279:ILE:CB	2.36	0.56
2:B:465:LEU:HB3	2:B:466:PRO:HD2	1.87	0.56
2:B:822:LYS:O	2:B:824:THR:N	2.39	0.56
2:D:856:ASN:HB3	2:D:859:PHE:HE2	1.71	0.56
1:A:38:ASN:HD21	1:A:484:SER:CB	2.19	0.56
1:C:855:MET:C	1:C:856:ARG:HD3	2.31	0.56
1:C:1083:ASP:N	1:C:1129:ILE:O	2.33	0.56
1:E:462:ASN:HB3	1:E:463:ASN:HA	1.87	0.56
2:F:393:THR:HG1	2:F:396:ASN:N	2.04	0.56
1:E:1131:ARG:HD2	1:E:1131:ARG:C	2.30	0.56
2:F:98:LEU:O	2:F:101:LEU:HB3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:SER:O	1:C:200:ASN:N	2.39	0.56
1:C:454:ILE:CD1	1:C:456:ASP:OD1	2.53	0.56
1:E:416:VAL:HG13	1:E:420:GLY:N	2.21	0.56
2:B:552:LYS:HB2	2:B:713:PHE:CE1	2.40	0.56
2:F:429:ILE:HG22	2:F:429:ILE:O	2.06	0.56
1:A:154:GLU:HB2	1:A:155:PRO:CD	2.35	0.56
1:C:857:TYR:HA	1:C:862:TYR:HA	1.88	0.56
1:C:899:ASN:OD1	1:C:1028:ASN:HB3	2.05	0.56
1:C:1044:ILE:HG22	1:C:1045:ARG:N	2.20	0.56
1:E:289:VAL:CB	1:E:290:GLN:HA	2.27	0.56
2:B:269:TYR:CE1	2:B:287:LEU:HB3	2.41	0.56
2:B:742:ASN:HA	2:B:745:THR:HG22	1.88	0.56
2:D:870:TYR:CE2	2:D:983:SER:OG	2.59	0.56
2:F:554:ILE:HG21	2:F:556:TRP:CE2	2.41	0.56
1:C:119:THR:H	1:C:120:PRO:CD	2.18	0.55
1:E:1163:TYR:O	1:E:1175:ILE:HG23	2.06	0.55
1:E:1211:LEU:HD12	1:E:1225:TYR:HB3	1.86	0.55
2:D:9:ILE:O	2:D:10:ASP:C	2.49	0.55
2:B:40:TRP:O	2:B:137:VAL:HA	2.06	0.55
2:B:1015:LEU:HB2	2:B:1071:VAL:HB	1.89	0.55
2:D:943:LEU:HD23	2:D:953:ASN:HA	1.88	0.55
2:F:428:LYS:C	2:F:430:PRO:HD2	2.31	0.55
2:F:545:SER:HA	2:F:550:ASP:N	2.21	0.55
1:E:376:ASN:HB3	1:E:381:LYS:HA	1.89	0.55
2:D:92:ASN:HB3	2:D:310:PHE:CZ	2.42	0.55
2:D:545:SER:HA	2:D:550:ASP:N	2.21	0.55
2:D:554:ILE:HG21	2:D:556:TRP:CE2	2.41	0.55
2:D:1023:LEU:HD13	2:D:1158:TRP:CZ3	2.41	0.55
2:F:269:TYR:CE1	2:F:287:LEU:HB3	2.41	0.55
1:A:67:SER:HA	1:A:158:PHE:CD2	2.41	0.55
1:C:452:LYS:HB2	1:C:651:LYS:HE2	1.87	0.55
1:C:1092:LEU:O	1:C:1094:PRO:HD3	2.06	0.55
2:B:9:ILE:O	2:B:10:ASP:C	2.49	0.55
2:F:9:ILE:O	2:F:10:ASP:C	2.49	0.55
2:F:498:TYR:OH	2:F:559:ARG:O	2.23	0.55
2:F:943:LEU:HD23	2:F:953:ASN:HA	1.89	0.55
1:A:742:GLN:O	1:A:744:GLU:N	2.40	0.55
1:C:427:ILE:HG22	1:C:428:GLU:N	2.22	0.55
1:C:475:PHE:C	2:D:1136:LYS:HE2	2.31	0.55
2:B:92:ASN:HB3	2:B:310:PHE:CZ	2.42	0.55
2:B:1023:LEU:HD13	2:B:1158:TRP:CZ3	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:895:TRP:O	2:D:896:GLU:HG2	2.05	0.55
2:F:1023:LEU:HD12	2:F:1024:PHE:N	2.22	0.55
1:A:1092:LEU:O	1:A:1094:PRO:HD3	2.07	0.55
1:C:462:ASN:HB3	1:C:463:ASN:HA	1.88	0.55
1:C:627:LEU:O	1:E:420:GLY:N	2.40	0.55
1:E:111:ASN:HA	1:E:147:ASN:OD1	2.07	0.55
2:B:9:ILE:HG23	2:B:10:ASP:H	1.71	0.55
2:B:98:LEU:O	2:B:101:LEU:HB3	2.07	0.55
2:B:469:TYR:CE2	2:B:562:ASN:HB2	2.41	0.55
2:D:23:SER:OG	2:D:29:PHE:HB2	2.07	0.55
2:F:81:ALA:O	2:F:82:THR:C	2.48	0.55
1:A:606:ILE:HG13	1:A:704:MET:HE3	1.89	0.55
1:A:737:LYS:O	1:A:738:TYR:O	2.24	0.55
2:B:502:ASN:O	2:B:506:ASP:HB2	2.06	0.55
1:A:119:THR:H	1:A:120:PRO:CD	2.19	0.55
1:A:829:SER:C	1:A:831:THR:H	2.15	0.55
1:A:1025:VAL:HG12	1:A:1026:SER:N	2.22	0.55
1:C:742:GLN:O	1:C:744:GLU:N	2.40	0.55
2:F:727:TYR:N	2:F:728:PRO:HD2	2.22	0.55
1:E:392:ASN:O	1:E:395:ILE:HG12	2.07	0.55
2:B:1149:HIS:NE2	2:B:1150:ASP:HB3	2.22	0.55
2:F:1072:GLN:O	2:F:1075:ASP:HB2	2.07	0.55
1:A:943:MET:HB3	1:A:947:ASN:HA	1.88	0.54
1:C:606:ILE:HD13	1:C:761:PHE:CE2	2.42	0.54
1:E:1044:ILE:HG22	1:E:1045:ARG:N	2.22	0.54
2:B:23:SER:OG	2:B:29:PHE:HB2	2.08	0.54
2:B:544:ILE:HD13	2:B:575:LYS:HG2	1.88	0.54
2:D:98:LEU:O	2:D:101:LEU:HB3	2.07	0.54
1:C:67:SER:HA	1:C:158:PHE:CD2	2.43	0.54
1:C:467:ASP:OD1	1:C:468:LEU:N	2.40	0.54
1:C:1053:GLU:HG3	1:C:1053:GLU:O	2.07	0.54
1:E:606:ILE:HD13	1:E:761:PHE:CE2	2.42	0.54
1:E:824:PRO:HB3	2:F:952:ALA:HB2	1.89	0.54
2:B:88:ARG:NE	2:B:339:TYR:OH	2.41	0.54
2:B:870:TYR:CE2	2:B:983:SER:OG	2.59	0.54
2:D:1142:TRP:N	2:D:1142:TRP:CD1	2.75	0.54
2:F:583:ILE:O	2:F:586:LYS:HE3	2.08	0.54
1:C:1150:ILE:HG22	1:C:1162:LEU:HD12	1.88	0.54
1:E:480:ALA:N	1:E:481:PRO:HD3	2.23	0.54
2:B:545:SER:HA	2:B:550:ASP:N	2.21	0.54
2:B:1072:GLN:O	2:B:1075:ASP:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:269:TYR:CE2	2:F:288:GLU:HA	2.43	0.54
2:F:990:ASN:O	2:F:991:SER:C	2.50	0.54
1:A:236:GLN:HB3	1:A:241:ILE:CD1	2.37	0.54
1:A:1163:TYR:O	1:A:1175:ILE:HG23	2.06	0.54
1:C:606:ILE:HG13	1:C:704:MET:HE3	1.89	0.54
1:E:1150:ILE:HG22	1:E:1162:LEU:HD12	1.88	0.54
2:D:429:ILE:O	2:D:429:ILE:HG22	2.08	0.54
1:C:309:LEU:CD2	1:C:319:VAL:HG12	2.37	0.54
1:E:899:ASN:OD1	1:E:1028:ASN:HB3	2.07	0.54
1:A:416:VAL:HG13	1:A:420:GLY:N	2.23	0.54
1:E:309:LEU:CD2	1:E:319:VAL:HG12	2.36	0.54
1:E:427:ILE:HG22	1:E:428:GLU:N	2.23	0.54
2:B:429:ILE:O	2:B:429:ILE:HG22	2.07	0.54
1:A:227:ILE:CD1	1:A:271:ILE:HA	2.38	0.54
1:A:735:THR:O	1:A:911:LYS:NZ	2.38	0.54
1:C:568:GLN:O	1:C:569:ALA:CB	2.56	0.54
1:C:737:LYS:O	1:C:738:TYR:O	2.24	0.54
1:E:737:LYS:O	1:E:738:TYR:O	2.25	0.54
2:B:381:MET:HE3	2:B:471:GLN:CD	2.33	0.54
2:B:990:ASN:O	2:B:991:SER:C	2.50	0.54
2:F:502:ASN:O	2:F:506:ASP:N	2.38	0.54
1:C:242:THR:HG22	1:C:435:PHE:O	2.08	0.54
2:B:14:ASP:OD1	2:B:16:LYS:N	2.41	0.54
2:B:615:LEU:HB3	2:B:767:ASN:ND2	2.23	0.54
2:D:239:ASP:OD2	2:D:318:TYR:N	2.41	0.54
2:D:755:ILE:CG2	2:D:759:GLU:HB2	2.37	0.54
2:F:526:TRP:CZ2	2:F:530:ILE:HD11	2.42	0.54
2:F:742:ASN:HA	2:F:745:THR:HG22	1.90	0.54
1:A:443:TYR:CD1	1:A:444:ASN:N	2.75	0.54
1:A:857:TYR:OH	1:A:860:ASP:HA	2.08	0.54
1:A:892:ASN:N	1:A:892:ASN:OD1	2.40	0.54
1:E:857:TYR:OH	1:E:860:ASP:HA	2.07	0.54
2:B:727:TYR:N	2:B:728:PRO:HD2	2.23	0.54
2:B:863:LEU:HD23	2:B:864:THR:HG23	1.90	0.54
2:F:856:ASN:HB3	2:F:859:PHE:HE2	1.72	0.54
1:A:111:ASN:HA	1:A:147:ASN:OD1	2.08	0.54
1:C:705:TYR:C	1:C:705:TYR:HD1	2.12	0.54
2:D:1015:LEU:HB2	2:D:1071:VAL:HB	1.90	0.54
2:F:502:ASN:O	2:F:506:ASP:HB2	2.08	0.54
1:C:86:ILE:HG13	1:C:364:LEU:HD21	1.90	0.53
1:C:297:ASN:N	1:C:298:PRO:CD	2.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:605:TYR:O	1:E:605:TYR:CD1	2.61	0.53
2:B:153:TYR:HD2	2:B:165:MET:HB2	1.73	0.53
2:D:273:ILE:O	2:D:276:ASN:HB3	2.08	0.53
1:C:289:VAL:HB	1:C:290:GLN:CB	2.38	0.53
1:C:480:ALA:N	1:C:481:PRO:HD3	2.23	0.53
2:B:859:PHE:CD1	2:B:968:ILE:HD12	2.43	0.53
2:D:817:GLY:HA2	2:D:826:VAL:HG21	1.91	0.53
2:F:23:SER:OG	2:F:29:PHE:HB2	2.07	0.53
2:F:254:TYR:O	2:F:258:THR:HG22	2.08	0.53
2:F:755:ILE:CG2	2:F:759:GLU:HB2	2.37	0.53
1:E:38:ASN:HD21	1:E:484:SER:CB	2.20	0.53
1:E:289:VAL:HB	1:E:290:GLN:CB	2.37	0.53
1:E:1083:ASP:N	1:E:1129:ILE:O	2.32	0.53
2:B:803:LEU:HD23	2:B:803:LEU:C	2.33	0.53
2:D:101:LEU:HD11	2:D:293:ILE:HD12	1.90	0.53
1:A:45:ARG:HG3	1:A:74:LEU:HD23	1.89	0.53
1:A:278:ASP:N	1:A:278:ASP:OD1	2.40	0.53
1:A:547:GLU:HB2	1:A:550:LYS:HG3	1.90	0.53
1:A:606:ILE:HD13	1:A:761:PHE:CE2	2.43	0.53
1:A:836:LEU:HD11	2:B:945:PHE:CE1	2.44	0.53
1:A:1149:TYR:CD1	1:A:1183:ARG:HD2	2.43	0.53
1:C:236:GLN:HB3	1:C:241:ILE:CD1	2.37	0.53
1:C:447:ASN:N	1:C:447:ASN:OD1	2.40	0.53
1:E:45:ARG:HG3	1:E:74:LEU:HD23	1.89	0.53
1:E:597:ALA:HB2	2:F:939:LYS:HB3	1.90	0.53
2:B:755:ILE:CG2	2:B:759:GLU:HB2	2.37	0.53
2:D:428:LYS:C	2:D:430:PRO:HD2	2.33	0.53
2:F:694:ASN:O	2:F:697:ARG:HD2	2.08	0.53
2:F:803:LEU:HD23	2:F:803:LEU:C	2.33	0.53
1:A:297:ASN:N	1:A:298:PRO:CD	2.70	0.53
1:C:111:ASN:HA	1:C:147:ASN:OD1	2.09	0.53
1:E:382:VAL:O	1:E:382:VAL:HG13	2.08	0.53
2:D:206:ASN:ND2	2:D:208:ASN:HB2	2.23	0.53
2:D:269:TYR:CE1	2:D:287:LEU:HB3	2.44	0.53
2:F:817:GLY:HA2	2:F:826:VAL:HG21	1.91	0.53
2:F:859:PHE:CD1	2:F:968:ILE:HD12	2.43	0.53
1:A:1012:ILE:O	2:B:779:ILE:HD12	2.09	0.53
1:C:227:ILE:CD1	1:C:271:ILE:HA	2.39	0.53
1:C:829:SER:C	1:C:831:THR:H	2.17	0.53
2:D:277:ASN:HB3	2:D:281:ASN:CB	2.39	0.53
2:D:1072:GLN:O	2:D:1075:ASP:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:544:ILE:HD13	2:F:575:LYS:HG2	1.91	0.53
2:F:895:TRP:O	2:F:896:GLU:HG2	2.08	0.53
1:A:1083:ASP:N	1:A:1129:ILE:O	2.32	0.53
1:C:382:VAL:O	1:C:382:VAL:HG13	2.08	0.53
2:B:254:TYR:O	2:B:258:THR:HG22	2.08	0.53
2:B:554:ILE:CG2	2:B:556:TRP:CE2	2.92	0.53
2:D:166:LEU:HD12	2:D:196:SER:HB2	1.89	0.53
2:D:694:ASN:O	2:D:697:ARG:HD2	2.09	0.53
2:D:1149:HIS:NE2	2:D:1150:ASP:HB3	2.24	0.53
2:F:14:ASP:O	2:F:15:ASN:HB2	2.09	0.53
2:F:206:ASN:ND2	2:F:208:ASN:HB2	2.24	0.53
1:A:568:GLN:O	1:A:569:ALA:CB	2.56	0.53
1:C:735:THR:O	1:C:911:LYS:NZ	2.39	0.53
1:C:1149:TYR:CD1	1:C:1183:ARG:HD2	2.44	0.53
1:C:1174:THR:HA	1:C:1220:VAL:HG12	1.90	0.53
2:B:273:ILE:O	2:B:276:ASN:HB3	2.08	0.53
1:A:855:MET:C	1:A:856:ARG:HD3	2.33	0.53
1:C:605:TYR:O	1:C:605:TYR:CD1	2.61	0.53
2:B:227:LEU:HD11	2:B:231:ASP:HB2	1.91	0.53
2:B:239:ASP:OD2	2:B:318:TYR:N	2.41	0.53
2:B:534:TYR:CE1	2:B:538:ILE:HD12	2.44	0.53
2:D:551:THR:HG21	2:D:716:ASN:HB3	1.91	0.53
2:D:822:LYS:O	2:D:824:THR:N	2.41	0.53
2:F:273:ILE:O	2:F:276:ASN:HB3	2.08	0.53
2:F:1017:TYR:O	2:F:1018:ASN:CB	2.57	0.53
1:A:274:ASN:HA	1:A:277:ASN:ND2	2.25	0.53
1:A:823:ILE:HG23	1:A:824:PRO:HD2	1.91	0.53
1:C:45:ARG:HG3	1:C:74:LEU:HD23	1.90	0.53
1:E:467:ASP:OD1	1:E:468:LEU:N	2.42	0.53
2:B:583:ILE:O	2:B:586:LYS:HE3	2.09	0.53
2:D:863:LEU:HD23	2:D:864:THR:HG23	1.91	0.53
2:D:1093:THR:HG22	2:D:1097:ARG:O	2.08	0.53
2:D:1138:GLN:HB3	2:D:1139:ASP:C	2.34	0.53
1:A:467:ASP:OD1	1:A:468:LEU:N	2.42	0.52
1:A:1108:ILE:O	1:A:1110:ASN:N	2.42	0.52
1:C:682:TYR:CE2	1:C:825:PHE:HA	2.45	0.52
1:E:1053:GLU:O	1:E:1053:GLU:HG3	2.07	0.52
2:B:101:LEU:HD11	2:B:293:ILE:HD12	1.90	0.52
2:D:381:MET:HE3	2:D:471:GLN:CD	2.35	0.52
2:F:1015:LEU:HB2	2:F:1071:VAL:HB	1.90	0.52
1:A:38:ASN:HD21	1:A:484:SER:HB2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:THR:O	1:A:212:HIS:HB3	2.09	0.52
1:C:38:ASN:HD21	1:C:484:SER:CB	2.23	0.52
1:C:273:THR:O	1:C:276:LEU:N	2.42	0.52
1:E:34:ASN:HB2	1:E:40:TRP:CH2	2.44	0.52
1:E:289:VAL:HB	1:E:290:GLN:HB3	1.90	0.52
2:B:858:TYR:OH	2:B:866:ASN:O	2.27	0.52
2:D:583:ILE:O	2:D:586:LYS:HE3	2.08	0.52
1:C:443:TYR:CD1	1:C:444:ASN:N	2.76	0.52
1:C:1108:ILE:O	1:C:1110:ASN:N	2.43	0.52
1:E:1174:THR:HA	1:E:1220:VAL:HG12	1.92	0.52
2:D:40:TRP:O	2:D:137:VAL:HA	2.09	0.52
2:D:254:TYR:O	2:D:258:THR:HG22	2.09	0.52
2:F:568:ASN:OD1	2:F:569:SER:N	2.42	0.52
2:F:726:ILE:C	2:F:728:PRO:HD2	2.34	0.52
1:A:382:VAL:HG13	1:A:382:VAL:O	2.09	0.52
1:A:632:ILE:HG23	1:A:633:LEU:N	2.24	0.52
1:A:818:THR:O	1:A:819:LEU:HG	2.09	0.52
1:A:1053:GLU:HG3	1:A:1053:GLU:O	2.09	0.52
1:E:443:TYR:CD1	1:E:444:ASN:N	2.77	0.52
1:E:480:ALA:N	1:E:481:PRO:CD	2.73	0.52
1:E:1092:LEU:O	1:E:1094:PRO:HD3	2.08	0.52
2:B:421:VAL:O	2:B:421:VAL:HG12	2.09	0.52
2:D:21:VAL:CG1	2:D:22:ARG:N	2.72	0.52
2:D:502:ASN:O	2:D:506:ASP:HB2	2.09	0.52
2:F:14:ASP:OD1	2:F:16:LYS:N	2.42	0.52
2:F:166:LEU:HD12	2:F:196:SER:HB2	1.90	0.52
2:F:552:LYS:HB2	2:F:713:PHE:CE1	2.44	0.52
1:A:462:ASN:CB	1:A:463:ASN:HA	2.38	0.52
1:E:242:THR:HG22	1:E:435:PHE:O	2.10	0.52
1:A:86:ILE:HG13	1:A:364:LEU:HD21	1.92	0.52
1:A:273:THR:O	1:A:276:LEU:N	2.42	0.52
1:C:289:VAL:HB	1:C:290:GLN:HB3	1.90	0.52
1:E:606:ILE:HG13	1:E:704:MET:HE3	1.91	0.52
1:E:836:LEU:CB	2:F:995:LEU:HD11	2.40	0.52
2:D:794:ILE:O	2:D:795:LYS:C	2.53	0.52
1:C:944:ARG:CG	1:C:1026:SER:HA	2.39	0.52
1:E:738:TYR:HA	1:E:743:ILE:CG1	2.38	0.52
2:B:726:ILE:C	2:B:728:PRO:HD2	2.35	0.52
2:D:727:TYR:N	2:D:728:PRO:HD2	2.25	0.52
2:F:21:VAL:CG1	2:F:121:ASN:HA	2.39	0.52
2:F:1137:ASN:CB	2:F:1142:TRP:HE1	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:ASP:OD1	1:A:206:PRO:HD2	2.10	0.52
1:A:899:ASN:OD1	1:A:1028:ASN:HB3	2.09	0.52
1:A:1174:THR:HA	1:A:1220:VAL:HG12	1.90	0.52
1:E:1043:GLY:C	1:E:1044:ILE:HG13	2.35	0.52
2:B:21:VAL:CG1	2:B:22:ARG:N	2.73	0.52
2:B:1093:THR:HG22	2:B:1097:ARG:O	2.09	0.52
2:B:1138:GLN:HB3	2:B:1139:ASP:C	2.34	0.52
2:D:411:HIS:HA	2:D:624:PHE:HE1	1.74	0.52
2:D:421:VAL:O	2:D:421:VAL:HG12	2.10	0.52
1:A:199:ILE:HA	1:A:705:TYR:CE2	2.39	0.52
1:E:481:PRO:HG2	1:E:483:LEU:HD21	1.92	0.52
2:B:251:ILE:O	2:B:252:ASP:CB	2.58	0.52
2:B:1137:ASN:CB	2:B:1142:TRP:HE1	2.20	0.52
2:D:1017:TYR:O	2:D:1018:ASN:CB	2.57	0.52
2:F:863:LEU:HD23	2:F:864:THR:HG23	1.92	0.52
1:A:738:TYR:HA	1:A:743:ILE:CG1	2.40	0.52
1:C:41:ILE:HG22	1:C:150:ILE:HB	1.92	0.52
1:C:209:THR:O	1:C:212:HIS:HB3	2.10	0.52
1:E:209:THR:O	1:E:212:HIS:HB3	2.10	0.52
1:E:829:SER:C	1:E:831:THR:H	2.18	0.52
2:D:381:MET:HE2	2:D:383:SER:HB2	1.92	0.52
2:D:917:ASN:C	2:D:918:ILE:HG13	2.35	0.52
2:F:277:ASN:HB3	2:F:281:ASN:CB	2.39	0.52
2:F:1093:THR:HG22	2:F:1097:ARG:O	2.09	0.52
1:A:286:LEU:O	1:A:287:SER:C	2.52	0.51
1:C:682:TYR:CD2	1:C:825:PHE:HD1	2.28	0.51
1:E:82:ARG:HG3	1:E:364:LEU:HD11	1.92	0.51
1:E:462:ASN:CB	1:E:463:ASN:HA	2.39	0.51
2:B:185:PRO:O	2:B:186:ALA:C	2.53	0.51
2:D:571:VAL:O	2:D:574:PHE:HB3	2.10	0.51
2:F:41:ILE:HG22	2:F:138:ILE:HB	1.92	0.51
2:F:534:TYR:CE1	2:F:538:ILE:HD12	2.45	0.51
2:F:722:PHE:HA	2:F:726:ILE:HD12	1.92	0.51
2:F:822:LYS:O	2:F:824:THR:N	2.42	0.51
1:A:854:ASN:CB	1:A:865:THR:HG22	2.40	0.51
1:A:1143:ARG:HH21	1:A:1143:ARG:CG	2.23	0.51
1:E:297:ASN:N	1:E:298:PRO:CD	2.73	0.51
1:E:568:GLN:O	1:E:569:ALA:CB	2.58	0.51
2:B:151:ILE:HD11	2:B:167:GLU:HB2	1.91	0.51
2:B:1140:TYR:CE2	2:B:1142:TRP:CD2	2.98	0.51
2:D:534:TYR:CE1	2:D:538:ILE:HD12	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:421:VAL:O	2:F:421:VAL:HG12	2.10	0.51
1:A:392:ASN:O	1:A:395:ILE:HG12	2.10	0.51
1:A:1025:VAL:CG1	1:A:1026:SER:N	2.73	0.51
1:C:205:ASP:OD1	1:C:206:PRO:HD2	2.10	0.51
1:E:896:SER:C	1:E:897:GLU:HG3	2.35	0.51
2:D:14:ASP:OD1	2:D:16:LYS:N	2.43	0.51
2:D:88:ARG:NE	2:D:339:TYR:OH	2.43	0.51
2:D:502:ASN:O	2:D:506:ASP:N	2.41	0.51
2:F:88:ARG:NE	2:F:339:TYR:OH	2.43	0.51
1:A:166:SER:HB3	1:A:498:ILE:HB	1.92	0.51
1:A:376:ASN:HB3	1:A:381:LYS:HA	1.92	0.51
1:E:67:SER:HA	1:E:158:PHE:CD2	2.46	0.51
2:B:155:LYS:O	2:B:156:GLU:C	2.54	0.51
2:B:381:MET:HE2	2:B:383:SER:HB2	1.92	0.51
2:B:923:ILE:O	2:B:925:ASN:N	2.33	0.51
2:F:185:PRO:O	2:F:186:ALA:C	2.53	0.51
1:C:1025:VAL:HG12	1:C:1026:SER:N	2.25	0.51
1:E:38:ASN:HD21	1:E:484:SER:HB2	1.76	0.51
1:E:227:ILE:CD1	1:E:271:ILE:HA	2.40	0.51
2:B:262:PHE:CZ	2:B:293:ILE:O	2.63	0.51
2:B:1017:TYR:O	2:B:1018:ASN:CB	2.59	0.51
2:B:1042:ILE:O	2:B:1099:GLN:HA	2.11	0.51
2:F:381:MET:HE2	2:F:383:SER:HB2	1.92	0.51
1:A:857:TYR:HA	1:A:862:TYR:HA	1.93	0.51
1:C:215:ILE:HG22	1:C:219:HIS:CE1	2.45	0.51
1:C:363:LEU:HD21	1:C:375:TYR:OH	2.10	0.51
1:C:376:ASN:HB3	1:C:381:LYS:HA	1.93	0.51
1:E:855:MET:C	1:E:856:ARG:HD3	2.36	0.51
2:B:277:ASN:HB3	2:B:281:ASN:CB	2.39	0.51
2:B:567:ASN:O	2:B:568:ASN:C	2.53	0.51
2:B:817:GLY:HA2	2:B:826:VAL:HG21	1.92	0.51
2:F:21:VAL:CG1	2:F:22:ARG:N	2.73	0.51
2:F:858:TYR:OH	2:F:866:ASN:O	2.29	0.51
1:A:785:TYR:O	1:A:786:ASP:C	2.53	0.51
1:C:220:GLY:CA	1:C:225:LYS:HE3	2.41	0.51
1:C:462:ASN:CB	1:C:463:ASN:HA	2.40	0.51
1:C:795:ASN:C	1:C:795:ASN:OD1	2.54	0.51
1:E:273:THR:O	1:E:276:LEU:N	2.44	0.51
1:E:682:TYR:CD2	1:E:825:PHE:HD1	2.29	0.51
1:E:972:LYS:HB2	2:F:772:LEU:HD21	1.93	0.51
2:B:14:ASP:O	2:B:15:ASN:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:251:ILE:O	2:D:252:ASP:CB	2.59	0.51
2:D:872:TRP:HB2	2:D:980:GLU:HB3	1.92	0.51
1:A:113:TYR:HB3	1:A:178:PHE:HB3	1.93	0.51
1:A:453:GLU:C	1:A:454:ILE:HG22	2.36	0.51
1:C:480:ALA:N	1:C:481:PRO:CD	2.74	0.51
1:E:86:ILE:HG13	1:E:364:LEU:HD21	1.93	0.51
1:E:144:LEU:HA	1:E:487:LYS:HA	1.93	0.51
1:E:823:ILE:HG23	1:E:824:PRO:HD2	1.92	0.51
2:B:22:ARG:HD2	2:B:27:ASP:O	2.11	0.51
2:B:154:LYS:HD3	2:B:157:TYR:CE2	2.45	0.51
2:D:81:ALA:O	2:D:82:THR:C	2.53	0.51
2:F:482:LEU:HD22	2:F:499:SER:HB3	1.93	0.51
2:F:1022:GLU:HG2	2:F:1023:LEU:N	2.25	0.51
1:A:481:PRO:HG2	1:A:483:LEU:HD21	1.93	0.51
1:C:392:ASN:O	1:C:395:ILE:HG12	2.10	0.51
2:D:815:VAL:C	2:D:816:ILE:HG13	2.36	0.51
2:D:859:PHE:CD1	2:D:968:ILE:HD12	2.46	0.51
2:D:1122:LEU:HD21	2:D:1158:TRP:HZ2	1.75	0.51
2:F:763:LEU:HA	2:F:766:GLN:HB2	1.92	0.51
1:C:47:VAL:O	1:C:47:VAL:HG12	2.11	0.51
1:C:547:GLU:HB2	1:C:550:LYS:HG3	1.92	0.51
1:C:854:ASN:CB	1:C:865:THR:HG22	2.41	0.51
1:E:363:LEU:HD21	1:E:375:TYR:OH	2.11	0.51
2:B:146:ILE:HD13	2:B:330:TYR:CZ	2.46	0.51
2:B:1007:ILE:HG22	2:B:1015:LEU:HD12	1.93	0.51
1:A:363:LEU:HD21	1:A:375:TYR:OH	2.11	0.50
1:A:1087:TYR:N	1:A:1243:ILE:O	2.45	0.50
1:C:143:ILE:HG22	1:C:144:LEU:N	2.26	0.50
1:C:1093:LYS:HB3	1:C:1096:ASN:HB2	1.91	0.50
1:E:1108:ILE:O	1:E:1110:ASN:N	2.44	0.50
2:B:9:ILE:O	2:B:11:SER:N	2.44	0.50
2:B:153:TYR:CD2	2:B:165:MET:HB2	2.45	0.50
2:B:568:ASN:OD1	2:B:569:SER:N	2.44	0.50
2:B:583:ILE:HG23	2:B:644:GLN:NE2	2.26	0.50
2:B:815:VAL:C	2:B:816:ILE:HG13	2.36	0.50
2:D:568:ASN:OD1	2:D:569:SER:N	2.43	0.50
2:D:726:ILE:C	2:D:728:PRO:HD2	2.36	0.50
2:F:101:LEU:HD11	2:F:293:ILE:HD12	1.93	0.50
2:F:571:VAL:O	2:F:574:PHE:HB3	2.11	0.50
2:F:824:THR:HA	2:F:856:ASN:HB2	1.92	0.50
1:A:215:ILE:HG22	1:A:219:HIS:CE1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:GLU:CB	1:C:155:PRO:HD2	2.41	0.50
1:E:143:ILE:HG22	1:E:144:LEU:N	2.26	0.50
1:E:291:VAL:HA	1:E:292:SER:HB2	1.93	0.50
1:E:453:GLU:C	1:E:454:ILE:HG22	2.35	0.50
2:B:347:GLY:O	2:B:351:THR:HB	2.11	0.50
2:F:154:LYS:HD3	2:F:157:TYR:CE2	2.47	0.50
2:F:381:MET:HE3	2:F:471:GLN:CD	2.36	0.50
2:F:1138:GLN:HB3	2:F:1139:ASP:C	2.36	0.50
1:A:447:ASN:N	1:A:447:ASN:OD1	2.42	0.50
1:C:632:ILE:HG23	1:C:633:LEU:N	2.26	0.50
1:C:823:ILE:HG23	1:C:824:PRO:HD2	1.92	0.50
1:C:836:LEU:HD21	2:D:945:PHE:HE1	1.75	0.50
2:B:372:LEU:O	2:B:379:VAL:HA	2.11	0.50
2:B:1022:GLU:HG2	2:B:1023:LEU:N	2.26	0.50
2:D:544:ILE:HD13	2:D:575:LYS:HG2	1.92	0.50
2:D:858:TYR:OH	2:D:866:ASN:O	2.30	0.50
2:D:1022:GLU:HG2	2:D:1023:LEU:N	2.26	0.50
1:A:482:GLY:C	1:A:483:LEU:HG	2.36	0.50
1:A:896:SER:C	1:A:897:GLU:HG3	2.36	0.50
1:E:857:TYR:HA	1:E:862:TYR:HA	1.93	0.50
2:B:205:PRO:HD3	2:B:230:ILE:HD11	1.94	0.50
2:B:694:ASN:O	2:B:697:ARG:HD2	2.10	0.50
2:D:269:TYR:CE2	2:D:288:GLU:HA	2.47	0.50
2:D:888:SER:HB3	2:D:968:ILE:HG12	1.94	0.50
2:F:151:ILE:HD11	2:F:167:GLU:HB2	1.94	0.50
2:F:262:PHE:CZ	2:F:293:ILE:O	2.64	0.50
2:F:554:ILE:CG2	2:F:556:TRP:CE2	2.94	0.50
2:F:1149:HIS:NE2	2:F:1150:ASP:HB3	2.26	0.50
1:A:143:ILE:HG22	1:A:144:LEU:N	2.27	0.50
1:A:144:LEU:HA	1:A:487:LYS:HA	1.93	0.50
1:A:154:GLU:CB	1:A:155:PRO:HD2	2.42	0.50
1:C:82:ARG:HG3	1:C:364:LEU:HD11	1.94	0.50
1:E:45:ARG:NH1	1:E:154:GLU:O	2.45	0.50
1:E:447:ASN:OD1	1:E:447:ASN:N	2.43	0.50
1:E:482:GLY:C	1:E:483:LEU:HG	2.37	0.50
1:E:944:ARG:CG	1:E:1026:SER:HA	2.41	0.50
1:E:1093:LYS:HB3	1:E:1096:ASN:HB2	1.93	0.50
2:B:482:LEU:HD22	2:B:499:SER:HB3	1.94	0.50
2:D:277:ASN:HA	2:D:281:ASN:HA	1.92	0.50
2:F:22:ARG:HD2	2:F:27:ASP:O	2.11	0.50
2:F:923:ILE:O	2:F:925:ASN:N	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:ASN:HA	1:A:664:ILE:HG22	1.94	0.50
1:C:795:ASN:OD1	1:C:796:TYR:N	2.44	0.50
2:B:374:ASN:C	2:B:374:ASN:OD1	2.54	0.50
2:D:1137:ASN:CB	2:D:1142:TRP:HE1	2.20	0.50
1:A:610:LEU:CD1	1:A:704:MET:HE2	2.41	0.50
1:A:836:LEU:HD21	2:B:945:PHE:HE1	1.75	0.50
1:A:864:ASP:C	1:A:864:ASP:OD1	2.55	0.50
1:C:34:ASN:HB2	1:C:40:TRP:CH2	2.47	0.50
1:C:45:ARG:NH1	1:C:154:GLU:O	2.44	0.50
1:C:1143:ARG:HH21	1:C:1143:ARG:CG	2.24	0.50
1:E:661:ASN:HA	1:E:664:ILE:HG22	1.93	0.50
2:B:9:ILE:HG13	2:B:10:ASP:N	2.27	0.50
2:B:251:ILE:O	2:B:252:ASP:HB2	2.12	0.50
2:F:932:VAL:C	2:F:933:ILE:HG13	2.37	0.50
1:A:45:ARG:NH1	1:A:154:GLU:O	2.45	0.50
1:A:90:ILE:O	1:A:93:ARG:HB3	2.12	0.50
1:C:113:TYR:HB3	1:C:178:PHE:HB3	1.93	0.50
1:C:738:TYR:HA	1:C:743:ILE:CG1	2.42	0.50
1:E:818:THR:O	1:E:819:LEU:HG	2.12	0.50
1:E:836:LEU:HD21	2:F:945:PHE:HE1	1.76	0.50
1:E:989:LYS:HG2	1:E:1076:TRP:HA	1.94	0.50
2:D:262:PHE:CZ	2:D:293:ILE:O	2.65	0.50
2:D:932:VAL:C	2:D:933:ILE:HG13	2.36	0.50
2:F:92:ASN:HB3	2:F:310:PHE:CZ	2.46	0.50
2:F:551:THR:HG21	2:F:716:ASN:HB3	1.94	0.50
2:F:1008:ARG:HA	2:F:1014:ILE:HA	1.94	0.50
1:A:46:ASN:OD1	1:A:151:MET:HG3	2.12	0.50
1:A:82:ARG:HG3	1:A:364:LEU:HD11	1.94	0.50
1:A:242:THR:HG22	1:A:435:PHE:O	2.11	0.50
1:A:573:VAL:HA	1:A:576:ILE:HD12	1.94	0.50
1:C:453:GLU:C	1:C:454:ILE:HG22	2.37	0.50
2:B:436:ASP:CA	2:B:437:ILE:HB	2.25	0.50
2:D:658:ALA:O	2:D:662:LEU:HG	2.12	0.50
2:D:1140:TYR:CE2	2:D:1142:TRP:CD2	3.00	0.50
2:F:277:ASN:HA	2:F:281:ASN:HA	1.93	0.50
1:A:607:GLY:HA2	1:A:612:ILE:HG13	1.94	0.49
1:A:897:GLU:HG2	1:A:1032:LYS:CB	2.38	0.49
1:A:897:GLU:CG	1:A:1032:LYS:HD3	2.42	0.49
1:A:1090:ASN:HB2	1:A:1240:TRP:CZ3	2.47	0.49
1:E:41:ILE:HG22	1:E:150:ILE:HB	1.93	0.49
2:B:763:LEU:HA	2:B:766:GLN:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:9:ILE:O	2:D:11:SER:N	2.45	0.49
2:D:9:ILE:HG21	2:D:76:ASP:HB2	1.94	0.49
2:D:274:LYS:C	2:D:276:ASN:H	2.20	0.49
2:D:482:LEU:HD22	2:D:499:SER:HB3	1.93	0.49
2:D:877:LYS:HB3	2:D:878:GLN:CB	2.42	0.49
1:A:634:LEU:HD23	1:A:696:GLN:CD	2.37	0.49
2:B:41:ILE:HG22	2:B:138:ILE:HB	1.94	0.49
2:D:14:ASP:O	2:D:15:ASN:HB2	2.12	0.49
2:D:21:VAL:HG12	2:D:22:ARG:N	2.26	0.49
2:D:388:ASP:OD1	2:D:388:ASP:N	2.42	0.49
2:F:251:ILE:O	2:F:252:ASP:CB	2.60	0.49
2:F:888:SER:HB3	2:F:968:ILE:HG12	1.94	0.49
1:A:836:LEU:HD13	2:B:991:SER:HA	1.94	0.49
1:A:940:ILE:O	1:A:951:LYS:HA	2.13	0.49
1:E:547:GLU:HB2	1:E:550:LYS:HG3	1.94	0.49
2:B:867:PHE:CD1	2:B:867:PHE:C	2.91	0.49
2:B:888:SER:HB3	2:B:968:ILE:HG12	1.95	0.49
2:D:554:ILE:CG2	2:D:556:TRP:CE2	2.95	0.49
1:E:143:ILE:CG2	1:E:144:LEU:N	2.75	0.49
1:E:785:TYR:O	1:E:786:ASP:C	2.55	0.49
2:B:677:ASN:CG	2:D:849:ASN:ND2	2.70	0.49
2:B:856:ASN:O	2:B:857:ASP:C	2.55	0.49
2:D:290:LYS:O	2:D:290:LYS:HG2	2.13	0.49
2:D:347:GLY:O	2:D:351:THR:HB	2.13	0.49
2:D:803:LEU:HD23	2:D:803:LEU:C	2.37	0.49
2:D:824:THR:HA	2:D:856:ASN:HB2	1.94	0.49
2:F:877:LYS:HB3	2:F:878:GLN:CB	2.42	0.49
2:F:1007:ILE:HG22	2:F:1015:LEU:HD12	1.93	0.49
1:A:795:ASN:OD1	1:A:796:TYR:N	2.45	0.49
1:C:38:ASN:HD21	1:C:484:SER:HB2	1.77	0.49
1:C:90:ILE:O	1:C:93:ARG:HB3	2.13	0.49
1:C:738:TYR:C	1:C:740:ILE:N	2.70	0.49
1:C:896:SER:C	1:C:897:GLU:HG3	2.36	0.49
1:C:1188:VAL:CG1	1:C:1199:MET:HB2	2.43	0.49
1:E:607:GLY:HA2	1:E:612:ILE:CG1	2.42	0.49
2:D:151:ILE:HD11	2:D:167:GLU:HB2	1.94	0.49
2:D:706:ALA:O	2:D:709:ASN:HB2	2.13	0.49
2:D:827:GLU:O	2:D:852:ILE:HG23	2.12	0.49
1:A:41:ILE:HG22	1:A:150:ILE:HB	1.93	0.49
1:A:1093:LYS:HB3	1:A:1096:ASN:HB2	1.94	0.49
1:C:607:GLY:HA2	1:C:612:ILE:HG13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:166:SER:HB3	1:E:498:ILE:HB	1.94	0.49
2:B:717:ALA:O	2:B:721:VAL:HG23	2.12	0.49
2:B:722:PHE:HA	2:B:726:ILE:HD12	1.93	0.49
2:B:755:ILE:HG23	2:B:759:GLU:HB2	1.95	0.49
2:D:755:ILE:HG23	2:D:759:GLU:HB2	1.95	0.49
2:F:155:LYS:O	2:F:156:GLU:C	2.55	0.49
1:A:607:GLY:HA2	1:A:612:ILE:CG1	2.43	0.49
1:A:795:ASN:OD1	1:A:795:ASN:C	2.55	0.49
1:A:989:LYS:HG2	1:A:1076:TRP:HA	1.94	0.49
1:A:1122:TYR:HE1	1:A:1244:SER:O	1.95	0.49
1:C:199:ILE:HA	1:C:705:TYR:CE2	2.42	0.49
1:C:892:ASN:N	1:C:892:ASN:OD1	2.45	0.49
1:E:113:TYR:HB3	1:E:178:PHE:HB3	1.93	0.49
1:E:607:GLY:HA2	1:E:612:ILE:HG13	1.95	0.49
2:B:64:TYR:HE2	2:B:363:ILE:HD12	1.78	0.49
2:B:274:LYS:C	2:B:276:ASN:H	2.19	0.49
2:B:922:ASN:C	2:B:923:ILE:HG13	2.37	0.49
2:B:1095:ASN:HB2	2:B:1097:ARG:HB2	1.95	0.49
2:D:22:ARG:HD2	2:D:27:ASP:O	2.12	0.49
2:D:41:ILE:HG22	2:D:138:ILE:HB	1.94	0.49
2:D:153:TYR:HD2	2:D:165:MET:HB2	1.77	0.49
2:D:154:LYS:HD3	2:D:157:TYR:CE2	2.47	0.49
2:D:717:ALA:O	2:D:721:VAL:HG23	2.13	0.49
2:F:274:LYS:C	2:F:276:ASN:H	2.21	0.49
2:F:347:GLY:O	2:F:351:THR:HB	2.12	0.49
2:F:424:GLU:O	2:F:428:LYS:N	2.44	0.49
2:F:518:ASP:O	2:F:680:ILE:HD11	2.12	0.49
1:A:34:ASN:HB2	1:A:40:TRP:CH2	2.48	0.49
1:A:700:ARG:HA	1:A:703:GLN:HB2	1.95	0.49
1:A:738:TYR:C	1:A:740:ILE:N	2.71	0.49
1:A:854:ASN:HB2	1:A:865:THR:CG2	2.43	0.49
1:E:154:GLU:CB	1:E:155:PRO:HD2	2.40	0.49
1:E:205:ASP:OD1	1:E:206:PRO:HD2	2.13	0.49
2:B:541:THR:O	2:B:542:GLN:CB	2.60	0.49
2:B:806:TYR:O	2:B:806:TYR:CD1	2.65	0.49
2:D:23:SER:HB2	2:D:47:TYR:CZ	2.47	0.49
2:F:203:ILE:HG22	2:F:254:TYR:OH	2.12	0.49
2:F:755:ILE:HG23	2:F:759:GLU:HB2	1.95	0.49
1:C:143:ILE:CG2	1:C:144:LEU:N	2.75	0.49
1:C:331:LEU:HB2	1:C:332:TYR:HD2	1.77	0.49
1:C:785:TYR:O	1:C:786:ASP:C	2.54	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:940:ILE:O	1:C:951:LYS:HA	2.12	0.49
1:E:864:ASP:C	1:E:864:ASP:OD1	2.55	0.49
2:B:393:THR:OG1	2:B:396:ASN:N	2.46	0.49
2:B:872:TRP:HB2	2:B:980:GLU:HB3	1.94	0.49
2:D:763:LEU:HA	2:D:766:GLN:HB2	1.95	0.49
1:A:143:ILE:CG2	1:A:144:LEU:N	2.76	0.49
1:A:398:PRO:C	1:A:399:ILE:HG13	2.38	0.49
2:B:277:ASN:HA	2:B:281:ASN:HA	1.94	0.49
2:B:815:VAL:HG12	2:B:816:ILE:N	2.28	0.49
2:B:932:VAL:C	2:B:933:ILE:HG13	2.37	0.49
2:F:153:TYR:HD2	2:F:165:MET:HB2	1.77	0.49
2:F:815:VAL:C	2:F:816:ILE:HG13	2.37	0.49
1:C:278:ASP:OD1	1:C:278:ASP:N	2.43	0.48
1:C:627:LEU:O	1:E:419:LYS:HG2	2.12	0.48
1:C:854:ASN:HB2	1:C:865:THR:CG2	2.43	0.48
1:C:879:TYR:O	1:C:888:PHE:HA	2.13	0.48
1:C:1025:VAL:CG1	1:C:1026:SER:N	2.76	0.48
1:C:1108:ILE:CG2	1:C:1217:ASP:HA	2.43	0.48
1:E:944:ARG:O	1:E:946:ASN:N	2.46	0.48
2:B:1020:THR:HA	2:B:1059:PHE:O	2.12	0.48
2:F:8:ASN:O	2:F:9:ILE:C	2.55	0.48
2:F:552:LYS:C	2:F:713:PHE:CE1	2.91	0.48
1:C:482:GLY:C	1:C:483:LEU:HG	2.38	0.48
1:C:864:ASP:C	1:C:864:ASP:OD1	2.56	0.48
1:E:46:ASN:OD1	1:E:151:MET:HG3	2.12	0.48
1:E:47:VAL:O	1:E:47:VAL:HG12	2.12	0.48
2:B:877:LYS:HB3	2:B:878:GLN:CB	2.42	0.48
2:D:251:ILE:O	2:D:252:ASP:HB2	2.13	0.48
2:D:518:ASP:O	2:D:680:ILE:HD11	2.12	0.48
2:F:207:ASP:N	2:F:207:ASP:OD1	2.46	0.48
2:F:658:ALA:O	2:F:662:LEU:HG	2.13	0.48
1:A:17:THR:HG22	1:A:34:ASN:HB3	1.94	0.48
1:A:220:GLY:CA	1:A:225:LYS:HE3	2.43	0.48
1:A:480:ALA:N	1:A:481:PRO:HD3	2.29	0.48
1:C:548:GLN:HB2	1:C:549:PRO:HD3	1.95	0.48
1:C:818:THR:O	1:C:819:LEU:HG	2.13	0.48
1:C:1087:TYR:N	1:C:1243:ILE:O	2.46	0.48
1:E:940:ILE:O	1:E:951:LYS:HA	2.13	0.48
2:B:206:ASN:ND2	2:B:208:ASN:HB2	2.27	0.48
2:B:424:GLU:O	2:B:428:LYS:N	2.46	0.48
2:D:64:TYR:HE2	2:D:363:ILE:HD12	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:9:ILE:O	2:F:11:SER:N	2.46	0.48
2:F:21:VAL:HG12	2:F:22:ARG:N	2.28	0.48
2:F:1140:TYR:CE2	2:F:1142:TRP:CD2	3.02	0.48
1:C:94:ILE:HG23	1:C:211:MET:HE3	1.95	0.48
1:C:573:VAL:HA	1:C:576:ILE:HD12	1.95	0.48
1:C:607:GLY:HA2	1:C:612:ILE:CG1	2.43	0.48
1:E:17:THR:HG22	1:E:34:ASN:HB3	1.95	0.48
1:E:376:ASN:O	1:E:381:LYS:HB3	2.13	0.48
2:B:552:LYS:CB	2:B:713:PHE:HE1	2.26	0.48
2:D:372:LEU:O	2:D:379:VAL:HA	2.14	0.48
2:D:1008:ARG:HA	2:D:1014:ILE:HA	1.96	0.48
1:A:936:GLU:HA	1:A:954:LEU:O	2.14	0.48
1:A:1212:LEU:O	1:A:1238:CYS:HA	2.12	0.48
1:C:46:ASN:OD1	1:C:151:MET:HG3	2.12	0.48
1:E:892:ASN:OD1	1:E:892:ASN:N	2.45	0.48
1:E:972:LYS:CB	2:F:772:LEU:HD11	2.44	0.48
1:E:1025:VAL:HG12	1:E:1026:SER:N	2.27	0.48
2:B:402:ILE:HG12	2:B:593:LYS:CB	2.44	0.48
2:B:827:GLU:O	2:B:852:ILE:HG23	2.12	0.48
2:D:552:LYS:CB	2:D:713:PHE:HE1	2.26	0.48
2:D:1007:ILE:HG22	2:D:1015:LEU:HD12	1.95	0.48
2:F:615:LEU:HB3	2:F:767:ASN:ND2	2.28	0.48
1:A:47:VAL:O	1:A:47:VAL:HG12	2.13	0.48
1:A:94:ILE:HG23	1:A:211:MET:HE3	1.94	0.48
1:C:231:CYS:CB	1:C:249:ILE:HD12	2.43	0.48
1:C:398:PRO:C	1:C:399:ILE:HG13	2.38	0.48
1:C:475:PHE:C	2:D:1136:LYS:CE	2.87	0.48
1:C:1122:TYR:HE1	1:C:1244:SER:O	1.97	0.48
1:E:440:GLU:O	1:E:443:TYR:CD1	2.67	0.48
1:E:854:ASN:CB	1:E:865:THR:HG22	2.43	0.48
1:E:1122:TYR:HE1	1:E:1244:SER:O	1.97	0.48
2:B:502:ASN:O	2:B:506:ASP:N	2.42	0.48
2:B:570:PHE:O	2:B:573:GLU:HB2	2.13	0.48
2:B:645:TYR:O	2:B:646:PHE:C	2.56	0.48
2:F:567:ASN:O	2:F:568:ASN:C	2.57	0.48
2:F:570:PHE:O	2:F:573:GLU:HB2	2.14	0.48
2:F:867:PHE:C	2:F:867:PHE:CD1	2.91	0.48
1:E:220:GLY:CA	1:E:225:LYS:HE3	2.44	0.48
1:E:423:LYS:HD2	2:D:510:PHE:CE2	2.48	0.48
1:E:700:ARG:HA	1:E:703:GLN:HB2	1.95	0.48
2:B:518:ASP:O	2:B:680:ILE:HD11	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:794:ILE:O	2:B:795:LYS:C	2.56	0.48
2:D:552:LYS:C	2:D:713:PHE:CE1	2.92	0.48
2:F:23:SER:HB2	2:F:47:TYR:CZ	2.49	0.48
2:F:794:ILE:O	2:F:795:LYS:C	2.56	0.48
1:A:291:VAL:HA	1:A:292:SER:HB2	1.95	0.48
1:A:944:ARG:CG	1:A:1026:SER:HA	2.42	0.48
1:E:215:ILE:HG22	1:E:219:HIS:CE1	2.48	0.48
1:E:548:GLN:HB2	1:E:549:PRO:HD3	1.96	0.48
1:E:634:LEU:HD23	1:E:696:GLN:CD	2.39	0.48
2:B:1122:LEU:HD21	2:B:1158:TRP:HZ2	1.76	0.48
2:D:153:TYR:CD2	2:D:165:MET:HB2	2.48	0.48
2:D:567:ASN:O	2:D:568:ASN:C	2.54	0.48
2:D:1042:ILE:O	2:D:1099:GLN:HA	2.13	0.48
2:F:232:PHE:CZ	2:F:240:TYR:HA	2.49	0.48
1:A:944:ARG:O	1:A:946:ASN:N	2.47	0.48
1:C:836:LEU:HD13	2:D:991:SER:HA	1.96	0.48
1:E:897:GLU:CG	1:E:1032:LYS:HD3	2.44	0.48
2:B:203:ILE:HG22	2:B:203:ILE:O	2.13	0.48
2:D:146:ILE:HD13	2:D:330:TYR:CZ	2.49	0.48
2:D:615:LEU:HB3	2:D:767:ASN:ND2	2.29	0.48
2:D:645:TYR:O	2:D:646:PHE:C	2.55	0.48
2:D:684:ASN:O	2:D:687:LEU:N	2.47	0.48
2:F:15:ASN:OD1	2:F:126:LYS:CB	2.62	0.48
2:F:475:ILE:HG21	2:F:497:VAL:HG22	1.95	0.48
2:F:1020:THR:HA	2:F:1059:PHE:O	2.14	0.48
1:C:661:ASN:HA	1:C:664:ILE:HG22	1.95	0.48
1:C:944:ARG:O	1:C:946:ASN:N	2.47	0.48
1:C:1088:LEU:HD23	1:C:1089:LEU:N	2.29	0.48
1:E:1143:ARG:HH21	1:E:1143:ARG:CG	2.26	0.48
2:B:21:VAL:HG12	2:B:22:ARG:N	2.29	0.48
2:B:64:TYR:CD2	2:B:64:TYR:N	2.81	0.48
2:B:571:VAL:O	2:B:574:PHE:HB3	2.14	0.48
2:B:1008:ARG:HA	2:B:1014:ILE:HA	1.96	0.48
2:D:1095:ASN:HB2	2:D:1097:ARG:HB2	1.95	0.48
2:F:856:ASN:O	2:F:857:ASP:C	2.56	0.48
2:F:1042:ILE:O	2:F:1099:GLN:HA	2.14	0.48
1:A:468:LEU:C	1:A:468:LEU:HD12	2.39	0.47
1:C:166:SER:HB3	1:C:498:ILE:HB	1.95	0.47
1:E:90:ILE:O	1:E:93:ARG:HB3	2.14	0.47
1:E:795:ASN:OD1	1:E:795:ASN:C	2.57	0.47
2:B:203:ILE:HG22	2:B:254:TYR:OH	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:232:PHE:CZ	2:B:240:TYR:HA	2.49	0.47
2:B:913:GLY:O	2:B:914:ASN:C	2.57	0.47
2:F:583:ILE:HG23	2:F:644:GLN:NE2	2.29	0.47
2:F:815:VAL:HG12	2:F:816:ILE:N	2.29	0.47
1:A:929:LYS:HA	1:A:932:ASN:HB2	1.96	0.47
1:E:682:TYR:CE2	1:E:825:PHE:HA	2.49	0.47
1:E:879:TYR:O	1:E:888:PHE:HA	2.13	0.47
2:B:551:THR:HG21	2:B:716:ASN:HB3	1.95	0.47
2:D:205:PRO:HD3	2:D:230:ILE:HD11	1.96	0.47
2:D:945:PHE:CD1	2:D:950:LEU:HA	2.49	0.47
2:D:991:SER:O	2:D:994:ILE:HB	2.13	0.47
2:F:306:PHE:O	2:F:307:SER:C	2.57	0.47
2:F:631:TYR:O	2:F:634:LEU:HB2	2.14	0.47
2:F:1122:LEU:HD21	2:F:1158:TRP:HZ2	1.75	0.47
1:A:138:ASN:ND2	1:A:140:SER:OG	2.47	0.47
1:A:270:ASP:O	1:A:273:THR:HG22	2.14	0.47
1:C:634:LEU:HD23	1:C:696:GLN:CD	2.38	0.47
1:C:936:GLU:HA	1:C:954:LEU:O	2.14	0.47
1:E:854:ASN:HB2	1:E:865:THR:CG2	2.43	0.47
1:E:911:LYS:O	1:E:999:ARG:NE	2.47	0.47
2:B:290:LYS:O	2:B:290:LYS:HG2	2.14	0.47
2:B:402:ILE:HG12	2:B:593:LYS:HB2	1.96	0.47
2:B:541:THR:HA	2:B:553:ILE:O	2.14	0.47
2:B:554:ILE:HB	2:B:557:ILE:CD1	2.44	0.47
2:B:923:ILE:C	2:B:925:ASN:H	2.18	0.47
2:D:1020:THR:HA	2:D:1059:PHE:O	2.14	0.47
2:F:205:PRO:HD3	2:F:230:ILE:HD11	1.96	0.47
2:F:269:TYR:HD1	2:F:287:LEU:HD23	1.79	0.47
2:F:717:ALA:O	2:F:721:VAL:HG23	2.14	0.47
2:F:923:ILE:C	2:F:925:ASN:H	2.21	0.47
1:A:203:ILE:HD13	1:A:396:ILE:HG21	1.96	0.47
1:A:603:VAL:CG1	1:A:605:TYR:CE2	2.98	0.47
1:C:286:LEU:O	1:C:287:SER:C	2.58	0.47
1:C:716:LYS:O	1:C:719:ILE:HG22	2.14	0.47
1:E:231:CYS:HB2	1:E:249:ILE:HD12	1.97	0.47
2:D:192:CYS:O	2:D:195:LYS:HB3	2.14	0.47
2:D:815:VAL:HG12	2:D:816:ILE:N	2.29	0.47
2:F:1095:ASN:HB2	2:F:1097:ARG:HB2	1.96	0.47
1:A:456:ASP:HA	1:A:669:ASN:HD21	1.79	0.47
1:A:528:VAL:HG13	1:A:528:VAL:O	2.15	0.47
1:C:17:THR:HG22	1:C:34:ASN:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:ASN:ND2	1:C:140:SER:OG	2.47	0.47
1:C:949:GLY:O	1:C:963:LEU:HD12	2.15	0.47
1:E:1087:TYR:N	1:E:1243:ILE:O	2.47	0.47
1:E:1108:ILE:CG2	1:E:1217:ASP:HA	2.44	0.47
2:B:428:LYS:C	2:B:430:PRO:CD	2.88	0.47
2:F:239:ASP:OD2	2:F:318:TYR:N	2.43	0.47
2:F:402:ILE:HG12	2:F:593:LYS:HB2	1.97	0.47
2:F:827:GLU:O	2:F:852:ILE:HG23	2.14	0.47
1:A:431:ASN:O	1:A:434:LEU:HB2	2.14	0.47
1:A:912:TYR:O	1:A:913:LYS:HB3	2.15	0.47
1:A:1229:MET:O	1:A:1231:ASP:N	2.48	0.47
1:C:467:ASP:OD1	1:C:467:ASP:C	2.57	0.47
1:C:897:GLU:CG	1:C:1032:LYS:HD3	2.44	0.47
1:E:186:PHE:CE2	1:E:188:PRO:HB3	2.48	0.47
2:B:706:ALA:O	2:B:709:ASN:HB2	2.13	0.47
2:B:991:SER:O	2:B:994:ILE:HB	2.15	0.47
2:D:155:LYS:O	2:D:156:GLU:C	2.57	0.47
2:D:238:ILE:O	2:D:239:ASP:C	2.55	0.47
2:D:271:ILE:HG23	2:D:272:LYS:N	2.30	0.47
2:D:424:GLU:O	2:D:428:LYS:N	2.47	0.47
2:D:976:ASN:C	2:D:977:VAL:HG23	2.40	0.47
2:F:173:PHE:HA	2:F:333:ILE:HB	1.96	0.47
1:A:548:GLN:HB2	1:A:549:PRO:HD3	1.96	0.47
1:A:716:LYS:O	1:A:719:ILE:HG22	2.15	0.47
1:A:778:LYS:HA	1:A:782:LEU:HB2	1.96	0.47
1:C:203:ILE:HD13	1:C:396:ILE:HG21	1.97	0.47
1:C:291:VAL:HA	1:C:292:SER:HB2	1.97	0.47
1:C:376:ASN:O	1:C:381:LYS:HB3	2.15	0.47
1:C:911:LYS:O	1:C:999:ARG:NE	2.47	0.47
1:E:270:ASP:O	1:E:273:THR:HG22	2.15	0.47
1:E:278:ASP:OD1	1:E:278:ASP:N	2.43	0.47
1:E:610:LEU:CD1	1:E:704:MET:HE2	2.43	0.47
1:E:633:LEU:O	1:E:700:ARG:NH2	2.45	0.47
2:B:210:ASN:HB3	2:B:228:ASP:HA	1.97	0.47
2:B:269:TYR:HD1	2:B:287:LEU:HD23	1.79	0.47
2:B:1069:GLN:O	2:B:1070:TYR:CD2	2.68	0.47
2:B:1122:LEU:C	2:B:1122:LEU:HD12	2.40	0.47
2:D:203:ILE:HG22	2:D:254:TYR:OH	2.14	0.47
2:D:541:THR:HA	2:D:553:ILE:O	2.15	0.47
2:F:9:ILE:HG21	2:F:76:ASP:HB2	1.97	0.47
2:F:290:LYS:HG2	2:F:290:LYS:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:388:ASP:OD1	2:F:388:ASP:N	2.44	0.47
2:F:706:ALA:O	2:F:709:ASN:HB2	2.14	0.47
1:A:231:CYS:HB2	1:A:249:ILE:HD12	1.97	0.47
1:C:1092:LEU:HD11	1:C:1234:ASN:O	2.15	0.47
1:E:632:ILE:HG23	1:E:633:LEU:N	2.28	0.47
1:E:738:TYR:C	1:E:740:ILE:N	2.72	0.47
1:E:795:ASN:OD1	1:E:796:TYR:N	2.48	0.47
2:B:13:VAL:HG12	2:B:14:ASP:H	1.77	0.47
2:D:868:SER:HA	2:D:933:ILE:O	2.14	0.47
2:F:251:ILE:O	2:F:252:ASP:HB2	2.14	0.47
1:A:911:LYS:O	1:A:999:ARG:NE	2.47	0.47
1:C:857:TYR:HB2	1:C:862:TYR:CE1	2.50	0.47
1:E:94:ILE:HG23	1:E:211:MET:HE3	1.95	0.47
1:E:331:LEU:HB2	1:E:332:TYR:HD2	1.80	0.47
1:E:398:PRO:C	1:E:399:ILE:HG13	2.40	0.47
1:E:1092:LEU:HD11	1:E:1234:ASN:O	2.15	0.47
2:B:15:ASN:OD1	2:B:126:LYS:CB	2.63	0.47
2:B:629:ILE:O	2:B:630:TYR:C	2.58	0.47
2:B:658:ALA:O	2:B:662:LEU:HG	2.14	0.47
2:B:876:LEU:HD21	2:B:978:TYR:CD2	2.50	0.47
2:D:9:ILE:HG13	2:D:10:ASP:N	2.29	0.47
1:A:903:ASN:C	1:A:903:ASN:OD1	2.59	0.47
1:A:942:CYS:SG	1:A:1025:VAL:CG1	3.03	0.47
1:A:949:GLY:O	1:A:963:LEU:HD12	2.15	0.47
1:C:231:CYS:HB2	1:C:249:ILE:HD12	1.97	0.47
1:C:270:ASP:O	1:C:273:THR:HG22	2.15	0.47
2:B:305:TYR:CE1	2:B:418:LEU:CD1	2.97	0.47
2:B:475:ILE:HG21	2:B:497:VAL:HG22	1.96	0.47
2:D:1003:ASN:CG	2:D:1003:ASN:O	2.57	0.47
2:F:238:ILE:O	2:F:239:ASP:C	2.57	0.47
2:F:541:THR:HA	2:F:553:ILE:O	2.15	0.47
2:F:738:ILE:O	2:F:739:LYS:C	2.58	0.47
2:F:876:LEU:HD21	2:F:978:TYR:CD2	2.50	0.47
1:A:480:ALA:N	1:A:481:PRO:CD	2.78	0.46
1:A:1132:VAL:HG23	1:A:1149:TYR:CE2	2.50	0.46
1:A:1188:VAL:CG1	1:A:1199:MET:HB2	2.45	0.46
1:C:535:VAL:HG12	1:C:536:ASN:N	2.30	0.46
2:B:45:ARG:HG3	2:B:141:PRO:O	2.15	0.46
2:B:106:ILE:HG22	2:B:107:PRO:O	2.14	0.46
2:D:922:ASN:C	2:D:923:ILE:HG13	2.40	0.46
2:F:146:ILE:HD13	2:F:330:TYR:CZ	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:922:ASN:C	2:F:923:ILE:HG13	2.39	0.46
1:A:186:PHE:CE2	1:A:188:PRO:HB3	2.51	0.46
1:A:297:ASN:N	1:A:298:PRO:HD3	2.30	0.46
1:C:440:GLU:O	1:C:443:TYR:CD1	2.68	0.46
1:C:470:GLN:HG3	2:D:1028:PHE:CE1	2.50	0.46
1:C:1090:ASN:HB2	1:C:1240:TRP:CZ3	2.50	0.46
1:E:154:GLU:CB	1:E:155:PRO:CD	2.94	0.46
1:E:528:VAL:O	1:E:528:VAL:HG13	2.15	0.46
1:E:735:THR:O	1:E:911:LYS:NZ	2.40	0.46
1:E:824:PRO:HB2	2:F:952:ALA:HB2	1.97	0.46
1:E:1025:VAL:CG1	1:E:1026:SER:N	2.78	0.46
2:D:570:PHE:O	2:D:573:GLU:HB2	2.15	0.46
2:D:631:TYR:O	2:D:634:LEU:HB2	2.15	0.46
2:D:722:PHE:HA	2:D:726:ILE:HD12	1.96	0.46
2:D:1093:THR:OG1	2:D:1094:THR:N	2.49	0.46
2:F:629:ILE:O	2:F:630:TYR:C	2.58	0.46
1:A:1043:GLY:C	1:A:1044:ILE:HG13	2.39	0.46
1:C:528:VAL:O	1:C:528:VAL:HG13	2.15	0.46
1:E:920:TRP:HB2	1:E:1045:ARG:CD	2.45	0.46
1:E:1188:VAL:CG1	1:E:1199:MET:HB2	2.45	0.46
2:B:917:ASN:C	2:B:918:ILE:HG13	2.40	0.46
2:B:923:ILE:C	2:B:925:ASN:N	2.72	0.46
2:D:856:ASN:O	2:D:857:ASP:C	2.58	0.46
2:D:990:ASN:O	2:D:993:GLU:N	2.48	0.46
2:F:45:ARG:HG3	2:F:141:PRO:O	2.15	0.46
2:F:1003:ASN:O	2:F:1003:ASN:CG	2.58	0.46
1:A:376:ASN:O	1:A:381:LYS:HB3	2.15	0.46
1:A:879:TYR:O	1:A:888:PHE:HA	2.16	0.46
1:C:606:ILE:CG2	1:C:621:PHE:CE2	2.98	0.46
1:E:345:VAL:HG13	1:E:387:GLN:HE22	1.81	0.46
1:E:573:VAL:HA	1:E:576:ILE:HD12	1.97	0.46
1:E:1132:VAL:HG23	1:E:1149:TYR:CE2	2.50	0.46
2:B:23:SER:HB2	2:B:47:TYR:CZ	2.50	0.46
2:B:530:ILE:O	2:B:531:PHE:C	2.59	0.46
2:D:106:ILE:HG22	2:D:107:PRO:O	2.15	0.46
2:D:846:THR:HG23	2:D:847:GLY:N	2.31	0.46
2:F:153:TYR:CD2	2:F:165:MET:HB2	2.50	0.46
2:F:859:PHE:HD1	2:F:968:ILE:HD12	1.80	0.46
2:F:867:PHE:CZ	2:F:935:ILE:HD12	2.50	0.46
1:A:22:LYS:CG	1:A:23:PRO:HD2	2.45	0.46
1:A:1088:LEU:HD23	1:A:1089:LEU:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:LYS:CG	1:C:23:PRO:HD2	2.45	0.46
1:C:469:ASP:O	1:C:472:ILE:HB	2.15	0.46
1:C:571:LEU:O	1:C:575:TRP:N	2.42	0.46
2:B:141:PRO:HA	2:B:169:TRP:HB3	1.96	0.46
2:B:192:CYS:O	2:B:195:LYS:HB3	2.15	0.46
2:B:305:TYR:CZ	2:B:418:LEU:CD1	2.99	0.46
2:B:552:LYS:C	2:B:713:PHE:CE1	2.93	0.46
2:B:868:SER:HA	2:B:933:ILE:O	2.16	0.46
2:B:1007:ILE:HG12	2:B:1072:GLN:C	2.41	0.46
2:B:1142:TRP:CD1	2:B:1142:TRP:H	2.32	0.46
2:D:13:VAL:HG12	2:D:14:ASP:H	1.80	0.46
2:D:185:PRO:O	2:D:186:ALA:C	2.57	0.46
2:D:610:ASP:OD1	2:D:611:LEU:HD13	2.15	0.46
2:F:14:ASP:O	2:F:15:ASN:CB	2.64	0.46
2:F:872:TRP:HB2	2:F:980:GLU:HB3	1.97	0.46
1:A:179:GLY:HA2	1:A:220:GLY:O	2.15	0.46
1:A:987:ILE:C	1:A:989:LYS:N	2.73	0.46
1:C:179:GLY:HA2	1:C:220:GLY:O	2.15	0.46
1:C:903:ASN:C	1:C:903:ASN:OD1	2.59	0.46
1:C:932:ASN:HA	1:C:956:HIS:CE1	2.51	0.46
1:C:989:LYS:HG2	1:C:1076:TRP:HA	1.97	0.46
2:B:269:TYR:CE2	2:B:288:GLU:HA	2.51	0.46
2:B:989:ILE:HG22	2:B:990:ASN:N	2.30	0.46
2:D:203:ILE:HG22	2:D:203:ILE:O	2.16	0.46
2:D:1003:ASN:HB3	2:D:1116:ILE:CD1	2.46	0.46
2:F:271:ILE:HG23	2:F:272:LYS:N	2.30	0.46
2:F:806:TYR:O	2:F:806:TYR:CD1	2.69	0.46
1:A:231:CYS:CB	1:A:249:ILE:HD12	2.46	0.46
1:A:286:LEU:O	1:A:289:VAL:HG13	2.16	0.46
1:C:211:MET:HE1	1:C:343:PHE:CZ	2.51	0.46
1:C:942:CYS:SG	1:C:1025:VAL:CG1	3.04	0.46
1:E:873:ASN:N	1:E:899:ASN:O	2.39	0.46
1:E:949:GLY:O	1:E:963:LEU:HD12	2.16	0.46
1:E:981:ASN:ND2	2:F:414:ASN:HB3	2.28	0.46
2:B:207:ASP:OD1	2:B:207:ASP:N	2.48	0.46
2:D:475:ILE:HG21	2:D:497:VAL:HG22	1.96	0.46
2:F:586:LYS:O	2:F:641:TYR:CZ	2.69	0.46
2:F:991:SER:O	2:F:994:ILE:HB	2.16	0.46
1:A:382:VAL:HG11	1:A:868:TYR:CE1	2.51	0.46
1:A:1108:ILE:CG2	1:A:1217:ASP:HA	2.46	0.46
1:E:286:LEU:O	1:E:289:VAL:HG13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:456:ASP:HA	1:E:669:ASN:HD21	1.80	0.46
2:B:1007:ILE:CG2	2:B:1015:LEU:HD12	2.46	0.46
2:D:515:LYS:HB3	2:D:516:PRO:HD2	1.97	0.46
2:D:1003:ASN:HB3	2:D:1116:ILE:HD13	1.97	0.46
2:F:554:ILE:HB	2:F:557:ILE:CD1	2.45	0.46
1:A:468:LEU:HD12	1:A:471:VAL:HG22	1.98	0.46
1:A:937:TYR:CE1	1:A:954:LEU:HB2	2.51	0.46
1:C:297:ASN:N	1:C:298:PRO:HD3	2.31	0.46
1:E:231:CYS:CB	1:E:249:ILE:HD12	2.45	0.46
1:E:1010:ASN:HB3	2:F:780:GLN:HG3	1.97	0.46
1:E:1212:LEU:O	1:E:1238:CYS:HA	2.16	0.46
2:B:867:PHE:CZ	2:B:935:ILE:HD12	2.51	0.46
2:D:173:PHE:HA	2:D:333:ILE:HB	1.98	0.46
2:F:51:LEU:HB3	2:F:66:SER:HA	1.97	0.46
2:F:402:ILE:HG12	2:F:593:LYS:CB	2.45	0.46
2:F:1003:ASN:HB3	2:F:1116:ILE:CD1	2.46	0.46
1:A:664:ILE:HG23	1:A:665:LYS:N	2.31	0.46
1:A:1127:VAL:HG11	1:A:1150:ILE:HG23	1.97	0.46
1:C:627:LEU:O	1:E:420:GLY:HA3	2.16	0.46
1:C:1168:THR:HG22	1:C:1170:ASN:H	1.80	0.46
2:B:610:ASP:OD1	2:B:611:LEU:HD13	2.16	0.46
2:D:298:ILE:HA	2:D:301:LEU:HD12	1.98	0.46
2:D:806:TYR:CD1	2:D:806:TYR:O	2.69	0.46
2:D:1135:ILE:HG22	2:D:1136:LYS:N	2.31	0.46
2:F:106:ILE:HG22	2:F:107:PRO:O	2.16	0.46
2:F:428:LYS:C	2:F:430:PRO:CD	2.89	0.46
1:A:456:ASP:HA	1:A:669:ASN:ND2	2.31	0.45
1:C:345:VAL:HG13	1:C:387:GLN:HE22	1.81	0.45
1:C:468:LEU:O	1:C:469:ASP:C	2.59	0.45
1:C:610:LEU:O	1:C:611:ASN:C	2.58	0.45
1:C:664:ILE:HG23	1:C:665:LYS:N	2.31	0.45
1:C:778:LYS:HA	1:C:782:LEU:HB2	1.98	0.45
1:E:773:LEU:O	1:E:774:ILE:C	2.59	0.45
1:E:972:LYS:HB2	2:F:772:LEU:HD11	1.98	0.45
1:E:972:LYS:CD	2:F:772:LEU:HD11	2.46	0.45
2:B:21:VAL:CG1	2:B:121:ASN:HA	2.43	0.45
2:B:51:LEU:HB3	2:B:66:SER:HA	1.98	0.45
2:B:846:THR:HG23	2:B:847:GLY:N	2.31	0.45
2:F:298:ILE:HA	2:F:301:LEU:HD12	1.97	0.45
2:F:552:LYS:C	2:F:713:PHE:HE1	2.24	0.45
2:F:709:ASN:O	2:F:710:ILE:C	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:868:SER:HA	2:F:933:ILE:O	2.16	0.45
2:F:989:ILE:HG22	2:F:990:ASN:N	2.31	0.45
1:A:535:VAL:HG12	1:A:536:ASN:N	2.32	0.45
1:A:912:TYR:O	1:A:913:LYS:CB	2.64	0.45
1:A:1143:ARG:O	1:A:1144:LYS:C	2.59	0.45
1:C:468:LEU:C	1:C:468:LEU:HD12	2.41	0.45
1:C:625:LEU:O	1:C:626:GLU:C	2.59	0.45
1:C:897:GLU:HG2	1:C:1032:LYS:CB	2.44	0.45
1:E:468:LEU:O	1:E:469:ASP:C	2.60	0.45
1:E:606:ILE:CG2	1:E:621:PHE:CE2	2.99	0.45
1:E:903:ASN:C	1:E:903:ASN:OD1	2.59	0.45
1:E:1168:THR:HG22	1:E:1170:ASN:H	1.80	0.45
2:B:1149:HIS:CE1	2:B:1150:ASP:CB	3.00	0.45
2:D:269:TYR:HD1	2:D:287:LEU:HD23	1.81	0.45
2:F:269:TYR:HE2	2:F:288:GLU:CG	2.29	0.45
2:F:552:LYS:CB	2:F:713:PHE:HE1	2.30	0.45
1:A:469:ASP:O	1:A:472:ILE:HB	2.15	0.45
1:A:771:MET:HA	1:A:774:ILE:CG2	2.46	0.45
1:C:942:CYS:SG	1:C:1026:SER:HB3	2.56	0.45
1:C:1106:LEU:HD12	1:C:1175:ILE:HB	1.97	0.45
1:E:603:VAL:CG1	1:E:605:TYR:CE2	2.99	0.45
2:B:298:ILE:O	2:B:301:LEU:HB2	2.17	0.45
2:D:15:ASN:OD1	2:D:126:LYS:CB	2.64	0.45
2:D:867:PHE:CB	2:D:985:LEU:O	2.64	0.45
2:F:579:PRO:C	2:F:581:SER:N	2.74	0.45
2:F:866:ASN:O	2:F:867:PHE:HB3	2.16	0.45
1:A:1092:LEU:HD11	1:A:1234:ASN:O	2.16	0.45
1:C:21:ILE:HG12	1:C:134:ILE:HG22	1.98	0.45
1:C:448:ILE:O	1:C:449:ASN:O	2.35	0.45
1:C:597:ALA:HB2	2:D:939:LYS:HB3	1.98	0.45
1:E:778:LYS:HA	1:E:782:LEU:HB2	1.97	0.45
1:E:836:LEU:HD11	2:F:945:PHE:CE1	2.52	0.45
1:E:942:CYS:SG	1:E:1026:SER:HB3	2.57	0.45
2:B:990:ASN:O	2:B:993:GLU:N	2.49	0.45
2:F:594:ILE:CG2	2:F:595:LYS:N	2.79	0.45
1:A:192:PHE:CE1	1:A:204:GLN:HB3	2.51	0.45
1:A:203:ILE:CD1	1:A:396:ILE:HG21	2.46	0.45
1:A:440:GLU:O	1:A:443:TYR:CD1	2.69	0.45
1:A:606:ILE:CG2	1:A:621:PHE:CE2	3.00	0.45
1:C:160:THR:HA	1:C:185:THR:O	2.17	0.45
1:C:275:LEU:HD11	1:C:279:TYR:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:576:ILE:HG12	1:C:719:ILE:HD11	1.97	0.45
1:C:1012:ILE:O	2:D:779:ILE:HD12	2.17	0.45
1:E:199:ILE:HA	1:E:705:TYR:CE2	2.45	0.45
1:E:203:ILE:HD13	1:E:396:ILE:HG21	1.97	0.45
1:E:716:LYS:O	1:E:719:ILE:HG22	2.16	0.45
1:E:1127:VAL:HG11	1:E:1150:ILE:HG23	1.99	0.45
2:B:173:PHE:HA	2:B:333:ILE:HB	1.98	0.45
2:B:1142:TRP:H	2:B:1142:TRP:HD1	1.65	0.45
2:F:192:CYS:O	2:F:195:LYS:HB3	2.16	0.45
2:F:917:ASN:C	2:F:918:ILE:HG13	2.42	0.45
1:A:92:ASN:O	1:A:96:ASN:HB2	2.17	0.45
1:A:625:LEU:O	1:A:626:GLU:C	2.60	0.45
1:A:857:TYR:HB2	1:A:862:TYR:CE1	2.51	0.45
1:C:427:ILE:HD12	1:C:521:PHE:CD1	2.52	0.45
1:C:720:GLU:HA	1:C:723:TYR:HB3	1.99	0.45
1:E:981:ASN:HB3	1:E:1117:LEU:HB3	1.99	0.45
2:B:43:PRO:HA	2:B:78:PHE:CE2	2.51	0.45
2:D:402:ILE:HG12	2:D:593:LYS:CB	2.46	0.45
2:D:709:ASN:O	2:D:710:ILE:C	2.60	0.45
2:F:203:ILE:HG22	2:F:203:ILE:O	2.15	0.45
1:A:275:LEU:HD11	1:A:279:TYR:CE2	2.51	0.45
1:A:345:VAL:HG13	1:A:387:GLN:HE22	1.80	0.45
1:A:467:ASP:OD1	1:A:467:ASP:C	2.58	0.45
1:C:456:ASP:HA	1:C:669:ASN:HD21	1.81	0.45
1:C:484:SER:O	1:C:485:ASP:CB	2.64	0.45
2:B:541:THR:O	2:B:542:GLN:HB3	2.16	0.45
2:B:646:PHE:O	2:B:647:ASP:C	2.59	0.45
2:B:727:TYR:N	2:B:728:PRO:CD	2.80	0.45
2:B:738:ILE:HA	2:B:741:ILE:HD12	1.99	0.45
2:D:102:ILE:HG12	2:D:197:LEU:HD11	1.98	0.45
2:D:646:PHE:O	2:D:647:ASP:C	2.60	0.45
2:F:684:ASN:O	2:F:687:LEU:N	2.50	0.45
2:F:734:MET:HA	2:F:737:CYS:SG	2.57	0.45
1:A:427:ILE:CG2	1:A:428:GLU:N	2.79	0.45
1:A:1168:THR:HG22	1:A:1170:ASN:H	1.82	0.45
1:C:92:ASN:O	1:C:96:ASN:HB2	2.16	0.45
1:C:249:ILE:O	1:C:250:GLU:C	2.57	0.45
1:C:416:VAL:CG1	1:C:420:GLY:N	2.80	0.45
1:E:610:LEU:O	1:E:611:ASN:C	2.60	0.45
2:B:9:ILE:HG21	2:B:76:ASP:HB2	1.98	0.45
2:B:631:TYR:O	2:B:634:LEU:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:730:PHE:O	2:B:734:MET:HG2	2.17	0.45
2:B:1116:ILE:HG23	2:B:1117:PHE:N	2.29	0.45
2:D:43:PRO:HA	2:D:78:PHE:CE2	2.52	0.45
2:D:583:ILE:HG23	2:D:644:GLN:NE2	2.32	0.45
2:D:730:PHE:O	2:D:734:MET:HG2	2.17	0.45
2:F:1003:ASN:HB3	2:F:1116:ILE:HD13	1.98	0.45
1:A:206:PRO:O	1:A:209:THR:N	2.50	0.45
1:C:144:LEU:HA	1:C:487:LYS:HA	1.99	0.45
1:C:194:PHE:N	1:C:194:PHE:CD1	2.85	0.45
1:C:203:ILE:CD1	1:C:396:ILE:HG21	2.47	0.45
1:E:416:VAL:CG1	1:E:420:GLY:N	2.80	0.45
1:E:467:ASP:OD1	1:E:467:ASP:C	2.59	0.45
1:E:576:ILE:HG12	1:E:719:ILE:HD11	1.98	0.45
1:E:852:VAL:HG11	1:E:906:ILE:HG23	1.99	0.45
2:B:684:ASN:O	2:B:687:LEU:N	2.49	0.45
2:B:965:SER:C	2:B:967:ILE:H	2.24	0.45
2:D:64:TYR:CD2	2:D:64:TYR:N	2.85	0.45
2:D:232:PHE:CZ	2:D:240:TYR:HA	2.52	0.45
2:D:402:ILE:HG12	2:D:593:LYS:HB2	1.99	0.45
2:D:579:PRO:C	2:D:581:SER:N	2.75	0.45
2:F:530:ILE:O	2:F:531:PHE:C	2.60	0.45
2:F:610:ASP:OD1	2:F:611:LEU:HD13	2.17	0.45
2:F:738:ILE:HA	2:F:741:ILE:HD12	1.98	0.45
2:F:913:GLY:O	2:F:914:ASN:C	2.59	0.45
1:A:154:GLU:CB	1:A:155:PRO:CD	2.94	0.45
1:A:682:TYR:CE2	1:A:825:PHE:HA	2.52	0.45
1:A:942:CYS:SG	1:A:1026:SER:HB3	2.57	0.45
1:C:920:TRP:HB2	1:C:1045:ARG:CD	2.47	0.45
1:C:1143:ARG:O	1:C:1144:LYS:C	2.59	0.45
1:C:1212:LEU:O	1:C:1238:CYS:HA	2.16	0.45
1:E:193:ARG:NH2	1:E:196:ASP:OD1	2.50	0.45
1:E:423:LYS:HD2	2:D:510:PHE:CZ	2.52	0.45
1:E:1088:LEU:HD23	1:E:1089:LEU:N	2.31	0.45
2:B:14:ASP:O	2:B:15:ASN:CB	2.64	0.45
2:D:210:ASN:HB3	2:D:228:ASP:HA	1.99	0.45
2:D:298:ILE:O	2:D:301:LEU:HB2	2.17	0.45
2:D:679:ASN:O	2:D:680:ILE:C	2.60	0.45
2:D:1116:ILE:HG23	2:D:1117:PHE:N	2.32	0.45
2:F:423:ILE:O	2:F:423:ILE:CG2	2.64	0.45
2:F:870:TYR:HA	2:F:931:ILE:O	2.17	0.45
2:F:989:ILE:CG2	2:F:994:ILE:HG13	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:ILE:HD12	1:A:521:PHE:CD1	2.52	0.44
1:A:614:ASN:CB	1:A:617:GLN:OE1	2.66	0.44
1:A:633:LEU:O	1:A:700:ARG:NH2	2.46	0.44
1:C:154:GLU:CB	1:C:155:PRO:CD	2.94	0.44
1:C:1229:MET:O	1:C:1231:ASP:N	2.50	0.44
1:E:484:SER:O	1:E:485:ASP:CB	2.65	0.44
2:B:238:ILE:O	2:B:239:ASP:C	2.58	0.44
2:B:583:ILE:HG23	2:B:644:GLN:CD	2.42	0.44
2:B:824:THR:HA	2:B:856:ASN:HB2	1.99	0.44
2:B:870:TYR:HA	2:B:931:ILE:O	2.17	0.44
2:B:1056:PRO:O	2:B:1058:LYS:N	2.50	0.44
2:D:8:ASN:O	2:D:9:ILE:C	2.60	0.44
2:D:14:ASP:O	2:D:15:ASN:CB	2.65	0.44
2:D:51:LEU:HB3	2:D:66:SER:HA	1.98	0.44
2:D:1106:ASN:O	2:D:1107:ALA:C	2.59	0.44
2:F:1056:PRO:O	2:F:1058:LYS:N	2.50	0.44
1:A:576:ILE:HG12	1:A:719:ILE:HD11	1.99	0.44
1:A:603:VAL:HG13	1:A:605:TYR:CE2	2.52	0.44
1:C:635:GLU:C	1:C:636:PHE:CD2	2.96	0.44
1:C:1127:VAL:HG11	1:C:1150:ILE:HG23	1.99	0.44
1:E:535:VAL:HG11	1:E:551:ILE:HD12	1.99	0.44
1:E:554:PHE:HB3	1:E:608:LEU:HD12	1.99	0.44
2:B:271:ILE:HG23	2:B:272:LYS:N	2.32	0.44
2:B:866:ASN:O	2:B:867:PHE:HB3	2.18	0.44
2:B:976:ASN:C	2:B:977:VAL:HG23	2.42	0.44
2:D:35:VAL:O	2:D:36:ALA:HB2	2.17	0.44
2:D:415:TYR:O	2:D:416:SER:CB	2.65	0.44
2:D:594:ILE:CG2	2:D:595:LYS:N	2.80	0.44
2:D:859:PHE:HD1	2:D:968:ILE:HD12	1.82	0.44
2:D:867:PHE:CD1	2:D:867:PHE:C	2.95	0.44
2:F:64:TYR:HE2	2:F:363:ILE:HD12	1.81	0.44
1:A:331:LEU:HB2	1:A:332:TYR:HD2	1.81	0.44
1:C:220:GLY:HA2	1:C:225:LYS:HE3	1.99	0.44
1:C:441:ASN:C	1:C:441:ASN:HD22	2.25	0.44
1:C:700:ARG:HA	1:C:703:GLN:HB2	1.98	0.44
1:E:22:LYS:CG	1:E:23:PRO:HD2	2.47	0.44
1:E:448:ILE:O	1:E:449:ASN:O	2.36	0.44
1:E:912:TYR:O	1:E:913:LYS:CB	2.65	0.44
2:B:622:ASN:O	2:B:625:TYR:N	2.50	0.44
2:D:45:ARG:HG3	2:D:141:PRO:O	2.18	0.44
2:D:866:ASN:O	2:D:867:PHE:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:913:GLY:O	2:D:914:ASN:C	2.60	0.44
2:F:99:LEU:C	2:F:101:LEU:H	2.25	0.44
2:F:372:LEU:O	2:F:379:VAL:HA	2.17	0.44
1:A:535:VAL:HG11	1:A:551:ILE:HD12	1.99	0.44
1:A:908:TYR:HB3	1:A:1025:VAL:CG2	2.47	0.44
1:C:331:LEU:CB	1:C:332:TYR:CD2	3.01	0.44
1:C:908:TYR:HB3	1:C:1025:VAL:CG2	2.47	0.44
1:E:469:ASP:O	1:E:472:ILE:HB	2.17	0.44
1:E:664:ILE:HG23	1:E:665:LYS:N	2.30	0.44
1:E:1090:ASN:HB2	1:E:1240:TRP:CZ3	2.53	0.44
2:B:1122:LEU:HD21	2:B:1158:TRP:CE2	2.53	0.44
2:D:306:PHE:O	2:D:307:SER:C	2.60	0.44
2:D:1056:PRO:O	2:D:1058:LYS:N	2.50	0.44
2:F:480:ILE:HG21	2:F:497:VAL:HG23	2.00	0.44
2:F:846:THR:HG23	2:F:847:GLY:N	2.32	0.44
2:F:880:THR:CB	2:F:901:ASN:HA	2.48	0.44
2:F:923:ILE:C	2:F:925:ASN:N	2.76	0.44
2:F:1036:ILE:HD12	2:F:1045:SER:HB3	1.99	0.44
2:F:1142:TRP:CD1	2:F:1142:TRP:H	2.34	0.44
1:A:522:TYR:O	1:A:525:ALA:HB3	2.16	0.44
1:A:636:PHE:HD2	1:A:696:GLN:OE1	2.01	0.44
1:C:186:PHE:CE2	1:C:188:PRO:HB3	2.53	0.44
1:C:286:LEU:O	1:C:289:VAL:HG13	2.17	0.44
1:C:1043:GLY:C	1:C:1044:ILE:HG13	2.42	0.44
1:E:21:ILE:HG12	1:E:134:ILE:HG22	2.00	0.44
2:B:211:ILE:O	2:B:226:GLU:HA	2.18	0.44
2:B:1135:ILE:HG22	2:B:1136:LYS:N	2.32	0.44
2:D:554:ILE:HB	2:D:557:ILE:CD1	2.48	0.44
2:D:626:LEU:HD22	2:D:734:MET:HE1	2.00	0.44
2:F:1013:GLU:O	2:F:1014:ILE:CB	2.66	0.44
1:A:468:LEU:O	1:A:469:ASP:C	2.59	0.44
1:A:681:VAL:O	1:A:682:TYR:C	2.61	0.44
1:A:916:SER:OG	1:A:1054:LEU:HG	2.18	0.44
2:B:102:ILE:HG12	2:B:197:LEU:HD11	1.99	0.44
2:B:298:ILE:HA	2:B:301:LEU:HD12	1.99	0.44
2:B:1003:ASN:CG	2:B:1003:ASN:O	2.61	0.44
2:D:141:PRO:HA	2:D:169:TRP:HB3	1.99	0.44
2:F:727:TYR:N	2:F:728:PRO:CD	2.80	0.44
2:F:1007:ILE:CG2	2:F:1015:LEU:HD12	2.47	0.44
1:A:920:TRP:HB2	1:A:1045:ARG:CD	2.48	0.44
1:C:912:TYR:O	1:C:913:LYS:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1044:ILE:CG2	1:C:1045:ARG:N	2.80	0.44
1:E:203:ILE:CD1	1:E:396:ILE:HG21	2.47	0.44
2:B:285:LEU:O	2:B:288:GLU:N	2.51	0.44
2:B:877:LYS:CB	2:B:878:GLN:HB3	2.47	0.44
2:D:552:LYS:C	2:D:713:PHE:HE1	2.26	0.44
2:D:990:ASN:HB3	2:D:993:GLU:OE2	2.17	0.44
1:A:193:ARG:NH2	1:A:196:ASP:OD1	2.51	0.44
1:A:287:SER:HA	1:A:317:TYR:CD2	2.53	0.44
1:A:395:ILE:HG13	1:A:396:ILE:HG23	2.00	0.44
1:A:484:SER:O	1:A:485:ASP:CB	2.66	0.44
1:A:987:ILE:O	1:A:989:LYS:N	2.51	0.44
1:A:1044:ILE:CG2	1:A:1045:ARG:N	2.80	0.44
1:C:380:LEU:HD23	1:C:385:ARG:HD3	2.00	0.44
1:C:431:ASN:O	1:C:434:LEU:HB2	2.17	0.44
1:C:916:SER:OG	1:C:1054:LEU:HG	2.18	0.44
1:C:1132:VAL:HG23	1:C:1149:TYR:CE2	2.52	0.44
1:C:1153:VAL:HG23	1:C:1159:LEU:CD2	2.48	0.44
1:E:299:TYR:HA	1:E:302:ILE:HG22	1.99	0.44
1:E:468:LEU:C	1:E:468:LEU:HD12	2.43	0.44
2:B:99:LEU:C	2:B:101:LEU:N	2.76	0.44
2:B:153:TYR:HB2	2:B:165:MET:O	2.18	0.44
2:B:579:PRO:C	2:B:581:SER:N	2.71	0.44
2:F:645:TYR:O	2:F:646:PHE:C	2.58	0.44
1:A:21:ILE:HG12	1:A:134:ILE:HG22	2.00	0.44
1:A:554:PHE:HB3	1:A:608:LEU:HD12	1.99	0.44
1:A:610:LEU:HG	1:A:704:MET:HE1	2.00	0.44
1:C:18:ILE:C	1:C:19:LEU:HD23	2.43	0.44
1:C:476:ASN:N	2:D:1136:LYS:CE	2.81	0.44
1:C:773:LEU:O	1:C:774:ILE:C	2.61	0.44
1:E:92:ASN:O	1:E:96:ASN:HB2	2.18	0.44
1:E:431:ASN:O	1:E:434:LEU:HB2	2.17	0.44
1:E:571:LEU:O	1:E:575:TRP:N	2.42	0.44
1:E:942:CYS:SG	1:E:1025:VAL:CG1	3.06	0.44
1:E:1229:MET:O	1:E:1231:ASP:N	2.51	0.44
2:B:106:ILE:N	2:B:290:LYS:HD3	2.33	0.44
2:D:374:ASN:OD1	2:D:374:ASN:C	2.60	0.44
2:D:530:ILE:O	2:D:531:PHE:C	2.61	0.44
2:D:867:PHE:CZ	2:D:935:ILE:HD12	2.52	0.44
2:F:108:PHE:HB3	2:F:162:MET:CG	2.46	0.44
2:F:945:PHE:CD1	2:F:950:LEU:HA	2.53	0.44
2:F:1142:TRP:H	2:F:1142:TRP:HD1	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:610:LEU:O	1:A:611:ASN:C	2.59	0.43
1:C:427:ILE:CG2	1:C:428:GLU:N	2.81	0.43
1:C:636:PHE:HD2	1:C:696:GLN:OE1	2.00	0.43
1:C:727:THR:O	1:C:728:LEU:CB	2.65	0.43
1:E:161:ASN:HA	1:E:213:GLU:CD	2.43	0.43
1:E:535:VAL:HG12	1:E:536:ASN:N	2.31	0.43
1:E:571:LEU:O	1:E:572:PHE:C	2.60	0.43
2:B:173:PHE:O	2:B:333:ILE:N	2.51	0.43
2:B:1003:ASN:HB3	2:B:1116:ILE:HD13	2.00	0.43
2:D:870:TYR:HA	2:D:931:ILE:O	2.18	0.43
2:F:227:LEU:HD11	2:F:231:ASP:CB	2.48	0.43
2:F:298:ILE:O	2:F:301:LEU:HB2	2.17	0.43
2:F:305:TYR:CE1	2:F:418:LEU:CD1	3.01	0.43
1:A:299:TYR:HA	1:A:302:ILE:HG22	1.99	0.43
1:A:416:VAL:CG1	1:A:420:GLY:N	2.81	0.43
1:C:522:TYR:O	1:C:525:ALA:HB3	2.18	0.43
1:C:554:PHE:HB3	1:C:608:LEU:HD12	2.00	0.43
1:E:361:SER:OG	1:E:397:LYS:HE2	2.17	0.43
1:E:857:TYR:HB2	1:E:862:TYR:CE1	2.53	0.43
2:B:501:LEU:HD22	2:B:537:ASP:HB3	2.00	0.43
2:D:629:ILE:O	2:D:630:TYR:C	2.59	0.43
2:D:804:SER:HB3	2:D:819:THR:HG22	1.99	0.43
2:D:962:ILE:O	2:D:962:ILE:CG2	2.66	0.43
2:F:141:PRO:HA	2:F:169:TRP:HB3	2.00	0.43
2:F:415:TYR:O	2:F:416:SER:CB	2.65	0.43
2:F:501:LEU:HD22	2:F:537:ASP:HB3	2.00	0.43
1:A:873:ASN:N	1:A:899:ASN:O	2.39	0.43
1:C:299:TYR:HA	1:C:302:ILE:HG22	2.00	0.43
1:E:522:TYR:O	1:E:525:ALA:HB3	2.18	0.43
1:E:993:VAL:HG12	1:E:994:THR:N	2.33	0.43
2:B:99:LEU:C	2:B:101:LEU:H	2.25	0.43
2:B:400:ASN:OD1	2:B:400:ASN:N	2.50	0.43
2:B:799:SER:HB2	2:B:800:PRO:HD2	1.99	0.43
2:B:962:ILE:O	2:B:962:ILE:CG2	2.65	0.43
2:F:540:GLU:HB3	2:F:555:PRO:CD	2.49	0.43
2:F:1135:ILE:HG22	2:F:1136:LYS:N	2.33	0.43
1:A:211:MET:HE1	1:A:343:PHE:CZ	2.53	0.43
1:A:454:ILE:HD12	1:A:456:ASP:OD1	2.19	0.43
1:A:727:THR:O	1:A:728:LEU:CB	2.66	0.43
1:C:836:LEU:HD11	2:D:945:PHE:CE1	2.54	0.43
1:C:929:LYS:HA	1:C:932:ASN:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:625:LEU:O	1:E:626:GLU:C	2.60	0.43
1:E:771:MET:HA	1:E:774:ILE:CG2	2.45	0.43
1:E:833:ASP:HB3	1:E:835:ILE:HD12	2.01	0.43
1:E:1095:ASN:O	1:E:1112:ARG:N	2.40	0.43
2:B:27:ASP:OD1	2:B:27:ASP:N	2.50	0.43
2:B:515:LYS:HB3	2:B:516:PRO:HD2	1.98	0.43
2:B:552:LYS:C	2:B:713:PHE:HE1	2.25	0.43
2:B:709:ASN:O	2:B:710:ILE:C	2.61	0.43
2:B:738:ILE:O	2:B:739:LYS:C	2.61	0.43
2:B:806:TYR:O	2:B:816:ILE:HA	2.19	0.43
2:D:295:VAL:O	2:D:296:LYS:C	2.61	0.43
2:D:296:LYS:HA	2:D:299:TRP:HE3	1.84	0.43
2:F:89:ILE:O	2:F:95:GLY:HA3	2.18	0.43
2:F:645:TYR:OH	2:F:721:VAL:HG21	2.19	0.43
2:F:976:ASN:C	2:F:977:VAL:HG23	2.43	0.43
1:A:361:SER:OG	1:A:397:LYS:HE2	2.18	0.43
1:A:836:LEU:CB	2:B:995:LEU:HD11	2.47	0.43
1:A:981:ASN:HB3	1:A:1117:LEU:HB3	2.01	0.43
1:E:456:ASP:HA	1:E:669:ASN:ND2	2.34	0.43
1:E:987:ILE:C	1:E:989:LYS:N	2.76	0.43
2:B:105:ALA:HA	2:B:290:LYS:CD	2.48	0.43
2:B:146:ILE:HD13	2:B:330:TYR:CE2	2.54	0.43
2:B:234:ILE:O	2:B:235:SER:C	2.60	0.43
2:B:972:SER:O	2:B:972:SER:OG	2.36	0.43
2:B:1142:TRP:N	2:B:1142:TRP:HD1	2.16	0.43
2:D:35:VAL:CG1	2:D:36:ALA:H	2.29	0.43
2:D:246:ASN:HA	2:D:247:PRO:HA	1.83	0.43
2:D:428:LYS:C	2:D:430:PRO:CD	2.92	0.43
2:D:738:ILE:HA	2:D:741:ILE:HD12	1.99	0.43
2:D:876:LEU:HD21	2:D:978:TYR:CD2	2.53	0.43
2:F:707:ILE:O	2:F:708:ASN:C	2.62	0.43
1:A:380:LEU:HD23	1:A:385:ARG:HD3	2.01	0.43
1:C:4:ILE:HD11	1:C:95:ASN:HB2	2.01	0.43
1:C:193:ARG:NH2	1:C:196:ASP:OD1	2.51	0.43
1:C:571:LEU:O	1:C:572:PHE:C	2.60	0.43
1:E:179:GLY:HA2	1:E:220:GLY:O	2.17	0.43
1:E:522:TYR:CZ	1:E:611:ASN:HB2	2.53	0.43
1:E:617:GLN:OE1	1:E:617:GLN:N	2.47	0.43
1:E:632:ILE:HG23	1:E:633:LEU:HG	2.01	0.43
1:E:883:THR:HG23	1:E:884:ASN:H	1.84	0.43
2:B:81:ALA:O	2:B:84:LYS:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:21:VAL:CG1	2:D:121:ASN:HA	2.46	0.43
2:D:269:TYR:HE2	2:D:288:GLU:CG	2.31	0.43
1:C:456:ASP:HA	1:C:669:ASN:ND2	2.34	0.43
1:C:633:LEU:O	1:C:700:ARG:NH2	2.47	0.43
1:E:249:ILE:O	1:E:250:GLU:C	2.61	0.43
1:E:863:VAL:HG12	1:E:864:ASP:N	2.33	0.43
1:E:912:TYR:O	1:E:913:LYS:HB3	2.16	0.43
1:E:1106:LEU:HD12	1:E:1175:ILE:HB	1.99	0.43
1:E:1232:HIS:CB	1:E:1236:ASN:HD21	2.32	0.43
2:B:1013:GLU:O	2:B:1014:ILE:CB	2.66	0.43
2:D:923:ILE:C	2:D:925:ASN:N	2.77	0.43
1:A:660:LYS:CG	1:A:661:ASN:N	2.82	0.43
1:A:824:PRO:HB3	2:B:952:ALA:HB2	2.00	0.43
1:C:36:MET:HE2	1:C:36:MET:HB3	1.94	0.43
1:C:627:LEU:HG	1:E:419:LYS:O	2.18	0.43
1:C:863:VAL:HG12	1:C:864:ASP:N	2.34	0.43
1:C:898:VAL:O	1:C:1030:LEU:HA	2.18	0.43
1:C:990:TRP:HZ3	1:C:1044:ILE:HA	1.83	0.43
1:C:994:THR:HB	1:C:1006:TYR:HB2	2.00	0.43
1:E:38:ASN:HB3	1:E:147:ASN:HB2	2.00	0.43
1:E:118:ASN:HA	1:E:119:THR:CB	2.41	0.43
1:E:262:ILE:CD1	1:E:690:MET:HB3	2.49	0.43
1:E:423:LYS:NZ	2:D:514:ASP:OD1	2.41	0.43
1:E:603:VAL:HG13	1:E:605:TYR:CE2	2.54	0.43
1:E:897:GLU:HG2	1:E:1032:LYS:CB	2.42	0.43
2:B:13:VAL:CG1	2:B:14:ASP:N	2.82	0.43
2:B:1003:ASN:HB3	2:B:1116:ILE:CD1	2.48	0.43
2:F:43:PRO:HA	2:F:78:PHE:CE2	2.54	0.43
2:F:400:ASN:N	2:F:400:ASN:OD1	2.51	0.43
2:F:972:SER:O	2:F:972:SER:OG	2.35	0.43
2:F:990:ASN:O	2:F:993:GLU:N	2.51	0.43
1:A:452:LYS:CB	1:A:651:LYS:HE2	2.49	0.43
1:C:250:GLU:O	1:C:254:THR:N	2.43	0.43
1:C:682:TYR:HE2	1:C:825:PHE:HA	1.83	0.43
1:C:943:MET:CE	1:C:947:ASN:HB3	2.49	0.43
2:B:423:ILE:O	2:B:423:ILE:CG2	2.64	0.43
2:B:859:PHE:HD1	2:B:968:ILE:HD12	1.81	0.43
2:D:13:VAL:HG13	2:D:19:ALA:HA	2.01	0.43
2:D:523:TYR:O	2:D:524:TYR:C	2.60	0.43
2:D:854:PHE:HE2	2:D:970:LEU:HB2	1.83	0.43
2:D:917:ASN:O	2:D:918:ILE:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1093:THR:HG23	2:D:1095:ASN:N	2.34	0.43
2:F:13:VAL:HG12	2:F:14:ASP:H	1.82	0.43
2:F:626:LEU:HD22	2:F:734:MET:HE1	1.99	0.43
2:F:867:PHE:CB	2:F:985:LEU:O	2.65	0.43
1:A:730:GLU:O	1:A:732:ASN:N	2.52	0.43
1:A:994:THR:HB	1:A:1006:TYR:HB2	2.00	0.43
1:C:632:ILE:HG23	1:C:633:LEU:HG	2.01	0.43
1:C:1226:TYR:N	1:C:1226:TYR:CD2	2.87	0.43
1:E:173:PRO:HB2	1:E:178:PHE:HB2	2.01	0.43
1:E:838:SER:O	1:E:842:LYS:HB3	2.19	0.43
1:E:916:SER:OG	1:E:1054:LEU:HG	2.18	0.43
2:B:289:GLN:NE2	2:B:423:ILE:HG22	2.34	0.43
2:D:1007:ILE:CG2	2:D:1015:LEU:HD12	2.49	0.43
2:F:190:ILE:O	2:F:191:LYS:C	2.61	0.43
2:F:249:TRP:H	2:F:249:TRP:CD1	2.37	0.43
2:F:289:GLN:NE2	2:F:292:LYS:HE3	2.34	0.43
2:F:429:ILE:N	2:F:430:PRO:HD3	2.34	0.43
2:F:554:ILE:HG21	2:F:556:TRP:CZ2	2.54	0.43
1:A:191:SER:HB2	1:A:360:LEU:HD11	2.01	0.42
1:A:448:ILE:O	1:A:449:ASN:O	2.36	0.42
1:A:912:TYR:N	1:A:912:TYR:CD1	2.83	0.42
1:A:1106:LEU:HD12	1:A:1175:ILE:HB	2.00	0.42
1:C:196:ASP:OD2	1:C:196:ASP:N	2.52	0.42
1:C:382:VAL:HG11	1:C:868:TYR:CE1	2.54	0.42
1:E:468:LEU:HD12	1:E:471:VAL:HG22	2.01	0.42
1:E:660:LYS:CG	1:E:661:ASN:N	2.82	0.42
1:E:936:GLU:HA	1:E:954:LEU:O	2.19	0.42
1:E:1153:VAL:HG23	1:E:1159:LEU:CD2	2.48	0.42
2:B:35:VAL:O	2:B:36:ALA:HB2	2.19	0.42
2:B:586:LYS:O	2:B:641:TYR:CZ	2.72	0.42
2:B:679:ASN:O	2:B:680:ILE:C	2.61	0.42
2:D:211:ILE:O	2:D:226:GLU:HA	2.19	0.42
2:D:254:TYR:O	2:D:258:THR:HB	2.19	0.42
2:D:989:ILE:HG22	2:D:990:ASN:N	2.34	0.42
2:F:973:ASP:O	2:F:975:ASN:N	2.51	0.42
2:F:1093:THR:HB	2:F:1099:GLN:CD	2.44	0.42
1:A:36:MET:HE2	1:A:36:MET:HB3	1.92	0.42
1:A:453:GLU:HG3	1:A:454:ILE:HB	2.01	0.42
1:A:497:TYR:O	1:A:498:ILE:C	2.62	0.42
1:A:581:VAL:O	1:A:582:ASP:C	2.63	0.42
1:E:138:ASN:ND2	1:E:140:SER:OG	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:296:LYS:HA	2:B:299:TRP:HE3	1.84	0.42
2:B:989:ILE:CG2	2:B:994:ILE:HG13	2.50	0.42
2:D:106:ILE:N	2:D:290:LYS:HD3	2.34	0.42
2:D:502:ASN:O	2:D:503:ASN:C	2.62	0.42
2:F:9:ILE:HG13	2:F:10:ASP:N	2.34	0.42
2:F:211:ILE:O	2:F:226:GLU:HA	2.19	0.42
1:A:194:PHE:N	1:A:194:PHE:CD1	2.87	0.42
1:A:571:LEU:O	1:A:572:PHE:C	2.63	0.42
1:C:361:SER:OG	1:C:397:LYS:HE2	2.19	0.42
1:C:912:TYR:O	1:C:913:LYS:CB	2.67	0.42
1:C:1188:VAL:HG22	1:C:1201:PHE:CE1	2.54	0.42
1:E:274:ASN:HA	1:E:277:ASN:ND2	2.34	0.42
1:E:610:LEU:HG	1:E:704:MET:HE1	2.01	0.42
2:B:266:LYS:HA	2:B:291:PHE:CE1	2.55	0.42
2:B:480:ILE:HG21	2:B:497:VAL:HG23	2.01	0.42
2:B:626:LEU:HD22	2:B:734:MET:HE1	1.99	0.42
2:B:645:TYR:OH	2:B:721:VAL:HG21	2.19	0.42
2:D:1098:ILE:HD12	2:D:1143:VAL:CG1	2.50	0.42
2:D:1122:LEU:C	2:D:1122:LEU:HD12	2.43	0.42
2:F:210:ASN:HB3	2:F:228:ASP:HA	1.99	0.42
1:A:160:THR:HA	1:A:185:THR:O	2.19	0.42
1:A:990:TRP:HZ3	1:A:1044:ILE:HA	1.84	0.42
1:C:416:VAL:HG13	1:C:420:GLY:CA	2.50	0.42
1:C:920:TRP:O	1:C:1044:ILE:HA	2.19	0.42
1:E:297:ASN:N	1:E:298:PRO:HD3	2.33	0.42
1:E:597:ALA:HA	2:F:939:LYS:HD3	2.01	0.42
1:E:1083:ASP:HB2	1:E:1128:LYS:HE3	2.01	0.42
2:D:289:GLN:NE2	2:D:423:ILE:HG22	2.35	0.42
2:D:855:THR:HG22	2:D:967:ILE:HG12	2.02	0.42
2:D:877:LYS:CB	2:D:878:GLN:HB3	2.47	0.42
2:D:1103:ASN:C	2:D:1105:ASN:H	2.28	0.42
2:F:295:VAL:O	2:F:296:LYS:C	2.61	0.42
2:F:411:HIS:CA	2:F:624:PHE:HE1	2.32	0.42
2:F:877:LYS:CB	2:F:878:GLN:HB3	2.47	0.42
2:F:962:ILE:O	2:F:962:ILE:CG2	2.66	0.42
2:F:1116:ILE:HG23	2:F:1117:PHE:N	2.34	0.42
1:C:194:PHE:N	1:C:194:PHE:HD1	2.18	0.42
1:C:535:VAL:HG11	1:C:551:ILE:HD12	2.00	0.42
1:E:497:TYR:O	1:E:498:ILE:C	2.62	0.42
1:E:727:THR:O	1:E:728:LEU:CB	2.66	0.42
1:E:987:ILE:O	1:E:989:LYS:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1012:ILE:O	2:F:779:ILE:HD12	2.19	0.42
1:E:1044:ILE:CG2	1:E:1045:ARG:N	2.82	0.42
2:B:94:VAL:O	2:B:95:GLY:C	2.62	0.42
2:B:234:ILE:O	2:B:302:ASN:HB2	2.19	0.42
2:B:242:LEU:CD1	2:B:638:TRP:CG	3.03	0.42
2:B:415:TYR:O	2:B:416:SER:CB	2.67	0.42
2:F:949:ILE:HG22	2:F:950:LEU:C	2.45	0.42
2:F:1106:ASN:O	2:F:1107:ALA:C	2.62	0.42
1:A:287:SER:HB3	1:A:317:TYR:H	1.84	0.42
1:A:720:GLU:HA	1:A:723:TYR:HB3	2.02	0.42
1:A:993:VAL:HG12	1:A:994:THR:N	2.35	0.42
1:C:1127:VAL:CG1	1:C:1128:LYS:N	2.82	0.42
1:E:15:ASP:HA	1:E:16:ARG:HA	1.77	0.42
1:E:427:ILE:CG2	1:E:428:GLU:N	2.82	0.42
2:B:306:PHE:O	2:B:307:SER:C	2.61	0.42
2:D:727:TYR:N	2:D:728:PRO:CD	2.82	0.42
2:F:242:LEU:CD1	2:F:638:TRP:CG	3.02	0.42
2:F:276:ASN:O	2:F:277:ASN:HB3	2.20	0.42
2:F:583:ILE:HG23	2:F:644:GLN:CD	2.45	0.42
1:A:617:GLN:OE1	1:A:617:GLN:N	2.47	0.42
1:A:932:ASN:HA	1:A:956:HIS:CE1	2.55	0.42
1:C:926:TYR:HD1	1:C:1247:HIS:O	2.03	0.42
1:E:170:ASN:HD21	2:B:377:ASN:ND2	2.18	0.42
1:E:250:GLU:O	1:E:254:THR:N	2.44	0.42
1:E:730:GLU:O	1:E:732:ASN:N	2.52	0.42
2:B:707:ILE:O	2:B:708:ASN:C	2.61	0.42
2:B:1097:ARG:NE	2:B:1142:TRP:CE3	2.87	0.42
2:D:586:LYS:O	2:D:641:TYR:CZ	2.73	0.42
2:D:995:LEU:O	2:D:996:THR:C	2.61	0.42
2:F:99:LEU:C	2:F:101:LEU:N	2.75	0.42
2:F:945:PHE:HA	2:F:949:ILE:O	2.20	0.42
1:A:305:GLU:OE1	1:A:305:GLU:HA	2.20	0.42
1:A:436:PHE:CD1	1:A:437:VAL:N	2.86	0.42
1:A:845:LYS:C	1:A:847:ILE:H	2.27	0.42
1:C:262:ILE:CD1	1:C:690:MET:HB3	2.50	0.42
1:C:452:LYS:CB	1:C:651:LYS:HE2	2.50	0.42
1:C:617:GLN:OE1	1:C:617:GLN:N	2.48	0.42
1:C:660:LYS:CG	1:C:661:ASN:N	2.82	0.42
1:C:981:ASN:HB3	1:C:1117:LEU:HB3	2.02	0.42
1:C:1232:HIS:CB	1:C:1236:ASN:HD21	2.32	0.42
1:E:15:ASP:HA	1:E:136:PHE:HZ	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1143:ARG:O	1:E:1144:LYS:C	2.62	0.42
2:B:13:VAL:HG13	2:B:19:ALA:HA	2.01	0.42
2:B:60:ASP:C	2:B:62:GLY:H	2.28	0.42
2:B:755:ILE:HG22	2:B:760:LYS:HG3	2.01	0.42
2:B:905:VAL:HA	2:B:918:ILE:O	2.20	0.42
2:B:1106:ASN:O	2:B:1107:ALA:C	2.62	0.42
2:D:153:TYR:HB2	2:D:165:MET:O	2.19	0.42
2:F:349:ILE:C	2:F:351:THR:H	2.27	0.42
1:A:220:GLY:HA2	1:A:225:LYS:HE3	2.01	0.42
1:A:1111:ILE:HG23	1:A:1111:ILE:O	2.20	0.42
1:A:1153:VAL:HG23	1:A:1159:LEU:CD2	2.50	0.42
1:C:38:ASN:HB3	1:C:147:ASN:HB2	2.02	0.42
1:C:395:ILE:HG13	1:C:396:ILE:HG23	2.02	0.42
1:C:716:LYS:C	1:C:716:LYS:HD3	2.44	0.42
1:C:838:SER:O	1:C:842:LYS:HB3	2.20	0.42
1:E:196:ASP:OD2	1:E:196:ASP:N	2.53	0.42
2:B:108:PHE:CG	2:B:109:PRO:HD2	2.55	0.42
2:B:276:ASN:O	2:B:277:ASN:HB3	2.20	0.42
2:B:381:MET:CE	2:B:471:GLN:CD	2.92	0.42
2:B:945:PHE:CD1	2:B:950:LEU:HA	2.55	0.42
2:B:1093:THR:HG23	2:B:1095:ASN:N	2.35	0.42
2:D:554:ILE:HG21	2:D:556:TRP:CZ2	2.54	0.42
2:D:1149:HIS:CE1	2:D:1150:ASP:CB	3.02	0.42
2:F:266:LYS:HA	2:F:291:PHE:CE1	2.55	0.42
2:F:374:ASN:OD1	2:F:374:ASN:C	2.62	0.42
2:F:515:LYS:HB3	2:F:516:PRO:HD2	2.01	0.42
2:F:709:ASN:O	2:F:713:PHE:HD2	2.02	0.42
1:A:427:ILE:CD1	1:A:521:PHE:CD1	3.03	0.42
1:A:522:TYR:CZ	1:A:611:ASN:HB2	2.53	0.42
1:A:575:TRP:O	1:A:576:ILE:C	2.62	0.42
1:C:993:VAL:HG12	1:C:994:THR:N	2.35	0.42
1:C:1103:ASP:OD1	1:C:1103:ASP:N	2.36	0.42
1:E:4:ILE:HD11	1:E:95:ASN:HB2	2.02	0.42
1:E:39:ILE:HG12	1:E:148:VAL:HB	2.02	0.42
1:E:908:TYR:HB3	1:E:1025:VAL:CG2	2.49	0.42
1:E:1227:THR:HG22	2:F:806:TYR:CD2	2.54	0.42
2:B:729:LYS:O	2:B:730:PHE:C	2.62	0.42
2:B:734:MET:HA	2:B:737:CYS:SG	2.60	0.42
2:B:990:ASN:HB3	2:B:993:GLU:OE2	2.19	0.42
2:B:1093:THR:OG1	2:B:1094:THR:N	2.52	0.42
2:D:27:ASP:N	2:D:27:ASP:OD1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:81:ALA:O	2:D:84:LYS:N	2.52	0.42
2:D:308:LYS:HA	2:D:789:TYR:CE2	2.55	0.42
2:D:1122:LEU:HD21	2:D:1158:TRP:CE2	2.55	0.42
2:F:285:LEU:C	2:F:287:LEU:N	2.77	0.42
1:C:427:ILE:CD1	1:C:521:PHE:CD1	3.02	0.41
1:C:518:ASN:OD1	1:C:518:ASN:C	2.62	0.41
1:E:36:MET:HE2	1:E:36:MET:HB3	1.90	0.41
1:E:581:VAL:O	1:E:582:ASP:C	2.62	0.41
1:E:636:PHE:HD2	1:E:696:GLN:OE1	2.03	0.41
1:E:943:MET:CE	1:E:947:ASN:HB3	2.50	0.41
2:B:973:ASP:O	2:B:975:ASN:N	2.50	0.41
2:D:806:TYR:CE2	2:D:817:GLY:C	2.98	0.41
2:F:71:THR:OG1	2:F:74:GLU:HG2	2.20	0.41
2:F:679:ASN:O	2:F:680:ILE:C	2.63	0.41
2:F:855:THR:HG22	2:F:967:ILE:HG12	2.02	0.41
2:F:855:THR:HA	2:F:966:ASP:O	2.19	0.41
2:F:1122:LEU:HD21	2:F:1158:TRP:CE2	2.54	0.41
1:C:192:PHE:CE1	1:C:204:GLN:HB3	2.55	0.41
1:C:468:LEU:HD12	1:C:471:VAL:HG22	2.02	0.41
1:C:522:TYR:CZ	1:C:611:ASN:HB2	2.54	0.41
1:E:216:HIS:CE1	1:E:250:GLU:HG3	2.54	0.41
1:E:720:GLU:HA	1:E:723:TYR:HB3	2.02	0.41
2:B:71:THR:OG1	2:B:74:GLU:HG2	2.19	0.41
2:B:453:ILE:CG1	2:B:454:THR:H	2.32	0.41
2:B:917:ASN:O	2:B:918:ILE:HG13	2.20	0.41
2:B:1122:LEU:HD21	2:B:1158:TRP:NE1	2.35	0.41
2:D:89:ILE:O	2:D:95:GLY:HA3	2.21	0.41
2:D:622:ASN:O	2:D:625:TYR:N	2.53	0.41
2:D:828:TYR:HB2	2:D:829:PRO:HD2	2.02	0.41
2:D:1097:ARG:NE	2:D:1142:TRP:CE3	2.89	0.41
2:F:321:ALA:HB1	2:F:388:ASP:HB3	2.02	0.41
2:F:580:ILE:H	2:F:580:ILE:HG13	1.66	0.41
1:A:22:LYS:HG3	1:A:23:PRO:HD2	2.01	0.41
1:A:1143:ARG:HB2	1:A:1146:ASP:OD1	2.20	0.41
1:C:161:ASN:HA	1:C:213:GLU:CD	2.46	0.41
1:C:912:TYR:CD1	1:C:912:TYR:N	2.87	0.41
1:C:1232:HIS:HB3	1:C:1236:ASN:HD21	1.85	0.41
1:E:286:LEU:O	1:E:287:SER:C	2.62	0.41
1:E:436:PHE:CD1	1:E:437:VAL:N	2.85	0.41
1:E:778:LYS:HA	1:E:782:LEU:HD12	2.02	0.41
1:E:789:VAL:O	1:E:790:LYS:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1010:ASN:HB3	2:F:780:GLN:CG	2.50	0.41
2:B:245:THR:HB	2:B:631:TYR:CE1	2.55	0.41
2:D:308:LYS:HA	2:D:789:TYR:CD2	2.56	0.41
2:D:799:SER:HB2	2:D:800:PRO:HD2	2.02	0.41
2:D:1093:THR:HB	2:D:1099:GLN:CD	2.45	0.41
2:F:308:LYS:HA	2:F:789:TYR:CE2	2.55	0.41
2:F:502:ASN:O	2:F:505:MET:N	2.54	0.41
2:F:730:PHE:O	2:F:734:MET:HG2	2.20	0.41
1:A:38:ASN:HB3	1:A:147:ASN:HB2	2.03	0.41
1:A:584:THR:HG22	1:A:750:LYS:HD2	2.02	0.41
1:A:789:VAL:HG12	1:A:793:LEU:HD12	2.03	0.41
1:A:838:SER:O	1:A:842:LYS:HB3	2.21	0.41
1:A:852:VAL:HG11	1:A:906:ILE:HG23	2.03	0.41
1:A:1000:LEU:N	1:A:1000:LEU:HD12	2.36	0.41
1:C:102:ILE:O	1:C:103:LEU:C	2.64	0.41
1:C:238:ASN:CG	1:C:239:PRO:CD	2.87	0.41
1:C:249:ILE:HG23	1:C:263:ILE:CD1	2.51	0.41
1:C:497:TYR:O	1:C:498:ILE:C	2.63	0.41
1:E:614:ASN:CB	1:E:617:GLN:OE1	2.68	0.41
1:E:1188:VAL:HG22	1:E:1201:PHE:CE1	2.55	0.41
2:B:431:PRO:O	2:B:432:ILE:C	2.64	0.41
2:B:526:TRP:O	2:B:529:ALA:HB3	2.20	0.41
2:B:540:GLU:HB3	2:B:555:PRO:CD	2.50	0.41
2:B:554:ILE:HG21	2:B:556:TRP:CZ2	2.54	0.41
2:B:860:GLU:O	2:B:861:ASN:HB2	2.20	0.41
2:B:885:LEU:HG	2:B:886:ILE:CD1	2.22	0.41
2:D:46:TYR:HB3	2:D:142:GLY:HA2	2.02	0.41
2:D:71:THR:OG1	2:D:74:GLU:HG2	2.19	0.41
2:D:254:TYR:O	2:D:258:THR:CG2	2.69	0.41
2:D:289:GLN:NE2	2:D:292:LYS:HE3	2.36	0.41
2:D:645:TYR:OH	2:D:721:VAL:HG21	2.21	0.41
2:F:35:VAL:O	2:F:36:ALA:HB2	2.19	0.41
2:F:46:TYR:HB3	2:F:142:GLY:HA2	2.03	0.41
2:F:269:TYR:CZ	2:F:288:GLU:HB2	2.55	0.41
2:F:423:ILE:HG23	2:F:426:ILE:HB	2.02	0.41
2:F:603:MET:HE3	2:F:611:LEU:HD12	2.02	0.41
2:F:637:TRP:O	2:F:638:TRP:C	2.62	0.41
2:F:860:GLU:O	2:F:861:ASN:HB2	2.21	0.41
2:F:1069:GLN:O	2:F:1070:TYR:CD2	2.74	0.41
1:A:297:ASN:N	1:A:297:ASN:OD1	2.49	0.41
1:A:1001:GLY:HA2	1:A:1018:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:ASN:HA	1:C:277:ASN:ND2	2.36	0.41
1:C:614:ASN:HB2	1:C:617:GLN:HE22	1.85	0.41
1:C:730:GLU:O	1:C:732:ASN:N	2.53	0.41
1:C:835:ILE:HG23	2:D:949:ILE:HA	2.03	0.41
1:E:199:ILE:O	1:E:201:GLU:CD	2.63	0.41
1:E:395:ILE:HG13	1:E:396:ILE:HG23	2.03	0.41
1:E:456:ASP:OD1	1:E:456:ASP:N	2.52	0.41
1:E:932:ASN:HA	1:E:956:HIS:CE1	2.56	0.41
1:E:1127:VAL:CG1	1:E:1128:LYS:N	2.84	0.41
2:B:190:ILE:O	2:B:191:LYS:C	2.64	0.41
2:B:594:ILE:CG2	2:B:595:LYS:N	2.83	0.41
2:B:709:ASN:O	2:B:712:LYS:N	2.53	0.41
2:B:730:PHE:CE2	2:B:734:MET:HG3	2.55	0.41
2:D:423:ILE:HG23	2:D:426:ILE:HB	2.01	0.41
2:D:654:LYS:HA	2:D:657:LEU:HD12	2.02	0.41
2:F:88:ARG:O	2:F:91:ASN:HB2	2.20	0.41
2:F:646:PHE:O	2:F:647:ASP:C	2.64	0.41
2:F:755:ILE:HG22	2:F:760:LYS:HG3	2.03	0.41
2:F:799:SER:HB2	2:F:800:PRO:HD2	2.02	0.41
2:F:1098:ILE:HD12	2:F:1143:VAL:CG1	2.51	0.41
1:A:102:ILE:O	1:A:103:LEU:C	2.64	0.41
1:A:199:ILE:O	1:A:201:GLU:CD	2.64	0.41
1:A:863:VAL:HG12	1:A:864:ASP:N	2.36	0.41
1:A:883:THR:HG23	1:A:884:ASN:H	1.85	0.41
1:A:1002:ASP:OD1	1:A:1002:ASP:N	2.53	0.41
1:A:1083:ASP:HB2	1:A:1128:LYS:HE3	2.02	0.41
1:A:1127:VAL:CG1	1:A:1128:LYS:N	2.83	0.41
1:C:603:VAL:CG1	1:C:605:TYR:CE2	3.04	0.41
1:C:700:ARG:O	1:C:701:LYS:C	2.61	0.41
1:E:238:ASN:CG	1:E:239:PRO:CD	2.80	0.41
1:E:1111:ILE:HG23	1:E:1111:ILE:O	2.20	0.41
2:B:185:PRO:O	2:B:188:GLU:N	2.53	0.41
2:B:583:ILE:HD11	2:B:645:TYR:CE2	2.55	0.41
2:B:709:ASN:O	2:B:713:PHE:HD2	2.03	0.41
2:B:828:TYR:HB2	2:B:829:PRO:HD2	2.02	0.41
2:B:1140:TYR:CE2	2:B:1142:TRP:CE2	3.09	0.41
2:D:501:LEU:HD22	2:D:537:ASP:HB3	2.01	0.41
2:D:755:ILE:HG22	2:D:760:LYS:HG3	2.03	0.41
2:D:945:PHE:HA	2:D:949:ILE:O	2.20	0.41
2:F:553:ILE:CG2	2:F:554:ILE:N	2.83	0.41
2:F:731:THR:O	2:F:735:GLU:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1097:ARG:NE	2:F:1142:TRP:CE3	2.89	0.41
1:A:682:TYR:CD2	1:A:825:PHE:HD1	2.38	0.41
1:C:470:GLN:HG3	2:D:1028:PHE:HE1	1.86	0.41
1:C:789:VAL:O	1:C:790:LYS:C	2.63	0.41
1:C:1233:THR:C	1:C:1235:SER:H	2.27	0.41
1:E:1233:THR:C	1:E:1235:SER:H	2.28	0.41
2:B:11:SER:CB	2:B:12:PRO:HA	2.51	0.41
2:B:35:VAL:CG1	2:B:36:ALA:H	2.30	0.41
2:B:60:ASP:C	2:B:62:GLY:N	2.79	0.41
2:B:254:TYR:O	2:B:258:THR:HB	2.21	0.41
2:B:295:VAL:O	2:B:296:LYS:C	2.63	0.41
2:B:423:ILE:HG23	2:B:426:ILE:HB	2.02	0.41
2:B:507:TYR:O	2:B:508:LEU:C	2.61	0.41
2:F:68:PHE:CD2	2:F:68:PHE:C	2.99	0.41
2:F:102:ILE:HG12	2:F:197:LEU:HD11	2.03	0.41
2:F:182:TYR:CE2	2:F:351:THR:HG22	2.56	0.41
2:F:185:PRO:O	2:F:188:GLU:N	2.53	0.41
1:A:15:ASP:HA	1:A:16:ARG:HA	1.75	0.41
1:A:143:ILE:CD1	1:A:491:THR:HG23	2.50	0.41
1:A:755:MET:HE3	1:A:758:ILE:HB	2.03	0.41
1:A:775:ASN:O	1:A:776:GLU:C	2.62	0.41
1:A:829:SER:C	1:A:831:THR:N	2.79	0.41
1:A:1127:VAL:HG13	1:A:1151:ASN:O	2.21	0.41
1:A:1188:VAL:HG22	1:A:1201:PHE:CE1	2.55	0.41
1:C:436:PHE:CD1	1:C:437:VAL:N	2.83	0.41
1:C:610:LEU:CD1	1:C:704:MET:HE2	2.44	0.41
1:C:1083:ASP:HB2	1:C:1128:LYS:HE3	2.03	0.41
1:E:416:VAL:HG13	1:E:420:GLY:CA	2.51	0.41
2:B:681:SER:HB3	2:B:684:ASN:HD22	1.85	0.41
2:D:99:LEU:C	2:D:101:LEU:N	2.79	0.41
2:D:480:ILE:HG21	2:D:497:VAL:HG23	2.02	0.41
2:D:583:ILE:HD11	2:D:645:TYR:CE2	2.55	0.41
2:F:13:VAL:HG13	2:F:19:ALA:HA	2.03	0.41
1:A:773:LEU:O	1:A:774:ILE:C	2.62	0.41
1:A:962:THR:HA	1:A:972:LYS:HG2	2.03	0.41
1:A:989:LYS:HE2	1:A:1075:PHE:CE2	2.55	0.41
1:A:1137:THR:OG1	2:B:1109:ILE:HG21	2.21	0.41
1:A:1190:MET:CE	1:A:1199:MET:HB3	2.51	0.41
1:C:74:LEU:N	1:C:79:GLU:OE1	2.49	0.41
1:C:116:ASN:OD1	1:C:116:ASN:N	2.54	0.41
1:C:331:LEU:HB2	1:C:332:TYR:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:627:LEU:O	1:E:419:LYS:CG	2.69	0.41
1:C:641:LEU:HD12	1:E:614:ASN:ND2	2.35	0.41
1:C:645:ILE:HD12	1:C:785:TYR:HB2	2.03	0.41
1:C:769:TYR:O	1:C:772:LYS:HB2	2.21	0.41
1:E:192:PHE:CE1	1:E:204:GLN:HB3	2.56	0.41
1:E:220:GLY:HA2	1:E:225:LYS:HE3	2.03	0.41
1:E:382:VAL:HG11	1:E:868:TYR:CE1	2.56	0.41
1:E:912:TYR:CD1	1:E:912:TYR:N	2.87	0.41
1:E:929:LYS:HA	1:E:932:ASN:HB2	2.02	0.41
1:E:989:LYS:CG	1:E:1076:TRP:HA	2.50	0.41
2:B:197:LEU:N	2:B:197:LEU:HD12	2.36	0.41
2:B:491:SER:O	2:B:495:SER:N	2.54	0.41
2:B:789:TYR:CE2	2:B:793:LEU:CD1	3.03	0.41
2:B:1147:LEU:HD12	2:B:1147:LEU:N	2.36	0.41
2:D:105:ALA:HA	2:D:290:LYS:CD	2.50	0.41
2:D:108:PHE:CG	2:D:109:PRO:HD2	2.55	0.41
2:D:235:SER:O	2:D:314:MET:HE1	2.20	0.41
2:D:242:LEU:CD1	2:D:638:TRP:CG	3.04	0.41
2:D:453:ILE:CG1	2:D:454:THR:H	2.33	0.41
2:D:709:ASN:O	2:D:713:PHE:HD2	2.03	0.41
2:D:710:ILE:HG23	2:D:714:PHE:CE2	2.56	0.41
2:D:734:MET:HA	2:D:737:CYS:SG	2.60	0.41
2:D:847:GLY:O	2:D:848:ALA:C	2.64	0.41
2:D:855:THR:HA	2:D:966:ASP:O	2.20	0.41
2:D:1008:ARG:HD2	2:D:1012:GLU:HB3	2.02	0.41
2:F:35:VAL:CG1	2:F:36:ALA:H	2.31	0.41
2:F:106:ILE:N	2:F:290:LYS:HD3	2.36	0.41
2:F:146:ILE:HD13	2:F:330:TYR:CE2	2.56	0.41
2:F:832:ILE:H	2:F:832:ILE:HG13	1.75	0.41
1:A:778:LYS:HA	1:A:782:LEU:HD12	2.02	0.41
1:A:1067:PRO:O	1:A:1068:ASN:O	2.38	0.41
1:C:297:ASN:N	1:C:297:ASN:OD1	2.49	0.41
1:C:444:ASN:CG	1:C:445:ASP:N	2.79	0.41
1:C:1227:THR:C	1:C:1228:HIS:CG	2.99	0.41
1:E:160:THR:HA	1:E:185:THR:O	2.21	0.41
1:E:452:LYS:CB	1:E:651:LYS:HE2	2.50	0.41
1:E:775:ASN:O	1:E:776:GLU:C	2.64	0.41
2:B:269:TYR:HE2	2:B:288:GLU:CG	2.34	0.41
2:B:502:ASN:O	2:B:505:MET:N	2.54	0.41
2:B:855:THR:HA	2:B:966:ASP:O	2.21	0.41
2:B:1098:ILE:HD12	2:B:1143:VAL:CG1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:112:ASN:O	2:D:113:ASN:CG	2.64	0.41
2:D:234:ILE:O	2:D:235:SER:C	2.64	0.41
2:D:276:ASN:O	2:D:277:ASN:HB3	2.21	0.41
2:D:400:ASN:N	2:D:400:ASN:OD1	2.54	0.41
2:D:624:PHE:O	2:D:625:TYR:C	2.62	0.41
2:D:1069:GLN:O	2:D:1070:TYR:CD2	2.74	0.41
2:F:285:LEU:O	2:F:288:GLU:N	2.54	0.41
1:A:4:ILE:HD11	1:A:95:ASN:HB2	2.02	0.40
1:A:196:ASP:N	1:A:196:ASP:OD2	2.54	0.40
1:A:989:LYS:CG	1:A:1076:TRP:HA	2.50	0.40
1:C:225:LYS:HA	1:C:228:THR:OG1	2.21	0.40
1:C:610:LEU:HG	1:C:704:MET:HE1	2.03	0.40
1:C:717:THR:O	1:C:718:ILE:C	2.64	0.40
1:E:20:TYR:HA	1:E:30:TYR:O	2.21	0.40
1:E:211:MET:HE1	1:E:343:PHE:CZ	2.55	0.40
1:E:388:ASN:HB3	1:E:391:LEU:HB3	2.01	0.40
1:E:898:VAL:O	1:E:1030:LEU:HA	2.22	0.40
2:B:554:ILE:CG2	2:B:556:TRP:NE1	2.84	0.40
2:D:108:PHE:HB3	2:D:162:MET:CG	2.47	0.40
2:D:207:ASP:OD1	2:D:207:ASP:N	2.52	0.40
2:D:923:ILE:O	2:D:925:ASN:N	2.39	0.40
2:F:108:PHE:CG	2:F:109:PRO:HD2	2.56	0.40
2:F:254:TYR:O	2:F:258:THR:HB	2.21	0.40
2:F:624:PHE:O	2:F:625:TYR:C	2.64	0.40
1:C:614:ASN:CB	1:C:617:GLN:OE1	2.68	0.40
1:C:833:ASP:HB3	1:C:835:ILE:HD12	2.03	0.40
2:B:429:ILE:N	2:B:430:PRO:HD3	2.34	0.40
2:B:470:LEU:HD11	2:B:654:LYS:HB3	2.04	0.40
2:B:624:PHE:O	2:B:625:TYR:C	2.62	0.40
2:D:497:VAL:HG12	2:D:498:TYR:N	2.35	0.40
2:F:583:ILE:HD11	2:F:645:TYR:CE2	2.56	0.40
2:F:854:PHE:HE2	2:F:970:LEU:HB2	1.87	0.40
2:F:880:THR:HB	2:F:901:ASN:HA	2.03	0.40
2:F:965:SER:C	2:F:967:ILE:H	2.28	0.40
2:F:990:ASN:HB3	2:F:993:GLU:OE2	2.20	0.40
1:A:632:ILE:HG23	1:A:633:LEU:HG	2.02	0.40
1:A:792:TYR:CD2	1:A:792:TYR:C	2.99	0.40
1:A:926:TYR:HD1	1:A:1247:HIS:O	2.04	0.40
1:A:1213:GLY:HA3	1:A:1225:TYR:CE2	2.57	0.40
1:C:39:ILE:HG12	1:C:148:VAL:HB	2.04	0.40
1:C:293:ASN:C	1:C:295:GLN:H	2.28	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:GLU:OE1	1:C:305:GLU:HA	2.20	0.40
1:C:897:GLU:HG2	1:C:1032:LYS:HD3	2.04	0.40
1:C:903:ASN:OD1	1:C:904:ASP:N	2.54	0.40
1:E:635:GLU:C	1:E:636:PHE:CD2	2.99	0.40
1:E:1125:ILE:HD12	1:E:1125:ILE:HA	1.93	0.40
2:B:8:ASN:O	2:B:9:ILE:C	2.64	0.40
2:B:107:PRO:HG2	2:B:118:ARG:CB	2.50	0.40
2:D:197:LEU:HD12	2:D:197:LEU:N	2.36	0.40
2:F:205:PRO:CD	2:F:230:ILE:HD11	2.52	0.40
2:F:246:ASN:HA	2:F:247:PRO:HA	1.84	0.40
2:F:254:TYR:O	2:F:258:THR:CG2	2.69	0.40
2:F:298:ILE:HA	2:F:301:LEU:CD1	2.52	0.40
2:F:469:TYR:CE1	2:F:562:ASN:HB2	2.55	0.40
2:F:541:THR:O	2:F:542:GLN:HB3	2.21	0.40
1:A:614:ASN:HB2	1:A:617:GLN:HE22	1.86	0.40
1:A:833:ASP:HB3	1:A:835:ILE:HD12	2.03	0.40
1:A:834:LYS:O	1:A:835:ILE:C	2.64	0.40
1:A:1084:LYS:HB3	1:A:1086:TYR:CE2	2.57	0.40
1:C:824:PRO:HB2	2:D:952:ALA:HB2	2.03	0.40
1:C:845:LYS:C	1:C:847:ILE:H	2.28	0.40
1:C:937:TYR:CE1	1:C:954:LEU:HB2	2.57	0.40
1:C:945:ASP:C	1:C:947:ASN:H	2.28	0.40
1:E:102:ILE:O	1:E:103:LEU:C	2.64	0.40
1:E:225:LYS:HA	1:E:228:THR:OG1	2.22	0.40
1:E:305:GLU:OE1	1:E:305:GLU:HA	2.21	0.40
1:E:681:VAL:O	1:E:682:TYR:C	2.64	0.40
1:E:717:THR:O	1:E:718:ILE:C	2.64	0.40
1:E:789:VAL:HG12	1:E:793:LEU:HD12	2.03	0.40
1:E:920:TRP:O	1:E:1044:ILE:HA	2.21	0.40
2:B:589:ILE:HG13	2:B:641:TYR:OH	2.22	0.40
2:B:603:MET:HE3	2:B:611:LEU:HD12	2.03	0.40
2:F:87:GLN:O	2:F:88:ARG:C	2.64	0.40
2:F:253:LYS:O	2:F:254:TYR:C	2.64	0.40
2:F:507:TYR:O	2:F:508:LEU:C	2.65	0.40
2:F:828:TYR:HB2	2:F:829:PRO:HD2	2.04	0.40
1:A:39:ILE:HG12	1:A:148:VAL:HB	2.04	0.40
1:C:22:LYS:HG3	1:C:23:PRO:HD2	2.02	0.40
1:C:873:ASN:N	1:C:899:ASN:O	2.41	0.40
1:C:1163:TYR:CZ	1:C:1176:LYS:HB2	2.56	0.40
1:E:169:ASN:OD1	2:B:461:THR:HA	2.20	0.40
1:E:427:ILE:HD12	1:E:521:PHE:CD1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:541:ILE:O	1:E:542:ASP:C	2.63	0.40
1:E:975:PHE:CE2	1:E:977:TYR:HB3	2.57	0.40
1:E:1000:LEU:N	1:E:1000:LEU:HD12	2.36	0.40
2:B:373:ILE:HG22	2:B:379:VAL:HG22	2.04	0.40
2:B:403:ILE:HA	2:B:404:PRO:HD3	1.95	0.40
2:B:654:LYS:HA	2:B:657:LEU:HD12	2.02	0.40
2:D:13:VAL:CG1	2:D:14:ASP:N	2.84	0.40
2:D:245:THR:HB	2:D:631:TYR:CE1	2.56	0.40
2:D:271:ILE:CG2	2:D:272:LYS:N	2.84	0.40
2:D:540:GLU:HB3	2:D:555:PRO:CD	2.52	0.40
2:D:589:ILE:HG13	2:D:641:TYR:OH	2.21	0.40
2:D:603:MET:HE3	2:D:611:LEU:HD12	2.02	0.40
2:D:1056:PRO:O	2:D:1057:LEU:C	2.65	0.40
2:F:92:ASN:O	2:F:95:GLY:N	2.55	0.40
2:F:153:TYR:HB2	2:F:165:MET:O	2.21	0.40
2:F:1007:ILE:HG12	2:F:1072:GLN:C	2.47	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:ARG:NH2	1:C:420:GLY:O[3_564]	2.16	0.04

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	1225/1252 (98%)	999 (82%)	159 (13%)	67 (6%)	1 7
1	C	1225/1252 (98%)	995 (81%)	166 (14%)	64 (5%)	1 8
1	E	1225/1252 (98%)	997 (81%)	162 (13%)	66 (5%)	1 7
2	B	1084/1163 (93%)	832 (77%)	183 (17%)	69 (6%)	1 5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	1084/1163 (93%)	835 (77%)	179 (16%)	70 (6%)	1	5
2	F	1084/1163 (93%)	838 (77%)	177 (16%)	69 (6%)	1	5
All	All	6927/7245 (96%)	5496 (79%)	1026 (15%)	405 (6%)	1	6

All (405) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	THR
1	A	199	ILE
1	A	291	VAL
1	A	419	LYS
1	A	449	ASN
1	A	469	ASP
1	A	483	LEU
1	A	485	ASP
1	A	490	LEU
1	A	499	PRO
1	A	738	TYR
1	A	740	ILE
1	A	743	ILE
1	A	928	ASN
1	A	978	GLY
1	A	979	ASN
1	A	1068	ASN
1	A	1074	ASP
1	A	1103	ASP
1	A	1104	SER
1	A	1109	ASN
1	A	1156	LYS
1	C	119	THR
1	C	199	ILE
1	C	291	VAL
1	C	419	LYS
1	C	449	ASN
1	C	469	ASP
1	C	483	LEU
1	C	485	ASP
1	C	490	LEU
1	C	499	PRO
1	C	738	TYR
1	C	740	ILE

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Mol	Chain	Res	Type
1	C	743	ILE
1	C	928	ASN
1	C	978	GLY
1	C	979	ASN
1	C	1068	ASN
1	C	1074	ASP
1	C	1103	ASP
1	C	1104	SER
1	C	1109	ASN
1	C	1156	LYS
1	E	119	THR
1	E	199	ILE
1	E	291	VAL
1	E	419	LYS
1	E	449	ASN
1	E	469	ASP
1	E	483	LEU
1	E	485	ASP
1	E	490	LEU
1	E	499	PRO
1	E	738	TYR
1	E	740	ILE
1	E	743	ILE
1	E	928	ASN
1	E	978	GLY
1	E	979	ASN
1	E	1068	ASN
1	E	1074	ASP
1	E	1103	ASP
1	E	1104	SER
1	E	1109	ASN
1	E	1156	LYS
2	B	9	ILE
2	B	10	ASP
2	B	36	ALA
2	B	37	PRO
2	B	155	LYS
2	B	252	ASP
2	B	253	LYS
2	B	273	ILE
2	B	277	ASN
2	B	279	ILE

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Mol	Chain	Res	Type
2	B	285	LEU
2	B	416	SER
2	B	439	PRO
2	B	480	ILE
2	B	604	LEU
2	B	709	ASN
2	B	848	ALA
2	B	856	ASN
2	B	861	ASN
2	B	914	ASN
2	B	991	SER
2	B	1057	LEU
2	B	1102	ASP
2	B	1107	ALA
2	B	1128	ASN
2	D	9	ILE
2	D	10	ASP
2	D	36	ALA
2	D	37	PRO
2	D	155	LYS
2	D	252	ASP
2	D	253	LYS
2	D	273	ILE
2	D	277	ASN
2	D	279	ILE
2	D	285	LEU
2	D	416	SER
2	D	439	PRO
2	D	480	ILE
2	D	604	LEU
2	D	709	ASN
2	D	848	ALA
2	D	856	ASN
2	D	861	ASN
2	D	914	ASN
2	D	991	SER
2	D	1057	LEU
2	D	1102	ASP
2	D	1128	ASN
2	F	9	ILE
2	F	10	ASP
2	F	36	ALA

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Mol	Chain	Res	Type
2	F	37	PRO
2	F	155	LYS
2	F	252	ASP
2	F	253	LYS
2	F	273	ILE
2	F	277	ASN
2	F	279	ILE
2	F	285	LEU
2	F	416	SER
2	F	439	PRO
2	F	480	ILE
2	F	604	LEU
2	F	709	ASN
2	F	848	ALA
2	F	856	ASN
2	F	861	ASN
2	F	914	ASN
2	F	991	SER
2	F	1057	LEU
2	F	1102	ASP
2	F	1107	ALA
2	F	1128	ASN
1	A	362	ASN
1	A	417	SER
1	A	420	GLY
1	A	444	ASN
1	A	530	GLU
1	A	569	ALA
1	A	611	ASN
1	A	728	LEU
1	A	731	LYS
1	A	739	ASP
1	A	742	GLN
1	A	819	LEU
1	A	835	ILE
1	A	1116	LEU
1	A	1230	ARG
1	C	362	ASN
1	C	417	SER
1	C	420	GLY
1	C	444	ASN
1	C	530	GLU

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Mol	Chain	Res	Type
1	C	569	ALA
1	C	611	ASN
1	C	728	LEU
1	C	731	LYS
1	C	739	ASP
1	C	742	GLN
1	C	819	LEU
1	C	835	ILE
1	C	1027	ASP
1	C	1116	LEU
1	C	1230	ARG
1	E	362	ASN
1	E	417	SER
1	E	420	GLY
1	E	444	ASN
1	E	530	GLU
1	E	569	ALA
1	E	611	ASN
1	E	728	LEU
1	E	731	LYS
1	E	739	ASP
1	E	742	GLN
1	E	819	LEU
1	E	835	ILE
1	E	1116	LEU
1	E	1230	ARG
2	B	15	ASN
2	B	81	ALA
2	B	114	THR
2	B	419	ASP
2	B	501	LEU
2	B	540	GLU
2	B	676	GLU
2	B	710	ILE
2	B	811	GLN
2	B	822	LYS
2	B	947	ASP
2	B	1012	GLU
2	B	1014	ILE
2	D	15	ASN
2	D	81	ALA
2	D	114	THR

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Mol	Chain	Res	Type
2	D	419	ASP
2	D	501	LEU
2	D	540	GLU
2	D	676	GLU
2	D	710	ILE
2	D	811	GLN
2	D	822	LYS
2	D	947	ASP
2	D	1012	GLU
2	D	1014	ILE
2	D	1107	ALA
2	F	15	ASN
2	F	81	ALA
2	F	114	THR
2	F	419	ASP
2	F	501	LEU
2	F	540	GLU
2	F	676	GLU
2	F	710	ILE
2	F	811	GLN
2	F	822	LYS
2	F	947	ASP
2	F	1012	GLU
2	F	1014	ILE
1	A	138	ASN
1	A	293	ASN
1	A	398	PRO
1	A	451	PRO
1	A	507	SER
1	A	583	PHE
1	A	648	PHE
1	A	666	ALA
1	A	1027	ASP
1	C	138	ASN
1	C	293	ASN
1	C	398	PRO
1	C	451	PRO
1	C	507	SER
1	C	583	PHE
1	C	648	PHE
1	C	666	ALA
1	E	138	ASN

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Mol	Chain	Res	Type
1	E	293	ASN
1	E	398	PRO
1	E	451	PRO
1	E	507	SER
1	E	583	PHE
1	E	648	PHE
1	E	666	ALA
1	E	1027	ASP
1	E	1083	ASP
2	B	16	LYS
2	B	113	ASN
2	B	153	TYR
2	B	154	LYS
2	B	276	ASN
2	B	542	GLN
2	B	857	ASP
2	B	922	ASN
2	B	924	SER
2	B	972	SER
2	B	1018	ASN
2	D	16	LYS
2	D	113	ASN
2	D	153	TYR
2	D	154	LYS
2	D	276	ASN
2	D	296	LYS
2	D	417	TYR
2	D	542	GLN
2	D	922	ASN
2	D	924	SER
2	D	972	SER
2	D	1018	ASN
2	F	16	LYS
2	F	113	ASN
2	F	154	LYS
2	F	276	ASN
2	F	417	TYR
2	F	922	ASN
2	F	924	SER
2	F	972	SER
2	F	1018	ASN
1	A	454	ILE

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Mol	Chain	Res	Type
1	A	488	LEU
1	A	498	ILE
1	A	913	LYS
1	A	915	PHE
1	A	927	ASP
1	A	1083	ASP
1	A	1117	LEU
1	C	454	ILE
1	C	488	LEU
1	C	498	ILE
1	C	913	LYS
1	C	927	ASP
1	C	1083	ASP
1	C	1117	LEU
1	E	468	LEU
1	E	498	ILE
1	E	913	LYS
1	E	927	ASP
1	E	988	ASN
2	B	66	SER
2	B	296	LYS
2	B	417	TYR
2	B	442	LYS
2	B	680	ILE
2	B	1093	THR
2	B	1140	TYR
2	B	1147	LEU
2	D	275	ASN
2	D	295	VAL
2	D	442	LYS
2	D	680	ILE
2	D	857	ASP
2	D	878	GLN
2	D	1093	THR
2	D	1140	TYR
2	D	1147	LEU
2	F	153	TYR
2	F	275	ASN
2	F	295	VAL
2	F	296	LYS
2	F	442	LYS
2	F	542	GLN

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Mol	Chain	Res	Type
2	F	857	ASP
2	F	1140	TYR
2	F	1147	LEU
1	A	146	PRO
1	A	292	SER
1	A	400	THR
1	A	468	LEU
1	A	791	THR
1	A	910	ASN
1	A	988	ASN
1	A	1139	ASP
1	C	50	THR
1	C	146	PRO
1	C	292	SER
1	C	468	LEU
1	C	791	THR
1	C	915	PHE
1	C	988	ASN
1	C	1094	PRO
1	E	146	PRO
1	E	292	SER
1	E	400	THR
1	E	454	ILE
1	E	488	LEU
1	E	791	THR
1	E	910	ASN
1	E	915	PHE
1	E	1094	PRO
1	E	1117	LEU
2	B	275	ASN
2	B	295	VAL
2	B	433	ASN
2	B	478	ASN
2	B	878	GLN
2	D	14	ASP
2	D	66	SER
2	D	328	LYS
2	D	433	ASN
2	D	478	ASN
2	F	66	SER
2	F	433	ASN
2	F	478	ASN

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Mol	Chain	Res	Type
2	F	680	ILE
2	F	878	GLN
2	F	1093	THR
1	A	1094	PRO
1	E	50	THR
2	B	14	ASP
2	B	328	LYS
2	B	429	ILE
2	B	1101	VAL
2	D	186	ALA
2	D	429	ILE
2	D	1101	VAL
2	F	14	ASP
2	F	328	LYS
2	F	1101	VAL
1	C	604	PRO
2	B	251	ILE
2	D	142	GLY
2	D	251	ILE
2	F	142	GLY
2	F	251	ILE
2	F	429	ILE
1	A	604	PRO
1	C	239	PRO
2	B	93	VAL
2	B	142	GLY
2	D	93	VAL
2	F	93	VAL
1	A	154	GLU
1	A	803	ILE
1	C	803	ILE
1	E	604	PRO
1	A	239	PRO
1	E	803	ILE
1	E	154	GLU

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1125/1155 (97%)	1013 (90%)	112 (10%)	7	25
1	C	1125/1155 (97%)	1014 (90%)	111 (10%)	7	26
1	E	1125/1155 (97%)	1012 (90%)	113 (10%)	7	25
2	B	990/1103 (90%)	911 (92%)	79 (8%)	11	33
2	D	990/1103 (90%)	912 (92%)	78 (8%)	11	34
2	F	990/1103 (90%)	911 (92%)	79 (8%)	11	33
All	All	6345/6774 (94%)	5773 (91%)	572 (9%)	9	29

All (572) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ARG
1	A	17	THR
1	A	19	LEU
1	A	50	THR
1	A	53	GLN
1	A	65	ASP
1	A	108	SER
1	A	122	ASN
1	A	136	PHE
1	A	144	LEU
1	A	159	GLU
1	A	180	SER
1	A	191	SER
1	A	194	PHE
1	A	196	ASP
1	A	197	ASN
1	A	201	GLU
1	A	221	LEU
1	A	230	THR
1	A	258	ASN
1	A	273	THR
1	A	278	ASP
1	A	287	SER
1	A	290	GLN
1	A	305	GLU
1	A	336	GLU
1	A	348	ARG
1	A	354	GLN

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Mol	Chain	Res	Type
1	A	402	ARG
1	A	421	ILE
1	A	428	GLU
1	A	436	PHE
1	A	440	GLU
1	A	441	ASN
1	A	443	TYR
1	A	447	ASN
1	A	452	LYS
1	A	456	ASP
1	A	465	GLU
1	A	468	LEU
1	A	486	GLU
1	A	487	LYS
1	A	491	THR
1	A	506	THR
1	A	507	SER
1	A	532	GLU
1	A	533	ASN
1	A	591	SER
1	A	598	ASP
1	A	608	LEU
1	A	625	LEU
1	A	634	LEU
1	A	658	ASP
1	A	674	ARG
1	A	690	MET
1	A	696	GLN
1	A	703	GLN
1	A	705	TYR
1	A	716	LYS
1	A	725	SER
1	A	733	GLU
1	A	734	LEU
1	A	735	THR
1	A	738	TYR
1	A	755	MET
1	A	781	LYS
1	A	795	ASN
1	A	821	ASN
1	A	831	THR
1	A	838	SER

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Mol	Chain	Res	Type
1	A	839	TYR
1	A	842	LYS
1	A	855	MET
1	A	869	ASP
1	A	874	ILE
1	A	886	ASN
1	A	887	GLN
1	A	892	ASN
1	A	893	ASP
1	A	897	GLU
1	A	903	ASN
1	A	904	ASP
1	A	907	ILE
1	A	918	SER
1	A	930	ILE
1	A	931	VAL
1	A	933	VAL
1	A	938	THR
1	A	1002	ASP
1	A	1016	SER
1	A	1020	LEU
1	A	1027	ASP
1	A	1037	SER
1	A	1040	ARG
1	A	1045	ARG
1	A	1053	GLU
1	A	1081	LEU
1	A	1088	LEU
1	A	1099	ASP
1	A	1101	ARG
1	A	1103	ASP
1	A	1104	SER
1	A	1105	THR
1	A	1129	ILE
1	A	1134	ASN
1	A	1143	ARG
1	A	1169	THR
1	A	1197	CYS
1	A	1205	ASN
1	A	1217	ASP
1	A	1230	ARG
1	A	1250	GLN

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Mol	Chain	Res	Type
1	C	16	ARG
1	C	17	THR
1	C	19	LEU
1	C	50	THR
1	C	53	GLN
1	C	65	ASP
1	C	108	SER
1	C	122	ASN
1	C	136	PHE
1	C	144	LEU
1	C	159	GLU
1	C	180	SER
1	C	191	SER
1	C	194	PHE
1	C	196	ASP
1	C	197	ASN
1	C	201	GLU
1	C	221	LEU
1	C	230	THR
1	C	258	ASN
1	C	273	THR
1	C	278	ASP
1	C	290	GLN
1	C	305	GLU
1	C	336	GLU
1	C	348	ARG
1	C	354	GLN
1	C	402	ARG
1	C	421	ILE
1	C	422	ARG
1	C	428	GLU
1	C	436	PHE
1	C	440	GLU
1	C	441	ASN
1	C	443	TYR
1	C	447	ASN
1	C	452	LYS
1	C	456	ASP
1	C	465	GLU
1	C	468	LEU
1	C	486	GLU
1	C	487	LYS

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Mol	Chain	Res	Type
1	C	491	THR
1	C	506	THR
1	C	532	GLU
1	C	533	ASN
1	C	591	SER
1	C	598	ASP
1	C	608	LEU
1	C	625	LEU
1	C	634	LEU
1	C	658	ASP
1	C	674	ARG
1	C	690	MET
1	C	696	GLN
1	C	703	GLN
1	C	705	TYR
1	C	716	LYS
1	C	725	SER
1	C	732	ASN
1	C	733	GLU
1	C	734	LEU
1	C	735	THR
1	C	738	TYR
1	C	755	MET
1	C	781	LYS
1	C	795	ASN
1	C	821	ASN
1	C	831	THR
1	C	838	SER
1	C	839	TYR
1	C	842	LYS
1	C	855	MET
1	C	869	ASP
1	C	874	ILE
1	C	886	ASN
1	C	887	GLN
1	C	892	ASN
1	C	893	ASP
1	C	897	GLU
1	C	903	ASN
1	C	904	ASP
1	C	907	ILE
1	C	930	ILE

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Mol	Chain	Res	Type
1	C	931	VAL
1	C	933	VAL
1	C	938	THR
1	C	1002	ASP
1	C	1016	SER
1	C	1020	LEU
1	C	1027	ASP
1	C	1037	SER
1	C	1040	ARG
1	C	1045	ARG
1	C	1053	GLU
1	C	1081	LEU
1	C	1088	LEU
1	C	1099	ASP
1	C	1101	ARG
1	C	1103	ASP
1	C	1104	SER
1	C	1105	THR
1	C	1129	ILE
1	C	1134	ASN
1	C	1143	ARG
1	C	1169	THR
1	C	1197	CYS
1	C	1205	ASN
1	C	1217	ASP
1	C	1230	ARG
1	C	1250	GLN
1	E	16	ARG
1	E	17	THR
1	E	19	LEU
1	E	50	THR
1	E	53	GLN
1	E	65	ASP
1	E	108	SER
1	E	122	ASN
1	E	136	PHE
1	E	144	LEU
1	E	159	GLU
1	E	180	SER
1	E	191	SER
1	E	194	PHE
1	E	196	ASP

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Mol	Chain	Res	Type
1	E	197	ASN
1	E	201	GLU
1	E	221	LEU
1	E	230	THR
1	E	258	ASN
1	E	273	THR
1	E	278	ASP
1	E	290	GLN
1	E	297	ASN
1	E	305	GLU
1	E	336	GLU
1	E	348	ARG
1	E	354	GLN
1	E	367	SER
1	E	402	ARG
1	E	421	ILE
1	E	422	ARG
1	E	428	GLU
1	E	436	PHE
1	E	440	GLU
1	E	441	ASN
1	E	443	TYR
1	E	447	ASN
1	E	452	LYS
1	E	456	ASP
1	E	465	GLU
1	E	468	LEU
1	E	486	GLU
1	E	487	LYS
1	E	491	THR
1	E	506	THR
1	E	507	SER
1	E	532	GLU
1	E	533	ASN
1	E	591	SER
1	E	598	ASP
1	E	608	LEU
1	E	625	LEU
1	E	634	LEU
1	E	658	ASP
1	E	674	ARG
1	E	690	MET

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Mol	Chain	Res	Type
1	E	696	GLN
1	E	703	GLN
1	E	705	TYR
1	E	716	LYS
1	E	725	SER
1	E	733	GLU
1	E	734	LEU
1	E	735	THR
1	E	738	TYR
1	E	755	MET
1	E	781	LYS
1	E	795	ASN
1	E	821	ASN
1	E	831	THR
1	E	838	SER
1	E	839	TYR
1	E	842	LYS
1	E	855	MET
1	E	869	ASP
1	E	874	ILE
1	E	886	ASN
1	E	887	GLN
1	E	892	ASN
1	E	893	ASP
1	E	897	GLU
1	E	903	ASN
1	E	904	ASP
1	E	907	ILE
1	E	930	ILE
1	E	931	VAL
1	E	933	VAL
1	E	938	THR
1	E	1002	ASP
1	E	1016	SER
1	E	1020	LEU
1	E	1027	ASP
1	E	1037	SER
1	E	1040	ARG
1	E	1045	ARG
1	E	1053	GLU
1	E	1081	LEU
1	E	1088	LEU

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Mol	Chain	Res	Type
1	E	1099	ASP
1	E	1101	ARG
1	E	1103	ASP
1	E	1104	SER
1	E	1105	THR
1	E	1129	ILE
1	E	1134	ASN
1	E	1143	ARG
1	E	1169	THR
1	E	1197	CYS
1	E	1205	ASN
1	E	1217	ASP
1	E	1230	ARG
1	E	1250	GLN
2	B	14	ASP
2	B	23	SER
2	B	27	ASP
2	B	39	ILE
2	B	41	ILE
2	B	63	ILE
2	B	68	PHE
2	B	70	SER
2	B	74	GLU
2	B	82	THR
2	B	152	TYR
2	B	153	TYR
2	B	207	ASP
2	B	253	LYS
2	B	258	THR
2	B	267	ASN
2	B	273	ILE
2	B	293	ILE
2	B	300	GLU
2	B	304	SER
2	B	319	ASN
2	B	335	TYR
2	B	351	THR
2	B	374	ASN
2	B	400	ASN
2	B	418	LEU
2	B	435	GLU
2	B	438	TYR

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Mol	Chain	Res	Type
2	B	453	ILE
2	B	481	ASN
2	B	483	SER
2	B	484	SER
2	B	491	SER
2	B	499	SER
2	B	504	THR
2	B	518	ASP
2	B	566	THR
2	B	570	PHE
2	B	580	ILE
2	B	588	ASN
2	B	601	SER
2	B	643	SER
2	B	656	VAL
2	B	678	SER
2	B	697	ARG
2	B	703	SER
2	B	754	ASN
2	B	756	ASN
2	B	763	LEU
2	B	791	GLU
2	B	793	LEU
2	B	830	LYS
2	B	832	ILE
2	B	845	LEU
2	B	855	THR
2	B	856	ASN
2	B	863	LEU
2	B	865	ASN
2	B	876	LEU
2	B	899	PHE
2	B	910	ASP
2	B	954	GLU
2	B	958	GLU
2	B	969	SER
2	B	971	LEU
2	B	986	ASN
2	B	1002	LEU
2	B	1013	GLU
2	B	1024	PHE
2	B	1030	GLU

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Mol	Chain	Res	Type
2	B	1075	ASP
2	B	1095	ASN
2	B	1097	ARG
2	B	1140	TYR
2	B	1142	TRP
2	B	1145	CYS
2	B	1147	LEU
2	B	1148	ASN
2	B	1158	TRP
2	D	14	ASP
2	D	23	SER
2	D	27	ASP
2	D	39	ILE
2	D	41	ILE
2	D	63	ILE
2	D	68	PHE
2	D	70	SER
2	D	82	THR
2	D	152	TYR
2	D	153	TYR
2	D	207	ASP
2	D	253	LYS
2	D	258	THR
2	D	267	ASN
2	D	273	ILE
2	D	300	GLU
2	D	304	SER
2	D	319	ASN
2	D	335	TYR
2	D	351	THR
2	D	374	ASN
2	D	400	ASN
2	D	418	LEU
2	D	435	GLU
2	D	438	TYR
2	D	453	ILE
2	D	481	ASN
2	D	483	SER
2	D	484	SER
2	D	491	SER
2	D	499	SER
2	D	504	THR

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Mol	Chain	Res	Type
2	D	518	ASP
2	D	566	THR
2	D	570	PHE
2	D	580	ILE
2	D	588	ASN
2	D	601	SER
2	D	643	SER
2	D	656	VAL
2	D	678	SER
2	D	691	THR
2	D	697	ARG
2	D	703	SER
2	D	754	ASN
2	D	756	ASN
2	D	763	LEU
2	D	791	GLU
2	D	793	LEU
2	D	830	LYS
2	D	832	ILE
2	D	845	LEU
2	D	855	THR
2	D	856	ASN
2	D	863	LEU
2	D	865	ASN
2	D	876	LEU
2	D	899	PHE
2	D	910	ASP
2	D	954	GLU
2	D	958	GLU
2	D	969	SER
2	D	971	LEU
2	D	986	ASN
2	D	1002	LEU
2	D	1013	GLU
2	D	1024	PHE
2	D	1030	GLU
2	D	1075	ASP
2	D	1095	ASN
2	D	1097	ARG
2	D	1140	TYR
2	D	1142	TRP
2	D	1145	CYS

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Mol	Chain	Res	Type
2	D	1147	LEU
2	D	1148	ASN
2	D	1158	TRP
2	F	14	ASP
2	F	23	SER
2	F	27	ASP
2	F	39	ILE
2	F	41	ILE
2	F	63	ILE
2	F	68	PHE
2	F	70	SER
2	F	74	GLU
2	F	152	TYR
2	F	153	TYR
2	F	207	ASP
2	F	248	TYR
2	F	253	LYS
2	F	258	THR
2	F	267	ASN
2	F	300	GLU
2	F	304	SER
2	F	319	ASN
2	F	335	TYR
2	F	351	THR
2	F	374	ASN
2	F	400	ASN
2	F	418	LEU
2	F	435	GLU
2	F	438	TYR
2	F	453	ILE
2	F	481	ASN
2	F	483	SER
2	F	484	SER
2	F	491	SER
2	F	499	SER
2	F	504	THR
2	F	518	ASP
2	F	566	THR
2	F	570	PHE
2	F	580	ILE
2	F	588	ASN
2	F	601	SER

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Mol	Chain	Res	Type
2	F	610	ASP
2	F	643	SER
2	F	656	VAL
2	F	678	SER
2	F	697	ARG
2	F	754	ASN
2	F	756	ASN
2	F	763	LEU
2	F	791	GLU
2	F	793	LEU
2	F	830	LYS
2	F	832	ILE
2	F	845	LEU
2	F	855	THR
2	F	856	ASN
2	F	863	LEU
2	F	865	ASN
2	F	876	LEU
2	F	899	PHE
2	F	910	ASP
2	F	928	TRP
2	F	954	GLU
2	F	958	GLU
2	F	969	SER
2	F	971	LEU
2	F	986	ASN
2	F	996	THR
2	F	1002	LEU
2	F	1013	GLU
2	F	1024	PHE
2	F	1030	GLU
2	F	1075	ASP
2	F	1095	ASN
2	F	1097	ARG
2	F	1140	TYR
2	F	1142	TRP
2	F	1145	CYS
2	F	1147	LEU
2	F	1148	ASN
2	F	1158	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (101) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	38	ASN
1	A	111	ASN
1	A	125	HIS
1	A	197	ASN
1	A	235	GLN
1	A	441	ASN
1	A	489	ASN
1	A	669	ASN
1	A	711	GLN
1	A	886	ASN
1	A	957	ASN
1	A	1008	ASN
1	A	1022	ASN
1	A	1060	GLN
1	A	1170	ASN
1	A	1236	ASN
1	C	8	ASN
1	C	38	ASN
1	C	111	ASN
1	C	125	HIS
1	C	197	ASN
1	C	235	GLN
1	C	441	ASN
1	C	466	ASN
1	C	489	ASN
1	C	589	GLN
1	C	669	ASN
1	C	820	ASN
1	C	886	ASN
1	C	957	ASN
1	C	1008	ASN
1	C	1022	ASN
1	C	1048	ASN
1	C	1060	GLN
1	C	1170	ASN
1	C	1236	ASN
1	E	8	ASN
1	E	38	ASN
1	E	111	ASN
1	E	125	HIS
1	E	170	ASN
1	E	197	ASN

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Mol	Chain	Res	Type
1	E	235	GLN
1	E	261	ASN
1	E	414	ASN
1	E	441	ASN
1	E	466	ASN
1	E	489	ASN
1	E	669	ASN
1	E	886	ASN
1	E	957	ASN
1	E	1008	ASN
1	E	1022	ASN
1	E	1048	ASN
1	E	1060	GLN
1	E	1236	ASN
2	B	171	GLN
2	B	208	ASN
2	B	289	GLN
2	B	452	ASN
2	B	623	ASN
2	B	677	ASN
2	B	684	ASN
2	B	689	ASN
2	B	702	GLN
2	B	724	ASN
2	B	762	HIS
2	B	865	ASN
2	B	892	ASN
2	B	1034	ASN
2	B	1137	ASN
2	D	171	GLN
2	D	208	ASN
2	D	289	GLN
2	D	452	ASN
2	D	636	GLN
2	D	677	ASN
2	D	684	ASN
2	D	689	ASN
2	D	702	GLN
2	D	724	ASN
2	D	762	HIS
2	D	849	ASN
2	D	865	ASN

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Mol	Chain	Res	Type
2	D	1034	ASN
2	D	1137	ASN
2	F	208	ASN
2	F	289	GLN
2	F	452	ASN
2	F	636	GLN
2	F	677	ASN
2	F	684	ASN
2	F	689	ASN
2	F	701	ASN
2	F	702	GLN
2	F	762	HIS
2	F	892	ASN
2	F	976	ASN
2	F	1034	ASN
2	F	1137	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 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 [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9	
1	A	1235/1252 (98%)	-1.57	0	100	100	53, 120, 189, 296	0
1	C	1235/1252 (98%)	-1.54	0	100	100	46, 129, 207, 364	0
1	E	1235/1252 (98%)	-1.55	0	100	100	62, 143, 214, 391	0
2	B	1114/1163 (95%)	-1.58	0	100	100	37, 109, 179, 274	0
2	D	1114/1163 (95%)	-1.59	0	100	100	48, 129, 194, 278	0
2	F	1114/1163 (95%)	-1.50	1 (0%)	92	86	51, 143, 220, 328	0
All	All	7047/7245 (97%)	-1.56	1 (0%)	100	100	37, 129, 203, 391	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	1158	TRP	2.5

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	A	1301	1/1	1.00	0.01	86,86,86,86	0
3	ZN	C	1301	1/1	1.00	0.01	83,83,83,83	0
3	ZN	E	1301	1/1	1.00	0.01	99,99,99,99	0

6.5 Other polymers [i](#)

There are no such residues in this entry.