



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:09 PM UTC

PDB ID : 1TR2 / pdb_00001tr2
Title : Crystal structure of human full-length vinculin (residues 1-1066)
Authors : Borgon, R.A.; Vornrhein, C.; Bricogne, G.; Bois, P.R.; Izard, T.
Deposited on : 2004-06-19
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	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

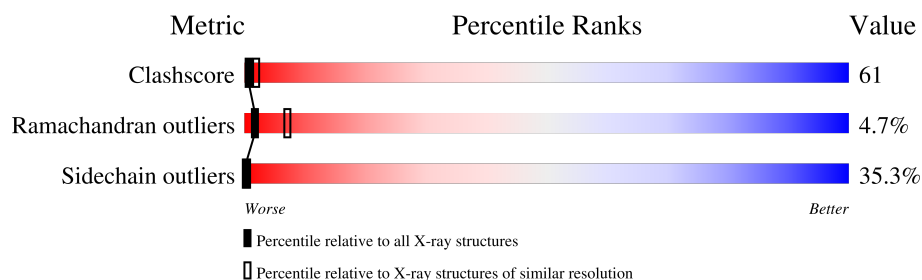
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

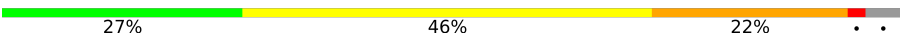
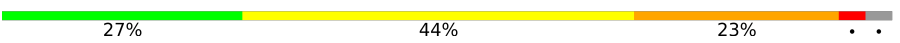
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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	1066	 27% 46% 22% . .
1	B	1066	 27% 44% 23% . .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16033 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 VINCULIN ISOFORM 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1028	Total	C	N	O	S	Se	99	8	0
			7908	4876	1436	1550	10	36			
1	B	1029	Total	C	N	O	S	Se	117	7	0
			7907	4873	1438	1550	10	36			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	initiating methionine	UNP P18206
A	26	MSE	MET	modified residue	UNP P18206
A	74	MSE	MET	modified residue	UNP P18206
A	94	MSE	MET	modified residue	UNP P18206
A	154	MSE	MET	modified residue	UNP P18206
A	168	MSE	MET	modified residue	UNP P18206
A	171	MSE	MET	modified residue	UNP P18206
A	174	MSE	MET	modified residue	UNP P18206
A	190	MSE	MET	modified residue	UNP P18206
A	195	MSE	MET	modified residue	UNP P18206
A	209	MSE	MET	modified residue	UNP P18206
A	237	MSE	MET	modified residue	UNP P18206
A	266	MSE	MET	modified residue	UNP P18206
A	327	MSE	MET	modified residue	UNP P18206
A	331	MSE	MET	modified residue	UNP P18206
A	350	MSE	MET	modified residue	UNP P18206
A	377	MSE	MET	modified residue	UNP P18206
A	533	MSE	MET	modified residue	UNP P18206
A	534	MSE	MET	modified residue	UNP P18206
A	587	MSE	MET	modified residue	UNP P18206
A	591	MSE	MET	modified residue	UNP P18206
A	698	MSE	MET	modified residue	UNP P18206
A	709	MSE	MET	modified residue	UNP P18206
A	741	MSE	MET	modified residue	UNP P18206
A	748	MSE	MET	modified residue	UNP P18206

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Chain	Residue	Modelled	Actual	Comment	Reference
A	797	MSE	MET	modified residue	UNP P18206
A	799	MSE	MET	modified residue	UNP P18206
A	898	MSE	MET	modified residue	UNP P18206
A	899	MSE	MET	modified residue	UNP P18206
A	900	MSE	MET	modified residue	UNP P18206
A	926	MSE	MET	modified residue	UNP P18206
A	930	MSE	MET	modified residue	UNP P18206
A	933	MSE	MET	modified residue	UNP P18206
A	1005	MSE	MET	modified residue	UNP P18206
A	1022	MSE	MET	modified residue	UNP P18206
A	1031	MSE	MET	modified residue	UNP P18206
B	1	MSE	MET	initiating methionine	UNP P18206
B	26	MSE	MET	modified residue	UNP P18206
B	74	MSE	MET	modified residue	UNP P18206
B	94	MSE	MET	modified residue	UNP P18206
B	154	MSE	MET	modified residue	UNP P18206
B	168	MSE	MET	modified residue	UNP P18206
B	171	MSE	MET	modified residue	UNP P18206
B	174	MSE	MET	modified residue	UNP P18206
B	190	MSE	MET	modified residue	UNP P18206
B	195	MSE	MET	modified residue	UNP P18206
B	209	MSE	MET	modified residue	UNP P18206
B	237	MSE	MET	modified residue	UNP P18206
B	266	MSE	MET	modified residue	UNP P18206
B	327	MSE	MET	modified residue	UNP P18206
B	331	MSE	MET	modified residue	UNP P18206
B	350	MSE	MET	modified residue	UNP P18206
B	377	MSE	MET	modified residue	UNP P18206
B	533	MSE	MET	modified residue	UNP P18206
B	534	MSE	MET	modified residue	UNP P18206
B	587	MSE	MET	modified residue	UNP P18206
B	591	MSE	MET	modified residue	UNP P18206
B	698	MSE	MET	modified residue	UNP P18206
B	709	MSE	MET	modified residue	UNP P18206
B	741	MSE	MET	modified residue	UNP P18206
B	748	MSE	MET	modified residue	UNP P18206
B	797	MSE	MET	modified residue	UNP P18206
B	799	MSE	MET	modified residue	UNP P18206
B	898	MSE	MET	modified residue	UNP P18206
B	899	MSE	MET	modified residue	UNP P18206
B	900	MSE	MET	modified residue	UNP P18206
B	926	MSE	MET	modified residue	UNP P18206

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Chain	Residue	Modelled	Actual	Comment	Reference
B	930	MSE	MET	modified residue	UNP P18206
B	933	MSE	MET	modified residue	UNP P18206
B	1005	MSE	MET	modified residue	UNP P18206
B	1022	MSE	MET	modified residue	UNP P18206
B	1031	MSE	MET	modified residue	UNP P18206

- Molecule 2 is water.

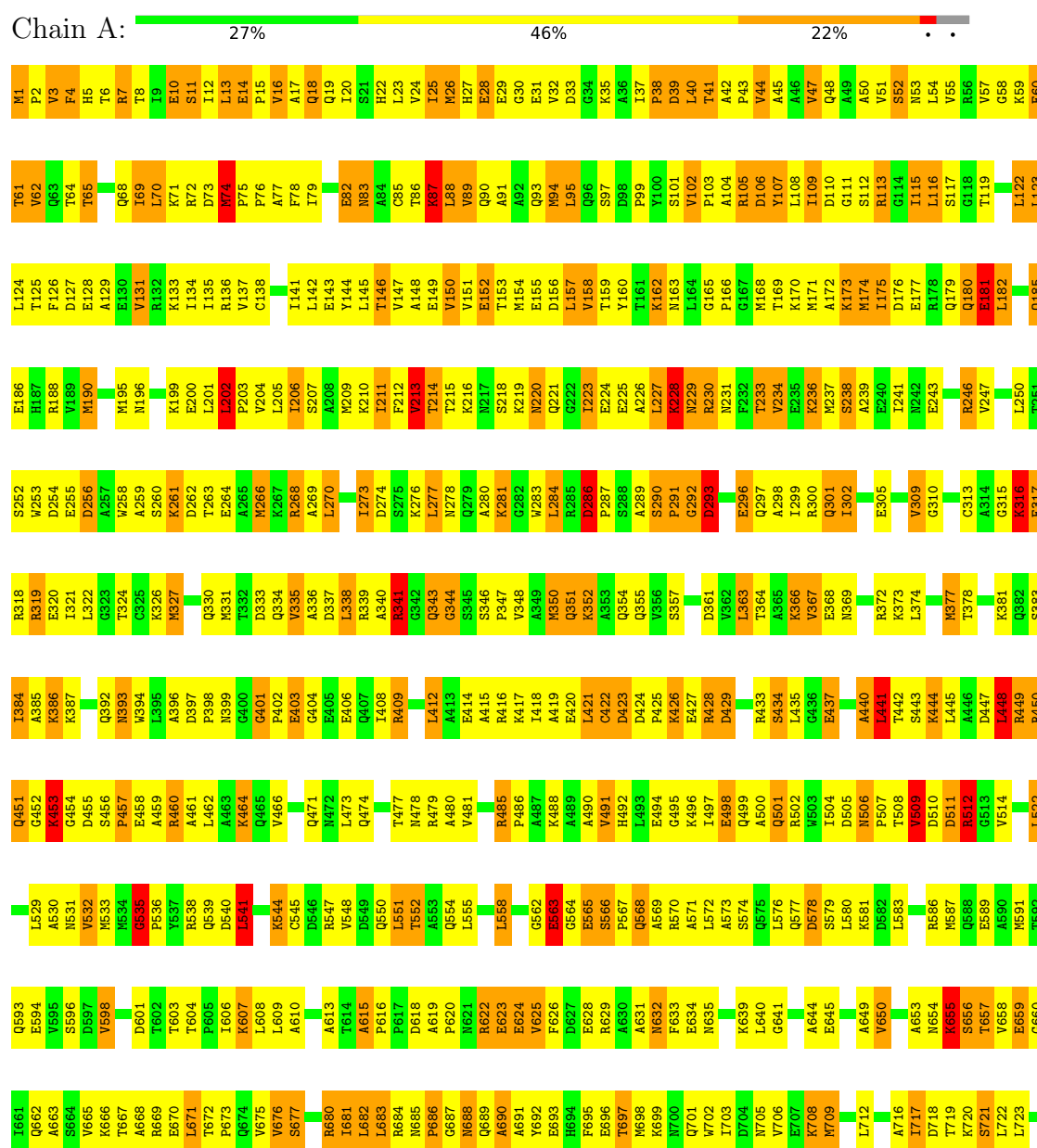
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	108	Total	O	0	0
			108	108		
2	B	110	Total	O	0	0
			110	110		

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: VINCULIN ISOFORM 1





Response	Percentage
Good job	27%
Not a good job	44%
Don't know	23%
Other	2%
No answer	2%



TRP TYR GLN	L995	K996	T997	L998	S999	T1000	V1001	K1002	A1003	T1004	M1005	L1006	G1007	R1008											D597	V598	F599	S600											T603	T604	P605	L606	K607	L608	L609	A610	V611	A612	A613	T614	A615	P616	F617	D618	A619	P620	F626	D627	E628	R629											M632	F633	E634	M635													K639	L640	G641	A644	E645											A648	A649	V650											A653	K654	K655	S656	T657	V658	E659	G660	I661	Q662	A663							
	R925	M926	A927	L928	L929	M930	A931	E932	M933	S934	R935	L936	V937											D800	A801	K802	A803	V804											N807	I808	S809	D810	P811	N812	L813	Q814	K815	S816	F817	L749	E750	A751											T754	S755	I756	A757	R758	R759	A760	N761	R762	I763	L764	L765	V766	A767	K768	R769	E770	V771	E772											D776	R780											K784	A785	A786	S787	D788	E789	L790	S791	K792	T793	I794	S795	P796	V797	V798	M799													
	PR0	PR0	LEU	PR0	GLU	GLY	VAL	PR0	PR0	PR0	PR0	ARG	PR0	PR0	PR0	P877	P878	E879	E880	K881	D882	E883	E884	F885	P886	E887	Q888	K889											E892	E893	R894	T894	N895	Q896	P897	N898	M899	N900	A901	A902	R903	Q904	L905	H906	D907	E908	A909	R910	K911	W912	S913	S914	K915	G916	N917	D918	I919	I920	A921													K924																																																		
											R925	M926	A927	L928	L929	M930	A931	E932	M933	S934	R935	L936	V937											G940	S941	G942	T943	K944	R945	A946	L947	I948	Q949	C950											D953	L954	A955	K956	A957	S958	D959	E960	V961	T962	R963	L964											E967											C972	T973	D974	K975	R976	I977	R978											L981											C985	E986	R987	I988	P989	T990											T993
										K1035	E1036											M1031	Q1032											E1042	S1045	I1046	K1047	I1048	R1049	T1050	D1051	A1052	G1053	F1054	T1055	L1056	R1057											R1060	K1061	T1062	PR0																																																																							

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.74Å 154.08Å 108.95Å 90.00° 90.44° 90.00°	Depositor
Resolution (Å)	56.86 – 2.90	Depositor
% Data completeness (in resolution range)	100.0 (56.86-2.90)	Depositor
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	BUSTER-TNT 1.1.1	Depositor
R, R_{free}	0.232 , 0.300	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16033	wwPDB-VP
Average B, all atoms (Å ²)	92.0	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	0.51	0/7994	1.06	42/10720 (0.4%)
1	B	0.51	0/7992	1.05	53/10717 (0.5%)
All	All	0.51	0/15986	1.05	95/21437 (0.4%)

There are no bond length outliers.

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	675	VAL	N-CA-C	-11.51	102.53	111.62
1	A	794	ILE	N-CA-C	11.27	121.02	110.42
1	A	107	TYR	N-CA-C	-9.30	101.36	112.89
1	A	615	ALA	CA-C-N	9.29	129.95	120.38
1	A	615	ALA	C-N-CA	9.29	129.95	120.38
1	B	686	PRO	N-CA-C	-8.78	105.55	114.68
1	A	877	PRO	CA-C-N	8.07	127.64	119.24
1	A	877	PRO	C-N-CA	8.07	127.64	119.24
1	B	461	ALA	N-CA-C	-7.99	103.09	112.92
1	B	401	GLY	CA-C-N	7.79	127.44	119.19
1	B	401	GLY	C-N-CA	7.79	127.44	119.19
1	B	615	ALA	CA-C-N	7.44	128.05	120.38
1	B	615	ALA	C-N-CA	7.44	128.05	120.38
1	A	1054	PHE	CA-CB-CG	7.34	121.14	113.80
1	B	716	ALA	N-CA-C	-7.18	104.78	113.97
1	A	1049	ARG	N-CA-C	7.16	120.23	108.99
1	B	1	MSE	CA-C-N	-7.11	110.95	119.84
1	B	1	MSE	C-N-CA	-7.11	110.95	119.84
1	A	511	ASP	N-CA-C	-7.10	104.77	113.50
1	A	401	GLY	CA-C-N	6.90	128.47	119.84
1	A	401	GLY	C-N-CA	6.90	128.47	119.84
1	B	290	SER	CA-C-N	6.76	128.29	119.84
1	B	290	SER	C-N-CA	6.76	128.29	119.84
1	A	649	ALA	N-CA-C	6.73	118.31	110.97
1	A	352	LYS	N-CA-C	-6.69	105.65	113.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	824	ILE	N-CA-C	-6.52	104.29	110.42
1	B	202	LEU	CA-C-N	6.51	126.74	119.32
1	B	202	LEU	C-N-CA	6.51	126.74	119.32
1	A	202	LEU	CA-C-N	6.46	125.96	119.24
1	A	202	LEU	C-N-CA	6.46	125.96	119.24
1	A	578	ASP	N-CA-C	-6.42	105.75	113.97
1	A	624	GLU	N-CA-C	-6.17	105.66	113.43
1	B	107	TYR	N-CA-C	-6.13	105.45	113.17
1	B	798	VAL	N-CA-C	6.12	116.87	110.62
1	A	181	GLU	N-CA-C	6.08	120.70	113.28
1	B	106	ASP	N-CA-C	-6.05	105.20	114.16
1	B	23	LEU	N-CA-C	-6.03	105.18	112.54
1	B	462	LEU	N-CA-C	-5.95	104.18	112.45
1	B	352	LYS	N-CA-C	-5.94	106.07	113.55
1	B	98	ASP	CA-C-N	5.90	127.22	119.84
1	B	98	ASP	C-N-CA	5.90	127.22	119.84
1	B	653	ALA	N-CA-C	5.88	119.05	108.17
1	A	514	VAL	N-CA-C	5.88	117.33	110.62
1	A	805	ALA	N-CA-C	-5.84	104.83	111.14
1	B	96	GLN	N-CA-C	-5.83	105.01	111.71
1	B	165	GLY	CA-C-N	5.80	125.00	118.97
1	B	165	GLY	C-N-CA	5.80	125.00	118.97
1	B	181	GLU	N-CA-C	5.77	120.39	113.23
1	B	509	VAL	N-CA-C	5.75	117.62	108.87
1	B	241	ILE	N-CA-C	-5.75	104.75	110.62
1	A	273	ILE	N-CA-C	-5.69	104.80	111.00
1	B	309	VAL	N-CA-C	-5.69	105.55	111.58
1	A	655	LYS	N-CA-C	-5.63	105.51	112.38
1	A	541	LEU	N-CA-C	-5.59	104.88	110.97
1	A	290	SER	CA-C-N	5.56	126.79	119.84
1	A	290	SER	C-N-CA	5.56	126.79	119.84
1	B	252	SER	N-CA-C	5.44	115.74	108.23
1	B	460	ARG	N-CA-C	-5.44	106.49	113.02
1	B	616	PRO	CA-N-CD	-5.37	104.48	112.00
1	A	690	ALA	N-CA-C	-5.37	106.24	112.89
1	B	456	SER	CA-C-N	-5.35	113.16	119.84
1	B	456	SER	C-N-CA	-5.35	113.16	119.84
1	A	409[A]	ARG	N-CA-C	-5.33	105.13	111.69
1	A	409[B]	ARG	N-CA-C	-5.33	105.13	111.69
1	A	838	GLN	N-CA-C	5.30	118.13	110.28
1	A	510	ASP	N-CA-C	5.29	116.77	109.15
1	B	31	GLU	N-CA-C	-5.28	107.49	114.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	MSE	CA-C-N	5.28	125.82	120.38
1	A	74	MSE	C-N-CA	5.28	125.82	120.38
1	B	619	ALA	CA-C-N	5.24	125.14	119.85
1	B	619	ALA	C-N-CA	5.24	125.14	119.85
1	B	87	LYS	N-CA-C	-5.23	106.92	113.72
1	B	362	VAL	N-CA-C	-5.21	105.63	110.53
1	A	344	GLY	N-CA-C	-5.21	107.86	114.16
1	B	800	ASP	N-CA-C	-5.21	105.67	112.23
1	B	813	LEU	N-CA-C	-5.20	107.00	113.55
1	B	511	ASP	N-CA-C	-5.18	107.01	113.38
1	A	509	VAL	N-CA-C	5.17	116.25	109.21
1	B	649	ALA	N-CA-C	5.17	117.70	111.40
1	B	654	ASN	N-CA-C	-5.15	99.82	110.80
1	B	284	LEU	N-CA-C	-5.13	106.53	112.89
1	B	446	ALA	N-CA-C	-5.11	105.41	111.69
1	A	927	ALA	N-CA-C	-5.10	105.41	110.97
1	B	514	VAL	N-CA-C	5.10	115.82	110.62
1	A	89	VAL	N-CA-C	-5.09	104.72	111.09
1	A	87	LYS	N-CA-C	-5.09	107.10	113.72
1	B	89	VAL	N-CA-C	-5.08	104.74	111.09
1	A	716	ALA	N-CA-C	-5.07	107.23	113.41
1	B	794	ILE	N-CA-C	5.05	119.83	109.34
1	A	535	GLY	CA-C-N	5.04	124.83	119.28
1	A	535	GLY	C-N-CA	5.04	124.83	119.28
1	B	691	ALA	N-CA-C	-5.03	105.99	112.68
1	B	655	LYS	CA-C-N	5.03	131.15	121.54
1	B	655	LYS	C-N-CA	5.03	131.15	121.54
1	A	801	ALA	N-CA-C	-5.01	106.01	111.82

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7908	0	8065	937	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	7907	0	8072	979	0
2	A	108	0	0	12	0
2	B	110	0	0	12	0
All	All	16033	0	16137	1911	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 61.

All (1911) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:THR:HG21	1:B:70:LEU:HD22	1.21	1.18
1:A:74:MSE:HE3	1:A:122:LEU:HD21	1.18	1.18
1:B:913:SER:HB2	1:B:915:LYS:HG3	1.24	1.17
1:B:729:ALA:HA	1:B:732:LYS:HD3	1.24	1.16
1:B:215:THR:HG22	1:B:223:ILE:HG13	1.26	1.16
1:A:732:LYS:HE2	1:A:736:LYS:HE2	1.28	1.14
1:A:898:MSE:HE1	1:A:1023:LEU:HD23	1.30	1.14
1:A:65:THR:HG21	1:A:70:LEU:HD22	1.19	1.12
1:A:426:LYS:HE3	1:A:427:GLU:HG3	1.23	1.10
1:B:153:THR:HB	1:B:156:ASP:HB2	1.12	1.08
1:B:697:THR:HG22	1:B:698:MSE:HE2	1.35	1.08
1:A:153:THR:HB	1:A:156:ASP:HB2	1.10	1.08
1:A:807:ASN:HB3	1:A:810:ASP:HB3	1.37	1.07
1:B:20:ILE:HD11	1:B:115:ILE:HG12	1.09	1.06
1:B:807:ASN:ND2	1:B:807:ASN:H	1.45	1.06
1:A:53:ASN:HB3	1:B:288:SER:HB2	1.35	1.06
1:A:913:SER:HB2	1:A:915:LYS:HG2	1.35	1.03
1:B:613:ALA:HB1	1:B:682:LEU:HD12	1.41	1.02
1:A:158:VAL:HG13	1:A:162:LYS:HE3	1.41	1.02
1:A:281:LYS:HA	1:A:284:LEU:HD12	1.40	1.01
1:B:216:LYS:HA	1:B:223:ILE:HG12	1.40	1.01
1:A:74:MSE:CE	1:A:122:LEU:HD21	1.91	1.01
1:B:158:VAL:HG13	1:B:162:LYS:HE3	1.45	0.99
1:A:445:LEU:HB2	1:A:462:LEU:HD23	1.45	0.99
1:A:441:LEU:HA	1:A:444:LYS:HZ2	1.28	0.98
1:B:256:ASP:HA	1:B:258:TRP:CZ3	1.98	0.98
1:A:770:GLU:HG2	1:A:835:PHE:HE1	1.29	0.97
1:B:898:MSE:HE1	1:B:1023:LEU:HD23	1.47	0.96
1:A:491:VAL:HG11	1:A:658:VAL:HG11	1.44	0.96
1:A:215:THR:HG22	1:A:223:ILE:HG13	1.46	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:811:PRO:HB3	1:A:815:LYS:HE2	1.47	0.95
1:A:589:GLU:HG2	1:A:593:GLN:HE21	1.30	0.94
1:A:441:LEU:HD23	1:A:441:LEU:H	1.33	0.94
1:B:589:GLU:HG2	1:B:593:GLN:HE21	1.27	0.94
1:B:671:LEU:HD23	1:B:671:LEU:H	1.33	0.94
1:A:20:ILE:HD11	1:A:115:ILE:HG12	1.49	0.93
1:A:109:ILE:HD13	1:A:1008[B]:ARG:HH21	1.29	0.93
1:A:113:ARG:HB2	1:A:1004:THR:HG21	1.51	0.93
1:A:447:ASP:HA	1:A:450:ARG:HD2	1.50	0.93
1:B:897:PRO:HB2	1:B:1024:VAL:HG11	1.47	0.93
1:B:738:LYS:HA	1:B:741:MSE:HE2	1.50	0.93
1:B:22:HIS:HA	1:B:25:ILE:HG13	1.47	0.93
1:B:31:GLU:HA	1:B:105:ARG:NH2	1.84	0.92
1:B:936:LEU:HB3	1:B:943:THR:HG23	1.49	0.92
1:A:778:LYS:HD2	1:A:1049:ARG:HH12	1.35	0.92
1:B:913:SER:HB2	1:B:915:LYS:CG	2.00	0.92
1:B:448:LEU:HA	1:B:451:GLN:HG2	1.51	0.92
1:A:69:ILE:H	1:A:69:ILE:HD12	1.33	0.91
1:B:40:LEU:HB2	1:B:43:PRO:CG	1.98	0.91
1:A:453:LYS:H	1:A:453:LYS:HD2	1.34	0.91
1:B:1:MSE:HE1	1:B:1018:GLN:NE2	1.86	0.91
1:A:409[B]:ARG:NH2	1:A:442:THR:HB	1.86	0.91
1:B:75:PRO:HA	1:B:78:PHE:CD2	2.06	0.91
1:A:770:GLU:HG2	1:A:835:PHE:CE1	2.05	0.90
1:A:960:GLU:HG2	1:A:963:ARG:HH21	1.36	0.90
1:B:74:MSE:HE3	1:B:122:LEU:HD21	1.54	0.90
1:B:138:CYS:SG	1:B:171:MSE:HE3	2.10	0.90
1:A:51:VAL:HG11	1:A:115:ILE:HD12	1.53	0.90
1:B:906:HIS:HB2	1:B:927:ALA:HB1	1.52	0.90
1:B:926:MSE:HA	1:B:929:LEU:HB2	1.53	0.90
1:B:40:LEU:HB2	1:B:43:PRO:HG2	1.50	0.90
1:B:215:THR:HG23	1:B:220:ASN:HB2	1.52	0.90
1:B:116:LEU:HD13	1:B:1001:VAL:HG23	1.53	0.90
1:B:793:THR:HG23	1:B:824:ILE:HG12	1.52	0.90
1:B:179:GLN:HA	1:B:182:LEU:HD22	1.50	0.90
1:B:445:LEU:HB2	1:B:462:LEU:HD23	1.54	0.90
1:A:28:GLU:HG2	1:A:945:ARG:HE	1.37	0.90
1:A:491:VAL:CG1	1:A:658:VAL:HG11	2.01	0.89
1:A:138:CYS:SG	1:A:171:MSE:HE3	2.12	0.89
1:A:74:MSE:HE2	1:A:78:PHE:CZ	2.07	0.89
1:B:153:THR:HG22	1:B:154:MSE:H	1.36	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:533:MSE:CE	1:B:541:LEU:HD12	2.01	0.89
1:B:807:ASN:H	1:B:807:ASN:HD22	0.94	0.89
1:A:914:SER:N	1:A:915:LYS:HE2	1.88	0.89
1:A:675:VAL:HG22	1:A:698:MSE:HB3	1.54	0.88
1:A:789:GLU:HG2	1:A:830:LYS:NZ	1.88	0.88
1:B:281:LYS:HA	1:B:284:LEU:HD12	1.55	0.88
1:B:770:GLU:HG2	1:B:835:PHE:HE1	1.38	0.88
1:A:688:ASN:O	1:A:690:ALA:N	2.07	0.88
1:A:936:LEU:HB3	1:A:943:THR:HG23	1.56	0.88
1:A:75:PRO:HA	1:A:78:PHE:CD2	2.08	0.87
1:B:216:LYS:CA	1:B:223:ILE:HG12	2.03	0.87
1:A:641:GLY:HA2	1:A:709:MSE:HE1	1.56	0.87
1:B:69:ILE:HD12	1:B:69:ILE:H	1.40	0.87
1:B:807:ASN:HD22	1:B:807:ASN:N	1.73	0.87
1:A:558:LEU:HD22	1:A:569:ALA:HB2	1.53	0.87
1:A:153:THR:HB	1:A:156:ASP:CB	2.03	0.87
1:B:95:LEU:HD21	1:B:105:ARG:HG3	1.57	0.86
1:B:27:HIS:CD2	1:B:108:LEU:HD23	2.10	0.86
1:A:153:THR:HG22	1:A:154:MSE:H	1.39	0.86
1:B:898:MSE:HE1	1:B:1023:LEU:CD2	2.04	0.86
1:A:220:ASN:HD22	1:A:220:ASN:H	1.21	0.86
1:B:113:ARG:HB3	1:B:1004:THR:CG2	2.05	0.86
1:B:394:TRP:HE1	1:B:401:GLY:H	1.22	0.86
1:A:441:LEU:HA	1:A:444:LYS:NZ	1.90	0.86
1:B:558:LEU:HD22	1:B:569:ALA:HB2	1.56	0.86
1:B:94:MSE:HE2	1:B:104:ALA:HB2	1.55	0.86
1:B:276:LYS:HE3	1:B:301:GLN:HE21	1.40	0.86
1:A:926:MSE:HA	1:A:929:LEU:HB2	1.56	0.86
1:B:1005:MSE:HE1	1:B:1015:GLU:HG2	1.58	0.86
1:B:530:ALA:HA	1:B:533:MSE:HE3	1.58	0.85
1:A:70:LEU:HG	1:A:74:MSE:HG3	1.57	0.85
1:B:22:HIS:HA	1:B:25:ILE:CG1	2.06	0.85
1:B:412:LEU:HB3	1:B:435:LEU:HD22	1.58	0.85
1:A:259:ALA:HA	1:A:485:ARG:HH12	1.42	0.85
1:B:394:TRP:CD1	1:B:404:GLY:HA3	2.12	0.85
1:B:945:ARG:NH2	1:B:946:ALA:HB2	1.91	0.85
1:A:1024:VAL:O	1:A:1028:GLN:HG3	1.76	0.85
1:B:149:GLU:HA	1:B:230:ARG:NH2	1.92	0.84
1:A:65:THR:HG21	1:A:70:LEU:CD2	2.06	0.84
1:B:74:MSE:CE	1:B:122:LEU:HD21	2.06	0.84
1:B:738:LYS:HA	1:B:741:MSE:CE	2.07	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:729:ALA:CA	1:B:732:LYS:HD3	2.08	0.84
1:B:807:ASN:ND2	1:B:807:ASN:N	2.25	0.84
1:B:533:MSE:HE1	1:B:541:LEU:HD12	1.60	0.84
1:B:40:LEU:O	1:B:43:PRO:HD2	1.78	0.84
1:A:266:MSE:HG3	1:A:309:VAL:HG22	1.60	0.83
1:B:341[B]:ARG:HG3	1:B:343:GLN:CD	2.04	0.83
1:A:917:ASN:HA	1:A:1056:LEU:HD23	1.59	0.83
1:A:289:ALA:HB3	1:A:339:ARG:HH12	1.43	0.83
1:A:933:MSE:HG3	1:A:950:CYS:SG	2.18	0.83
1:B:924:LYS:HZ1	1:B:1061:LYS:HE3	1.43	0.83
1:B:441:LEU:HD23	1:B:441:LEU:H	1.42	0.82
1:B:14:GLU:HA	1:B:997:ILE:HD11	1.60	0.82
1:B:448:LEU:HA	1:B:451:GLN:CG	2.09	0.82
1:A:37:ILE:HD13	1:A:105:ARG:HG2	1.61	0.82
1:B:47:VAL:HG12	1:B:115:ILE:HD13	1.60	0.82
1:A:276:LYS:HE3	1:A:301:GLN:NE2	1.94	0.82
1:A:74:MSE:HE3	1:A:122:LEU:CD2	2.06	0.82
1:A:143:GLU:O	1:A:146:THR:HB	1.78	0.82
1:A:276:LYS:HE3	1:A:301:GLN:HE21	1.42	0.82
1:B:644:ALA:CB	1:B:709:MSE:HE2	2.09	0.82
1:A:448:LEU:HA	1:A:451:GLN:HG2	1.60	0.82
1:B:444:LYS:HB2	1:B:444:LYS:HZ2	1.43	0.82
1:B:75:PRO:HA	1:B:78:PHE:CE2	2.15	0.81
1:A:27:HIS:NE2	1:A:109:ILE:HB	1.94	0.81
1:B:936:LEU:HB3	1:B:943:THR:CG2	2.10	0.81
1:A:179:GLN:HA	1:A:182:LEU:HD22	1.63	0.81
1:A:297[B]:GLN:HG2	1:A:298:ALA:N	1.96	0.81
1:B:205:LEU:HB2	1:B:237:MSE:HE1	1.62	0.81
1:B:297:GLN:NE2	1:B:297:GLN:HA	1.94	0.81
1:A:732:LYS:CE	1:A:736:LYS:HE2	2.09	0.80
1:A:936:LEU:HB3	1:A:943:THR:CG2	2.10	0.80
1:A:789:GLU:HG2	1:A:830:LYS:HZ2	1.42	0.80
1:A:836:GLN:NE2	1:A:837:PRO:HD2	1.96	0.80
1:B:594:GLU:O	1:B:598:VAL:HG23	1.82	0.80
1:B:53:ASN:O	1:B:57:VAL:HG22	1.81	0.80
1:B:563:GLU:HG3	1:B:564:GLY:N	1.96	0.80
1:B:216:LYS:HB2	1:B:223:ILE:CG2	2.11	0.80
1:B:506:ASN:HB2	1:B:509:VAL:HG13	1.64	0.80
1:B:932:GLU:HB2	2:B:1132:HOH:O	1.82	0.80
1:A:671:LEU:HD23	1:A:671:LEU:H	1.47	0.80
1:A:811:PRO:CB	1:A:815:LYS:HE2	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:708:LYS:O	1:A:712:LEU:HG	1.83	0.79
1:B:653:ALA:O	1:B:655:LYS:N	2.15	0.79
1:B:20:ILE:HD11	1:B:115:ILE:CG1	2.04	0.79
1:B:20:ILE:CD1	1:B:115:ILE:HG12	2.04	0.79
1:B:529:LEU:O	1:B:532:VAL:HG12	1.82	0.79
1:B:654:ASN:HB2	1:B:657:THR:CG2	2.12	0.79
1:A:215:THR:HG22	1:A:223:ILE:CG1	2.11	0.79
1:A:220:ASN:HD22	1:A:220:ASN:N	1.78	0.79
1:B:546:ASP:O	1:B:550[A]:GLN:HG3	1.82	0.79
1:A:547:ARG:O	1:A:551:LEU:HD23	1.83	0.79
1:A:793:THR:HG23	1:A:824:ILE:HG12	1.64	0.79
1:A:152:GLU:HB3	1:A:216:LYS:NZ	1.97	0.79
1:B:116:LEU:HD13	1:B:1001:VAL:CG2	2.13	0.79
1:B:895:ASN:HB2	1:B:937:VAL:HG11	1.63	0.79
1:B:913:SER:CB	1:B:915:LYS:HG3	2.10	0.79
1:A:914:SER:H	1:A:915:LYS:HE2	1.47	0.79
1:A:149:GLU:HA	1:A:230:ARG:NH2	1.99	0.78
1:A:944:LYS:HD3	1:A:1007:GLY:HA2	1.63	0.78
1:B:127:ASP:O	1:B:131:VAL:HG23	1.82	0.78
1:B:635:ASN:O	1:B:639:LYS:HE3	1.83	0.78
1:A:205:LEU:HB2	1:A:237:MSE:HE1	1.66	0.78
1:B:113:ARG:HB3	1:B:1004:THR:HG21	1.62	0.78
1:B:512:ARG:CB	1:B:512:ARG:HH11	1.95	0.78
1:B:113:ARG:HD2	1:B:1004:THR:HG23	1.64	0.78
1:B:324:THR:HG21	1:B:363:LEU:HG	1.62	0.78
1:A:75:PRO:HB2	1:A:76:PRO:HD3	1.65	0.78
1:B:247:VAL:HA	1:B:250:LEU:HD13	1.64	0.78
1:B:1024:VAL:O	1:B:1028:GLN:HG3	1.82	0.78
1:B:153:THR:HB	1:B:156:ASP:CB	2.06	0.78
1:B:770:GLU:HG2	1:B:835:PHE:CE1	2.18	0.78
1:A:529:LEU:O	1:A:532:VAL:HG12	1.84	0.78
1:A:608:LEU:HD23	1:A:629:ARG:CZ	2.14	0.78
1:B:202:LEU:HB3	1:B:203:PRO:HD3	1.65	0.78
1:B:836:GLN:NE2	1:B:837:PRO:HD2	1.99	0.78
1:A:283:TRP:HH2	1:A:336:ALA:HB2	1.48	0.78
1:B:729:ALA:HA	1:B:732:LYS:CD	2.10	0.78
1:A:4:PHE:HZ	1:A:998:LEU:HD21	1.49	0.77
1:A:429:ASP:O	1:A:433:ARG:HG2	1.83	0.77
1:B:563:GLU:HG3	1:B:565:GLU:H	1.48	0.77
1:B:741:MSE:HA	1:B:808:ILE:HD13	1.65	0.77
1:B:86:THR:O	1:B:90:GLN:HG2	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:635:ASN:O	1:A:639:LYS:HE3	1.84	0.77
1:A:316:LYS:O	1:A:320:GLU:HG3	1.85	0.77
1:A:880:GLU:HG3	1:A:915:LYS:CE	2.13	0.77
1:A:906:HIS:HB2	1:A:927:ALA:HB1	1.65	0.77
1:A:913:SER:HB2	1:A:915:LYS:CG	2.13	0.77
1:A:1045:SER:O	1:A:1048:ILE:HD12	1.84	0.77
1:B:216:LYS:HB2	1:B:223:ILE:HG21	1.63	0.77
1:B:789:GLU:HG2	1:B:830:LYS:NZ	1.99	0.77
1:B:211:ILE:CG1	1:B:690:ALA:O	2.31	0.77
1:B:457:PRO:CD	1:B:460:ARG:HG3	2.15	0.77
1:A:127:ASP:O	1:A:131:VAL:HG23	1.84	0.77
1:B:1057:ARG:HG2	1:B:1057:ARG:HH11	1.49	0.76
1:B:4:PHE:HZ	1:B:998:LEU:HD21	1.50	0.76
1:B:760:ALA:CB	1:B:794:ILE:HD11	2.16	0.76
1:A:7:ARG:HG3	1:A:7:ARG:HH11	1.51	0.76
1:A:94:MSE:HG3	1:A:104:ALA:HB1	1.67	0.76
1:A:958:SER:HB3	2:A:1089:HOH:O	1.84	0.76
1:B:8:THR:O	1:B:12:ILE:HG13	1.86	0.76
1:B:776:ASP:O	1:B:780:ARG:HG3	1.85	0.76
1:A:550:GLN:O	1:A:554:GLN:HG3	1.84	0.76
1:B:424:ASP:HB3	1:B:427:GLU:HG2	1.66	0.76
1:B:897:PRO:HB2	1:B:1024:VAL:CG1	2.16	0.76
1:B:944:LYS:HE2	1:B:1006:LEU:O	1.85	0.76
1:A:555:LEU:HD23	1:A:555:LEU:O	1.86	0.76
1:A:568:GLN:HE21	1:A:568:GLN:H	1.33	0.76
1:B:495:GLY:O	1:B:499:GLN:HG3	1.86	0.76
1:B:653:ALA:HB1	1:B:658:VAL:HG23	1.68	0.76
1:A:40:LEU:HB2	1:A:43:PRO:HG2	1.67	0.75
1:A:506:ASN:HB2	1:A:509:VAL:HG13	1.67	0.75
1:A:906:HIS:CE1	1:A:910:ARG:HG3	2.21	0.75
1:B:29:GLU:HG2	1:B:945:ARG:HD3	1.67	0.75
1:B:563:GLU:CG	1:B:565:GLU:H	1.98	0.75
1:B:31:GLU:HG3	1:B:105:ARG:CZ	2.16	0.75
1:B:398:PRO:HB3	1:B:454:GLY:O	1.85	0.75
1:B:149:GLU:HA	1:B:230:ARG:CZ	2.16	0.75
1:A:287:PRO:HG3	1:A:350:MSE:HG2	1.68	0.75
1:B:59:LYS:HA	1:B:62:VAL:CG2	2.16	0.75
1:A:795:SER:O	1:A:798:VAL:HG22	1.87	0.75
1:A:37:ILE:HB	1:A:95:LEU:HD11	1.69	0.74
1:A:109:ILE:HD13	1:A:1008[B]:ARG:NH2	2.02	0.74
1:A:1032:GLN:HA	1:A:1035:LYS:HD2	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:GLU:OE1	1:B:942:GLY:HA2	1.85	0.74
1:A:702:TRP:CZ3	1:A:706:VAL:HG21	2.22	0.74
1:B:225:GLU:HB3	1:B:681:ILE:HG13	1.68	0.74
1:B:921:ALA:O	1:B:925:ARG:HG3	1.87	0.74
1:A:898:MSE:HE1	1:A:1023:LEU:CD2	2.13	0.74
1:B:507:PRO:CG	1:B:555:LEU:HD21	2.17	0.74
1:B:811:PRO:HB3	1:B:815:LYS:HE2	1.69	0.74
1:A:205:LEU:HD13	1:A:234:VAL:HG23	1.68	0.74
1:B:666:LYS:HE2	1:B:670:GLU:OE2	1.87	0.74
1:B:94:MSE:CE	1:B:104:ALA:HB2	2.18	0.74
1:B:882:ASP:CG	1:B:1061:LYS:HZ1	1.96	0.74
1:B:793:THR:CG2	1:B:824:ILE:HG12	2.17	0.74
1:B:25:ILE:CG2	1:B:945:ARG:HG3	2.17	0.74
1:B:511:ASP:O	1:B:512:ARG:HB2	1.86	0.74
1:A:51:VAL:O	1:A:55:VAL:HG23	1.87	0.74
1:B:74:MSE:HE2	1:B:78:PHE:CZ	2.23	0.73
1:A:256:ASP:HB3	1:A:259:ALA:HB2	1.67	0.73
1:A:798:VAL:O	1:A:802:LYS:HG3	1.88	0.73
1:B:154:MSE:HE1	1:B:158:VAL:HG23	1.70	0.73
1:B:143:GLU:O	1:B:146:THR:HB	1.88	0.73
1:B:301:GLN:O	1:B:305:GLU:HG2	1.88	0.73
1:A:40:LEU:CB	1:A:43:PRO:HG2	2.17	0.73
1:A:75:PRO:HA	1:A:78:PHE:CE2	2.24	0.73
1:A:444:LYS:HZ2	1:A:444:LYS:HB2	1.53	0.73
1:A:447:ASP:HA	1:A:450:ARG:HH11	1.52	0.73
1:A:506:ASN:CB	1:A:509:VAL:HG13	2.18	0.73
1:A:670:GLU:O	1:A:673:PRO:HD2	1.89	0.73
1:A:793:THR:HG23	1:A:824:ILE:CG1	2.19	0.73
1:B:895:ASN:CB	1:B:937:VAL:HG11	2.19	0.73
1:A:738:LYS:HA	1:A:741:MSE:HE2	1.71	0.73
1:A:147:VAL:O	1:A:150:VAL:HG12	1.88	0.73
1:B:272:SER:O	1:B:276:LYS:HG3	1.89	0.73
1:A:440:ALA:C	1:A:444:LYS:HD3	2.12	0.73
1:A:608:LEU:HD23	1:A:629:ARG:NH2	2.03	0.73
1:B:142:LEU:HD23	1:B:238:SER:HB3	1.70	0.73
1:B:318:ARG:O	1:B:322:LEU:HG	1.87	0.73
1:B:394:TRP:HE1	1:B:401:GLY:N	1.87	0.73
1:A:53:ASN:HB3	1:B:288:SER:CB	2.18	0.73
1:A:202:LEU:HB3	1:A:203:PRO:HD3	1.71	0.73
1:B:152:GLU:HB3	1:B:216:LYS:NZ	2.04	0.73
1:B:908:GLU:O	1:B:911:LYS:HG3	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:THR:HG21	1:B:70:LEU:CD2	2.10	0.72
1:B:154:MSE:O	1:B:154:MSE:HE3	1.88	0.72
1:B:394:TRP:NE1	1:B:401:GLY:H	1.87	0.72
1:B:558:LEU:CD2	1:B:569:ALA:HB2	2.19	0.72
1:B:744:ILE:HA	1:B:808:ILE:HG21	1.70	0.72
1:A:201:LEU:HB3	1:A:237:MSE:HE2	1.70	0.72
1:A:281:LYS:HA	1:A:284:LEU:CD1	2.16	0.72
1:B:158:VAL:HG13	1:B:162:LYS:CE	2.19	0.72
1:B:201:LEU:HB3	1:B:237:MSE:HE2	1.71	0.72
1:A:448:LEU:HA	1:A:451:GLN:CG	2.17	0.72
1:A:511:ASP:O	1:A:512:ARG:HB2	1.88	0.72
1:B:824:ILE:O	1:B:828:VAL:HG13	1.89	0.72
1:B:911:LYS:O	1:B:1060:ARG:HG2	1.89	0.72
1:A:780:ARG:O	1:A:784:LYS:HB2	1.89	0.72
1:B:27:HIS:NE2	1:B:108:LEU:HB3	2.04	0.72
1:B:665:VAL:HG22	1:B:709:MSE:CE	2.19	0.72
1:A:225:GLU:OE1	1:A:677:SER:HB2	1.89	0.72
1:A:908:GLU:O	1:A:911:LYS:HG3	1.90	0.72
1:B:398:PRO:HB3	1:B:460:ARG:HH21	1.52	0.72
1:B:737:CYS:HG	1:B:817:PHE:HZ	1.36	0.72
1:A:209:MSE:O	1:A:213:VAL:HG23	1.89	0.72
1:A:403:GLU:CD	1:A:403:GLU:H	1.98	0.72
1:A:769:ARG:NH1	1:A:976:ARG:NH2	2.37	0.72
1:B:445:LEU:HD21	1:B:449:ARG:NE	2.05	0.72
1:B:898:MSE:HE1	1:B:1023:LEU:CG	2.20	0.72
1:A:744:ILE:HA	1:A:808:ILE:HG21	1.72	0.72
1:B:215:THR:CG2	1:B:223:ILE:HG13	2.14	0.72
1:B:269:ALA:O	1:B:273:ILE:HG13	1.90	0.72
1:B:506:ASN:CB	1:B:509:VAL:HG13	2.20	0.72
1:A:37:ILE:CD1	1:A:105:ARG:HE	2.03	0.71
1:B:277:LEU:O	1:B:281:LYS:HG3	1.90	0.71
1:A:718:ASP:HB3	1:A:721:SER:OG	1.90	0.71
1:B:115:ILE:O	1:B:119:THR:HG23	1.90	0.71
1:B:211:ILE:HG21	1:B:681:ILE:HD13	1.72	0.71
1:B:266:MSE:HG3	1:B:309:VAL:HG22	1.70	0.71
1:B:906:HIS:HB2	1:B:927:ALA:CB	2.20	0.71
1:A:498:GLU:HG2	1:A:499:GLN:N	2.05	0.71
1:A:589:GLU:O	1:A:593:GLN:HG2	1.90	0.71
1:A:960:GLU:O	1:A:964:LEU:HG	1.91	0.71
1:B:324:THR:CG2	1:B:363:LEU:HG	2.20	0.71
1:A:86:THR:O	1:A:90:GLN:HG2	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:776:ASP:O	1:A:780:ARG:HG3	1.90	0.71
1:B:660:GLY:O	1:B:663:ALA:HB3	1.90	0.71
1:A:457:PRO:HB3	1:A:460:ARG:HG2	1.73	0.71
1:B:681:ILE:O	1:B:684:ARG:HG3	1.91	0.71
1:B:960:GLU:HG2	1:B:963[B]:ARG:NH2	2.06	0.71
1:A:434:SER:O	1:A:437:GLU:HG2	1.90	0.71
1:B:51:VAL:O	1:B:55:VAL:HG23	1.91	0.71
1:B:383:SER:OG	1:B:387:LYS:HE2	1.90	0.71
1:B:731:LYS:HG3	1:B:825:LEU:HD11	1.71	0.71
1:A:269:ALA:O	1:A:273:ILE:HG13	1.91	0.71
1:A:944:LYS:HD3	1:A:1007:GLY:CA	2.20	0.71
1:B:211:ILE:HD11	1:B:691:ALA:HA	1.73	0.71
1:B:281:LYS:HA	1:B:284:LEU:CD1	2.21	0.71
1:B:504:ILE:CD1	1:B:576:LEU:HD23	2.20	0.71
1:B:1045:SER:O	1:B:1048:ILE:HG13	1.91	0.71
1:A:87:LYS:HE2	1:A:107:TYR:HA	1.73	0.70
1:A:398:PRO:O	1:A:449:ARG:HG2	1.91	0.70
1:B:17:ALA:O	1:B:1000:THR:HG21	1.90	0.70
1:B:793:THR:HG23	1:B:824:ILE:CG1	2.20	0.70
1:B:960:GLU:O	1:B:964:LEU:HG	1.91	0.70
1:A:124:LEU:HD12	1:A:124:LEU:O	1.92	0.70
1:A:158:VAL:HG13	1:A:162:LYS:CE	2.19	0.70
1:A:154:MSE:O	1:A:154:MSE:HE3	1.91	0.70
1:B:457:PRO:HD2	1:B:460:ARG:HG3	1.73	0.70
1:A:924:LYS:O	1:A:928:LEU:HD12	1.91	0.70
1:B:74:MSE:HG2	1:B:125:THR:HG21	1.73	0.70
1:B:95:LEU:CD1	1:B:104:ALA:HB1	2.22	0.70
1:B:341[B]:ARG:HG3	1:B:343:GLN:NE2	2.07	0.70
1:B:654:ASN:O	1:B:656:SER:N	2.25	0.70
1:B:589:GLU:O	1:B:593:GLN:HG2	1.91	0.70
1:A:113:ARG:HB2	1:A:1004:THR:CG2	2.21	0.70
1:A:812:GLY:N	1:A:815:LYS:HG2	2.06	0.70
1:B:26:MSE:HE3	1:B:40:LEU:HD23	1.73	0.70
1:B:936:LEU:N	1:B:936:LEU:HD23	2.06	0.70
1:A:671:LEU:HD23	1:A:671:LEU:N	2.06	0.70
1:A:530:ALA:HA	1:A:533:MSE:HE3	1.72	0.70
1:B:215:THR:HG22	1:B:223:ILE:CG1	2.12	0.70
1:B:25:ILE:HG22	1:B:945:ARG:HG3	1.72	0.69
1:B:653:ALA:CB	1:B:658:VAL:HG23	2.22	0.69
1:B:665:VAL:HG22	1:B:709:MSE:HE3	1.73	0.69
1:A:152:GLU:HB3	1:A:216:LYS:HZ2	1.55	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:ARG:NH1	2:A:1080:HOH:O	2.24	0.69
1:B:507:PRO:HG2	1:B:555:LEU:HD21	1.74	0.69
1:A:1013:ASP:O	1:A:1017:GLU:HG2	1.92	0.69
1:A:28:GLU:HG2	1:A:945:ARG:NE	2.06	0.69
1:A:37:ILE:CD1	1:A:105:ARG:HG2	2.23	0.69
1:B:403:GLU:H	1:B:403:GLU:CD	2.01	0.69
1:B:608:LEU:HD12	1:B:608:LEU:H	1.57	0.69
1:B:1018:GLN:HG2	1:B:1019:ALA:N	2.05	0.69
1:A:58:GLY:O	1:A:62:VAL:HG22	1.92	0.69
1:A:613:ALA:HA	1:A:683:LEU:HD23	1.73	0.69
1:A:318:ARG:O	1:A:322:LEU:HG	1.93	0.69
1:B:26:MSE:CE	1:B:40:LEU:HD23	2.23	0.69
1:B:124:LEU:O	1:B:124:LEU:HD12	1.92	0.69
1:B:635:ASN:C	1:B:639:LYS:HE3	2.17	0.69
1:A:544:LYS:HD2	1:A:586:ARG:NE	2.08	0.69
1:A:1054:PHE:H	1:A:1054:PHE:HD1	1.39	0.69
1:B:185:GLN:OE1	1:B:188:ARG:HD3	1.93	0.69
1:B:444:LYS:HB2	1:B:444:LYS:NZ	2.07	0.69
1:B:726:SER:O	1:B:730:ILE:HG13	1.93	0.69
1:B:926:MSE:HE1	1:B:958:SER:HA	1.74	0.69
1:A:936:LEU:HD23	1:A:936:LEU:N	2.07	0.69
1:A:964:LEU:O	1:A:968:VAL:HG23	1.92	0.69
1:B:147:VAL:O	1:B:150:VAL:HG12	1.92	0.69
1:B:441:LEU:HA	1:B:444:LYS:NZ	2.07	0.69
1:B:670:GLU:O	1:B:673:PRO:HD2	1.93	0.68
1:A:444:LYS:NZ	1:A:444:LYS:HB2	2.07	0.68
1:A:613:ALA:HB1	1:A:682:LEU:HD21	1.76	0.68
1:B:457:PRO:O	1:B:460:ARG:HB2	1.93	0.68
1:A:1:MSE:HB2	1:A:1018:GLN:CD	2.18	0.68
1:B:1013:ASP:O	1:B:1017:GLU:HG2	1.92	0.68
1:A:40:LEU:N	1:A:40:LEU:HD23	2.08	0.68
1:A:343:GLN:NE2	2:A:1141:HOH:O	2.27	0.68
1:A:364:THR:O	1:A:368[A]:GLU:HG3	1.93	0.68
1:A:929:LEU:HD11	1:A:953:ASP:HB3	1.76	0.68
1:B:276:LYS:HE3	1:B:301:GLN:NE2	2.07	0.68
1:A:635:ASN:C	1:A:639:LYS:HE3	2.16	0.68
1:B:289:ALA:HB3	1:B:339:ARG:HH12	1.58	0.68
1:B:563:GLU:HG3	1:B:564:GLY:H	1.57	0.68
1:A:667:THR:HG23	1:A:671:LEU:HD21	1.76	0.68
1:A:812:GLY:H	1:A:815:LYS:CG	2.06	0.68
1:A:412:LEU:HB3	1:A:435:LEU:HD22	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:GLY:O	1:A:454:GLY:N	2.27	0.68
1:B:498:GLU:HG2	1:B:499:GLN:N	2.06	0.68
1:B:505:ASP:C	1:B:507:PRO:HD3	2.18	0.68
1:A:74:MSE:HG2	1:A:125:THR:HG21	1.74	0.68
1:A:318:ARG:HH11	1:A:318:ARG:HG3	1.59	0.68
1:A:381:LYS:HE2	1:A:478:ASN:OD1	1.93	0.68
1:A:960:GLU:HG2	1:A:963:ARG:NH2	2.08	0.68
1:B:330:GLN:O	1:B:333:ASP:HB2	1.94	0.68
1:B:408:ILE:O	1:B:412:LEU:HG	1.94	0.68
1:B:895:ASN:HB2	1:B:937:VAL:CG1	2.23	0.68
1:A:1048:ILE:HD13	1:A:1048:ILE:O	1.95	0.67
1:B:233:THR:HG22	1:B:237:MSE:HE3	1.76	0.67
1:B:943:THR:O	1:B:945:ARG:N	2.27	0.67
1:B:47:VAL:HG12	1:B:115:ILE:CD1	2.24	0.67
1:B:74:MSE:HE3	1:B:122:LEU:CD2	2.23	0.67
1:B:1050:THR:O	1:B:1052:ALA:N	2.27	0.67
1:A:563:GLU:HB3	1:A:566:SER:OG	1.94	0.67
1:B:440:ALA:C	1:B:444:LYS:HD3	2.19	0.67
1:A:37:ILE:HB	1:A:95:LEU:CD1	2.24	0.67
1:A:95:LEU:HD13	1:A:99:PRO:HA	1.75	0.67
1:A:533:MSE:CE	1:A:541:LEU:HD12	2.24	0.67
1:B:671:LEU:HD23	1:B:671:LEU:N	2.07	0.67
1:A:75:PRO:HA	1:A:78:PHE:HD2	1.53	0.67
1:A:153:THR:HG22	1:A:154:MSE:N	2.08	0.67
1:A:283:TRP:CH2	1:A:336:ALA:HB2	2.29	0.67
1:B:47:VAL:CG1	1:B:115:ILE:HD13	2.23	0.67
1:B:124:LEU:O	1:B:128:GLU:HG3	1.95	0.67
1:B:756:ILE:CG2	1:B:797:MSE:HE2	2.24	0.67
1:A:263:THR:HG21	1:A:378:THR:OG1	1.94	0.67
1:A:793:THR:HG21	1:A:824:ILE:HA	1.75	0.67
1:B:129:ALA:O	1:B:133:LYS:HE3	1.95	0.67
1:A:27:HIS:HE2	1:A:109:ILE:HB	1.58	0.67
1:B:654:ASN:HB2	1:B:657:THR:HG23	1.76	0.67
1:A:215:THR:CG2	1:A:223:ILE:HG13	2.21	0.67
1:A:926:MSE:HE1	1:A:958:SER:HA	1.76	0.67
1:B:70:LEU:O	1:B:74:MSE:HB2	1.94	0.67
1:B:75:PRO:HA	1:B:78:PHE:HD2	1.57	0.67
1:A:149:GLU:HA	1:A:230:ARG:CZ	2.25	0.67
1:A:551:LEU:HB2	1:A:576:LEU:HD13	1.77	0.67
1:A:812:GLY:H	1:A:815:LYS:HG2	1.59	0.67
1:B:153:THR:HG22	1:B:154:MSE:N	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:LYS:CE	1:A:107:TYR:HA	2.24	0.67
1:A:887:GLU:HB3	1:A:903:ARG:HH21	1.60	0.67
1:B:454:GLY:O	1:B:460:ARG:NE	2.27	0.67
1:B:930:MSE:HG3	1:B:1031:MSE:SE	2.44	0.67
1:B:283:TRP:HH2	1:B:336:ALA:HB2	1.58	0.66
1:B:398:PRO:O	1:B:449:ARG:HG2	1.94	0.66
1:B:717:ILE:HG21	1:B:722:LEU:HB2	1.77	0.66
1:A:811:PRO:HB3	1:A:815:LYS:CE	2.23	0.66
1:A:893:VAL:HG22	1:A:938:ARG:HD3	1.76	0.66
1:B:566:SER:HB3	1:B:567:PRO:HD2	1.77	0.66
1:B:613:ALA:CB	1:B:682:LEU:HD12	2.21	0.66
1:B:812:GLY:N	1:B:815:LYS:HG2	2.10	0.66
1:A:47:VAL:HG12	1:A:115:ILE:HD13	1.76	0.66
1:A:807:ASN:HB3	1:A:810:ASP:CB	2.20	0.66
1:B:236:LYS:N	1:B:236:LYS:HE3	2.10	0.66
1:B:839:GLU:OE1	1:B:839:GLU:HA	1.95	0.66
1:A:898:MSE:CE	1:A:1024:VAL:HA	2.25	0.66
1:B:336:ALA:HA	1:B:339:ARG:HD2	1.76	0.66
1:B:684:ARG:NE	1:B:684:ARG:O	2.28	0.66
1:A:327:MSE:O	1:A:331:MSE:HG3	1.95	0.66
1:B:316:LYS:O	1:B:320:GLU:HG3	1.95	0.66
1:B:406:GLU:OE1	1:B:409:ARG:NH1	2.28	0.66
1:B:658:VAL:HG13	1:B:662:GLN:NE2	2.11	0.66
1:A:644:ALA:HB2	1:A:709:MSE:HE2	1.77	0.66
1:A:943:THR:O	1:A:945:ARG:N	2.29	0.66
1:B:40:LEU:HD22	1:B:44:VAL:HG23	1.77	0.66
1:B:58:GLY:O	1:B:62:VAL:HG22	1.95	0.66
1:B:717:ILE:CG2	1:B:722:LEU:HB2	2.26	0.66
1:B:910:ARG:HD3	2:B:1167:HOH:O	1.94	0.66
1:A:289:ALA:HB3	1:A:339:ARG:NH1	2.10	0.66
1:A:490:ALA:O	1:A:496:LYS:HE3	1.95	0.66
1:B:364:THR:O	1:B:368:GLU:HG3	1.96	0.66
1:B:772:GLU:O	1:B:975:LYS:NZ	2.29	0.66
1:B:1:MSE:HE1	1:B:1018:GLN:HE22	1.57	0.66
1:A:90:GLN:C	1:A:94:MSE:HE3	2.20	0.65
1:B:457:PRO:HG2	1:B:460:ARG:CG	2.26	0.65
1:B:512:ARG:HH11	1:B:512:ARG:CG	2.08	0.65
1:B:554:GLN:NE2	2:B:1176:HOH:O	2.29	0.65
1:A:233:THR:CG2	1:A:237:MSE:HE3	2.26	0.65
1:A:422:CYS:O	1:A:428:ARG:NH2	2.29	0.65
1:B:65:THR:CG2	1:B:70:LEU:HD22	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:GLU:O	1:B:321:ILE:HG13	1.96	0.65
1:A:608:LEU:H	1:A:608:LEU:HD12	1.61	0.65
1:A:1004:THR:O	1:A:1008[B]:ARG:NH2	2.29	0.65
1:B:317:GLU:CD	1:B:317:GLU:H	2.03	0.65
1:B:760:ALA:HB3	1:B:794:ILE:HD11	1.78	0.65
1:A:613:ALA:HB1	1:A:682:LEU:CD2	2.25	0.65
1:B:27:HIS:NE2	1:B:108:LEU:HD23	2.11	0.65
1:B:266:MSE:HE3	1:B:309:VAL:HG13	1.78	0.65
1:A:660:GLY:O	1:A:663:ALA:HB3	1.96	0.65
1:A:20:ILE:O	1:A:24:VAL:HG23	1.97	0.65
1:A:500:ALA:O	1:A:504:ILE:HG12	1.96	0.65
1:B:16:VAL:HG12	1:B:17:ALA:N	2.10	0.65
1:B:22:HIS:HA	1:B:25:ILE:CD1	2.26	0.65
1:B:297:GLN:NE2	2:B:1099:HOH:O	2.29	0.65
1:B:459:ALA:O	1:B:462:LEU:HB2	1.96	0.65
1:A:626:PHE:CZ	1:A:680:ARG:HG2	2.32	0.65
1:B:62:VAL:HA	1:B:70:LEU:HD21	1.77	0.65
1:B:186:GLU:O	1:B:190:MSE:HG3	1.97	0.65
1:B:216:LYS:N	1:B:223:ILE:HG12	2.11	0.65
1:B:266:MSE:CE	1:B:309:VAL:HG13	2.27	0.65
1:B:628:GLU:O	1:B:632:ASN:ND2	2.30	0.65
1:A:319:ARG:HD3	2:A:1134:HOH:O	1.96	0.65
1:A:589:GLU:HG2	1:A:593:GLN:NE2	2.09	0.65
1:B:343:GLN:N	1:B:343:GLN:OE1	2.29	0.65
1:B:544:LYS:HD2	1:B:586:ARG:NE	2.10	0.65
1:B:760:ALA:HB1	1:B:794:ILE:HD11	1.78	0.65
1:A:53:ASN:O	1:A:57:VAL:HG22	1.97	0.65
1:A:205:LEU:O	1:A:209:MSE:HG3	1.97	0.65
1:A:256:ASP:OD1	1:A:485:ARG:NH2	2.29	0.65
1:B:547:ARG:NH2	1:B:575:GLN:HG2	2.12	0.65
1:B:719:THR:HG22	1:B:723:LEU:CD2	2.26	0.65
1:B:960:GLU:HG2	1:B:963[A]:ARG:HH21	1.62	0.65
1:A:91:ALA:HB2	1:A:107:TYR:CB	2.27	0.65
1:A:880:GLU:HG3	1:A:915:LYS:HD2	1.78	0.65
1:B:40:LEU:HD22	1:B:43:PRO:HG2	1.79	0.65
1:B:207:SER:HB3	1:B:694:HIS:CE1	2.31	0.65
1:B:533:MSE:HE3	1:B:541:LEU:HD12	1.78	0.65
1:B:608:LEU:HD23	1:B:629:ARG:NH2	2.12	0.65
1:B:733:ASP:OD2	1:B:759:ARG:NH1	2.29	0.65
1:A:37:ILE:HD12	1:A:105:ARG:HE	1.62	0.64
1:B:441:LEU:HA	1:B:444:LYS:HZ2	1.60	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:644:ALA:HB3	1:B:709:MSE:HE2	1.79	0.64
1:B:1005:MSE:CE	1:B:1015:GLU:HG2	2.26	0.64
1:A:74:MSE:O	1:A:77:ALA:HB3	1.97	0.64
1:A:403:GLU:O	1:A:406:GLU:N	2.30	0.64
1:B:589:GLU:HG2	1:B:593:GLN:NE2	2.06	0.64
1:B:667:THR:CG2	1:B:671:LEU:HD21	2.26	0.64
1:B:793:THR:HG21	1:B:824:ILE:HA	1.78	0.64
1:A:27:HIS:ND1	2:A:1154:HOH:O	2.30	0.64
1:A:409[B]:ARG:HH22	1:A:442:THR:HB	1.60	0.64
1:A:512:ARG:CB	1:A:512:ARG:HH11	2.11	0.64
1:A:566:SER:HB3	1:A:567:PRO:HD2	1.80	0.64
1:A:594:GLU:O	1:A:598:VAL:HG23	1.98	0.64
1:B:440:ALA:O	1:B:443:SER:N	2.30	0.64
1:B:789:GLU:HG2	1:B:830:LYS:HZ1	1.62	0.64
1:A:211:ILE:HD11	1:A:690:ALA:O	1.96	0.64
1:A:898:MSE:HE3	1:A:1024:VAL:HG22	1.78	0.64
1:A:944:LYS:CD	1:A:1007:GLY:HA2	2.27	0.64
1:B:812:GLY:H	1:B:815:LYS:CG	2.10	0.64
1:B:898:MSE:CE	1:B:1023:LEU:HD23	2.24	0.64
1:A:287:PRO:HB3	1:A:344:GLY:O	1.96	0.64
1:B:798:VAL:O	1:B:802:LYS:HG3	1.97	0.64
1:A:62:VAL:HA	1:A:70:LEU:HD21	1.79	0.64
1:A:815:LYS:O	1:A:819:ASP:HB3	1.97	0.64
1:B:28:GLU:CD	1:B:942:GLY:HA2	2.23	0.64
1:B:815:LYS:O	1:B:819:ASP:HB3	1.98	0.64
1:A:266:MSE:HE3	1:A:309:VAL:HG13	1.80	0.64
1:A:619:ALA:O	1:A:622:ARG:HB2	1.98	0.64
1:A:756:ILE:CG2	1:A:797:MSE:HE2	2.27	0.64
1:B:341[B]:ARG:NE	1:B:343:GLN:NE2	2.46	0.64
1:B:837:PRO:O	1:B:839:GLU:N	2.31	0.64
1:A:158:VAL:O	1:A:162:LYS:HG3	1.97	0.64
1:A:247:VAL:HA	1:A:250:LEU:HD13	1.79	0.64
1:A:281:LYS:NZ	1:A:361:ASP:OD2	2.31	0.64
1:B:209:MSE:O	1:B:212:PHE:HB3	1.98	0.64
1:B:412:LEU:N	1:B:412:LEU:HD23	2.12	0.64
1:B:564:GLY:HA2	1:B:569:ALA:HB1	1.79	0.64
1:B:1057:ARG:HG2	1:B:1057:ARG:NH1	2.13	0.64
1:B:207:SER:OG	1:B:694:HIS:ND1	2.29	0.64
1:B:1014:GLU:HA	1:B:1017:GLU:CG	2.27	0.64
1:B:281:LYS:NZ	1:B:361:ASP:OD2	2.31	0.63
1:B:708:LYS:O	1:B:712:LEU:HG	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:GLU:O	1:A:213:VAL:HG13	1.98	0.63
1:A:449:ARG:HA	1:A:453:LYS:HA	1.80	0.63
1:A:1052:ALA:O	1:A:1053:GLY:C	2.40	0.63
1:B:795:SER:OG	1:B:796:PRO:HD3	1.98	0.63
1:A:108:LEU:O	1:A:112:SER:N	2.32	0.63
1:A:233:THR:HG22	1:A:237:MSE:HE3	1.79	0.63
1:B:28:GLU:HG2	1:B:944:LYS:HB2	1.80	0.63
1:B:83:ASN:OD1	1:B:83:ASN:N	2.31	0.63
1:B:901:ALA:HB1	1:B:1031:MSE:HG3	1.79	0.63
1:A:453:LYS:HD2	1:A:453:LYS:N	2.10	0.63
1:B:682:LEU:O	1:B:682:LEU:HD22	1.98	0.63
1:A:18:GLN:NE2	1:A:22[B]:HIS:NE2	2.47	0.63
1:A:448:LEU:CD1	1:A:448:LEU:H	2.11	0.63
1:A:633:PHE:CD2	1:A:676:VAL:HG23	2.32	0.63
1:B:236:LYS:HE3	1:B:236:LYS:CA	2.29	0.63
1:B:257:ALA:HB2	2:B:1115:HOH:O	1.97	0.63
1:B:454:GLY:C	1:B:457:PRO:HD2	2.23	0.63
1:B:718:ASP:HB3	1:B:721:SER:OG	1.99	0.63
1:B:811:PRO:CB	1:B:815:LYS:HE2	2.28	0.63
1:A:505:ASP:C	1:A:507:PRO:HD3	2.23	0.63
1:B:394:TRP:CG	1:B:404:GLY:HA3	2.34	0.63
1:B:734:LEU:O	1:B:738:LYS:HG3	1.98	0.63
1:B:335:VAL:HG12	1:B:336:ALA:N	2.14	0.63
1:A:266:MSE:CE	1:A:309:VAL:HG13	2.29	0.63
1:A:880:GLU:HG3	1:A:915:LYS:NZ	2.14	0.63
1:B:318:ARG:HH11	1:B:318:ARG:HG3	1.63	0.63
1:B:441:LEU:HD23	1:B:441:LEU:N	2.14	0.63
1:B:499:GLN:NE2	1:B:514:VAL:HG11	2.14	0.63
1:B:731:LYS:HG3	1:B:825:LEU:CD1	2.29	0.63
1:B:905:LEU:HD12	1:B:1031:MSE:SE	2.49	0.63
1:A:258:TRP:HB3	1:A:488:LYS:HE2	1.81	0.62
1:A:812:GLY:CA	1:A:815:LYS:HG2	2.28	0.62
1:B:667:THR:O	1:B:670:GLU:N	2.26	0.62
1:A:833:GLU:O	1:A:835:PHE:N	2.32	0.62
1:B:14:GLU:N	1:B:15:PRO:HD2	2.14	0.62
1:B:70:LEU:HG	1:B:74:MSE:HG3	1.81	0.62
1:B:907:ASP:O	1:B:910:ARG:HG3	1.98	0.62
1:A:947:LEU:O	1:A:947:LEU:HD22	1.99	0.62
1:B:59:LYS:HA	1:B:62:VAL:HG23	1.81	0.62
1:A:22[A]:HIS:HD2	1:A:23:LEU:HD23	1.63	0.62
1:B:29:GLU:CG	1:B:945:ARG:HD3	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:THR:HG21	1:B:222:GLY:CA	2.29	0.62
1:B:886:PRO:CG	1:B:928:LEU:HD23	2.29	0.62
1:A:2:PRO:O	1:A:1022:MSE:HE1	2.00	0.62
1:A:610:ALA:HA	1:A:695:PHE:CZ	2.35	0.62
1:B:283:TRP:CZ2	1:B:296:GLU:HG2	2.33	0.62
1:B:347:PRO:HA	1:B:350:MSE:HE1	1.82	0.62
1:B:551:LEU:HB2	1:B:576:LEU:HD13	1.80	0.62
1:A:70:LEU:O	1:A:74:MSE:HB2	1.99	0.62
1:A:91:ALA:HB2	1:A:107:TYR:HB3	1.82	0.62
1:A:109:ILE:CD1	1:A:1008[B]:ARG:HH21	2.10	0.62
1:A:283:TRP:CZ2	1:A:296:GLU:HG2	2.34	0.62
1:A:613:ALA:CB	1:A:682:LEU:HD21	2.29	0.62
1:A:1:MSE:HE2	1:A:1:MSE:O	1.99	0.62
1:A:115:ILE:O	1:A:119:THR:HG23	2.00	0.62
1:A:205:LEU:CD1	1:A:234:VAL:HG23	2.29	0.62
1:A:530:ALA:C	1:A:532:VAL:H	2.08	0.62
1:A:793:THR:CG2	1:A:824:ILE:HG12	2.29	0.62
1:A:944:LYS:CE	1:A:1007:GLY:HA2	2.29	0.62
1:B:2:PRO:O	1:B:1022:MSE:HE1	1.98	0.62
1:B:225:GLU:OE1	1:B:225:GLU:HA	1.98	0.62
1:B:1050:THR:C	1:B:1052:ALA:H	2.07	0.62
1:A:7:ARG:HH11	1:A:7:ARG:CG	2.10	0.62
1:A:330:GLN:O	1:A:333:ASP:HB2	2.00	0.62
1:A:445:LEU:HD12	1:A:462:LEU:HB3	1.80	0.62
1:B:613:ALA:HB1	1:B:682:LEU:CD1	2.23	0.62
1:B:795:SER:O	1:B:798:VAL:HG22	2.00	0.62
1:B:924:LYS:HZ1	1:B:1061:LYS:CE	2.10	0.62
1:A:958:SER:O	1:A:961:VAL:HG23	2.00	0.62
1:B:701:GLN:O	1:B:704:ASP:HB2	2.00	0.62
1:B:940:GLY:O	1:B:944:LYS:NZ	2.31	0.62
1:A:441:LEU:H	1:A:441:LEU:CD2	2.05	0.62
1:B:667:THR:HG23	1:B:671:LEU:HD21	1.81	0.62
1:A:369:ASN:O	1:A:373:LYS:HG3	2.00	0.61
1:A:910:ARG:O	1:A:1061:LYS:HD3	2.00	0.61
1:B:960:GLU:HG2	1:B:963[B]:ARG:HH21	1.64	0.61
1:A:408:ILE:O	1:A:412:LEU:HG	2.00	0.61
1:A:290:SER:O	1:A:292:GLY:N	2.33	0.61
1:A:884:GLU:HG3	1:A:885:PHE:H	1.65	0.61
1:B:51:VAL:HG11	1:B:115:ILE:HD12	1.82	0.61
1:B:684:ARG:NH2	1:B:686:PRO:HB3	2.16	0.61
1:A:335:VAL:HG12	1:A:336:ALA:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:944:LYS:HE2	1:A:1007:GLY:HA2	1.81	0.61
1:B:176:ASP:O	1:B:179:GLN:HG3	2.00	0.61
1:B:310:GLY:O	1:B:318:ARG:HG2	2.00	0.61
1:B:444:LYS:O	1:B:448:LEU:HD13	1.99	0.61
1:B:74:MSE:O	1:B:77:ALA:HB3	2.01	0.61
1:B:93:GLN:HG2	1:B:94:MSE:H	1.65	0.61
1:B:958:SER:O	1:B:961:VAL:HG23	2.01	0.61
1:A:69:ILE:HD12	1:A:69:ILE:N	2.11	0.61
1:A:424:ASP:OD1	1:A:427:GLU:HB2	2.01	0.61
1:A:568:GLN:C	1:A:570:ARG:H	2.08	0.61
1:B:95:LEU:HD11	1:B:104:ALA:HB1	1.81	0.61
1:A:558:LEU:CD2	1:A:569:ALA:HB2	2.27	0.61
1:A:666:LYS:HE2	1:A:670:GLU:OE2	2.01	0.61
1:A:756:ILE:HG22	1:A:797:MSE:HE2	1.83	0.61
1:A:885:PHE:CZ	1:A:899:MSE:HE3	2.36	0.61
1:B:168:MSE:CE	1:B:202:LEU:HB2	2.31	0.61
1:B:744:ILE:HD12	1:B:744:ILE:N	2.14	0.61
1:B:769:ARG:NH1	1:B:976:ARG:NH2	2.49	0.61
1:A:447:ASP:CA	1:A:450:ARG:HD2	2.29	0.61
1:B:122:LEU:HD13	1:B:126:PHE:HE1	1.64	0.61
1:B:547:ARG:HD2	1:B:551:LEU:HD21	1.83	0.61
1:B:1014:GLU:HA	1:B:1017:GLU:HG2	1.83	0.61
1:A:170:LYS:O	1:A:174:MSE:HG3	2.00	0.61
1:A:227:LEU:CD1	1:A:230:ARG:HH12	2.14	0.61
1:B:452:GLY:C	1:B:454:GLY:H	2.08	0.61
1:A:374:LEU:HD12	1:A:374:LEU:O	2.01	0.60
1:A:825:LEU:O	1:A:828:VAL:HG22	2.01	0.60
1:B:59:LYS:O	1:B:62:VAL:HG23	2.01	0.60
1:A:41:THR:O	1:A:45:ALA:HB2	2.00	0.60
1:A:65:THR:CG2	1:A:70:LEU:HD22	2.13	0.60
1:A:258:TRP:CD1	1:A:488:LYS:HD2	2.36	0.60
1:A:573:ALA:O	1:A:577:GLN:HG2	2.01	0.60
1:A:719:THR:O	1:A:723:LEU:HD23	2.01	0.60
1:A:1049:ARG:HG3	1:A:1050:THR:H	1.67	0.60
1:B:218:SER:OG	1:B:220:ASN:ND2	2.35	0.60
1:B:898:MSE:HE1	1:B:1023:LEU:HG	1.84	0.60
1:B:913:SER:CB	1:B:915:LYS:HE3	2.31	0.60
1:B:300:ARG:HG3	2:B:1099:HOH:O	2.01	0.60
1:A:808:ILE:O	1:A:814:GLN:NE2	2.35	0.60
1:B:87:LYS:HG3	1:B:87:LYS:O	2.02	0.60
1:A:4:PHE:HZ	1:A:998:LEU:CD2	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ILE:HD12	1:A:37:ILE:H	1.67	0.60
1:A:286:ASP:O	1:A:339:ARG:NH2	2.35	0.60
1:A:444:LYS:O	1:A:448:LEU:HD13	2.01	0.60
1:B:836:GLN:C	1:B:838:GLN:H	2.07	0.60
1:A:683:LEU:O	1:A:683:LEU:HD13	2.00	0.60
1:B:327:MSE:O	1:B:331:MSE:HG3	2.02	0.60
1:A:533:MSE:HE1	1:A:541:LEU:HD12	1.84	0.60
1:B:152:GLU:HB3	1:B:216:LYS:HZ2	1.65	0.60
1:B:445:LEU:O	1:B:445:LEU:HD23	2.02	0.60
1:A:87:LYS:HG3	1:A:87:LYS:O	2.01	0.59
1:A:880:GLU:HG3	1:A:915:LYS:CD	2.31	0.59
1:A:972:CYS:SG	1:A:1044:ALA:HB1	2.42	0.59
1:B:697:THR:HG22	1:B:698:MSE:CE	2.21	0.59
1:A:48:GLN:O	1:A:52:SER:HB3	2.01	0.59
1:A:69:ILE:HG22	1:A:73:ASP:OD2	2.01	0.59
1:A:512:ARG:HH11	1:A:512:ARG:CG	2.16	0.59
1:A:734:LEU:O	1:A:738:LYS:HG3	2.01	0.59
1:A:930:MSE:HG3	1:A:1031:MSE:SE	2.52	0.59
1:B:7:ARG:HH11	1:B:7:ARG:HG3	1.67	0.59
1:B:75:PRO:HB2	1:B:76:PRO:HD3	1.84	0.59
1:B:211:ILE:HG12	1:B:690:ALA:O	2.00	0.59
1:A:59:LYS:HA	1:A:62:VAL:CG2	2.32	0.59
1:A:459:ALA:O	1:A:462:LEU:N	2.34	0.59
1:A:760:ALA:CB	1:A:794:ILE:HD11	2.32	0.59
1:B:209:MSE:O	1:B:213:VAL:HG23	2.01	0.59
1:A:1:MSE:HB2	1:A:1018:GLN:NE2	2.17	0.59
1:A:317:GLU:H	1:A:317:GLU:CD	2.07	0.59
1:A:666:LYS:O	1:A:669:ARG:HB2	2.02	0.59
1:B:40:LEU:HB2	1:B:43:PRO:HG3	1.82	0.59
1:B:69:ILE:HG22	1:B:73:ASP:OD2	2.03	0.59
1:B:113:ARG:HB3	1:B:1004:THR:HG23	1.83	0.59
1:B:211:ILE:HD11	1:B:690:ALA:O	2.02	0.59
1:B:1001:VAL:HG12	1:B:1002:LYS:N	2.16	0.59
1:A:681:ILE:HG22	1:A:682:LEU:N	2.16	0.59
1:A:839:GLU:HA	2:A:1161:HOH:O	2.02	0.59
1:A:83:ASN:OD1	1:A:83:ASN:N	2.35	0.59
1:A:564:GLY:O	1:A:565:GLU:HG3	2.02	0.59
1:A:738:LYS:HA	1:A:741:MSE:CE	2.31	0.59
1:B:7:ARG:HH11	1:B:7:ARG:CG	2.16	0.59
1:B:253:TRP:CD1	1:B:1025:HIS:HD2	2.21	0.59
1:A:16:VAL:HG12	1:A:17:ALA:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:GLN:OE1	1:A:188:ARG:HD3	2.02	0.59
1:B:256:ASP:OD1	1:B:258:TRP:HZ3	1.86	0.59
1:B:887:GLU:HA	1:B:887:GLU:OE1	2.01	0.59
1:A:42:ALA:N	1:A:43:PRO:HD2	2.18	0.59
1:A:336:ALA:HA	1:A:339:ARG:HD2	1.84	0.59
1:A:377:MSE:HE3	1:A:421:LEU:HD23	1.83	0.59
1:B:215:THR:HG21	1:B:222:GLY:HA3	1.84	0.59
1:B:897:PRO:CB	1:B:1024:VAL:HG11	2.26	0.59
1:A:79:ILE:HG12	2:A:1097:HOH:O	2.03	0.58
1:A:215:THR:HG23	1:A:220:ASN:ND2	2.17	0.58
1:A:641:GLY:HA2	1:A:709:MSE:CE	2.31	0.58
1:B:22:HIS:CE1	1:B:23:LEU:HD23	2.38	0.58
1:B:40:LEU:O	1:B:43:PRO:CD	2.48	0.58
1:B:720:LYS:HD3	1:B:837:PRO:HD3	1.84	0.58
1:B:917:ASN:HA	1:B:1056:LEU:HD23	1.84	0.58
1:A:216:LYS:HA	1:A:223:ILE:HG12	1.84	0.58
1:B:293:ASP:N	1:B:293:ASP:OD1	2.33	0.58
1:A:94:MSE:HG3	1:A:104:ALA:CB	2.33	0.58
1:A:129:ALA:O	1:A:133:LYS:HE3	2.03	0.58
1:A:1001:VAL:HG12	1:A:1002:LYS:N	2.18	0.58
1:B:667:THR:O	1:B:670:GLU:HB2	2.02	0.58
1:A:51:VAL:HG11	1:A:115:ILE:CD1	2.30	0.58
1:A:536:PRO:O	1:A:540:ASP:N	2.34	0.58
1:B:253:TRP:O	1:B:255:GLU:HG2	2.03	0.58
1:B:563:GLU:HG2	1:B:565:GLU:HB2	1.84	0.58
1:A:14:GLU:N	1:A:15:PRO:HD2	2.19	0.58
1:A:530:ALA:CA	1:A:533:MSE:HE3	2.33	0.58
1:B:933:MSE:HG3	1:B:950:CYS:SG	2.43	0.58
1:A:53:ASN:CB	1:B:288:SER:HB2	2.21	0.58
1:B:137:VAL:O	1:B:141:ILE:HG12	2.04	0.58
1:B:270:LEU:HD21	1:B:367:VAL:HG23	1.84	0.58
1:A:206:ILE:HG22	1:A:207:SER:N	2.17	0.58
1:A:209:MSE:O	1:A:212:PHE:HB3	2.04	0.58
1:A:644:ALA:CB	1:A:709:MSE:HE2	2.32	0.58
1:A:658:VAL:HG13	1:A:662:GLN:NE2	2.18	0.58
1:A:906:HIS:O	1:A:910:ARG:HB2	2.04	0.58
1:A:112:SER:O	1:A:115:ILE:HG23	2.03	0.58
1:A:186:GLU:H	1:A:186:GLU:CD	2.12	0.58
1:A:394:TRP:CD1	1:A:404:GLY:HA3	2.39	0.58
1:A:702:TRP:CH2	1:A:706:VAL:HG21	2.38	0.58
1:A:896:GLN:HG3	1:A:897:PRO:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:898:MSE:CG	1:A:1024:VAL:HG13	2.34	0.58
1:A:926:MSE:HE2	1:A:957:ALA:CB	2.34	0.58
1:A:986:GLU:HG2	2:A:1151:HOH:O	2.02	0.58
1:A:176:ASP:O	1:A:179:GLN:HG3	2.03	0.58
1:A:726:SER:O	1:A:730:ILE:HG13	2.02	0.58
1:B:154:MSE:CE	1:B:158:VAL:HB	2.34	0.58
1:B:202:LEU:CB	1:B:203:PRO:HD3	2.34	0.58
1:B:741:MSE:SE	1:B:814:GLN:HB3	2.53	0.58
1:A:548:VAL:HG13	1:A:576:LEU:HD11	1.84	0.58
1:A:885:PHE:CE2	1:A:903:ARG:HG3	2.39	0.58
1:B:227:LEU:HD21	1:B:230:ARG:NH2	2.19	0.58
1:B:756:ILE:HG22	1:B:797:MSE:HE2	1.85	0.58
1:B:896:GLN:HG3	1:B:897:PRO:N	2.18	0.58
1:A:87:LYS:HE2	1:A:107:TYR:CA	2.33	0.57
1:A:653:ALA:HB1	1:A:657:THR:OG1	2.04	0.57
1:A:882:ASP:OD2	1:A:924:LYS:NZ	2.30	0.57
1:A:1054:PHE:N	1:A:1054:PHE:CD1	2.71	0.57
1:B:4:PHE:HZ	1:B:998:LEU:CD2	2.15	0.57
1:B:218:SER:HB3	1:B:220:ASN:CG	2.29	0.57
1:A:473:LEU:O	1:A:477:THR:HG23	2.03	0.57
1:A:811:PRO:C	1:A:813:LEU:H	2.12	0.57
1:B:281:LYS:CA	1:B:284:LEU:HD12	2.33	0.57
1:B:548:VAL:O	1:B:552:THR:OG1	2.23	0.57
1:B:902:ALA:HB2	1:B:930:MSE:HB3	1.86	0.57
1:A:1:MSE:HE3	1:A:3:VAL:HG23	1.85	0.57
1:A:154:MSE:HE1	1:A:158:VAL:HG23	1.86	0.57
1:A:456:SER:O	1:A:458:GLU:N	2.37	0.57
1:A:717:ILE:CG2	1:A:722:LEU:HB2	2.34	0.57
1:B:69:ILE:HD12	1:B:69:ILE:N	2.16	0.57
1:B:133:LYS:HD3	1:B:136:ARG:NH2	2.20	0.57
1:B:244:ILE:O	1:B:248:LEU:HD12	2.04	0.57
1:B:530:ALA:C	1:B:532:VAL:H	2.12	0.57
1:B:924:LYS:NZ	1:B:1061:LYS:HE3	2.17	0.57
1:A:440:ALA:O	1:A:443:SER:N	2.30	0.57
1:A:667:THR:O	1:A:670:GLU:N	2.35	0.57
1:B:216:LYS:HB2	1:B:223:ILE:HG23	1.86	0.57
1:B:523:VAL:HG13	1:B:545:CYS:HB3	1.85	0.57
1:B:886:PRO:HD3	1:B:928:LEU:HD23	1.86	0.57
1:A:338:LEU:N	1:A:338:LEU:HD23	2.20	0.57
1:A:501:GLN:HA	1:A:501:GLN:NE2	2.20	0.57
1:A:576:LEU:O	1:A:579:SER:N	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:790:LEU:O	1:B:793:THR:HG22	2.04	0.57
1:A:741:MSE:HA	1:A:808:ILE:HD13	1.85	0.57
1:B:88:LEU:HD11	1:B:111:GLY:O	2.04	0.57
1:B:227:LEU:HD13	1:B:230:ARG:HH12	1.70	0.57
1:B:362:VAL:O	1:B:365:ALA:HB3	2.04	0.57
1:B:454:GLY:C	1:B:460:ARG:HE	2.11	0.57
1:B:477:THR:O	1:B:481:VAL:HG23	2.03	0.57
1:B:501:GLN:HA	1:B:501:GLN:NE2	2.18	0.57
1:B:930:MSE:HG2	1:B:954:ILE:CD1	2.35	0.57
1:B:1020:THR:O	1:B:1024:VAL:HG23	2.04	0.57
1:A:437:GLU:O	1:A:441:LEU:HG	2.04	0.57
1:B:227:LEU:HD22	1:B:230:ARG:NH1	2.20	0.57
1:B:812:GLY:CA	1:B:815:LYS:HG2	2.35	0.57
1:A:568:GLN:H	1:A:568:GLN:NE2	2.03	0.57
1:A:905:LEU:HD12	1:A:1031:MSE:SE	2.55	0.57
1:B:945:ARG:CZ	1:B:946:ALA:HB2	2.35	0.57
1:A:69:ILE:H	1:A:69:ILE:CD1	2.10	0.57
1:B:732:LYS:HG2	1:B:733:ASP:N	2.19	0.57
1:A:441:LEU:HD23	1:A:441:LEU:N	2.12	0.57
1:A:897:PRO:HB2	1:A:1024:VAL:HG11	1.87	0.57
1:B:492:HIS:HB3	1:B:655:LYS:HD3	1.85	0.57
1:B:1002:LYS:HZ1	1:B:1020:THR:HG1	1.50	0.57
1:A:8:THR:O	1:A:12:ILE:HG13	2.05	0.56
1:B:985:CYS:O	1:B:989:PRO:HD2	2.04	0.56
1:A:40:LEU:HB2	1:A:44:VAL:HG23	1.88	0.56
1:B:170:LYS:O	1:B:174:MSE:HG3	2.04	0.56
1:B:665:VAL:CG2	1:B:709:MSE:HE3	2.35	0.56
1:B:671:LEU:HD13	1:B:701:GLN:HG2	1.86	0.56
1:A:293:ASP:OD1	1:A:293:ASP:N	2.33	0.56
1:A:604:THR:HA	1:A:607:LYS:HD3	1.86	0.56
1:A:610:ALA:HA	1:A:695:PHE:HZ	1.70	0.56
1:A:685:ASN:N	1:A:686:PRO:HD3	2.20	0.56
1:A:778:LYS:HD2	1:A:1049:ARG:NH1	2.14	0.56
1:A:898:MSE:HE2	1:A:1024:VAL:HA	1.87	0.56
1:B:152:GLU:O	1:B:213:VAL:HG13	2.05	0.56
1:B:376:ALA:CB	1:B:421:LEU:HD21	2.36	0.56
1:B:608:LEU:HD12	1:B:608:LEU:N	2.21	0.56
1:B:653:ALA:O	1:B:654:ASN:C	2.48	0.56
1:A:258:TRP:CB	1:A:488:LYS:HE2	2.35	0.56
1:B:205:LEU:O	1:B:209:MSE:HG3	2.04	0.56
1:B:289:ALA:HB3	1:B:339:ARG:NH1	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:547:ARG:O	1:B:551:LEU:HD23	2.06	0.56
1:B:604:THR:O	1:B:607:LYS:HB2	2.06	0.56
1:B:807:ASN:HB2	1:B:810:ASP:HB3	1.87	0.56
1:B:812:GLY:H	1:B:815:LYS:HG2	1.66	0.56
1:A:20:ILE:HD12	1:A:116:LEU:CD2	2.36	0.56
1:A:347:PRO:HA	1:A:350:MSE:HE1	1.88	0.56
1:A:744:ILE:HA	1:A:808:ILE:CG2	2.35	0.56
1:A:760:ALA:HB3	1:A:794:ILE:HD11	1.86	0.56
1:B:224:GLU:OE1	1:B:228:LYS:NZ	2.38	0.56
1:B:886:PRO:HG3	1:B:928:LEU:HD23	1.88	0.56
1:B:893:VAL:O	1:B:893:VAL:HG13	2.06	0.56
1:B:398:PRO:CB	1:B:460:ARG:HH21	2.19	0.56
1:B:913:SER:HB3	1:B:915:LYS:HE3	1.87	0.56
1:A:412:LEU:HD23	1:A:412:LEU:N	2.20	0.56
1:A:533:MSE:O	1:A:538:ARG:NH1	2.39	0.56
1:A:566:SER:CB	1:A:567:PRO:HD2	2.36	0.56
1:A:744:ILE:HG22	1:A:744:ILE:O	2.04	0.56
1:A:947:LEU:HD22	1:A:947:LEU:C	2.30	0.56
1:B:458:GLU:HG2	1:B:459:ALA:N	2.21	0.56
1:A:281:LYS:CA	1:A:284:LEU:HD12	2.24	0.56
1:B:85:CYS:O	1:B:89:VAL:HG23	2.05	0.56
1:B:122:LEU:O	1:B:122:LEU:HD22	2.05	0.56
1:B:675:VAL:HG22	1:B:698:MSE:HB3	1.86	0.56
1:B:926:MSE:HE2	1:B:957:ALA:C	2.31	0.56
1:B:1014:GLU:HA	1:B:1017:GLU:CD	2.29	0.56
1:B:1032:GLN:HA	1:B:1035:LYS:HD2	1.88	0.56
1:B:1049:ARG:O	1:B:1051:ASP:N	2.39	0.56
1:A:258:TRP:CG	1:A:488:LYS:HE2	2.40	0.56
1:A:447:ASP:O	1:A:449:ARG:N	2.38	0.56
1:B:447:ASP:O	1:B:451:GLN:HG2	2.06	0.56
1:A:337:ASP:O	1:A:340:ALA:HB3	2.06	0.56
1:A:887:GLU:HB3	1:A:903:ARG:NH2	2.20	0.56
1:A:913:SER:HB2	1:A:915:LYS:CE	2.36	0.56
1:A:212:PHE:CE1	1:A:227:LEU:HD23	2.40	0.55
1:B:13:LEU:HD11	1:B:119:THR:OG1	2.05	0.55
1:A:124:LEU:O	1:A:128:GLU:HG3	2.06	0.55
1:B:227:LEU:CD1	1:B:230:ARG:HH12	2.19	0.55
1:B:334:GLN:O	1:B:337:ASP:HB3	2.06	0.55
1:B:41:THR:O	1:B:45:ALA:HB2	2.06	0.55
1:B:157:LEU:HD23	1:B:157:LEU:C	2.31	0.55
1:B:216:LYS:HA	1:B:223:ILE:CG1	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:LYS:O	1:B:376:ALA:HB3	2.07	0.55
1:B:744:ILE:O	1:B:744:ILE:HG22	2.06	0.55
1:A:25:ILE:O	1:A:29:GLU:HB2	2.06	0.55
1:A:441:LEU:N	1:A:444:LYS:HD3	2.20	0.55
1:A:719:THR:HG22	1:A:723:LEU:HD23	1.88	0.55
1:B:112:SER:O	1:B:115:ILE:HG23	2.07	0.55
1:B:501:GLN:OE1	1:B:577:GLN:HG3	2.06	0.55
1:A:2:PRO:HB2	1:A:4:PHE:CE2	2.42	0.55
1:A:276:LYS:CE	1:A:301:GLN:HE21	2.17	0.55
1:A:401:GLY:O	1:A:403:GLU:N	2.40	0.55
1:A:665:VAL:O	1:A:669:ARG:HD2	2.07	0.55
1:A:1055:THR:HG22	1:A:1056:LEU:H	1.71	0.55
1:B:253:TRP:CD1	1:B:1025:HIS:CD2	2.94	0.55
1:B:445:LEU:HD23	1:B:445:LEU:C	2.31	0.55
1:B:253:TRP:CE2	1:B:1025:HIS:CD2	2.95	0.55
1:A:236:LYS:HA	1:A:236:LYS:HE3	1.89	0.55
1:A:377:MSE:HE3	1:A:421:LEU:CD2	2.37	0.55
1:B:22:HIS:HB2	1:B:25:ILE:CD1	2.35	0.55
1:B:266:MSE:SE	1:B:374:LEU:HD23	2.56	0.55
1:B:316:LYS:HB2	1:B:317:GLU:OE2	2.07	0.55
1:B:374:LEU:HD12	1:B:374:LEU:O	2.07	0.55
1:B:445:LEU:HD12	1:B:462:LEU:HB3	1.89	0.55
1:B:461:ALA:HB1	2:B:1084:HOH:O	2.07	0.55
1:A:570:ARG:HH22	1:A:577:GLN:HE22	1.54	0.55
1:B:290:SER:O	1:B:292:GLY:N	2.40	0.55
1:B:456:SER:N	1:B:457:PRO:CD	2.70	0.55
1:B:737:CYS:SG	1:B:817:PHE:HZ	2.28	0.55
1:A:744:ILE:HD12	1:A:744:ILE:N	2.21	0.55
1:A:833:GLU:O	1:A:836:GLN:HB2	2.07	0.55
1:B:924:LYS:O	1:B:928:LEU:HD12	2.06	0.55
1:A:922:ALA:O	1:A:926:MSE:HG2	2.07	0.55
1:B:346:SER:OG	1:B:347:PRO:HD2	2.06	0.55
1:B:767:ALA:O	1:B:771:VAL:HG23	2.06	0.55
1:B:800:ASP:O	1:B:804:VAL:HG23	2.07	0.55
1:B:641:GLY:HA2	1:B:709:MSE:HE1	1.90	0.54
1:B:899:MSE:HB2	1:B:934:SER:OG	2.06	0.54
1:B:990:THR:HA	2:B:1128:HOH:O	2.06	0.54
1:A:26:MSE:HE3	1:A:40:LEU:HD13	1.89	0.54
1:A:570:ARG:HH12	1:A:577:GLN:NE2	2.06	0.54
1:A:775:GLU:HG3	1:A:975:LYS:HE3	1.88	0.54
1:B:158:VAL:O	1:B:162:LYS:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:LEU:HD11	1:A:230:ARG:HH12	1.72	0.54
1:A:790:LEU:O	1:A:790:LEU:HD12	2.06	0.54
1:B:744:ILE:HA	1:B:808:ILE:CG2	2.34	0.54
1:A:152:GLU:HB3	1:A:216:LYS:HZ1	1.70	0.54
1:A:246:ARG:NH2	1:A:254:ASP:OD1	2.41	0.54
1:A:492:HIS:CD2	1:A:495:GLY:H	2.26	0.54
1:A:885:PHE:CE2	1:A:899:MSE:HE3	2.43	0.54
1:A:893:VAL:HG13	1:A:893:VAL:O	2.08	0.54
1:A:896:GLN:CB	1:A:897:PRO:HD3	2.38	0.54
1:A:939:GLY:HA2	1:A:1006:LEU:CG	2.37	0.54
1:A:1014:GLU:HA	1:A:1017:GLU:CG	2.38	0.54
1:B:22:HIS:CB	1:B:25:ILE:HD11	2.37	0.54
1:B:136:ARG:HD2	2:B:1126:HOH:O	2.07	0.54
1:B:237:MSE:O	1:B:241:ILE:HG13	2.08	0.54
1:B:342:GLY:C	1:B:344:GLY:H	2.15	0.54
1:B:789:GLU:HG2	1:B:830:LYS:HZ2	1.70	0.54
1:A:501:GLN:O	1:A:504:ILE:HB	2.08	0.54
1:A:507:PRO:HG2	1:A:555:LEU:HD21	1.88	0.54
1:A:717:ILE:HG21	1:A:722:LEU:HB2	1.89	0.54
1:B:13:LEU:CD2	1:B:123:LEU:HD23	2.37	0.54
1:B:351:GLN:NE2	1:B:351:GLN:HA	2.21	0.54
1:A:511:ASP:OD1	1:A:511:ASP:N	2.31	0.54
1:A:626:PHE:CE1	1:A:680:ARG:HG2	2.43	0.54
1:A:719:THR:HG22	1:A:723:LEU:CD2	2.38	0.54
1:B:69:ILE:H	1:B:69:ILE:CD1	2.18	0.54
1:B:233:THR:CG2	1:B:237:MSE:HE3	2.37	0.54
1:A:318:ARG:HG3	1:A:318:ARG:NH1	2.21	0.54
1:A:457:PRO:CB	1:A:460:ARG:HG2	2.37	0.54
1:A:157:LEU:HD23	1:A:157:LEU:C	2.32	0.54
1:A:409[B]:ARG:HH21	1:A:442:THR:HB	1.71	0.54
1:A:913:SER:CA	1:A:915:LYS:HE2	2.38	0.54
1:B:457:PRO:CG	1:B:460:ARG:HG3	2.38	0.54
1:B:836:GLN:C	1:B:838:GLN:N	2.66	0.54
1:B:1018:GLN:O	1:B:1021:GLU:HB2	2.08	0.54
1:A:533:MSE:HE3	1:A:541:LEU:HD12	1.89	0.54
1:A:898:MSE:HE3	1:A:1024:VAL:CA	2.37	0.54
1:B:211:ILE:CD1	1:B:690:ALA:O	2.56	0.54
1:B:279:GLN:OE1	1:B:294:ALA:HB1	2.08	0.54
1:B:457:PRO:HG2	1:B:460:ARG:HG3	1.90	0.54
1:B:910:ARG:O	1:B:1061:LYS:HD2	2.08	0.54
1:B:212:PHE:C	1:B:214:THR:H	2.16	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:LYS:CE	1:B:301:GLN:HE21	2.16	0.54
1:B:490:ALA:O	1:B:496:LYS:HE3	2.08	0.54
1:A:74:MSE:HG2	1:A:125:THR:CG2	2.38	0.53
1:A:237:MSE:O	1:A:241:ILE:HG13	2.08	0.53
1:A:898:MSE:HE3	1:A:1024:VAL:HA	1.89	0.53
1:B:338:LEU:HD23	1:B:338:LEU:N	2.23	0.53
1:B:430:ASP:OD1	1:B:433[B]:ARG:NH2	2.41	0.53
1:B:947:LEU:C	1:B:947:LEU:HD22	2.33	0.53
1:A:384:ILE:HG12	1:A:414:GLU:HB3	1.90	0.53
1:A:393:ASN:N	1:A:393:ASN:ND2	2.55	0.53
1:A:495:GLY:O	1:A:499:GLN:HG3	2.08	0.53
1:A:1054:PHE:HD1	1:A:1054:PHE:N	2.04	0.53
1:A:171:MSE:O	1:A:175:ILE:HG13	2.09	0.53
1:A:298:ALA:O	1:A:302:ILE:HD12	2.08	0.53
1:B:341[B]:ARG:CZ	1:B:343:GLN:HE21	2.20	0.53
1:B:732:LYS:NZ	1:B:733:ASP:OD1	2.40	0.53
1:B:811:PRO:C	1:B:813:LEU:H	2.15	0.53
1:A:14:GLU:HG2	1:A:993:THR:HG23	1.90	0.53
1:A:555:LEU:HD23	1:A:555:LEU:C	2.34	0.53
1:A:567:PRO:HD2	1:A:568:GLN:NE2	2.23	0.53
1:A:807:ASN:ND2	1:A:810:ASP:HB2	2.23	0.53
1:B:152:GLU:HB3	1:B:216:LYS:HZ1	1.72	0.53
1:B:260:SER:OG	1:B:261:LYS:N	2.40	0.53
1:A:641:GLY:CA	1:A:709:MSE:HE1	2.32	0.53
1:A:918:ASP:HB2	1:A:964:LEU:HD13	1.90	0.53
1:A:97:SER:O	1:A:99:PRO:HD3	2.09	0.53
1:A:842:PHE:N	1:A:842:PHE:CD1	2.77	0.53
1:B:57:VAL:HA	1:B:60:GLU:HG3	1.90	0.53
1:B:218:SER:O	1:B:219:LYS:HB2	2.08	0.53
1:B:258:TRP:C	1:B:258:TRP:HE3	2.15	0.53
1:B:544:LYS:HD2	1:B:586:ARG:HE	1.73	0.53
1:B:547:ARG:HD2	1:B:551:LEU:CD2	2.39	0.53
1:A:26:MSE:O	1:A:29:GLU:N	2.42	0.53
1:A:28:GLU:HA	2:A:1154:HOH:O	2.08	0.53
1:A:144:TYR:CE2	1:A:160:TYR:CD1	2.97	0.53
1:A:448:LEU:CD1	1:A:448:LEU:N	2.72	0.53
1:A:453:LYS:HB2	1:A:455:ASP:OD1	2.09	0.53
1:A:772:GLU:O	1:A:975:LYS:NZ	2.35	0.53
1:B:343:GLN:CD	1:B:343:GLN:H	2.14	0.53
1:B:608:LEU:HD23	1:B:629:ARG:CZ	2.38	0.53
1:B:673:PRO:C	1:B:675:VAL:H	2.17	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ARG:CG	1:A:7:ARG:NH1	2.72	0.53
1:A:151:VAL:O	1:A:212:PHE:HE2	1.92	0.53
1:A:913:SER:C	1:A:915:LYS:HE2	2.33	0.53
1:A:917:ASN:OD1	1:A:1056:LEU:HD22	2.09	0.53
1:B:256:ASP:HA	1:B:258:TRP:CE3	2.42	0.53
1:B:363:LEU:O	1:B:367:VAL:HG13	2.09	0.53
1:B:760:ALA:HB3	1:B:794:ILE:CD1	2.38	0.53
1:B:880:GLU:O	1:B:881:LYS:HD2	2.09	0.53
1:B:947:LEU:HD22	1:B:947:LEU:O	2.09	0.53
1:A:91:ALA:HB2	1:A:107:TYR:HB2	1.91	0.53
1:A:236:LYS:HE3	1:A:236:LYS:CA	2.39	0.53
1:B:104:ALA:C	1:B:106:ASP:H	2.17	0.53
1:A:334:GLN:O	1:A:337:ASP:HB3	2.08	0.52
1:B:318:ARG:HG3	1:B:318:ARG:NH1	2.23	0.52
1:B:906:HIS:CB	1:B:927:ALA:HB1	2.32	0.52
1:B:963[B]:ARG:HG3	2:B:1095:HOH:O	2.09	0.52
1:A:216:LYS:HB2	1:A:223:ILE:HG21	1.92	0.52
1:A:833:GLU:C	1:A:835:PHE:H	2.17	0.52
1:B:563:GLU:CG	1:B:565:GLU:HB2	2.39	0.52
1:B:1048:ILE:HD12	1:B:1048:ILE:O	2.09	0.52
1:A:419:ALA:O	1:A:422:CYS:HB2	2.09	0.52
1:A:603:THR:O	1:A:606:ILE:HG22	2.08	0.52
1:A:655:LYS:HG2	1:A:659:GLU:OE2	2.09	0.52
1:A:688:ASN:O	1:A:691:ALA:N	2.27	0.52
1:A:898:MSE:HG3	1:A:1024:VAL:HG13	1.90	0.52
1:B:144:TYR:CE2	1:B:160:TYR:CD1	2.97	0.52
1:B:402:PRO:HD2	1:B:403:GLU:OE2	2.09	0.52
1:B:654:ASN:HB2	1:B:657:THR:HG21	1.90	0.52
1:B:919:ILE:HD11	1:B:964:LEU:HB2	1.92	0.52
1:A:698:MSE:HE2	1:A:698:MSE:HA	1.90	0.52
1:B:68:GLN:O	1:B:72:ARG:HG2	2.10	0.52
1:B:74:MSE:HG2	1:B:125:THR:CG2	2.38	0.52
1:B:223:ILE:C	1:B:225:GLU:H	2.17	0.52
1:B:685:ASN:C	1:B:687:GLY:H	2.16	0.52
1:A:224:GLU:O	1:A:228:LYS:HD3	2.09	0.52
1:A:253:TRP:CD2	1:A:1025:HIS:CD2	2.98	0.52
1:A:604:THR:O	1:A:607:LYS:HB2	2.09	0.52
1:A:987:ARG:O	1:A:991:ILE:HG13	2.10	0.52
1:B:551:LEU:CD1	1:B:575:GLN:HB3	2.40	0.52
1:A:883:GLU:HA	1:A:883:GLU:OE1	2.09	0.52
1:B:551:LEU:CD2	1:B:551:LEU:N	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:734:LEU:HD13	1:B:822:TYR:CE1	2.44	0.52
1:A:144:TYR:CE2	1:A:160:TYR:CE1	2.98	0.52
1:A:220:ASN:OD1	1:A:685:ASN:OD1	2.27	0.52
1:A:424:ASP:OD1	1:A:424:ASP:O	2.27	0.52
1:B:283:TRP:CH2	1:B:336:ALA:HB2	2.41	0.52
1:B:457:PRO:HG2	1:B:460:ARG:HG2	1.91	0.52
1:B:530:ALA:CA	1:B:533:MSE:HE3	2.34	0.52
1:B:555:LEU:O	1:B:555:LEU:HD23	2.10	0.52
1:A:75:PRO:HB2	1:A:76:PRO:CD	2.36	0.52
1:A:87:LYS:NZ	1:A:107:TYR:HA	2.24	0.52
1:B:15:PRO:O	1:B:18:GLN:N	2.39	0.52
1:B:113:ARG:CZ	1:B:1005:MSE:HB3	2.40	0.52
1:B:535:GLY:O	1:B:539:GLN:OE1	2.28	0.52
1:A:142:LEU:HD23	1:A:238:SER:HB3	1.91	0.52
1:A:692:TYR:O	1:A:696:GLU:HB2	2.09	0.52
1:B:93:GLN:HG2	1:B:94:MSE:HG3	1.91	0.52
1:B:144:TYR:CE2	1:B:160:TYR:CE1	2.98	0.52
1:A:42:ALA:H	1:A:43:PRO:HD2	1.75	0.52
1:A:218:SER:O	1:A:219:LYS:HB2	2.11	0.52
1:A:341:ARG:CB	1:A:343:GLN:HE21	2.23	0.52
1:A:458:GLU:CG	1:A:459:ALA:N	2.73	0.52
1:B:538[A]:ARG:HH11	1:B:539:GLN:HE22	1.57	0.52
1:A:574:SER:HA	1:A:577:GLN:HG2	1.92	0.51
1:A:800:ASP:O	1:A:804:VAL:HG23	2.10	0.51
1:B:122:LEU:HD22	1:B:122:LEU:C	2.35	0.51
1:B:205:LEU:HD13	1:B:234:VAL:HG23	1.90	0.51
1:B:808:ILE:O	1:B:814:GLN:NE2	2.43	0.51
1:B:933:MSE:HE2	1:B:947:LEU:HD21	1.92	0.51
1:A:220:ASN:H	1:A:220:ASN:ND2	2.00	0.51
1:A:1020:THR:O	1:A:1024:VAL:HG23	2.10	0.51
1:B:14:GLU:HA	1:B:997:ILE:CD1	2.34	0.51
1:B:93:GLN:CG	1:B:94:MSE:N	2.72	0.51
1:B:154:MSE:O	1:B:157:LEU:N	2.43	0.51
1:B:754:THR:HG22	1:B:758:ARG:HH21	1.76	0.51
1:B:780:ARG:O	1:B:784:LYS:HB2	2.09	0.51
1:A:30:GLY:O	1:A:105:ARG:NH2	2.43	0.51
1:A:59:LYS:O	1:A:62:VAL:HG23	2.10	0.51
1:A:212:PHE:C	1:A:214:THR:H	2.19	0.51
1:A:535:GLY:O	1:A:539:GLN:OE1	2.28	0.51
1:A:793:THR:CG2	1:A:824:ILE:HA	2.40	0.51
1:A:1014:GLU:HA	1:A:1017:GLU:CD	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:LEU:CD2	1:B:238:SER:HB3	2.39	0.51
1:B:236:LYS:HE3	1:B:236:LYS:HA	1.90	0.51
1:B:328:LEU:HD22	1:B:356:VAL:HG13	1.92	0.51
1:B:910:ARG:HA	1:B:924:LYS:HE2	1.91	0.51
1:A:216:LYS:HD3	1:A:216:LYS:C	2.35	0.51
1:A:896:GLN:HB3	1:A:897:PRO:HD3	1.93	0.51
1:B:216:LYS:C	1:B:216:LYS:HD3	2.36	0.51
1:B:634:GLU:HG3	1:B:676:VAL:HG21	1.92	0.51
1:A:123:LEU:HA	1:A:126:PHE:HD1	1.75	0.51
1:A:460:ARG:C	1:A:462:LEU:H	2.19	0.51
1:A:548:VAL:O	1:A:552:THR:OG1	2.29	0.51
1:A:1014:GLU:HA	1:A:1017:GLU:HG2	1.91	0.51
1:B:22:HIS:HA	1:B:25:ILE:HD11	1.91	0.51
1:B:22:HIS:CA	1:B:25:ILE:HG13	2.30	0.51
1:B:290:SER:O	1:B:293:ASP:OD1	2.28	0.51
1:B:563:GLU:HG3	1:B:565:GLU:N	2.24	0.51
1:B:886:PRO:CD	1:B:928:LEU:HD23	2.41	0.51
1:A:165:GLY:N	1:A:166:PRO:HD2	2.26	0.51
1:A:363:LEU:O	1:A:367:VAL:HG13	2.11	0.51
1:A:688:ASN:C	1:A:690:ALA:H	2.17	0.51
1:A:731:LYS:NZ	1:A:731:LYS:HB3	2.25	0.51
1:A:985:CYS:O	1:A:989:PRO:HD2	2.10	0.51
1:B:397:ASP:C	1:B:399:ASN:H	2.19	0.51
1:A:749:LEU:C	1:A:749:LEU:HD13	2.36	0.51
1:A:895:ASN:OD1	1:A:895:ASN:O	2.28	0.51
1:A:445:LEU:HD21	1:A:449:ARG:NE	2.25	0.51
1:B:684:ARG:HH22	1:B:686:PRO:HB3	1.76	0.51
1:B:885:PHE:CZ	1:B:899:MSE:HE3	2.46	0.51
1:A:460:ARG:O	1:A:464:LYS:HB2	2.11	0.51
1:B:297:GLN:HA	1:B:297:GLN:HE21	1.71	0.51
1:B:423:ASP:O	1:B:425:PRO:HD3	2.11	0.51
1:B:454:GLY:HA3	1:B:460:ARG:HE	1.75	0.51
1:B:568:GLN:C	1:B:570:ARG:H	2.19	0.51
1:A:790:LEU:O	1:A:793:THR:HG22	2.11	0.51
1:A:955:ALA:HA	1:A:958:SER:HB2	1.93	0.51
1:A:998:LEU:HB3	1:A:1023:LEU:HD12	1.93	0.51
1:B:885:PHE:CE2	1:B:899:MSE:HE3	2.46	0.51
1:B:943:THR:C	1:B:945:ARG:H	2.18	0.51
1:B:1004:THR:HG22	1:B:1005:MSE:HG3	1.93	0.51
1:A:75:PRO:O	1:A:79:ILE:HD13	2.11	0.50
1:A:506:ASN:HB3	1:A:509:VAL:HG13	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:667:THR:CG2	1:A:671:LEU:HD21	2.41	0.50
1:B:179:GLN:O	1:B:188:ARG:NE	2.45	0.50
1:B:232:PHE:CE1	1:B:674:GLN:NE2	2.79	0.50
1:B:898:MSE:HE3	1:B:1024:VAL:N	2.26	0.50
1:A:74:MSE:HB2	1:A:75:PRO:HD3	1.94	0.50
1:A:122:LEU:HD22	1:A:122:LEU:C	2.36	0.50
1:A:794:ILE:O	1:A:798:VAL:HG13	2.11	0.50
1:A:929:LEU:CD1	1:A:953:ASP:HB3	2.41	0.50
1:A:1050:THR:HG23	1:A:1050:THR:O	2.12	0.50
1:A:301:GLN:O	1:A:305:GLU:HG2	2.10	0.50
1:A:754:THR:HG22	1:A:758:ARG:HH21	1.76	0.50
1:A:915:LYS:CD	1:A:915:LYS:H	2.22	0.50
1:B:747:GLN:HG3	1:B:748:MSE:N	2.25	0.50
1:A:258:TRP:CE3	1:A:261:LYS:HE2	2.47	0.50
1:A:316:LYS:HB2	1:A:317:GLU:OE2	2.09	0.50
1:A:569:ALA:HB1	2:A:1138:HOH:O	2.12	0.50
1:B:606:ILE:CD1	1:B:699:LYS:HG3	2.41	0.50
1:B:665:VAL:O	1:B:669:ARG:HD2	2.10	0.50
1:B:881:LYS:HG2	2:B:1136:HOH:O	2.12	0.50
1:A:79:ILE:O	1:A:83:ASN:OD1	2.29	0.50
1:A:157:LEU:HD23	1:A:158:VAL:N	2.25	0.50
1:A:270:LEU:N	1:A:270:LEU:HD23	2.26	0.50
1:A:933:MSE:C	1:A:935:ARG:H	2.20	0.50
1:A:935:ARG:HB2	1:A:936:LEU:HD23	1.94	0.50
1:B:207:SER:CB	1:B:694:HIS:ND1	2.75	0.50
1:B:756:ILE:HG21	1:B:797:MSE:HE2	1.92	0.50
1:B:61:THR:O	1:B:65:THR:HB	2.10	0.50
1:B:333:ASP:O	1:B:337:ASP:HB2	2.11	0.50
1:B:460:ARG:NH1	1:B:460:ARG:HB3	2.27	0.50
1:B:785:ALA:O	1:B:788:ASP:HB2	2.11	0.50
1:B:896:GLN:CB	1:B:897:PRO:HD3	2.42	0.50
1:B:913:SER:HB2	1:B:915:LYS:HE3	1.93	0.50
1:A:568:GLN:O	1:A:572:LEU:HB2	2.11	0.50
1:A:785:ALA:O	1:A:788:ASP:HB2	2.12	0.50
1:B:138:CYS:HG	1:B:171:MSE:HE3	1.77	0.50
1:B:287:PRO:HG3	1:B:350:MSE:HG2	1.94	0.50
1:B:895:ASN:OD1	1:B:895:ASN:O	2.29	0.50
1:A:618:ASP:OD1	1:A:618:ASP:O	2.29	0.50
1:B:215:THR:HG21	1:B:223:ILE:N	2.26	0.50
1:B:454:GLY:CA	1:B:460:ARG:HE	2.25	0.50
1:B:608:LEU:H	1:B:608:LEU:CD1	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:839:GLU:N	1:B:840:PRO:CD	2.75	0.50
1:A:939:GLY:HA2	1:A:1006:LEU:HG	1.92	0.49
1:B:40:LEU:C	1:B:43:PRO:HD2	2.35	0.49
1:B:258:TRP:C	1:B:258:TRP:CE3	2.90	0.49
1:B:403:GLU:O	1:B:406:GLU:N	2.44	0.49
1:A:113:ARG:NH1	1:A:1005:MSE:HE2	2.27	0.49
1:A:234:VAL:O	1:A:238:SER:OG	2.29	0.49
1:A:952:LYS:NZ	1:B:623[B]:GLU:OE2	2.44	0.49
1:A:1004:THR:HG22	1:A:1005:MSE:HG3	1.93	0.49
1:A:1013:ASP:N	1:A:1013:ASP:OD1	2.44	0.49
1:B:558:LEU:HD22	1:B:569:ALA:CB	2.37	0.49
1:A:70:LEU:HD23	1:A:70:LEU:C	2.37	0.49
1:A:136:ARG:HG3	1:A:136:ARG:NH1	2.26	0.49
1:A:682:LEU:HD12	1:A:682:LEU:O	2.11	0.49
1:A:836:GLN:CD	1:A:837:PRO:HD2	2.37	0.49
1:B:458:GLU:C	1:B:460:ARG:H	2.20	0.49
1:A:313:CYS:O	1:A:486:PRO:HG3	2.12	0.49
1:A:68:GLN:O	1:A:72:ARG:HG2	2.11	0.49
1:A:122:LEU:HD22	1:A:122:LEU:O	2.12	0.49
1:A:626:PHE:CZ	1:A:680:ARG:CG	2.95	0.49
1:A:926:MSE:HE2	1:A:957:ALA:C	2.38	0.49
1:B:229:ASN:OD1	1:B:229:ASN:N	2.45	0.49
1:B:885:PHE:CE2	1:B:903:ARG:HG3	2.46	0.49
1:B:894:ILE:CG2	1:B:895:ASN:N	2.75	0.49
1:B:932:GLU:O	1:B:936:LEU:HG	2.13	0.49
1:A:85:CYS:O	1:A:89:VAL:HG23	2.12	0.49
1:A:90:GLN:O	1:A:94:MSE:HE3	2.12	0.49
1:A:745:GLN:HG3	1:A:748:MSE:HB2	1.95	0.49
1:A:747:GLN:HG3	1:A:748:MSE:N	2.27	0.49
1:A:898:MSE:HE3	1:A:1024:VAL:CG2	2.43	0.49
1:A:901:ALA:HB1	1:A:1031:MSE:HG3	1.93	0.49
1:A:1018:GLN:HG2	1:A:1019:ALA:N	2.24	0.49
1:B:79:ILE:O	1:B:83:ASN:OD1	2.29	0.49
1:A:453:LYS:H	1:A:453:LYS:CD	2.09	0.49
1:A:479:ARG:HB3	2:A:1164:HOH:O	2.11	0.49
1:B:31:GLU:HG3	1:B:105:ARG:NH1	2.27	0.49
1:B:580:LEU:O	1:B:583:LEU:N	2.46	0.49
1:B:790:LEU:O	1:B:790:LEU:HD12	2.13	0.49
1:A:109:ILE:HD13	1:A:1008[B]:ARG:HE	1.78	0.49
1:A:631:ALA:O	1:A:633:PHE:N	2.45	0.49
1:B:14:GLU:HB3	1:B:15:PRO:HD3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:LEU:HD11	1:B:111:GLY:C	2.38	0.49
1:A:136:ARG:HG3	1:A:136:ARG:HH11	1.78	0.49
1:A:333:ASP:O	1:A:337:ASP:HB2	2.13	0.49
1:A:912:TRP:O	1:A:1061:LYS:HD2	2.13	0.49
1:B:654:ASN:O	1:B:657:THR:N	2.36	0.49
1:A:168:MSE:CE	1:A:202:LEU:HB2	2.43	0.49
1:A:216:LYS:HB2	1:A:223:ILE:CG2	2.43	0.49
1:A:769:ARG:HH11	1:A:976:ARG:NH2	2.08	0.49
1:A:944:LYS:HE2	1:A:1006:LEU:O	2.13	0.49
1:B:376:ALA:HB1	1:B:421:LEU:HD21	1.95	0.49
1:B:799:MSE:HE2	1:B:799:MSE:HB2	1.77	0.49
1:B:815:LYS:CD	1:B:815:LYS:N	2.76	0.49
1:A:911:LYS:O	1:A:1060:ARG:HG2	2.13	0.48
1:B:43:PRO:O	1:B:46:ALA:HB3	2.13	0.48
1:B:894:ILE:HD13	1:B:934:SER:O	2.13	0.48
1:B:898:MSE:CE	1:B:1024:VAL:HA	2.43	0.48
1:A:310:GLY:O	1:A:318:ARG:HG2	2.13	0.48
1:A:634:GLU:HG3	1:A:676:VAL:HG21	1.96	0.48
1:A:665:VAL:HG22	1:A:709:MSE:HE3	1.95	0.48
1:A:838:GLN:CD	1:A:839:GLU:H	2.21	0.48
1:B:641:GLY:O	1:B:645:GLU:HG3	2.13	0.48
1:B:841:ASP:OD1	1:B:841:ASP:N	2.40	0.48
1:B:1014:GLU:CA	1:B:1017:GLU:HG2	2.43	0.48
1:B:1055:THR:HG22	1:B:1056:LEU:H	1.78	0.48
1:A:457:PRO:CA	1:A:460:ARG:HG2	2.44	0.48
1:A:477:THR:O	1:A:481:VAL:HG23	2.12	0.48
1:B:2:PRO:HB2	1:B:1022:MSE:SE	2.63	0.48
1:B:22:HIS:HB2	1:B:25:ILE:HD12	1.94	0.48
1:B:159:THR:HA	1:B:162:LYS:HZ1	1.77	0.48
1:B:530:ALA:O	1:B:532:VAL:N	2.45	0.48
1:B:744:ILE:N	1:B:744:ILE:CD1	2.75	0.48
1:A:448:LEU:H	1:A:448:LEU:HD13	1.77	0.48
1:A:530:ALA:O	1:A:532:VAL:N	2.45	0.48
1:A:898:MSE:CE	1:A:1023:LEU:HD23	2.23	0.48
1:B:14:GLU:HG2	1:B:993:THR:CG2	2.43	0.48
1:B:566:SER:CB	1:B:567:PRO:HD2	2.41	0.48
1:B:974:ASP:CG	1:B:977:ILE:HG13	2.39	0.48
1:A:126:PHE:O	1:A:129:ALA:HB3	2.13	0.48
1:A:769:ARG:NH1	1:A:976:ARG:HH22	2.12	0.48
1:B:29:GLU:HG2	1:B:945:ARG:CD	2.38	0.48
1:B:434:SER:O	1:B:438:ILE:HG13	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:437:GLU:O	1:B:441:LEU:HG	2.14	0.48
1:B:903:ARG:O	1:B:907:ASP:OD2	2.31	0.48
1:A:74:MSE:CE	1:A:78:PHE:CZ	2.91	0.48
1:A:544:LYS:HD2	1:A:586:ARG:HE	1.76	0.48
1:B:253:TRP:CD2	1:B:1025:HIS:CD2	3.02	0.48
1:B:341[B]:ARG:CZ	1:B:343:GLN:NE2	2.77	0.48
1:B:369:ASN:CG	1:B:373:LYS:HE2	2.38	0.48
1:B:384:ILE:HG12	1:B:414:GLU:HB3	1.95	0.48
1:B:422:CYS:O	1:B:428:ARG:NH2	2.45	0.48
1:A:530:ALA:C	1:A:532:VAL:N	2.71	0.48
1:A:622:ARG:NH1	1:A:683:LEU:HD13	2.28	0.48
1:A:741:MSE:SE	1:A:814:GLN:HB3	2.64	0.48
1:A:906:HIS:HB2	1:A:927:ALA:CB	2.40	0.48
1:B:42:ALA:N	1:B:43:PRO:HD2	2.29	0.48
1:B:159:THR:HA	1:B:162:LYS:NZ	2.29	0.48
1:B:807:ASN:CB	1:B:810:ASP:HB3	2.42	0.48
1:A:87:LYS:HZ1	1:A:107:TYR:HA	1.79	0.48
1:A:173:LYS:O	1:A:177:GLU:HG3	2.14	0.48
1:A:644:ALA:CB	1:A:709:MSE:CE	2.91	0.48
1:A:898:MSE:HG2	1:A:1024:VAL:HG13	1.96	0.48
1:A:921:ALA:O	1:A:925:ARG:HG3	2.14	0.48
1:B:502:ARG:O	1:B:505:ASP:HB2	2.14	0.48
1:A:123:LEU:HA	1:A:126:PHE:CD1	2.49	0.48
1:A:697:THR:HG22	1:A:698:MSE:HE2	1.95	0.48
1:A:838:GLN:NE2	1:A:838:GLN:HA	2.27	0.48
1:B:262:ASP:OD2	1:B:485:ARG:HD2	2.12	0.48
1:B:377:MSE:HB3	1:B:481:VAL:HG13	1.95	0.48
1:B:466:VAL:HG12	1:B:467:ALA:N	2.29	0.48
1:B:754:THR:HG22	1:B:758:ARG:NH2	2.29	0.48
1:B:880:GLU:CG	1:B:881:LYS:N	2.77	0.48
1:A:460:ARG:NH2	2:A:1097:HOH:O	2.43	0.48
1:A:919:ILE:CD1	1:A:964:LEU:HB2	2.44	0.48
1:B:321:ILE:HG12	1:B:366:LYS:HD2	1.96	0.48
1:B:667:THR:HG22	1:B:671:LEU:HD21	1.95	0.48
1:B:833:GLU:O	1:B:836:GLN:HB2	2.14	0.48
1:B:902:ALA:HB1	1:B:927:ALA:O	2.13	0.48
1:A:60:GLU:O	1:A:64:THR:OG1	2.31	0.47
1:A:146:THR:HG22	1:A:147:VAL:N	2.27	0.47
1:A:744:ILE:HG13	1:A:808:ILE:CG2	2.44	0.47
1:A:769:ARG:NH1	1:A:976:ARG:HH21	2.11	0.47
1:B:331:MSE:HE1	1:B:355:GLN:HG2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:551:LEU:HD23	1:B:551:LEU:H	1.77	0.47
1:B:840:PRO:C	1:B:842:PHE:H	2.20	0.47
1:B:933:MSE:C	1:B:935:ARG:H	2.21	0.47
1:A:253:TRP:CZ3	1:A:1022:MSE:HG2	2.49	0.47
1:A:321:ILE:HG12	1:A:366:LYS:HD2	1.96	0.47
1:A:498:GLU:CG	1:A:499:GLN:N	2.75	0.47
1:A:682:LEU:HB2	1:A:691:ALA:HB1	1.95	0.47
1:A:1008[A]:ARG:CZ	1:A:1008[A]:ARG:HB2	2.44	0.47
1:B:10:GLU:HG2	1:B:11:SER:N	2.26	0.47
1:B:294:ALA:O	1:B:297:GLN:HB2	2.15	0.47
1:B:598:VAL:HG12	1:B:640:LEU:HD23	1.95	0.47
1:A:94:MSE:H	1:A:94:MSE:HG2	1.46	0.47
1:A:512:ARG:CG	1:A:512:ARG:NH1	2.77	0.47
1:A:658:VAL:CG1	1:A:662:GLN:NE2	2.77	0.47
1:A:683:LEU:HD13	1:A:683:LEU:C	2.40	0.47
1:A:685:ASN:N	1:A:686:PRO:CD	2.77	0.47
1:B:750:VAL:CG1	1:B:751:ALA:N	2.77	0.47
1:B:972:CYS:O	1:B:978:ARG:NH2	2.47	0.47
1:A:142:LEU:O	1:A:145:LEU:HB2	2.14	0.47
1:B:454:GLY:HA2	1:B:457:PRO:CG	2.44	0.47
1:A:1:MSE:HE3	1:A:3:VAL:CG2	2.44	0.47
1:A:566:SER:CB	1:A:567:PRO:CD	2.93	0.47
1:B:48:GLN:O	1:B:52:SER:HB3	2.13	0.47
1:B:74:MSE:HE1	1:B:122:LEU:HD21	1.94	0.47
1:B:564:GLY:CA	1:B:569:ALA:HB1	2.45	0.47
1:A:153:THR:CG2	1:A:154:MSE:H	2.18	0.47
1:A:223:ILE:HA	1:A:226:ALA:HB3	1.95	0.47
1:A:429:ASP:OD2	1:A:433:ARG:NH2	2.47	0.47
1:A:675:VAL:CG2	1:A:698:MSE:HB3	2.36	0.47
1:A:1014:GLU:CA	1:A:1017:GLU:HG2	2.45	0.47
1:B:456:SER:N	1:B:457:PRO:HD2	2.30	0.47
1:B:501:GLN:O	1:B:502:ARG:C	2.58	0.47
1:B:603:THR:O	1:B:606:ILE:HG22	2.14	0.47
1:A:88:LEU:HD11	1:A:111:GLY:C	2.39	0.47
1:A:122:LEU:HD13	1:A:126:PHE:HE1	1.80	0.47
1:A:324:THR:HG21	1:A:363:LEU:HG	1.96	0.47
1:A:337:ASP:O	1:A:340:ALA:N	2.35	0.47
1:A:447:ASP:C	1:A:449:ARG:H	2.23	0.47
1:A:626:PHE:CE1	1:A:680:ARG:CG	2.97	0.47
1:A:744:ILE:HG13	1:A:808:ILE:HG22	1.97	0.47
1:A:913:SER:CB	1:A:915:LYS:HG2	2.25	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:936:LEU:HD12	1:A:947:LEU:HA	1.96	0.47
1:B:13:LEU:CD2	1:B:123:LEU:CD2	2.93	0.47
1:B:31:GLU:HA	1:B:105:ARG:HH21	1.73	0.47
1:B:211:ILE:CD1	1:B:681:ILE:HG21	2.45	0.47
1:B:253:TRP:CG	1:B:1025:HIS:CD2	3.03	0.47
1:B:253:TRP:C	1:B:255:GLU:H	2.21	0.47
1:B:377:MSE:HE3	1:B:421:LEU:HD23	1.96	0.47
1:B:682:LEU:HD22	1:B:685:ASN:HB3	1.96	0.47
1:B:929:LEU:O	1:B:950:CYS:SG	2.73	0.47
1:A:82:GLU:O	1:A:86:THR:HG23	2.15	0.47
1:A:131:VAL:O	1:A:135:ILE:HG13	2.15	0.47
1:A:215:THR:HG23	1:A:220:ASN:HD21	1.78	0.47
1:B:448:LEU:HA	1:B:451:GLN:HG3	1.94	0.47
1:B:555:LEU:HD23	1:B:555:LEU:C	2.40	0.47
1:A:227:LEU:CD1	1:A:230:ARG:NH1	2.78	0.47
1:A:227:LEU:HD22	1:A:227:LEU:HA	1.61	0.47
1:A:394:TRP:CG	1:A:404:GLY:HA3	2.50	0.47
1:A:447:ASP:O	1:A:450:ARG:HG3	2.15	0.47
1:A:563:GLU:H	1:A:563:GLU:HG2	1.45	0.47
1:A:619:ALA:HA	1:A:620:PRO:HD3	1.81	0.47
1:A:885:PHE:CZ	1:A:899:MSE:CE	2.98	0.47
1:B:563:GLU:HG2	1:B:565:GLU:H	1.76	0.47
1:B:595:VAL:HG11	1:B:717:ILE:HD11	1.97	0.47
1:B:611:VAL:HG12	1:B:612:ALA:N	2.29	0.47
1:B:790:LEU:HD12	1:B:793:THR:CG2	2.45	0.47
1:A:202:LEU:CB	1:A:203:PRO:HD3	2.44	0.47
1:A:243:GLU:OE1	1:A:243:GLU:HA	2.15	0.47
1:A:622:ARG:CZ	1:A:683:LEU:HD13	2.44	0.47
1:B:10:GLU:O	1:B:14:GLU:HB2	2.15	0.47
1:B:93:GLN:HG2	1:B:94:MSE:N	2.29	0.47
1:B:227:LEU:O	1:B:231:ASN:HB2	2.15	0.47
1:B:402:PRO:O	1:B:406:GLU:HB2	2.15	0.47
1:B:544:LYS:HD3	1:B:582:ASP:OD2	2.14	0.47
1:A:815:LYS:CD	1:A:815:LYS:N	2.78	0.46
1:A:833:GLU:C	1:A:835:PHE:N	2.74	0.46
1:A:894:ILE:CG2	1:A:895:ASN:N	2.77	0.46
1:B:24:VAL:O	1:B:27:HIS:HB2	2.15	0.46
1:B:247:VAL:CA	1:B:250:LEU:HD13	2.39	0.46
1:B:256:ASP:CG	1:B:259:ALA:HB2	2.39	0.46
1:B:929:LEU:HD11	1:B:953:ASP:HB3	1.97	0.46
1:A:104:ALA:C	1:A:106:ASP:H	2.22	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:LEU:HD22	1:A:270:LEU:HA	1.71	0.46
1:A:369:ASN:OD1	1:A:372:ARG:NH2	2.48	0.46
1:A:440:ALA:O	1:A:442:THR:N	2.48	0.46
1:B:74:MSE:CE	1:B:78:PHE:CZ	2.97	0.46
1:B:277:LEU:HD23	1:B:277:LEU:HA	1.68	0.46
1:B:460:ARG:HH11	1:B:460:ARG:HA	1.80	0.46
1:A:74:MSE:CB	1:A:75:PRO:HD3	2.46	0.46
1:A:397:ASP:C	1:A:399:ASN:H	2.22	0.46
1:A:427:GLU:OE1	1:A:480:ALA:HA	2.15	0.46
1:A:886:PRO:C	1:A:887:GLU:HG3	2.39	0.46
1:B:6:THR:HG22	1:B:182:LEU:HD12	1.96	0.46
1:B:143:GLU:HG2	1:B:144:TYR:N	2.29	0.46
1:B:223:ILE:HG13	1:B:223:ILE:H	1.50	0.46
1:A:10:GLU:HG2	1:A:11:SER:N	2.29	0.46
1:A:47:VAL:HG12	1:A:115:ILE:CD1	2.44	0.46
1:A:110:ASP:OD1	1:A:1008[B]:ARG:NH1	2.49	0.46
1:A:743:ASN:HB2	1:A:745:GLN:NE2	2.31	0.46
1:B:84:ALA:O	1:B:88:LEU:HD12	2.15	0.46
1:B:885:PHE:CE2	1:B:899:MSE:CE	2.99	0.46
1:B:919:ILE:CD1	1:B:964:LEU:HB2	2.46	0.46
1:A:5:HIS:CD2	1:A:6:THR:HG23	2.50	0.46
1:A:28:GLU:OE1	1:A:944:LYS:HD2	2.15	0.46
1:B:45:ALA:O	1:B:48:GLN:HB3	2.16	0.46
1:B:63:GLN:C	1:B:65:THR:H	2.22	0.46
1:B:619:ALA:HA	1:B:620:PRO:HD3	1.79	0.46
1:A:506:ASN:C	1:A:508:THR:H	2.22	0.46
1:A:793:THR:HG23	1:A:824:ILE:HG13	1.97	0.46
1:A:930:MSE:HG2	1:A:954:ILE:CD1	2.46	0.46
1:B:190:MSE:HE2	1:B:247:VAL:HG21	1.97	0.46
1:B:754:THR:CG2	1:B:758:ARG:HH21	2.29	0.46
1:A:20:ILE:CD1	1:A:115:ILE:HG23	2.45	0.46
1:A:346:SER:O	1:A:350:MSE:HE2	2.16	0.46
1:A:445:LEU:HD23	1:A:445:LEU:C	2.40	0.46
1:A:744:ILE:N	1:A:744:ILE:CD1	2.78	0.46
1:A:769:ARG:HH11	1:A:976:ARG:HH21	1.64	0.46
1:A:915:LYS:CD	1:A:915:LYS:N	2.78	0.46
1:A:59:LYS:HA	1:A:62:VAL:HG23	1.97	0.46
1:A:150:VAL:O	1:A:150:VAL:HG13	2.14	0.46
1:A:324:THR:CG2	1:A:363:LEU:HG	2.45	0.46
1:A:731:LYS:NZ	1:A:731:LYS:CB	2.78	0.46
1:A:824:ILE:HG22	1:A:825:LEU:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:HIS:CE1	1:B:23:LEU:CD2	2.99	0.46
1:B:40:LEU:CD2	1:B:43:PRO:HG2	2.45	0.46
1:B:102:VAL:N	1:B:103:PRO:CD	2.79	0.46
1:B:225:GLU:HB3	1:B:681:ILE:CG1	2.41	0.46
1:B:369:ASN:OD1	1:B:372:ARG:NH2	2.49	0.46
1:B:452:GLY:O	1:B:454:GLY:N	2.49	0.46
1:B:512:ARG:CG	1:B:512:ARG:NH1	2.71	0.46
1:A:448:LEU:N	1:A:448:LEU:HD12	2.30	0.46
1:A:741:MSE:O	1:A:744:ILE:HD12	2.16	0.46
1:B:623[B]:GLU:OE2	1:B:624:GLU:HG3	2.16	0.46
1:B:648:ALA:O	1:B:658:VAL:HG22	2.15	0.46
1:A:401:GLY:HA3	1:A:403:GLU:OE1	2.15	0.46
1:A:601:ASP:OD2	1:A:604:THR:OG1	2.22	0.46
1:A:988:ILE:HB	1:A:989:PRO:HD3	1.98	0.46
1:B:54:LEU:HD13	1:B:122:LEU:HD12	1.96	0.46
1:B:458:GLU:O	1:B:459:ALA:HB3	2.15	0.46
1:B:604:THR:HA	1:B:607:LYS:HD3	1.98	0.46
1:B:811:PRO:HB3	1:B:815:LYS:CE	2.43	0.46
1:B:933:MSE:HE2	1:B:947:LEU:CD2	2.45	0.46
1:A:377:MSE:CE	1:A:418:ILE:HA	2.46	0.45
1:A:760:ALA:HB3	1:A:794:ILE:CD1	2.46	0.45
1:A:836:GLN:OE1	1:A:836:GLN:HA	2.13	0.45
1:A:906:HIS:NE2	1:A:910:ARG:HG3	2.31	0.45
1:A:995:LEU:O	1:A:995:LEU:HD13	2.16	0.45
1:B:625:VAL:CG1	1:B:626:PHE:N	2.80	0.45
1:B:734:LEU:HD22	1:B:818:LEU:CD2	2.45	0.45
1:B:936:LEU:N	1:B:936:LEU:CD2	2.77	0.45
1:A:220:ASN:N	1:A:220:ASN:ND2	2.51	0.45
1:A:350:MSE:HE3	1:A:350:MSE:HB2	1.61	0.45
1:A:623:GLU:OE1	1:A:623:GLU:HA	2.16	0.45
1:B:749:LEU:HD13	1:B:749:LEU:C	2.41	0.45
1:A:122:LEU:HD23	1:A:122:LEU:HA	1.63	0.45
1:A:506:ASN:O	1:A:508:THR:N	2.50	0.45
1:A:622:ARG:NH1	1:A:683:LEU:CD1	2.80	0.45
1:A:644:ALA:HB3	1:A:709:MSE:CE	2.46	0.45
1:A:20:ILE:HD11	1:A:115:ILE:CG2	2.46	0.45
1:A:343:GLN:H	1:A:343:GLN:HG3	1.55	0.45
1:A:501:GLN:O	1:A:502:ARG:C	2.59	0.45
1:A:593:GLN:HG2	1:A:593:GLN:H	1.58	0.45
1:B:189:VAL:O	1:B:192:VAL:N	2.49	0.45
1:B:227:LEU:HD22	1:B:227:LEU:HA	1.71	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354[A]:GLN:HG2	1:B:355:GLN:N	2.32	0.45
1:B:731:LYS:NZ	1:B:731:LYS:CB	2.79	0.45
1:B:995:LEU:HD13	1:B:995:LEU:C	2.41	0.45
1:A:172:ALA:HB2	1:A:195:MSE:HE2	1.98	0.45
1:A:615:ALA:HA	1:A:616:PRO:HD2	1.59	0.45
1:A:893:VAL:CG2	1:A:938:ARG:HD3	2.44	0.45
1:B:108:LEU:O	1:B:112:SER:N	2.49	0.45
1:B:131:VAL:O	1:B:135:ILE:HG13	2.17	0.45
1:B:157:LEU:HD23	1:B:158:VAL:N	2.32	0.45
1:B:168:MSE:HE3	1:B:202:LEU:HB2	1.98	0.45
1:B:419:ALA:O	1:B:422:CYS:HB2	2.16	0.45
1:B:836:GLN:HE22	1:B:837:PRO:HD2	1.79	0.45
1:A:61:THR:O	1:A:65:THR:HB	2.16	0.45
1:A:87:LYS:NZ	1:A:107:TYR:O	2.45	0.45
1:A:225:GLU:O	1:A:229:ASN:OD1	2.34	0.45
1:A:277:LEU:HA	1:A:277:LEU:HD23	1.43	0.45
1:A:331:MSE:HE1	1:A:355:GLN:HG2	1.97	0.45
1:A:456:SER:O	1:A:458:GLU:HG2	2.16	0.45
1:A:756:ILE:HG22	1:A:797:MSE:CE	2.46	0.45
1:A:880:GLU:HG3	1:A:915:LYS:HE3	1.97	0.45
1:B:154:MSE:HE3	1:B:158:VAL:HB	1.97	0.45
1:B:335:VAL:C	1:B:337:ASP:N	2.72	0.45
1:B:499:GLN:NE2	1:B:514:VAL:CG1	2.80	0.45
1:B:618:ASP:OD1	1:B:618:ASP:O	2.35	0.45
1:A:180:GLN:HE21	1:B:358:GLN:CD	2.24	0.45
1:A:341:ARG:HB3	1:A:343:GLN:HE21	1.82	0.45
1:B:819:ASP:OD1	1:B:823:ARG:NH1	2.50	0.45
1:A:280:ALA:HB1	1:A:299:ILE:HG13	1.99	0.45
1:A:506:ASN:C	1:A:508:THR:N	2.75	0.45
1:B:277:LEU:HD13	1:B:281:LYS:HE2	1.99	0.45
1:A:101:SER:O	1:A:105:ARG:HD2	2.17	0.45
1:A:266:MSE:CG	1:A:309:VAL:HG22	2.41	0.45
1:A:270:LEU:HD21	1:A:367:VAL:HG23	1.99	0.45
1:B:70:LEU:C	1:B:70:LEU:HD23	2.40	0.45
1:B:223:ILE:C	1:B:225:GLU:N	2.75	0.45
1:B:523:VAL:HG12	1:B:527:HIS:CE1	2.51	0.45
1:A:27:HIS:ND1	1:A:27:HIS:C	2.75	0.45
1:A:734:LEU:HD13	1:A:822:TYR:CE1	2.52	0.45
1:A:993:THR:O	1:A:996:LYS:HB2	2.17	0.45
1:B:615:ALA:HA	1:B:616:PRO:HD2	1.71	0.45
1:B:1005:MSE:HE1	1:B:1015:GLU:CG	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1053:GLY:O	1:B:1054:PHE:HD1	1.99	0.45
1:A:95:LEU:HD21	1:A:105:ARG:HG3	1.99	0.44
1:A:544:LYS:H	1:A:544:LYS:HG2	1.42	0.44
1:B:95:LEU:HD11	1:B:104:ALA:CB	2.45	0.44
1:B:190:MSE:HE1	1:B:246:ARG:HH12	1.83	0.44
1:A:444:LYS:NZ	1:A:444:LYS:CB	2.78	0.44
1:A:551:LEU:CB	1:A:576:LEU:HD13	2.45	0.44
1:A:633:PHE:HD2	1:A:676:VAL:HG23	1.79	0.44
1:B:445:LEU:HD23	1:B:449:ARG:HD2	1.99	0.44
1:B:551:LEU:HD11	1:B:575:GLN:HB3	1.98	0.44
1:B:604:THR:N	1:B:605:PRO:HD2	2.32	0.44
1:B:633:PHE:CE2	1:B:676:VAL:HG23	2.52	0.44
1:B:734:LEU:CD2	1:B:818:LEU:HD23	2.47	0.44
1:A:102:VAL:N	1:A:103:PRO:CD	2.80	0.44
1:A:943:THR:O	1:A:946:ALA:N	2.50	0.44
1:B:369:ASN:O	1:B:373:LYS:HG3	2.16	0.44
1:B:743:ASN:HB2	1:B:745:GLN:NE2	2.32	0.44
1:B:744:ILE:HG13	1:B:808:ILE:CG2	2.47	0.44
1:B:836:GLN:OE1	1:B:836:GLN:HA	2.07	0.44
1:A:14:GLU:HG2	1:A:993:THR:CG2	2.48	0.44
1:A:87:LYS:NZ	1:A:107:TYR:CA	2.81	0.44
1:A:622:ARG:O	1:A:623:GLU:CB	2.64	0.44
1:A:880:GLU:CG	1:A:915:LYS:NZ	2.81	0.44
1:B:331:MSE:HE2	1:B:331:MSE:HB3	1.95	0.44
1:B:397:ASP:C	1:B:399:ASN:N	2.75	0.44
1:B:417:LYS:HZ2	1:B:417:LYS:HG3	1.64	0.44
1:B:595:VAL:HG11	1:B:717:ILE:CD1	2.48	0.44
1:B:658:VAL:HG13	1:B:662:GLN:HE21	1.81	0.44
1:B:904:GLN:HB3	1:B:1035:LYS:HE2	2.00	0.44
1:B:1004:THR:HG22	1:B:1005:MSE:CG	2.46	0.44
1:A:201:LEU:C	1:A:237:MSE:HE2	2.42	0.44
1:A:706:VAL:O	1:A:709:MSE:N	2.51	0.44
1:B:63:GLN:O	1:B:65:THR:N	2.44	0.44
1:B:153:THR:CG2	1:B:154:MSE:H	2.18	0.44
1:B:512:ARG:HH11	1:B:512:ARG:HB3	1.77	0.44
1:B:947:LEU:C	1:B:949:GLN:N	2.75	0.44
1:B:990:THR:O	1:B:994:GLN:HG2	2.18	0.44
1:A:27:HIS:ND1	1:A:27:HIS:O	2.50	0.44
1:A:71:LYS:O	1:A:75:PRO:HG2	2.18	0.44
1:A:204:VAL:HG22	1:A:698:MSE:HE1	1.99	0.44
1:A:825:LEU:C	1:A:828:VAL:HG22	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1004:THR:HG22	1:A:1005:MSE:CG	2.47	0.44
1:B:506:ASN:C	1:B:508:THR:H	2.25	0.44
1:B:1014:GLU:HA	1:B:1017:GLU:OE2	2.18	0.44
1:A:626:PHE:CD1	1:A:626:PHE:C	2.94	0.44
1:A:1030:LEU:O	1:A:1034:VAL:HG23	2.18	0.44
1:B:448:LEU:N	1:B:448:LEU:CD1	2.80	0.44
1:A:447:ASP:C	1:A:449:ARG:N	2.75	0.44
1:B:27:HIS:CE1	1:B:108:LEU:HB3	2.53	0.44
1:B:266:MSE:HE2	1:B:309:VAL:HG13	2.00	0.44
1:B:341[B]:ARG:CG	1:B:343:GLN:NE2	2.79	0.44
1:B:538[A]:ARG:HD2	1:B:539:GLN:NE2	2.33	0.44
1:B:570:ARG:HD2	1:B:570:ARG:HA	1.72	0.44
1:B:912:TRP:HB2	1:B:920:ILE:HG13	2.00	0.44
1:A:45:ALA:O	1:A:48:GLN:HB3	2.18	0.44
1:A:129:ALA:C	1:A:133:LYS:HE3	2.43	0.44
1:A:159:THR:HA	1:A:162:LYS:NZ	2.32	0.44
1:A:420:GLU:C	1:A:422:CYS:H	2.25	0.44
1:A:580:LEU:O	1:A:583:LEU:N	2.51	0.44
1:A:898:MSE:HE3	1:A:1024:VAL:N	2.33	0.44
1:B:154:MSE:C	1:B:156:ASP:N	2.75	0.44
1:B:211:ILE:HG13	1:B:690:ALA:O	2.16	0.44
1:B:445:LEU:HD21	1:B:449:ARG:HE	1.80	0.44
1:B:795:SER:N	1:B:796:PRO:CD	2.80	0.44
1:B:930:MSE:HG2	1:B:954:ILE:HD11	1.98	0.44
1:A:4:PHE:CZ	1:A:998:LEU:HD21	2.40	0.43
1:A:317:GLU:O	1:A:321:ILE:HG13	2.18	0.43
1:A:351:GLN:NE2	1:A:351:GLN:HA	2.32	0.43
1:A:383:SER:O	1:A:386:LYS:HG3	2.17	0.43
1:A:448:LEU:HA	1:A:451:GLN:HG3	1.98	0.43
1:A:898:MSE:CE	1:A:1024:VAL:CA	2.96	0.43
1:A:899:MSE:HG3	1:A:903:ARG:NH1	2.33	0.43
1:B:177:GLU:O	1:B:180:GLN:HB2	2.18	0.43
1:B:233:THR:CG2	1:B:237:MSE:CE	2.96	0.43
1:B:374:LEU:C	1:B:376:ALA:N	2.76	0.43
1:B:506:ASN:C	1:B:508:THR:N	2.74	0.43
1:B:626:PHE:CD1	1:B:627:ASP:N	2.86	0.43
1:B:885:PHE:HA	1:B:886:PRO:HD3	1.67	0.43
1:B:943:THR:O	1:B:946:ALA:N	2.50	0.43
1:B:1057:ARG:NH1	1:B:1057:ARG:CG	2.81	0.43
1:A:68:GLN:HB3	1:A:396:ALA:HB1	2.00	0.43
1:A:384:ILE:HD11	1:A:415:ALA:CA	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:MSE:HE3	1:A:591:MSE:HB3	1.96	0.43
1:A:769:ARG:HH12	1:A:976:ARG:NH2	2.14	0.43
1:B:653:ALA:HB1	1:B:658:VAL:CG2	2.42	0.43
1:B:666:LYS:O	1:B:669:ARG:HB2	2.17	0.43
1:A:447:ASP:HA	1:A:450:ARG:NH1	2.29	0.43
1:A:606:ILE:CD1	1:A:699:LYS:HG3	2.48	0.43
1:A:914:SER:H	1:A:915:LYS:CE	2.26	0.43
1:B:40:LEU:CD2	1:B:44:VAL:HG23	2.46	0.43
1:B:94:MSE:H	1:B:94:MSE:HG3	1.40	0.43
1:B:547:ARG:O	1:B:550[A]:GLN:HB2	2.17	0.43
1:B:656:SER:O	1:B:659:GLU:HB2	2.18	0.43
1:A:40:LEU:N	1:A:40:LEU:CD2	2.79	0.43
1:A:87:LYS:NZ	1:A:107:TYR:C	2.77	0.43
1:A:227:LEU:HD13	1:A:230:ARG:NH1	2.33	0.43
1:A:227:LEU:O	1:A:231:ASN:HB2	2.18	0.43
1:A:236:LYS:O	1:A:239:ALA:HB3	2.19	0.43
1:A:280:ALA:HB1	1:A:299:ILE:CG1	2.48	0.43
1:A:576:LEU:C	1:A:578:ASP:H	2.25	0.43
1:A:760:ALA:HB1	1:A:794:ILE:HD11	2.00	0.43
1:A:825:LEU:HA	1:A:828:VAL:HG22	2.00	0.43
1:A:885:PHE:CE2	1:A:899:MSE:CE	3.01	0.43
1:B:59:LYS:CA	1:B:62:VAL:HG23	2.48	0.43
1:B:207:SER:HG	1:B:694:HIS:CG	2.31	0.43
1:B:395:LEU:HD13	1:B:467:ALA:HB2	2.01	0.43
1:B:793:THR:CG2	1:B:824:ILE:HA	2.47	0.43
1:A:223:ILE:HG13	1:A:223:ILE:H	1.44	0.43
1:A:229:ASN:OD1	1:A:229:ASN:N	2.50	0.43
1:A:291:PRO:HB3	1:A:336:ALA:HB1	2.01	0.43
1:A:501:GLN:NE2	1:A:501:GLN:CA	2.82	0.43
1:A:625:VAL:CG1	1:A:626:PHE:N	2.81	0.43
1:A:633:PHE:CE2	1:A:676:VAL:HG23	2.53	0.43
1:A:654:ASN:C	1:A:656:SER:N	2.75	0.43
1:A:750:VAL:CG1	1:A:751:ALA:N	2.80	0.43
1:B:42:ALA:H	1:B:43:PRO:HD2	1.83	0.43
1:B:158:VAL:HG12	1:B:159:THR:N	2.34	0.43
1:B:185:GLN:O	1:B:189:VAL:HG23	2.18	0.43
1:B:227:LEU:CD2	1:B:230:ARG:NH1	2.82	0.43
1:B:286:ASP:C	1:B:288:SER:H	2.26	0.43
1:B:350:MSE:HE3	1:B:350:MSE:HB2	1.80	0.43
1:B:406:GLU:OE1	1:B:406:GLU:HA	2.17	0.43
1:B:896:GLN:HB3	1:B:897:PRO:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:GLU:HB3	1:A:15:PRO:HD3	2.01	0.43
1:A:186:GLU:O	1:A:190:MSE:HG3	2.18	0.43
1:A:212:PHE:O	1:A:214:THR:N	2.41	0.43
1:A:258:TRP:CE2	1:A:488:LYS:HD3	2.53	0.43
1:A:309:VAL:HG11	1:A:367:VAL:HB	2.01	0.43
1:A:728:GLU:OE2	1:A:731:LYS:HE3	2.18	0.43
1:A:1002:LYS:NZ	1:A:1020:THR:OG1	2.51	0.43
1:B:216:LYS:CB	1:B:223:ILE:HG21	2.41	0.43
1:B:460:ARG:HH11	1:B:460:ARG:CA	2.31	0.43
1:B:501:GLN:NE2	1:B:501:GLN:CA	2.78	0.43
1:B:738:LYS:CA	1:B:741:MSE:HE2	2.36	0.43
1:B:838:GLN:O	1:B:838:GLN:HG2	2.18	0.43
1:A:420:GLU:C	1:A:422:CYS:N	2.76	0.43
1:A:496:LYS:HD2	1:A:522:LEU:HD13	2.01	0.43
1:A:568:GLN:HA	1:A:571:ALA:HB3	2.01	0.43
1:A:836:GLN:HE22	1:A:837:PRO:HD2	1.81	0.43
1:A:950:CYS:O	1:A:954:ILE:HG13	2.18	0.43
1:B:56:ARG:HG2	1:B:57:VAL:N	2.34	0.43
1:B:123:LEU:HA	1:B:126:PHE:HD1	1.82	0.43
1:B:154:MSE:HE1	1:B:158:VAL:CG2	2.42	0.43
1:B:215:THR:HG21	1:B:222:GLY:C	2.43	0.43
1:B:301:GLN:O	1:B:304:ASP:HB3	2.19	0.43
1:B:537:TYR:O	1:B:537:TYR:HD1	2.00	0.43
1:B:719:THR:HG22	1:B:723:LEU:HD21	1.97	0.43
1:B:955:ALA:HA	1:B:958:SER:HB2	2.01	0.43
1:A:541:LEU:HD23	1:A:541:LEU:HA	1.80	0.43
1:A:756:ILE:HG21	1:A:797:MSE:HE2	1.97	0.43
1:B:15:PRO:O	1:B:18:GLN:CB	2.67	0.43
1:B:98:ASP:HA	1:B:99:PRO:HD2	1.69	0.43
1:B:144:TYR:HE2	1:B:160:TYR:CD1	2.37	0.43
1:B:263:THR:HG22	1:B:374:LEU:HG	2.00	0.43
1:B:285:ARG:O	1:B:286:ASP:HB2	2.19	0.43
1:B:335:VAL:C	1:B:337:ASP:H	2.26	0.43
1:B:994:GLN:HG2	1:B:994:GLN:H	1.56	0.43
1:A:10:GLU:O	1:A:14:GLU:HB2	2.19	0.43
1:A:454:GLY:C	1:A:456:SER:N	2.76	0.43
1:A:641:GLY:O	1:A:645:GLU:HG3	2.19	0.43
1:A:936:LEU:HD23	1:A:936:LEU:H	1.83	0.43
1:A:1042:GLU:HA	1:A:1045:SER:HB3	2.00	0.43
1:B:61:THR:CG2	1:B:70:LEU:HD11	2.48	0.43
1:B:177:GLU:H	1:B:177:GLU:HG3	1.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:LEU:N	1:B:203:PRO:CD	2.82	0.43
1:B:270:LEU:HD21	1:B:367:VAL:CG2	2.49	0.43
1:B:900:MSE:HE3	1:B:904:GLN:HE22	1.84	0.43
1:A:39:ASP:C	1:A:40:LEU:HD23	2.43	0.43
1:A:149:GLU:C	1:A:151:VAL:H	2.27	0.43
1:A:698:MSE:O	1:A:701:GLN:HB3	2.19	0.43
1:A:811:PRO:C	1:A:813:LEU:N	2.77	0.43
1:B:7:ARG:CG	1:B:7:ARG:NH1	2.78	0.43
1:B:122:LEU:HD23	1:B:122:LEU:HA	1.83	0.43
1:B:270:LEU:HD22	1:B:270:LEU:HA	1.71	0.43
1:B:466:VAL:CG1	1:B:467:ALA:N	2.82	0.43
1:B:926:MSE:HE2	1:B:957:ALA:CB	2.49	0.43
1:B:936:LEU:HD12	1:B:947:LEU:HA	2.01	0.43
1:A:613:ALA:O	1:A:682:LEU:HD11	2.18	0.42
1:A:978:ARG:O	1:A:982:LEU:HG	2.19	0.42
1:B:759:ARG:O	1:B:763:ILE:HG13	2.19	0.42
1:A:221:GLN:O	1:A:684:ARG:HB3	2.19	0.42
1:A:460:ARG:C	1:A:462:LEU:N	2.74	0.42
1:A:650:VAL:O	1:A:650:VAL:CG2	2.66	0.42
1:A:1042:GLU:HB2	1:A:1058:TRP:CD2	2.54	0.42
1:B:15:PRO:O	1:B:18:GLN:HB2	2.18	0.42
1:B:22:HIS:O	1:B:26:MSE:HG2	2.18	0.42
1:B:212:PHE:CE1	1:B:227:LEU:HD23	2.53	0.42
1:B:667:THR:O	1:B:668:ALA:C	2.62	0.42
1:B:882:ASP:O	1:B:883:GLU:O	2.37	0.42
1:B:950:CYS:O	1:B:954:ILE:HG13	2.20	0.42
1:A:61:THR:CG2	1:A:70:LEU:HD11	2.50	0.42
1:A:122:LEU:HD13	1:A:126:PHE:CE1	2.53	0.42
1:A:343:GLN:HB2	1:A:346:SER:HB2	2.01	0.42
1:A:485:ARG:HE	1:A:485:ARG:HB2	1.60	0.42
1:A:607:LYS:O	1:A:610:ALA:N	2.52	0.42
1:A:1049:ARG:HG3	1:A:1050:THR:N	2.33	0.42
1:A:423:ASP:O	1:A:425:PRO:HD3	2.19	0.42
1:A:566:SER:HB3	1:A:567:PRO:CD	2.49	0.42
1:A:658:VAL:HG13	1:A:662:GLN:HE21	1.85	0.42
1:A:804:VAL:O	1:A:804:VAL:HG12	2.20	0.42
1:A:899:MSE:HE2	1:A:903:ARG:NH2	2.34	0.42
1:A:1018:GLN:O	1:A:1021:GLU:HB2	2.20	0.42
1:B:60:GLU:O	1:B:64:THR:OG1	2.37	0.42
1:B:91:ALA:C	1:B:93:GLN:H	2.28	0.42
1:B:1050:THR:C	1:B:1052:ALA:N	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:PHE:C	1:A:214:THR:N	2.77	0.42
1:A:268:ARG:CZ	1:A:669:ARG:HH11	2.32	0.42
1:A:331:MSE:HE2	1:A:331:MSE:HB3	1.88	0.42
1:A:667:THR:O	1:A:668:ALA:C	2.62	0.42
1:B:59:LYS:C	1:B:62:VAL:HG23	2.44	0.42
1:B:126:PHE:O	1:B:129:ALA:HB3	2.19	0.42
1:B:445:LEU:HD11	1:B:463:ALA:HB2	2.01	0.42
1:B:530:ALA:C	1:B:532:VAL:N	2.77	0.42
1:A:37:ILE:CG2	1:A:38:PRO:CD	2.97	0.42
1:A:262:ASP:OD2	1:A:485:ARG:HD2	2.20	0.42
1:A:568:GLN:C	1:A:570:ARG:N	2.74	0.42
1:A:671:LEU:H	1:A:671:LEU:CD2	2.19	0.42
1:A:804:VAL:HG12	1:A:808:ILE:HA	2.02	0.42
1:A:915:LYS:N	1:A:915:LYS:HD3	2.35	0.42
1:B:14:GLU:CA	1:B:997:ILE:HD11	2.41	0.42
1:B:571:ALA:O	1:B:575:GLN:HB2	2.19	0.42
1:B:883:GLU:CG	1:B:884:GLU:H	2.32	0.42
1:B:1001:VAL:CG1	1:B:1002:LYS:N	2.81	0.42
1:B:1002:LYS:NZ	1:B:1020:THR:OG1	2.29	0.42
1:A:152:GLU:OE1	1:A:216:LYS:NZ	2.30	0.42
1:A:284:LEU:HD13	1:A:357:SER:HB2	2.01	0.42
1:A:440:ALA:HB3	1:A:441:LEU:HD23	2.00	0.42
1:B:28:GLU:OE2	1:B:944:LYS:NZ	2.30	0.42
1:B:94:MSE:HE2	1:B:94:MSE:HB2	1.96	0.42
1:B:512:ARG:NH1	1:B:512:ARG:HG3	2.34	0.42
1:B:626:PHE:CD1	1:B:626:PHE:C	2.97	0.42
1:B:898:MSE:HE3	1:B:1024:VAL:CA	2.49	0.42
1:A:529:LEU:CD1	1:A:587:MSE:HB3	2.49	0.42
1:A:650:VAL:O	1:A:650:VAL:HG22	2.18	0.42
1:A:685:ASN:O	1:A:686:PRO:O	2.37	0.42
1:B:212:PHE:C	1:B:214:THR:N	2.77	0.42
1:B:815:LYS:N	1:B:815:LYS:HD3	2.34	0.42
1:B:896:GLN:CG	1:B:897:PRO:HD3	2.50	0.42
1:B:988:ILE:HG22	1:B:989:PRO:N	2.34	0.42
1:B:1005:MSE:HE2	1:B:1015:GLU:CD	2.45	0.42
1:A:14:GLU:HB3	1:A:15:PRO:CD	2.50	0.42
1:A:137:VAL:O	1:A:141:ILE:HG12	2.19	0.42
1:A:168:MSE:HE2	1:A:202:LEU:HD12	2.01	0.42
1:A:185:GLN:O	1:A:188:ARG:HB2	2.20	0.42
1:A:440:ALA:HB1	1:A:444:LYS:HD2	2.02	0.42
1:A:745:GLN:O	1:A:748:MSE:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:754:THR:HG22	1:A:758:ARG:NH2	2.35	0.42
1:B:54:LEU:HD23	1:B:54:LEU:HA	1.73	0.42
1:B:504:ILE:HD12	1:B:576:LEU:HD23	2.01	0.42
1:B:756:ILE:HG22	1:B:797:MSE:CE	2.49	0.42
1:B:924:LYS:NZ	1:B:1061:LYS:NZ	2.67	0.42
1:B:1053:GLY:C	1:B:1054:PHE:HD1	2.27	0.42
1:A:148:ALA:O	1:A:209:MSE:HE1	2.19	0.42
1:A:278:ASN:O	1:A:281:LYS:N	2.51	0.42
1:A:785:ALA:O	1:A:788:ASP:N	2.49	0.42
1:A:795:SER:N	1:A:796:PRO:CD	2.83	0.42
1:B:79:ILE:N	1:B:79:ILE:CD1	2.83	0.42
1:B:236:LYS:O	1:B:239:ALA:HB3	2.20	0.42
1:B:505:ASP:O	1:B:507:PRO:HD3	2.20	0.42
1:B:974:ASP:OD1	1:B:977:ILE:HG13	2.20	0.42
1:A:1:MSE:HA	1:A:1018:GLN:OE1	2.19	0.41
1:A:926:MSE:HE2	1:A:957:ALA:HB3	2.01	0.41
1:A:984:VAL:O	1:A:984:VAL:HG12	2.20	0.41
1:B:182:LEU:HD13	1:B:182:LEU:N	2.35	0.41
1:B:189:VAL:HG12	1:B:193:ASN:OD1	2.19	0.41
1:B:205:LEU:CD1	1:B:234:VAL:HG23	2.50	0.41
1:B:582:ASP:O	1:B:586:ARG:HB2	2.20	0.41
1:B:737:CYS:SG	1:B:817:PHE:CZ	3.09	0.41
1:A:807:ASN:CB	1:A:810:ASP:HB3	2.27	0.41
1:A:896:GLN:CG	1:A:897:PRO:HD3	2.49	0.41
1:A:919:ILE:HD11	1:A:964:LEU:HB2	2.02	0.41
1:B:196:ASN:O	1:B:199:LYS:HB2	2.19	0.41
1:B:458:GLU:HG2	1:B:459:ALA:H	1.83	0.41
1:A:78:PHE:O	1:A:82:GLU:OE1	2.38	0.41
1:A:154:MSE:C	1:A:156:ASP:N	2.76	0.41
1:A:162:LYS:HG3	1:A:162:LYS:H	1.68	0.41
1:A:287:PRO:HG3	1:A:350:MSE:CG	2.45	0.41
1:A:888:GLN:H	1:A:888:GLN:HG2	1.37	0.41
1:B:227:LEU:HD22	1:B:230:ARG:CZ	2.50	0.41
1:B:298:ALA:O	1:B:302:ILE:HD12	2.20	0.41
1:B:444:LYS:NZ	1:B:444:LYS:CB	2.81	0.41
1:B:1018:GLN:O	1:B:1021:GLU:N	2.53	0.41
1:A:458:GLU:HG2	1:A:459:ALA:N	2.36	0.41
1:A:506:ASN:HB3	1:A:509:VAL:CG1	2.51	0.41
1:B:14:GLU:N	1:B:15:PRO:CD	2.82	0.41
1:B:202:LEU:CB	1:B:203:PRO:CD	2.98	0.41
1:B:376:ALA:HB3	1:B:421:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:566:SER:CB	1:B:567:PRO:CD	2.98	0.41
1:B:655:LYS:HA	1:B:655:LYS:HD2	1.34	0.41
1:B:811:PRO:HA	1:B:814:GLN:HG3	2.02	0.41
1:B:894:ILE:HA	1:B:934:SER:O	2.20	0.41
1:B:930:MSE:O	1:B:933:MSE:N	2.42	0.41
1:A:19:GLN:O	1:A:22[A]:HIS:HB3	2.20	0.41
1:A:385:ALA:HA	1:A:474:GLN:HE22	1.86	0.41
1:A:401:GLY:C	1:A:403:GLU:N	2.76	0.41
1:A:441:LEU:HA	1:A:444:LYS:CE	2.51	0.41
1:A:919:ILE:HG23	1:A:961:VAL:HG12	2.02	0.41
1:B:14:GLU:HB3	1:B:15:PRO:CD	2.50	0.41
1:B:22:HIS:CB	1:B:25:ILE:CD1	2.95	0.41
1:B:916:GLY:O	1:B:1057:ARG:HB2	2.20	0.41
1:A:290:SER:O	1:A:293:ASP:OD1	2.38	0.41
1:A:1014:GLU:C	1:A:1017:GLU:HG2	2.46	0.41
1:B:174:MSE:HE2	1:B:174:MSE:HB3	1.73	0.41
1:B:178:ARG:HA	1:B:178:ARG:HD2	1.89	0.41
1:B:501:GLN:O	1:B:504:ILE:N	2.53	0.41
1:B:732:LYS:O	1:B:736:LYS:HG3	2.21	0.41
1:B:829:ALA:O	1:B:833:GLU:OE2	2.39	0.41
1:B:894:ILE:HD13	1:B:894:ILE:HA	1.95	0.41
1:A:74:MSE:HE2	1:A:74:MSE:HB3	1.98	0.41
1:A:88:LEU:CD2	1:A:108:LEU:CD1	2.99	0.41
1:A:377:MSE:HE1	1:A:418:ILE:HA	2.02	0.41
1:A:633:PHE:HD2	1:A:676:VAL:CG2	2.34	0.41
1:A:939:GLY:HA2	1:A:1006:LEU:HD11	2.03	0.41
1:B:20:ILE:CD1	1:B:115:ILE:CG2	2.99	0.41
1:B:22:HIS:CA	1:B:25:ILE:HD11	2.51	0.41
1:B:40:LEU:O	1:B:43:PRO:HG2	2.21	0.41
1:B:212:PHE:O	1:B:214:THR:N	2.44	0.41
1:B:461:ALA:O	1:B:465:GLN:HB3	2.21	0.41
1:B:506:ASN:HB3	1:B:509:VAL:HG13	1.97	0.41
1:B:996:LYS:O	1:B:999:SER:N	2.54	0.41
1:A:75:PRO:CA	1:A:78:PHE:CE2	3.00	0.41
1:A:196:ASN:O	1:A:199:LYS:HB2	2.21	0.41
1:A:335:VAL:C	1:A:337:ASP:N	2.78	0.41
1:A:460:ARG:HG3	1:A:461:ALA:N	2.36	0.41
1:A:491:VAL:HG11	1:A:658:VAL:CG1	2.32	0.41
1:A:512:ARG:NH1	1:A:512:ARG:HG3	2.35	0.41
1:A:545:CYS:C	1:A:547:ARG:N	2.78	0.41
1:B:458:GLU:C	1:B:460:ARG:N	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:583:LEU:HD23	1:B:583:LEU:HA	1.72	0.41
1:B:733:ASP:HB3	1:B:756:ILE:HG13	2.03	0.41
1:B:1001:VAL:O	1:B:1004:THR:N	2.51	0.41
1:A:20:ILE:HD12	1:A:116:LEU:HD21	2.02	0.41
1:A:190:MSE:HE2	1:A:247:VAL:HG21	2.02	0.41
1:A:201:LEU:HD23	1:A:201:LEU:HA	1.86	0.41
1:A:744:ILE:HD12	1:A:744:ILE:H	1.86	0.41
1:A:896:GLN:HG3	1:A:897:PRO:CD	2.51	0.41
1:A:933:MSE:HE2	1:A:947:LEU:HD21	2.03	0.41
1:B:1:MSE:O	1:B:3:VAL:N	2.54	0.41
1:B:152:GLU:OE1	1:B:216:LYS:NZ	2.35	0.41
1:B:153:THR:O	1:B:213:VAL:HG11	2.20	0.41
1:B:626:PHE:O	1:B:629:ARG:N	2.43	0.41
1:B:644:ALA:HB2	1:B:709:MSE:HE2	1.95	0.41
1:B:731:LYS:CB	1:B:731:LYS:HZ2	2.33	0.41
1:A:13:LEU:HD13	1:A:13:LEU:HA	1.84	0.41
1:A:69:ILE:N	1:A:69:ILE:CD1	2.80	0.41
1:B:14:GLU:CB	1:B:15:PRO:CD	2.99	0.41
1:B:154:MSE:CE	1:B:158:VAL:CG2	2.98	0.41
1:B:243:GLU:OE2	1:B:246:ARG:NH1	2.53	0.41
1:B:500:ALA:O	1:B:504:ILE:HG12	2.21	0.41
1:B:924:LYS:NZ	1:B:1061:LYS:CE	2.80	0.41
1:A:37:ILE:CD1	1:A:105:ARG:NE	2.80	0.40
1:A:87:LYS:HZ3	1:A:107:TYR:C	2.26	0.40
1:A:179:GLN:C	1:A:181:GLU:N	2.78	0.40
1:A:218:SER:HB3	1:A:220:ASN:ND2	2.36	0.40
1:A:576:LEU:C	1:A:578:ASP:N	2.77	0.40
1:A:731:LYS:HB3	1:A:731:LYS:HZ2	1.86	0.40
1:A:895:ASN:HB2	1:A:937:VAL:HG11	2.04	0.40
1:B:335:VAL:O	1:B:337:ASP:N	2.54	0.40
1:B:734:LEU:CD2	1:B:818:LEU:CD2	2.99	0.40
1:B:811:PRO:CA	1:B:815:LYS:HE2	2.51	0.40
1:A:426:LYS:HG2	1:A:427:GLU:N	2.27	0.40
1:A:460:ARG:HG3	1:A:461:ALA:H	1.86	0.40
1:A:640:LEU:HD23	1:A:640:LEU:HA	1.93	0.40
1:B:40:LEU:CB	1:B:43:PRO:HG2	2.36	0.40
1:B:133:LYS:CD	1:B:136:ARG:HH21	2.34	0.40
1:B:347:PRO:HA	1:B:350:MSE:CE	2.49	0.40
1:B:434:SER:O	1:B:437:GLU:HG2	2.21	0.40
1:B:666:LYS:O	1:B:667:THR:C	2.63	0.40
1:B:697:THR:CG2	1:B:698:MSE:HE2	2.26	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:811:PRO:C	1:B:813:LEU:N	2.79	0.40
1:A:20:ILE:CD1	1:A:115:ILE:CG2	2.99	0.40
1:A:154:MSE:O	1:A:157:LEU:N	2.55	0.40
1:A:574:SER:HA	1:A:577:GLN:HE21	1.85	0.40
1:A:658:VAL:CG1	1:A:662:GLN:HE22	2.34	0.40
1:A:672:THR:O	1:A:676:VAL:HB	2.22	0.40
1:B:190:MSE:HE2	1:B:247:VAL:CG2	2.52	0.40
1:B:733:ASP:OD2	1:B:755:SER:OG	2.35	0.40
1:B:880:GLU:HG2	1:B:881:LYS:N	2.34	0.40
1:A:26:MSE:HA	1:A:29:GLU:HB2	2.02	0.40
1:A:210:LYS:C	1:A:212:PHE:N	2.79	0.40
1:A:717:ILE:HG22	1:A:722:LEU:HB2	2.03	0.40
1:A:896:GLN:CB	1:A:897:PRO:CD	2.99	0.40
1:B:227:LEU:CD2	1:B:230:ARG:CZ	2.99	0.40
1:B:377:MSE:HG2	1:B:421:LEU:HD23	2.04	0.40
1:B:412:LEU:N	1:B:412:LEU:CD2	2.80	0.40
1:B:491:VAL:CG1	1:B:658:VAL:HG11	2.51	0.40
1:B:506:ASN:O	1:B:508:THR:N	2.54	0.40
1:B:901:ALA:HB1	1:B:1031:MSE:CG	2.49	0.40
1:A:452:GLY:C	1:A:454:GLY:H	2.29	0.40
1:A:583:LEU:HD12	1:A:583:LEU:HA	1.93	0.40
1:A:910:ARG:HH12	1:A:1061:LYS:HE2	1.86	0.40
1:B:316:LYS:CB	2:B:1108:HOH:O	2.68	0.40
1:B:566:SER:HB3	1:B:567:PRO:CD	2.48	0.40
1:B:731:LYS:NZ	1:B:731:LYS:HB3	2.36	0.40
1:B:898:MSE:HE3	1:B:1024:VAL:HA	2.03	0.40
1:B:919:ILE:HG23	1:B:961:VAL:HG12	2.04	0.40
1:B:996:LYS:O	1:B:998:LEU:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1032/1066 (97%)	849 (82%)	140 (14%)	43 (4%)	2	9
1	B	1032/1066 (97%)	849 (82%)	130 (13%)	53 (5%)	1	6
All	All	2064/2132 (97%)	1698 (82%)	270 (13%)	96 (5%)	2	7

All (96) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	ASP
1	A	402	PRO
1	A	441	LEU
1	A	453	LYS
1	A	686	PRO
1	A	689	GLN
1	A	834	ALA
1	A	896	GLN
1	A	944	LYS
1	B	456	SER
1	B	531	ASN
1	B	655	LYS
1	B	838	GLN
1	B	881	LYS
1	B	883	GLU
1	B	887	GLU
1	B	893	VAL
1	B	896	GLN
1	B	944	LYS
1	B	1050	THR
1	B	1051	ASP
1	A	213	VAL
1	A	291	PRO
1	A	315	GLY
1	A	316	LYS
1	A	440	ALA
1	A	448	LEU
1	A	457	PRO
1	A	531	ASN
1	A	535	GLY
1	A	563	GLU
1	A	632	ASN
1	A	687	GLY
1	A	688	ASN
1	A	705	ASN

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Mol	Chain	Res	Type
1	A	890	ALA
1	A	939	GLY
1	B	34	GLY
1	B	41	THR
1	B	101	SER
1	B	213	VAL
1	B	291	PRO
1	B	335	VAL
1	B	440	ALA
1	B	441	LEU
1	B	535	GLY
1	B	622	ARG
1	B	654	ASN
1	B	656	SER
1	B	997	ILE
1	A	50	ALA
1	A	116	LEU
1	A	150	VAL
1	A	228	LYS
1	A	335	VAL
1	A	341	ARG
1	A	512	ARG
1	A	656	SER
1	B	30	GLY
1	B	38	PRO
1	B	116	LEU
1	B	253	TRP
1	B	254	ASP
1	B	316	LYS
1	B	451	GLN
1	B	600	SER
1	B	667	THR
1	B	689	GLN
1	B	892	GLU
1	A	38	PRO
1	A	1051	ASP
1	A	1052	ALA
1	B	64	THR
1	B	228	LYS
1	B	315	GLY
1	B	343	GLN
1	B	452	GLY

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Mol	Chain	Res	Type
1	B	453	LYS
1	B	841	ASP
1	A	293	ASP
1	B	50	ALA
1	B	150	VAL
1	B	286	ASP
1	B	663	ALA
1	B	92	ALA
1	B	457	PRO
1	B	910	ARG
1	A	286	ASP
1	A	840	PRO
1	B	292	GLY
1	B	989	PRO
1	A	562	GLY
1	A	292	GLY
1	A	744	ILE
1	A	891	GLY
1	B	744	ILE

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	850/842 (101%)	557 (66%)	293 (34%)	0	0
1	B	850/842 (101%)	543 (64%)	307 (36%)	0	0
All	All	1700/1684 (101%)	1100 (65%)	600 (35%)	0	0

All (600) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	3	VAL
1	A	4	PHE
1	A	7	ARG

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Mol	Chain	Res	Type
1	A	10	GLU
1	A	11	SER
1	A	13	LEU
1	A	14	GLU
1	A	16	VAL
1	A	18	GLN
1	A	25	ILE
1	A	26	MSE
1	A	28	GLU
1	A	31	GLU
1	A	32	VAL
1	A	35	LYS
1	A	39	ASP
1	A	40	LEU
1	A	41	THR
1	A	44	VAL
1	A	47	VAL
1	A	52	SER
1	A	54	LEU
1	A	60	GLU
1	A	61	THR
1	A	62	VAL
1	A	65	THR
1	A	69	ILE
1	A	70	LEU
1	A	74	MSE
1	A	82	GLU
1	A	83	ASN
1	A	87	LYS
1	A	88	LEU
1	A	93	GLN
1	A	94	MSE
1	A	95	LEU
1	A	102	VAL
1	A	105	ARG
1	A	106	ASP
1	A	109	ILE
1	A	113	ARG
1	A	115	ILE
1	A	117	SER
1	A	122	LEU
1	A	123	LEU

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Mol	Chain	Res	Type
1	A	131	VAL
1	A	134	ILE
1	A	146	THR
1	A	152	GLU
1	A	155	GLU
1	A	157	LEU
1	A	158	VAL
1	A	162	LYS
1	A	163	ASN
1	A	169	THR
1	A	173	LYS
1	A	174	MSE
1	A	175	ILE
1	A	180	GLN
1	A	181	GLU
1	A	182	LEU
1	A	185	GLN
1	A	190	MSE
1	A	200	GLU
1	A	202	LEU
1	A	206	ILE
1	A	211	ILE
1	A	213	VAL
1	A	214	THR
1	A	220	ASN
1	A	223	ILE
1	A	227	LEU
1	A	228	LYS
1	A	229	ASN
1	A	230	ARG
1	A	233	THR
1	A	234	VAL
1	A	236	LYS
1	A	238	SER
1	A	246	ARG
1	A	252	SER
1	A	255	GLU
1	A	256	ASP
1	A	260	SER
1	A	261	LYS
1	A	264	GLU
1	A	266	MSE

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Mol	Chain	Res	Type
1	A	268	ARG
1	A	270	LEU
1	A	274	ASP
1	A	277	LEU
1	A	281	LYS
1	A	284	LEU
1	A	286	ASP
1	A	293	ASP
1	A	296	GLU
1	A	301	GLN
1	A	302	ILE
1	A	309	VAL
1	A	316	LYS
1	A	317	GLU
1	A	319	ARG
1	A	326	LYS
1	A	327	MSE
1	A	338	LEU
1	A	341	ARG
1	A	343	GLN
1	A	348	VAL
1	A	350	MSE
1	A	351	GLN
1	A	352	LYS
1	A	354[A]	GLN
1	A	354[B]	GLN
1	A	363	LEU
1	A	366	LYS
1	A	367	VAL
1	A	377	MSE
1	A	384	ILE
1	A	386	LYS
1	A	387	LYS
1	A	392	GLN
1	A	393	ASN
1	A	403	GLU
1	A	412	LEU
1	A	416	ARG
1	A	417	LYS
1	A	421	LEU
1	A	422	CYS
1	A	423	ASP

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Mol	Chain	Res	Type
1	A	426	LYS
1	A	428	ARG
1	A	429	ASP
1	A	434	SER
1	A	437	GLU
1	A	441	LEU
1	A	444	LYS
1	A	448	LEU
1	A	449	ARG
1	A	450	ARG
1	A	451	GLN
1	A	453	LYS
1	A	460	ARG
1	A	464	LYS
1	A	466	VAL
1	A	471	GLN
1	A	485	ARG
1	A	491	VAL
1	A	497	ILE
1	A	498	GLU
1	A	501	GLN
1	A	506	ASN
1	A	509	VAL
1	A	512	ARG
1	A	522	LEU
1	A	532	VAL
1	A	541	LEU
1	A	544	LYS
1	A	551	LEU
1	A	552	THR
1	A	558	LEU
1	A	563	GLU
1	A	565	GLU
1	A	566	SER
1	A	568	GLN
1	A	581	LYS
1	A	596	SER
1	A	598	VAL
1	A	607	LYS
1	A	609	LEU
1	A	622	ARG
1	A	623	GLU

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Mol	Chain	Res	Type
1	A	624	GLU
1	A	625	VAL
1	A	628	GLU
1	A	632	ASN
1	A	650	VAL
1	A	655	LYS
1	A	657	THR
1	A	659	GLU
1	A	671	LEU
1	A	676	VAL
1	A	677	SER
1	A	680	ARG
1	A	681	ILE
1	A	682	LEU
1	A	683	LEU
1	A	693	GLU
1	A	697	THR
1	A	703	ILE
1	A	708	LYS
1	A	709	MSE
1	A	717	ILE
1	A	720	LYS
1	A	721	SER
1	A	726	SER
1	A	731	LYS
1	A	732	LYS
1	A	734	LEU
1	A	739	VAL
1	A	745	GLN
1	A	749	LEU
1	A	750	VAL
1	A	759	ARG
1	A	762	ARG
1	A	765	LEU
1	A	768	LYS
1	A	772	GLU
1	A	784	LYS
1	A	787	SER
1	A	789	GLU
1	A	791	SER
1	A	793	THR
1	A	794	ILE

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Mol	Chain	Res	Type
1	A	795	SER
1	A	798	VAL
1	A	799	MSE
1	A	808	ILE
1	A	813	LEU
1	A	814	GLN
1	A	815	LYS
1	A	819	ASP
1	A	830	LYS
1	A	831	VAL
1	A	832	ARG
1	A	833	GLU
1	A	836	GLN
1	A	838	GLN
1	A	839	GLU
1	A	841	ASP
1	A	842	PHE
1	A	879	GLU
1	A	880	GLU
1	A	881	LYS
1	A	887	GLU
1	A	888	GLN
1	A	889	LYS
1	A	900	MSE
1	A	905	LEU
1	A	910	ARG
1	A	914	SER
1	A	915	LYS
1	A	919	ILE
1	A	920	ILE
1	A	926	MSE
1	A	933	MSE
1	A	936	LEU
1	A	938	ARG
1	A	944	LYS
1	A	947	LEU
1	A	949	GLN
1	A	954	ILE
1	A	956	LYS
1	A	958	SER
1	A	960	GLU
1	A	961	VAL

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Mol	Chain	Res	Type
1	A	963	ARG
1	A	967	GLU
1	A	978	ARG
1	A	979	THR
1	A	981	LEU
1	A	986	GLU
1	A	992	SER
1	A	994	GLN
1	A	997	ILE
1	A	999	SER
1	A	1001	VAL
1	A	1002	LYS
1	A	1004	THR
1	A	1005	MSE
1	A	1006	LEU
1	A	1008[A]	ARG
1	A	1008[B]	ARG
1	A	1009	THR
1	A	1011	ILE
1	A	1013	ASP
1	A	1016	SER
1	A	1018	GLN
1	A	1020	THR
1	A	1026	ASN
1	A	1036	GLU
1	A	1042	GLU
1	A	1045	SER
1	A	1046	ILE
1	A	1048	ILE
1	A	1050	THR
1	A	1054	PHE
1	A	1055	THR
1	A	1056	LEU
1	A	1057[A]	ARG
1	A	1057[B]	ARG
1	A	1060	ARG
1	A	1061	LYS
1	B	1	MSE
1	B	3	VAL
1	B	4	PHE
1	B	7	ARG
1	B	10	GLU

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Mol	Chain	Res	Type
1	B	11	SER
1	B	12	ILE
1	B	13	LEU
1	B	14	GLU
1	B	16	VAL
1	B	18	GLN
1	B	22	HIS
1	B	25	ILE
1	B	26	MSE
1	B	27	HIS
1	B	28	GLU
1	B	32	VAL
1	B	33	ASP
1	B	35	LYS
1	B	37	ILE
1	B	40	LEU
1	B	41	THR
1	B	47	VAL
1	B	52	SER
1	B	54	LEU
1	B	60	GLU
1	B	61	THR
1	B	62	VAL
1	B	65	THR
1	B	69	ILE
1	B	70	LEU
1	B	74	MSE
1	B	79	ILE
1	B	82	GLU
1	B	83	ASN
1	B	87	LYS
1	B	88	LEU
1	B	90	GLN
1	B	94	MSE
1	B	102	VAL
1	B	105	ARG
1	B	106	ASP
1	B	109	ILE
1	B	113	ARG
1	B	115	ILE
1	B	122	LEU
1	B	123	LEU

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Mol	Chain	Res	Type
1	B	124	LEU
1	B	133	LYS
1	B	134	ILE
1	B	139	LYS
1	B	143	GLU
1	B	146	THR
1	B	152	GLU
1	B	154	MSE
1	B	155	GLU
1	B	157	LEU
1	B	158	VAL
1	B	162	LYS
1	B	163	ASN
1	B	169	THR
1	B	173	LYS
1	B	175	ILE
1	B	180	GLN
1	B	181	GLU
1	B	182	LEU
1	B	185	GLN
1	B	186	GLU
1	B	190	MSE
1	B	200	GLU
1	B	202	LEU
1	B	206	ILE
1	B	211	ILE
1	B	213	VAL
1	B	214	THR
1	B	223	ILE
1	B	225	GLU
1	B	227	LEU
1	B	228	LYS
1	B	229	ASN
1	B	230	ARG
1	B	236	LYS
1	B	238	SER
1	B	244	ILE
1	B	248	LEU
1	B	252	SER
1	B	256	ASP
1	B	258	TRP
1	B	260	SER

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Mol	Chain	Res	Type
1	B	261	LYS
1	B	264	GLU
1	B	266	MSE
1	B	268	ARG
1	B	270	LEU
1	B	274	ASP
1	B	277	LEU
1	B	281	LYS
1	B	284	LEU
1	B	296	GLU
1	B	297	GLN
1	B	301	GLN
1	B	302	ILE
1	B	309	VAL
1	B	316	LYS
1	B	317	GLU
1	B	319	ARG
1	B	326	LYS
1	B	327	MSE
1	B	343	GLN
1	B	345	SER
1	B	348	VAL
1	B	350	MSE
1	B	351	GLN
1	B	352	LYS
1	B	354[A]	GLN
1	B	354[B]	GLN
1	B	363	LEU
1	B	366	LYS
1	B	367	VAL
1	B	373	LYS
1	B	377	MSE
1	B	384	ILE
1	B	386	LYS
1	B	387	LYS
1	B	392	GLN
1	B	393	ASN
1	B	399	ASN
1	B	403	GLU
1	B	412	LEU
1	B	417	LYS
1	B	421	LEU

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Mol	Chain	Res	Type
1	B	422	CYS
1	B	423	ASP
1	B	426	LYS
1	B	428	ARG
1	B	429	ASP
1	B	433[A]	ARG
1	B	433[B]	ARG
1	B	434	SER
1	B	437	GLU
1	B	441	LEU
1	B	444	LYS
1	B	447	ASP
1	B	448	LEU
1	B	450	ARG
1	B	451	GLN
1	B	458	GLU
1	B	464	LYS
1	B	465	GLN
1	B	466	VAL
1	B	471	GLN
1	B	484	SER
1	B	485	ARG
1	B	491	VAL
1	B	497	ILE
1	B	498	GLU
1	B	501	GLN
1	B	506	ASN
1	B	509	VAL
1	B	512	ARG
1	B	522	LEU
1	B	532	VAL
1	B	541	LEU
1	B	544	LYS
1	B	551	LEU
1	B	552	THR
1	B	558	LEU
1	B	561	ARG
1	B	563	GLU
1	B	565	GLU
1	B	566	SER
1	B	568	GLN
1	B	575	GLN

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Mol	Chain	Res	Type
1	B	577	GLN
1	B	581	LYS
1	B	583	LEU
1	B	593	GLN
1	B	596	SER
1	B	598	VAL
1	B	607	LYS
1	B	609	LEU
1	B	611	VAL
1	B	624	GLU
1	B	625	VAL
1	B	650	VAL
1	B	655	LYS
1	B	658	VAL
1	B	659	GLU
1	B	671	LEU
1	B	674	GLN
1	B	675	VAL
1	B	676	VAL
1	B	681	ILE
1	B	682	LEU
1	B	683	LEU
1	B	684	ARG
1	B	685	ASN
1	B	688	ASN
1	B	689	GLN
1	B	692	TYR
1	B	693	GLU
1	B	697	THR
1	B	703	ILE
1	B	705	ASN
1	B	706	VAL
1	B	708	LYS
1	B	709	MSE
1	B	717	ILE
1	B	720	LYS
1	B	721	SER
1	B	723	LEU
1	B	726	SER
1	B	731	LYS
1	B	732	LYS
1	B	734	LEU

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Mol	Chain	Res	Type
1	B	739	VAL
1	B	744	ILE
1	B	745	GLN
1	B	749	LEU
1	B	750	VAL
1	B	754	THR
1	B	759	ARG
1	B	762	ARG
1	B	765	LEU
1	B	768	LYS
1	B	772	GLU
1	B	784	LYS
1	B	787	SER
1	B	789	GLU
1	B	791	SER
1	B	793	THR
1	B	794	ILE
1	B	798	VAL
1	B	799	MSE
1	B	807	ASN
1	B	808	ILE
1	B	813	LEU
1	B	814	GLN
1	B	816	SER
1	B	819	ASP
1	B	830	LYS
1	B	831	VAL
1	B	832	ARG
1	B	833	GLU
1	B	836	GLN
1	B	839	GLU
1	B	841	ASP
1	B	879	GLU
1	B	880	GLU
1	B	881	LYS
1	B	882	ASP
1	B	887	GLU
1	B	888	GLN
1	B	889	LYS
1	B	900	MSE
1	B	905	LEU
1	B	910	ARG

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Mol	Chain	Res	Type
1	B	914	SER
1	B	915	LYS
1	B	919	ILE
1	B	920	ILE
1	B	926	MSE
1	B	933	MSE
1	B	936	LEU
1	B	944	LYS
1	B	945	ARG
1	B	947	LEU
1	B	949	GLN
1	B	954	ILE
1	B	956	LYS
1	B	958	SER
1	B	960	GLU
1	B	961	VAL
1	B	967	GLU
1	B	976	ARG
1	B	977	ILE
1	B	978	ARG
1	B	981	LEU
1	B	986	GLU
1	B	987	ARG
1	B	994	GLN
1	B	997	ILE
1	B	999	SER
1	B	1001	VAL
1	B	1002	LYS
1	B	1004	THR
1	B	1005	MSE
1	B	1008	ARG
1	B	1011	ILE
1	B	1012	SER
1	B	1013	ASP
1	B	1016	SER
1	B	1018	GLN
1	B	1020	THR
1	B	1026	ASN
1	B	1036	GLU
1	B	1042	GLU
1	B	1045	SER
1	B	1046	ILE

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Mol	Chain	Res	Type
1	B	1048	ILE
1	B	1050	THR
1	B	1051	ASP
1	B	1055	THR
1	B	1056	LEU
1	B	1057	ARG
1	B	1060	ARG
1	B	1062	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	180	GLN
1	A	184	HIS
1	A	193	ASN
1	A	220	ASN
1	A	221	GLN
1	A	279	GLN
1	A	301	GLN
1	A	343	GLN
1	A	351	GLN
1	A	379	ASN
1	A	471	GLN
1	A	472	ASN
1	A	474	GLN
1	A	492	HIS
1	A	506	ASN
1	A	550	GLN
1	A	568	GLN
1	A	577	GLN
1	A	593	GLN
1	A	662	GLN
1	A	705	ASN
1	A	904	GLN
1	A	994	GLN
1	A	1025	HIS
1	A	1026	ASN
1	B	19	GLN
1	B	27	HIS
1	B	93	GLN
1	B	179	GLN

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Mol	Chain	Res	Type
1	B	180	GLN
1	B	220	ASN
1	B	297	GLN
1	B	301	GLN
1	B	351	GLN
1	B	471	GLN
1	B	472	ASN
1	B	539	GLN
1	B	575	GLN
1	B	588	GLN
1	B	593	GLN
1	B	662	GLN
1	B	685	ASN
1	B	688	ASN
1	B	701	GLN
1	B	705	ASN
1	B	807	ASN
1	B	814	GLN
1	B	888	GLN
1	B	895	ASN
1	B	904	GLN
1	B	949	GLN
1	B	994	GLN
1	B	1018	GLN
1	B	1026	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.