



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:27 PM UTC

PDB ID : 2C9M / pdb_00002c9m
Title : Structure of (SR) Calcium-ATPase in the Ca₂E1 state solved in a P1 crystal form.
Authors : Lund Jensen, A.-M.; Sorensen, T.L.-M.; Olesen, C.; Moller, J.V.; Nissen, P.
Deposited on : 2005-12-13
Resolution : 3.00 Å(reported)

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

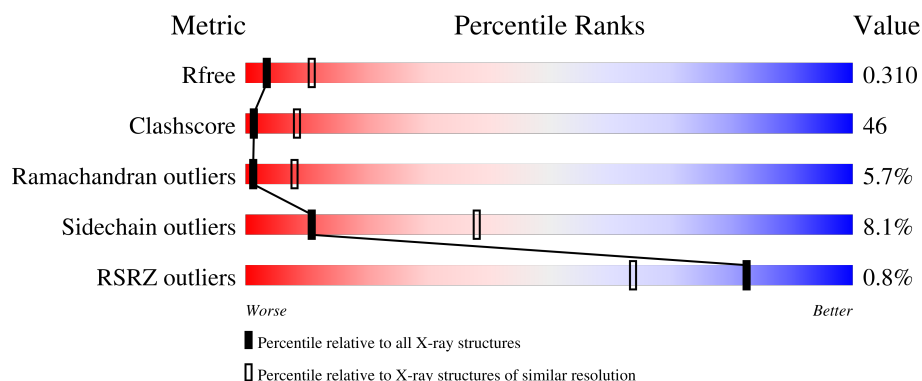
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	994	36% 53% 10% .
1	B	994	35% 53% 10% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15351 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 SARCOPLASMIC/ENDOPLASMIC RETICULUM CALCIUM ATPASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	994	Total	C	N	O	S	0	0	0
			7670	4876	1287	1450	57			
1	B	994	Total	C	N	O	S	0	0	0
			7670	4876	1287	1450	57			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Ca	0	0
			4	4		
2	B	3	Total	Ca	0	0
			3	3		

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	K	0	0
			1	1		
3	B	1	Total	K	0	0
			1	1		

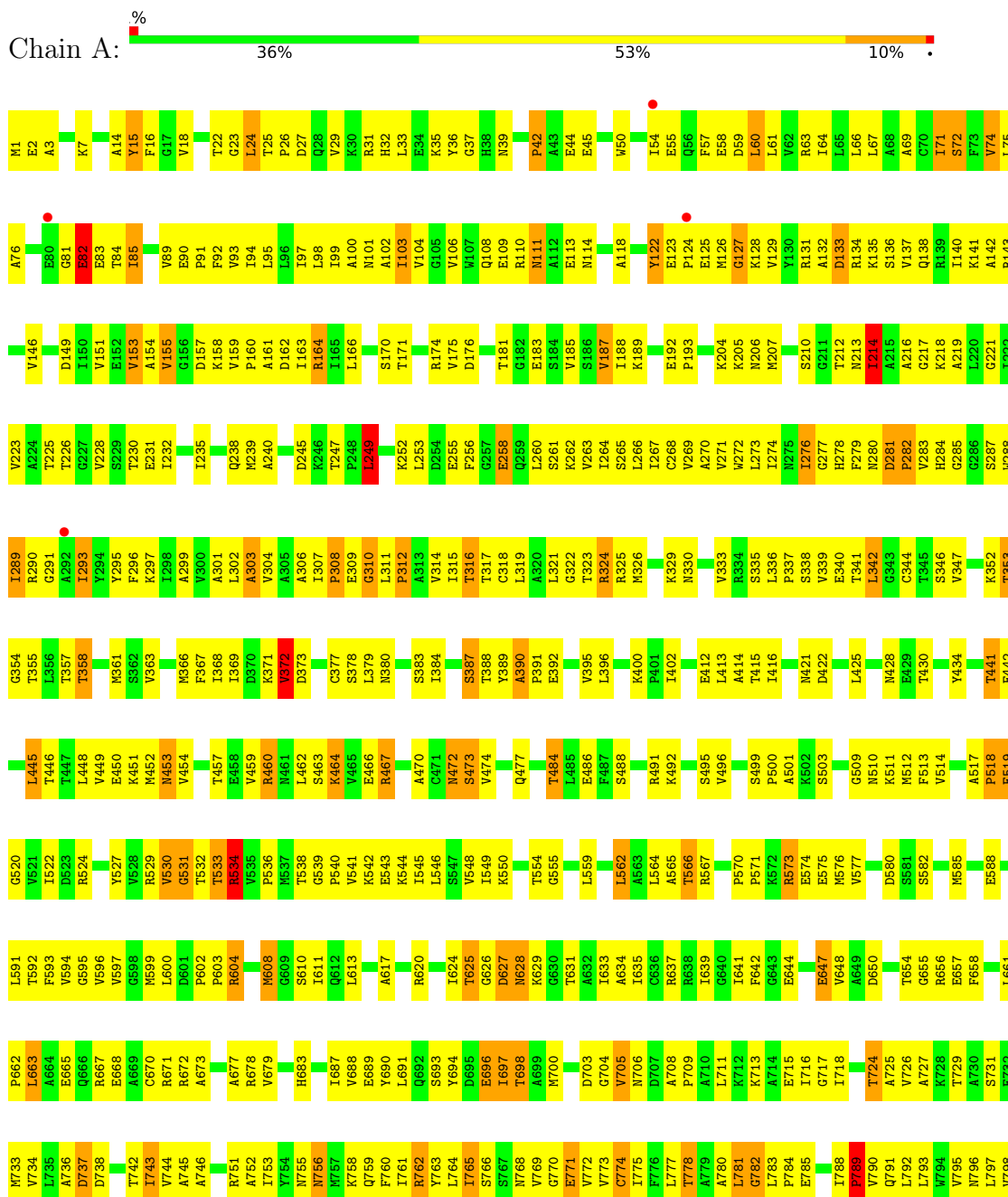
- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

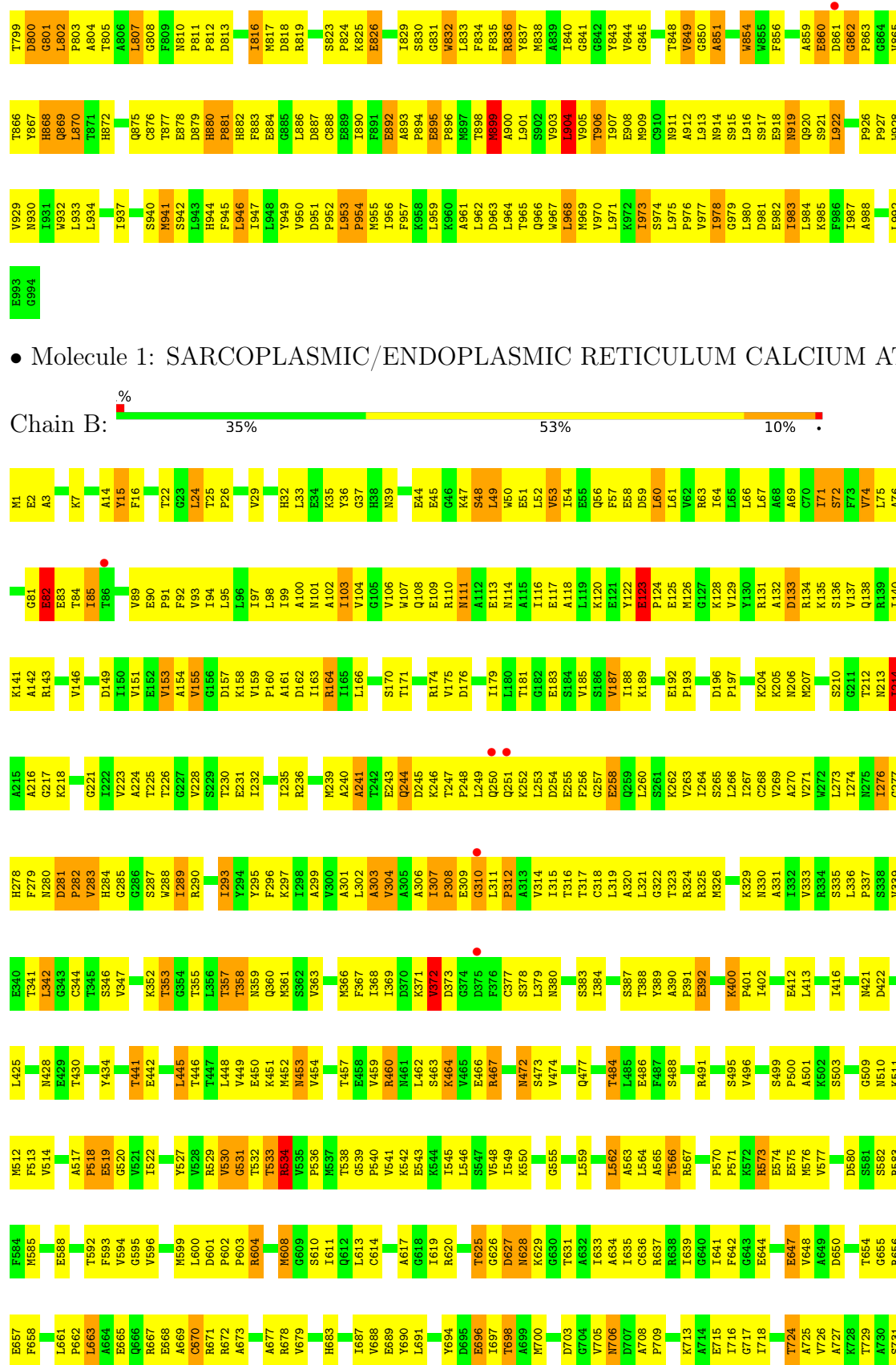
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	B	1	Total	Cl	0	0
			1	1		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: SARCOPLASMIC/ENDOPLASMIC RETICULUM CALCIUM ATPASE 1





W832	L933	L934	I937	C938	L939	S940	M941	S942	L943	H944	F945	L946	L947	L948	Y949	V950	D951	P952	L953	P954	M955	I956	F957	K958	L959	K960	A961	L962	D963	L964	T965	Q966	W967	L968	M969	V970	L971	K972	I973	S974	L975	P976	V977	I978	G979	L980	D981	E982	I983	L984	K985	F986	I987	A988	L992	E993	G994	L792	L793	L794	L795	L796	L797	L798	L799	D800	G801	L802	N810	P811	P812	D813	L814	M817	S823	E826	P827	S830	G831	W832	L833	F834	P835	R836	T837	M838	A839	T840	C841	G842	T843	W844	G845	A846	T847	T848	W849	G850	A851	A852	A853	W854	W855	F856	M857	Y858	A859	G862	P863	G864	W865						
																																																										E732	M733	V734	L735	A736	D737	D738	N739	F740	S741	T742	I743	V744	A745	A746	V747	E748	E749	G750	R751	A752	I753	W754	N755	W756	M757	K758	Q759	F760	I761	R762	T763	L764	I765	S766	S767	N768	V769	G770	E771	V772	V773	C774	I775	F776	L777	T778	A779	A780	L781	G782	L783	F784	E785	A786	L787	I788	P789	V790	Q791
																																																										T866	Y867	H868	Q869	L870	T871	H872	F873	T877	P881	H882	F883	E884	G885	L886	D887	C888	E889	I890	F891	E892	A893	P894	E895	P896	M897	T898	M899	A900	L901	S902	V903	L904	V905	T906	I907	E908	M909	C910	N911	A912	L913	N914	S915	L916	S917	E918	N919	Q920	S921	L922	P926	P927	W928	V929	N930	I931			
																																																										L792	L793	W794	V795	L796	L797	V798	T799	D800	G801	L802	N810	P811	D812	D813	L814	N817	S823	E826	P827	S830	G831	W832	L833	F834	P835	R836	T837	M838	A839	T840	C841	G842	T843	W844	G845	A846	T847	T848	W849	G850	A851	A852	A853	W854	W855	F856	M857	Y858	A859	G862	P863	G864	W865						

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	64.95Å 81.28Å 131.01Å 97.64° 99.94° 95.22°	Depositor
Resolution (Å)	15.00 – 3.00 15.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	80.4 (15.00-3.00) 79.7 (15.00-3.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 2.99Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.266 , 0.317 0.262 , 0.310	Depositor DCC
R_{free} test set	1158 reflections (2.56%)	wwPDB-VP
Wilson B-factor (Å ²)	75.2	Xtriage
Anisotropy	0.441	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 49.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	15351	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, CA, K

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	0.62	0/7811	1.10	51/10592 (0.5%)
1	B	0.60	0/7811	1.08	54/10592 (0.5%)
All	All	0.61	0/15622	1.09	105/21184 (0.5%)

There are no bond length outliers.

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	870	LEU	N-CA-C	-9.76	100.47	112.38
1	A	922	LEU	N-CA-C	-9.54	101.64	113.18
1	A	869	GLN	N-CA-C	-9.50	102.29	112.93
1	A	159	VAL	CA-C-N	9.23	128.88	119.56
1	A	159	VAL	C-N-CA	9.23	128.88	119.56
1	B	922	LEU	N-CA-C	-9.11	102.15	113.18
1	B	826	GLU	CA-C-N	8.90	130.97	119.84
1	B	826	GLU	C-N-CA	8.90	130.97	119.84
1	B	159	VAL	CA-C-N	8.72	128.37	119.56
1	B	159	VAL	C-N-CA	8.72	128.37	119.56
1	A	892	GLU	N-CA-C	-8.06	103.91	114.31
1	A	625	THR	N-CA-C	7.74	119.89	108.60
1	B	800	ASP	N-CA-C	-7.55	102.30	112.26
1	A	862	GLY	CA-C-N	7.53	127.20	119.82
1	A	862	GLY	C-N-CA	7.53	127.20	119.82
1	B	123	GLU	CA-C-N	7.51	129.23	119.84
1	B	123	GLU	C-N-CA	7.51	129.23	119.84
1	A	296	PHE	N-CA-C	-7.49	102.27	111.40
1	B	296	PHE	N-CA-C	-7.38	102.39	111.40
1	B	71	ILE	N-CA-C	-7.27	105.55	111.81
1	A	532	THR	N-CA-C	-7.27	102.41	113.89
1	A	71	ILE	N-CA-C	-7.19	105.63	111.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	800	ASP	N-CA-C	-7.17	95.52	110.80
1	B	532	THR	N-CA-C	-7.09	102.69	113.89
1	B	625	THR	N-CA-C	7.07	118.92	108.60
1	A	324	ARG	N-CA-C	-6.95	103.63	111.07
1	B	258	GLU	N-CA-C	-6.95	105.43	114.04
1	A	826	GLU	CA-C-N	6.75	126.71	120.03
1	A	826	GLU	C-N-CA	6.75	126.71	120.03
1	A	978	ILE	N-CA-C	-6.68	103.28	110.23
1	A	771	GLU	N-CA-C	-6.61	102.72	111.24
1	B	978	ILE	N-CA-C	-6.58	103.38	110.23
1	B	117	GLU	N-CA-C	-6.56	105.41	113.41
1	B	892	GLU	N-CA-C	-6.54	103.56	113.89
1	B	126	MET	N-CA-C	6.47	119.28	110.35
1	B	750	GLY	N-CA-C	-6.47	105.00	112.50
1	A	258	GLU	N-CA-C	-6.46	105.30	113.43
1	B	811	PRO	CA-C-N	6.38	127.81	119.84
1	B	811	PRO	C-N-CA	6.38	127.81	119.84
1	A	851	ALA	N-CA-C	-6.37	104.46	112.93
1	A	835	PHE	N-CA-C	-6.26	104.15	110.97
1	A	217	GLY	N-CA-C	6.25	118.42	112.04
1	A	624	ILE	N-CA-C	-6.24	99.48	108.53
1	B	360	GLN	N-CA-C	-6.24	98.24	108.41
1	B	849	VAL	N-CA-C	-6.21	104.69	110.53
1	A	82	GLU	CA-CB-CG	6.15	126.40	114.10
1	B	49	LEU	N-CA-C	-6.12	105.07	112.54
1	A	390	ALA	CA-C-N	6.06	127.41	119.84
1	A	390	ALA	C-N-CA	6.06	127.41	119.84
1	B	217	GLY	N-CA-C	6.03	119.63	112.33
1	B	968	LEU	N-CA-C	-6.02	105.43	112.89
1	B	865	VAL	N-CA-C	6.01	121.85	109.34
1	A	968	LEU	N-CA-C	-5.94	105.53	112.89
1	B	324	ARG	N-CA-C	-5.87	104.79	111.07
1	A	899	MET	N-CA-C	-5.85	105.64	112.89
1	B	517	ALA	CA-C-N	5.80	127.09	119.84
1	B	517	ALA	C-N-CA	5.80	127.09	119.84
1	A	249	LEU	N-CA-C	-5.79	105.31	112.90
1	A	453	ASN	N-CA-C	-5.77	104.16	110.91
1	A	808	GLY	N-CA-C	-5.77	108.33	114.67
1	A	919	ASN	N-CA-C	5.70	119.44	111.30
1	A	373	ASP	N-CA-C	5.64	118.15	111.33
1	B	826	GLU	N-CA-C	-5.64	99.52	108.82
1	B	82	GLU	CA-CB-CG	5.63	125.36	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	670	CYS	N-CA-C	5.60	118.14	111.71
1	B	310	GLY	N-CA-C	5.59	121.73	115.08
1	B	244	GLN	N-CA-C	-5.58	99.64	108.73
1	A	291	GLY	N-CA-C	-5.56	107.77	114.66
1	A	310	GLY	N-CA-C	5.54	121.67	115.08
1	B	453	ASN	N-CA-C	-5.52	104.46	110.91
1	B	373	ASP	N-CA-C	5.48	117.96	111.33
1	B	74	VAL	N-CA-C	5.43	115.88	110.23
1	A	778	THR	N-CA-C	-5.41	104.27	111.24
1	B	164	ARG	N-CA-C	-5.39	98.97	108.20
1	A	628	ASN	N-CA-C	-5.38	101.50	110.17
1	A	74	VAL	N-CA-C	5.38	115.82	110.23
1	B	919	ASN	N-CA-C	5.37	118.98	111.30
1	A	517	ALA	CA-C-N	5.34	126.52	119.84
1	A	517	ALA	C-N-CA	5.34	126.52	119.84
1	B	400	LYS	CA-C-N	5.34	125.10	119.76
1	B	400	LYS	C-N-CA	5.34	125.10	119.76
1	B	899	MET	N-CA-C	-5.33	106.28	112.89
1	B	390	ALA	CA-C-N	5.32	126.49	119.84
1	B	390	ALA	C-N-CA	5.32	126.49	119.84
1	A	400	LYS	CA-C-N	5.31	125.07	119.76
1	A	400	LYS	C-N-CA	5.31	125.07	119.76
1	B	628	ASN	N-CA-C	-5.27	102.25	110.42
1	A	697	ILE	N-CA-C	-5.27	101.94	108.89
1	A	255	GLU	N-CA-C	-5.26	106.12	112.54
1	A	245	ASP	N-CA-C	-5.24	102.25	110.36
1	A	164	ARG	N-CA-C	-5.21	99.30	108.20
1	A	801	GLY	N-CA-C	5.15	125.38	113.18
1	B	738	ASP	N-CA-C	-5.14	105.84	113.40
1	A	983	ILE	N-CA-C	-5.14	106.67	111.45
1	A	293	ILE	N-CA-C	-5.11	108.14	113.10
1	B	293	ILE	N-CA-C	-5.11	108.14	113.10
1	B	107	TRP	N-CA-C	-5.08	105.45	111.69
1	A	214	ILE	N-CA-C	5.07	115.99	108.23
1	A	387	SER	N-CA-C	5.07	118.55	111.30
1	A	870	LEU	N-CA-C	-5.07	106.60	112.89
1	B	754	TYR	N-CA-C	-5.05	103.83	111.56
1	B	852	ALA	N-CA-C	-5.03	105.25	111.33
1	B	255	GLU	N-CA-C	-5.02	106.41	112.54
1	B	224	ALA	N-CA-C	-5.01	103.28	111.04
1	B	214	ILE	N-CA-C	5.00	115.89	108.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7670	0	7764	684	0
1	B	7670	0	7766	725	0
2	A	4	0	0	0	0
2	B	3	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	1	0
4	B	1	0	0	0	0
All	All	15351	0	15530	1409	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 46.

All (1409) 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:830:SER:HB3	1:B:833:LEU:HB2	1.40	1.03
1:A:372:VAL:HG13	1:A:377:CYS:HB3	1.44	0.99
1:A:263:VAL:HG12	1:A:267:ILE:HD11	1.44	0.97
1:B:941:MET:HE3	1:B:941:MET:HA	1.44	0.97
1:B:372:VAL:HG13	1:B:377:CYS:HB3	1.46	0.97
1:A:941:MET:HE3	1:A:941:MET:HA	1.46	0.96
1:B:559:LEU:HD23	1:B:600:LEU:HB3	1.47	0.95
1:A:559:LEU:HD23	1:A:600:LEU:HB3	1.47	0.95
1:B:47:LYS:HB3	1:B:51:GLU:HB3	1.46	0.94
1:A:214:ILE:HD13	1:A:214:ILE:H	1.33	0.94
1:B:263:VAL:HG12	1:B:267:ILE:HD11	1.48	0.93
1:A:658:PHE:HA	1:A:661:LEU:HD12	1.49	0.93
1:A:629:LYS:O	1:A:633:ILE:HG13	1.70	0.92
1:B:907:ILE:HD12	1:B:974:SER:HA	1.50	0.92
1:B:767:SER:HB3	1:B:911:ASN:HD22	1.36	0.91
1:B:658:PHE:HA	1:B:661:LEU:HD12	1.50	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:VAL:HG12	1:B:151:VAL:HG22	1.50	0.90
1:A:24:LEU:HD13	1:A:149:ASP:HA	1.51	0.90
1:A:759:GLN:HE21	1:A:917:SER:HA	1.35	0.90
1:B:214:ILE:HD13	1:B:214:ILE:H	1.37	0.90
1:A:755:ASN:O	1:A:759:GLN:HG3	1.72	0.90
1:B:904:LEU:O	1:B:907:ILE:HG22	1.70	0.90
1:B:756:ASN:HA	1:B:759:GLN:HE21	1.37	0.89
1:B:980:LEU:HA	1:B:983:ILE:HD12	1.53	0.89
1:B:629:LYS:O	1:B:633:ILE:HG13	1.73	0.88
1:A:904:LEU:O	1:A:907:ILE:HG22	1.74	0.87
1:A:679:VAL:HG13	1:A:683:HIS:HB2	1.55	0.87
1:B:567:ARG:HD3	1:B:570:PRO:HA	1.57	0.87
1:B:24:LEU:HD13	1:B:149:ASP:HA	1.54	0.87
1:A:773:VAL:CG2	1:A:845:GLY:HA3	2.05	0.87
1:B:783:LEU:HD13	1:B:870:LEU:HD11	1.55	0.87
1:A:773:VAL:HG23	1:A:845:GLY:HA3	1.55	0.86
1:B:679:VAL:HG13	1:B:683:HIS:HB2	1.56	0.86
1:B:311:LEU:HB3	1:B:312:PRO:HD3	1.58	0.86
1:A:567:ARG:HD3	1:A:570:PRO:HA	1.56	0.86
1:B:530:VAL:HG12	1:B:531:GLY:H	1.39	0.86
1:A:530:VAL:HG12	1:A:531:GLY:H	1.41	0.86
1:B:920:GLN:O	1:B:985:LYS:HD3	1.76	0.86
1:B:319:LEU:HD11	1:B:339:VAL:CG2	2.06	0.85
1:B:319:LEU:HD11	1:B:339:VAL:HG21	1.57	0.85
1:A:783:LEU:HD22	1:A:784:PRO:HD2	1.57	0.85
1:A:813:ASP:OD1	1:A:917:SER:HB2	1.76	0.85
1:A:42:PRO:HG2	1:A:44:GLU:OE1	1.77	0.84
1:A:125:GLU:CD	1:A:158:LYS:HB3	2.03	0.84
1:A:769:VAL:HG13	1:A:841:GLY:HA3	1.58	0.84
1:A:788:ILE:HG12	1:A:791:GLN:NE2	1.92	0.84
1:B:798:VAL:HG13	1:B:940:SER:HB3	1.59	0.84
1:A:980:LEU:HA	1:A:983:ILE:HD12	1.59	0.83
1:B:886:LEU:HD11	1:B:890:ILE:HD11	1.58	0.83
1:B:798:VAL:O	1:B:909:MET:HE1	1.79	0.83
1:B:767:SER:HB3	1:B:911:ASN:ND2	1.93	0.82
1:A:844:VAL:HG12	1:A:907:ILE:HG12	1.61	0.82
1:B:767:SER:CB	1:B:911:ASN:HD22	1.93	0.81
1:A:125:GLU:HB3	1:A:142:ALA:HB2	1.61	0.81
1:A:311:LEU:HB3	1:A:312:PRO:HD3	1.62	0.81
1:A:679:VAL:CG1	1:A:683:HIS:HB2	2.10	0.81
1:A:907:ILE:HD12	1:A:974:SER:HA	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:775:ILE:HD11	1:B:787:LEU:HD12	1.62	0.81
1:A:920:GLN:O	1:A:985:LYS:HD3	1.81	0.81
1:A:193:PRO:HD3	4:A:1000:CL:CL	2.18	0.80
1:B:679:VAL:CG1	1:B:683:HIS:HB2	2.12	0.79
1:A:759:GLN:NE2	1:A:917:SER:HA	1.97	0.79
1:A:881:PRO:HG2	1:A:882:HIS:H	1.45	0.79
1:A:111:ASN:HD22	1:A:111:ASN:H	1.31	0.79
1:B:49:LEU:HB3	1:B:254:ASP:HB3	1.64	0.78
1:B:111:ASN:HD22	1:B:111:ASN:H	1.32	0.78
1:A:756:ASN:HA	1:A:759:GLN:OE1	1.83	0.78
1:B:276:ILE:HA	1:B:279:PHE:CE2	2.18	0.78
1:A:802:LEU:HB3	1:A:803:PRO:HD3	1.65	0.78
1:A:102:ALA:O	1:A:106:VAL:HG22	1.83	0.77
1:B:907:ILE:HA	1:B:974:SER:HB3	1.64	0.77
1:B:102:ALA:O	1:B:106:VAL:HG22	1.83	0.77
1:B:573:ARG:HH11	1:B:573:ARG:HG3	1.50	0.77
1:A:276:ILE:HA	1:A:279:PHE:CE2	2.20	0.77
1:B:580:ASP:OD2	1:B:582:SER:HB3	1.85	0.77
1:B:887:ASP:HB2	1:B:890:ILE:HG23	1.64	0.77
1:A:580:ASP:OD2	1:A:582:SER:HB3	1.84	0.76
1:B:69:ALA:HA	1:B:297:LYS:HZ1	1.50	0.76
1:B:814:LEU:HG	1:B:920:GLN:HE21	1.49	0.76
1:B:794:TRP:HD1	1:B:901:LEU:HD11	1.49	0.76
1:B:278:HIS:HA	1:B:281:ASP:OD2	1.86	0.76
1:A:811:PRO:HG2	1:A:929:VAL:HG12	1.67	0.76
1:A:565:ALA:HA	1:A:594:VAL:HG23	1.67	0.76
1:A:125:GLU:OE2	1:A:158:LYS:HB3	1.86	0.75
1:A:769:VAL:O	1:A:773:VAL:HG13	1.85	0.75
1:B:565:ALA:HA	1:B:594:VAL:HG23	1.69	0.75
1:B:795:VAL:HG13	1:B:904:LEU:HG	1.69	0.75
1:A:347:VAL:HG22	1:A:620:ARG:HB2	1.69	0.75
1:A:129:VAL:HG12	1:A:151:VAL:HG22	1.66	0.75
1:A:2:GLU:CD	1:A:3:ALA:H	1.94	0.75
1:A:75:LEU:HD12	1:A:76:ALA:N	2.01	0.75
1:B:811:PRO:HG2	1:B:929:VAL:HG12	1.69	0.75
1:A:573:ARG:HG3	1:A:573:ARG:HH11	1.50	0.74
1:B:318:CYS:SG	1:B:756:ASN:HB3	2.27	0.74
1:A:69:ALA:HA	1:A:297:LYS:HZ1	1.52	0.74
1:A:267:ILE:HG21	1:A:772:VAL:HG11	1.69	0.74
1:B:928:TRP:HA	1:B:934:LEU:HD11	1.69	0.74
1:A:697:ILE:HA	1:A:715:GLU:HG2	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:HIS:HA	1:A:281:ASP:OD2	1.88	0.74
1:B:2:GLU:CD	1:B:3:ALA:H	1.95	0.74
1:A:763:TYR:HB2	1:A:915:SER:OG	1.88	0.74
1:B:918:GLU:C	1:B:919:ASN:HD22	1.94	0.74
1:A:907:ILE:HA	1:A:974:SER:HB3	1.69	0.73
1:A:387:SER:HB3	1:A:602:PRO:CG	2.19	0.73
1:B:314:VAL:HG21	1:B:760:PHE:CE2	2.23	0.73
1:B:441:THR:HG22	1:B:599:MET:SD	2.28	0.73
1:B:75:LEU:HD12	1:B:76:ALA:N	2.02	0.73
1:B:678:ARG:HG3	1:B:678:ARG:HH11	1.54	0.73
1:B:161:ALA:HA	1:B:210:SER:HB2	1.70	0.72
1:B:697:ILE:HA	1:B:715:GLU:HG2	1.70	0.72
1:A:647:GLU:CD	1:A:647:GLU:H	1.97	0.72
1:B:962:LEU:HB3	1:B:966:GLN:HB3	1.71	0.72
1:B:95:LEU:O	1:B:99:ILE:HG12	1.90	0.72
1:B:941:MET:HA	1:B:941:MET:CE	2.18	0.72
1:A:175:VAL:HG22	1:A:214:ILE:HG22	1.72	0.72
1:A:678:ARG:HG3	1:A:678:ARG:HH11	1.55	0.72
1:A:941:MET:HA	1:A:941:MET:CE	2.19	0.72
1:A:446:THR:O	1:A:449:VAL:HG22	1.89	0.72
1:A:825:LYS:HG3	1:A:826:GLU:H	1.55	0.72
1:A:95:LEU:O	1:A:99:ILE:HG12	1.90	0.71
1:B:788:ILE:HB	1:B:789:PRO:HD2	1.71	0.71
1:A:823:SER:HB2	1:A:825:LYS:HG2	1.71	0.71
1:B:647:GLU:H	1:B:647:GLU:CD	1.98	0.71
1:A:100:ALA:HA	1:A:103:ILE:HG22	1.72	0.71
1:A:918:GLU:C	1:A:919:ASN:HD22	1.98	0.71
1:B:310:GLY:O	1:B:314:VAL:HG23	1.90	0.71
1:A:367:PHE:CD2	1:A:379:LEU:HD13	2.25	0.71
1:B:756:ASN:HA	1:B:759:GLN:NE2	2.06	0.71
1:B:367:PHE:CD2	1:B:379:LEU:HD13	2.25	0.71
1:B:769:VAL:HG12	1:B:841:GLY:HA3	1.71	0.71
1:A:559:LEU:CD2	1:A:600:LEU:HB3	2.20	0.71
1:B:175:VAL:HG22	1:B:214:ILE:HG22	1.73	0.71
1:B:763:TYR:HB2	1:B:915:SER:OG	1.91	0.71
1:B:840:ILE:HD13	1:B:980:LEU:HD23	1.73	0.71
1:B:347:VAL:CG2	1:B:696:GLU:HG2	2.20	0.71
1:B:617:ALA:HB1	1:B:751:ARG:HH12	1.54	0.70
1:A:81:GLY:C	1:A:82:GLU:OE1	2.35	0.70
1:A:416:ILE:HD11	1:A:594:VAL:HG21	1.73	0.70
1:A:449:VAL:HG21	1:A:472:ASN:ND2	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:ILE:HG21	1:B:772:VAL:HG11	1.73	0.70
1:A:50:TRP:HB2	1:A:55:GLU:CD	2.16	0.70
1:A:281:ASP:HB3	1:A:282:PRO:HD2	1.73	0.70
1:A:310:GLY:O	1:A:314:VAL:HG23	1.91	0.70
1:A:319:LEU:HD11	1:A:339:VAL:CG2	2.22	0.70
1:A:988:ALA:HA	1:A:992:LEU:HD12	1.73	0.70
1:A:111:ASN:HD22	1:A:111:ASN:N	1.88	0.70
1:B:346:SER:OG	1:B:696:GLU:HG3	1.91	0.70
1:B:988:ALA:HA	1:B:992:LEU:HD12	1.74	0.70
1:A:926:PRO:O	1:A:929:VAL:HG23	1.91	0.70
1:B:755:ASN:O	1:B:759:GLN:HG3	1.92	0.69
1:B:281:ASP:HB3	1:B:282:PRO:HD2	1.73	0.69
1:A:25:THR:HG22	1:A:132:ALA:HB2	1.73	0.69
1:B:926:PRO:O	1:B:929:VAL:HG23	1.93	0.69
1:A:962:LEU:HB3	1:A:966:GLN:HB3	1.74	0.69
1:B:111:ASN:HD22	1:B:111:ASN:N	1.89	0.69
1:B:347:VAL:HG22	1:B:620:ARG:HB2	1.74	0.69
1:B:899:MET:HG2	1:B:962:LEU:HD21	1.73	0.69
1:B:917:SER:OG	1:B:920:GLN:HB2	1.91	0.69
1:A:122:TYR:O	1:A:124:PRO:HD3	1.93	0.69
1:A:413:LEU:C	1:A:413:LEU:HD23	2.17	0.69
1:A:459:VAL:HA	1:A:462:LEU:HD12	1.74	0.68
1:B:100:ALA:HA	1:B:103:ILE:HG22	1.74	0.68
1:B:783:LEU:CD1	1:B:870:LEU:HD11	2.23	0.68
1:A:311:LEU:HA	1:A:760:PHE:CE1	2.28	0.68
1:A:342:LEU:HD12	1:A:716:ILE:HD13	1.73	0.68
1:B:319:LEU:CD1	1:B:339:VAL:HG21	2.22	0.68
1:B:416:ILE:HD11	1:B:594:VAL:HG21	1.74	0.68
1:B:628:ASN:HB3	1:B:678:ARG:HH22	1.58	0.68
1:B:832:TRP:O	1:B:835:PHE:HB3	1.94	0.68
1:B:870:LEU:C	1:B:870:LEU:HD12	2.19	0.68
1:B:446:THR:O	1:B:449:VAL:HG22	1.92	0.67
1:A:336:LEU:N	1:A:337:PRO:HD2	2.09	0.67
1:B:47:LYS:HD3	1:B:51:GLU:O	1.95	0.67
1:B:559:LEU:CD2	1:B:600:LEU:HB3	2.22	0.67
1:B:25:THR:HG22	1:B:132:ALA:HB2	1.75	0.67
1:A:326:MET:CE	1:A:333:VAL:HG21	2.25	0.67
1:A:742:THR:O	1:A:745:ALA:N	2.27	0.67
1:A:778:THR:HG22	1:A:849:VAL:HG13	1.76	0.67
1:A:811:PRO:HG2	1:A:929:VAL:CG1	2.24	0.67
1:B:359:ASN:HA	1:B:601:ASP:OD1	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:459:VAL:HA	1:B:462:LEU:HD12	1.77	0.67
1:B:662:PRO:HD2	1:B:665:GLU:HB2	1.76	0.67
1:B:671:ARG:HB3	1:B:694:TYR:CE2	2.30	0.67
1:B:387:SER:HB3	1:B:602:PRO:CG	2.24	0.67
1:A:271:VAL:HA	1:A:274:ILE:HG12	1.76	0.67
1:A:366:MET:HE1	1:A:452:MET:HE3	1.76	0.67
1:B:336:LEU:N	1:B:337:PRO:HD2	2.10	0.67
1:A:631:THR:O	1:A:634:ALA:HB3	1.95	0.67
1:A:946:LEU:C	1:A:946:LEU:HD23	2.19	0.67
1:B:413:LEU:C	1:B:413:LEU:HD23	2.20	0.66
1:B:688:VAL:CG2	1:B:700:MET:HE2	2.25	0.66
1:B:946:LEU:HD23	1:B:946:LEU:C	2.20	0.66
1:A:308:PRO:HB2	1:A:764:LEU:HD12	1.76	0.66
1:A:928:TRP:HA	1:A:934:LEU:HD11	1.77	0.66
1:B:539:GLY:N	1:B:540:PRO:HD2	2.10	0.66
1:B:306:ALA:O	1:B:768:ASN:ND2	2.28	0.66
1:A:975:LEU:N	1:A:976:PRO:HD2	2.11	0.66
1:A:100:ALA:HB1	1:A:797:LEU:HD11	1.77	0.66
1:A:210:SER:HB3	1:A:230:THR:HG21	1.76	0.66
1:A:54:ILE:HD12	1:A:55:GLU:N	2.10	0.66
1:A:662:PRO:HD2	1:A:665:GLU:HB2	1.78	0.66
1:A:412:GLU:OE1	1:A:529:ARG:HD2	1.95	0.66
1:A:441:THR:HG22	1:A:599:MET:SD	2.36	0.66
1:B:210:SER:HB3	1:B:230:THR:HG21	1.78	0.66
1:A:230:THR:CG2	1:A:232:ILE:HG22	2.26	0.65
1:A:899:MET:HG2	1:A:962:LEU:HD21	1.77	0.65
1:B:357:THR:HA	1:B:603:PRO:HA	1.77	0.65
1:B:944:HIS:O	1:B:947:ILE:HG22	1.95	0.65
1:A:161:ALA:HA	1:A:210:SER:HB2	1.76	0.65
1:A:162:ASP:OD1	1:A:230:THR:HG23	1.96	0.65
1:B:347:VAL:HG23	1:B:696:GLU:HG2	1.77	0.65
1:B:495:SER:HB3	1:B:514:VAL:HA	1.78	0.65
1:A:317:THR:HG22	1:A:321:LEU:HD12	1.77	0.65
1:A:319:LEU:HD11	1:A:339:VAL:HG21	1.78	0.65
1:A:442:GLU:O	1:A:445:LEU:HB2	1.96	0.65
1:A:495:SER:HB3	1:A:514:VAL:HA	1.78	0.65
1:B:271:VAL:HA	1:B:274:ILE:HG12	1.78	0.65
1:B:317:THR:HG22	1:B:321:LEU:HD12	1.79	0.65
1:B:975:LEU:N	1:B:976:PRO:HD2	2.12	0.65
1:A:539:GLY:N	1:A:540:PRO:HD2	2.12	0.65
1:A:944:HIS:O	1:A:947:ILE:HG22	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ALA:CB	1:A:797:LEU:HD11	2.27	0.65
1:B:118:ALA:C	1:B:120:LYS:H	2.04	0.65
1:B:342:LEU:HD12	1:B:716:ILE:HD13	1.79	0.65
1:B:857:MET:HE3	1:B:858:TYR:HE1	1.60	0.65
1:B:893:ALA:O	1:B:896:PRO:HD2	1.96	0.65
1:B:442:GLU:O	1:B:445:LEU:HB2	1.97	0.65
1:A:82:GLU:OE1	1:A:82:GLU:N	2.30	0.65
1:B:267:ILE:CG2	1:B:772:VAL:HG11	2.28	0.64
1:A:780:ALA:C	1:A:782:GLY:H	2.05	0.64
1:B:82:GLU:OE1	1:B:82:GLU:N	2.30	0.64
1:B:783:LEU:HD13	1:B:870:LEU:CD1	2.26	0.64
1:A:628:ASN:HB3	1:A:678:ARG:HH22	1.62	0.64
1:B:49:LEU:HB3	1:B:254:ASP:CB	2.28	0.64
1:B:230:THR:CG2	1:B:232:ILE:HG22	2.26	0.64
1:B:610:SER:HB3	1:B:744:VAL:HG21	1.79	0.64
1:B:775:ILE:CD1	1:B:787:LEU:HD12	2.27	0.64
1:B:898:THR:OG1	1:B:959:LEU:HA	1.97	0.64
1:A:770:GLY:HA2	1:A:841:GLY:O	1.96	0.64
1:A:347:VAL:CG2	1:A:696:GLU:HG2	2.27	0.64
1:B:518:PRO:O	1:B:522:ILE:HG12	1.98	0.64
1:B:759:GLN:OE1	1:B:917:SER:HA	1.96	0.64
1:B:883:PHE:O	1:B:884:GLU:HG2	1.97	0.64
1:A:688:VAL:CG2	1:A:700:MET:HE2	2.28	0.64
1:A:770:GLY:HA3	1:A:844:VAL:CG2	2.28	0.64
1:B:449:VAL:HG21	1:B:472:ASN:ND2	2.12	0.64
1:B:962:LEU:HB3	1:B:966:GLN:CB	2.28	0.64
1:B:162:ASP:OD1	1:B:230:THR:HG23	1.97	0.64
1:B:962:LEU:HA	1:B:966:GLN:OE1	1.97	0.64
1:A:263:VAL:O	1:A:267:ILE:HG13	1.97	0.64
1:A:459:VAL:HG23	1:A:460:ARG:H	1.61	0.64
1:A:467:ARG:HG2	1:A:467:ARG:HH11	1.62	0.64
1:A:629:LYS:HD2	1:A:657:GLU:OE1	1.98	0.64
1:A:798:VAL:HG13	1:A:940:SER:HB3	1.78	0.64
1:B:895:GLU:N	1:B:896:PRO:HD2	2.13	0.64
1:A:559:LEU:HD21	1:A:600:LEU:HD13	1.80	0.63
1:A:762:ARG:HG3	1:A:837:TYR:CE1	2.33	0.63
1:B:60:LEU:HD12	1:B:60:LEU:O	1.98	0.63
1:B:886:LEU:HD11	1:B:890:ILE:CD1	2.29	0.63
1:B:907:ILE:CA	1:B:974:SER:HB3	2.29	0.63
1:A:449:VAL:CG2	1:A:472:ASN:ND2	2.61	0.63
1:B:530:VAL:O	1:B:531:GLY:C	2.41	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:628:ASN:HD21	1:B:631:THR:HG23	1.63	0.63
1:B:766:SER:O	1:B:769:VAL:HG12	1.97	0.63
1:B:894:PRO:HG2	1:B:895:GLU:OE2	1.99	0.63
1:A:679:VAL:HG13	1:A:683:HIS:CB	2.26	0.63
1:A:271:VAL:C	1:A:273:LEU:H	2.05	0.63
1:A:843:TYR:OH	1:A:976:PRO:HG2	1.99	0.63
1:B:330:ASN:HB3	1:B:736:ALA:HB3	1.79	0.63
1:A:118:ALA:HB1	1:A:324:ARG:HE	1.63	0.63
1:B:631:THR:O	1:B:634:ALA:HB3	1.99	0.63
1:B:25:THR:O	1:B:29:VAL:HG23	1.98	0.63
1:B:467:ARG:HH11	1:B:467:ARG:HG2	1.64	0.62
1:A:97:ILE:HG21	1:A:793:LEU:HB3	1.82	0.62
1:A:610:SER:HB3	1:A:744:VAL:HG21	1.81	0.62
1:B:230:THR:HG21	1:B:232:ILE:HG22	1.81	0.62
1:B:326:MET:CE	1:B:333:VAL:HG21	2.28	0.62
1:B:412:GLU:OE1	1:B:529:ARG:HD2	1.99	0.62
1:B:658:PHE:HA	1:B:661:LEU:CD1	2.26	0.62
1:A:708:ALA:HB3	1:A:709:PRO:HD3	1.80	0.62
1:A:867:TYR:C	1:A:869:GLN:H	2.07	0.62
1:A:25:THR:O	1:A:29:VAL:HG23	1.98	0.62
1:A:230:THR:HG21	1:A:232:ILE:HG22	1.82	0.62
1:A:879:ASP:C	1:A:881:PRO:HD3	2.24	0.62
1:B:1:MET:O	1:B:1:MET:HG3	1.98	0.62
1:B:559:LEU:HD21	1:B:600:LEU:HD13	1.81	0.62
1:A:369:ILE:N	1:A:369:ILE:HD12	2.13	0.62
1:A:947:ILE:HG12	1:A:957:PHE:CE2	2.34	0.62
1:A:962:LEU:HB3	1:A:966:GLN:CB	2.30	0.62
1:B:957:PHE:O	1:B:959:LEU:HG	1.99	0.62
1:A:230:THR:HG22	1:A:232:ILE:H	1.64	0.62
1:B:683:HIS:O	1:B:687:ILE:HG13	2.00	0.62
1:A:100:ALA:HA	1:A:103:ILE:CG2	2.30	0.62
1:A:264:ILE:HA	1:A:267:ILE:HD12	1.81	0.62
1:A:330:ASN:HB3	1:A:736:ALA:HB3	1.81	0.61
1:A:843:TYR:CD2	1:A:843:TYR:C	2.78	0.61
1:B:742:THR:O	1:B:745:ALA:N	2.33	0.61
1:A:658:PHE:HA	1:A:661:LEU:CD1	2.27	0.61
1:B:639:ILE:HD11	1:B:641:ILE:HD12	1.83	0.61
1:B:679:VAL:HG13	1:B:683:HIS:CB	2.28	0.61
1:B:369:ILE:HD12	1:B:369:ILE:N	2.15	0.61
1:A:24:LEU:HD22	1:A:149:ASP:HB3	1.82	0.61
1:A:898:THR:OG1	1:A:959:LEU:HA	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:769:VAL:CG1	1:A:841:GLY:HA3	2.28	0.61
1:A:448:LEU:O	1:A:452:MET:HG3	2.00	0.61
1:A:263:VAL:HG12	1:A:267:ILE:CD1	2.25	0.61
1:A:367:PHE:CE1	1:A:596:VAL:HB	2.36	0.61
1:B:214:ILE:H	1:B:214:ILE:CD1	2.13	0.61
1:B:836:ARG:HD3	1:B:984:LEU:HD12	1.82	0.61
1:A:57:PHE:O	1:A:61:LEU:HG	2.01	0.61
1:A:907:ILE:CA	1:A:974:SER:HB3	2.31	0.61
1:A:953:LEU:H	1:A:954:PRO:HD2	1.65	0.61
1:B:240:ALA:O	1:B:241:ALA:C	2.44	0.61
1:A:895:GLU:H	1:A:895:GLU:CD	2.05	0.61
1:A:947:ILE:HG12	1:A:957:PHE:CD2	2.36	0.61
1:B:271:VAL:C	1:B:273:LEU:H	2.07	0.60
1:B:449:VAL:CG2	1:B:472:ASN:ND2	2.63	0.60
1:B:484:THR:HB	1:B:496:VAL:HG12	1.81	0.60
1:B:843:TYR:O	1:B:846:ALA:HB3	2.00	0.60
1:A:962:LEU:HA	1:A:966:GLN:OE1	2.01	0.60
1:B:459:VAL:HG23	1:B:460:ARG:H	1.65	0.60
1:A:50:TRP:HB2	1:A:55:GLU:OE2	2.01	0.60
1:A:518:PRO:O	1:A:522:ILE:HG12	2.02	0.60
1:B:212:THR:HG22	1:B:213:ASN:N	2.15	0.60
1:B:263:VAL:O	1:B:267:ILE:HG13	2.00	0.60
1:A:650:ASP:HB2	1:A:672:ARG:NH2	2.16	0.60
1:B:93:VAL:HB	1:B:790:VAL:HG11	1.83	0.60
1:B:708:ALA:HB3	1:B:709:PRO:HD3	1.82	0.60
1:B:834:PHE:O	1:B:838:MET:HG2	2.01	0.60
1:A:1:MET:O	1:A:1:MET:HG3	2.02	0.60
1:A:347:VAL:HG23	1:A:696:GLU:HG2	1.82	0.60
1:A:917:SER:OG	1:A:920:GLN:HB2	2.01	0.60
1:A:214:ILE:H	1:A:214:ILE:CD1	2.11	0.60
1:A:628:ASN:HD21	1:A:631:THR:HG23	1.66	0.60
1:A:642:PHE:CD2	1:A:648:VAL:HG11	2.36	0.60
1:A:905:VAL:HG12	1:A:941:MET:HE1	1.84	0.60
1:A:957:PHE:O	1:A:959:LEU:HG	2.01	0.60
1:B:100:ALA:HA	1:B:103:ILE:CG2	2.32	0.60
1:A:212:THR:HG22	1:A:213:ASN:N	2.16	0.60
1:A:484:THR:HB	1:A:496:VAL:HG12	1.84	0.60
1:B:788:ILE:HB	1:B:789:PRO:CD	2.31	0.60
1:B:905:VAL:HG12	1:B:941:MET:HE1	1.84	0.60
1:A:683:HIS:O	1:A:687:ILE:HG13	2.01	0.60
1:B:462:LEU:HD22	1:B:466:GLU:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:762:ARG:CZ	1:B:836:ARG:NH1	2.64	0.60
1:B:726:VAL:HG13	1:B:727:ALA:N	2.16	0.60
1:A:94:ILE:HD12	1:A:95:LEU:N	2.17	0.59
1:A:346:SER:OG	1:A:696:GLU:HG3	2.01	0.59
1:A:387:SER:HB3	1:A:602:PRO:HG3	1.83	0.59
1:A:671:ARG:HB3	1:A:694:TYR:CE2	2.37	0.59
1:B:81:GLY:C	1:B:82:GLU:OE1	2.45	0.59
1:B:116:ILE:HD13	1:B:320:ALA:HB2	1.84	0.59
1:A:249:LEU:O	1:A:253:LEU:HB2	2.02	0.59
1:A:372:VAL:HG13	1:A:377:CYS:CB	2.25	0.59
1:A:22:THR:HG22	1:A:135:LYS:NZ	2.18	0.59
1:A:311:LEU:HA	1:A:760:PHE:HE1	1.65	0.59
1:B:367:PHE:CE2	1:B:379:LEU:HD13	2.38	0.59
1:B:947:ILE:HG12	1:B:957:PHE:CE2	2.37	0.59
1:A:758:LYS:HE3	1:A:833:LEU:HD21	1.84	0.59
1:B:134:ARG:HG3	1:B:134:ARG:HH11	1.67	0.59
1:A:355:THR:HA	1:A:738:ASP:O	2.02	0.59
1:A:60:LEU:HD12	1:A:60:LEU:O	2.03	0.59
1:A:697:ILE:HG23	1:A:715:GLU:HG2	1.85	0.59
1:B:52:LEU:HD12	1:B:56:GLN:OE1	2.03	0.59
1:B:629:LYS:HD2	1:B:657:GLU:OE1	2.02	0.59
1:A:367:PHE:CE2	1:A:379:LEU:HD13	2.37	0.59
1:B:22:THR:HG22	1:B:135:LYS:NZ	2.18	0.59
1:B:24:LEU:HD22	1:B:149:ASP:HB3	1.85	0.59
1:B:725:ALA:O	1:B:729:THR:HG23	2.03	0.59
1:B:953:LEU:H	1:B:954:PRO:HD2	1.68	0.59
1:A:223:VAL:HG11	1:A:226:THR:HG22	1.85	0.58
1:B:131:ARG:HH11	1:B:131:ARG:HG3	1.67	0.58
1:B:654:THR:HA	1:B:677:ALA:O	2.03	0.58
1:A:600:LEU:O	1:A:600:LEU:HD23	2.03	0.58
1:A:825:LYS:HG3	1:A:826:GLU:N	2.17	0.58
1:B:230:THR:HG22	1:B:232:ILE:H	1.67	0.58
1:B:603:PRO:HB3	1:B:639:ILE:HG22	1.83	0.58
1:B:94:ILE:HD12	1:B:95:LEU:N	2.18	0.58
1:B:264:ILE:HA	1:B:267:ILE:HD12	1.84	0.58
1:B:688:VAL:HG23	1:B:700:MET:HE2	1.86	0.58
1:B:788:ILE:HG12	1:B:791:GLN:HG3	1.86	0.58
1:B:212:THR:CG2	1:B:213:ASN:N	2.67	0.58
1:B:650:ASP:HB2	1:B:672:ARG:NH2	2.18	0.58
1:B:50:TRP:CZ2	1:B:311:LEU:HD23	2.38	0.58
1:B:154:ALA:O	1:B:214:ILE:HD11	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:VAL:HG11	1:B:226:THR:HG22	1.85	0.58
1:B:282:PRO:O	1:B:284:HIS:N	2.37	0.58
1:A:361:MET:HE3	1:A:599:MET:HB2	1.84	0.58
1:B:57:PHE:O	1:B:61:LEU:HG	2.04	0.58
1:B:573:ARG:HG3	1:B:573:ARG:NH1	2.17	0.58
1:B:770:GLY:CA	1:B:841:GLY:O	2.52	0.58
1:A:726:VAL:HG13	1:A:727:ALA:N	2.18	0.58
1:B:933:LEU:O	1:B:937:ILE:HG13	2.04	0.58
1:A:140:ILE:HD12	1:A:141:LYS:H	1.69	0.57
1:B:39:ASN:HB3	1:B:143:ARG:HA	1.86	0.57
1:B:762:ARG:NH2	1:B:918:GLU:O	2.37	0.57
1:B:900:ALA:O	1:B:903:VAL:N	2.36	0.57
1:B:244:GLN:HE21	1:B:247:THR:CG2	2.17	0.57
1:B:847:ALA:HB1	1:B:973:ILE:HD12	1.85	0.57
1:A:39:ASN:HB3	1:A:143:ARG:HA	1.86	0.57
1:A:134:ARG:HH11	1:A:134:ARG:HG3	1.67	0.57
1:A:539:GLY:O	1:A:543:GLU:HG2	2.04	0.57
1:B:146:VAL:O	1:B:149:ASP:OD2	2.22	0.57
1:B:947:ILE:HG12	1:B:957:PHE:CD2	2.40	0.57
1:A:462:LEU:HD22	1:A:466:GLU:HB3	1.85	0.57
1:B:2:GLU:CD	1:B:3:ALA:N	2.62	0.57
1:B:326:MET:HE1	1:B:333:VAL:HG21	1.85	0.57
1:B:474:VAL:HA	1:B:477:GLN:HE21	1.70	0.57
1:A:770:GLY:O	1:A:773:VAL:HG22	2.04	0.57
1:B:530:VAL:HG12	1:B:531:GLY:N	2.16	0.57
1:A:639:ILE:HD11	1:A:641:ILE:HD12	1.87	0.57
1:B:116:ILE:CD1	1:B:320:ALA:HB2	2.35	0.57
1:B:308:PRO:HB3	1:B:764:LEU:HG	1.87	0.57
1:A:2:GLU:CD	1:A:3:ALA:N	2.62	0.57
1:A:125:GLU:OE1	1:A:158:LYS:HB3	2.04	0.57
1:A:783:LEU:CD2	1:A:784:PRO:HD2	2.31	0.57
1:A:950:VAL:O	1:A:954:PRO:HD2	2.05	0.57
1:B:263:VAL:HG12	1:B:267:ILE:CD1	2.28	0.57
1:A:800:ASP:O	1:A:802:LEU:N	2.37	0.57
1:B:353:THR:CG2	1:B:353:THR:O	2.53	0.57
1:B:367:PHE:HA	1:B:380:ASN:O	2.04	0.57
1:B:539:GLY:O	1:B:543:GLU:HG2	2.05	0.57
1:B:567:ARG:HD3	1:B:570:PRO:CA	2.32	0.57
1:A:742:THR:O	1:A:743:ILE:C	2.48	0.57
1:A:867:TYR:O	1:A:869:GLN:N	2.38	0.57
1:A:879:ASP:O	1:A:880:HIS:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:LEU:HB3	1:B:254:ASP:CG	2.30	0.57
1:B:448:LEU:O	1:B:452:MET:HG3	2.05	0.57
1:B:762:ARG:CZ	1:B:836:ARG:HH12	2.18	0.57
1:B:812:PRO:O	1:B:813:ASP:O	2.23	0.57
1:A:763:TYR:CE1	1:A:912:ALA:HB2	2.40	0.56
1:A:950:VAL:HG12	1:A:952:PRO:HD2	1.87	0.56
1:B:279:PHE:HE1	1:B:295:TYR:HB2	1.69	0.56
1:B:336:LEU:O	1:B:339:VAL:HG22	2.05	0.56
1:B:366:MET:HE1	1:B:452:MET:HE3	1.87	0.56
1:A:573:ARG:HG3	1:A:573:ARG:NH1	2.17	0.56
1:B:881:PRO:HD2	1:B:883:PHE:HE2	1.69	0.56
1:A:33:LEU:O	1:A:37:GLY:N	2.38	0.56
1:A:137:VAL:HG12	1:A:138:GLN:N	2.20	0.56
1:A:488:SER:OG	1:A:491:ARG:NH1	2.39	0.56
1:A:836:ARG:HH11	1:A:836:ARG:CG	2.17	0.56
1:B:950:VAL:O	1:B:954:PRO:HD2	2.05	0.56
1:A:131:ARG:HG3	1:A:131:ARG:HH11	1.71	0.56
1:A:154:ALA:O	1:A:214:ILE:HD11	2.06	0.56
1:A:335:SER:OG	1:A:337:PRO:HG2	2.05	0.56
1:A:770:GLY:HA3	1:A:844:VAL:HG23	1.88	0.56
1:A:834:PHE:O	1:A:838:MET:HG2	2.06	0.56
1:A:968:LEU:HD23	1:A:968:LEU:O	2.05	0.56
1:B:628:ASN:HD21	1:B:631:THR:CG2	2.17	0.56
1:B:968:LEU:O	1:B:968:LEU:HD23	2.05	0.56
1:A:50:TRP:HB2	1:A:55:GLU:OE1	2.04	0.56
1:A:282:PRO:O	1:A:284:HIS:N	2.39	0.56
1:A:428:ASN:OD1	1:A:430:THR:HB	2.04	0.56
1:A:530:VAL:O	1:A:531:GLY:C	2.49	0.56
1:A:900:ALA:O	1:A:903:VAL:N	2.38	0.56
1:A:988:ALA:CA	1:A:992:LEU:HD12	2.35	0.56
1:B:857:MET:HE3	1:B:858:TYR:CE1	2.39	0.56
1:A:25:THR:HB	1:A:26:PRO:HD2	1.87	0.56
1:A:264:ILE:C	1:A:266:LEU:H	2.14	0.56
1:A:903:VAL:HA	1:A:970:VAL:HG13	1.88	0.56
1:A:66:LEU:HD12	1:A:94:ILE:HD11	1.86	0.56
1:B:137:VAL:HG12	1:B:138:GLN:H	1.70	0.56
1:B:361:MET:HE3	1:B:599:MET:HB2	1.87	0.56
1:B:950:VAL:HG12	1:B:952:PRO:HD2	1.87	0.56
1:A:832:TRP:CZ2	1:A:988:ALA:HB2	2.41	0.56
1:A:137:VAL:HG12	1:A:138:GLN:H	1.71	0.56
1:A:146:VAL:O	1:A:149:ASP:OD2	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:774:CYS:SG	1:A:775:ILE:N	2.79	0.56
1:B:260:LEU:HD11	1:B:765:ILE:HD11	1.88	0.56
1:B:306:ALA:HA	1:B:768:ASN:HD21	1.70	0.55
1:B:777:LEU:HA	1:B:780:ALA:HB3	1.87	0.55
1:B:899:MET:O	1:B:903:VAL:HG23	2.05	0.55
1:A:950:VAL:C	1:A:952:PRO:HD2	2.31	0.55
1:A:962:LEU:CD2	1:A:966:GLN:HB3	2.37	0.55
1:B:325:ARG:NH1	1:B:812:PRO:HG3	2.21	0.55
1:A:389:TYR:HB3	1:A:425:LEU:HD21	1.88	0.55
1:A:567:ARG:HD3	1:A:570:PRO:CA	2.31	0.55
1:B:89:VAL:O	1:B:93:VAL:HG23	2.06	0.55
1:A:628:ASN:HD21	1:A:631:THR:CG2	2.20	0.55
1:B:66:LEU:HD12	1:B:94:ILE:HD11	1.86	0.55
1:B:372:VAL:HG13	1:B:377:CYS:CB	2.28	0.55
1:A:252:LYS:NZ	1:A:826:GLU:O	2.40	0.55
1:A:329:LYS:O	1:A:330:ASN:HB2	2.06	0.55
1:B:367:PHE:CE1	1:B:596:VAL:HB	2.42	0.55
1:A:192:GLU:HB3	1:A:193:PRO:HD2	1.88	0.55
1:A:325:ARG:NH1	1:A:812:PRO:HG3	2.21	0.55
1:A:872:HIS:O	1:A:875:GLN:HG2	2.06	0.55
1:B:25:THR:HB	1:B:26:PRO:HD2	1.88	0.55
1:B:256:PHE:C	1:B:258:GLU:H	2.15	0.55
1:B:276:ILE:HA	1:B:279:PHE:CD2	2.41	0.55
1:B:771:GLU:O	1:B:775:ILE:HG12	2.06	0.55
1:B:814:LEU:HG	1:B:920:GLN:NE2	2.20	0.55
1:A:851:ALA:CB	1:A:903:VAL:HG21	2.37	0.55
1:B:137:VAL:HG12	1:B:138:GLN:N	2.21	0.55
1:B:428:ASN:OD1	1:B:430:THR:HB	2.07	0.55
1:A:128:LYS:O	1:A:151:VAL:HG13	2.07	0.55
1:A:212:THR:CG2	1:A:213:ASN:N	2.70	0.55
1:A:913:LEU:HD22	1:A:927:PRO:HB3	1.89	0.55
1:B:855:TRP:CZ2	1:B:895:GLU:HB2	2.42	0.55
1:A:153:VAL:O	1:A:218:LYS:HA	2.06	0.55
1:A:530:VAL:HG12	1:A:531:GLY:N	2.19	0.55
1:A:725:ALA:O	1:A:729:THR:HG23	2.07	0.55
1:A:848:THR:C	1:A:850:GLY:H	2.15	0.55
1:B:54:ILE:HG23	1:B:307:ILE:CG2	2.37	0.55
1:B:903:VAL:HA	1:B:970:VAL:HG13	1.89	0.55
1:A:737:ASP:OD1	1:A:737:ASP:N	2.40	0.54
1:A:823:SER:CB	1:A:825:LYS:HG2	2.37	0.54
1:B:697:ILE:HG23	1:B:715:GLU:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:748:GLU:HB2	1:B:817:MET:SD	2.47	0.54
1:A:302:LEU:HA	1:A:792:LEU:HD13	1.89	0.54
1:B:413:LEU:HG	1:B:564:LEU:CD1	2.37	0.54
1:B:988:ALA:CA	1:B:992:LEU:HD12	2.37	0.54
1:A:474:VAL:HA	1:A:477:GLN:HE21	1.71	0.54
1:A:880:HIS:N	1:A:881:PRO:CD	2.71	0.54
1:B:140:ILE:HD12	1:B:141:LYS:H	1.73	0.54
1:B:628:ASN:HA	1:B:678:ARG:NH1	2.22	0.54
1:A:326:MET:HE1	1:A:333:VAL:HG21	1.88	0.54
1:A:513:PHE:CD1	1:A:566:THR:HG23	2.42	0.54
1:B:389:TYR:HB3	1:B:425:LEU:HD21	1.89	0.54
1:B:571:PRO:HG2	1:B:576:MET:SD	2.48	0.54
1:A:367:PHE:O	1:A:368:ILE:HG23	2.08	0.54
1:B:315:ILE:HG12	1:B:757:MET:HG3	1.90	0.54
1:B:488:SER:OG	1:B:491:ARG:NH1	2.41	0.54
1:B:724:THR:HB	1:B:726:VAL:HG12	1.88	0.54
1:A:836:ARG:HD3	1:A:984:LEU:CD1	2.38	0.54
1:B:155:VAL:HG13	1:B:216:ALA:HA	1.88	0.54
1:B:355:THR:HA	1:B:738:ASP:O	2.07	0.54
1:B:562:LEU:O	1:B:596:VAL:HG13	2.07	0.54
1:B:742:THR:O	1:B:743:ILE:C	2.51	0.54
1:B:840:ILE:HG22	1:B:841:GLY:N	2.23	0.54
1:A:155:VAL:HG13	1:A:216:ALA:HA	1.89	0.54
1:A:276:ILE:HA	1:A:279:PHE:CD2	2.42	0.54
1:A:724:THR:HB	1:A:726:VAL:HG12	1.89	0.54
1:B:826:GLU:O	1:B:827:PRO:O	2.26	0.54
1:B:962:LEU:CD2	1:B:966:GLN:HB3	2.38	0.54
1:A:176:ASP:O	1:A:212:THR:HG23	2.07	0.54
1:A:214:ILE:HD13	1:A:214:ILE:N	2.14	0.54
1:A:678:ARG:HG3	1:A:678:ARG:NH1	2.22	0.54
1:B:50:TRP:CE3	1:B:257:GLY:HA3	2.42	0.54
1:A:571:PRO:HG2	1:A:576:MET:SD	2.48	0.54
1:A:688:VAL:HG23	1:A:700:MET:HE2	1.90	0.54
1:B:718:ILE:HG12	1:B:733:MET:HE2	1.90	0.54
1:B:794:TRP:HZ2	1:B:944:HIS:HA	1.72	0.54
1:A:164:ARG:HA	1:A:207:MET:SD	2.48	0.54
1:A:726:VAL:HG13	1:A:727:ALA:H	1.72	0.54
1:B:153:VAL:O	1:B:218:LYS:HA	2.07	0.54
1:B:192:GLU:HB3	1:B:193:PRO:HD2	1.90	0.54
1:B:726:VAL:HG13	1:B:727:ALA:H	1.72	0.54
1:B:122:TYR:O	1:B:123:GLU:C	2.50	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:PRO:CB	1:B:764:LEU:HG	2.38	0.53
1:B:893:ALA:C	1:B:896:PRO:HD2	2.33	0.53
1:A:628:ASN:HA	1:A:678:ARG:NH1	2.23	0.53
1:A:755:ASN:OD1	1:A:819:ARG:NH2	2.40	0.53
1:B:53:VAL:HG12	1:B:53:VAL:O	2.08	0.53
1:B:765:ILE:HG21	1:B:837:TYR:HD2	1.73	0.53
1:B:903:VAL:HG22	1:B:973:ILE:HG21	1.90	0.53
1:B:920:GLN:OE1	1:B:920:GLN:HA	2.08	0.53
1:A:627:ASP:O	1:A:678:ARG:HG2	2.09	0.53
1:A:868:HIS:C	1:A:870:LEU:H	2.17	0.53
1:A:903:VAL:CG2	1:A:973:ILE:HG21	2.39	0.53
1:B:176:ASP:O	1:B:212:THR:HG23	2.08	0.53
1:A:89:VAL:O	1:A:93:VAL:HG23	2.07	0.53
1:A:264:ILE:O	1:A:266:LEU:N	2.42	0.53
1:A:654:THR:HA	1:A:677:ALA:O	2.09	0.53
1:A:823:SER:C	1:A:825:LYS:H	2.16	0.53
1:B:104:VAL:HG21	1:B:797:LEU:HD11	1.91	0.53
1:A:204:LYS:C	1:A:206:ASN:H	2.15	0.53
1:B:264:ILE:C	1:B:266:LEU:H	2.16	0.53
1:B:322:GLY:HA3	1:B:753:ILE:HD11	1.91	0.53
1:B:513:PHE:CD1	1:B:566:THR:HG23	2.44	0.53
1:B:950:VAL:C	1:B:952:PRO:HD2	2.34	0.53
1:A:279:PHE:HE1	1:A:295:TYR:HB2	1.72	0.53
1:A:788:ILE:HB	1:A:789:PRO:HD2	1.90	0.53
1:A:798:VAL:O	1:A:909:MET:HE1	2.09	0.53
1:B:689:GLU:CD	1:B:713:LYS:HZ1	2.16	0.53
1:A:751:ARG:CB	1:A:816:ILE:HD11	2.38	0.53
1:B:82:GLU:HB2	1:B:83:GLU:OE1	2.09	0.53
1:A:110:ARG:HG3	1:A:110:ARG:HH11	1.73	0.53
1:B:98:LEU:HA	1:B:101:ASN:HD22	1.72	0.53
1:B:794:TRP:CZ2	1:B:944:HIS:HA	2.43	0.53
1:A:358:THR:HG23	1:A:602:PRO:O	2.08	0.53
1:A:916:LEU:HD11	1:A:927:PRO:HA	1.91	0.53
1:B:656:ARG:HG2	1:B:656:ARG:HH11	1.73	0.53
1:B:762:ARG:NH2	1:B:836:ARG:HH12	2.07	0.53
1:A:367:PHE:HA	1:A:380:ASN:O	2.09	0.53
1:B:953:LEU:C	1:B:955:MET:H	2.17	0.53
1:A:880:HIS:HA	1:A:883:PHE:CD2	2.45	0.52
1:B:123:GLU:O	1:B:123:GLU:HG2	2.09	0.52
1:B:836:ARG:HD3	1:B:984:LEU:CD1	2.40	0.52
1:B:843:TYR:C	1:B:843:TYR:CD2	2.87	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:LEU:HA	1:A:101:ASN:HD22	1.73	0.52
1:B:154:ALA:O	1:B:214:ILE:CG1	2.58	0.52
1:B:246:LYS:HA	1:B:251:GLN:HG3	1.90	0.52
1:B:263:VAL:O	1:B:264:ILE:C	2.53	0.52
1:B:867:TYR:CG	1:B:868:HIS:N	2.78	0.52
1:B:913:LEU:HD22	1:B:927:PRO:HB3	1.91	0.52
1:B:799:THR:HB	1:B:908:GLU:OE1	2.09	0.52
1:A:256:PHE:C	1:A:258:GLU:H	2.17	0.52
1:A:459:VAL:HG23	1:A:460:ARG:N	2.23	0.52
1:B:369:ILE:HA	1:B:379:LEU:HD23	1.91	0.52
1:B:459:VAL:HG23	1:B:460:ARG:N	2.25	0.52
1:B:745:ALA:O	1:B:746:ALA:C	2.52	0.52
1:A:336:LEU:O	1:A:339:VAL:HG22	2.09	0.52
1:A:765:ILE:HG21	1:A:837:TYR:CD2	2.44	0.52
1:B:228:VAL:HG22	1:B:228:VAL:O	2.09	0.52
1:B:311:LEU:HB3	1:B:312:PRO:CD	2.34	0.52
1:A:491:ARG:HE	1:A:588:GLU:CD	2.18	0.52
1:A:920:GLN:OE1	1:A:920:GLN:HA	2.10	0.52
1:B:522:ILE:HD12	1:B:545:ILE:HG21	1.92	0.52
1:B:717:GLY:C	1:B:731:SER:HB2	2.35	0.52
1:A:69:ALA:O	1:A:91:PRO:HG3	2.10	0.52
1:A:72:SER:HA	1:A:293:ILE:CD1	2.39	0.52
1:A:953:LEU:C	1:A:955:MET:H	2.18	0.52
1:B:306:ALA:C	1:B:768:ASN:HD21	2.16	0.52
1:B:501:ALA:C	1:B:503:SER:H	2.17	0.52
1:A:751:ARG:C	1:A:816:ILE:HD11	2.34	0.52
1:B:50:TRP:C	1:B:52:LEU:H	2.18	0.52
1:B:627:ASP:O	1:B:678:ARG:HG2	2.10	0.52
1:B:895:GLU:OE2	1:B:960:LYS:HG2	2.10	0.52
1:A:932:TRP:H	1:A:932:TRP:CD1	2.28	0.52
1:B:290:ARG:O	1:B:293:ILE:HG12	2.09	0.52
1:B:600:LEU:HD23	1:B:600:LEU:O	2.09	0.52
1:B:916:LEU:HD11	1:B:927:PRO:HA	1.91	0.52
1:A:689:GLU:CD	1:A:713:LYS:HZ1	2.18	0.52
1:A:825:LYS:CG	1:A:826:GLU:H	2.21	0.52
1:A:844:VAL:HG23	1:A:845:GLY:H	1.74	0.52
1:A:975:LEU:N	1:A:976:PRO:CD	2.73	0.52
1:B:620:ARG:NH2	1:B:670:CYS:O	2.42	0.52
1:B:862:GLY:O	1:B:865:VAL:HG13	2.10	0.52
1:B:100:ALA:O	1:B:104:VAL:HG23	2.10	0.51
1:B:747:VAL:HG12	1:B:748:GLU:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:763:TYR:CE1	1:B:912:ALA:HB2	2.45	0.51
1:A:384:ILE:N	1:A:384:ILE:HD12	2.25	0.51
1:B:174:ARG:HA	1:B:187:VAL:O	2.11	0.51
1:B:335:SER:OG	1:B:337:PRO:HG2	2.09	0.51
1:B:402:ILE:HD12	1:B:402:ILE:O	2.10	0.51
1:B:668:GLU:OE2	1:B:671:ARG:NH1	2.40	0.51
1:B:787:LEU:HD13	1:B:792:LEU:HD23	1.91	0.51
1:A:54:ILE:HD12	1:A:54:ILE:C	2.35	0.51
1:A:559:LEU:CD2	1:A:600:LEU:HD13	2.40	0.51
1:A:762:ARG:HG3	1:A:837:TYR:HE1	1.75	0.51
1:A:763:TYR:CD1	1:A:912:ALA:HA	2.45	0.51
1:A:795:VAL:HG22	1:A:901:LEU:CD1	2.40	0.51
1:A:876:CYS:C	1:A:888:CYS:SG	2.92	0.51
1:B:717:GLY:O	1:B:731:SER:HB2	2.11	0.51
1:B:887:ASP:CB	1:B:890:ILE:HG23	2.36	0.51
1:A:363:VAL:HG11	1:A:448:LEU:HD22	1.93	0.51
1:A:791:GLN:O	1:A:795:VAL:HG23	2.11	0.51
1:B:784:PRO:HA	1:B:873:PHE:CE2	2.46	0.51
1:A:467:ARG:HH11	1:A:467:ARG:CG	2.24	0.51
1:A:836:ARG:NH1	1:A:836:ARG:HG2	2.24	0.51
1:B:72:SER:O	1:B:75:LEU:HG	2.08	0.51
1:A:903:VAL:HG22	1:A:973:ILE:HG21	1.92	0.51
1:B:110:ARG:HH11	1:B:110:ARG:HG3	1.75	0.51
1:B:214:ILE:HD13	1:B:214:ILE:N	2.17	0.51
1:B:367:PHE:O	1:B:368:ILE:HG23	2.10	0.51
1:B:759:GLN:C	1:B:761:ILE:N	2.68	0.51
1:A:69:ALA:HA	1:A:297:LYS:NZ	2.25	0.51
1:A:100:ALA:O	1:A:104:VAL:HG23	2.11	0.51
1:A:319:LEU:CD1	1:A:339:VAL:HG21	2.40	0.51
1:A:44:GLU:OE2	1:A:45:GLU:HG3	2.11	0.51
1:A:122:TYR:O	1:A:124:PRO:CD	2.59	0.51
1:A:270:ALA:O	1:A:274:ILE:HG23	2.11	0.51
1:A:840:ILE:HD11	1:A:981:ASP:HB2	1.93	0.51
1:B:204:LYS:C	1:B:206:ASN:H	2.18	0.51
1:B:249:LEU:O	1:B:252:LYS:N	2.43	0.51
1:B:347:VAL:HG21	1:B:696:GLU:HG2	1.90	0.51
1:A:881:PRO:HG2	1:A:882:HIS:N	2.21	0.51
1:B:323:THR:HA	1:B:326:MET:HE3	1.92	0.51
1:B:974:SER:C	1:B:976:PRO:HD2	2.36	0.51
1:B:49:LEU:HD21	1:B:258:GLU:OE1	2.11	0.51
1:B:883:PHE:H	1:B:883:PHE:HD2	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:TYR:C	1:A:124:PRO:HD3	2.35	0.50
1:A:859:ALA:O	1:A:860:GLU:C	2.53	0.50
1:B:932:TRP:CD1	1:B:932:TRP:H	2.29	0.50
1:B:975:LEU:N	1:B:976:PRO:CD	2.74	0.50
1:B:116:ILE:O	1:B:116:ILE:HG22	2.10	0.50
1:B:154:ALA:O	1:B:214:ILE:HG13	2.11	0.50
1:B:157:ASP:O	1:B:214:ILE:HD13	2.12	0.50
1:B:269:VAL:HG12	1:B:269:VAL:O	2.12	0.50
1:A:111:ASN:H	1:A:111:ASN:ND2	2.05	0.50
1:A:271:VAL:C	1:A:273:LEU:N	2.70	0.50
1:A:459:VAL:O	1:A:460:ARG:C	2.55	0.50
1:A:522:ILE:HD12	1:A:545:ILE:HG21	1.92	0.50
1:A:843:TYR:HE2	1:A:907:ILE:HD11	1.75	0.50
1:A:881:PRO:CG	1:A:882:HIS:H	2.19	0.50
1:B:315:ILE:O	1:B:317:THR:N	2.45	0.50
1:B:953:LEU:C	1:B:955:MET:N	2.69	0.50
1:A:491:ARG:HD3	1:A:585:MET:HA	1.92	0.50
1:A:737:ASP:O	1:A:738:ASP:HB2	2.12	0.50
1:A:833:LEU:O	1:A:836:ARG:HB3	2.11	0.50
1:B:49:LEU:HD23	1:B:254:ASP:HB3	1.93	0.50
1:B:963:ASP:N	1:B:966:GLN:HB2	2.27	0.50
1:A:54:ILE:CG2	1:A:261:SER:HB3	2.41	0.50
1:A:72:SER:O	1:A:75:LEU:HG	2.09	0.50
1:A:258:GLU:O	1:A:262:LYS:HG2	2.12	0.50
1:A:501:ALA:C	1:A:503:SER:H	2.19	0.50
1:A:752:ALA:N	1:A:816:ILE:HD11	2.27	0.50
1:B:69:ALA:O	1:B:91:PRO:HG3	2.12	0.50
1:B:347:VAL:HB	1:B:698:THR:HG23	1.93	0.50
1:B:357:THR:HG23	1:B:601:ASP:OD2	2.12	0.50
1:B:363:VAL:HG11	1:B:448:LEU:HD22	1.94	0.50
1:B:484:THR:CB	1:B:496:VAL:HG12	2.42	0.50
1:B:753:ILE:HG22	1:B:753:ILE:O	2.11	0.50
1:B:921:SER:HA	1:B:982:GLU:OE2	2.12	0.50
1:B:953:LEU:O	1:B:955:MET:N	2.44	0.50
1:A:263:VAL:O	1:A:264:ILE:C	2.55	0.50
1:A:157:ASP:O	1:A:214:ILE:HD13	2.12	0.50
1:A:907:ILE:CG2	1:A:908:GLU:N	2.75	0.50
1:B:104:VAL:HG13	1:B:802:LEU:CD2	2.41	0.50
1:B:353:THR:O	1:B:353:THR:HG22	2.12	0.50
1:B:642:PHE:CD2	1:B:648:VAL:HG11	2.46	0.50
1:B:903:VAL:CG2	1:B:973:ILE:HG21	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ARG:CZ	1:A:206:ASN:HD22	2.25	0.50
1:A:290:ARG:O	1:A:293:ILE:HG12	2.11	0.50
1:A:907:ILE:HG23	1:A:908:GLU:N	2.27	0.50
1:A:974:SER:C	1:A:976:PRO:HD2	2.37	0.50
1:A:988:ALA:CB	1:A:992:LEU:HD12	2.41	0.50
1:B:111:ASN:H	1:B:111:ASN:ND2	2.06	0.50
1:B:368:ILE:HG22	1:B:595:GLY:HA3	1.94	0.50
1:B:387:SER:HB3	1:B:602:PRO:HG3	1.93	0.50
1:B:870:LEU:O	1:B:873:PHE:HB3	2.12	0.50
1:A:303:ALA:O	1:A:304:VAL:C	2.55	0.49
1:A:777:LEU:O	1:A:781:LEU:HG	2.11	0.49
1:A:832:TRP:CZ3	1:A:992:LEU:HD11	2.47	0.49
1:A:123:GLU:OE2	1:A:734:VAL:HG21	2.12	0.49
1:A:239:MET:HG3	1:A:240:ALA:H	1.77	0.49
1:A:347:VAL:HB	1:A:698:THR:HG23	1.94	0.49
1:A:963:ASP:N	1:A:966:GLN:HB2	2.27	0.49
1:B:72:SER:HA	1:B:293:ILE:CD1	2.41	0.49
1:B:491:ARG:HD3	1:B:585:MET:HA	1.93	0.49
1:B:718:ILE:HD13	1:B:743:ILE:HG12	1.94	0.49
1:B:869:GLN:C	1:B:871:THR:N	2.67	0.49
1:B:907:ILE:HG23	1:B:908:GLU:N	2.27	0.49
1:A:369:ILE:HA	1:A:379:LEU:HD23	1.94	0.49
1:A:620:ARG:NH2	1:A:691:LEU:HD21	2.27	0.49
1:B:122:TYR:O	1:B:124:PRO:N	2.45	0.49
1:B:559:LEU:CD2	1:B:600:LEU:HD13	2.41	0.49
1:A:228:VAL:O	1:A:228:VAL:HG22	2.12	0.49
1:A:463:SER:O	1:A:466:GLU:HB2	2.12	0.49
1:A:836:ARG:HH11	1:A:836:ARG:HG2	1.77	0.49
1:A:953:LEU:N	1:A:954:PRO:HD2	2.27	0.49
1:A:953:LEU:O	1:A:955:MET:N	2.44	0.49
1:B:342:LEU:HD12	1:B:716:ILE:CD1	2.41	0.49
1:A:342:LEU:HD12	1:A:716:ILE:CD1	2.40	0.49
1:B:264:ILE:O	1:B:266:LEU:N	2.46	0.49
1:B:303:ALA:O	1:B:304:VAL:C	2.56	0.49
1:B:491:ARG:HE	1:B:588:GLU:CD	2.21	0.49
1:A:269:VAL:HG12	1:A:269:VAL:O	2.13	0.49
1:A:780:ALA:O	1:A:782:GLY:N	2.43	0.49
1:A:884:GLU:C	1:A:886:LEU:H	2.20	0.49
1:B:104:VAL:HG13	1:B:802:LEU:HD21	1.93	0.49
1:B:258:GLU:O	1:B:262:LYS:HG2	2.13	0.49
1:A:333:VAL:HG11	1:A:339:VAL:CG1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:603:PRO:HB3	1:A:639:ILE:HG22	1.95	0.49
1:A:668:GLU:OE2	1:A:671:ARG:NH1	2.42	0.49
1:B:49:LEU:O	1:B:53:VAL:HG23	2.12	0.49
1:B:188:ILE:HG22	1:B:189:LYS:N	2.27	0.49
1:B:495:SER:CB	1:B:514:VAL:HG22	2.43	0.49
1:B:678:ARG:HG3	1:B:678:ARG:NH1	2.20	0.49
1:A:154:ALA:O	1:A:214:ILE:CG1	2.61	0.49
1:A:799:THR:HG21	1:A:908:GLU:HB2	1.93	0.49
1:B:249:LEU:O	1:B:250:GLN:C	2.56	0.49
1:B:333:VAL:HG11	1:B:339:VAL:CG1	2.43	0.49
1:B:577:VAL:HG23	1:B:577:VAL:O	2.13	0.49
1:B:783:LEU:HD13	1:B:784:PRO:HD3	1.95	0.49
1:A:204:LYS:O	1:A:206:ASN:N	2.43	0.49
1:A:770:GLY:HA3	1:A:844:VAL:HG21	1.92	0.49
1:A:953:LEU:C	1:A:955:MET:N	2.70	0.49
1:B:459:VAL:O	1:B:460:ARG:C	2.56	0.49
1:B:463:SER:O	1:B:466:GLU:HB2	2.12	0.49
1:A:287:SER:HB3	1:A:290:ARG:HD3	1.95	0.49
1:A:548:VAL:C	1:A:550:LYS:N	2.71	0.49
1:A:784:PRO:HG3	1:A:856:PHE:CE2	2.47	0.49
1:A:906:THR:HG22	1:A:974:SER:CB	2.42	0.49
1:A:188:ILE:HG22	1:A:189:LYS:N	2.27	0.48
1:A:289:ILE:O	1:A:293:ILE:HG23	2.13	0.48
1:A:369:ILE:N	1:A:369:ILE:CD1	2.76	0.48
1:A:509:GLY:O	1:A:511:LYS:HG2	2.13	0.48
1:A:530:VAL:HB	1:A:533:THR:OG1	2.12	0.48
1:A:949:TYR:N	1:A:949:TYR:CD1	2.81	0.48
1:B:620:ARG:NH2	1:B:691:LEU:HD21	2.28	0.48
1:B:635:ILE:O	1:B:639:ILE:HG12	2.13	0.48
1:A:163:ILE:CD1	1:A:223:VAL:HG22	2.43	0.48
1:A:230:THR:HG22	1:A:232:ILE:HG22	1.94	0.48
1:A:463:SER:OG	1:A:466:GLU:HG3	2.13	0.48
1:B:737:ASP:OD1	1:B:737:ASP:N	2.35	0.48
1:A:764:LEU:O	1:A:765:ILE:C	2.55	0.48
1:B:270:ALA:O	1:B:274:ILE:HG23	2.14	0.48
1:B:287:SER:HB3	1:B:290:ARG:HD3	1.95	0.48
1:B:289:ILE:O	1:B:293:ILE:HG23	2.13	0.48
1:A:323:THR:HA	1:A:326:MET:HE3	1.95	0.48
1:A:326:MET:HE3	1:A:333:VAL:HG21	1.94	0.48
1:B:134:ARG:HG3	1:B:134:ARG:NH1	2.29	0.48
1:B:164:ARG:HA	1:B:207:MET:SD	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:ILE:HD12	1:B:384:ILE:N	2.29	0.48
1:B:794:TRP:CH2	1:B:943:LEU:O	2.66	0.48
1:B:823:SER:HB2	1:B:826:GLU:HB2	1.94	0.48
1:B:869:GLN:HA	1:B:871:THR:HG22	1.94	0.48
1:A:859:ALA:O	1:A:861:ASP:N	2.47	0.48
1:B:33:LEU:O	1:B:37:GLY:N	2.42	0.48
1:B:293:ILE:O	1:B:297:LYS:HG3	2.13	0.48
1:B:756:ASN:CA	1:B:759:GLN:HE21	2.18	0.48
1:B:887:ASP:HB2	1:B:890:ILE:CG2	2.40	0.48
1:A:264:ILE:HD13	1:A:267:ILE:HD12	1.95	0.48
1:A:499:SER:O	1:A:500:PRO:C	2.57	0.48
1:A:642:PHE:CG	1:A:648:VAL:HG11	2.48	0.48
1:A:718:ILE:HG12	1:A:733:MET:HE2	1.94	0.48
1:B:1:MET:HE1	1:B:7:LYS:CD	2.43	0.48
1:B:539:GLY:N	1:B:540:PRO:CD	2.75	0.48
1:B:737:ASP:O	1:B:738:ASP:HB2	2.14	0.48
1:A:459:VAL:O	1:A:462:LEU:N	2.43	0.48
1:A:625:THR:OG1	1:A:626:GLY:N	2.46	0.48
1:B:66:LEU:C	1:B:66:LEU:HD23	2.38	0.48
1:B:548:VAL:C	1:B:550:LYS:N	2.71	0.48
1:A:247:THR:HB	1:A:340:GLU:OE1	2.13	0.48
1:A:368:ILE:HG22	1:A:595:GLY:HA3	1.96	0.48
1:A:921:SER:HA	1:A:982:GLU:OE2	2.13	0.48
1:A:930:ASN:C	1:A:930:ASN:OD1	2.57	0.48
1:B:271:VAL:C	1:B:273:LEU:N	2.72	0.48
1:B:280:ASN:OD1	1:B:281:ASP:N	2.47	0.48
1:A:134:ARG:HG3	1:A:134:ARG:NH1	2.29	0.48
1:A:854:TRP:O	1:A:859:ALA:HB2	2.13	0.48
1:A:867:TYR:C	1:A:869:GLN:N	2.72	0.48
1:B:22:THR:HG22	1:B:135:LYS:HZ3	1.79	0.48
1:B:134:ARG:HG2	1:B:136:SER:H	1.79	0.48
1:B:163:ILE:CD1	1:B:223:VAL:HG22	2.44	0.48
1:B:288:TRP:HD1	1:B:289:ILE:HG13	1.78	0.48
1:B:540:PRO:O	1:B:543:GLU:HB2	2.14	0.48
1:B:631:THR:O	1:B:635:ILE:HG13	2.13	0.48
1:A:1:MET:HB2	1:A:16:PHE:CZ	2.48	0.48
1:A:124:PRO:O	1:A:126:MET:HG2	2.14	0.48
1:A:280:ASN:OD1	1:A:281:ASP:N	2.47	0.48
1:A:315:ILE:O	1:A:317:THR:N	2.47	0.48
1:A:369:ILE:CD1	1:A:593:PHE:HE1	2.26	0.48
1:A:768:ASN:O	1:A:769:VAL:C	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:865:VAL:HG12	1:A:866:THR:N	2.28	0.48
1:B:762:ARG:O	1:B:762:ARG:HG2	2.14	0.48
1:B:899:MET:HG2	1:B:962:LEU:CD2	2.42	0.48
1:A:539:GLY:N	1:A:540:PRO:CD	2.77	0.47
1:B:214:ILE:HG12	1:B:214:ILE:O	2.13	0.47
1:B:264:ILE:HD13	1:B:267:ILE:HD12	1.95	0.47
1:B:317:THR:O	1:B:318:CYS:C	2.57	0.47
1:B:325:ARG:NH1	1:B:749:GLU:OE1	2.47	0.47
1:B:811:PRO:HG2	1:B:929:VAL:CG1	2.43	0.47
1:B:949:TYR:N	1:B:949:TYR:CD1	2.82	0.47
1:A:84:THR:O	1:A:85:ILE:HB	2.14	0.47
1:A:322:GLY:HA3	1:A:753:ILE:HD11	1.96	0.47
1:B:236:ARG:O	1:B:239:MET:HE2	2.13	0.47
1:B:530:VAL:HB	1:B:533:THR:OG1	2.13	0.47
1:B:942:SER:C	1:B:944:HIS:N	2.72	0.47
1:B:953:LEU:O	1:B:956:ILE:N	2.48	0.47
1:A:181:THR:C	1:A:183:GLU:H	2.22	0.47
1:A:311:LEU:HB3	1:A:312:PRO:CD	2.38	0.47
1:A:797:LEU:O	1:A:797:LEU:HD23	2.13	0.47
1:B:794:TRP:HH2	1:B:943:LEU:O	1.97	0.47
1:B:979:GLY:O	1:B:983:ILE:HG13	2.14	0.47
1:A:15:TYR:O	1:A:15:TYR:CD1	2.67	0.47
1:A:371:LYS:O	1:A:377:CYS:HB2	2.14	0.47
1:A:538:THR:HB	1:A:540:PRO:HD2	1.97	0.47
1:B:118:ALA:C	1:B:120:LYS:N	2.72	0.47
1:B:509:GLY:O	1:B:511:LYS:HG2	2.13	0.47
1:B:794:TRP:HE1	1:B:944:HIS:CE1	2.31	0.47
1:B:826:GLU:HA	1:B:827:PRO:HD2	1.66	0.47
1:A:346:SER:C	1:A:347:VAL:HG23	2.40	0.47
1:A:895:GLU:N	1:A:896:PRO:HD2	2.29	0.47
1:B:271:VAL:HG22	1:B:776:PHE:HE1	1.78	0.47
1:B:369:ILE:CD1	1:B:593:PHE:HE1	2.27	0.47
1:B:887:ASP:O	1:B:890:ILE:HG12	2.14	0.47
1:A:293:ILE:O	1:A:297:LYS:HG3	2.14	0.47
1:A:886:LEU:HD12	1:A:886:LEU:O	2.14	0.47
1:B:245:ASP:OD1	1:B:246:LYS:N	2.47	0.47
1:B:549:ILE:O	1:B:549:ILE:HG22	2.15	0.47
1:B:748:GLU:HG3	1:B:817:MET:HG2	1.96	0.47
1:B:756:ASN:HD21	1:B:810:ASN:HB2	1.80	0.47
1:A:249:LEU:HB2	1:A:340:GLU:CD	2.40	0.47
1:A:263:VAL:CG1	1:A:267:ILE:HD11	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:CYS:C	1:A:270:ALA:H	2.22	0.47
1:A:317:THR:O	1:A:318:CYS:C	2.58	0.47
1:A:449:VAL:O	1:A:453:ASN:N	2.37	0.47
1:A:823:SER:C	1:A:825:LYS:N	2.70	0.47
1:B:413:LEU:HG	1:B:564:LEU:HD12	1.96	0.47
1:B:467:ARG:HH11	1:B:467:ARG:CG	2.25	0.47
1:B:786:ALA:O	1:B:787:LEU:HG	2.15	0.47
1:A:288:TRP:HD1	1:A:289:ILE:HG13	1.79	0.47
1:A:467:ARG:HD2	1:A:467:ARG:O	2.15	0.47
1:A:953:LEU:O	1:A:956:ILE:N	2.48	0.47
1:B:181:THR:C	1:B:183:GLU:H	2.23	0.47
1:B:271:VAL:HG22	1:B:776:PHE:CE1	2.50	0.47
1:B:346:SER:C	1:B:347:VAL:HG23	2.40	0.47
1:B:369:ILE:N	1:B:369:ILE:CD1	2.77	0.47
1:B:402:ILE:HD12	1:B:402:ILE:C	2.40	0.47
1:A:413:LEU:HD23	1:A:413:LEU:O	2.15	0.47
1:A:470:ALA:O	1:A:473:SER:N	2.48	0.47
1:A:484:THR:CB	1:A:496:VAL:HG12	2.45	0.47
1:B:303:ALA:O	1:B:306:ALA:N	2.45	0.47
1:B:474:VAL:HA	1:B:477:GLN:NE2	2.30	0.47
1:A:335:SER:O	1:A:336:LEU:C	2.58	0.47
1:A:496:VAL:O	1:A:512:MET:HA	2.15	0.47
1:A:763:TYR:CD2	1:A:764:LEU:HD23	2.50	0.47
1:B:109:GLU:O	1:B:113:GLU:HG2	2.15	0.47
1:B:129:VAL:CG1	1:B:151:VAL:HG22	2.35	0.47
1:B:161:ALA:CA	1:B:210:SER:HB2	2.41	0.47
1:B:253:LEU:HD21	1:B:315:ILE:HD11	1.97	0.47
1:B:574:GLU:C	1:B:576:MET:H	2.22	0.47
1:B:895:GLU:N	1:B:896:PRO:CD	2.78	0.47
1:B:953:LEU:N	1:B:954:PRO:HD2	2.29	0.47
1:B:963:ASP:H	1:B:966:GLN:HB2	1.79	0.47
1:A:247:THR:CB	1:A:340:GLU:OE1	2.62	0.46
1:A:933:LEU:O	1:A:937:ILE:HG13	2.14	0.46
1:A:963:ASP:H	1:A:966:GLN:HB2	1.79	0.46
1:B:434:TYR:OH	1:B:464:LYS:HG3	2.15	0.46
1:B:755:ASN:O	1:B:756:ASN:C	2.56	0.46
1:A:354:GLY:O	1:A:604:ARG:HD2	2.15	0.46
1:A:836:ARG:HD3	1:A:984:LEU:HD13	1.96	0.46
1:B:1:MET:HB2	1:B:16:PHE:CZ	2.49	0.46
1:B:247:THR:H	1:B:251:GLN:CG	2.28	0.46
1:B:400:LYS:HA	1:B:401:PRO:HD3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:658:PHE:CA	1:B:661:LEU:HD12	2.35	0.46
1:B:913:LEU:O	1:B:922:LEU:HD21	2.15	0.46
1:A:66:LEU:C	1:A:66:LEU:HD23	2.40	0.46
1:A:949:TYR:N	1:A:949:TYR:HD1	2.13	0.46
1:B:496:VAL:O	1:B:512:MET:HA	2.15	0.46
1:B:538:THR:HB	1:B:540:PRO:HD2	1.98	0.46
1:B:836:ARG:HG2	1:B:836:ARG:HH11	1.80	0.46
1:B:840:ILE:O	1:B:843:TYR:N	2.49	0.46
1:A:264:ILE:C	1:A:266:LEU:N	2.73	0.46
1:A:335:SER:C	1:A:337:PRO:HD2	2.40	0.46
1:A:341:THR:O	1:A:344:CYS:N	2.34	0.46
1:A:474:VAL:HA	1:A:477:GLN:NE2	2.31	0.46
1:A:577:VAL:HG23	1:A:577:VAL:O	2.15	0.46
1:B:352:LYS:HD2	1:B:635:ILE:HG21	1.97	0.46
1:B:614:CYS:HB3	1:B:619:ILE:HB	1.97	0.46
1:A:867:TYR:CG	1:A:868:HIS:N	2.83	0.46
1:B:140:ILE:HG13	1:B:141:LYS:N	2.31	0.46
1:B:499:SER:O	1:B:500:PRO:C	2.57	0.46
1:B:837:TYR:HD1	1:B:837:TYR:H	1.64	0.46
1:B:988:ALA:CB	1:B:992:LEU:HD12	2.44	0.46
1:A:140:ILE:HG13	1:A:141:LYS:N	2.31	0.46
1:A:238:GLN:HG3	1:A:238:GLN:O	2.16	0.46
1:A:285:GLY:HA3	1:A:290:ARG:CZ	2.46	0.46
1:A:637:ARG:HA	1:A:642:PHE:O	2.15	0.46
1:A:751:ARG:NH2	1:A:819:ARG:O	2.44	0.46
1:A:895:GLU:N	1:A:895:GLU:OE1	2.25	0.46
1:B:774:CYS:SG	1:B:848:THR:HG21	2.56	0.46
1:B:906:THR:HG21	1:B:970:VAL:HG12	1.98	0.46
1:A:134:ARG:HG2	1:A:136:SER:H	1.80	0.46
1:A:154:ALA:O	1:A:214:ILE:HG13	2.15	0.46
1:B:306:ALA:HA	1:B:768:ASN:ND2	2.31	0.46
1:B:907:ILE:CG2	1:B:908:GLU:N	2.78	0.46
1:B:14:ALA:O	1:B:16:PHE:N	2.49	0.46
1:B:230:THR:HG22	1:B:232:ILE:HG22	1.96	0.46
1:B:795:VAL:CG1	1:B:904:LEU:HG	2.42	0.46
1:B:911:ASN:O	1:B:914:ASN:HB2	2.16	0.46
1:B:84:THR:O	1:B:85:ILE:HB	2.16	0.46
1:B:341:THR:O	1:B:344:CYS:N	2.35	0.46
1:B:413:LEU:HD23	1:B:413:LEU:O	2.16	0.46
1:B:442:GLU:O	1:B:445:LEU:N	2.48	0.46
1:B:637:ARG:HA	1:B:642:PHE:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:759:GLN:C	1:B:761:ILE:H	2.24	0.46
1:A:22:THR:HG22	1:A:135:LYS:HZ1	1.80	0.46
1:A:25:THR:HG22	1:A:132:ALA:CB	2.43	0.46
1:B:157:ASP:HB2	1:B:214:ILE:HD11	1.98	0.46
1:B:268:CYS:C	1:B:270:ALA:H	2.23	0.46
1:B:527:TYR:CD1	1:B:534:ARG:HD3	2.51	0.46
1:B:772:VAL:O	1:B:773:VAL:C	2.58	0.46
1:B:788:ILE:CB	1:B:789:PRO:CD	2.93	0.46
1:B:843:TYR:CD2	1:B:844:VAL:N	2.83	0.46
1:B:869:GLN:OE1	1:B:872:HIS:HD2	1.99	0.46
1:A:353:THR:O	1:A:353:THR:CG2	2.61	0.45
1:A:540:PRO:O	1:A:543:GLU:HB2	2.16	0.45
1:A:823:SER:O	1:A:826:GLU:HG2	2.15	0.45
1:A:844:VAL:HG23	1:A:845:GLY:N	2.30	0.45
1:B:335:SER:C	1:B:337:PRO:HD2	2.40	0.45
1:B:625:THR:OG1	1:B:626:GLY:N	2.49	0.45
1:B:855:TRP:CE3	1:B:856:PHE:HA	2.51	0.45
1:A:230:THR:HG22	1:A:232:ILE:N	2.29	0.45
1:A:352:LYS:HE2	1:A:627:ASP:OD1	2.16	0.45
1:A:510:ASN:O	1:A:511:LYS:HD3	2.17	0.45
1:A:654:THR:O	1:A:655:GLY:C	2.58	0.45
1:A:656:ARG:HH11	1:A:656:ARG:HG2	1.81	0.45
1:A:717:GLY:C	1:A:731:SER:HB2	2.42	0.45
1:A:829:ILE:HD13	1:A:837:TYR:CE2	2.51	0.45
1:B:15:TYR:O	1:B:15:TYR:CD1	2.69	0.45
1:B:158:LYS:O	1:B:160:PRO:HD3	2.17	0.45
1:B:357:THR:C	1:B:604:ARG:HG3	2.41	0.45
1:A:82:GLU:HB2	1:A:83:GLU:H	1.43	0.45
1:A:562:LEU:O	1:A:596:VAL:HG13	2.16	0.45
1:A:768:ASN:C	1:A:770:GLY:N	2.72	0.45
1:A:780:ALA:C	1:A:782:GLY:N	2.70	0.45
1:B:359:ASN:HA	1:B:601:ASP:CG	2.41	0.45
1:B:788:ILE:HG12	1:B:791:GLN:CG	2.46	0.45
1:B:791:GLN:HE22	1:B:897:MET:HE2	1.80	0.45
1:B:798:VAL:CG1	1:B:940:SER:HB3	2.39	0.45
1:A:75:LEU:HD12	1:A:76:ALA:CB	2.46	0.45
1:A:108:GLN:HB3	1:A:805:THR:OG1	2.15	0.45
1:A:449:VAL:CG2	1:A:450:GLU:N	2.79	0.45
1:A:608:MET:HE3	1:A:608:MET:HB3	1.82	0.45
1:A:718:ILE:HD13	1:A:743:ILE:HG12	1.99	0.45
1:A:764:LEU:C	1:A:768:ASN:HD22	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:877:THR:O	1:A:878:GLU:HB3	2.16	0.45
1:B:44:GLU:CD	1:B:44:GLU:O	2.59	0.45
1:B:154:ALA:O	1:B:214:ILE:CD1	2.64	0.45
1:B:230:THR:HG22	1:B:232:ILE:N	2.30	0.45
1:B:274:ILE:HD13	1:B:776:PHE:CZ	2.51	0.45
1:B:637:ARG:HD3	1:B:644:GLU:O	2.17	0.45
1:B:769:VAL:CG1	1:B:841:GLY:HA3	2.43	0.45
1:B:770:GLY:HA3	1:B:841:GLY:O	2.15	0.45
1:B:895:GLU:N	1:B:895:GLU:CD	2.74	0.45
1:A:1:MET:HE1	1:A:7:LYS:CD	2.47	0.45
1:A:413:LEU:HG	1:A:564:LEU:CD1	2.47	0.45
1:A:662:PRO:O	1:A:665:GLU:N	2.42	0.45
1:A:783:LEU:HD22	1:A:784:PRO:CD	2.39	0.45
1:B:903:VAL:HG13	1:B:973:ILE:CG2	2.46	0.45
1:B:949:TYR:N	1:B:949:TYR:HD1	2.13	0.45
1:A:301:ALA:O	1:A:302:LEU:C	2.59	0.45
1:A:895:GLU:O	1:A:899:MET:N	2.49	0.45
1:B:110:ARG:O	1:B:114:ASN:N	2.49	0.45
1:B:855:TRP:O	1:B:859:ALA:HB2	2.16	0.45
1:A:766:SER:O	1:A:769:VAL:HG12	2.17	0.45
1:A:942:SER:C	1:A:944:HIS:N	2.74	0.45
1:A:969:MET:O	1:A:970:VAL:C	2.60	0.45
1:B:85:ILE:HG22	1:B:85:ILE:O	2.17	0.45
1:B:352:LYS:HE2	1:B:627:ASP:OD1	2.16	0.45
1:B:467:ARG:HA	1:B:467:ARG:HD2	1.64	0.45
1:B:794:TRP:NE1	1:B:944:HIS:ND1	2.63	0.45
1:A:157:ASP:HB2	1:A:214:ILE:HD11	1.99	0.45
1:A:600:LEU:HD23	1:A:600:LEU:C	2.40	0.45
1:B:50:TRP:CE3	1:B:257:GLY:CA	3.00	0.45
1:B:75:LEU:HD12	1:B:76:ALA:CB	2.47	0.45
1:B:449:VAL:O	1:B:453:ASN:N	2.36	0.45
1:B:633:ILE:O	1:B:636:CYS:HB2	2.17	0.45
1:B:654:THR:O	1:B:655:GLY:C	2.59	0.45
1:B:930:ASN:OD1	1:B:930:ASN:C	2.60	0.45
1:A:66:LEU:HD12	1:A:94:ILE:CD1	2.47	0.45
1:A:100:ALA:CA	1:A:103:ILE:HG22	2.43	0.45
1:A:527:TYR:O	1:A:592:THR:HA	2.17	0.45
1:A:933:LEU:O	1:A:934:LEU:C	2.59	0.45
1:B:66:LEU:HD12	1:B:94:ILE:CD1	2.47	0.45
1:B:264:ILE:C	1:B:266:LEU:N	2.75	0.45
1:A:109:GLU:O	1:A:113:GLU:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ARG:O	1:A:114:ASN:N	2.49	0.45
1:A:140:ILE:CD1	1:A:141:LYS:H	2.30	0.45
1:B:14:ALA:C	1:B:16:PHE:N	2.75	0.45
1:B:131:ARG:HG3	1:B:131:ARG:NH1	2.30	0.45
1:B:231:GLU:OE1	1:B:231:GLU:HA	2.16	0.45
1:B:548:VAL:C	1:B:550:LYS:H	2.24	0.45
1:B:799:THR:HG21	1:B:908:GLU:HB2	1.99	0.45
1:B:980:LEU:HA	1:B:983:ILE:CD1	2.37	0.45
1:A:899:MET:SD	1:A:962:LEU:HD22	2.57	0.44
1:B:204:LYS:O	1:B:206:ASN:N	2.47	0.44
1:B:662:PRO:O	1:B:665:GLU:N	2.42	0.44
1:B:969:MET:O	1:B:970:VAL:C	2.60	0.44
1:A:85:ILE:HG22	1:A:85:ILE:O	2.17	0.44
1:A:717:GLY:O	1:A:731:SER:HB2	2.18	0.44
1:A:927:PRO:O	1:A:934:LEU:HD21	2.17	0.44
1:B:247:THR:H	1:B:251:GLN:HG2	1.81	0.44
1:B:335:SER:O	1:B:336:LEU:C	2.59	0.44
1:B:773:VAL:HG21	1:B:842:GLY:HA2	1.99	0.44
1:A:35:LYS:HE3	1:A:36:TYR:CZ	2.53	0.44
1:A:637:ARG:HD3	1:A:644:GLU:O	2.17	0.44
1:A:745:ALA:O	1:A:746:ALA:C	2.58	0.44
1:B:518:PRO:O	1:B:519:GLU:C	2.60	0.44
1:B:611:ILE:HD13	1:B:641:ILE:HG13	2.00	0.44
1:B:895:GLU:CD	1:B:895:GLU:H	2.24	0.44
1:B:977:VAL:HG13	1:B:978:ILE:N	2.32	0.44
1:A:39:ASN:HB3	1:A:142:ALA:O	2.17	0.44
1:A:402:ILE:HD12	1:A:402:ILE:O	2.16	0.44
1:B:767:SER:CB	1:B:911:ASN:ND2	2.64	0.44
1:B:832:TRP:CH2	1:B:992:LEU:HD11	2.53	0.44
1:A:390:ALA:HA	1:A:391:PRO:HD3	1.89	0.44
1:A:548:VAL:C	1:A:550:LYS:H	2.25	0.44
1:A:631:THR:O	1:A:635:ILE:HG13	2.17	0.44
1:A:778:THR:HG22	1:A:849:VAL:CG1	2.47	0.44
1:A:830:SER:O	1:A:831:GLY:C	2.60	0.44
1:A:899:MET:O	1:A:903:VAL:HG23	2.17	0.44
1:A:977:VAL:HG13	1:A:978:ILE:N	2.33	0.44
1:B:315:ILE:CG1	1:B:757:MET:HG3	2.48	0.44
1:B:608:MET:HE3	1:B:608:MET:HB3	1.86	0.44
1:B:650:ASP:OD1	1:B:650:ASP:N	2.50	0.44
1:B:771:GLU:O	1:B:774:CYS:HB3	2.17	0.44
1:B:893:ALA:O	1:B:896:PRO:CG	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:LYS:O	1:A:160:PRO:HD3	2.18	0.44
1:A:527:TYR:CD1	1:A:534:ARG:HD3	2.52	0.44
1:A:810:ASN:OD1	1:A:916:LEU:HD23	2.18	0.44
1:B:301:ALA:O	1:B:302:LEU:C	2.59	0.44
1:B:765:ILE:HG21	1:B:837:TYR:CD2	2.53	0.44
1:A:214:ILE:O	1:A:214:ILE:HG12	2.16	0.44
1:A:262:LYS:O	1:A:263:VAL:C	2.58	0.44
1:A:445:LEU:O	1:A:448:LEU:HB3	2.18	0.44
1:A:737:ASP:O	1:A:738:ASP:CB	2.65	0.44
1:B:39:ASN:HB3	1:B:142:ALA:O	2.17	0.44
1:B:97:ILE:HG21	1:B:793:LEU:HB3	1.99	0.44
1:B:519:GLU:O	1:B:520:GLY:C	2.59	0.44
1:B:541:VAL:C	1:B:543:GLU:N	2.75	0.44
1:A:247:THR:OG1	1:A:340:GLU:OE1	2.35	0.44
1:A:449:VAL:HG23	1:A:450:GLU:N	2.33	0.44
1:A:518:PRO:O	1:A:519:GLU:C	2.61	0.44
1:A:836:ARG:CG	1:A:836:ARG:NH1	2.78	0.44
1:B:44:GLU:O	1:B:45:GLU:C	2.61	0.44
1:B:128:LYS:HD2	1:B:137:VAL:HG11	2.00	0.44
1:B:392:GLU:O	1:B:451:LYS:HE2	2.18	0.44
1:B:617:ALA:HB1	1:B:751:ARG:NH1	2.26	0.44
1:B:755:ASN:HA	1:B:758:LYS:HB2	2.00	0.44
1:B:763:TYR:CD1	1:B:912:ALA:HA	2.52	0.44
1:B:765:ILE:HG22	1:B:766:SER:N	2.33	0.44
1:B:778:THR:HG22	1:B:849:VAL:HG13	1.99	0.44
1:B:849:VAL:C	1:B:851:ALA:H	2.24	0.44
1:A:299:ALA:C	1:A:301:ALA:N	2.75	0.44
1:A:549:ILE:O	1:A:549:ILE:HG22	2.17	0.44
1:A:869:GLN:NE2	1:A:872:HIS:CD2	2.86	0.44
1:A:892:GLU:O	1:A:893:ALA:C	2.61	0.44
1:A:962:LEU:HD23	1:A:966:GLN:HB3	2.00	0.44
1:B:48:SER:HB2	1:B:254:ASP:OD1	2.17	0.44
1:B:264:ILE:HA	1:B:267:ILE:CD1	2.47	0.44
1:B:881:PRO:O	1:B:882:HIS:HB2	2.18	0.44
1:A:110:ARG:HG3	1:A:110:ARG:NH1	2.33	0.43
1:A:512:MET:HB2	1:A:567:ARG:HB3	1.99	0.43
1:A:906:THR:CG2	1:A:974:SER:HB2	2.48	0.43
1:B:25:THR:HG22	1:B:132:ALA:CB	2.44	0.43
1:B:285:GLY:HA3	1:B:290:ARG:CZ	2.48	0.43
1:B:446:THR:HG23	1:B:472:ASN:ND2	2.33	0.43
1:B:539:GLY:H	1:B:540:PRO:HD2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:794:TRP:O	1:B:795:VAL:C	2.61	0.43
1:B:847:ALA:O	1:B:851:ALA:HB2	2.18	0.43
1:B:933:LEU:O	1:B:934:LEU:C	2.60	0.43
1:A:97:ILE:O	1:A:100:ALA:N	2.51	0.43
1:A:164:ARG:HH22	1:A:192:GLU:C	2.25	0.43
1:A:166:LEU:HG	1:A:221:GLY:HA2	1.99	0.43
1:B:706:ASN:HD22	1:B:706:ASN:HA	1.55	0.43
1:B:836:ARG:NH1	1:B:836:ARG:HG2	2.33	0.43
1:B:893:ALA:O	1:B:896:PRO:CD	2.63	0.43
1:A:388:THR:OG1	1:A:389:TYR:N	2.51	0.43
1:A:617:ALA:HB2	1:A:817:MET:O	2.18	0.43
1:A:802:LEU:C	1:A:804:ALA:N	2.74	0.43
1:A:832:TRP:CH2	1:A:992:LEU:HD11	2.53	0.43
1:A:841:GLY:HA2	1:A:844:VAL:CG2	2.49	0.43
1:B:170:SER:O	1:B:171:THR:C	2.61	0.43
1:B:542:LYS:O	1:B:546:LEU:HD12	2.19	0.43
1:B:840:ILE:O	1:B:841:GLY:C	2.61	0.43
1:A:131:ARG:HG3	1:A:131:ARG:NH1	2.32	0.43
1:A:574:GLU:C	1:A:576:MET:H	2.25	0.43
1:B:69:ALA:HA	1:B:297:LYS:NZ	2.27	0.43
1:A:239:MET:HG3	1:A:240:ALA:N	2.33	0.43
1:A:542:LYS:O	1:A:546:LEU:HD12	2.18	0.43
1:A:679:VAL:HG13	1:A:683:HIS:ND1	2.33	0.43
1:A:689:GLU:HB2	1:A:713:LYS:NZ	2.34	0.43
1:B:196:ASP:HA	1:B:197:PRO:HD2	1.92	0.43
1:B:355:THR:HG22	1:B:740:PHE:HB2	2.01	0.43
1:B:565:ALA:HB2	1:B:593:PHE:HA	2.00	0.43
1:A:311:LEU:CA	1:A:760:PHE:HE1	2.31	0.43
1:A:893:ALA:HA	1:A:894:PRO:HD3	1.80	0.43
1:A:894:PRO:HD2	1:A:895:GLU:OE1	2.19	0.43
1:B:164:ARG:CZ	1:B:206:ASN:HD22	2.32	0.43
1:B:378:SER:O	1:B:379:LEU:HD23	2.19	0.43
1:B:449:VAL:CG2	1:B:450:GLU:N	2.81	0.43
1:A:253:LEU:HD21	1:A:315:ILE:HD11	2.01	0.43
1:A:342:LEU:HD21	1:A:746:ALA:C	2.42	0.43
1:A:402:ILE:HD12	1:A:402:ILE:C	2.43	0.43
1:A:704:GLY:O	1:A:705:VAL:C	2.61	0.43
1:A:899:MET:HG2	1:A:962:LEU:CD2	2.46	0.43
1:B:32:HIS:O	1:B:36:TYR:HD2	2.01	0.43
1:B:314:VAL:O	1:B:315:ILE:C	2.61	0.43
1:B:358:THR:HG23	1:B:602:PRO:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:CYS:C	1:A:270:ALA:N	2.75	0.43
1:A:338:SER:C	1:A:340:GLU:N	2.71	0.43
1:A:932:TRP:H	1:A:932:TRP:HD1	1.67	0.43
1:A:946:LEU:C	1:A:946:LEU:CD2	2.90	0.43
1:B:832:TRP:CZ3	1:B:992:LEU:HD11	2.54	0.43
1:A:314:VAL:O	1:A:315:ILE:C	2.62	0.43
1:A:830:SER:O	1:A:833:LEU:N	2.51	0.43
1:B:100:ALA:CA	1:B:103:ILE:HG22	2.45	0.43
1:B:573:ARG:HD3	1:B:573:ARG:O	2.19	0.43
1:B:945:PHE:HE1	1:B:967:TRP:CZ2	2.36	0.43
1:A:264:ILE:HA	1:A:267:ILE:CD1	2.47	0.43
1:A:467:ARG:CG	1:A:467:ARG:NH1	2.82	0.43
1:B:248:PRO:O	1:B:252:LYS:HB2	2.19	0.43
1:B:299:ALA:C	1:B:301:ALA:N	2.76	0.43
1:A:378:SER:O	1:A:379:LEU:HD23	2.19	0.42
1:A:911:ASN:O	1:A:914:ASN:HB2	2.19	0.42
1:A:913:LEU:O	1:A:922:LEU:HD21	2.19	0.42
1:B:58:GLU:OE1	1:B:309:GLU:OE2	2.37	0.42
1:B:83:GLU:O	1:B:83:GLU:HG2	2.19	0.42
1:B:97:ILE:O	1:B:100:ALA:N	2.52	0.42
1:B:125:GLU:OE1	1:B:125:GLU:HA	2.18	0.42
1:B:600:LEU:HD23	1:B:600:LEU:C	2.43	0.42
1:B:798:VAL:O	1:B:798:VAL:HG12	2.19	0.42
1:A:654:THR:HG23	1:A:657:GLU:OE1	2.18	0.42
1:B:166:LEU:HG	1:B:221:GLY:HA2	2.01	0.42
1:B:228:VAL:O	1:B:228:VAL:CG2	2.67	0.42
1:B:342:LEU:HD21	1:B:746:ALA:C	2.43	0.42
1:B:832:TRP:CD1	1:B:833:LEU:N	2.87	0.42
1:B:946:LEU:C	1:B:946:LEU:CD2	2.90	0.42
1:A:14:ALA:O	1:A:16:PHE:N	2.52	0.42
1:A:154:ALA:O	1:A:214:ILE:CD1	2.67	0.42
1:A:879:ASP:C	1:A:881:PRO:CD	2.91	0.42
1:A:975:LEU:HD12	1:A:975:LEU:HA	1.90	0.42
1:B:271:VAL:CG2	1:B:776:PHE:HE1	2.32	0.42
1:B:315:ILE:C	1:B:317:THR:N	2.77	0.42
1:B:679:VAL:HG13	1:B:683:HIS:ND1	2.34	0.42
1:B:691:LEU:HA	1:B:691:LEU:HD23	1.82	0.42
1:B:762:ARG:NE	1:B:836:ARG:NH1	2.67	0.42
1:A:170:SER:O	1:A:171:THR:C	2.62	0.42
1:A:260:LEU:O	1:A:261:SER:C	2.62	0.42
1:A:434:TYR:OH	1:A:464:LYS:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:829:ILE:HD13	1:A:837:TYR:HE2	1.84	0.42
1:A:887:ASP:O	1:A:890:ILE:HG22	2.20	0.42
1:A:974:SER:O	1:A:977:VAL:HG12	2.18	0.42
1:B:59:ASP:O	1:B:63:ARG:HG3	2.19	0.42
1:A:14:ALA:C	1:A:16:PHE:N	2.76	0.42
1:A:94:ILE:HD12	1:A:94:ILE:C	2.44	0.42
1:A:541:VAL:C	1:A:543:GLU:N	2.75	0.42
1:A:650:ASP:OD1	1:A:650:ASP:N	2.51	0.42
1:A:679:VAL:HG13	1:A:683:HIS:CG	2.54	0.42
1:A:865:VAL:O	1:A:866:THR:HG23	2.20	0.42
1:A:945:PHE:HE1	1:A:967:TRP:CZ2	2.37	0.42
1:B:116:ILE:O	1:B:116:ILE:CG2	2.67	0.42
1:B:123:GLU:HA	1:B:124:PRO:HD2	1.76	0.42
1:B:329:LYS:O	1:B:330:ASN:HB2	2.19	0.42
1:B:656:ARG:HG2	1:B:656:ARG:NH1	2.34	0.42
1:A:83:GLU:HG2	1:A:83:GLU:O	2.19	0.42
1:A:303:ALA:O	1:A:306:ALA:N	2.50	0.42
1:A:353:THR:O	1:A:353:THR:HG22	2.20	0.42
1:A:711:LEU:HD23	1:A:711:LEU:HA	1.84	0.42
1:A:753:ILE:O	1:A:753:ILE:HG22	2.20	0.42
1:B:262:LYS:O	1:B:263:VAL:C	2.59	0.42
1:B:449:VAL:HG23	1:B:450:GLU:N	2.35	0.42
1:B:760:PHE:CD1	1:B:760:PHE:C	2.98	0.42
1:A:75:LEU:HD12	1:A:75:LEU:C	2.44	0.42
1:A:491:ARG:O	1:A:492:LYS:C	2.61	0.42
1:A:519:GLU:O	1:A:520:GLY:C	2.63	0.42
1:A:762:ARG:CG	1:A:837:TYR:CE1	3.01	0.42
1:A:851:ALA:HB2	1:A:903:VAL:HG21	2.01	0.42
1:B:35:LYS:HE3	1:B:36:TYR:CZ	2.55	0.42
1:B:306:ALA:CA	1:B:768:ASN:HD21	2.33	0.42
1:B:892:GLU:O	1:B:893:ALA:C	2.62	0.42
1:B:899:MET:SD	1:B:962:LEU:HD22	2.60	0.42
1:B:974:SER:O	1:B:977:VAL:HG12	2.19	0.42
1:A:288:TRP:CD1	1:A:289:ILE:H	2.37	0.42
1:A:495:SER:CB	1:A:514:VAL:HG22	2.50	0.42
1:A:765:ILE:HG21	1:A:837:TYR:HD2	1.85	0.42
1:A:798:VAL:CG1	1:A:940:SER:HB3	2.48	0.42
1:B:336:LEU:N	1:B:337:PRO:CD	2.81	0.42
1:B:512:MET:HB2	1:B:567:ARG:HB3	2.02	0.42
1:B:580:ASP:O	1:B:580:ASP:CG	2.63	0.42
1:B:668:GLU:O	1:B:669:ALA:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:964:LEU:O	1:B:968:LEU:HB2	2.19	0.42
1:A:54:ILE:HG22	1:A:261:SER:HB3	2.01	0.42
1:A:315:ILE:C	1:A:317:THR:N	2.77	0.42
1:A:946:LEU:HD23	1:A:946:LEU:O	2.19	0.42
1:B:110:ARG:HG3	1:B:110:ARG:NH1	2.35	0.42
1:B:231:GLU:O	1:B:235:ILE:HG12	2.20	0.42
1:B:510:ASN:O	1:B:511:LYS:HD3	2.19	0.42
1:B:757:MET:HE2	1:B:757:MET:HB3	1.94	0.42
1:B:833:LEU:O	1:B:836:ARG:HB3	2.20	0.42
1:A:2:GLU:CG	1:A:3:ALA:N	2.83	0.42
1:A:174:ARG:HA	1:A:187:VAL:O	2.20	0.42
1:A:347:VAL:HG21	1:A:696:GLU:HG2	1.98	0.42
1:A:395:VAL:C	1:A:396:LEU:HD12	2.44	0.42
1:A:449:VAL:HG21	1:A:472:ASN:CG	2.44	0.42
1:A:667:ARG:HA	1:A:690:TYR:CD1	2.55	0.42
1:A:884:GLU:C	1:A:886:LEU:N	2.78	0.42
1:A:886:LEU:HD12	1:A:886:LEU:C	2.44	0.42
1:B:268:CYS:C	1:B:270:ALA:N	2.76	0.42
1:B:276:ILE:HG12	1:B:279:PHE:HE2	1.85	0.42
1:B:388:THR:OG1	1:B:389:TYR:N	2.53	0.42
1:B:495:SER:HB3	1:B:514:VAL:HG22	2.01	0.42
1:B:932:TRP:H	1:B:932:TRP:HD1	1.68	0.42
1:A:24:LEU:HD13	1:A:149:ASP:CA	2.37	0.41
1:A:27:ASP:O	1:A:31:ARG:HB2	2.20	0.41
1:A:126:MET:HA	1:A:140:ILE:O	2.19	0.41
1:A:267:ILE:HG21	1:A:772:VAL:CG1	2.46	0.41
1:B:94:ILE:HG22	1:B:790:VAL:HG12	2.01	0.41
1:B:100:ALA:HB1	1:B:797:LEU:HD21	2.02	0.41
1:B:267:ILE:HG13	1:B:267:ILE:H	1.73	0.41
1:B:642:PHE:CG	1:B:648:VAL:HG11	2.55	0.41
1:A:59:ASP:O	1:A:63:ARG:HG3	2.20	0.41
1:A:276:ILE:HG12	1:A:279:PHE:HE2	1.85	0.41
1:A:336:LEU:N	1:A:337:PRO:CD	2.81	0.41
1:A:392:GLU:O	1:A:451:LYS:HE2	2.20	0.41
1:A:573:ARG:O	1:A:573:ARG:HD3	2.20	0.41
1:A:784:PRO:O	1:A:785:GLU:C	2.63	0.41
1:A:795:VAL:CG2	1:A:901:LEU:CD1	2.98	0.41
1:B:288:TRP:CD1	1:B:289:ILE:H	2.37	0.41
1:B:573:ARG:NH1	1:B:573:ARG:CG	2.83	0.41
1:B:811:PRO:HA	1:B:812:PRO:HD3	1.82	0.41
1:B:859:ALA:HB1	1:B:862:GLY:HA3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:927:PRO:O	1:B:934:LEU:HD21	2.19	0.41
1:A:231:GLU:O	1:A:235:ILE:HG12	2.20	0.41
1:A:903:VAL:HG13	1:A:973:ILE:CG2	2.50	0.41
1:B:89:VAL:HA	1:B:92:PHE:HD2	1.85	0.41
1:B:352:LYS:CD	1:B:635:ILE:HG21	2.51	0.41
1:B:798:VAL:O	1:B:909:MET:CE	2.57	0.41
1:B:851:ALA:O	1:B:852:ALA:C	2.62	0.41
1:B:855:TRP:CE3	1:B:856:PHE:N	2.89	0.41
1:A:58:GLU:OE1	1:A:309:GLU:OE2	2.39	0.41
1:A:218:LYS:O	1:A:219:ALA:HB2	2.21	0.41
1:A:352:LYS:CD	1:A:635:ILE:HG21	2.50	0.41
1:B:311:LEU:HA	1:B:760:PHE:CE1	2.55	0.41
1:B:358:THR:HG22	1:B:604:ARG:HA	2.01	0.41
1:B:467:ARG:HD2	1:B:467:ARG:O	2.20	0.41
1:B:754:TYR:CE2	1:B:758:LYS:HG3	2.55	0.41
1:B:900:ALA:O	1:B:901:LEU:C	2.63	0.41
1:B:926:PRO:HB2	1:B:928:TRP:CE2	2.55	0.41
1:A:866:THR:HG22	1:A:886:LEU:HD22	2.02	0.41
1:B:2:GLU:CG	1:B:3:ALA:N	2.83	0.41
1:B:735:LEU:HD13	1:B:739:ASN:O	2.19	0.41
1:B:792:LEU:O	1:B:793:LEU:C	2.64	0.41
1:B:939:LEU:O	1:B:939:LEU:HG	2.20	0.41
1:A:72:SER:HA	1:A:293:ILE:HD12	2.02	0.41
1:A:126:MET:O	1:A:127:GLY:C	2.62	0.41
1:A:161:ALA:CA	1:A:210:SER:HB2	2.46	0.41
1:A:253:LEU:O	1:A:256:PHE:HB3	2.21	0.41
1:A:662:PRO:O	1:A:663:LEU:C	2.62	0.41
1:A:755:ASN:HD21	1:A:819:ARG:HH12	1.68	0.41
1:A:893:ALA:C	1:A:896:PRO:HD2	2.45	0.41
1:A:964:LEU:O	1:A:968:LEU:HB2	2.20	0.41
1:B:563:ALA:HA	1:B:596:VAL:HG22	2.02	0.41
1:B:832:TRP:CZ2	1:B:988:ALA:HB2	2.55	0.41
1:A:125:GLU:OE1	1:A:158:LYS:HG2	2.20	0.41
1:A:840:ILE:O	1:A:843:TYR:N	2.50	0.41
1:A:862:GLY:HA2	1:A:863:PRO:HD3	1.80	0.41
1:B:342:LEU:HG	1:B:747:VAL:HA	2.02	0.41
1:B:782:GLY:O	1:B:783:LEU:O	2.38	0.41
1:A:74:VAL:O	1:A:75:LEU:C	2.62	0.41
1:A:81:GLY:CA	1:A:82:GLU:OE1	2.69	0.41
1:B:352:LYS:CD	1:B:635:ILE:HD13	2.51	0.41
1:B:795:VAL:HG22	1:B:901:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:962:LEU:HD23	1:B:966:GLN:CD	2.46	0.41
1:A:18:VAL:HG23	1:A:23:GLY:C	2.45	0.41
1:A:89:VAL:HA	1:A:92:PHE:HD2	1.86	0.41
1:A:140:ILE:CG1	1:A:141:LYS:N	2.84	0.41
1:A:311:LEU:O	1:A:312:PRO:C	2.63	0.41
1:A:366:MET:CB	1:A:597:VAL:HG12	2.51	0.41
1:A:611:ILE:HD13	1:A:641:ILE:HG13	2.02	0.41
1:A:906:THR:HG22	1:A:974:SER:OG	2.20	0.41
1:B:282:PRO:O	1:B:283:VAL:C	2.64	0.41
1:B:326:MET:HE3	1:B:333:VAL:HG21	2.02	0.41
1:B:527:TYR:O	1:B:592:THR:HA	2.21	0.41
1:B:737:ASP:O	1:B:738:ASP:CB	2.68	0.41
1:B:791:GLN:O	1:B:794:TRP:HB3	2.21	0.41
1:A:414:ALA:O	1:A:415:THR:C	2.64	0.41
1:A:565:ALA:HB2	1:A:593:PHE:HA	2.02	0.41
1:A:620:ARG:NH2	1:A:670:CYS:O	2.53	0.41
1:A:797:LEU:HD23	1:A:797:LEU:C	2.45	0.41
1:A:979:GLY:O	1:A:983:ILE:HG13	2.21	0.41
1:B:246:LYS:HA	1:B:251:GLN:CG	2.51	0.41
1:B:527:TYR:HA	1:B:536:PRO:HA	2.03	0.41
1:B:678:ARG:NH1	1:B:678:ARG:CG	2.83	0.41
1:A:125:GLU:HB3	1:A:142:ALA:CB	2.43	0.40
1:A:316:THR:O	1:A:316:THR:HG22	2.20	0.40
1:A:520:GLY:O	1:A:524:ARG:HG3	2.21	0.40
1:A:658:PHE:CA	1:A:661:LEU:HD12	2.35	0.40
1:A:988:ALA:HB2	1:A:992:LEU:HD12	2.03	0.40
1:B:108:GLN:OE1	1:B:310:GLY:HA2	2.21	0.40
1:B:326:MET:HB3	1:B:331:ALA:HB3	2.02	0.40
1:B:421:ASN:OD1	1:B:422:ASP:N	2.55	0.40
1:B:662:PRO:O	1:B:663:LEU:C	2.62	0.40
1:B:671:ARG:HB3	1:B:694:TYR:CD2	2.55	0.40
1:B:832:TRP:CD1	1:B:832:TRP:C	2.96	0.40
1:A:32:HIS:O	1:A:36:TYR:HD2	2.03	0.40
1:A:108:GLN:OE1	1:A:310:GLY:HA2	2.21	0.40
1:A:550:LYS:O	1:A:554:THR:HG23	2.21	0.40
1:A:580:ASP:O	1:A:580:ASP:CG	2.64	0.40
1:A:635:ILE:HG13	1:A:635:ILE:H	1.60	0.40
1:A:690:TYR:O	1:A:693:SER:OG	2.38	0.40
1:A:771:GLU:O	1:A:772:VAL:C	2.61	0.40
1:B:140:ILE:CG1	1:B:141:LYS:N	2.85	0.40
1:B:604:ARG:HE	1:B:604:ARG:HB3	1.72	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:628:ASN:O	1:B:629:LYS:C	2.64	0.40
1:B:667:ARG:HA	1:B:690:TYR:CD1	2.57	0.40
1:B:679:VAL:HG13	1:B:683:HIS:CG	2.56	0.40
1:B:770:GLY:HA2	1:B:841:GLY:O	2.21	0.40
1:B:838:MET:O	1:B:839:ALA:C	2.65	0.40
1:B:946:LEU:HD23	1:B:946:LEU:O	2.20	0.40
1:A:54:ILE:HA	1:A:57:PHE:CB	2.52	0.40
1:A:421:ASN:OD1	1:A:422:ASP:N	2.54	0.40
1:A:541:VAL:O	1:A:544:LYS:N	2.55	0.40
1:A:802:LEU:C	1:A:804:ALA:H	2.29	0.40
1:A:807:LEU:HD22	1:A:810:ASN:HD21	1.85	0.40
1:A:823:SER:O	1:A:825:LYS:N	2.55	0.40
1:B:74:VAL:O	1:B:75:LEU:C	2.62	0.40
1:B:75:LEU:HD12	1:B:75:LEU:C	2.46	0.40
1:B:247:THR:O	1:B:248:PRO:C	2.64	0.40
1:B:541:VAL:O	1:B:543:GLU:N	2.55	0.40
1:B:662:PRO:CD	1:B:665:GLU:HB2	2.47	0.40
1:B:688:VAL:HG23	1:B:700:MET:CE	2.50	0.40
1:B:855:TRP:CE2	1:B:895:GLU:HB2	2.56	0.40
1:B:906:THR:CG2	1:B:974:SER:HB2	2.50	0.40
1:A:24:LEU:O	1:A:132:ALA:N	2.53	0.40
1:A:319:LEU:HA	1:A:319:LEU:HD12	1.79	0.40
1:A:588:GLU:O	1:A:591:LEU:HD11	2.21	0.40
1:A:751:ARG:HB2	1:A:816:ILE:HD11	2.02	0.40
1:A:841:GLY:HA2	1:A:844:VAL:HG22	2.03	0.40
1:A:843:TYR:CD2	1:A:844:VAL:N	2.90	0.40
1:A:899:MET:HE1	1:A:969:MET:HB3	2.04	0.40
1:B:371:LYS:C	1:B:372:VAL:CG2	2.93	0.40
1:B:781:LEU:HD23	1:B:781:LEU:HA	1.82	0.40
1:B:962:LEU:HD23	1:B:966:GLN:HB3	2.03	0.40
1:A:81:GLY:HA2	1:A:82:GLU:OE1	2.22	0.40
1:A:926:PRO:HB2	1:A:928:TRP:CE2	2.56	0.40
1:A:962:LEU:HD23	1:A:966:GLN:CD	2.47	0.40
1:B:106:VAL:HA	1:B:109:GLU:HB2	2.03	0.40
1:B:371:LYS:O	1:B:377:CYS:HB2	2.22	0.40
1:B:459:VAL:O	1:B:462:LEU:N	2.48	0.40
1:B:583:ARG:HG3	1:B:583:ARG:HH11	1.86	0.40
1:B:792:LEU:O	1:B:795:VAL:N	2.55	0.40
1:B:877:THR:HA	1:B:888:CYS:SG	2.61	0.40
1:B:899:MET:HE1	1:B:969:MET:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	992/994 (100%)	785 (79%)	152 (15%)	55 (6%)	1	8
1	B	992/994 (100%)	774 (78%)	160 (16%)	58 (6%)	1	8
All	All	1984/1988 (100%)	1559 (79%)	312 (16%)	113 (6%)	1	8

All (113) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	ILE
1	A	205	LYS
1	A	283	VAL
1	A	518	PRO
1	A	519	GLU
1	A	801	GLY
1	A	860	GLU
1	A	868	HIS
1	A	880	HIS
1	A	881	PRO
1	B	85	ILE
1	B	205	LYS
1	B	241	ALA
1	B	283	VAL
1	B	518	PRO
1	B	519	GLU
1	B	789	PRO
1	B	813	ASP
1	B	827	PRO
1	B	865	VAL
1	A	82	GLU
1	A	127	GLY
1	A	265	SER
1	A	316	THR
1	A	342	LEU

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Mol	Chain	Res	Type
1	A	531	GLY
1	A	555	GLY
1	A	627	ASP
1	A	781	LEU
1	A	782	GLY
1	A	807	LEU
1	A	987	ILE
1	B	15	TYR
1	B	82	GLU
1	B	243	GLU
1	B	265	SER
1	B	316	THR
1	B	531	GLY
1	B	555	GLY
1	B	604	ARG
1	B	627	ASP
1	B	673	ALA
1	B	766	SER
1	B	797	LEU
1	B	866	THR
1	B	904	LEU
1	B	987	ILE
1	A	15	TYR
1	A	24	LEU
1	A	72	SER
1	A	133	ASP
1	A	307	ILE
1	A	534	ARG
1	A	575	GLU
1	A	604	ARG
1	A	673	ALA
1	A	703	ASP
1	A	904	LEU
1	B	24	LEU
1	B	72	SER
1	B	133	ASP
1	B	342	LEU
1	B	534	ARG
1	B	575	GLU
1	B	703	ASP
1	B	796	ASN
1	A	303	ALA

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Mol	Chain	Res	Type
1	A	372	VAL
1	A	460	ARG
1	A	533	THR
1	A	743	ILE
1	A	796	ASN
1	B	303	ALA
1	B	372	VAL
1	B	533	THR
1	B	743	ILE
1	B	783	LEU
1	A	42	PRO
1	A	282	PRO
1	A	789	PRO
1	A	802	LEU
1	A	961	ALA
1	B	48	SER
1	B	123	GLU
1	B	282	PRO
1	B	953	LEU
1	A	272	TRP
1	A	281	ASP
1	A	289	ILE
1	A	951	ASP
1	A	953	LEU
1	A	954	PRO
1	B	53	VAL
1	B	281	ASP
1	B	289	ILE
1	B	307	ILE
1	B	460	ARG
1	B	747	VAL
1	B	951	ASP
1	B	954	PRO
1	B	961	ALA
1	A	849	VAL
1	B	304	VAL
1	A	765	ILE
1	B	391	PRO
1	B	896	PRO
1	A	277	GLY
1	A	308	PRO
1	A	530	VAL

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Mol	Chain	Res	Type
1	B	277	GLY
1	B	530	VAL
1	B	905	VAL
1	B	308	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	840/840 (100%)	770 (92%)	70 (8%)	10	37
1	B	840/840 (100%)	774 (92%)	66 (8%)	11	39
All	All	1680/1680 (100%)	1544 (92%)	136 (8%)	11	38

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	LEU
1	A	64	ILE
1	A	67	LEU
1	A	71	ILE
1	A	82	GLU
1	A	90	GLU
1	A	103	ILE
1	A	111	ASN
1	A	122	TYR
1	A	133	ASP
1	A	153	VAL
1	A	155	VAL
1	A	185	VAL
1	A	187	VAL
1	A	214	ILE
1	A	225	THR
1	A	249	LEU
1	A	276	ILE
1	A	312	PRO

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Mol	Chain	Res	Type
1	A	353	THR
1	A	357	THR
1	A	358	THR
1	A	372	VAL
1	A	383	SER
1	A	441	THR
1	A	445	LEU
1	A	454	VAL
1	A	457	THR
1	A	464	LYS
1	A	467	ARG
1	A	472	ASN
1	A	473	SER
1	A	484	THR
1	A	486	GLU
1	A	534	ARG
1	A	536	PRO
1	A	562	LEU
1	A	566	THR
1	A	573	ARG
1	A	608	MET
1	A	613	LEU
1	A	647	GLU
1	A	663	LEU
1	A	696	GLU
1	A	698	THR
1	A	705	VAL
1	A	706	ASN
1	A	724	THR
1	A	737	ASP
1	A	756	ASN
1	A	761	ILE
1	A	762	ARG
1	A	774	CYS
1	A	789	PRO
1	A	790	VAL
1	A	816	ILE
1	A	818	ASP
1	A	824	PRO
1	A	832	TRP
1	A	836	ARG
1	A	854	TRP

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Mol	Chain	Res	Type
1	A	895	GLU
1	A	899	MET
1	A	904	LEU
1	A	906	THR
1	A	941	MET
1	A	946	LEU
1	A	965	THR
1	A	971	LEU
1	A	973	ILE
1	B	60	LEU
1	B	64	ILE
1	B	67	LEU
1	B	71	ILE
1	B	82	GLU
1	B	90	GLU
1	B	103	ILE
1	B	111	ASN
1	B	133	ASP
1	B	153	VAL
1	B	155	VAL
1	B	179	ILE
1	B	185	VAL
1	B	187	VAL
1	B	214	ILE
1	B	225	THR
1	B	276	ILE
1	B	312	PRO
1	B	353	THR
1	B	357	THR
1	B	358	THR
1	B	372	VAL
1	B	383	SER
1	B	392	GLU
1	B	441	THR
1	B	445	LEU
1	B	454	VAL
1	B	457	THR
1	B	464	LYS
1	B	467	ARG
1	B	472	ASN
1	B	473	SER
1	B	484	THR

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Mol	Chain	Res	Type
1	B	486	GLU
1	B	534	ARG
1	B	562	LEU
1	B	566	THR
1	B	573	ARG
1	B	608	MET
1	B	613	LEU
1	B	647	GLU
1	B	663	LEU
1	B	696	GLU
1	B	698	THR
1	B	705	VAL
1	B	706	ASN
1	B	724	THR
1	B	737	ASP
1	B	744	VAL
1	B	756	ASN
1	B	761	ILE
1	B	777	LEU
1	B	789	PRO
1	B	814	LEU
1	B	832	TRP
1	B	833	LEU
1	B	883	PHE
1	B	899	MET
1	B	904	LEU
1	B	906	THR
1	B	907	ILE
1	B	941	MET
1	B	946	LEU
1	B	965	THR
1	B	971	LEU
1	B	973	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	HIS
1	A	101	ASN
1	A	111	ASN
1	A	114	ASN
1	A	138	GLN

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Mol	Chain	Res	Type
1	A	284	HIS
1	A	359	ASN
1	A	472	ASN
1	A	477	GLN
1	A	612	GLN
1	A	706	ASN
1	A	759	GLN
1	A	768	ASN
1	A	810	ASN
1	A	869	GLN
1	A	872	HIS
1	A	914	ASN
1	A	919	ASN
1	B	38	HIS
1	B	39	ASN
1	B	101	ASN
1	B	111	ASN
1	B	114	ASN
1	B	138	GLN
1	B	201	ASN
1	B	244	GLN
1	B	251	GLN
1	B	284	HIS
1	B	472	ASN
1	B	477	GLN
1	B	510	ASN
1	B	612	GLN
1	B	706	ASN
1	B	756	ASN
1	B	768	ASN
1	B	791	GLN
1	B	872	HIS
1	B	882	HIS
1	B	911	ASN
1	B	914	ASN
1	B	919	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 11 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	994/994 (100%)	-0.13	5 (0%) 87 72	24, 73, 138, 174	0
1	B	994/994 (100%)	-0.02	10 (1%) 79 59	24, 77, 138, 175	0
All	All	1988/1988 (100%)	-0.07	15 (0%) 82 64	24, 75, 138, 175	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	864	GLY	3.2
1	A	124	PRO	3.1
1	B	767	SER	2.8
1	A	861	ASP	2.7
1	B	86	THR	2.6
1	B	973	ILE	2.5
1	B	853	ALA	2.5
1	B	882	HIS	2.4
1	A	292	ALA	2.3
1	B	250	GLN	2.3
1	A	54	ILE	2.2
1	B	310	GLY	2.1
1	A	80	GLU	2.1
1	B	251	GLN	2.0
1	B	375	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	K	A	997	1/1	0.68	0.20	91,91,91,91	0
3	K	B	997	1/1	0.79	0.17	69,69,69,69	0
2	CA	A	998	1/1	0.86	0.08	64,64,64,64	0
2	CA	B	995	1/1	0.89	0.07	70,70,70,70	0
4	CL	B	999	1/1	0.91	0.07	40,40,40,40	0
2	CA	B	998	1/1	0.93	0.11	84,84,84,84	0
2	CA	A	999	1/1	0.94	0.10	83,83,83,83	0
2	CA	B	996	1/1	0.94	0.14	52,52,52,52	0
2	CA	A	995	1/1	0.96	0.07	49,49,49,49	0
4	CL	A	1000	1/1	0.96	0.05	56,56,56,56	0
2	CA	A	996	1/1	0.96	0.12	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.