



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:37 PM UTC

PDB ID : 1UKL / pdb_00001ukl
Title : Crystal structure of Importin-beta and SREBP-2 complex
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Deposited on : 2003-08-26
Resolution : 3.00 Å(reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

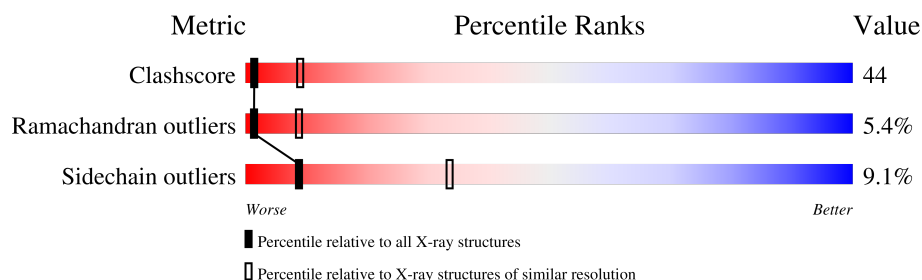
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	876	42% 48% 9% .
1	B	876	35% 51% 12% .
2	C	61	39% 46% 13% .
2	D	61	36% 48% 13% .
2	E	61	41% 43% 15% .
2	F	61	26% 52% 16% 5%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 15606 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 Importin beta-1 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	876	Total	C	N	O	S	0	0	0
			6807	4286	1141	1334	46			
1	B	876	Total	C	N	O	S	0	0	0
			6807	4286	1141	1334	46			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	388	MET	VAL	SEE REMARK 999	UNP P70168
B	388	MET	VAL	SEE REMARK 999	UNP P70168

- Molecule 2 is a protein called Sterol regulatory element binding protein-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	61	Total	C	N	O	Se	0	0	0
			498	313	93	89	3			
2	D	61	Total	C	N	O	Se	0	0	0
			498	313	93	89	3			
2	E	61	Total	C	N	O	Se	0	0	0
			498	313	93	89	3			
2	F	61	Total	C	N	O	Se	0	0	0
			498	313	93	89	3			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	358	MSE	MET	modified residue	UNP Q12772
C	364	MSE	MET	modified residue	UNP Q12772
C	392	MSE	MET	modified residue	UNP Q12772
D	358	MSE	MET	modified residue	UNP Q12772
D	364	MSE	MET	modified residue	UNP Q12772
D	392	MSE	MET	modified residue	UNP Q12772

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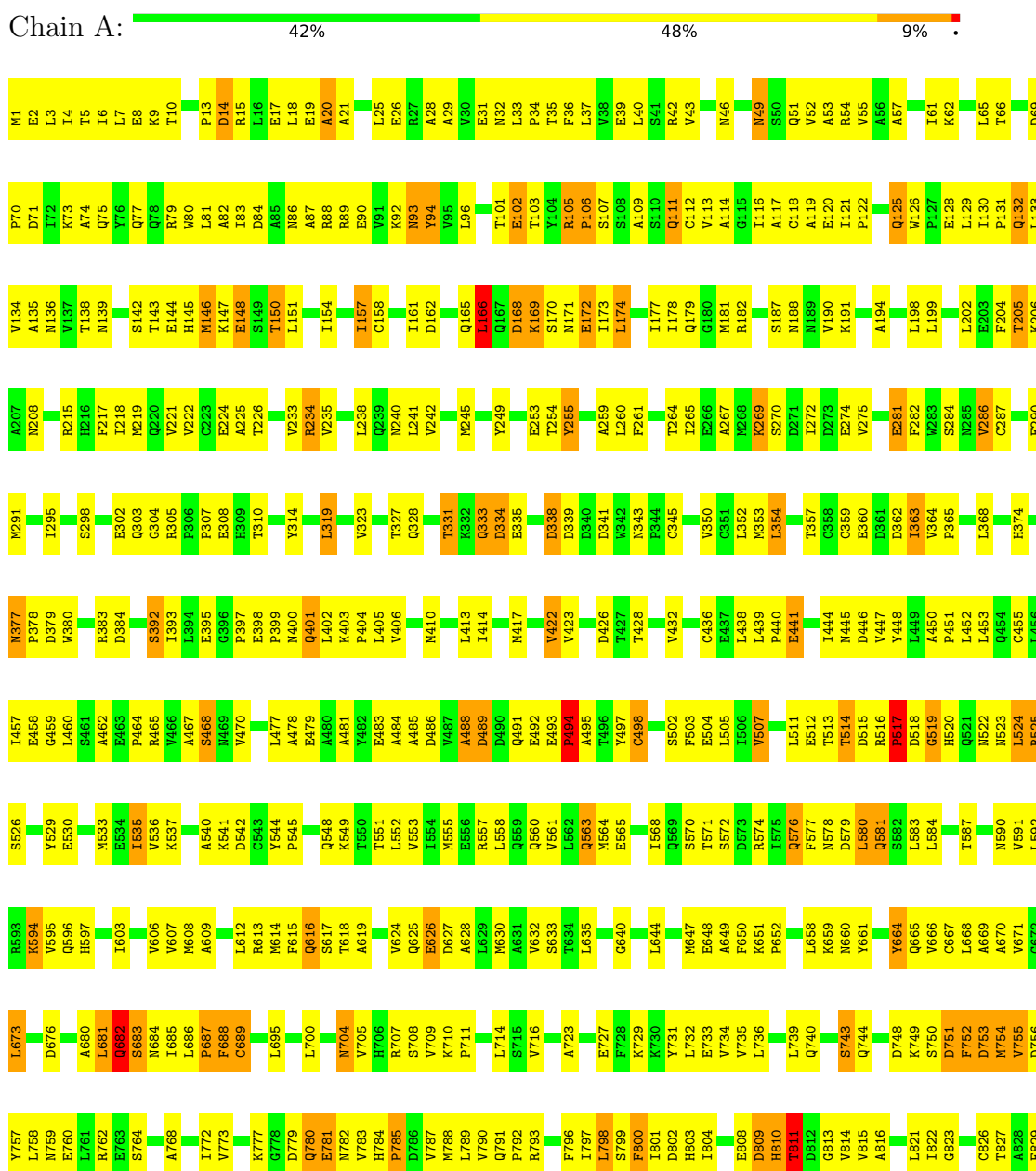
Chain	Residue	Modelled	Actual	Comment	Reference
E	358	MSE	MET	modified residue	UNP Q12772
E	364	MSE	MET	modified residue	UNP Q12772
E	392	MSE	MET	modified residue	UNP Q12772
F	358	MSE	MET	modified residue	UNP Q12772
F	364	MSE	MET	modified residue	UNP Q12772
F	392	MSE	MET	modified residue	UNP Q12772

3 Residue-property plots

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

Note EDS was not executed.

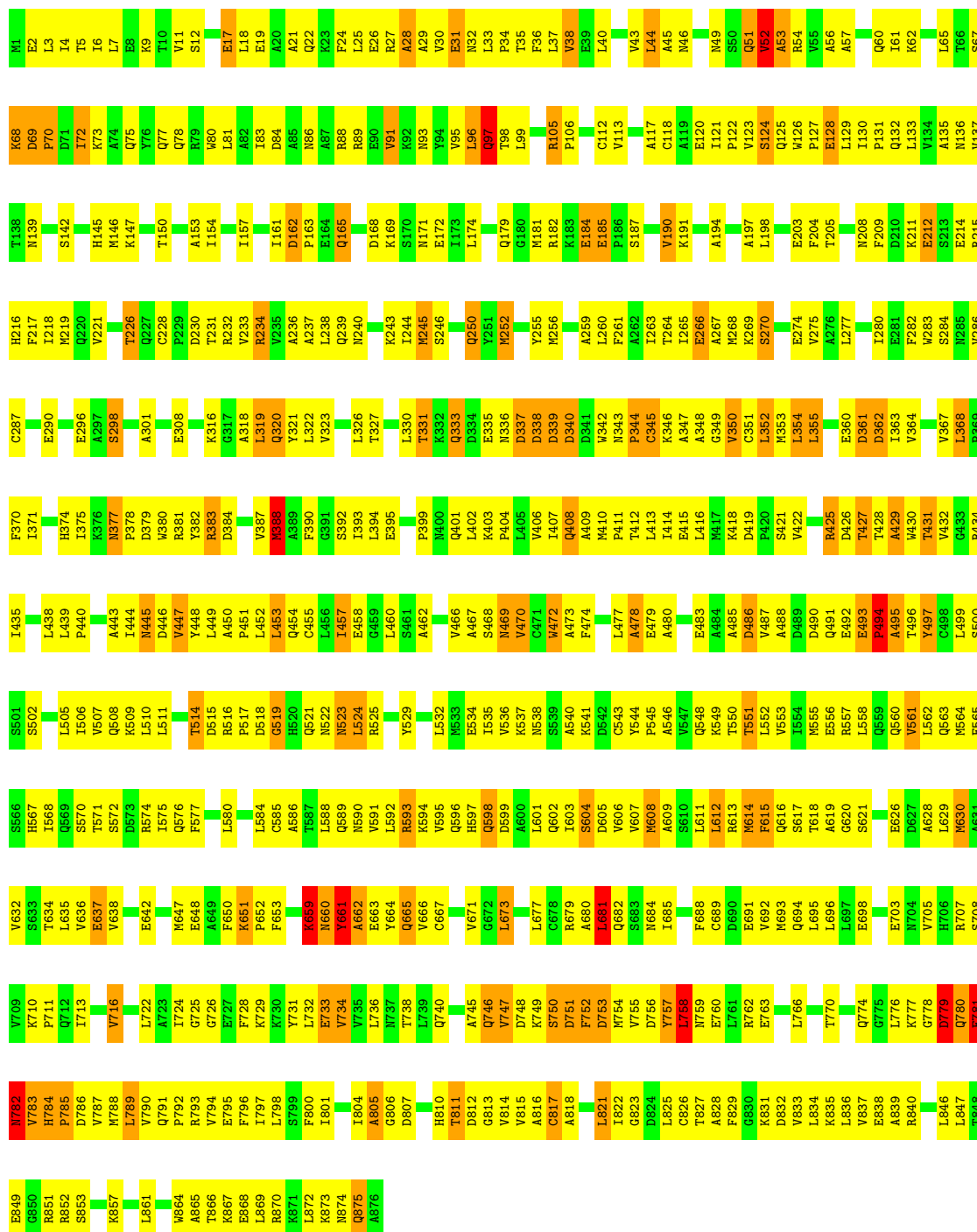
- Molecule 1: Importin beta-1 subunit



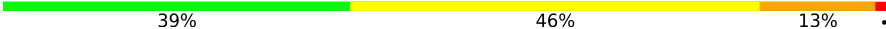


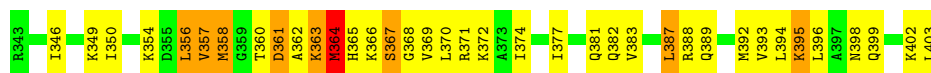
• Molecule 1: Importin beta-1 subunit

Chain B: 35% 51% 12%

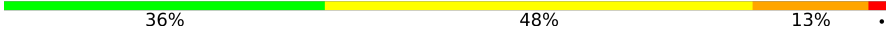


• Molecule 2: Sterol regulatory element binding protein-2

Chain C:  39% 46% 13% .



- Molecule 2: Sterol regulatory element binding protein-2

Chain D:  36% 48% 13% .

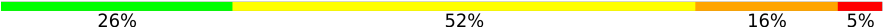


- Molecule 2: Sterol regulatory element binding protein-2

Chain E:  41% 43% 15% .



- Molecule 2: Sterol regulatory element binding protein-2

Chain F:  26% 52% 16% 5%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.09Å 113.28Å 240.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.00	Depositor
% Data completeness (in resolution range)	99.1 (19.99-3.00)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.239 , 0.297	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15606	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.58	4/6918 (0.1%)	1.08	49/9392 (0.5%)
1	B	0.59	3/6918 (0.0%)	1.19	82/9392 (0.9%)
2	C	0.81	4/498 (0.8%)	1.31	5/655 (0.8%)
2	D	0.67	3/498 (0.6%)	1.12	7/655 (1.1%)
2	E	0.96	4/498 (0.8%)	1.27	8/655 (1.2%)
2	F	0.88	4/498 (0.8%)	1.36	10/655 (1.5%)
All	All	0.62	22/15828 (0.1%)	1.16	161/21404 (0.8%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	358	MSE	CG-SE	-6.72	1.75	1.95
1	B	493	GLU	N-CA	-5.79	1.41	1.46
2	E	392	MSE	SE-CE	-5.58	1.78	1.95
1	A	681	LEU	CA-C	-5.52	1.48	1.52
2	F	358	MSE	SE-CE	-5.42	1.79	1.95
2	E	358	MSE	SE-CE	-5.40	1.79	1.95
2	F	364	MSE	SE-CE	-5.40	1.79	1.95
2	E	365	HIS	CA-C	-5.39	1.45	1.52
1	A	811	THR	N-CA	-5.38	1.39	1.46
2	C	358	MSE	CG-SE	-5.35	1.79	1.95
1	A	754	MET	C-N	5.35	1.40	1.33
2	C	364	MSE	SE-CE	-5.27	1.79	1.95
2	E	364	MSE	SE-CE	-5.27	1.79	1.95
2	F	348	ASP	N-CA	-5.17	1.38	1.46
2	C	358	MSE	SE-CE	-5.14	1.80	1.95
2	D	392	MSE	SE-CE	-5.07	1.80	1.95
2	D	392	MSE	CG-SE	-5.07	1.80	1.95
1	A	831	LYS	CA-C	-5.06	1.47	1.53
1	B	388	MET	SD-CE	5.06	1.92	1.79
2	D	364	MSE	CG-SE	-5.04	1.80	1.95
2	C	364	MSE	N-CA	-5.03	1.39	1.45
1	B	337	ASP	CA-C	-5.00	1.46	1.53

All (161) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	337	ASP	N-CA-C	11.79	123.53	107.73
2	C	362	ALA	CA-C-N	-11.56	106.47	122.77
2	C	362	ALA	C-N-CA	-11.56	106.47	122.77
1	B	70	PRO	CA-N-CD	-10.68	97.04	112.00
1	A	494	PRO	CA-N-CD	-10.55	97.23	112.00
1	A	682	GLN	OE1-CD-NE2	-10.39	112.21	122.60
1	B	780	GLN	OE1-CD-NE2	-9.95	112.65	122.60
1	B	333	GLN	OE1-CD-NE2	-9.94	112.66	122.60
1	B	51	GLN	OE1-CD-NE2	-9.93	112.67	122.60
1	B	665	GLN	OE1-CD-NE2	-9.83	112.77	122.60
2	F	399	GLN	OE1-CD-NE2	-9.77	112.83	122.60
1	B	250	GLN	OE1-CD-NE2	-9.63	112.97	122.60
2	E	368	GLY	N-CA-C	-9.56	90.53	113.18
1	A	491	GLN	OE1-CD-NE2	-9.45	113.15	122.60
1	B	746	GLN	OE1-CD-NE2	-9.38	113.22	122.60
1	B	491	GLN	OE1-CD-NE2	-9.36	113.24	122.60
1	B	615	PHE	N-CA-C	-9.25	101.89	113.55
1	B	784	HIS	CA-C-N	9.12	129.72	119.32
1	B	784	HIS	C-N-CA	9.12	129.72	119.32
1	A	106	PRO	N-CA-C	-9.00	105.32	114.68
2	C	363	LYS	N-CA-C	8.86	122.87	108.34
1	B	751	ASP	N-CA-C	-8.72	100.02	113.02
1	B	781	GLU	N-CA-C	-8.26	101.67	112.41
1	B	491	GLN	N-CA-C	-8.22	96.88	109.95
1	A	338	ASP	N-CA-C	-8.01	102.00	112.41
1	A	82	ALA	N-CA-C	-7.97	103.35	113.72
1	A	810	HIS	CA-C-N	7.93	134.46	122.65
1	A	810	HIS	C-N-CA	7.93	134.46	122.65
1	B	336	ASN	CA-C-N	-7.86	108.61	122.84
1	B	336	ASN	C-N-CA	-7.86	108.61	122.84
2	D	350	ILE	N-CA-C	-7.82	103.81	112.80
1	B	563	GLN	N-CA-C	-7.81	104.18	112.93
1	A	188	ASN	N-CA-C	-7.60	103.08	111.36
2	F	347	ASN	CA-C-N	-7.60	111.26	122.35
2	F	347	ASN	C-N-CA	-7.60	111.26	122.35
1	A	782	ASN	N-CA-C	-7.54	105.25	114.75
2	F	395	LYS	N-CA-C	-7.53	103.66	112.92
1	B	493	GLU	O-C-N	7.50	127.66	121.44
1	B	494	PRO	CA-N-CD	-7.40	101.64	112.00
1	B	70	PRO	N-CA-C	7.35	124.70	113.75
2	E	367	SER	CA-C-N	7.33	135.78	121.41
2	E	367	SER	C-N-CA	7.33	135.78	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	254	THR	N-CA-C	7.32	119.16	111.03
1	B	333	GLN	CG-CD-NE2	7.26	127.29	116.40
1	B	662	ALA	N-CA-C	-7.24	103.32	111.07
2	D	371	ARG	N-CA-C	-7.24	102.57	111.40
1	A	682	GLN	CG-CD-NE2	7.15	127.12	116.40
2	C	364	MSE	N-CA-C	-7.12	99.99	110.52
1	A	498	CYS	N-CA-C	7.06	120.99	112.38
1	B	614	MET	N-CA-C	-7.05	103.93	114.64
1	B	619	ALA	N-CA-C	-7.01	104.81	113.15
1	A	286	VAL	N-CA-C	-7.00	103.95	110.53
2	F	348	ASP	N-CA-C	-6.97	102.57	111.92
1	A	517	PRO	CA-N-CD	-6.97	102.24	112.00
1	A	810	HIS	O-C-N	6.93	130.87	122.84
1	B	250	GLN	CG-CD-NE2	6.77	126.56	116.40
1	B	337	ASP	CA-C-O	6.75	127.96	120.94
1	B	746	GLN	CG-CD-NE2	6.70	126.45	116.40
2	F	399	GLN	CG-CD-NE2	6.67	126.41	116.40
1	B	665	GLN	CG-CD-NE2	6.67	126.40	116.40
1	B	738	THR	N-CA-C	-6.62	105.74	113.88
1	B	51	GLN	CG-CD-NE2	6.61	126.32	116.40
1	B	472	TRP	N-CA-C	-6.60	103.70	111.03
1	B	510	LEU	N-CA-C	-6.59	104.89	113.12
1	A	831	LYS	O-C-N	6.56	129.86	122.32
1	B	491	GLN	CG-CD-NE2	6.55	126.23	116.40
1	B	780	GLN	CG-CD-NE2	6.55	126.23	116.40
2	C	357	VAL	N-CA-C	6.55	116.69	110.53
1	B	321	TYR	N-CA-C	-6.49	105.25	113.43
1	A	383	ARG	N-CA-C	-6.48	104.13	111.07
1	A	491	GLN	CG-CD-NE2	6.47	126.11	116.40
1	A	392	SER	N-CA-C	6.47	120.84	113.15
2	F	349	LYS	N-CA-C	-6.46	105.40	113.28
1	B	780	GLN	N-CA-C	6.46	119.23	108.96
1	B	69	ASP	CA-CB-CG	-6.41	106.19	112.60
1	B	763	GLU	N-CA-C	-6.39	104.23	111.07
1	B	429	ALA	N-CA-C	-6.38	104.75	112.54
1	A	94	TYR	N-CA-C	-6.37	104.56	112.90
2	D	347	ASN	N-CA-C	-6.32	106.53	114.56
2	D	357	VAL	N-CA-C	6.32	118.94	111.05
1	B	785	PRO	CA-N-CD	-6.27	103.22	112.00
1	B	747	VAL	O-C-N	6.26	129.50	122.68
1	A	305	ARG	CA-C-N	-6.25	113.94	120.38
1	A	305	ARG	C-N-CA	-6.25	113.94	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	53	ALA	N-CA-C	-6.24	105.32	113.12
1	A	426	ASP	N-CA-C	-6.19	104.16	111.03
1	B	338	ASP	N-CA-C	6.17	117.53	108.14
1	A	205	THR	N-CA-C	-6.16	103.84	113.02
1	A	809	ASP	CA-C-N	-6.15	112.03	122.67
1	A	809	ASP	C-N-CA	-6.15	112.03	122.67
2	F	396	LEU	N-CA-C	-6.13	105.83	113.55
1	A	704	ASN	N-CA-C	-6.11	104.54	112.23
1	A	52	VAL	N-CA-C	-6.07	107.33	113.47
1	B	128	GLU	N-CA-C	-6.07	107.11	114.75
1	A	393	ILE	N-CA-C	-6.06	106.41	112.17
1	A	755	VAL	CB-CA-C	-6.06	104.30	111.94
1	A	422	VAL	CB-CA-C	-6.06	104.21	111.97
1	B	339	ASP	CA-CB-CG	-6.04	106.56	112.60
1	A	363	ILE	N-CA-C	6.04	116.16	110.30
2	D	348	ASP	N-CA-C	-6.03	105.57	113.17
1	B	190	VAL	N-CA-C	-6.01	105.21	111.58
1	A	782	ASN	CB-CA-C	5.96	116.85	109.16
1	B	478	ALA	N-CA-C	-5.95	105.87	113.01
1	B	490	ASP	N-CA-C	-5.90	98.24	110.80
1	B	758	LEU	N-CA-C	-5.90	104.98	111.82
1	A	852	ARG	N-CA-C	-5.89	105.25	113.37
2	F	389	GLN	N-CA-C	-5.86	104.53	111.03
1	B	724	ILE	N-CA-C	5.85	117.79	112.29
1	B	38	VAL	N-CA-C	-5.85	105.12	113.07
1	B	284	SER	N-CA-C	-5.83	104.85	111.14
1	B	576	GLN	N-CA-C	-5.82	105.96	114.39
1	B	757	TYR	N-CA-C	-5.81	104.94	111.28
1	B	571	THR	N-CA-C	-5.81	104.95	111.28
1	B	779	ASP	N-CA-C	-5.77	102.74	110.24
1	B	784	HIS	O-C-N	5.75	127.94	121.32
1	A	810	HIS	CA-CB-CG	5.71	119.51	113.80
1	A	374	HIS	N-CA-C	5.70	120.36	113.17
1	B	91	VAL	N-CA-C	-5.68	104.96	110.42
1	A	377	ASN	CA-C-N	5.67	125.52	119.28
1	A	377	ASN	C-N-CA	5.67	125.52	119.28
2	E	365	HIS	O-C-N	5.61	130.05	122.59
1	A	571	THR	N-CA-C	-5.60	105.06	112.34
1	B	593	ARG	N-CA-C	-5.59	106.30	113.01
1	B	31	GLU	N-CA-C	-5.58	106.52	113.38
1	A	488	ALA	N-CA-C	-5.55	106.36	113.02
1	B	493	GLU	CA-C-O	5.53	126.65	120.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	691	GLU	N-CA-C	-5.50	105.19	111.07
1	B	491	GLN	CA-C-N	-5.47	111.08	121.54
1	B	491	GLN	C-N-CA	-5.47	111.08	121.54
1	A	284	SER	N-CA-C	-5.47	105.48	111.82
2	F	347	ASN	N-CA-C	5.45	115.32	108.45
1	B	383	ARG	N-CA-C	-5.40	104.81	111.40
1	A	393	ILE	CB-CA-C	-5.40	104.99	111.85
1	B	363	ILE	N-CA-C	5.39	118.66	111.44
1	A	172	GLU	N-CA-C	-5.38	105.11	110.97
1	B	681	LEU	N-CA-C	5.36	119.88	113.23
1	B	495	ALA	N-CA-C	-5.36	107.11	113.97
1	B	280	ILE	N-CA-C	-5.36	105.62	110.82
2	E	347	ASN	N-CA-C	-5.31	105.08	112.45
1	B	519	GLY	N-CA-C	5.29	119.04	112.64
1	B	337	ASP	O-C-N	5.23	128.82	122.75
1	B	364	VAL	CB-CA-C	-5.22	108.82	114.35
1	B	162	ASP	CA-C-N	5.21	124.88	119.56
1	B	162	ASP	C-N-CA	5.21	124.88	119.56
1	B	245	MET	N-CA-C	-5.20	105.69	111.36
2	D	370	LEU	N-CA-C	-5.18	106.96	113.28
1	A	401	GLN	N-CA-C	-5.16	107.12	113.41
1	A	446	ASP	N-CA-C	5.16	119.20	113.01
1	A	295	ILE	N-CA-C	-5.13	105.84	110.82
1	A	563	GLN	N-CA-C	-5.12	106.88	113.23
1	B	97	GLN	N-CA-C	-5.12	108.06	114.56
1	B	228	CYS	CA-C-N	5.09	124.88	119.28
1	B	228	CYS	C-N-CA	5.09	124.88	119.28
2	E	365	HIS	CA-C-O	5.08	127.78	120.51
2	E	392	MSE	N-CA-C	-5.08	104.68	111.24
1	B	457	ILE	N-CA-C	-5.05	104.74	111.05
2	D	400	LYS	N-CA-C	5.04	116.73	108.76
2	E	365	HIS	N-CA-C	5.01	121.48	110.80
1	A	810	HIS	CA-C-O	5.01	128.25	121.89
1	B	782	ASN	CA-C-N	-5.01	112.96	121.97
1	B	782	ASN	C-N-CA	-5.01	112.96	121.97

There are no chirality outliers.

There are no planarity outliers.

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	6807	0	6802	549	1
1	B	6807	0	6802	654	0
2	C	498	0	539	60	0
2	D	498	0	539	41	0
2	E	498	0	539	80	0
2	F	498	0	539	57	1
All	All	15606	0	15760	1385	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 44.

All (1385) 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:E:357:VAL:HG12	2:E:372:LYS:CE	1.52	1.39
1:A:870:ARG:NE	1:B:487:VAL:CG1	1.83	1.39
1:A:489:ASP:HB2	1:A:494:PRO:CD	1.63	1.26
1:A:870:ARG:NE	1:B:487:VAL:HG11	0.94	1.25
1:A:489:ASP:CB	1:A:494:PRO:HD3	1.68	1.23
2:E:357:VAL:CG1	2:E:372:LYS:HE3	1.69	1.22
1:B:748:ASP:OD2	1:B:754:MET:HE1	1.40	1.22
2:F:347:ASN:OD1	2:F:348:ASP:N	1.69	1.22
2:E:357:VAL:HG11	2:E:372:LYS:CG	1.72	1.19
2:E:357:VAL:HG11	2:E:372:LYS:HG3	1.25	1.18
1:B:783:VAL:O	1:B:783:VAL:CG1	1.92	1.18
2:E:357:VAL:CG1	2:E:372:LYS:CE	2.21	1.17
2:C:358:MSE:SE	2:C:364:MSE:SE	2.62	1.16
2:F:364:MSE:SE	2:F:365:HIS:CE1	2.49	1.15
1:A:796:PHE:O	1:A:799:SER:HB2	1.46	1.12
2:E:357:VAL:HG12	2:E:372:LYS:HE2	1.18	1.11
2:E:358:MSE:HB3	2:E:372:LYS:HE2	1.30	1.09
1:A:784:HIS:HD2	1:A:785:PRO:HD2	1.14	1.08
1:A:870:ARG:CZ	1:B:487:VAL:CG1	2.31	1.07
1:A:762:ARG:HD3	1:A:800:PHE:HE1	1.17	1.06
1:A:762:ARG:HD3	1:A:800:PHE:CE1	1.90	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:365:HIS:HD2	2:F:367:SER:HB3	1.19	1.06
1:A:870:ARG:CZ	1:B:487:VAL:HG11	1.86	1.06
1:A:870:ARG:HE	1:B:487:VAL:CG1	1.56	1.06
1:B:659:LYS:HE3	1:B:659:LYS:HA	1.34	1.05
2:E:357:VAL:HG12	2:E:358:MSE:H	1.17	1.04
2:F:347:ASN:CG	2:F:348:ASP:H	1.66	1.04
1:A:102:GLU:H	1:A:106:PRO:HG2	1.21	1.04
1:B:69:ASP:OD2	1:B:73:LYS:HE2	1.57	1.04
1:B:751:ASP:O	1:B:752:PHE:O	1.75	1.03
1:B:663:GLU:OE2	1:B:665:GLN:HB3	1.58	1.03
1:A:752:PHE:O	1:A:753:ASP:C	1.99	1.03
1:A:870:ARG:CD	1:B:487:VAL:HG11	1.90	1.01
1:B:663:GLU:OE2	1:B:665:GLN:CB	2.09	1.01
2:F:347:ASN:O	2:F:348:ASP:HB3	1.61	1.01
2:F:365:HIS:CD2	2:F:367:SER:HB3	1.96	1.01
1:A:514:THR:HG21	1:A:557:ARG:NH1	1.76	1.00
1:A:492:GLU:OE1	2:D:343:ARG:NH1	1.93	1.00
1:A:576:GLN:HA	1:A:576:GLN:HE21	1.27	1.00
1:B:777:LYS:HA	1:B:787:VAL:CG2	1.91	0.99
1:A:752:PHE:O	1:A:754:MET:N	1.95	0.99
2:D:370:LEU:HD23	2:D:370:LEU:N	1.77	0.99
1:A:752:PHE:O	1:A:755:VAL:N	1.95	0.99
2:E:358:MSE:HB3	2:E:372:LYS:CE	1.94	0.98
1:A:514:THR:HG21	1:A:557:ARG:HH12	1.28	0.98
1:B:335:GLU:OE2	1:B:380:TRP:HZ2	1.47	0.97
1:B:38:VAL:HA	1:B:91:VAL:HG22	1.45	0.97
1:B:30:VAL:HG12	1:B:32:ASN:H	1.30	0.97
2:E:357:VAL:HG12	2:E:372:LYS:HE3	1.27	0.96
1:B:608:MET:HE1	1:B:632:VAL:HG22	1.47	0.96
1:A:157:ILE:HG23	1:A:161:ILE:HD12	1.48	0.95
1:B:327:THR:HA	1:B:330:LEU:HD12	1.48	0.95
2:D:370:LEU:O	2:D:374:ILE:HD12	1.66	0.95
1:B:783:VAL:O	1:B:783:VAL:HG12	1.63	0.95
1:A:215:ARG:HD2	1:A:255:TYR:OH	1.67	0.95
1:A:338:ASP:HA	1:A:465:ARG:HH22	1.33	0.94
1:A:762:ARG:HD2	1:A:804:ILE:HD11	1.49	0.94
1:B:514:THR:HG21	1:B:557:ARG:HH12	1.33	0.94
1:B:749:LYS:HG3	1:B:750:SER:H	1.30	0.94
1:B:751:ASP:C	1:B:752:PHE:O	2.12	0.93
1:B:406:VAL:HG13	1:B:435:ILE:HD13	1.50	0.92
2:E:358:MSE:HE2	2:E:372:LYS:HG2	1.52	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:783:VAL:O	1:B:783:VAL:HG13	1.67	0.92
1:A:513:THR:O	1:A:516:ARG:HG3	1.70	0.92
1:B:337:ASP:O	1:B:338:ASP:OD1	1.88	0.92
1:B:606:VAL:O	1:B:609:ALA:HB3	1.70	0.91
2:D:370:LEU:HD23	2:D:370:LEU:H	1.32	0.91
1:B:130:ILE:HG22	1:B:169:LYS:HD2	1.53	0.91
1:A:102:GLU:HB3	1:A:106:PRO:HD3	1.50	0.91
1:A:489:ASP:HB2	1:A:494:PRO:HD3	0.92	0.90
1:A:515:ASP:O	1:A:516:ARG:HG2	1.69	0.90
1:A:762:ARG:CD	1:A:800:PHE:HE1	1.84	0.90
1:B:708:SER:O	1:B:711:PRO:HD2	1.71	0.90
1:A:135:ALA:HA	1:A:138:THR:HG22	1.53	0.90
2:E:357:VAL:HG12	2:E:358:MSE:N	1.80	0.90
2:E:358:MSE:CB	2:E:372:LYS:HE2	2.01	0.90
2:E:358:MSE:O	2:E:358:MSE:HG2	1.71	0.90
1:A:515:ASP:O	1:A:516:ARG:CG	2.21	0.89
2:E:358:MSE:HE2	2:E:372:LYS:CG	2.02	0.89
1:B:749:LYS:HG3	1:B:750:SER:N	1.85	0.89
1:A:644:LEU:HD22	1:A:684:ASN:HD21	1.37	0.89
1:A:784:HIS:CD2	1:A:785:PRO:HD2	2.06	0.89
1:A:568:ILE:HD13	1:A:574:ARG:HD2	1.56	0.88
2:C:361:ASP:OD1	2:C:361:ASP:O	1.90	0.88
1:B:169:LYS:HB2	1:B:172:GLU:HB2	1.53	0.88
1:A:181:MET:HE1	1:A:198:LEU:HD22	1.56	0.88
1:A:762:ARG:CD	1:A:800:PHE:CE1	2.55	0.87
2:E:346:ILE:HD12	2:E:349:LYS:HD2	1.57	0.86
1:B:494:PRO:O	1:B:541:LYS:HB2	1.76	0.86
1:B:335:GLU:OE2	1:B:380:TRP:CZ2	2.28	0.86
1:A:707:ARG:NH2	1:A:753:ASP:OD1	2.09	0.85
1:B:410:MET:O	1:B:414:ILE:HG13	1.77	0.85
1:A:84:ASP:HB3	1:A:87:ALA:HB2	1.57	0.85
1:A:489:ASP:HB2	1:A:494:PRO:CG	2.07	0.85
2:E:358:MSE:H	2:E:372:LYS:HE2	1.41	0.84
1:B:65:LEU:HB2	1:B:69:ASP:HB2	1.60	0.84
1:B:69:ASP:OD2	1:B:73:LYS:CE	2.25	0.84
1:A:644:LEU:HD22	1:A:684:ASN:ND2	1.93	0.84
1:B:33:LEU:HA	1:B:36:PHE:HB3	1.59	0.84
1:B:410:MET:HE1	1:B:452:LEU:HD13	1.60	0.84
1:B:483:GLU:HA	1:B:486:ASP:CG	2.01	0.84
1:B:27:ARG:HG2	1:B:28:ALA:N	1.91	0.84
1:B:478:ALA:HB2	1:B:535:ILE:HD12	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:357:VAL:HG23	2:C:358:MSE:HG3	1.60	0.84
2:E:354:LYS:HE3	2:E:361:ASP:HA	1.57	0.83
1:B:468:SER:HB3	2:E:343:ARG:HH22	1.43	0.83
1:A:787:VAL:HG23	1:A:788:MET:HE2	1.58	0.82
2:E:358:MSE:N	2:E:372:LYS:HE2	1.94	0.82
1:A:377:ASN:ND2	1:A:379:ASP:H	1.77	0.82
1:B:414:ILE:HG23	1:B:455:CYS:SG	2.19	0.82
1:B:65:LEU:HD23	1:B:65:LEU:H	1.42	0.82
1:B:430:TRP:HA	1:B:469:ASN:HD22	1.44	0.82
1:B:756:ASP:HA	1:B:759:ASN:HB2	1.62	0.82
1:A:684:ASN:O	1:A:687:PRO:HD2	1.78	0.82
1:A:799:SER:O	1:A:802:ASP:N	2.12	0.82
1:A:558:LEU:HD11	1:A:614:MET:HE1	1.62	0.81
2:F:364:MSE:SE	2:F:365:HIS:HE1	2.14	0.81
2:E:358:MSE:O	2:E:358:MSE:CG	2.29	0.81
1:B:483:GLU:HA	1:B:486:ASP:OD1	1.81	0.81
1:B:89:ARG:O	1:B:93:ASN:HB2	1.79	0.81
1:B:751:ASP:O	1:B:752:PHE:C	2.23	0.81
1:A:488:ALA:HA	1:B:870:ARG:HH12	1.46	0.80
1:A:544:TYR:HE1	1:A:595:VAL:HA	1.46	0.80
1:A:751:ASP:O	1:A:754:MET:N	2.13	0.80
2:D:345:SER:HB2	2:D:349:LYS:HB2	1.63	0.80
2:E:357:VAL:CG1	2:E:358:MSE:H	1.78	0.80
1:A:32:ASN:HB3	1:A:35:THR:HB	1.63	0.80
1:B:485:ALA:O	1:B:487:VAL:N	2.12	0.80
2:C:361:ASP:O	2:C:361:ASP:CG	2.24	0.80
1:A:377:ASN:HD22	1:A:378:PRO:N	1.79	0.80
1:B:105:ARG:HB3	1:B:106:PRO:CD	2.12	0.80
1:B:388:MET:HG2	1:B:427:THR:HG23	1.60	0.80
2:E:357:VAL:CG1	2:E:372:LYS:CG	2.59	0.80
1:A:808:GLU:O	1:A:810:HIS:N	2.15	0.80
1:A:516:ARG:HD3	1:A:524:LEU:CD1	2.13	0.79
1:A:51:GLN:HB2	1:A:105:ARG:HG3	1.63	0.79
1:B:483:GLU:HA	1:B:486:ASP:OD2	1.82	0.79
1:B:736:LEU:HB3	1:B:793:ARG:HH12	1.48	0.79
1:B:811:THR:HG22	1:B:813:GLY:H	1.46	0.79
1:B:777:LYS:HA	1:B:787:VAL:HG21	1.63	0.79
1:A:353:MET:CG	1:A:392:SER:HB2	2.13	0.79
2:E:398:ASN:HD21	2:E:401:ASN:HA	1.46	0.78
1:A:555:MET:SD	1:A:603:ILE:HG23	2.23	0.78
1:B:777:LYS:CA	1:B:787:VAL:CG2	2.60	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:ARG:NH1	1:B:28:ALA:H	1.81	0.78
1:B:327:THR:O	1:B:330:LEU:HB2	1.82	0.78
1:B:153:ALA:O	1:B:157:ILE:HG13	1.82	0.78
1:B:320:GLN:C	1:B:320:GLN:HE21	1.92	0.78
1:A:736:LEU:HD13	1:A:793:ARG:HE	1.50	0.77
1:B:27:ARG:NH1	1:B:28:ALA:HA	1.98	0.77
1:B:402:LEU:O	1:B:406:VAL:HG23	1.84	0.77
1:A:353:MET:HG2	1:A:392:SER:HB2	1.66	0.77
1:A:516:ARG:HD3	1:A:524:LEU:HD11	1.67	0.77
1:A:640:GLY:O	1:A:680:ALA:HB1	1.85	0.76
1:B:483:GLU:O	1:B:486:ASP:OD2	2.03	0.76
1:B:777:LYS:HD2	1:B:780:GLN:HE21	1.50	0.76
1:B:402:LEU:HD23	1:B:439:LEU:HD11	1.67	0.76
1:B:834:LEU:HB2	1:B:872:LEU:HD13	1.67	0.76
1:A:533:MET:HG2	1:A:590:ASN:HD22	1.50	0.76
1:B:831:LYS:HA	1:B:872:LEU:HD22	1.66	0.76
1:A:478:ALA:HB2	1:A:535:ILE:HD12	1.67	0.75
1:A:397:PRO:HB2	1:A:402:LEU:HD11	1.67	0.75
1:A:707:ARG:HG3	1:A:707:ARG:HH11	1.52	0.75
1:A:486:ASP:O	1:A:489:ASP:HB3	1.86	0.75
2:F:364:MSE:SE	2:F:365:HIS:ND1	2.68	0.75
1:A:102:GLU:N	1:A:106:PRO:HG2	1.98	0.75
1:B:256:MET:HA	1:B:260:LEU:HB2	1.67	0.75
1:B:169:LYS:C	1:B:171:ASN:H	1.95	0.75
1:B:261:PHE:CE1	1:B:265:ILE:HD11	2.22	0.74
1:B:753:ASP:OD1	2:E:372:LYS:NZ	2.19	0.74
1:A:34:PRO:HB3	1:A:83:ILE:HD11	1.68	0.74
1:A:489:ASP:CG	1:A:494:PRO:HD3	2.12	0.74
1:B:707:ARG:NH2	1:B:753:ASP:O	2.21	0.74
1:A:80:TRP:HE1	1:A:120:GLU:CG	2.00	0.74
1:B:99:LEU:HB2	1:B:146:MET:HE1	1.69	0.74
1:A:516:ARG:C	1:A:518:ASP:H	1.95	0.74
1:A:88:ARG:HD2	1:A:120:GLU:OE2	1.88	0.73
1:B:105:ARG:HB3	1:B:106:PRO:HD3	1.70	0.73
1:A:740:GLN:O	1:A:744:GLN:HG2	1.88	0.73
1:B:444:ILE:HA	1:B:449:LEU:HD13	1.68	0.73
2:F:365:HIS:HD2	2:F:367:SER:CB	1.98	0.73
2:D:370:LEU:N	2:D:370:LEU:CD2	2.52	0.73
2:E:357:VAL:HG11	2:E:372:LYS:HG2	1.68	0.73
1:A:96:LEU:HD11	1:A:132:GLN:HG2	1.70	0.73
1:B:40:LEU:HD23	1:B:43:VAL:HB	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:682:GLN:O	1:A:684:ASN:N	2.22	0.72
1:B:37:LEU:HD13	1:B:61:ILE:HG12	1.70	0.72
1:A:608:MET:HE1	1:A:632:VAL:HG22	1.69	0.72
1:A:667:CYS:O	1:A:671:VAL:HG23	1.88	0.72
1:B:27:ARG:O	1:B:29:ALA:N	2.19	0.72
1:B:353:MET:HG2	1:B:392:SER:HB2	1.72	0.72
1:A:495:ALA:O	1:A:542:ASP:HB3	1.90	0.72
1:A:756:ASP:CG	2:C:371:ARG:HH22	1.96	0.72
1:B:558:LEU:O	1:B:562:LEU:HD13	1.88	0.72
1:A:492:GLU:O	1:A:493:GLU:HG3	1.88	0.72
2:E:358:MSE:CE	2:E:372:LYS:HG2	2.19	0.72
1:B:679:ARG:CZ	2:F:343:ARG:N	2.53	0.72
1:A:417:MET:HG3	1:A:455:CYS:SG	2.29	0.72
1:A:551:THR:HG22	1:A:555:MET:HE2	1.72	0.72
1:A:544:TYR:CE1	1:A:595:VAL:HA	2.25	0.72
1:A:790:VAL:HG23	1:A:829:PHE:HZ	1.54	0.71
1:A:800:PHE:HA	1:A:803:HIS:HD2	1.53	0.71
1:B:667:CYS:O	1:B:671:VAL:HG23	1.89	0.71
1:B:174:LEU:HD13	1:B:205:THR:HG21	1.72	0.71
1:B:663:GLU:O	1:B:663:GLU:HG3	1.90	0.71
1:B:851:ARG:HH12	1:B:866:THR:HG21	1.56	0.71
1:A:682:GLN:O	1:A:685:ILE:N	2.16	0.71
1:B:126:TRP:N	1:B:127:PRO:HD3	2.06	0.71
1:A:551:THR:HG21	1:A:603:ILE:HD13	1.71	0.71
1:A:608:MET:HE3	1:A:635:LEU:HD23	1.70	0.71
2:F:365:HIS:CD2	2:F:368:GLY:H	2.07	0.71
1:A:172:GLU:H	1:A:172:GLU:CD	1.99	0.71
1:A:173:ILE:O	1:A:177:ILE:HG13	1.91	0.71
1:A:682:GLN:HA	1:A:723:ALA:HB1	1.73	0.71
1:B:162:ASP:O	1:B:165:GLN:HG3	1.90	0.71
1:B:430:TRP:CZ2	1:B:434:ARG:HD2	2.25	0.71
1:A:410:MET:HE1	1:A:452:LEU:HD13	1.72	0.71
1:B:736:LEU:HB3	1:B:793:ARG:NH1	2.06	0.70
1:A:83:ILE:HG12	1:A:84:ASP:H	1.56	0.70
1:B:65:LEU:CB	1:B:69:ASP:HB2	2.21	0.70
1:A:51:GLN:HB2	1:A:105:ARG:CG	2.19	0.70
1:A:36:PHE:O	1:A:40:LEU:HG	1.91	0.70
1:B:705:VAL:HB	1:B:710:LYS:NZ	2.05	0.70
2:F:368:GLY:O	2:F:372:LYS:HB2	1.92	0.70
1:A:5:THR:O	1:A:9:LYS:HG2	1.90	0.70
1:A:80:TRP:O	1:A:83:ILE:HG22	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:ARG:NH2	1:B:275:VAL:HG11	2.06	0.70
1:B:374:HIS:HB3	1:B:382:TYR:HB3	1.73	0.70
2:F:347:ASN:O	2:F:348:ASP:CB	2.32	0.70
1:A:51:GLN:CB	1:A:105:ARG:HG3	2.20	0.70
1:A:700:LEU:CD2	1:A:710:LYS:HG3	2.21	0.70
1:B:418:LYS:NZ	1:B:458:GLU:HG2	2.05	0.70
1:A:568:ILE:HD12	1:A:574:ARG:NH1	2.06	0.70
1:B:696:LEU:HD22	1:B:713:ILE:HG23	1.74	0.70
1:A:377:ASN:HD22	1:A:377:ASN:C	1.98	0.69
1:B:758:LEU:CD2	1:B:762:ARG:HE	2.05	0.69
2:C:346:ILE:O	2:C:350:ILE:HG12	1.92	0.69
1:B:467:ALA:O	1:B:470:VAL:HG12	1.92	0.69
1:A:174:LEU:O	1:A:178:ILE:HG13	1.92	0.69
1:A:444:ILE:HD12	1:A:481:ALA:HA	1.72	0.69
1:A:83:ILE:HG12	1:A:84:ASP:N	2.08	0.69
1:B:44:LEU:HD22	1:B:54:ARG:HB3	1.74	0.69
1:B:580:LEU:HD23	1:B:584:LEU:HG	1.75	0.69
1:B:410:MET:CE	1:B:452:LEU:HD13	2.23	0.69
2:D:370:LEU:O	2:D:374:ILE:CD1	2.39	0.68
1:A:84:ASP:HB3	1:A:87:ALA:CB	2.21	0.68
1:A:808:GLU:C	1:A:810:HIS:H	1.99	0.68
1:B:483:GLU:CA	1:B:486:ASP:OD2	2.41	0.68
1:A:62:LYS:O	1:A:66:THR:HG22	1.94	0.68
1:A:514:THR:CG2	1:A:557:ARG:HH12	2.05	0.68
1:B:575:ILE:HG22	1:B:575:ILE:O	1.92	0.68
1:B:588:LEU:HD21	1:B:607:VAL:HG23	1.75	0.68
1:B:49:ASN:HB2	1:B:54:ARG:HD2	1.74	0.68
2:F:403:LEU:H	2:F:403:LEU:HD23	1.59	0.68
1:B:136:ASN:ND2	1:B:146:MET:HE2	2.08	0.68
1:B:758:LEU:HD21	1:B:762:ARG:HE	1.58	0.68
2:D:403:LEU:HD12	2:D:403:LEU:H	1.59	0.68
1:A:88:ARG:HH12	1:A:92:LYS:HD3	1.59	0.68
1:B:122:PRO:HG3	1:B:165:GLN:HE22	1.59	0.68
1:B:591:VAL:O	1:B:595:VAL:HG13	1.94	0.68
1:A:174:LEU:HD22	1:A:178:ILE:HD11	1.76	0.68
1:A:830:GLY:O	1:A:872:LEU:HD13	1.94	0.68
1:A:142:SER:HB3	1:A:146:MET:HG2	1.76	0.67
2:E:358:MSE:CA	2:E:372:LYS:HE2	2.23	0.67
1:A:2:GLU:HB2	1:A:5:THR:OG1	1.94	0.67
1:A:752:PHE:C	1:A:754:MET:N	2.50	0.67
1:A:870:ARG:NH2	1:B:487:VAL:CG1	2.57	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:MET:HG3	1:B:255:TYR:CE1	2.28	0.67
1:B:557:ARG:O	1:B:561:VAL:HG23	1.95	0.67
2:E:354:LYS:CE	2:E:361:ASP:HA	2.23	0.67
1:A:644:LEU:CD2	1:A:684:ASN:HD21	2.07	0.67
1:A:80:TRP:HE1	1:A:120:GLU:CD	2.03	0.67
2:E:358:MSE:HE2	2:E:372:LYS:CD	2.25	0.67
1:A:700:LEU:HD22	1:A:710:LYS:HE3	1.76	0.67
1:B:21:ALA:HA	1:B:24:PHE:HB3	1.78	0.66
1:B:130:ILE:CG2	1:B:169:LYS:HD2	2.24	0.66
1:B:244:ILE:HG22	1:B:252:MET:HE3	1.76	0.66
1:B:445:ASN:O	1:B:447:VAL:N	2.28	0.66
1:B:834:LEU:HD21	1:B:873:LYS:HZ3	1.60	0.66
1:B:27:ARG:NH1	1:B:28:ALA:N	2.42	0.66
1:A:170:SER:O	1:A:174:LEU:HB2	1.96	0.66
1:A:328:GLN:O	1:A:331:THR:HB	1.95	0.66
1:B:244:ILE:HG22	1:B:252:MET:CE	2.25	0.66
1:B:615:PHE:HB3	1:B:653:PHE:CD1	2.30	0.66
1:B:851:ARG:NH1	1:B:866:THR:HG21	2.10	0.66
1:B:31:GLU:C	1:B:34:PRO:HD2	2.21	0.66
2:E:357:VAL:CG1	2:E:372:LYS:HE2	2.04	0.66
1:A:14:ASP:HB3	1:A:17:GLU:HB3	1.78	0.65
1:A:665:GLN:NE2	2:C:363:LYS:O	2.29	0.65
2:E:357:VAL:HG13	2:E:372:LYS:HE3	1.73	0.65
1:A:135:ALA:HA	1:A:138:THR:CG2	2.25	0.65
1:A:339:ASP:HB3	1:A:341:ASP:HB2	1.77	0.65
1:B:800:PHE:O	1:B:804:ILE:HG13	1.97	0.65
2:C:361:ASP:OD1	2:C:361:ASP:C	2.39	0.65
1:B:790:VAL:HG13	1:B:829:PHE:HZ	1.61	0.65
1:B:367:VAL:HG12	1:B:371:ILE:HD11	1.79	0.65
1:A:870:ARG:HE	1:B:487:VAL:HG11	0.83	0.65
1:A:15:ARG:NH1	1:A:18:LEU:HD12	2.11	0.65
1:A:494:PRO:O	1:A:541:LYS:HG2	1.97	0.65
1:A:511:LEU:O	1:A:514:THR:HB	1.96	0.65
1:B:287:CYS:HB2	1:B:354:LEU:CD1	2.27	0.65
1:B:511:LEU:HD22	1:B:553:VAL:HG11	1.78	0.65
1:B:580:LEU:HD23	1:B:580:LEU:O	1.97	0.65
1:A:516:ARG:C	1:A:518:ASP:N	2.54	0.65
2:C:388:ARG:HG3	2:D:387:LEU:HD11	1.78	0.65
1:B:462:ALA:H	1:B:516:ARG:HH12	1.45	0.64
2:F:396:LEU:HD13	2:F:397:ALA:N	2.12	0.64
1:B:532:LEU:O	1:B:535:ILE:HG22	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:758:LEU:O	1:B:762:ARG:HG3	1.96	0.64
1:A:867:LYS:HG3	1:A:870:ARG:HH22	1.61	0.64
1:B:169:LYS:C	1:B:171:ASN:N	2.54	0.64
1:B:568:ILE:CD1	1:B:574:ARG:HH11	2.09	0.64
1:A:544:TYR:N	1:A:545:PRO:HD2	2.13	0.64
1:A:748:ASP:C	1:A:750:SER:H	2.05	0.64
1:A:756:ASP:O	1:A:760:GLU:HG3	1.98	0.64
1:B:663:GLU:OE2	1:B:665:GLN:HB2	1.94	0.64
1:B:73:LYS:C	1:B:75:GLN:H	2.06	0.64
1:B:40:LEU:HD23	1:B:40:LEU:O	1.98	0.63
1:A:15:ARG:C	1:A:15:ARG:HD3	2.23	0.63
1:B:780:GLN:HE22	1:B:827:THR:CG2	2.12	0.63
1:B:40:LEU:HD22	1:B:44:LEU:HG	1.79	0.63
1:B:427:THR:HG22	1:B:427:THR:O	1.98	0.63
2:C:349:LYS:HZ2	2:D:367:SER:HB2	1.62	0.63
1:A:81:LEU:HD13	1:A:88:ARG:HD3	1.81	0.63
1:B:174:LEU:CD1	1:B:205:THR:HG21	2.29	0.63
1:B:496:THR:HG23	1:B:500:SER:OG	1.99	0.63
1:A:338:ASP:CA	1:A:465:ARG:HH22	2.08	0.62
1:A:218:ILE:O	1:A:222:VAL:HG23	1.99	0.62
1:A:489:ASP:HB2	1:A:494:PRO:HG3	1.80	0.62
1:A:603:ILE:HG22	1:A:607:VAL:HG23	1.80	0.62
1:B:27:ARG:NH1	1:B:28:ALA:CA	2.62	0.62
1:B:125:GLN:C	1:B:127:PRO:HD3	2.24	0.62
1:B:660:ASN:ND2	1:B:663:GLU:H	1.97	0.62
1:B:752:PHE:HE2	2:E:372:LYS:HZ2	1.45	0.62
2:C:357:VAL:HG23	2:C:358:MSE:N	2.14	0.62
1:B:838:GLU:C	1:B:840:ARG:H	2.06	0.62
2:C:358:MSE:CE	2:C:364:MSE:SE	2.97	0.62
2:C:366:LYS:O	2:C:367:SER:OG	2.17	0.62
1:A:650:PHE:C	1:A:652:PRO:HD2	2.24	0.62
1:A:686:LEU:HD11	1:A:727:GLU:HG2	1.80	0.62
1:B:327:THR:HA	1:B:330:LEU:CD1	2.27	0.62
2:C:374:ILE:HG12	2:D:353:LEU:HD13	1.81	0.62
2:C:395:LYS:HB3	2:C:395:LYS:NZ	2.14	0.62
1:B:132:GLN:HE21	1:B:132:GLN:HA	1.64	0.62
1:B:286:VAL:O	1:B:290:GLU:HG3	1.99	0.62
1:B:857:LYS:O	1:B:861:LEU:HB3	1.97	0.62
2:C:363:LYS:O	2:C:363:LYS:HG3	2.00	0.62
1:B:326:LEU:O	1:B:330:LEU:HG	1.99	0.62
1:B:590:ASN:N	1:B:590:ASN:HD22	1.95	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:834:LEU:HD22	1:B:872:LEU:HB3	1.80	0.62
1:A:444:ILE:CD1	1:A:481:ALA:HA	2.29	0.62
1:B:479:GLU:HA	1:B:538:ASN:HD22	1.63	0.62
2:F:377:ILE:O	2:F:381:GLN:HG3	2.00	0.62
1:A:514:THR:HG21	1:A:529:TYR:OH	2.00	0.62
1:B:343:ASN:ND2	1:B:345:CYS:H	1.97	0.62
1:B:758:LEU:HD11	1:B:762:ARG:NH2	2.15	0.62
2:C:367:SER:HB3	2:D:347:ASN:HB2	1.82	0.62
1:B:449:LEU:HG	1:B:453:LEU:HD12	1.81	0.61
1:B:514:THR:HG21	1:B:557:ARG:NH1	2.10	0.61
2:E:346:ILE:O	2:E:350:ILE:HG12	2.00	0.61
1:A:84:ASP:C	1:A:86:ASN:H	2.04	0.61
2:E:391:ASN:O	2:E:395:LYS:HB2	2.00	0.61
1:A:129:LEU:HD11	1:A:133:LEU:HD11	1.83	0.61
1:B:406:VAL:HG21	1:B:439:LEU:HD13	1.82	0.61
1:B:777:LYS:CD	1:B:780:GLN:HE21	2.12	0.61
2:C:349:LYS:NZ	2:D:367:SER:HB2	2.15	0.61
1:B:319:LEU:O	1:B:323:VAL:HG23	2.01	0.61
1:A:851:ARG:C	1:A:853:SER:H	2.06	0.61
1:A:102:GLU:HB3	1:A:106:PRO:CD	2.27	0.61
1:B:607:VAL:HG13	1:B:608:MET:H	1.65	0.61
1:A:42:ARG:HA	1:A:94:TYR:CE1	2.36	0.61
1:A:368:LEU:HD11	1:A:405:LEU:HD21	1.83	0.61
1:A:797:ILE:C	1:A:799:SER:N	2.58	0.61
1:B:184:GLU:O	1:B:185:GLU:C	2.42	0.61
1:B:468:SER:C	1:B:470:VAL:H	2.09	0.61
1:B:603:ILE:HG22	1:B:607:VAL:HG12	1.82	0.61
1:A:242:VAL:HG11	1:A:281:GLU:HG2	1.83	0.61
1:A:488:ALA:CA	1:B:870:ARG:HH12	2.14	0.61
1:B:73:LYS:HG2	1:B:77:GLN:HE21	1.65	0.61
1:A:339:ASP:C	1:A:341:ASP:H	2.07	0.60
1:A:338:ASP:HA	1:A:465:ARG:NH2	2.11	0.60
1:B:544:TYR:N	1:B:545:PRO:HD2	2.16	0.60
1:B:35:THR:HG22	1:B:35:THR:O	2.01	0.60
1:B:194:ALA:O	1:B:197:ALA:HB3	2.01	0.60
2:C:354:LYS:HG2	2:C:369:VAL:HG21	1.83	0.60
1:A:402:LEU:O	1:A:406:VAL:HG23	2.00	0.60
1:B:261:PHE:O	1:B:265:ILE:HG12	2.00	0.60
1:A:796:PHE:O	1:A:799:SER:CB	2.35	0.60
1:A:870:ARG:CZ	1:B:487:VAL:HG12	2.30	0.60
1:A:576:GLN:HA	1:A:576:GLN:NE2	2.07	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:374:ILE:HG22	2:D:378:LYS:HE2	1.83	0.60
1:A:533:MET:CG	1:A:590:ASN:HD22	2.15	0.60
1:B:215:ARG:HG2	1:B:255:TYR:OH	2.02	0.60
1:B:399:PRO:O	1:B:403:LYS:HG3	2.02	0.60
1:B:616:GLN:HG2	1:B:653:PHE:CZ	2.37	0.60
1:B:754:MET:HA	1:B:757:TYR:HB3	1.82	0.60
1:A:377:ASN:HD22	1:A:379:ASP:H	1.49	0.60
1:A:492:GLU:CD	2:D:343:ARG:NH1	2.60	0.60
1:B:163:PRO:HG3	1:B:204:PHE:CD1	2.37	0.60
1:B:663:GLU:HG3	1:B:666:VAL:HG23	1.84	0.59
1:B:133:LEU:O	1:B:150:THR:HG21	2.01	0.59
1:A:614:MET:O	1:A:618:THR:HB	2.02	0.59
1:A:668:LEU:HD21	1:A:709:VAL:HA	1.84	0.59
1:B:335:GLU:CD	1:B:380:TRP:HZ2	2.09	0.59
1:A:120:GLU:O	1:A:125:GLN:HB3	2.02	0.59
1:A:287:CYS:CB	1:A:354:LEU:HD13	2.32	0.59
1:A:560:GLN:HA	1:A:563:GLN:HE21	1.67	0.59
1:B:450:ALA:HB3	1:B:451:PRO:HD3	1.84	0.59
1:B:7:LEU:HD11	1:B:36:PHE:HZ	1.67	0.59
1:B:30:VAL:HG12	1:B:31:GLU:N	2.17	0.59
1:B:496:THR:HG23	1:B:500:SER:CB	2.32	0.59
1:B:430:TRP:CA	1:B:469:ASN:HD22	2.13	0.59
2:E:366:LYS:O	2:E:367:SER:HB3	2.03	0.59
1:A:125:GLN:OE1	1:A:126:TRP:HB2	2.03	0.59
1:B:78:GLN:OE1	1:B:81:LEU:HD12	2.03	0.59
1:A:363:ILE:HG23	1:A:364:VAL:N	2.17	0.59
2:D:364:MSE:SE	2:D:368:GLY:O	2.71	0.59
1:A:222:VAL:O	1:A:226:THR:HG23	2.02	0.59
1:A:414:ILE:O	1:A:417:MET:HB2	2.03	0.59
1:A:544:TYR:CZ	1:A:596:GLN:HG3	2.38	0.59
1:A:661:TYR:CE1	1:A:704:ASN:HB2	2.37	0.59
2:F:392:MSE:C	2:F:394:LEU:H	2.10	0.59
1:B:28:ALA:C	1:B:30:VAL:H	2.10	0.58
1:B:487:VAL:HG12	1:B:488:ALA:N	2.18	0.58
1:A:831:LYS:C	1:A:833:VAL:H	2.09	0.58
1:B:211:LYS:HD2	1:B:214:GLU:OE2	2.03	0.58
1:B:483:GLU:O	1:B:486:ASP:CG	2.46	0.58
1:B:708:SER:C	1:B:711:PRO:HD2	2.27	0.58
2:D:358:MSE:SE	2:D:372:LYS:HD2	2.53	0.58
1:A:29:ALA:HB1	1:A:33:LEU:HD13	1.85	0.58
1:B:588:LEU:O	1:B:591:VAL:HG22	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:357:VAL:CG1	2:E:372:LYS:HG3	2.18	0.58
1:A:120:GLU:HB3	1:A:125:GLN:OE1	2.04	0.58
1:A:303:GLN:O	1:A:304:GLY:C	2.44	0.58
1:A:558:LEU:HD11	1:A:614:MET:CE	2.32	0.58
1:A:43:VAL:HG13	1:A:49:ASN:ND2	2.18	0.58
1:B:444:ILE:HD12	1:B:444:ILE:N	2.19	0.58
1:A:265:ILE:O	1:A:269:LYS:HD2	2.04	0.58
1:A:797:ILE:C	1:A:799:SER:H	2.11	0.58
1:A:870:ARG:NH2	1:B:487:VAL:HG13	2.18	0.58
2:C:396:LEU:C	2:C:398:ASN:H	2.09	0.58
1:B:630:MET:HE3	1:B:630:MET:HA	1.86	0.58
1:A:661:TYR:CB	1:A:705:VAL:HG12	2.33	0.58
1:B:27:ARG:C	1:B:29:ALA:H	2.07	0.58
1:B:426:ASP:C	1:B:428:THR:H	2.10	0.58
1:A:682:GLN:O	1:A:683:SER:C	2.46	0.58
1:B:660:ASN:HD21	1:B:663:GLU:H	1.49	0.58
1:B:811:THR:HB	1:B:814:VAL:HG23	1.84	0.58
1:B:607:VAL:HG13	1:B:608:MET:N	2.19	0.57
1:A:117:ALA:C	1:A:119:ALA:H	2.12	0.57
1:B:411:PRO:HG3	1:B:448:TYR:CE1	2.39	0.57
1:B:483:GLU:CA	1:B:486:ASP:CG	2.77	0.57
1:B:748:ASP:OD2	1:B:754:MET:CE	2.32	0.57
2:C:346:ILE:CD1	2:D:367:SER:HB3	2.34	0.57
2:C:395:LYS:O	2:C:399:GLN:HB2	2.04	0.57
1:A:525:ARG:HG2	1:A:525:ARG:HH11	1.69	0.57
1:A:784:HIS:HD2	1:A:785:PRO:CD	2.02	0.57
1:B:128:GLU:O	1:B:131:PRO:HG2	2.04	0.57
1:B:394:LEU:HB3	1:B:438:LEU:HD12	1.86	0.57
1:B:694:GLN:HG3	1:B:698:GLU:OE2	2.05	0.57
1:A:800:PHE:HA	1:A:803:HIS:CD2	2.37	0.57
1:B:618:THR:C	1:B:620:GLY:H	2.10	0.57
2:E:377:ILE:HG21	2:F:356:LEU:HD13	1.86	0.57
2:F:389:GLN:HE21	2:F:389:GLN:C	2.13	0.57
1:A:756:ASP:OD1	2:C:371:ARG:NH2	2.37	0.57
1:B:367:VAL:O	1:B:371:ILE:HG13	2.05	0.57
1:B:660:ASN:C	1:B:662:ALA:H	2.12	0.57
1:B:779:ASP:OD1	1:B:779:ASP:N	2.38	0.57
1:A:54:ARG:HH22	1:A:101:THR:CG2	2.17	0.57
1:B:27:ARG:HH12	1:B:28:ALA:HA	1.68	0.57
1:B:552:LEU:O	1:B:555:MET:HB3	2.05	0.57
1:A:464:PRO:O	1:A:468:SER:HB2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:ALA:C	1:A:486:ASP:H	2.13	0.57
1:B:298:SER:O	1:B:301:ALA:HB3	2.04	0.57
1:B:377:ASN:HD22	1:B:378:PRO:N	2.03	0.57
1:B:756:ASP:HA	1:B:759:ASN:HD22	1.68	0.57
1:B:343:ASN:HB2	1:B:344:PRO:HD2	1.86	0.57
2:F:365:HIS:O	2:F:369:VAL:HG23	2.04	0.57
1:A:516:ARG:O	1:A:518:ASP:N	2.38	0.56
1:A:808:GLU:C	1:A:810:HIS:N	2.61	0.56
1:B:244:ILE:CG2	1:B:252:MET:CE	2.83	0.56
1:B:403:LYS:N	1:B:404:PRO:HD2	2.20	0.56
2:C:377:ILE:O	2:C:381:GLN:HG3	2.05	0.56
1:A:33:LEU:HB3	1:A:34:PRO:HD3	1.87	0.56
1:A:77:GLN:O	1:A:80:TRP:HB3	2.04	0.56
1:A:287:CYS:HB2	1:A:354:LEU:HD13	1.87	0.56
1:A:762:ARG:HD3	1:A:800:PHE:CZ	2.39	0.56
1:A:630:MET:HA	1:A:630:MET:HE2	1.87	0.56
1:A:802:ASP:O	1:A:803:HIS:C	2.47	0.56
1:B:485:ALA:C	1:B:487:VAL:N	2.62	0.56
1:B:598:GLN:O	1:B:602:GLN:HG3	2.05	0.56
1:B:681:LEU:O	1:B:684:ASN:HB2	2.06	0.56
1:B:805:ALA:HB2	1:B:846:LEU:HD22	1.87	0.56
1:A:618:THR:HG21	1:A:624:VAL:HG21	1.88	0.56
1:A:797:ILE:O	1:A:799:SER:N	2.39	0.56
1:A:109:ALA:O	1:A:113:VAL:HG23	2.05	0.56
1:A:122:PRO:HB3	1:A:165:GLN:HE22	1.71	0.56
1:B:616:GLN:HG2	1:B:653:PHE:HZ	1.71	0.56
1:B:659:LYS:HA	1:B:659:LYS:CE	2.17	0.56
1:A:681:LEU:O	1:A:682:GLN:CB	2.52	0.56
1:B:515:ASP:O	1:B:516:ARG:C	2.48	0.56
1:A:26:GLU:C	1:A:28:ALA:H	2.14	0.56
1:B:33:LEU:HA	1:B:36:PHE:CB	2.33	0.56
1:B:331:THR:C	1:B:333:GLN:OE1	2.49	0.56
1:B:804:ILE:C	1:B:806:GLY:H	2.13	0.56
1:B:4:ILE:HD12	1:B:4:ILE:N	2.21	0.56
1:B:360:GLU:O	1:B:362:ASP:N	2.39	0.56
1:B:663:GLU:CG	1:B:666:VAL:HG23	2.35	0.56
1:A:353:MET:HG3	1:A:392:SER:HB2	1.87	0.56
1:A:492:GLU:O	1:A:493:GLU:CG	2.54	0.56
1:A:830:GLY:O	1:A:872:LEU:HD22	2.06	0.56
1:B:593:ARG:HA	1:B:593:ARG:HH11	1.70	0.56
2:E:353:LEU:O	2:E:357:VAL:HG23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:VAL:HG22	1:B:91:VAL:CG2	2.36	0.56
1:B:525:ARG:HH12	1:B:580:LEU:HD12	1.69	0.56
1:B:681:LEU:HD23	1:B:681:LEU:N	2.20	0.56
1:B:784:HIS:HE2	1:B:786:ASP:CG	2.14	0.56
2:E:357:VAL:CG1	2:E:358:MSE:N	2.45	0.56
2:E:398:ASN:C	2:E:398:ASN:HD22	2.13	0.56
1:A:464:PRO:HB2	1:A:522:ASN:HD22	1.69	0.55
1:A:762:ARG:NH1	1:A:804:ILE:HG12	2.21	0.55
1:A:801:ILE:HD11	1:A:843:ILE:CD1	2.36	0.55
1:B:377:ASN:HD22	1:B:377:ASN:C	2.14	0.55
1:B:18:LEU:C	1:B:18:LEU:HD23	2.30	0.55
1:A:15:ARG:HD3	1:A:15:ARG:O	2.05	0.55
1:A:740:GLN:HG3	1:A:796:PHE:CZ	2.41	0.55
2:C:346:ILE:HD13	2:D:367:SER:HB3	1.87	0.55
2:C:394:LEU:O	2:D:394:LEU:HD13	2.06	0.55
1:A:580:LEU:O	1:A:584:LEU:HG	2.06	0.55
1:A:762:ARG:HD2	1:A:800:PHE:CE1	2.41	0.55
1:B:740:GLN:HG3	1:B:796:PHE:CZ	2.42	0.55
1:A:790:VAL:HG23	1:A:829:PHE:CZ	2.40	0.55
1:A:810:HIS:CD2	1:A:815:VAL:CG2	2.89	0.55
1:B:483:GLU:C	1:B:486:ASP:OD2	2.50	0.55
1:B:756:ASP:CA	1:B:759:ASN:HB2	2.35	0.55
2:E:351:ILE:HD12	2:E:352:GLU:N	2.21	0.55
1:A:151:LEU:HD13	1:A:194:ALA:HB2	1.89	0.55
1:A:489:ASP:HA	1:A:494:PRO:HA	1.88	0.55
1:B:21:ALA:O	1:B:25:LEU:HG	2.06	0.55
1:B:133:LEU:HD22	1:B:150:THR:HG23	1.88	0.55
1:B:343:ASN:HD22	1:B:345:CYS:H	1.55	0.55
1:B:118:CYS:O	1:B:122:PRO:HG2	2.07	0.55
1:B:123:VAL:HG12	1:B:123:VAL:O	2.06	0.55
1:B:834:LEU:HD22	1:B:872:LEU:CB	2.36	0.55
1:A:801:ILE:HD11	1:A:843:ILE:HD13	1.89	0.55
1:B:83:ILE:HB	1:B:88:ARG:HD3	1.88	0.55
1:B:377:ASN:ND2	1:B:379:ASP:H	2.04	0.55
1:B:468:SER:HB3	2:E:343:ARG:NH2	2.20	0.55
1:B:543:CYS:C	1:B:545:PRO:HD2	2.32	0.55
1:B:599:ASP:HA	1:B:602:GLN:HB2	1.88	0.55
1:A:102:GLU:HG3	1:A:103:THR:H	1.70	0.55
1:B:161:ILE:HG23	1:B:165:GLN:OE1	2.07	0.55
1:B:647:MET:O	1:B:651:LYS:HG3	2.07	0.55
2:E:358:MSE:HE2	2:E:372:LYS:HD3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:870:ARG:HH21	1:B:487:VAL:HG13	1.72	0.54
1:B:596:GLN:HE21	1:B:598:GLN:HG3	1.72	0.54
2:C:357:VAL:HG23	2:C:358:MSE:H	1.72	0.54
1:A:73:LYS:C	1:A:75:GLN:H	2.15	0.54
1:A:488:ALA:HA	1:B:870:ARG:NH1	2.21	0.54
1:A:516:ARG:O	1:A:519:GLY:N	2.27	0.54
1:B:129:LEU:HD11	1:B:133:LEU:HD11	1.89	0.54
1:B:394:LEU:HD12	1:B:434:ARG:HB3	1.88	0.54
1:B:429:ALA:HB2	1:B:466:VAL:HG13	1.89	0.54
1:A:286:VAL:O	1:A:290:GLU:HG3	2.08	0.54
1:B:86:ASN:HA	1:B:89:ARG:HH12	1.72	0.54
1:B:182:ARG:NE	1:B:184:GLU:HB2	2.23	0.54
1:B:390:PHE:O	1:B:393:ILE:HG12	2.07	0.54
1:B:426:ASP:C	1:B:428:THR:N	2.66	0.54
2:C:358:MSE:HG2	2:C:372:LYS:HD2	1.90	0.54
2:F:348:ASP:OD2	2:F:351:ILE:HG13	2.07	0.54
1:B:24:PHE:HE1	1:B:27:ARG:HE	1.54	0.54
1:A:42:ARG:HA	1:A:94:TYR:CZ	2.42	0.54
1:A:84:ASP:C	1:A:86:ASN:N	2.65	0.54
1:A:616:GLN:O	1:A:619:ALA:HB2	2.07	0.54
1:B:182:ARG:HG3	1:B:184:GLU:HB2	1.88	0.54
2:E:367:SER:HA	2:E:370:LEU:HB2	1.90	0.54
1:A:603:ILE:HG22	1:A:607:VAL:CG2	2.38	0.54
1:B:268:MET:HE2	1:B:283:TRP:CD1	2.43	0.54
1:A:302:GLU:O	1:A:303:GLN:HG3	2.08	0.54
1:A:714:LEU:HD12	1:A:714:LEU:H	1.73	0.54
1:B:150:THR:O	1:B:154:ILE:HG13	2.08	0.54
1:B:380:TRP:CZ2	1:B:381:ARG:NH1	2.75	0.54
1:B:753:ASP:OD1	2:E:358:MSE:HA	2.07	0.54
1:A:245:MET:HG3	1:A:282:PHE:CE1	2.42	0.54
1:B:154:ILE:HA	1:B:157:ILE:HD12	1.89	0.54
1:B:264:THR:HG21	1:B:282:PHE:CD2	2.42	0.54
1:B:375:ILE:O	1:B:383:ARG:HG2	2.08	0.54
1:A:592:LEU:O	1:A:595:VAL:HG22	2.08	0.54
2:F:370:LEU:C	2:F:372:LYS:H	2.16	0.54
1:B:430:TRP:CE2	1:B:434:ARG:HD2	2.43	0.54
1:B:507:VAL:HG11	1:B:550:THR:OG1	2.08	0.54
1:B:544:TYR:O	1:B:545:PRO:C	2.50	0.54
1:B:777:LYS:CA	1:B:787:VAL:HG21	2.34	0.54
1:A:4:ILE:HG22	1:A:4:ILE:O	2.07	0.53
1:A:117:ALA:O	1:A:121:ILE:HG13	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:GLU:HA	1:A:314:TYR:OH	2.07	0.53
1:A:729:LYS:HD3	1:A:789:LEU:HD13	1.90	0.53
1:B:174:LEU:HD13	1:B:205:THR:CG2	2.37	0.53
1:B:548:GLN:O	1:B:551:THR:HB	2.08	0.53
1:A:478:ALA:HB2	1:A:535:ILE:CD1	2.36	0.53
1:A:626:GLU:HB2	1:A:666:VAL:HG22	1.90	0.53
1:B:418:LYS:HZ2	1:B:458:GLU:HG2	1.72	0.53
1:B:450:ALA:HB3	1:B:451:PRO:CD	2.38	0.53
1:B:821:LEU:O	1:B:825:LEU:HG	2.08	0.53
1:B:826:CYS:C	1:B:828:ALA:H	2.16	0.53
1:A:150:THR:O	1:A:154:ILE:HG13	2.09	0.53
1:A:681:LEU:C	1:A:682:GLN:CG	2.78	0.53
1:A:756:ASP:OD2	2:C:371:ARG:NH2	2.41	0.53
1:B:483:GLU:C	1:B:486:ASP:CG	2.77	0.53
1:B:776:LEU:HD22	1:B:786:ASP:HB3	1.90	0.53
1:B:791:GLN:C	1:B:793:ARG:H	2.17	0.53
1:A:823:GLY:HA3	1:A:864:TRP:CZ3	2.43	0.53
1:B:130:ILE:N	1:B:131:PRO:HD2	2.23	0.53
1:B:266:GLU:HG2	1:B:267:ALA:N	2.23	0.53
1:B:444:ILE:HD12	1:B:444:ILE:H	1.74	0.53
2:C:366:LYS:C	2:C:367:SER:OG	2.52	0.53
2:C:366:LYS:C	2:C:368:GLY:H	2.14	0.53
1:B:43:VAL:C	1:B:45:ALA:H	2.17	0.53
1:B:777:LYS:CA	1:B:787:VAL:HG22	2.38	0.53
1:A:515:ASP:O	1:A:516:ARG:HG3	2.03	0.53
1:B:680:ALA:C	1:B:681:LEU:HD23	2.33	0.53
1:B:745:ALA:O	1:B:747:VAL:HG23	2.09	0.53
2:C:350:ILE:O	2:C:354:LYS:HG3	2.08	0.53
1:B:77:GLN:O	1:B:81:LEU:HG	2.08	0.53
1:B:473:ALA:O	1:B:477:LEU:HB2	2.09	0.53
1:B:778:GLY:O	1:B:779:ASP:C	2.50	0.53
1:A:681:LEU:O	1:A:682:GLN:HB2	2.09	0.53
1:A:867:LYS:HB2	1:A:867:LYS:NZ	2.24	0.53
1:B:604:SER:HA	1:B:607:VAL:CG1	2.39	0.53
1:B:827:THR:HG22	1:B:827:THR:O	2.08	0.53
1:B:404:PRO:O	1:B:408:GLN:HG2	2.10	0.53
1:B:561:VAL:HG21	1:B:580:LEU:HD22	1.91	0.53
1:B:707:ARG:HH12	1:B:754:MET:HG2	1.74	0.53
2:F:365:HIS:CD2	2:F:368:GLY:N	2.76	0.53
1:A:13:PRO:O	1:A:14:ASP:HB2	2.09	0.52
1:A:751:ASP:O	1:A:752:PHE:C	2.52	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:777:LYS:NZ	1:A:827:THR:HG21	2.24	0.52
1:B:181:MET:HE1	1:B:198:LEU:HB2	1.91	0.52
1:B:236:ALA:HA	1:B:239:GLN:OE1	2.08	0.52
1:B:265:ILE:O	1:B:268:MET:HB2	2.09	0.52
1:B:377:ASN:HD22	1:B:379:ASP:H	1.57	0.52
2:E:363:LYS:O	2:E:363:LYS:HG3	2.09	0.52
2:E:395:LYS:NZ	2:E:395:LYS:HB3	2.24	0.52
1:A:1:MET:HE1	1:A:20:ALA:HB1	1.90	0.52
1:A:121:ILE:N	1:A:122:PRO:CD	2.72	0.52
1:B:462:ALA:O	1:B:516:ARG:NH1	2.41	0.52
1:B:592:LEU:HA	1:B:595:VAL:HG22	1.91	0.52
1:B:596:GLN:O	1:B:597:HIS:C	2.52	0.52
1:B:589:GLN:HE22	1:B:630:MET:HB3	1.74	0.52
2:E:367:SER:OG	2:F:349:LYS:NZ	2.40	0.52
1:B:651:LYS:HB2	1:B:651:LYS:NZ	2.24	0.52
1:A:6:ILE:HG22	1:A:21:ALA:HB2	1.91	0.52
1:B:388:MET:HG2	1:B:427:THR:CG2	2.35	0.52
1:B:460:LEU:HD23	1:B:470:VAL:CG1	2.40	0.52
1:A:628:ALA:O	1:A:632:VAL:HG23	2.09	0.52
1:B:797:ILE:O	1:B:800:PHE:HB3	2.09	0.52
1:A:695:LEU:HD23	1:A:695:LEU:O	2.10	0.52
1:B:613:ARG:HD2	1:B:616:GLN:NE2	2.24	0.52
1:B:105:ARG:CB	1:B:106:PRO:CD	2.87	0.52
1:B:462:ALA:O	1:B:516:ARG:NH2	2.42	0.52
1:B:777:LYS:HA	1:B:787:VAL:HG23	1.84	0.52
1:B:777:LYS:N	1:B:787:VAL:HG22	2.25	0.52
1:A:681:LEU:C	1:A:682:GLN:HG3	2.34	0.52
1:A:707:ARG:O	1:A:711:PRO:HD3	2.10	0.52
1:B:462:ALA:H	1:B:516:ARG:NH1	2.08	0.52
1:A:445:ASN:OD1	1:A:447:VAL:HG23	2.10	0.52
1:A:485:ALA:O	1:A:488:ALA:HB3	2.10	0.52
1:A:516:ARG:HD3	1:A:524:LEU:HD12	1.91	0.52
1:B:434:ARG:HG3	1:B:472:TRP:HH2	1.74	0.52
1:A:122:PRO:HB3	1:A:165:GLN:NE2	2.24	0.51
1:B:91:VAL:O	1:B:95:VAL:HG23	2.10	0.51
1:B:268:MET:HE1	1:B:322:LEU:HD23	1.91	0.51
2:D:403:LEU:HD12	2:D:403:LEU:N	2.23	0.51
2:E:398:ASN:HD21	2:E:401:ASN:CA	2.17	0.51
2:E:398:ASN:ND2	2:E:401:ASN:H	2.08	0.51
2:E:346:ILE:CD1	2:F:367:SER:HA	2.40	0.51
1:A:380:TRP:HZ3	1:A:423:VAL:HG11	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:495:ALA:HA	1:B:541:LYS:HB3	1.92	0.51
2:D:350:ILE:HG22	2:D:369:VAL:HG11	1.92	0.51
2:E:346:ILE:CD1	2:E:349:LYS:HD2	2.37	0.51
1:A:103:THR:HA	1:A:145:HIS:CE1	2.45	0.51
1:A:513:THR:O	1:A:514:THR:C	2.53	0.51
1:A:651:LYS:N	1:A:652:PRO:HD2	2.25	0.51
1:B:333:GLN:O	1:B:381:ARG:NH2	2.43	0.51
2:C:395:LYS:HB3	2:C:395:LYS:HZ3	1.73	0.51
1:A:444:ILE:HD11	1:A:498:CYS:SG	2.50	0.51
1:A:801:ILE:HG13	1:A:802:ASP:N	2.25	0.51
1:B:51:GLN:C	1:B:53:ALA:H	2.18	0.51
1:B:695:LEU:O	1:B:696:LEU:C	2.54	0.51
2:C:389:GLN:O	2:C:392:MSE:N	2.38	0.51
2:F:389:GLN:HE21	2:F:390:GLU:N	2.08	0.51
1:A:398:GLU:OE1	1:A:400:ASN:HB2	2.10	0.51
1:A:514:THR:CG2	1:A:557:ARG:NH1	2.64	0.51
1:B:430:TRP:HA	1:B:469:ASN:ND2	2.21	0.51
1:B:801:ILE:O	1:B:804:ILE:HB	2.10	0.51
2:D:345:SER:HB2	2:D:349:LYS:CB	2.37	0.51
1:A:688:PHE:O	1:A:689:CYS:C	2.53	0.51
1:B:117:ALA:HB1	1:B:121:ILE:HD12	1.92	0.51
1:A:489:ASP:OD1	1:A:493:GLU:N	2.44	0.51
1:B:179:GLN:O	1:B:182:ARG:HG2	2.10	0.51
1:B:323:VAL:CG1	1:B:367:VAL:HG22	2.40	0.51
1:A:126:TRP:C	1:A:128:GLU:H	2.17	0.51
1:A:665:GLN:HE21	2:C:363:LYS:HG3	1.76	0.51
1:B:663:GLU:O	1:B:663:GLU:CG	2.58	0.51
1:B:836:LEU:O	1:B:840:ARG:HD2	2.11	0.51
1:A:19:GLU:C	1:A:21:ALA:N	2.67	0.50
1:A:537:LYS:O	1:A:594:LYS:HE3	2.11	0.50
1:A:756:ASP:OD1	2:C:372:LYS:HE2	2.10	0.50
1:B:37:LEU:HD13	1:B:61:ILE:CG1	2.38	0.50
1:A:831:LYS:C	1:A:833:VAL:N	2.67	0.50
1:A:851:ARG:C	1:A:853:SER:N	2.68	0.50
1:B:343:ASN:HD21	1:B:345:CYS:HB2	1.76	0.50
1:B:777:LYS:HD2	1:B:780:GLN:NE2	2.20	0.50
2:D:350:ILE:HG22	2:D:350:ILE:O	2.10	0.50
1:A:19:GLU:C	1:A:21:ALA:H	2.19	0.50
1:A:199:LEU:HD12	1:A:202:LEU:HD12	1.92	0.50
1:B:28:ALA:C	1:B:30:VAL:N	2.70	0.50
1:B:371:ILE:O	1:B:375:ILE:HB	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:345:SER:CB	2:D:349:LYS:HB2	2.38	0.50
1:A:102:GLU:CG	1:A:103:THR:H	2.25	0.50
1:A:811:THR:HG22	1:A:814:VAL:H	1.76	0.50
1:B:65:LEU:H	1:B:65:LEU:CD2	2.19	0.50
1:B:187:SER:OG	1:B:190:VAL:HG23	2.11	0.50
1:B:244:ILE:CG2	1:B:252:MET:HE1	2.42	0.50
1:B:453:LEU:HD21	1:B:499:LEU:HD22	1.94	0.50
1:B:632:VAL:O	1:B:636:VAL:HG23	2.11	0.50
2:E:358:MSE:CB	2:E:372:LYS:CE	2.72	0.50
2:E:376:TYR:O	2:E:379:TYR:HB3	2.12	0.50
2:F:371:ARG:HG3	2:F:371:ARG:HH11	1.77	0.50
1:A:467:ALA:O	1:A:470:VAL:HB	2.11	0.50
1:A:576:GLN:HE21	1:A:576:GLN:CA	2.06	0.50
1:B:181:MET:HE1	1:B:198:LEU:HD22	1.93	0.50
1:B:493:GLU:C	1:B:494:PRO:O	2.51	0.50
1:B:575:ILE:O	1:B:575:ILE:CG2	2.60	0.50
1:A:264:THR:O	1:A:267:ALA:HB3	2.11	0.50
1:A:811:THR:HG22	1:A:813:GLY:N	2.26	0.50
1:B:95:VAL:C	1:B:97:GLN:H	2.18	0.50
1:B:419:ASP:C	1:B:421:SER:H	2.20	0.50
1:B:511:LEU:CD2	1:B:553:VAL:HG11	2.42	0.50
2:E:346:ILE:HD11	2:F:367:SER:HA	1.93	0.50
1:A:105:ARG:H	1:A:106:PRO:HD3	1.77	0.50
1:A:144:GLU:CD	1:A:187:SER:HB2	2.37	0.50
1:A:395:GLU:HB2	1:A:438:LEU:HD13	1.94	0.50
1:A:867:LYS:HB2	1:A:867:LYS:HZ2	1.77	0.50
1:B:226:THR:O	1:B:234:ARG:HD3	2.12	0.50
1:B:756:ASP:O	1:B:760:GLU:N	2.42	0.50
1:A:3:LEU:HD12	1:A:3:LEU:N	2.27	0.50
1:A:88:ARG:NH1	1:A:92:LYS:HD3	2.25	0.50
1:A:591:VAL:HG23	1:A:592:LEU:N	2.27	0.50
1:A:762:ARG:CD	1:A:800:PHE:CZ	2.95	0.50
1:B:35:THR:HA	1:B:38:VAL:CG2	2.41	0.50
1:B:460:LEU:HD11	1:B:474:PHE:HE2	1.76	0.50
1:B:478:ALA:O	1:B:538:ASN:HB3	2.12	0.50
1:B:522:ASN:O	1:B:524:LEU:N	2.45	0.50
1:B:758:LEU:O	1:B:758:LEU:HD22	2.12	0.50
1:A:549:LYS:O	1:A:553:VAL:HG23	2.12	0.49
1:B:135:ALA:O	1:B:139:ASN:HB2	2.12	0.49
1:B:661:TYR:CD1	1:B:661:TYR:C	2.90	0.49
2:E:383:VAL:HG23	2:F:384:ASN:ND2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:366:LYS:O	2:F:370:LEU:HG	2.12	0.49
1:A:478:ALA:CB	1:A:535:ILE:HD12	2.41	0.49
1:B:35:THR:O	1:B:38:VAL:HB	2.12	0.49
1:B:426:ASP:O	1:B:428:THR:N	2.45	0.49
1:B:455:CYS:O	1:B:458:GLU:HB3	2.12	0.49
2:C:377:ILE:CG2	2:D:356:LEU:HD13	2.42	0.49
2:E:358:MSE:HE1	2:E:364:MSE:SE	2.62	0.49
1:A:707:ARG:HH22	1:A:753:ASP:CG	2.20	0.49
1:A:708:SER:O	1:A:711:PRO:HD2	2.12	0.49
1:B:590:ASN:N	1:B:590:ASN:ND2	2.61	0.49
2:C:366:LYS:C	2:C:367:SER:HG	2.19	0.49
1:A:518:ASP:O	1:A:520:HIS:N	2.45	0.49
1:A:710:LYS:HB3	1:A:711:PRO:HD3	1.94	0.49
1:B:30:VAL:HG12	1:B:31:GLU:H	1.78	0.49
1:B:73:LYS:C	1:B:75:GLN:N	2.68	0.49
1:B:525:ARG:NH1	1:B:580:LEU:HD12	2.27	0.49
1:A:117:ALA:HB1	1:A:121:ILE:HD11	1.94	0.49
1:A:485:ALA:O	1:A:488:ALA:N	2.43	0.49
1:A:681:LEU:O	1:A:682:GLN:HG3	2.12	0.49
1:A:867:LYS:HA	1:A:870:ARG:NH2	2.27	0.49
1:B:136:ASN:HD22	1:B:146:MET:CG	2.26	0.49
1:B:335:GLU:HG3	1:B:381:ARG:HH12	1.76	0.49
1:B:752:PHE:C	1:B:754:MET:N	2.68	0.49
1:B:770:THR:HG22	1:B:774:GLN:HE21	1.77	0.49
1:A:353:MET:O	1:A:357:THR:HG23	2.12	0.49
1:A:557:ARG:O	1:A:561:VAL:HG23	2.13	0.49
1:B:46:ASN:O	1:B:49:ASN:ND2	2.45	0.49
1:B:139:ASN:HB3	1:B:142:SER:OG	2.12	0.49
1:B:339:ASP:O	1:B:340:ASP:HB2	2.11	0.49
1:B:752:PHE:HE2	2:E:372:LYS:NZ	2.10	0.49
1:B:777:LYS:CE	1:B:780:GLN:NE2	2.76	0.49
2:C:377:ILE:HG21	2:D:356:LEU:HD13	1.93	0.49
1:A:616:GLN:CD	1:A:617:SER:N	2.70	0.49
1:B:182:ARG:CD	1:B:184:GLU:HB2	2.43	0.49
1:B:659:LYS:O	1:B:660:ASN:C	2.55	0.49
1:A:338:ASP:OD2	1:A:465:ARG:NH2	2.44	0.49
1:A:428:THR:O	1:A:432:VAL:HG23	2.13	0.49
1:B:44:LEU:HD11	1:B:57:ALA:HB3	1.95	0.49
1:A:799:SER:O	1:A:801:ILE:N	2.46	0.49
1:B:33:LEU:HB3	1:B:34:PRO:HD3	1.94	0.49
1:B:597:HIS:O	1:B:598:GLN:C	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:603:ILE:HG22	1:B:607:VAL:CG1	2.41	0.49
1:B:776:LEU:O	1:B:784:HIS:CD2	2.66	0.49
1:B:791:GLN:O	1:B:794:VAL:HG23	2.13	0.49
2:F:396:LEU:O	2:F:396:LEU:HD22	2.12	0.49
1:B:663:GLU:O	1:B:665:GLN:N	2.46	0.48
1:A:190:VAL:O	1:A:191:LYS:C	2.56	0.48
1:A:488:ALA:CB	1:B:870:ARG:HH12	2.26	0.48
1:A:756:ASP:CG	2:C:372:LYS:HE2	2.38	0.48
1:B:407:ILE:C	1:B:409:ALA:H	2.20	0.48
1:B:495:ALA:HA	1:B:541:LYS:CB	2.43	0.48
1:B:612:LEU:C	1:B:614:MET:H	2.22	0.48
1:B:838:GLU:C	1:B:840:ARG:N	2.71	0.48
1:A:7:LEU:HD23	1:A:25:LEU:HD11	1.95	0.48
1:A:484:ALA:C	1:A:486:ASP:N	2.69	0.48
1:A:560:GLN:O	1:A:564:MET:HB2	2.13	0.48
1:B:38:VAL:HG22	1:B:91:VAL:HG21	1.95	0.48
1:B:65:LEU:HD23	1:B:65:LEU:N	2.21	0.48
1:B:451:PRO:O	1:B:454:GLN:N	2.47	0.48
1:A:444:ILE:HG12	1:A:444:ILE:O	2.13	0.48
1:A:707:ARG:HG3	1:A:707:ARG:NH1	2.24	0.48
1:B:126:TRP:N	1:B:127:PRO:CD	2.76	0.48
2:E:370:LEU:O	2:E:374:ILE:HG13	2.14	0.48
1:A:86:ASN:O	1:A:89:ARG:HB3	2.13	0.48
1:A:689:CYS:HB3	1:A:731:TYR:OH	2.12	0.48
1:B:788:MET:O	1:B:790:VAL:N	2.46	0.48
1:A:69:ASP:O	1:A:71:ASP:N	2.47	0.48
1:A:399:PRO:O	1:A:403:LYS:HG3	2.13	0.48
1:A:661:TYR:HE1	1:A:704:ASN:HB2	1.76	0.48
1:B:19:GLU:HA	1:B:22:GLN:HE21	1.79	0.48
1:B:69:ASP:O	1:B:69:ASP:CG	2.56	0.48
2:D:364:MSE:HE2	2:D:365:HIS:CE1	2.48	0.48
1:A:62:LYS:HG3	1:A:112:CYS:SG	2.54	0.48
1:A:307:PRO:HG2	1:A:310:THR:HG22	1.96	0.48
1:B:237:ALA:O	1:B:240:ASN:HB2	2.14	0.48
1:B:444:ILE:O	1:B:445:ASN:HB2	2.13	0.48
1:B:682:GLN:O	1:B:685:ILE:HG22	2.14	0.48
1:B:752:PHE:HA	1:B:755:VAL:HG23	1.96	0.48
2:D:382:GLN:O	2:D:383:VAL:C	2.55	0.48
2:F:396:LEU:HD13	2:F:396:LEU:C	2.37	0.48
1:A:80:TRP:O	1:A:83:ILE:CG2	2.61	0.48
1:A:515:ASP:C	1:A:516:ARG:CG	2.84	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:801:ILE:O	1:A:804:ILE:HB	2.14	0.48
2:E:358:MSE:HB3	2:E:372:LYS:CD	2.43	0.48
1:A:168:ASP:O	1:A:170:SER:N	2.47	0.48
1:A:269:LYS:O	1:A:270:SER:C	2.56	0.48
1:B:268:MET:HE1	1:B:322:LEU:CD2	2.44	0.48
1:B:350:VAL:HG12	1:B:351:CYS:N	2.29	0.48
1:B:495:ALA:O	1:B:496:THR:OG1	2.28	0.48
1:B:804:ILE:C	1:B:806:GLY:N	2.71	0.48
1:A:51:GLN:HB2	1:A:105:ARG:CD	2.44	0.48
1:A:661:TYR:CG	1:A:705:VAL:HG12	2.48	0.48
1:A:700:LEU:HD23	1:A:710:LYS:HG3	1.94	0.48
1:A:789:LEU:O	1:A:792:PRO:HD2	2.14	0.48
2:D:364:MSE:HG3	2:D:365:HIS:H	1.78	0.48
1:A:591:VAL:HG23	1:A:592:LEU:H	1.79	0.47
1:A:784:HIS:O	1:A:787:VAL:HG22	2.13	0.47
1:A:798:LEU:O	1:A:801:ILE:HG12	2.14	0.47
1:B:233:VAL:O	1:B:234:ARG:C	2.57	0.47
1:B:318:ALA:O	1:B:322:LEU:HG	2.14	0.47
1:B:462:ALA:N	1:B:516:ARG:HH12	2.11	0.47
1:B:565:GLU:C	1:B:567:HIS:H	2.22	0.47
2:D:349:LYS:HG3	2:D:351:ILE:CG2	2.43	0.47
2:F:403:LEU:HD23	2:F:403:LEU:N	2.28	0.47
1:A:158:CYS:SG	1:A:204:PHE:HZ	2.37	0.47
1:A:736:LEU:HD13	1:A:793:ARG:NE	2.23	0.47
1:A:780:GLN:O	1:A:781:GLU:C	2.57	0.47
2:F:393:VAL:HG22	2:F:393:VAL:O	2.13	0.47
1:A:736:LEU:HD11	1:A:790:VAL:HG12	1.96	0.47
1:A:826:CYS:HA	1:A:830:GLY:HA2	1.96	0.47
1:B:33:LEU:C	1:B:35:THR:H	2.22	0.47
1:B:169:LYS:HD3	1:B:172:GLU:HB2	1.96	0.47
1:B:343:ASN:HB2	1:B:344:PRO:CD	2.45	0.47
1:B:394:LEU:CB	1:B:438:LEU:HD12	2.43	0.47
1:B:522:ASN:C	1:B:524:LEU:N	2.72	0.47
1:A:630:MET:HE3	1:A:669:ALA:HB1	1.96	0.47
1:A:810:HIS:HD2	1:A:815:VAL:CG2	2.27	0.47
1:B:440:PRO:CB	1:B:480:ALA:HB2	2.44	0.47
2:F:351:ILE:O	2:F:354:LYS:HB3	2.14	0.47
1:A:126:TRP:CE2	1:A:129:LEU:HB2	2.49	0.47
1:A:238:LEU:O	1:A:242:VAL:HG23	2.14	0.47
1:A:323:VAL:O	1:A:327:THR:HG23	2.15	0.47
1:A:682:GLN:C	1:A:684:ASN:N	2.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:777:LYS:HZ1	1:A:827:THR:HG21	1.79	0.47
1:A:868:GLU:OE1	1:A:868:GLU:HA	2.14	0.47
1:B:96:LEU:O	1:B:96:LEU:HG	2.15	0.47
1:B:96:LEU:HD22	1:B:126:TRP:CZ2	2.48	0.47
1:B:823:GLY:HA3	1:B:864:TRP:CZ3	2.50	0.47
1:A:37:LEU:HA	1:A:40:LEU:HD12	1.96	0.47
1:A:791:GLN:N	1:A:792:PRO:CD	2.78	0.47
1:B:129:LEU:C	1:B:131:PRO:HD2	2.38	0.47
1:B:374:HIS:HA	1:B:377:ASN:HB2	1.96	0.47
1:B:412:THR:O	1:B:415:GLU:HB2	2.14	0.47
2:D:400:LYS:O	2:D:401:ASN:HB3	2.15	0.47
1:A:90:GLU:O	1:A:94:TYR:HB2	2.15	0.47
1:A:686:LEU:N	1:A:687:PRO:CD	2.77	0.47
1:A:748:ASP:C	1:A:750:SER:N	2.72	0.47
1:A:755:VAL:O	1:A:759:ASN:ND2	2.47	0.47
1:B:316:LYS:O	1:B:319:LEU:HB2	2.15	0.47
1:B:449:LEU:HG	1:B:453:LEU:CD1	2.44	0.47
1:B:517:PRO:C	1:B:519:GLY:H	2.22	0.47
1:B:546:ALA:C	1:B:548:GLN:N	2.72	0.47
1:B:560:GLN:C	1:B:562:LEU:H	2.23	0.47
1:B:603:ILE:O	1:B:604:SER:C	2.58	0.47
1:B:780:GLN:HE22	1:B:827:THR:HG22	1.78	0.47
1:B:822:ILE:HA	1:B:825:LEU:HD12	1.97	0.47
1:B:861:LEU:O	1:B:865:ALA:HB2	2.14	0.47
2:E:354:LYS:NZ	2:E:361:ASP:HA	2.29	0.47
1:A:139:ASN:C	1:A:139:ASN:ND2	2.71	0.47
1:A:143:THR:O	1:A:146:MET:HB3	2.15	0.47
1:A:235:VAL:HG21	1:A:274:GLU:CG	2.45	0.47
1:A:777:LYS:HA	1:A:787:VAL:CG1	2.45	0.47
1:A:791:GLN:HB3	1:A:792:PRO:HD3	1.97	0.47
1:B:776:LEU:O	1:B:784:HIS:HD2	1.97	0.47
1:B:816:ALA:O	1:B:817:CYS:C	2.57	0.47
1:A:31:GLU:HG3	1:A:32:ASN:ND2	2.30	0.47
1:A:664:TYR:HB2	1:A:709:VAL:CG2	2.45	0.47
1:A:788:MET:O	1:A:791:GLN:HB2	2.14	0.47
1:B:570:SER:OG	1:B:572:SER:HB3	2.14	0.47
1:B:589:GLN:C	1:B:590:ASN:HD22	2.23	0.47
2:D:379:TYR:O	2:D:383:VAL:HG23	2.15	0.47
1:A:15:ARG:HH11	1:A:18:LEU:HD12	1.78	0.47
1:A:403:LYS:N	1:A:404:PRO:HD2	2.31	0.47
1:A:479:GLU:O	1:A:483:GLU:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:707:ARG:NH2	1:A:753:ASP:CG	2.72	0.47
1:A:816:ALA:HB1	1:A:857:LYS:HG2	1.97	0.47
1:B:96:LEU:HD22	1:B:126:TRP:HZ2	1.79	0.47
1:B:408:GLN:O	1:B:408:GLN:HG3	2.15	0.47
1:B:427:THR:O	1:B:427:THR:CG2	2.63	0.47
1:B:589:GLN:HG3	1:B:634:THR:OG1	2.15	0.47
1:A:33:LEU:HD22	1:A:79:ARG:HH21	1.80	0.46
1:B:5:THR:O	1:B:9:LYS:HE2	2.14	0.46
1:B:244:ILE:CG2	1:B:252:MET:HE3	2.43	0.46
1:B:401:GLN:O	1:B:401:GLN:HG3	2.15	0.46
1:B:419:ASP:O	1:B:425:ARG:NH1	2.48	0.46
2:F:380:LEU:HD23	2:F:380:LEU:HA	1.78	0.46
1:A:525:ARG:HG2	1:A:525:ARG:NH1	2.30	0.46
1:B:549:LYS:HA	1:B:552:LEU:HD12	1.97	0.46
1:B:607:VAL:O	1:B:608:MET:C	2.57	0.46
1:B:812:ASP:O	1:B:815:VAL:HB	2.15	0.46
1:A:21:ALA:HB1	1:A:25:LEU:CD1	2.45	0.46
1:A:174:LEU:HD22	1:A:178:ILE:CD1	2.45	0.46
1:A:617:SER:O	1:A:619:ALA:N	2.43	0.46
1:B:2:GLU:OE1	1:B:4:ILE:HD13	2.15	0.46
1:B:123:VAL:O	1:B:124:SER:C	2.58	0.46
1:B:867:LYS:O	1:B:870:ARG:HG2	2.16	0.46
2:C:387:LEU:N	2:C:387:LEU:HD23	2.30	0.46
1:A:54:ARG:HH22	1:A:101:THR:HG21	1.80	0.46
1:A:77:GLN:HG2	1:A:119:ALA:HB2	1.96	0.46
1:A:570:SER:C	1:A:572:SER:N	2.72	0.46
1:B:431:THR:O	1:B:435:ILE:HG13	2.14	0.46
1:B:562:LEU:C	1:B:564:MET:H	2.22	0.46
2:C:387:LEU:HD11	2:D:388:ARG:HE	1.79	0.46
2:E:377:ILE:O	2:E:381:GLN:HG3	2.16	0.46
1:A:118:CYS:HA	1:A:161:ILE:HG12	1.97	0.46
1:A:130:ILE:O	1:A:134:VAL:HG23	2.15	0.46
1:A:603:ILE:CG2	1:A:607:VAL:HG23	2.45	0.46
1:A:617:SER:C	1:A:619:ALA:H	2.22	0.46
1:A:661:TYR:HB2	1:A:705:VAL:HG12	1.97	0.46
1:B:230:ASP:OD1	1:B:232:ARG:N	2.49	0.46
2:C:374:ILE:CG1	2:D:353:LEU:HD13	2.45	0.46
2:F:397:ALA:HA	2:F:400:LYS:HD3	1.97	0.46
1:B:502:SER:O	1:B:506:ILE:HG13	2.16	0.46
2:E:391:ASN:OD1	2:F:391:ASN:HB2	2.15	0.46
1:A:35:THR:O	1:A:35:THR:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:MET:HE2	1:A:255:TYR:CD1	2.51	0.46
1:A:242:VAL:HG11	1:A:281:GLU:CG	2.46	0.46
1:B:28:ALA:HB1	1:B:33:LEU:CD2	2.46	0.46
1:B:40:LEU:CD2	1:B:44:LEU:HG	2.46	0.46
1:B:56:ALA:O	1:B:60:GLN:HG2	2.16	0.46
1:B:444:ILE:HG23	1:B:449:LEU:HD22	1.97	0.46
1:B:497:TYR:HD1	1:B:497:TYR:H	1.63	0.46
1:B:561:VAL:HG12	1:B:561:VAL:O	2.16	0.46
1:B:580:LEU:CD2	1:B:584:LEU:HG	2.45	0.46
1:A:514:THR:HG23	1:A:529:TYR:CE2	2.50	0.46
1:A:647:MET:HG2	1:A:688:PHE:CZ	2.50	0.46
1:A:658:LEU:HG	1:A:670:ALA:HB1	1.98	0.46
1:B:36:PHE:C	1:B:38:VAL:N	2.73	0.46
1:B:169:LYS:HD3	1:B:172:GLU:CB	2.45	0.46
1:B:695:LEU:O	1:B:698:GLU:N	2.49	0.46
1:B:732:LEU:HD22	1:B:736:LEU:HD11	1.98	0.46
2:C:358:MSE:HE1	2:C:364:MSE:SE	2.65	0.46
2:E:358:MSE:CE	2:E:372:LYS:CG	2.83	0.46
2:E:398:ASN:C	2:E:398:ASN:ND2	2.74	0.46
1:A:608:MET:O	1:A:612:LEU:HB2	2.16	0.46
1:B:618:THR:C	1:B:620:GLY:N	2.71	0.46
1:B:752:PHE:C	1:B:754:MET:H	2.24	0.46
1:A:241:LEU:HD13	1:A:260:LEU:HD22	1.97	0.46
1:B:27:ARG:HH11	1:B:28:ALA:HA	1.77	0.46
1:B:36:PHE:C	1:B:38:VAL:H	2.24	0.46
1:B:875:GLN:HA	1:B:875:GLN:OE1	2.16	0.46
2:E:371:ARG:HA	2:E:374:ILE:HD12	1.98	0.46
2:F:347:ASN:CG	2:F:348:ASP:N	2.32	0.46
2:E:349:LYS:NZ	2:F:367:SER:OG	2.42	0.45
1:B:3:LEU:H	1:B:4:ILE:HD12	1.80	0.45
1:B:80:TRP:HE1	1:B:120:GLU:CD	2.23	0.45
1:A:53:ALA:O	1:A:57:ALA:HB2	2.16	0.45
1:A:93:ASN:HA	1:A:96:LEU:HB3	1.96	0.45
1:B:756:ASP:HA	1:B:759:ASN:ND2	2.31	0.45
1:B:780:GLN:HE22	1:B:827:THR:HG21	1.80	0.45
2:C:402:LYS:HG3	2:C:403:LEU:N	2.31	0.45
1:A:436:CYS:SG	1:A:477:LEU:HD13	2.57	0.45
1:A:448:TYR:C	1:A:451:PRO:HD2	2.41	0.45
1:A:533:MET:HG2	1:A:590:ASN:ND2	2.26	0.45
1:A:552:LEU:HA	1:A:555:MET:HE3	1.98	0.45
1:A:659:LYS:O	1:A:661:TYR:CD2	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:VAL:HA	1:B:147:LYS:HG2	1.97	0.45
1:B:208:ASN:ND2	1:B:214:GLU:OE1	2.44	0.45
1:B:430:TRP:CZ2	1:B:434:ARG:CD	2.98	0.45
1:A:37:LEU:O	1:A:40:LEU:HB2	2.17	0.45
1:A:154:ILE:O	1:A:157:ILE:HB	2.16	0.45
1:A:609:ALA:O	1:A:613:ARG:HB3	2.16	0.45
1:A:673:LEU:HA	1:A:676:ASP:HB2	1.98	0.45
1:B:487:VAL:CG1	1:B:488:ALA:N	2.79	0.45
1:B:493:GLU:O	1:B:494:PRO:O	2.35	0.45
1:A:19:GLU:O	1:A:21:ALA:N	2.50	0.45
1:A:130:ILE:N	1:A:131:PRO:CD	2.79	0.45
1:A:287:CYS:O	1:A:291:MET:HG3	2.16	0.45
1:A:363:ILE:CG2	1:A:364:VAL:N	2.78	0.45
1:A:565:GLU:OE2	1:A:574:ARG:NH2	2.50	0.45
1:A:787:VAL:O	1:A:790:VAL:HG22	2.17	0.45
1:B:522:ASN:C	1:B:524:LEU:H	2.24	0.45
1:B:732:LEU:HD22	1:B:736:LEU:CD1	2.46	0.45
1:B:758:LEU:HD22	1:B:762:ARG:NE	2.31	0.45
1:B:867:LYS:C	1:B:869:LEU:H	2.25	0.45
1:A:147:LYS:O	1:A:148:GLU:C	2.60	0.45
1:B:370:PHE:CD1	1:B:370:PHE:C	2.94	0.45
1:B:407:ILE:HD13	1:B:407:ILE:HA	1.82	0.45
1:B:694:GLN:HE21	1:B:698:GLU:HG3	1.82	0.45
1:B:705:VAL:HB	1:B:710:LYS:HZ1	1.79	0.45
1:B:707:ARG:HH12	1:B:754:MET:CG	2.29	0.45
1:B:752:PHE:HE2	2:E:372:LYS:CE	2.29	0.45
2:C:350:ILE:HD12	2:C:370:LEU:HD21	1.98	0.45
2:E:358:MSE:SE	2:E:364:MSE:CE	3.15	0.45
1:A:29:ALA:O	1:A:33:LEU:N	2.49	0.45
1:A:401:GLN:O	1:A:405:LEU:HD13	2.17	0.45
1:B:122:PRO:HA	1:B:165:GLN:NE2	2.32	0.45
1:B:212:GLU:C	1:B:216:HIS:HD2	2.25	0.45
1:B:673:LEU:HD22	1:B:677:LEU:HG	1.99	0.45
1:B:758:LEU:HD22	1:B:762:ARG:HE	1.80	0.45
2:D:357:VAL:HG11	2:D:372:LYS:HB3	1.97	0.45
1:A:235:VAL:HG21	1:A:274:GLU:HG2	1.99	0.45
1:A:319:LEU:HD12	1:A:319:LEU:HA	1.81	0.45
1:B:194:ALA:O	1:B:197:ALA:N	2.50	0.45
1:B:351:CYS:O	1:B:355:LEU:HB2	2.17	0.45
1:B:731:TYR:O	1:B:732:LEU:C	2.60	0.45
1:A:33:LEU:N	1:A:34:PRO:CD	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ALA:C	1:A:119:ALA:N	2.75	0.45
1:A:334:ASP:O	1:A:335:GLU:C	2.59	0.45
1:A:503:PHE:CE2	1:A:507:VAL:HG11	2.50	0.45
1:A:626:GLU:O	1:A:630:MET:HG2	2.17	0.45
1:A:683:SER:N	1:A:723:ALA:O	2.50	0.45
1:B:529:TYR:OH	1:B:557:ARG:NH1	2.49	0.45
1:B:629:LEU:O	1:B:630:MET:C	2.60	0.45
1:B:787:VAL:O	1:B:790:VAL:HG12	2.17	0.45
1:A:707:ARG:HB2	1:A:757:TYR:CZ	2.52	0.44
1:A:748:ASP:O	1:A:750:SER:N	2.44	0.44
1:B:326:LEU:CD2	1:B:348:ALA:HA	2.47	0.44
1:B:335:GLU:HG2	1:B:380:TRP:CZ2	2.53	0.44
1:B:679:ARG:NE	2:F:343:ARG:N	2.65	0.44
1:B:864:TRP:O	1:B:868:GLU:HG2	2.17	0.44
1:A:233:VAL:O	1:A:234:ARG:C	2.60	0.44
1:B:72:ILE:O	1:B:75:GLN:HB3	2.17	0.44
1:B:565:GLU:HB2	1:B:577:PHE:CE1	2.52	0.44
1:B:770:THR:CG2	1:B:774:GLN:HE21	2.31	0.44
2:C:354:LYS:HG2	2:C:369:VAL:CG2	2.48	0.44
2:C:354:LYS:C	2:C:356:LEU:N	2.74	0.44
1:A:618:THR:HG22	1:A:618:THR:O	2.18	0.44
1:B:154:ILE:O	1:B:157:ILE:HB	2.18	0.44
1:B:238:LEU:O	1:B:239:GLN:C	2.61	0.44
1:B:589:GLN:NE2	1:B:630:MET:HB3	2.32	0.44
1:B:637:GLU:OE1	1:B:638:VAL:HA	2.17	0.44
1:B:749:LYS:CG	1:B:750:SER:N	2.69	0.44
1:A:81:LEU:CD1	1:A:88:ARG:HD3	2.45	0.44
1:A:458:GLU:O	1:A:459:GLY:C	2.60	0.44
1:A:798:LEU:HD23	1:A:798:LEU:HA	1.88	0.44
1:B:40:LEU:O	1:B:43:VAL:N	2.44	0.44
1:B:98:THR:O	1:B:99:LEU:C	2.59	0.44
1:B:410:MET:N	1:B:411:PRO:CD	2.80	0.44
1:B:457:ILE:HD13	1:B:505:LEU:HD23	2.00	0.44
1:B:544:TYR:O	1:B:548:GLN:N	2.47	0.44
1:B:651:LYS:N	1:B:652:PRO:CD	2.80	0.44
2:F:356:LEU:HD23	2:F:356:LEU:HA	1.84	0.44
2:F:392:MSE:C	2:F:394:LEU:N	2.74	0.44
1:A:15:ARG:HA	1:A:18:LEU:HG	2.00	0.44
2:E:348:ASP:O	2:E:351:ILE:HG13	2.17	0.44
1:A:25:LEU:HB3	1:A:36:PHE:HZ	1.83	0.44
1:A:540:ALA:C	1:A:542:ASP:H	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:846:LEU:HD23	1:A:846:LEU:C	2.43	0.44
1:B:468:SER:O	1:B:470:VAL:N	2.51	0.44
1:B:561:VAL:C	1:B:562:LEU:HD12	2.43	0.44
1:B:758:LEU:HD11	1:B:762:ARG:HH21	1.81	0.44
1:A:39:GLU:HA	1:A:42:ARG:HD3	1.99	0.44
1:A:54:ARG:O	1:A:57:ALA:HB3	2.18	0.44
1:A:105:ARG:H	1:A:106:PRO:CD	2.30	0.44
1:A:523:ASN:O	1:A:524:LEU:C	2.60	0.44
1:B:185:GLU:O	1:B:191:LYS:HE3	2.18	0.44
1:B:449:LEU:HD12	1:B:452:LEU:HD23	2.00	0.44
1:A:181:MET:HE1	1:A:198:LEU:CD2	2.39	0.44
1:B:51:GLN:O	1:B:52:VAL:HG12	2.17	0.44
1:B:61:ILE:HD12	1:B:112:CYS:SG	2.58	0.44
1:B:83:ILE:HG22	1:B:84:ASP:N	2.33	0.44
1:B:342:TRP:CZ2	1:B:347:ALA:HB2	2.53	0.44
2:C:396:LEU:C	2:C:398:ASN:N	2.75	0.44
2:F:361:ASP:O	2:F:362:ALA:HB2	2.17	0.44
1:A:57:ALA:O	1:A:61:ILE:HG13	2.18	0.43
1:A:377:ASN:ND2	1:A:377:ASN:C	2.69	0.43
1:A:615:PHE:CE1	1:A:625:GLN:HG2	2.53	0.43
1:B:24:PHE:C	1:B:26:GLU:H	2.26	0.43
1:B:187:SER:HB3	1:B:190:VAL:CG2	2.48	0.43
1:B:450:ALA:N	1:B:451:PRO:HD2	2.33	0.43
1:B:508:GLN:OE1	1:B:508:GLN:HA	2.18	0.43
1:A:55:VAL:HG21	1:A:105:ARG:HD2	1.99	0.43
1:A:711:PRO:O	1:A:764:SER:OG	2.30	0.43
1:B:168:ASP:OD1	1:B:169:LYS:HG2	2.18	0.43
1:B:360:GLU:O	1:B:361:ASP:C	2.61	0.43
1:B:572:SER:O	1:B:575:ILE:N	2.51	0.43
1:B:660:ASN:O	1:B:662:ALA:N	2.51	0.43
1:B:766:LEU:HD13	1:B:818:ALA:N	2.32	0.43
1:A:133:LEU:O	1:A:136:ASN:HB2	2.18	0.43
1:A:368:LEU:HD21	1:A:405:LEU:HD23	2.00	0.43
1:B:606:VAL:O	1:B:609:ALA:CB	2.54	0.43
1:B:608:MET:HG2	1:B:635:LEU:CD2	2.48	0.43
1:B:833:VAL:O	1:B:837:VAL:HG23	2.18	0.43
2:C:350:ILE:CD1	2:C:370:LEU:HD21	2.48	0.43
1:A:34:PRO:HG3	1:A:83:ILE:HG13	2.00	0.43
1:A:181:MET:O	1:A:182:ARG:C	2.61	0.43
1:A:199:LEU:HD12	1:A:199:LEU:HA	1.83	0.43
1:A:260:LEU:O	1:A:261:PHE:C	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:SER:C	1:B:470:VAL:N	2.71	0.43
1:B:647:MET:O	1:B:648:GLU:C	2.61	0.43
1:B:651:LYS:HB2	1:B:652:PRO:HD3	1.99	0.43
1:B:754:MET:HE2	1:B:754:MET:HB3	1.93	0.43
1:B:807:ASP:O	1:B:810:HIS:CD2	2.71	0.43
2:E:398:ASN:O	2:E:399:GLN:CG	2.66	0.43
1:A:51:GLN:HB2	1:A:105:ARG:HD2	1.99	0.43
1:A:120:GLU:HB3	1:A:125:GLN:CD	2.43	0.43
1:A:121:ILE:HD12	1:A:161:ILE:HD13	2.00	0.43
1:A:659:LYS:O	1:A:661:TYR:HD2	2.01	0.43
1:A:714:LEU:O	1:A:768:ALA:HB2	2.18	0.43
1:A:827:THR:HG22	1:A:827:THR:O	2.18	0.43
1:B:323:VAL:HG13	1:B:367:VAL:HG22	2.00	0.43
1:B:449:LEU:O	1:B:453:LEU:HD12	2.18	0.43
2:E:380:LEU:HA	2:E:383:VAL:HG22	2.00	0.43
1:A:174:LEU:HD12	1:A:208:ASN:ND2	2.33	0.43
1:A:440:PRO:HG2	1:A:441:GLU:H	1.84	0.43
1:A:465:ARG:HA	1:A:465:ARG:HD3	1.68	0.43
1:A:606:VAL:O	1:A:609:ALA:HB3	2.18	0.43
1:A:870:ARG:CZ	1:A:870:ARG:HB3	2.48	0.43
1:B:105:ARG:HG3	1:B:105:ARG:HH11	1.84	0.43
1:B:522:ASN:O	1:B:523:ASN:OD1	2.36	0.43
1:B:551:THR:HG22	1:B:552:LEU:N	2.34	0.43
2:F:371:ARG:HG3	2:F:371:ARG:NH1	2.34	0.43
1:A:338:ASP:CG	1:A:465:ARG:NH2	2.77	0.43
1:B:692:VAL:O	1:B:693:MET:C	2.61	0.43
1:B:798:LEU:HD11	1:B:833:VAL:HG13	2.00	0.43
2:C:366:LYS:H	2:C:366:LYS:HG2	1.55	0.43
2:F:354:LYS:HD2	2:F:354:LYS:C	2.44	0.43
1:A:69:ASP:C	1:A:71:ASP:H	2.27	0.43
1:A:112:CYS:C	1:A:114:ALA:N	2.75	0.43
1:A:139:ASN:C	1:A:139:ASN:HD22	2.27	0.43
1:A:739:LEU:O	1:A:743:SER:HB3	2.19	0.43
1:A:779:ASP:O	1:A:780:GLN:HG3	2.18	0.43
1:B:331:THR:HG23	1:B:331:THR:O	2.18	0.43
1:B:615:PHE:CE2	1:B:628:ALA:HB3	2.54	0.43
2:D:370:LEU:HA	2:D:373:ALA:HB3	1.99	0.43
2:F:389:GLN:C	2:F:389:GLN:NE2	2.76	0.43
1:A:8:GLU:C	1:A:10:THR:H	2.27	0.43
1:A:172:GLU:CD	1:A:172:GLU:N	2.72	0.43
1:A:439:LEU:O	1:A:440:PRO:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:846:LEU:HD12	1:B:849:GLU:OE1	2.18	0.43
2:C:365:HIS:O	2:C:369:VAL:HG23	2.19	0.43
2:D:402:LYS:O	2:D:403:LEU:C	2.62	0.43
2:F:402:LYS:O	2:F:403:LEU:O	2.37	0.43
1:A:46:ASN:HB3	1:A:49:ASN:ND2	2.33	0.43
1:A:135:ALA:CA	1:A:138:THR:HG22	2.38	0.43
1:A:505:LEU:HD12	1:A:505:LEU:O	2.19	0.43
1:A:533:MET:SD	1:A:590:ASN:ND2	2.92	0.43
1:B:33:LEU:C	1:B:35:THR:N	2.77	0.43
1:B:132:GLN:HA	1:B:132:GLN:NE2	2.31	0.43
1:B:592:LEU:HA	1:B:595:VAL:CG2	2.49	0.43
1:B:716:VAL:O	1:B:716:VAL:HG13	2.18	0.43
1:B:870:ARG:C	1:B:872:LEU:N	2.77	0.43
2:C:370:LEU:O	2:C:374:ILE:HG13	2.19	0.43
2:E:398:ASN:C	2:E:399:GLN:HG2	2.44	0.43
1:A:458:GLU:O	1:A:460:LEU:N	2.52	0.42
1:B:126:TRP:CD1	1:B:126:TRP:O	2.71	0.42
1:B:182:ARG:HD2	1:B:184:GLU:OE1	2.19	0.42
1:B:263:ILE:HG22	1:B:264:THR:N	2.33	0.42
1:B:287:CYS:CB	1:B:354:LEU:CD1	2.96	0.42
1:B:564:MET:HA	1:B:564:MET:HE3	2.00	0.42
2:E:358:MSE:SE	2:E:364:MSE:SE	3.37	0.42
2:F:403:LEU:H	2:F:403:LEU:CD2	2.30	0.42
1:A:34:PRO:CB	1:A:83:ILE:HD11	2.45	0.42
1:A:39:GLU:HA	1:A:42:ARG:CD	2.50	0.42
1:A:144:GLU:O	1:A:145:HIS:C	2.61	0.42
1:A:272:ILE:O	1:A:275:VAL:HB	2.19	0.42
1:A:751:ASP:O	1:A:754:MET:HB2	2.18	0.42
1:B:99:LEU:HB2	1:B:146:MET:CE	2.44	0.42
1:B:112:CYS:O	1:B:113:VAL:C	2.62	0.42
1:B:663:GLU:HG3	1:B:666:VAL:H	1.83	0.42
1:B:810:HIS:O	1:B:811:THR:C	2.62	0.42
2:F:348:ASP:OD1	2:F:351:ILE:HD11	2.18	0.42
1:A:217:PHE:O	1:A:221:VAL:HG23	2.19	0.42
1:A:587:THR:O	1:A:591:VAL:HG22	2.20	0.42
1:A:596:GLN:O	1:A:597:HIS:C	2.62	0.42
1:B:65:LEU:HB3	1:B:69:ASP:OD2	2.19	0.42
1:B:367:VAL:HG12	1:B:367:VAL:O	2.20	0.42
1:B:440:PRO:HB3	1:B:480:ALA:HB2	2.01	0.42
1:B:834:LEU:HD13	1:B:872:LEU:HD12	2.00	0.42
1:A:338:ASP:CB	1:A:465:ARG:HH22	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:ARG:CZ	1:B:275:VAL:HG11	2.49	0.42
1:B:269:LYS:O	1:B:270:SER:C	2.62	0.42
1:B:349:GLY:O	1:B:352:LEU:N	2.53	0.42
2:D:345:SER:C	2:D:349:LYS:HB2	2.44	0.42
1:B:136:ASN:ND2	1:B:146:MET:CE	2.81	0.42
1:B:205:THR:OG1	1:B:209:PHE:HE1	2.03	0.42
1:B:245:MET:HE3	1:B:256:MET:HE1	2.02	0.42
1:B:335:GLU:CG	1:B:380:TRP:HZ2	2.32	0.42
1:B:546:ALA:O	1:B:549:LYS:HG3	2.20	0.42
1:B:777:LYS:CB	1:B:787:VAL:HG21	2.49	0.42
1:B:831:LYS:O	1:B:834:LEU:N	2.51	0.42
2:F:349:LYS:C	2:F:351:ILE:N	2.75	0.42
1:A:34:PRO:HB3	1:A:83:ILE:CD1	2.44	0.42
1:A:772:ILE:O	1:A:773:VAL:C	2.61	0.42
1:B:457:ILE:HG22	1:B:509:LYS:HG2	2.01	0.42
2:F:396:LEU:HD22	2:F:396:LEU:C	2.45	0.42
1:A:6:ILE:HG22	1:A:21:ALA:CB	2.50	0.42
1:A:450:ALA:N	1:A:451:PRO:HD2	2.35	0.42
1:A:516:ARG:C	1:A:519:GLY:H	2.20	0.42
1:A:544:TYR:OH	1:A:596:GLN:N	2.35	0.42
1:A:847:LEU:O	1:A:851:ARG:HG3	2.20	0.42
1:B:51:GLN:C	1:B:53:ALA:N	2.77	0.42
1:B:266:GLU:O	1:B:267:ALA:C	2.62	0.42
1:B:353:MET:CG	1:B:392:SER:HB2	2.46	0.42
1:B:594:LYS:O	1:B:594:LYS:HG3	2.19	0.42
1:B:847:LEU:C	1:B:851:ARG:HH21	2.27	0.42
2:D:345:SER:OG	2:D:349:LYS:HD2	2.19	0.42
1:A:65:LEU:HD13	1:A:116:ILE:HG12	2.01	0.42
1:A:161:ILE:O	1:A:162:ASP:C	2.61	0.42
1:B:384:ASP:OD1	1:B:427:THR:OG1	2.33	0.42
1:B:444:ILE:H	1:B:444:ILE:CD1	2.31	0.42
1:B:615:PHE:CZ	1:B:628:ALA:HB3	2.55	0.42
1:B:733:GLU:O	1:B:734:VAL:C	2.62	0.42
1:B:777:LYS:HE3	1:B:780:GLN:NE2	2.35	0.42
1:A:166:LEU:C	1:A:168:ASP:N	2.76	0.42
1:A:338:ASP:CG	1:A:465:ARG:HH22	2.28	0.42
1:A:514:THR:O	1:A:525:ARG:HD3	2.19	0.42
1:A:668:LEU:CD2	1:A:709:VAL:HA	2.50	0.42
1:A:787:VAL:HG23	1:A:788:MET:CE	2.40	0.42
1:B:7:LEU:C	1:B:9:LYS:H	2.27	0.42
1:B:256:MET:HE2	1:B:256:MET:HB2	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:LEU:HD12	1:B:319:LEU:HA	1.84	0.42
1:B:368:LEU:HD23	1:B:368:LEU:HA	1.89	0.42
1:B:556:GLU:O	1:B:557:ARG:C	2.63	0.42
1:B:604:SER:O	1:B:605:ASP:C	2.62	0.42
1:B:729:LYS:HG2	1:B:789:LEU:CD1	2.49	0.42
2:C:357:VAL:CG2	2:C:358:MSE:N	2.82	0.42
1:A:8:GLU:OE1	1:A:53:ALA:HB2	2.20	0.42
1:A:359:CYS:O	1:A:360:GLU:C	2.63	0.42
1:A:544:TYR:N	1:A:545:PRO:CD	2.82	0.42
1:A:578:ASN:O	1:A:581:GLN:HB3	2.20	0.42
1:B:608:MET:HE2	1:B:611:LEU:HD12	2.01	0.42
1:B:726:GLY:C	1:B:728:PHE:H	2.27	0.42
1:B:790:VAL:O	1:B:793:ARG:HB2	2.19	0.42
1:B:831:LYS:HE2	1:B:872:LEU:O	2.20	0.42
1:A:169:LYS:HB2	1:A:172:GLU:OE1	2.20	0.41
1:B:613:ARG:O	1:B:617:SER:HB2	2.20	0.41
1:B:781:GLU:O	1:B:782:ASN:HB2	2.20	0.41
1:B:791:GLN:N	1:B:792:PRO:HD2	2.35	0.41
1:A:34:PRO:CG	1:A:83:ILE:HG13	2.50	0.41
1:A:146:MET:HE2	1:A:150:THR:OG1	2.20	0.41
1:A:151:LEU:HA	1:A:154:ILE:HD12	2.02	0.41
1:A:826:CYS:SG	1:A:869:LEU:HD23	2.60	0.41
1:A:870:ARG:HG2	1:A:870:ARG:HH11	1.85	0.41
1:B:6:ILE:O	1:B:6:ILE:HG22	2.20	0.41
1:B:69:ASP:OD1	1:B:69:ASP:C	2.61	0.41
1:B:169:LYS:O	1:B:169:LYS:HG3	2.20	0.41
1:B:217:PHE:O	1:B:221:VAL:HG23	2.19	0.41
1:B:326:LEU:HD22	1:B:348:ALA:O	2.20	0.41
1:B:337:ASP:CG	1:B:338:ASP:N	2.71	0.41
1:B:440:PRO:O	1:B:443:ALA:HB3	2.20	0.41
2:C:393:VAL:C	2:C:395:LYS:H	2.28	0.41
1:A:338:ASP:OD2	1:A:338:ASP:O	2.39	0.41
1:A:762:ARG:HD2	1:A:804:ILE:CD1	2.36	0.41
1:A:822:ILE:O	1:A:823:GLY:C	2.63	0.41
1:B:27:ARG:HH11	1:B:28:ALA:N	2.14	0.41
1:B:811:THR:C	1:B:813:GLY:N	2.74	0.41
1:A:665:GLN:NE2	2:C:363:LYS:HG3	2.35	0.41
1:B:182:ARG:CG	1:B:184:GLU:HB2	2.51	0.41
1:B:647:MET:HE2	1:B:688:PHE:CE1	2.55	0.41
1:B:758:LEU:HD22	1:B:762:ARG:HG3	2.02	0.41
1:B:857:LYS:O	1:B:861:LEU:CB	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:TRP:HA	1:A:128:GLU:OE1	2.21	0.41
1:A:695:LEU:HD23	1:A:695:LEU:C	2.45	0.41
1:B:33:LEU:N	1:B:34:PRO:CD	2.84	0.41
1:B:86:ASN:HA	1:B:89:ARG:NH1	2.35	0.41
1:B:804:ILE:O	1:B:806:GLY:N	2.53	0.41
1:B:861:LEU:O	1:B:865:ALA:CB	2.69	0.41
2:E:366:LYS:O	2:E:367:SER:CB	2.67	0.41
1:A:120:GLU:CD	1:A:125:GLN:HE22	2.28	0.41
1:A:333:GLN:OE1	1:A:384:ASP:OD2	2.38	0.41
1:A:362:ASP:O	1:A:365:PRO:HG2	2.20	0.41
1:B:126:TRP:O	1:B:128:GLU:N	2.46	0.41
1:B:174:LEU:HD21	1:B:218:ILE:HD11	2.03	0.41
1:B:497:TYR:CD1	1:B:540:ALA:HB2	2.56	0.41
1:A:80:TRP:HE1	1:A:120:GLU:HG3	1.79	0.41
1:A:125:GLN:HG2	1:A:126:TRP:H	1.86	0.41
1:A:365:PRO:HG3	2:E:392:MSE:CE	2.51	0.41
1:A:734:VAL:HG23	1:A:735:VAL:N	2.36	0.41
1:B:663:GLU:C	1:B:665:GLN:N	2.79	0.41
2:C:366:LYS:C	2:C:368:GLY:N	2.78	0.41
2:E:358:MSE:N	2:E:372:LYS:CE	2.76	0.41
1:A:21:ALA:HB1	1:A:25:LEU:HD12	2.03	0.41
1:A:458:GLU:C	1:A:460:LEU:N	2.79	0.41
1:A:685:ILE:C	1:A:687:PRO:HD2	2.46	0.41
1:B:387:VAL:HG11	1:B:428:THR:OG1	2.21	0.41
1:B:434:ARG:HG2	1:B:434:ARG:HH11	1.86	0.41
1:B:509:LYS:HD3	1:B:509:LYS:HA	1.92	0.41
2:D:382:GLN:O	2:D:385:HIS:N	2.54	0.41
1:A:146:MET:HA	1:A:146:MET:HE3	2.02	0.41
1:A:179:GLN:O	1:A:182:ARG:HG2	2.21	0.41
1:A:512:GLU:O	1:A:515:ASP:HB2	2.20	0.41
1:A:540:ALA:HB3	1:A:542:ASP:OD1	2.21	0.41
1:A:565:GLU:HB2	1:A:577:PHE:CZ	2.56	0.41
1:A:867:LYS:CG	1:A:870:ARG:HH22	2.31	0.41
1:B:7:LEU:HD11	1:B:36:PHE:CZ	2.50	0.41
1:B:395:GLU:HB2	1:B:438:LEU:HD13	2.01	0.41
1:B:451:PRO:O	1:B:455:CYS:N	2.49	0.41
1:B:536:VAL:O	1:B:537:LYS:C	2.63	0.41
1:B:585:CYS:O	1:B:586:ALA:C	2.63	0.41
1:B:740:GLN:HA	1:B:796:PHE:CE2	2.56	0.41
1:B:758:LEU:CD2	1:B:762:ARG:NE	2.76	0.41
2:C:354:LYS:C	2:C:356:LEU:H	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:352:GLU:HA	2:F:355:ASP:OD2	2.21	0.41
1:A:205:THR:O	1:A:206:LYS:C	2.62	0.41
1:A:360:GLU:O	1:A:363:ILE:HG22	2.21	0.41
1:A:488:ALA:HB2	1:B:870:ARG:HH22	1.86	0.41
1:A:548:GLN:O	1:A:549:LYS:C	2.64	0.41
1:A:686:LEU:CD1	1:A:727:GLU:HG2	2.50	0.41
1:B:27:ARG:CG	1:B:28:ALA:N	2.73	0.41
1:B:277:LEU:HD23	1:B:277:LEU:HA	1.83	0.41
1:B:524:LEU:HD13	1:B:524:LEU:C	2.45	0.41
1:A:224:GLU:O	1:A:226:THR:N	2.54	0.40
1:A:259:ALA:O	1:A:260:LEU:C	2.62	0.40
1:A:626:GLU:HB2	1:A:666:VAL:CG2	2.50	0.40
1:A:850:GLY:O	1:A:859:LYS:HA	2.20	0.40
1:B:28:ALA:O	1:B:33:LEU:HD23	2.21	0.40
1:B:401:GLN:O	1:B:401:GLN:CG	2.69	0.40
1:B:479:GLU:HA	1:B:538:ASN:ND2	2.33	0.40
1:B:740:GLN:HG3	1:B:796:PHE:CE2	2.56	0.40
2:C:382:GLN:O	2:C:383:VAL:C	2.64	0.40
1:A:287:CYS:HB3	1:A:354:LEU:HD13	2.03	0.40
1:B:444:ILE:N	1:B:444:ILE:CD1	2.84	0.40
1:B:612:LEU:O	1:B:616:GLN:HG3	2.22	0.40
2:C:360:THR:O	2:C:361:ASP:HB3	2.21	0.40
2:E:380:LEU:HB2	2:F:380:LEU:HD13	2.03	0.40
1:A:51:GLN:NE2	1:A:105:ARG:NE	2.69	0.40
1:A:62:LYS:HG2	1:A:111:GLN:HB3	2.02	0.40
1:A:89:ARG:HG3	1:A:89:ARG:HH11	1.86	0.40
1:A:105:ARG:C	1:A:107:SER:H	2.26	0.40
1:A:202:LEU:HD11	1:A:240:ASN:HD22	1.85	0.40
1:A:249:TYR:CD1	1:A:249:TYR:C	2.99	0.40
1:A:343:ASN:HD21	1:A:345:CYS:HB3	1.86	0.40
1:A:350:VAL:HA	1:A:353:MET:HE3	2.03	0.40
1:A:453:LEU:O	1:A:457:ILE:HG13	2.22	0.40
1:A:648:GLU:C	1:A:650:PHE:H	2.29	0.40
1:B:460:LEU:HD11	1:B:474:PHE:CE2	2.56	0.40
2:E:396:LEU:C	2:E:398:ASN:H	2.29	0.40
1:A:363:ILE:O	1:A:364:VAL:C	2.65	0.40
1:A:859:LYS:HB2	1:A:859:LYS:HE3	1.89	0.40
1:B:27:ARG:HG2	1:B:27:ARG:HH11	1.86	0.40
1:B:335:GLU:CG	1:B:380:TRP:CZ2	3.04	0.40
1:B:448:TYR:C	1:B:451:PRO:HD2	2.47	0.40
1:B:784:HIS:NE2	1:B:786:ASP:CG	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:826:CYS:C	1:B:828:ALA:N	2.78	0.40
1:B:831:LYS:O	1:B:833:VAL:N	2.54	0.40
2:F:357:VAL:HG12	2:F:358:MSE:N	2.37	0.40
1:A:73:LYS:C	1:A:75:GLN:N	2.80	0.40
1:A:514:THR:CG2	1:A:529:TYR:CZ	3.05	0.40
1:A:579:ASP:O	1:A:583:LEU:HG	2.21	0.40
1:A:859:LYS:O	1:A:863:THR:OG1	2.39	0.40
1:B:428:THR:C	1:B:430:TRP:N	2.78	0.40
1:B:599:ASP:O	1:B:603:ILE:N	2.55	0.40
2:F:370:LEU:O	2:F:374:ILE:HG13	2.22	0.40
2:F:385:HIS:O	2:F:388:ARG:HG2	2.21	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:171:ASN:CB	2:F:402:LYS:NZ[4_556]	1.72	0.48

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	874/876 (100%)	695 (80%)	146 (17%)	33 (4%)	2	15
1	B	874/876 (100%)	671 (77%)	143 (16%)	60 (7%)	1	5
2	C	59/61 (97%)	47 (80%)	12 (20%)	0	100	100
2	D	59/61 (97%)	45 (76%)	8 (14%)	6 (10%)	0	2
2	E	59/61 (97%)	48 (81%)	8 (14%)	3 (5%)	1	10
2	F	59/61 (97%)	45 (76%)	8 (14%)	6 (10%)	0	2
All	All	1984/1996 (99%)	1551 (78%)	325 (16%)	108 (5%)	1	9

All (108) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	166	LEU
1	A	168	ASP
1	A	169	LYS
1	A	462	ALA
1	A	683	SER
1	A	752	PHE
1	A	753	ASP
1	A	809	ASP
1	B	28	ALA
1	B	52	VAL
1	B	212	GLU
1	B	340	ASP
1	B	446	ASP
1	B	486	ASP
1	B	523	ASN
1	B	604	SER
1	B	621	SER
1	B	660	ASN
1	B	752	PHE
1	B	874	ASN
2	D	366	LYS
2	E	357	VAL
2	E	361	ASP
2	E	365	HIS
2	F	345	SER
2	F	357	VAL
2	F	365	HIS
2	F	402	LYS
1	A	49	ASN
1	A	225	ALA
1	A	519	GLY
1	A	800	PHE
1	A	830	GLY
1	B	12	SER
1	B	68	LYS
1	B	252	MET
1	B	259	ALA
1	B	270	SER
1	B	361	ASP
1	B	445	ASN
1	B	469	ASN
1	B	664	TYR

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Mol	Chain	Res	Type
1	B	689	CYS
1	B	725	GLY
1	B	733	GLU
1	B	746	GLN
1	B	750	SER
1	B	789	LEU
1	B	811	THR
1	B	852	ARG
1	B	853	SER
2	D	397	ALA
2	D	398	ASN
2	D	401	ASN
2	F	364	MSE
2	F	393	VAL
1	A	14	ASP
1	A	70	PRO
1	A	74	ALA
1	A	132	GLN
1	A	616	GLN
1	A	660	ASN
1	A	682	GLN
1	A	749	LYS
1	A	780	GLN
1	B	17	GLU
1	B	44	LEU
1	B	96	LEU
1	B	105	ARG
1	B	344	PRO
1	B	427	THR
1	B	659	LYS
1	B	805	ALA
1	B	832	ASP
1	B	875	GLN
2	D	367	SER
1	A	93	ASN
1	A	733	GLU
1	A	781	GLU
1	A	832	ASP
1	B	72	ILE
1	B	184	GLU
1	B	518	ASP
1	B	598	GLN

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Mol	Chain	Res	Type
1	B	650	PHE
1	B	661	TYR
1	B	782	ASN
1	B	795	GLU
1	A	20	ALA
1	A	517	PRO
1	A	649	ALA
1	A	798	LEU
1	B	62	LYS
1	B	124	SER
1	B	185	GLU
1	B	408	GLN
1	B	416	LEU
1	B	524	LEU
1	B	839	ALA
2	D	361	ASP
1	A	664	TYR
1	A	783	VAL
1	B	11	VAL
1	B	431	THR
1	B	561	VAL
1	B	734	VAL
1	B	494	PRO
1	A	105	ARG

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	753/753 (100%)	689 (92%)	64 (8%)	10	36
1	B	753/753 (100%)	682 (91%)	71 (9%)	8	32
2	C	56/53 (106%)	50 (89%)	6 (11%)	6	26
2	D	56/53 (106%)	51 (91%)	5 (9%)	9	34
2	E	56/53 (106%)	52 (93%)	4 (7%)	13	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	56/53 (106%)	49 (88%)	7 (12%)	4	20
All	All	1730/1718 (101%)	1573 (91%)	157 (9%)	9	33

All (157) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	GLU
1	A	111	GLN
1	A	125	GLN
1	A	146	MET
1	A	148	GLU
1	A	150	THR
1	A	157	ILE
1	A	166	LEU
1	A	174	LEU
1	A	234	ARG
1	A	255	TYR
1	A	269	LYS
1	A	281	GLU
1	A	298	SER
1	A	308	GLU
1	A	319	LEU
1	A	331	THR
1	A	333	GLN
1	A	334	ASP
1	A	352	LEU
1	A	354	LEU
1	A	413	LEU
1	A	422	VAL
1	A	441	GLU
1	A	468	SER
1	A	489	ASP
1	A	494	PRO
1	A	497	TYR
1	A	502	SER
1	A	504	GLU
1	A	507	VAL
1	A	514	THR
1	A	517	PRO
1	A	524	LEU
1	A	525	ARG
1	A	526	SER

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Mol	Chain	Res	Type
1	A	530	GLU
1	A	535	ILE
1	A	536	VAL
1	A	576	GLN
1	A	580	LEU
1	A	581	GLN
1	A	594	LYS
1	A	626	GLU
1	A	627	ASP
1	A	633	SER
1	A	673	LEU
1	A	687	PRO
1	A	688	PHE
1	A	689	CYS
1	A	716	VAL
1	A	732	LEU
1	A	743	SER
1	A	751	ASP
1	A	758	LEU
1	A	785	PRO
1	A	811	THR
1	A	821	LEU
1	A	831	LYS
1	A	832	ASP
1	A	840	ARG
1	A	860	THR
1	A	863	THR
1	A	867	LYS
1	B	17	GLU
1	B	52	VAL
1	B	67	SER
1	B	68	LYS
1	B	70	PRO
1	B	97	GLN
1	B	145	HIS
1	B	165	GLN
1	B	203	GLU
1	B	226	THR
1	B	231	THR
1	B	234	ARG
1	B	243	LYS
1	B	246	SER

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Mol	Chain	Res	Type
1	B	250	GLN
1	B	266	GLU
1	B	274	GLU
1	B	296	GLU
1	B	298	SER
1	B	308	GLU
1	B	319	LEU
1	B	320	GLN
1	B	331	THR
1	B	345	CYS
1	B	346	LYS
1	B	350	VAL
1	B	352	LEU
1	B	354	LEU
1	B	355	LEU
1	B	362	ASP
1	B	368	LEU
1	B	377	ASN
1	B	388	MET
1	B	413	LEU
1	B	422	VAL
1	B	425	ARG
1	B	432	VAL
1	B	447	VAL
1	B	453	LEU
1	B	470	VAL
1	B	492	GLU
1	B	494	PRO
1	B	497	TYR
1	B	514	THR
1	B	521	GLN
1	B	534	GLU
1	B	551	THR
1	B	601	LEU
1	B	608	MET
1	B	612	LEU
1	B	626	GLU
1	B	630	MET
1	B	637	GLU
1	B	642	GLU
1	B	651	LYS
1	B	659	LYS

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Mol	Chain	Res	Type
1	B	661	TYR
1	B	673	LEU
1	B	681	LEU
1	B	703	GLU
1	B	716	VAL
1	B	722	LEU
1	B	753	ASP
1	B	758	LEU
1	B	779	ASP
1	B	781	GLU
1	B	783	VAL
1	B	785	PRO
1	B	817	CYS
1	B	821	LEU
1	B	835	LYS
2	C	356	LEU
2	C	361	ASP
2	C	364	MSE
2	C	367	SER
2	C	387	LEU
2	C	395	LYS
2	D	351	ILE
2	D	364	MSE
2	D	369	VAL
2	D	370	LEU
2	D	399	GLN
2	E	346	ILE
2	E	364	MSE
2	E	395	LYS
2	E	398	ASN
2	F	356	LEU
2	F	363	LYS
2	F	364	MSE
2	F	383	VAL
2	F	389	GLN
2	F	396	LEU
2	F	403	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN

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Mol	Chain	Res	Type
1	A	32	ASN
1	A	49	ASN
1	A	111	GLN
1	A	139	ASN
1	A	141	ASN
1	A	159	GLN
1	A	196	ASN
1	A	208	ASN
1	A	220	GLN
1	A	240	ASN
1	A	278	GLN
1	A	328	GLN
1	A	336	ASN
1	A	366	HIS
1	A	377	ASN
1	A	401	GLN
1	A	520	HIS
1	A	523	ASN
1	A	538	ASN
1	A	563	GLN
1	A	576	GLN
1	A	590	ASN
1	A	596	GLN
1	A	597	HIS
1	A	625	GLN
1	A	660	ASN
1	A	665	GLN
1	A	684	ASN
1	A	702	ASN
1	A	737	ASN
1	A	740	GLN
1	A	741	GLN
1	A	759	ASN
1	A	784	HIS
1	A	803	HIS
1	A	856	ASN
1	A	874	ASN
1	B	22	GLN
1	B	32	ASN
1	B	75	GLN
1	B	97	GLN
1	B	132	GLN

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Mol	Chain	Res	Type
1	B	141	ASN
1	B	159	GLN
1	B	165	GLN
1	B	167	GLN
1	B	179	GLN
1	B	220	GLN
1	B	240	ASN
1	B	320	GLN
1	B	343	ASN
1	B	377	ASN
1	B	454	GLN
1	B	469	ASN
1	B	522	ASN
1	B	548	GLN
1	B	560	GLN
1	B	578	ASN
1	B	589	GLN
1	B	590	ASN
1	B	596	GLN
1	B	602	GLN
1	B	625	GLN
1	B	660	ASN
1	B	694	GLN
1	B	759	ASN
1	B	774	GLN
1	B	780	GLN
1	B	791	GLN
2	C	401	ASN
2	D	347	ASN
2	D	381	GLN
2	D	385	HIS
2	D	391	ASN
2	D	398	ASN
2	E	398	ASN
2	F	365	HIS
2	F	389	GLN
2	F	398	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.