



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:10 AM UTC

PDB ID : 1F4H / pdb_00001f4h
Title : E. COLI (LACZ) BETA-GALACTOSIDASE (ORTHORHOMBIC)
Authors : Juers, D.H.; Jacobson, R.H.; Wigley, D.; Zhang, X.J.; Huber, R.E.; Tronrud, D.E.; Matthews, B.W.
Deposited on : 2000-06-07
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

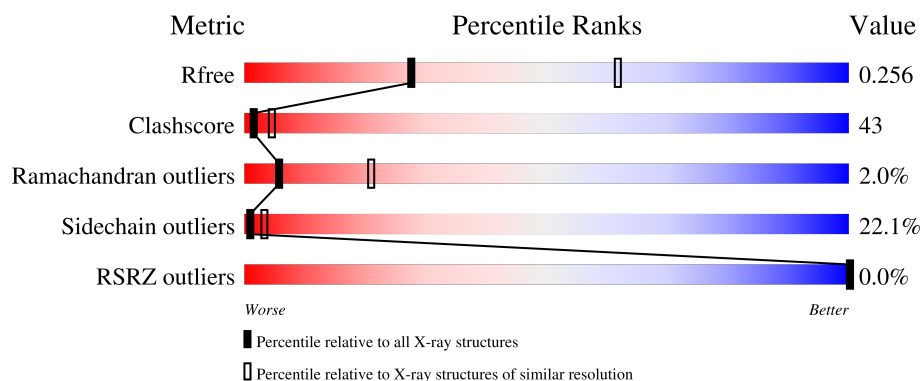
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	1021	32% 46% 19% .
1	B	1021	26% 49% 21% .
1	C	1021	31% 44% 21% .
1	D	1021	33% 45% 19% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 33805 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 BETA-GALACTOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1021	Total	C	N	O	S	84	7	0
			8238	5209	1466	1525	38			
1	B	1021	Total	C	N	O	S	84	7	0
			8238	5209	1466	1525	38			
1	C	1021	Total	C	N	O	S	84	7	0
			8238	5209	1466	1525	38			
1	D	1021	Total	C	N	O	S	84	7	0
			8238	5209	1466	1525	38			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		
2	B	2	Total	Mg	0	0
			2	2		
2	C	2	Total	Mg	0	0
			2	2		
2	D	2	Total	Mg	0	0
			2	2		

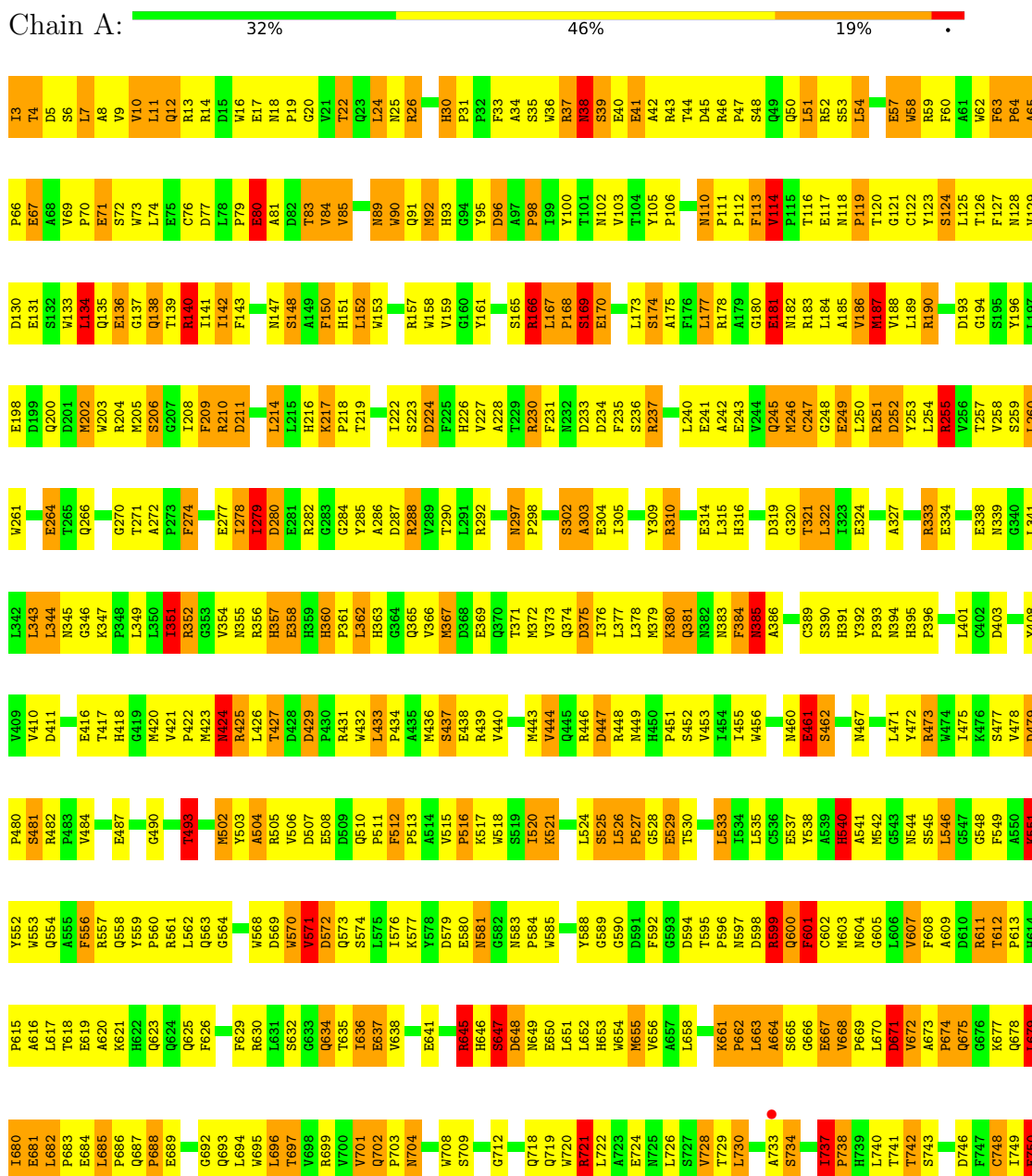
- Molecule 3 is water.

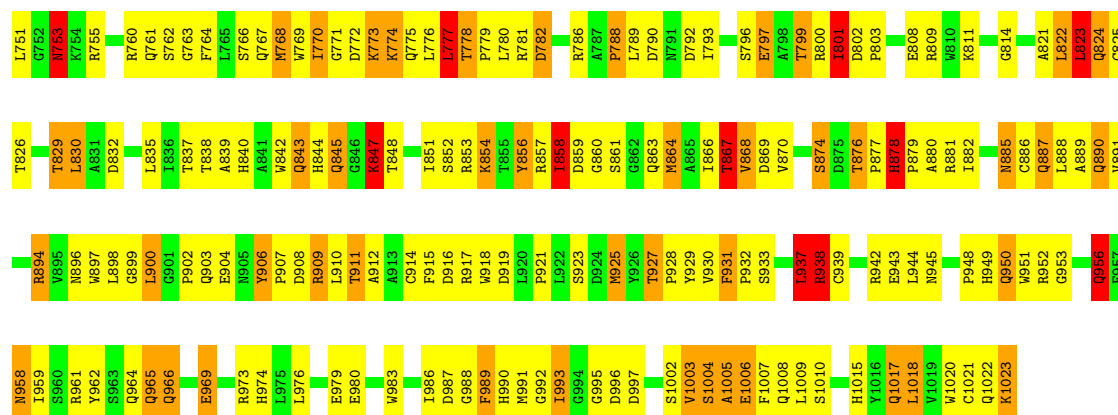
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	211	Total	O	0	0
			211	211		
3	B	202	Total	O	0	0
			202	202		
3	C	220	Total	O	0	0
			220	220		
3	D	212	Total	O	0	0
			212	212		

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.

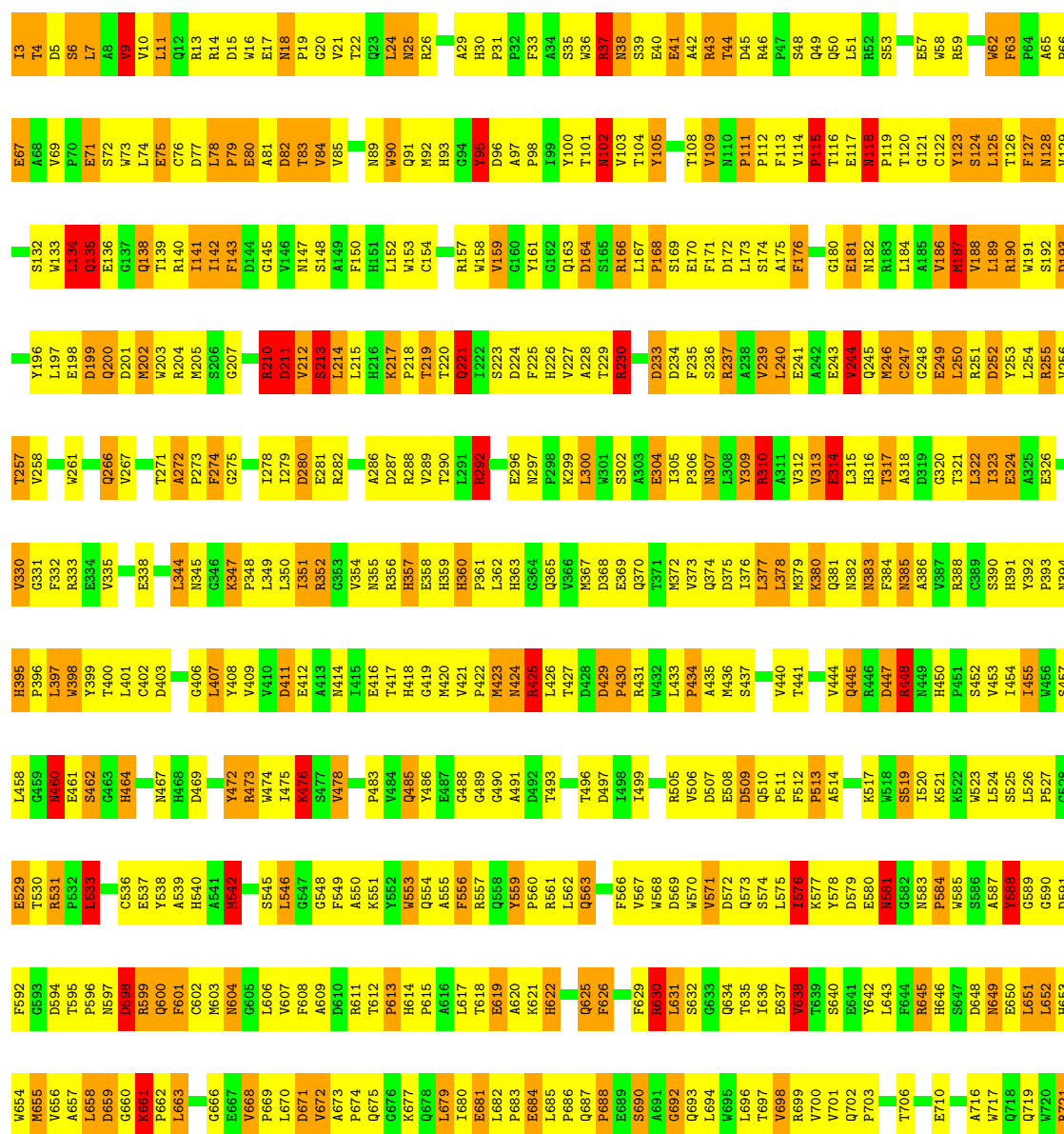
• Molecule 1: BETA-GALACTOSIDASE



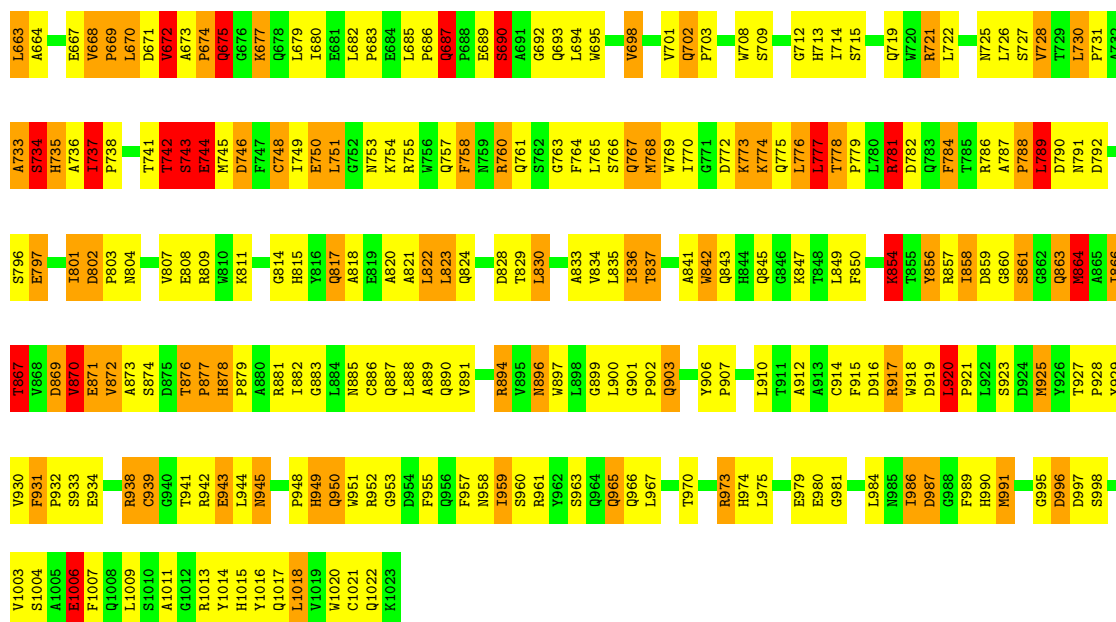


• Molecule 1: BETA-GALACTOSIDASE

Chain B: 26% 49% 21% •

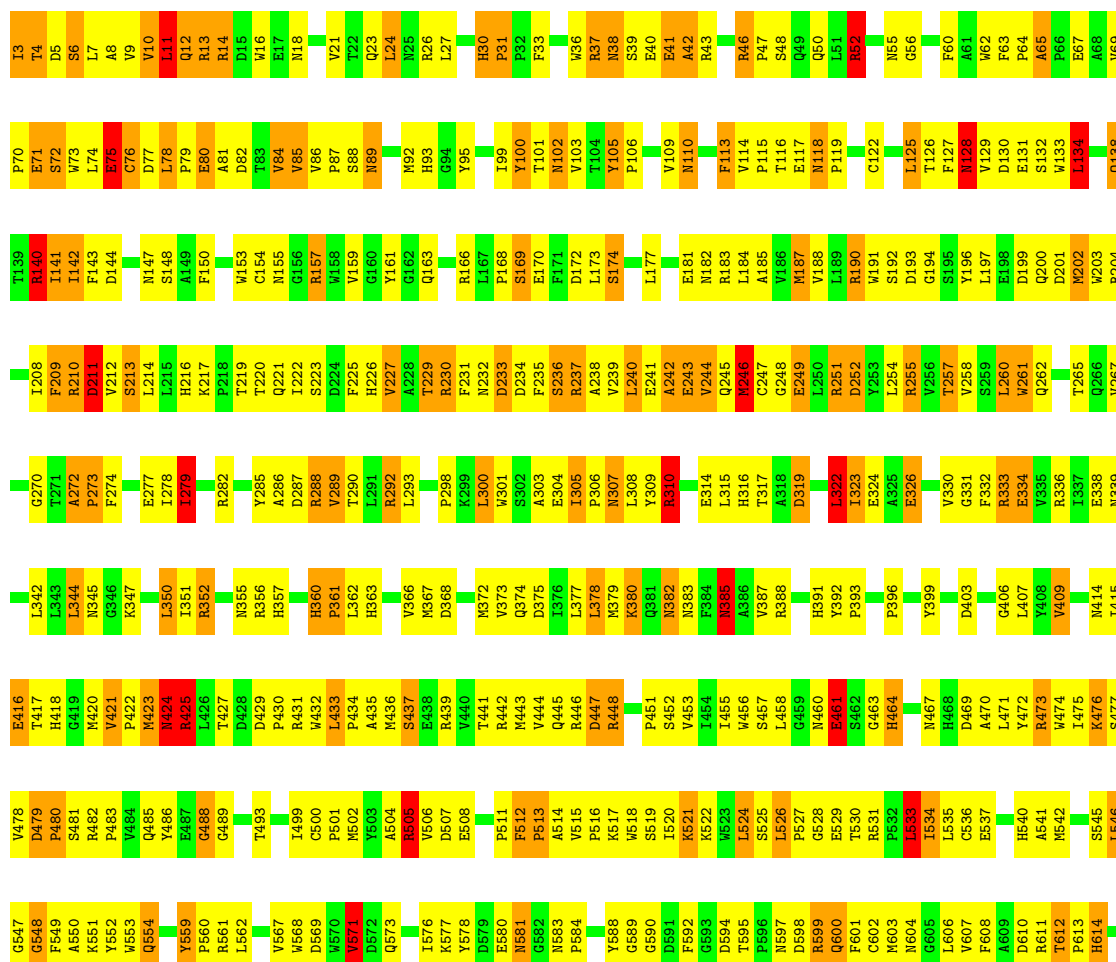






• Molecule 1: BETA-GALACTOSIDASE

Chain D: 33% 45% 19%



R894	R895	R896	R897	P902	Q903	E904	N905	Y906	P907	D908	R909	L910	T911	A912	A913	W918	D919	L920	P921	L922	S923	D924	M925	Y926	T927	P928	Y929	V930	F931	P932	S933	E934	N935	G936	L937	R938	T941	R942	E943	L944	N945	Y946	G947	H948	Q949	Q950	W951	R952	G953	D954	F955	Q956	F957	N958	T959	S960		
R894	V895	N896	W897	P902	Q903	E904	N905	Y906	P907	D908	R909	L910	T911	A912	A913	W918	D919	L920	P921	L922	S923	D924	M925	Y926	T927	P928	Y929	V930	F931	P932	S933	E934	N935	G936	L937	R938	T941	R942	E943	L944	N945	Y946	G947	H948	Q949	Q950	W951	R952	G953	D954	F955	Q956	F957	N958	T959	S960		
T826	A827	D828	T829	L830	V834	L835	L836	T837	T838	H844	Q845	G846	K847	T848	L849	F850	L851	S852	R853	K854	T855	Y856	R857	L858	D859	G860	S861	G862	Q863	M864	T867	V868	D869	V870	E871	V872	A873	S874	D875	T876	P877	H878	P879	A880	R881	L882	Q883	L884	N885	C886	Q887	L888	A889	Q890	E893			
F758	N759	R760	Q761	S762	G763	F764	L765	S766	Q767	M768	W769	L770	G771	D772	K773	K774	Q775	L776	L777	T778	P779	L780	R781	G782	Q783	F784	T785	R786	A787	P788	D792	I793	G794	E797	A798	T799	R800	S801	D802	P803	N804	E808	R809	W810	K811	G814	H815	Y816	E819	L822	L823	Q824	C825					
P883	E684	L685	P686	Q687	P688	E689	S690	A691	Q692	Q693	G694	W695	L696	Q697	W698	L699	G700	Q701	Q702	P703	N704	A705	T706	A707	W708	S709	A710	A711	W712	A713	A714	A715	A716	A717	R721	E724	L730	P731	A732	A733	S734	T737	P738	H739	L740	T742	S743	E744	H745	D746	F747	C748	I749	E750	L751	R755	W756	Q757
L617	T618	E619	A620	K621	Q624	Q625	F626	R630	L631	S632	G633	Q634	T635	I636	E637	V638	T639	L643	F644	R645	H646	S647	D648	N649	E650	L651	L652	H653	W654	M655	V656	A657	L658	K661	P662	L663	A664	S665	G666	E667	V668	P669	L670	D671	V672	A673	P674	Q675	G676	K677	Q678	L679	E680	E681	L682			

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	153.40Å 173.40Å 204.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.80 25.00 – 2.82	Depositor EDS
% Data completeness (in resolution range)	88.0 (25.00-2.80) 80.3 (25.00-2.82)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.80Å)	Xtrriage
Refinement program	TNT 5E	Depositor
R, R_{free}	0.137 , 0.279 0.125 , 0.256	Depositor DCC
R_{free} test set	1590 reflections (1.50%)	wwPDB-VP
Wilson B-factor (Å ²)	40.7	Xtrriage
Anisotropy	0.148	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 156.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	33805	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.86 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2179e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.38	20/8515 (0.2%)	1.97	235/11615 (2.0%)
1	B	1.34	11/8515 (0.1%)	2.01	273/11615 (2.4%)
1	C	1.34	19/8515 (0.2%)	1.97	248/11615 (2.1%)
1	D	1.36	20/8515 (0.2%)	1.99	250/11615 (2.2%)
All	All	1.35	70/34060 (0.2%)	1.99	1006/46460 (2.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	4	0
1	B	1	0
1	C	4	1
1	D	3	0
All	All	12	1

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	479	ASP	C-N	-7.97	1.27	1.33
1	D	749	ILE	N-CA	-6.92	1.38	1.46
1	A	258	VAL	CA-C	-6.38	1.45	1.52
1	D	679	LEU	CA-C	-6.37	1.45	1.52
1	A	376	ILE	CA-CB	-6.34	1.47	1.54
1	C	353	GLY	CA-C	-6.30	1.46	1.52
1	C	513	PRO	N-CA	-6.22	1.39	1.47
1	D	31	PRO	CA-C	-6.21	1.48	1.52
1	A	41	GLU	CA-C	-6.15	1.45	1.52
1	D	749	ILE	CA-C	-6.15	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	479	ASP	C-N	-6.07	1.26	1.33
1	C	414	ASN	CA-C	-5.99	1.46	1.53
1	C	119	PRO	N-CA	-5.89	1.39	1.47
1	A	334	GLU	CA-C	-5.86	1.45	1.52
1	A	280	ASP	CG-OD2	5.86	1.36	1.25
1	A	170	GLU	CA-C	-5.84	1.45	1.52
1	B	187	MET	CA-C	-5.81	1.45	1.52
1	D	350	LEU	C-N	-5.80	1.27	1.33
1	B	344	LEU	CA-C	-5.70	1.46	1.52
1	B	102	ASN	C-O	5.70	1.28	1.23
1	D	738	PRO	N-CA	-5.66	1.40	1.47
1	C	483	PRO	N-CA	-5.66	1.40	1.47
1	C	309	TYR	CA-C	-5.66	1.46	1.52
1	A	858	ILE	CA-CB	-5.64	1.47	1.54
1	C	381	GLN	CA-C	-5.61	1.44	1.52
1	D	534	ILE	C-O	-5.60	1.18	1.24
1	B	723	ALA	CA-C	-5.57	1.46	1.52
1	C	214	LEU	N-CA	-5.52	1.39	1.46
1	A	249	GLU	C-N	-5.52	1.26	1.33
1	B	288	ARG	CA-C	-5.47	1.45	1.52
1	B	249	GLU	CA-C	-5.42	1.46	1.52
1	D	301	TRP	CA-C	-5.41	1.46	1.52
1	C	344	LEU	CA-C	-5.41	1.46	1.52
1	B	840	HIS	CA-C	-5.40	1.46	1.52
1	D	479	ASP	CG-OD2	5.40	1.35	1.25
1	A	951	TRP	CA-C	-5.38	1.46	1.52
1	D	351	ILE	N-CA	-5.38	1.40	1.46
1	B	527	PRO	CA-C	-5.36	1.47	1.52
1	A	327	ALA	C-O	5.32	1.30	1.23
1	B	749	ILE	CA-C	-5.32	1.46	1.52
1	C	454	ILE	CA-CB	-5.30	1.48	1.54
1	A	770	ILE	CA-C	-5.26	1.48	1.53
1	C	30	HIS	CA-C	-5.24	1.46	1.52
1	D	249	GLU	CD-OE2	5.23	1.35	1.25
1	D	261	TRP	C-N	-5.23	1.26	1.33
1	A	343	LEU	CA-C	-5.21	1.46	1.52
1	D	835	LEU	N-CA	-5.21	1.39	1.46
1	C	114	VAL	N-CA	-5.21	1.40	1.46
1	C	917	ARG	N-CA	-5.20	1.39	1.46
1	D	938	ARG	CA-C	-5.19	1.47	1.53
1	C	352	ARG	CA-C	-5.17	1.45	1.53
1	D	951	TRP	CA-C	-5.13	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	527	PRO	CA-C	-5.12	1.46	1.52
1	C	373	VAL	CA-CB	-5.12	1.48	1.54
1	A	427	THR	CA-C	-5.09	1.45	1.52
1	A	687	GLN	C-N	5.08	1.39	1.33
1	B	748	CYS	CA-C	-5.07	1.46	1.52
1	A	868	VAL	CA-C	-5.06	1.46	1.52
1	D	30	HIS	CA-C	-5.05	1.46	1.52
1	C	113	PHE	CA-C	-5.05	1.46	1.52
1	C	261	TRP	CA-C	-5.04	1.46	1.52
1	A	222	ILE	CA-CB	-5.04	1.48	1.54
1	A	688	PRO	CA-C	-5.03	1.46	1.52
1	A	802	ASP	CG-OD2	5.03	1.34	1.25
1	D	226	HIS	CA-C	-5.03	1.46	1.52
1	A	167	LEU	CA-C	5.02	1.59	1.52
1	B	250	LEU	N-CA	-5.01	1.40	1.46
1	D	227	VAL	CA-CB	-5.01	1.47	1.54
1	D	305	ILE	CA-CB	-5.01	1.47	1.54
1	D	625	GLN	CA-C	5.00	1.58	1.52

All (1006) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	385	ASN	N-CA-CB	-12.32	92.58	110.81
1	A	385	ASN	CB-CA-C	-12.19	89.17	109.65
1	B	385	ASN	CB-CA-C	-11.71	88.75	109.24
1	D	479	ASP	CA-C-N	11.21	132.15	120.04
1	D	479	ASP	C-N-CA	11.21	132.15	120.04
1	D	938	ARG	N-CA-CB	10.92	129.84	110.95
1	A	424	ASN	CB-CA-C	-10.86	87.29	109.99
1	D	31	PRO	O-C-N	10.85	126.25	121.15
1	A	777	LEU	N-CA-C	-10.76	100.43	114.31
1	A	297	ASN	O-C-N	10.64	126.42	121.53
1	C	128	ASN	CA-CB-CG	-10.46	102.14	112.60
1	C	113	PHE	CA-CB-CG	-10.39	103.41	113.80
1	C	672	VAL	CB-CA-C	-10.18	95.47	110.33
1	A	110	ASN	CA-CB-CG	-10.06	102.54	112.60
1	C	737	ILE	N-CA-CB	10.02	125.23	111.21
1	D	363	HIS	CA-CB-CG	-9.93	103.87	113.80
1	C	352	ARG	CA-C-N	-9.88	113.52	121.82
1	C	352	ARG	C-N-CA	-9.88	113.52	121.82
1	D	777	LEU	N-CA-C	-9.77	101.71	114.31
1	B	313	VAL	CA-C-N	-9.74	109.56	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	313	VAL	C-N-CA	-9.74	109.56	123.00
1	C	63	PHE	CA-C-N	9.61	129.24	119.82
1	C	63	PHE	C-N-CA	9.61	129.24	119.82
1	D	323	ILE	O-C-N	9.49	129.28	121.98
1	A	211	ASP	CA-CB-CG	-9.39	103.21	112.60
1	C	63	PHE	CA-CB-CG	-9.29	104.51	113.80
1	A	601	PHE	CA-CB-CG	-9.29	104.51	113.80
1	D	949	HIS	CA-CB-CG	-9.26	104.55	113.80
1	D	571	VAL	CB-CA-C	-9.23	98.00	111.19
1	D	421	VAL	CB-CA-C	-9.21	100.86	110.16
1	B	150	PHE	CA-CB-CG	-9.19	104.61	113.80
1	B	988	GLY	N-CA-C	-9.19	101.37	112.49
1	C	118	ASN	CA-C-O	9.19	128.95	119.49
1	C	297	ASN	CB-CA-C	-9.08	103.10	111.00
1	D	307	ASN	CA-CB-CG	-9.05	103.55	112.60
1	B	248	GLY	CA-C-N	-9.00	110.80	122.77
1	B	248	GLY	C-N-CA	-9.00	110.80	122.77
1	C	423	MET	CA-C-N	8.99	132.68	120.54
1	C	423	MET	C-N-CA	8.99	132.68	120.54
1	B	186	VAL	CA-C-N	-8.96	110.37	123.00
1	B	186	VAL	C-N-CA	-8.96	110.37	123.00
1	B	188	VAL	N-CA-C	8.95	120.62	107.37
1	B	668	VAL	CA-C-N	8.95	129.30	119.90
1	B	668	VAL	C-N-CA	8.95	129.30	119.90
1	B	307	ASN	CA-CB-CG	8.92	121.52	112.60
1	B	945	ASN	CA-CB-CG	-8.90	103.70	112.60
1	C	110	ASN	N-CA-CB	8.89	122.34	110.79
1	B	272	ALA	N-CA-C	8.81	116.15	108.22
1	C	588	TYR	N-CA-C	8.80	119.55	108.19
1	C	781	ARG	N-CA-C	8.79	122.52	109.24
1	B	63	PHE	CA-C-N	8.77	128.49	119.19
1	B	63	PHE	C-N-CA	8.77	128.49	119.19
1	D	638	VAL	CB-CA-C	-8.76	100.37	110.96
1	A	168	PRO	CB-CA-C	-8.75	99.52	110.98
1	D	339	ASN	CA-CB-CG	-8.75	103.85	112.60
1	B	920	LEU	CA-C-N	8.72	128.48	119.76
1	B	920	LEU	C-N-CA	8.72	128.48	119.76
1	B	164	ASP	N-CA-CB	8.70	125.19	110.49
1	A	7	LEU	N-CA-C	-8.66	101.84	111.28
1	B	172	ASP	CA-CB-CG	-8.59	104.01	112.60
1	A	166	ARG	N-CA-CB	8.53	123.24	110.53
1	C	449	ASN	CA-CB-CG	8.52	121.12	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	291	LEU	CB-CA-C	8.41	123.72	109.50
1	A	938	ARG	N-CA-CB	8.40	123.96	110.77
1	B	625	GLN	N-CA-C	8.40	121.44	110.43
1	C	118	ASN	OD1-CG-ND2	8.40	131.00	122.60
1	D	89	ASN	CA-CB-CG	-8.38	104.22	112.60
1	A	142	ILE	N-CA-C	8.37	120.18	108.12
1	A	570	TRP	N-CA-C	8.33	120.28	111.03
1	C	870	VAL	N-CA-C	8.32	121.86	108.97
1	D	748	CYS	CA-C-N	-8.30	111.60	123.06
1	D	748	CYS	C-N-CA	-8.30	111.60	123.06
1	B	1004	SER	N-CA-CB	8.29	122.15	109.97
1	A	687	GLN	CB-CA-C	8.25	122.39	110.02
1	B	352	ARG	CA-C-N	-8.22	115.15	122.47
1	B	352	ARG	C-N-CA	-8.22	115.15	122.47
1	D	1011	ALA	N-CA-C	8.19	120.29	111.36
1	C	167	LEU	CA-C-N	8.19	128.50	119.90
1	C	167	LEU	C-N-CA	8.19	128.50	119.90
1	C	248	GLY	CA-C-N	-8.19	111.06	122.93
1	C	248	GLY	C-N-CA	-8.19	111.06	122.93
1	A	423	MET	CA-C-N	8.17	135.44	121.14
1	A	423	MET	C-N-CA	8.17	135.44	121.14
1	D	668	VAL	C-N-CD	-8.12	91.69	125.00
1	A	187	MET	N-CA-CB	8.11	122.41	110.49
1	C	512	PHE	CA-CB-CG	-8.08	105.72	113.80
1	D	105	TYR	CA-C-N	8.07	128.01	119.05
1	D	105	TYR	C-N-CA	8.07	128.01	119.05
1	D	651	LEU	CB-CA-C	-8.06	95.78	109.72
1	B	622	HIS	CA-CB-CG	-8.05	105.75	113.80
1	A	686	PRO	CA-C-N	-7.97	108.36	122.48
1	A	686	PRO	C-N-CA	-7.97	108.36	122.48
1	A	385	ASN	N-CA-CB	-7.94	97.01	110.51
1	A	528	GLY	CA-C-N	7.91	132.37	121.05
1	A	528	GLY	C-N-CA	7.91	132.37	121.05
1	B	423	MET	CA-C-N	7.88	131.49	120.29
1	B	423	MET	C-N-CA	7.88	131.49	120.29
1	C	4	THR	N-CA-C	-7.86	103.58	113.02
1	B	588	TYR	N-CA-C	7.80	118.28	108.45
1	A	737	ILE	CB-CA-C	7.80	125.55	111.36
1	B	604	ASN	CA-CB-CG	-7.79	104.81	112.60
1	D	52[A]	ARG	N-CA-C	7.79	121.61	109.07
1	D	52[B]	ARG	N-CA-C	7.79	121.61	109.07
1	B	949	HIS	CA-CB-CG	-7.79	106.01	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	221	GLN	N-CA-C	7.79	119.84	108.86
1	A	258	VAL	O-C-N	7.78	131.04	123.03
1	D	128	ASN	CA-CB-CG	-7.74	104.86	112.60
1	B	395	HIS	CA-C-N	7.67	129.43	119.84
1	B	395	HIS	C-N-CA	7.67	129.43	119.84
1	B	576	ILE	N-CA-C	7.67	119.64	109.21
1	D	524	LEU	O-C-N	7.66	130.06	122.09
1	A	235	PHE	CA-CB-CG	-7.65	106.15	113.80
1	C	555	ALA	N-CA-C	-7.64	102.08	111.40
1	B	309	TYR	CA-C-N	-7.64	110.81	122.81
1	B	309	TYR	C-N-CA	-7.64	110.81	122.81
1	D	988	GLY	N-CA-C	-7.64	103.13	113.37
1	D	750	GLU	N-CA-CB	7.63	124.01	110.80
1	B	614	HIS	N-CA-C	-7.63	100.45	110.07
1	C	734	SER	CA-C-N	-7.63	107.70	120.68
1	C	734	SER	C-N-CA	-7.63	107.70	120.68
1	B	448	ARG	N-CA-C	7.62	122.24	112.34
1	A	927	THR	CA-C-N	7.62	129.36	119.84
1	A	927	THR	C-N-CA	7.62	129.36	119.84
1	A	956	GLN	N-CA-C	-7.62	97.84	109.95
1	B	176	PHE	CA-CB-CG	-7.61	106.19	113.80
1	A	190	ARG	N-CA-CB	7.60	121.09	110.07
1	B	823	LEU	N-CA-C	-7.59	104.62	114.04
1	B	903[A]	GLN	N-CA-C	7.59	120.13	110.33
1	B	903[B]	GLN	N-CA-C	7.59	120.13	110.33
1	A	671	ASP	CA-CB-CG	7.59	120.19	112.60
1	C	118	ASN	CB-CG-ND2	-7.58	105.02	116.40
1	A	909	ARG	CA-C-N	-7.58	110.03	122.08
1	A	909	ARG	C-N-CA	-7.58	110.03	122.08
1	D	680	ILE	CB-CA-C	7.58	120.49	111.32
1	D	319	ASP	CA-CB-CG	7.57	120.17	112.60
1	D	383	ASN	N-CA-C	7.56	122.45	113.23
1	D	209	PHE	CA-CB-CG	-7.53	106.27	113.80
1	D	424	ASN	CB-CA-C	-7.53	96.70	110.63
1	A	689	GLU	N-CA-C	-7.52	102.75	112.23
1	B	630	ARG	CA-C-N	-7.51	112.35	122.72
1	B	630	ARG	C-N-CA	-7.51	112.35	122.72
1	B	1011	ALA	N-CA-C	7.51	120.34	111.71
1	A	903[A]	GLN	N-CA-C	7.50	121.58	110.48
1	A	903[B]	GLN	N-CA-C	7.50	121.58	110.48
1	A	701	VAL	N-CA-C	7.47	119.24	108.48
1	B	870	VAL	N-CA-C	7.47	119.84	108.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	744	GLU	CB-CA-C	7.47	122.64	109.65
1	D	188	VAL	N-CA-CB	-7.46	102.39	110.53
1	B	447	ASP	CA-CB-CG	-7.46	105.14	112.60
1	B	787	ALA	CA-C-N	7.45	129.16	119.84
1	B	787	ALA	C-N-CA	7.45	129.16	119.84
1	D	423	MET	CA-C-N	7.44	131.00	120.28
1	D	423	MET	C-N-CA	7.44	131.00	120.28
1	C	878	HIS	CA-CB-CG	-7.43	106.37	113.80
1	A	687	GLN	CB-CG-CD	-7.40	100.02	112.60
1	B	835	LEU	CA-C-N	-7.40	113.43	122.90
1	B	835	LEU	C-N-CA	-7.40	113.43	122.90
1	A	30	HIS	CA-CB-CG	-7.39	106.41	113.80
1	B	25	ASN	N-CA-C	7.36	121.67	111.74
1	B	249	GLU	O-C-N	7.34	131.59	123.22
1	D	102	ASN	CA-CB-CG	7.32	119.92	112.60
1	C	290	THR	CA-C-N	-7.31	110.21	122.64
1	C	290	THR	C-N-CA	-7.31	110.21	122.64
1	A	209	PHE	CA-CB-CG	-7.30	106.50	113.80
1	C	777	LEU	N-CA-C	-7.30	104.89	114.31
1	C	949	HIS	CA-CB-CG	-7.28	106.53	113.80
1	D	265	THR	N-CA-CB	-7.27	98.02	109.87
1	A	645	ARG	N-CA-C	7.26	121.12	110.59
1	A	793	ILE	CB-CA-C	-7.26	102.50	111.87
1	A	375	ASP	CA-CB-CG	-7.24	105.36	112.60
1	B	509	ASP	CA-CB-CG	7.22	119.82	112.60
1	B	249	GLU	CA-C-N	7.22	132.19	121.72
1	B	249	GLU	C-N-CA	7.22	132.19	121.72
1	C	571	VAL	CB-CA-C	-7.21	99.88	110.62
1	A	702	GLN	OE1-CD-NE2	7.18	129.78	122.60
1	C	30	HIS	O-C-N	7.18	128.67	121.56
1	A	782	ASP	CA-CB-CG	7.17	119.77	112.60
1	B	385	ASN	CA-CB-CG	7.17	119.77	112.60
1	C	1007	PHE	CA-CB-CG	-7.16	106.64	113.80
1	C	735	HIS	N-CA-C	7.14	121.23	112.23
1	C	570	TRP	N-CA-C	7.12	118.93	111.03
1	B	102	ASN	CA-CB-CG	7.12	119.72	112.60
1	D	142	ILE	N-CA-C	7.12	118.14	107.75
1	B	649	ASN	N-CA-C	-7.11	102.02	110.41
1	B	672	VAL	CB-CA-C	-7.11	100.11	110.63
1	D	644	PHE	CA-CB-CG	-7.11	106.69	113.80
1	D	592	PHE	CA-CB-CG	-7.08	106.72	113.80
1	C	5	ASP	N-CA-C	-7.07	104.53	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	553	TRP	CA-CB-CG	-7.06	100.19	113.60
1	C	93	HIS	CA-CB-CG	-7.06	106.74	113.80
1	C	291	LEU	N-CA-CB	7.06	122.13	110.63
1	D	383	ASN	CA-CB-CG	-7.06	105.54	112.60
1	C	147	ASN	N-CA-CB	-7.05	99.70	110.77
1	C	817	GLN	N-CA-CB	7.05	121.01	110.65
1	D	42	ALA	N-CA-C	-7.04	103.22	111.03
1	B	290	THR	CA-C-N	-7.03	111.55	122.87
1	B	290	THR	C-N-CA	-7.03	111.55	122.87
1	D	31	PRO	N-CA-CB	7.03	106.88	103.22
1	D	118	ASN	N-CA-CB	-7.03	98.67	111.03
1	D	128	ASN	N-CA-C	7.02	120.68	109.24
1	B	411	ASP	CA-CB-CG	7.02	119.62	112.60
1	B	603	MET	N-CA-C	7.02	118.43	108.54
1	B	187	MET	N-CA-CB	7.01	121.59	110.65
1	B	348	PRO	N-CA-CB	7.01	107.93	103.23
1	C	864	MET	N-CA-C	7.01	120.16	108.73
1	C	927	THR	CB-CA-C	6.99	117.93	110.17
1	B	344	LEU	N-CA-CB	6.99	121.55	110.65
1	B	649	ASN	O-C-N	6.98	129.09	122.18
1	D	249	GLU	CA-C-O	6.96	128.02	120.43
1	A	688	PRO	CB-CA-C	-6.96	100.99	110.60
1	B	1000	SER	O-C-N	6.96	126.72	121.85
1	D	784	PHE	CA-CB-CG	-6.96	106.84	113.80
1	C	151	HIS	CA-CB-CG	-6.95	106.85	113.80
1	C	903[A]	GLN	N-CA-C	6.94	119.92	110.55
1	C	903[B]	GLN	N-CA-C	6.94	119.92	110.55
1	A	38	ASN	N-CA-CB	6.93	122.09	110.79
1	D	770	ILE	CB-CA-C	-6.93	101.98	110.99
1	A	363	HIS	CA-CB-CG	-6.93	106.87	113.80
1	A	384	PHE	CA-CB-CG	-6.92	106.88	113.80
1	C	79	PRO	CA-C-N	6.92	131.19	120.82
1	C	79	PRO	C-N-CA	6.92	131.19	120.82
1	D	209	PHE	N-CA-C	6.91	121.56	113.20
1	D	323	ILE	CB-CA-C	-6.90	104.91	111.05
1	B	856	TYR	CA-C-N	-6.89	113.07	122.86
1	B	856	TYR	C-N-CA	-6.89	113.07	122.86
1	C	517	LYS	CB-CA-C	6.88	122.94	111.51
1	D	464	HIS	CA-CB-CG	-6.88	106.92	113.80
1	D	691	ALA	N-CA-C	-6.88	101.41	110.43
1	D	909	ARG	CA-C-N	-6.86	111.28	121.99
1	D	909	ARG	C-N-CA	-6.86	111.28	121.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	65	ALA	N-CA-C	6.86	114.30	108.13
1	D	322	LEU	CA-C-N	-6.85	115.90	123.16
1	D	322	LEU	C-N-CA	-6.85	115.90	123.16
1	D	506	VAL	N-CA-C	6.84	116.93	110.30
1	C	306	PRO	N-CA-CB	6.84	107.39	102.81
1	C	576	ILE	N-CA-C	6.84	117.91	108.89
1	D	745	MET	CB-CA-C	-6.84	96.59	109.72
1	D	541	ALA	N-CA-C	6.83	122.00	112.72
1	B	725	ASN	CA-CB-CG	-6.83	105.77	112.60
1	D	965	GLN	N-CA-CB	6.82	120.11	109.94
1	D	927	THR	CA-C-N	6.82	128.37	119.84
1	D	927	THR	C-N-CA	6.82	128.37	119.84
1	B	429	ASP	O-C-N	6.82	127.62	121.35
1	D	855	THR	CA-C-N	-6.82	112.50	122.65
1	D	855	THR	C-N-CA	-6.82	112.50	122.65
1	C	750	GLU	N-CA-CB	6.81	124.20	111.53
1	C	581	ASN	N-CA-CB	6.81	120.34	110.47
1	B	176	PHE	N-CA-C	-6.81	105.53	114.31
1	C	600	GLN	N-CA-CB	6.79	121.82	110.41
1	D	82	ASP	CA-CB-CG	6.79	119.39	112.60
1	A	352	ARG	CA-C-N	-6.79	116.13	122.17
1	A	352	ARG	C-N-CA	-6.79	116.13	122.17
1	A	687	GLN	CA-C-O	-6.78	113.35	119.86
1	C	568	TRP	CA-CB-CG	-6.77	100.73	113.60
1	D	956	GLN	N-CA-C	-6.77	98.89	109.72
1	A	65	ALA	O-C-N	6.75	127.85	121.71
1	B	150	PHE	N-CA-C	6.74	119.11	108.79
1	C	538	TYR	CA-C-O	-6.74	113.92	121.40
1	A	674	PRO	CB-CA-C	-6.72	103.02	111.56
1	B	540	HIS	CA-CB-CG	-6.72	107.08	113.80
1	B	612	THR	CB-CA-C	6.72	117.57	109.31
1	C	980	GLU	N-CA-CB	6.72	121.84	110.49
1	B	113	PHE	CA-CB-CG	-6.71	107.09	113.80
1	B	142	ILE	CB-CA-C	-6.70	98.85	110.65
1	D	787	ALA	CA-C-N	6.70	127.10	119.93
1	D	787	ALA	C-N-CA	6.70	127.10	119.93
1	D	863	GLN	N-CA-CB	-6.70	99.53	110.59
1	A	151	HIS	CA-CB-CG	-6.69	107.11	113.80
1	C	402	CYS	CA-CB-SG	-6.69	99.01	114.40
1	C	820	ALA	N-CA-C	6.68	119.35	110.53
1	B	210	ARG	N-CA-CB	6.68	120.96	110.87
1	D	868	VAL	N-CA-C	6.68	118.10	108.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	563	GLN	N-CA-C	6.68	120.41	112.93
1	D	190	ARG	N-CA-CB	6.68	120.04	110.16
1	C	649	ASN	N-CA-C	-6.67	102.54	110.41
1	A	249	GLU	CA-C-N	6.67	130.18	120.71
1	A	249	GLU	C-N-CA	6.67	130.18	120.71
1	A	134	LEU	N-CA-CB	6.66	120.92	110.46
1	A	583	ASN	CB-CA-C	6.66	118.26	108.87
1	A	506	VAL	CB-CA-C	-6.66	103.49	111.81
1	B	118	ASN	CB-CA-C	6.66	123.50	111.12
1	D	361	PRO	CB-CA-C	-6.65	100.58	111.56
1	A	605	GLY	CA-C-N	6.65	133.43	121.92
1	A	605	GLY	C-N-CA	6.65	133.43	121.92
1	B	233	ASP	N-CA-CB	6.64	120.61	109.78
1	C	317	THR	N-CA-C	-6.64	101.97	110.53
1	A	159	VAL	N-CA-C	6.63	117.26	111.56
1	A	980	GLU	N-CA-CB	6.63	120.43	110.22
1	C	753	ASN	CA-C-N	6.63	130.23	120.95
1	C	753	ASN	C-N-CA	6.63	130.23	120.95
1	C	516	PRO	CB-CA-C	-6.62	102.30	110.98
1	B	777	LEU	N-CA-C	-6.62	105.33	113.41
1	C	104	THR	CA-C-N	-6.60	110.65	120.68
1	C	104	THR	C-N-CA	-6.60	110.65	120.68
1	D	4	THR	N-CA-C	-6.60	105.23	113.28
1	A	98	PRO	N-CA-C	-6.60	98.88	112.47
1	B	181	GLU	N-CA-C	6.60	119.93	110.10
1	B	105	TYR	CA-C-N	6.59	126.84	119.32
1	B	105	TYR	C-N-CA	6.59	126.84	119.32
1	D	231	PHE	CA-CB-CG	-6.59	107.21	113.80
1	B	18	ASN	CA-C-N	6.58	127.42	120.12
1	B	18	ASN	C-N-CA	6.58	127.42	120.12
1	D	760	ARG	N-CA-CB	6.58	121.90	110.39
1	B	212	VAL	CA-CB-CG1	-6.57	99.23	110.40
1	C	327	ALA	N-CA-C	6.57	118.19	108.60
1	D	863	GLN	CA-C-N	-6.56	113.87	123.05
1	D	863	GLN	C-N-CA	-6.56	113.87	123.05
1	C	126	THR	N-CA-C	6.55	119.20	108.52
1	A	447	ASP	CA-CB-CG	-6.55	106.05	112.60
1	B	626	PHE	CA-CB-CG	-6.55	107.25	113.80
1	A	90	TRP	N-CA-C	6.54	120.36	112.38
1	C	280	ASP	N-CA-C	6.52	116.66	108.45
1	B	722	LEU	CA-C-N	-6.51	110.67	121.80
1	B	722	LEU	C-N-CA	-6.51	110.67	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	801	ILE	N-CA-C	6.50	117.66	108.36
1	B	527	PRO	N-CA-CB	6.50	108.50	103.30
1	D	251	ARG	NE-CZ-NH2	-6.50	113.35	119.20
1	D	614	HIS	N-CA-C	-6.50	101.34	110.31
1	A	264	GLU	CA-C-O	6.50	125.92	118.97
1	D	18	ASN	CA-C-N	6.48	127.31	120.12
1	D	18	ASN	C-N-CA	6.48	127.31	120.12
1	A	527	PRO	N-CA-CB	6.47	108.95	103.25
1	D	680	ILE	N-CA-C	6.47	117.01	106.72
1	A	303	ALA	N-CA-C	-6.46	104.33	111.82
1	C	46	ARG	C-N-CD	-6.46	98.53	125.00
1	C	176	PHE	CA-CB-CG	-6.44	107.36	113.80
1	C	758	PHE	CB-CA-C	-6.44	100.47	110.78
1	C	789	LEU	N-CA-C	-6.44	100.45	110.17
1	A	911	THR	N-CA-C	6.43	118.30	111.28
1	D	559	TYR	CA-C-O	6.43	124.76	119.36
1	D	1018	LEU	CA-C-N	-6.43	114.94	123.17
1	D	1018	LEU	C-N-CA	-6.43	114.94	123.17
1	A	680	ILE	N-CA-C	6.42	117.13	107.75
1	A	516	PRO	CB-CA-C	-6.42	101.25	110.75
1	A	41	GLU	CB-CA-C	-6.42	100.76	110.90
1	C	931	PHE	CA-C-N	6.41	126.44	119.90
1	C	931	PHE	C-N-CA	6.41	126.44	119.90
1	B	802	ASP	CA-CB-CG	-6.40	106.20	112.60
1	B	716	ALA	CB-CA-C	-6.39	97.70	110.42
1	A	385	ASN	CA-CB-CG	-6.39	106.21	112.60
1	A	826	THR	N-CA-C	6.38	118.80	108.34
1	B	601	PHE	CA-CB-CG	-6.38	107.42	113.80
1	D	244	VAL	N-CA-C	6.38	117.10	108.17
1	D	764	PHE	CA-CB-CG	-6.38	107.42	113.80
1	C	743	SER	CA-C-N	-6.38	111.23	122.26
1	C	743	SER	C-N-CA	-6.38	111.23	122.26
1	A	181	GLU	N-CA-C	6.36	118.94	109.59
1	C	1006	GLU	CG-CD-OE2	-6.36	103.77	118.40
1	C	424	ASN	CB-CA-C	-6.36	100.64	110.81
1	A	867	THR	CA-C-N	-6.35	114.11	122.94
1	A	867	THR	C-N-CA	-6.35	114.11	122.94
1	C	134	LEU	N-CA-CB	6.35	119.87	110.53
1	C	432	TRP	CA-CB-CG	-6.33	101.56	113.60
1	A	274	PHE	CA-CB-CG	-6.33	107.47	113.80
1	B	360	HIS	CA-CB-CG	-6.33	107.47	113.80
1	D	513	PRO	N-CA-CB	6.32	108.92	103.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	482	ARG	O-C-N	6.31	125.75	121.71
1	B	533	LEU	CB-CA-C	6.31	120.53	110.19
1	C	130	ASP	CA-CB-CG	-6.30	106.30	112.60
1	B	424	ASN	CA-CB-CG	-6.30	106.30	112.60
1	B	757	GLN	CA-C-N	-6.30	114.39	122.77
1	B	757	GLN	C-N-CA	-6.30	114.39	122.77
1	A	847	LYS	N-CA-C	-6.29	97.55	108.69
1	A	376	ILE	CB-CA-C	-6.28	103.84	111.88
1	A	479	ASP	CA-C-N	6.28	125.96	119.56
1	A	479	ASP	C-N-CA	6.28	125.96	119.56
1	A	748	CYS	CA-C-N	-6.28	114.39	123.06
1	A	748	CYS	C-N-CA	-6.28	114.39	123.06
1	D	360	HIS	CA-CB-CG	-6.28	107.53	113.80
1	B	455	ILE	CB-CA-C	-6.27	99.89	111.18
1	A	829	THR	N-CA-CB	6.27	120.41	110.57
1	A	702	GLN	CA-CB-CG	-6.26	101.58	114.10
1	A	360	HIS	CA-C-N	6.25	127.66	119.84
1	A	360	HIS	C-N-CA	6.25	127.66	119.84
1	C	36	TRP	N-CA-C	-6.25	101.02	110.28
1	D	661	LYS	O-C-N	6.25	128.72	121.47
1	B	571	VAL	CB-CA-C	-6.24	103.22	111.70
1	B	747	PHE	N-CA-C	-6.24	97.01	107.80
1	B	523	TRP	O-C-N	-6.23	115.51	122.12
1	B	249	GLU	N-CA-CB	6.23	120.58	110.42
1	B	127	PHE	O-C-N	6.23	130.08	123.42
1	A	989	PHE	CA-CB-CG	-6.22	107.58	113.80
1	C	867	THR	N-CA-CB	-6.21	101.39	110.84
1	D	21	VAL	CB-CA-C	-6.20	103.82	111.08
1	A	26	ARG	CD-NE-CZ	-6.20	115.72	124.40
1	D	226	HIS	CB-CA-C	-6.20	97.54	109.37
1	C	233	ASP	CA-CB-CG	6.19	118.79	112.60
1	D	745	MET	CA-C-N	-6.19	111.21	121.80
1	D	745	MET	C-N-CA	-6.19	111.21	121.80
1	D	520	ILE	N-CA-C	6.19	116.97	110.72
1	C	167	LEU	O-C-N	6.19	126.38	121.55
1	A	366	VAL	CB-CA-C	-6.18	103.48	110.96
1	C	1003	VAL	N-CA-CB	6.18	119.14	111.41
1	A	360	HIS	CA-CB-CG	-6.18	107.62	113.80
1	A	385	ASN	OD1-CG-ND2	6.18	128.78	122.60
1	D	46	ARG	CA-C-N	6.17	127.55	119.84
1	D	46	ARG	C-N-CA	6.17	127.55	119.84
1	B	511	PRO	N-CA-CB	6.16	106.84	102.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	320	GLY	CA-C-N	-6.15	112.38	121.24
1	B	320	GLY	C-N-CA	-6.15	112.38	121.24
1	A	386	ALA	N-CA-CB	-6.14	101.00	111.69
1	B	460	ASN	CA-CB-CG	6.14	118.74	112.60
1	B	230	ARG	CB-CA-C	-6.14	99.02	109.51
1	A	878	HIS	CA-C-O	6.13	125.52	119.75
1	B	207	GLY	N-CA-C	6.13	118.89	110.56
1	B	559	TYR	CA-C-O	6.12	124.50	119.36
1	B	864	MET	N-CA-CB	6.12	120.19	110.57
1	C	802	ASP	N-CA-CB	6.12	119.29	110.11
1	D	764	PHE	CA-C-N	-6.12	111.67	122.07
1	D	764	PHE	C-N-CA	-6.12	111.67	122.07
1	D	37	ARG	CB-CA-C	6.11	121.05	110.72
1	B	274	PHE	CA-CB-CG	-6.09	107.71	113.80
1	C	451	PRO	N-CA-CB	6.09	110.12	103.30
1	D	690	SER	N-CA-C	6.09	118.15	110.24
1	C	725	ASN	CA-CB-CG	-6.08	106.52	112.60
1	B	37	ARG	CB-CA-C	6.08	121.09	110.64
1	D	826	THR	CA-C-N	-6.08	114.33	122.72
1	D	826	THR	C-N-CA	-6.08	114.33	122.72
1	B	245	GLN	CB-CG-CD	-6.08	102.27	112.60
1	C	369	GLU	N-CA-C	6.07	118.39	111.11
1	B	78	LEU	CA-C-N	6.06	127.42	119.84
1	B	78	LEU	C-N-CA	6.06	127.42	119.84
1	B	394	ASN	CA-CB-CG	6.06	118.66	112.60
1	B	533	LEU	N-CA-CB	6.06	120.06	110.55
1	C	568	TRP	CB-CA-C	-6.06	100.92	110.79
1	D	181	GLU	N-CA-C	6.06	118.52	109.25
1	C	300	LEU	N-CA-C	6.04	119.75	110.20
1	D	927	THR	O-C-N	6.04	128.00	121.12
1	B	553	TRP	CA-CB-CG	-6.04	102.13	113.60
1	A	612	THR	N-CA-CB	6.03	119.19	109.90
1	D	704	ASN	N-CA-C	6.03	119.47	109.46
1	A	424	ASN	N-CA-CB	-6.02	100.58	110.40
1	A	54	LEU	CA-C-O	6.02	127.06	119.95
1	C	39	SER	N-CA-C	6.02	118.61	111.33
1	D	957	PHE	N-CA-C	6.02	117.39	108.60
1	C	197	LEU	N-CA-CB	-6.02	101.23	110.44
1	D	141	ILE	N-CA-C	6.02	117.14	108.48
1	A	47	PRO	N-CA-CB	6.02	108.58	103.35
1	B	193	ASP	CA-CB-CG	-6.01	106.58	112.60
1	D	737	ILE	N-CA-CB	6.01	119.63	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	598	ASP	N-CA-CB	6.00	121.01	111.17
1	A	802	ASP	CA-C-N	5.99	126.42	119.47
1	A	802	ASP	C-N-CA	5.99	126.42	119.47
1	C	479	ASP	CA-C-O	5.99	125.25	119.62
1	D	30	HIS	O-C-N	5.99	128.21	121.32
1	D	30	HIS	CA-C-N	5.99	123.97	119.66
1	D	30	HIS	C-N-CA	5.99	123.97	119.66
1	D	877	PRO	N-CA-CB	5.99	108.64	103.31
1	B	692	GLY	O-C-N	5.99	129.04	123.35
1	C	613	PRO	CB-CA-C	-5.99	103.14	110.98
1	B	840	HIS	CA-CB-CG	-5.98	107.82	113.80
1	C	226	HIS	CB-CA-C	-5.98	97.55	109.33
1	A	358	GLU	O-C-N	5.98	130.22	122.87
1	D	222	ILE	CB-CA-C	-5.98	103.73	110.96
1	A	671	ASP	CB-CA-C	5.97	125.75	111.83
1	A	572	ASP	CA-CB-CG	5.97	118.57	112.60
1	B	791	ASN	CA-CB-CG	5.97	118.57	112.60
1	D	931	PHE	CA-C-N	5.97	126.32	119.93
1	D	931	PHE	C-N-CA	5.97	126.32	119.93
1	B	82	ASP	CA-C-N	-5.97	112.96	121.50
1	B	82	ASP	C-N-CA	-5.97	112.96	121.50
1	A	583	ASN	N-CA-C	-5.96	102.56	110.07
1	C	669	PRO	CB-CA-C	-5.95	103.77	111.39
1	D	804	ASN	CA-CB-CG	-5.95	106.65	112.60
1	A	341	LEU	N-CA-C	5.94	119.16	109.59
1	B	509	ASP	N-CA-CB	5.94	120.09	110.41
1	A	320	GLY	N-CA-C	5.93	123.23	115.40
1	B	671	ASP	CA-CB-CG	5.93	118.53	112.60
1	B	200	GLN	N-CA-C	5.92	119.05	110.28
1	B	920	LEU	O-C-N	5.92	126.00	121.85
1	A	1003	VAL	N-CA-C	5.92	116.65	108.84
1	B	581	ASN	CA-CB-CG	5.92	118.52	112.60
1	C	168	PRO	N-CA-CB	5.91	108.56	103.36
1	A	351	ILE	N-CA-C	5.91	116.04	108.12
1	A	738	PRO	CA-C-N	-5.91	113.34	122.09
1	A	738	PRO	C-N-CA	-5.91	113.34	122.09
1	D	279	ILE	CB-CA-C	5.91	116.97	111.30
1	D	248	GLY	CA-C-N	-5.91	114.57	122.72
1	D	248	GLY	C-N-CA	-5.91	114.57	122.72
1	A	424	ASN	OD1-CG-ND2	5.90	128.50	122.60
1	D	957	PHE	CA-CB-CG	-5.90	107.90	113.80
1	D	964	GLN	N-CA-CB	5.90	118.89	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	357	HIS	CA-CB-CG	5.89	119.69	113.80
1	A	193	ASP	N-CA-C	-5.89	105.35	112.54
1	B	186	VAL	N-CA-C	5.89	116.35	107.75
1	D	829	THR	N-CA-CB	5.89	119.79	110.55
1	A	175	ALA	CB-CA-C	-5.88	100.63	110.81
1	B	576	ILE	N-CA-CB	5.88	118.31	110.26
1	B	386	ALA	N-CA-C	5.88	118.11	109.24
1	A	906	TYR	N-CA-CB	5.87	118.27	109.82
1	A	753	ASN	N-CA-C	-5.87	106.16	113.38
1	C	886	CYS	CA-C-N	-5.87	114.84	123.05
1	C	886	CYS	C-N-CA	-5.87	114.84	123.05
1	D	856	TYR	CA-C-N	-5.86	113.71	122.39
1	D	856	TYR	C-N-CA	-5.86	113.71	122.39
1	B	476	LYS	N-CA-CB	5.86	119.24	110.22
1	D	118	ASN	OD1-CG-ND2	5.84	128.44	122.60
1	C	593	GLY	N-CA-C	-5.84	107.82	115.47
1	B	491	ALA	N-CA-CB	5.84	120.35	110.49
1	C	30	HIS	N-CA-C	-5.83	102.88	108.07
1	C	629	PHE	CA-CB-CG	-5.83	107.97	113.80
1	D	744	GLU	N-CA-C	5.83	118.11	111.11
1	B	661	LYS	CA-C-O	5.83	126.89	119.54
1	A	560	PRO	CA-N-CD	-5.82	103.85	112.00
1	D	110	ASN	CA-CB-CG	-5.82	106.78	112.60
1	C	629	PHE	CB-CA-C	-5.82	97.83	109.35
1	C	1003	VAL	CA-C-N	-5.81	111.97	120.75
1	C	1003	VAL	C-N-CA	-5.81	111.97	120.75
1	A	964	GLN	N-CA-C	-5.81	105.03	111.71
1	B	478	VAL	N-CA-C	5.81	115.99	110.53
1	A	688	PRO	CA-C-N	-5.81	110.81	120.68
1	A	688	PRO	C-N-CA	-5.81	110.81	120.68
1	B	219	THR	N-CA-CB	5.81	118.76	110.16
1	C	274	PHE	CA-CB-CG	-5.81	107.99	113.80
1	B	1005	ALA	O-C-N	5.81	128.82	122.20
1	C	927	THR	CA-C-O	5.81	124.93	119.59
1	A	1006	GLU	N-CA-CB	5.80	120.54	110.39
1	D	100	TYR	CA-CB-CG	-5.80	103.46	113.90
1	D	553	TRP	CA-CB-CG	-5.80	102.58	113.60
1	B	836	ILE	N-CA-CB	5.80	117.99	111.21
1	D	941	THR	CA-CB-OG1	-5.80	100.90	109.60
1	A	788	PRO	N-CA-CB	5.79	108.35	103.25
1	C	170	GLU	N-CA-CB	5.78	120.00	110.69
1	B	462	SER	N-CA-CB	-5.78	103.56	111.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	876	THR	CA-CB-CG2	5.78	120.33	110.50
1	D	671	ASP	CA-CB-CG	5.78	118.38	112.60
1	C	854	LYS	N-CA-C	5.78	118.27	109.95
1	B	424	ASN	CB-CA-C	-5.77	101.03	110.85
1	C	424	ASN	CA-CB-CG	-5.77	106.83	112.60
1	D	996	ASP	N-CA-C	-5.77	104.37	111.75
1	D	802	ASP	CA-C-N	5.76	125.86	119.87
1	D	802	ASP	C-N-CA	5.76	125.86	119.87
1	C	687	GLN	CA-C-N	5.76	127.04	119.84
1	C	687	GLN	C-N-CA	5.76	127.04	119.84
1	C	901	GLY	N-CA-C	-5.76	100.59	112.34
1	B	314	GLU	N-CA-CB	5.76	119.61	110.57
1	B	757	GLN	N-CA-C	5.76	118.18	107.99
1	D	229	THR	N-CA-C	5.76	118.27	108.02
1	B	115	PRO	CA-N-CD	-5.75	103.94	112.00
1	C	220	THR	CB-CA-C	5.75	120.17	110.79
1	D	550	ALA	N-CA-CB	5.75	118.57	110.12
1	A	697	THR	CA-C-O	-5.75	114.15	120.24
1	B	280	ASP	CA-CB-CG	5.75	118.35	112.60
1	D	300	LEU	N-CA-C	5.75	119.46	110.32
1	B	829	THR	N-CA-CB	5.75	119.57	110.55
1	A	444	VAL	CB-CA-C	-5.74	104.53	111.88
1	B	244	VAL	N-CA-C	5.74	116.75	108.48
1	A	187	MET	N-CA-C	5.74	118.63	108.24
1	D	223	SER	CB-CA-C	5.74	119.73	109.29
1	A	792	ASP	CA-CB-CG	5.74	118.33	112.60
1	B	41	GLU	N-CA-C	-5.73	105.03	111.28
1	B	136	GLU	N-CA-C	5.73	116.94	108.86
1	C	464	HIS	CA-C-N	-5.73	117.01	121.82
1	C	464	HIS	C-N-CA	-5.73	117.01	121.82
1	C	579	ASP	CA-CB-CG	5.73	118.33	112.60
1	D	554	GLN	CB-CA-C	5.73	120.42	110.68
1	A	557	ARG	NE-CZ-NH2	-5.72	114.05	119.20
1	A	932	PRO	N-CA-CB	5.72	108.28	103.25
1	C	84	VAL	CB-CA-C	-5.72	105.30	111.59
1	B	22	THR	N-CA-C	-5.72	106.29	113.72
1	C	159	VAL	CB-CA-C	-5.71	105.06	111.80
1	C	991	MET	N-CA-C	5.71	117.67	110.24
1	B	224	ASP	CA-CB-CG	5.71	118.31	112.60
1	B	289	VAL	CA-C-N	-5.70	114.95	122.99
1	B	289	VAL	C-N-CA	-5.70	114.95	122.99
1	D	242	ALA	CA-C-N	-5.70	115.14	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	242	ALA	C-N-CA	-5.70	115.14	123.00
1	A	249	GLU	CG-CD-OE2	-5.70	105.30	118.40
1	A	479	ASP	CA-C-O	5.69	127.82	121.22
1	D	396	PRO	N-CA-CB	5.69	109.53	103.39
1	A	792	ASP	CA-C-N	5.69	127.66	120.72
1	A	792	ASP	C-N-CA	5.69	127.66	120.72
1	A	961	ARG	N-CA-C	-5.69	103.17	111.30
1	C	125	LEU	N-CA-C	5.69	117.74	108.76
1	A	439	ARG	N-CA-C	-5.68	106.18	113.23
1	C	537	GLU	N-CA-CB	5.68	120.18	110.57
1	B	97	ALA	N-CA-CB	5.68	116.90	110.03
1	D	113	PHE	CA-CB-CG	-5.67	108.12	113.80
1	A	636	ILE	CB-CA-C	-5.67	103.13	110.84
1	B	332	PHE	N-CA-C	5.66	117.92	109.59
1	A	142	ILE	N-CA-CB	-5.66	103.25	111.52
1	B	1007	PHE	N-CA-CB	-5.66	102.30	110.56
1	C	744	GLU	N-CA-CB	5.66	118.97	110.53
1	A	114	VAL	N-CA-CB	-5.66	103.29	111.21
1	D	550	ALA	N-CA-C	5.65	117.44	111.28
1	C	943	GLU	CA-C-O	5.65	127.03	120.14
1	C	927	THR	CA-C-N	5.65	126.90	119.84
1	C	927	THR	C-N-CA	5.65	126.90	119.84
1	D	672	VAL	CB-CA-C	-5.64	101.81	110.50
1	A	438	GLU	CA-C-N	-5.64	111.73	121.66
1	A	438	GLU	C-N-CA	-5.64	111.73	121.66
1	B	300	LEU	N-CA-C	5.64	119.44	109.96
1	A	679	LEU	N-CA-C	5.64	117.88	109.25
1	D	1018	LEU	CB-CA-C	-5.64	100.49	109.80
1	A	186	VAL	N-CA-C	5.63	115.71	107.37
1	A	900	LEU	N-CA-CB	5.63	118.57	110.06
1	D	260	LEU	CA-C-O	5.63	126.33	120.30
1	C	124	SER	CA-C-N	-5.63	110.83	121.63
1	C	124	SER	C-N-CA	-5.63	110.83	121.63
1	C	240	LEU	CA-C-N	-5.63	114.83	122.77
1	C	240	LEU	C-N-CA	-5.63	114.83	122.77
1	C	65	ALA	CA-C-O	5.62	124.75	119.13
1	D	612	THR	N-CA-CB	5.62	118.56	109.90
1	C	1006	GLU	CG-CD-OE1	5.62	131.34	118.40
1	D	607	VAL	CA-CB-CG1	-5.62	100.84	110.40
1	D	447	ASP	CA-C-O	5.62	125.23	119.05
1	A	376	ILE	N-CA-C	5.61	116.25	110.36
1	C	566	PHE	CA-CB-CG	-5.61	108.19	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	989	PHE	N-CA-C	5.61	118.59	109.06
1	C	610	ASP	N-CA-C	-5.61	106.29	113.02
1	D	750	GLU	CB-CA-C	5.61	119.84	109.70
1	B	83	THR	N-CA-CB	5.60	118.63	109.95
1	C	410	VAL	CB-CA-C	-5.60	104.14	111.81
1	A	823	LEU	N-CA-C	-5.60	105.57	112.90
1	D	798	ALA	CA-C-N	5.59	130.19	120.68
1	D	798	ALA	C-N-CA	5.59	130.19	120.68
1	C	160	GLY	N-CA-C	5.59	118.75	110.42
1	B	880	ALA	N-CA-C	-5.58	105.73	112.54
1	B	619	GLU	N-CA-C	-5.58	105.29	111.71
1	B	980	GLU	N-CA-CB	5.58	119.92	110.49
1	A	206	SER	N-CA-C	5.58	117.45	109.14
1	C	626	PHE	N-CA-CB	5.58	118.97	110.44
1	C	227	VAL	O-C-N	5.57	128.93	122.97
1	C	748	CYS	N-CA-CB	5.57	119.32	110.57
1	A	150	PHE	CA-CB-CG	-5.57	108.23	113.80
1	D	210	ARG	NE-CZ-NH1	5.57	127.07	121.50
1	D	764	PHE	N-CA-C	5.57	118.78	110.14
1	A	272	ALA	CB-CA-C	-5.57	102.87	110.22
1	C	675	GLN	CB-CG-CD	-5.57	103.14	112.60
1	A	284	GLY	CA-C-N	-5.57	113.54	121.50
1	A	284	GLY	C-N-CA	-5.57	113.54	121.50
1	B	187	MET	CB-CA-C	5.57	119.40	110.16
1	B	765	LEU	CA-C-N	5.57	128.01	120.38
1	B	765	LEU	C-N-CA	5.57	128.01	120.38
1	A	750	GLU	O-C-N	5.56	130.06	123.33
1	D	310	ARG	N-CA-CB	5.56	119.51	110.77
1	D	933	SER	CA-C-N	-5.56	112.88	121.56
1	D	933	SER	C-N-CA	-5.56	112.88	121.56
1	B	638	VAL	N-CA-CB	-5.56	103.69	111.25
1	A	321	THR	CB-CA-C	5.56	118.57	109.90
1	D	967	LEU	CA-C-N	5.56	127.67	120.44
1	D	967	LEU	C-N-CA	5.56	127.67	120.44
1	C	55	ASN	N-CA-CB	5.55	118.56	109.95
1	D	811	LYS	N-CA-CB	5.55	118.02	109.91
1	A	249	GLU	CB-CG-CD	-5.55	103.16	112.60
1	A	255	ARG	CA-CB-CG	-5.54	103.03	114.10
1	B	306	PRO	N-CA-CB	5.54	106.42	102.65
1	C	549	PHE	CA-CB-CG	-5.54	108.27	113.80
1	B	168	PRO	N-CA-C	5.53	119.55	111.03
1	D	1018	LEU	N-CA-C	5.53	119.00	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	460	ASN	CA-CB-CG	5.53	118.13	112.60
1	C	621	LYS	CA-C-N	5.53	128.14	120.29
1	C	621	LYS	C-N-CA	5.53	128.14	120.29
1	B	192	SER	CA-C-O	-5.52	115.53	121.38
1	D	75	GLU	CA-C-O	5.52	126.45	120.55
1	D	526	LEU	N-CA-C	-5.51	102.26	110.20
1	B	750	GLU	N-CA-CB	5.51	121.78	111.53
1	B	407	LEU	CA-C-N	-5.51	113.55	121.42
1	B	407	LEU	C-N-CA	-5.51	113.55	121.42
1	C	842	TRP	N-CA-CB	5.50	119.60	110.52
1	D	382	ASN	CA-CB-CG	-5.50	107.10	112.60
1	D	834	VAL	CA-C-N	-5.50	115.35	123.05
1	D	834	VAL	C-N-CA	-5.50	115.35	123.05
1	D	172	ASP	CB-CA-C	-5.50	101.27	110.29
1	B	245	GLN	N-CA-CB	5.50	120.48	111.08
1	A	571	VAL	CB-CA-C	-5.49	103.33	111.19
1	D	159	VAL	N-CA-C	5.49	116.89	111.67
1	D	662	PRO	O-C-N	5.49	130.04	122.64
1	A	272	ALA	O-C-N	5.48	126.70	121.71
1	B	135	GLN	O-C-N	5.48	128.41	122.11
1	B	859	ASP	CA-C-N	5.48	127.04	120.13
1	B	859	ASP	C-N-CA	5.48	127.04	120.13
1	C	675	GLN	CA-C-N	-5.48	116.64	122.67
1	C	675	GLN	C-N-CA	-5.48	116.64	122.67
1	B	213	SER	N-CA-C	5.48	117.30	109.14
1	A	770	ILE	N-CA-C	-5.47	98.16	106.42
1	D	626	PHE	N-CA-C	5.47	119.80	113.18
1	C	226	HIS	ND1-CE1-NE2	5.46	113.86	108.40
1	A	611	ARG	CA-C-O	5.46	126.40	120.12
1	C	168	PRO	N-CA-C	5.46	119.05	110.80
1	D	724	GLU	CA-C-N	-5.46	115.41	123.05
1	D	724	GLU	C-N-CA	-5.46	115.41	123.05
1	D	931	PHE	CB-CA-C	5.46	115.90	110.33
1	A	358	GLU	CA-C-N	5.46	131.50	122.33
1	A	358	GLU	C-N-CA	5.46	131.50	122.33
1	C	482	ARG	CD-NE-CZ	-5.46	116.76	124.40
1	A	1004	SER	N-CA-CB	5.46	118.41	109.95
1	D	731	PRO	N-CA-CB	5.45	108.18	103.27
1	C	501	PRO	CB-CA-C	-5.45	102.69	110.75
1	D	257	THR	CA-C-N	-5.45	115.85	123.10
1	D	257	THR	C-N-CA	-5.45	115.85	123.10
1	D	512	PHE	CA-CB-CG	-5.45	108.35	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	ARG	N-CA-C	5.45	120.08	113.38
1	D	634	GLN	CA-C-O	5.45	125.09	119.97
1	A	504	ALA	CB-CA-C	5.44	119.55	109.54
1	C	713	HIS	CA-C-N	-5.44	116.08	123.10
1	C	713	HIS	C-N-CA	-5.44	116.08	123.10
1	C	877	PRO	N-CA-CB	5.44	108.50	103.39
1	A	980	GLU	N-CA-C	5.44	117.97	111.71
1	B	763	GLY	N-CA-C	-5.44	108.35	115.47
1	C	518	TRP	CB-CA-C	-5.44	98.34	110.19
1	C	945	ASN	CA-CB-CG	-5.44	107.16	112.60
1	D	661	LYS	N-CA-CB	5.44	120.60	111.03
1	A	556	PHE	O-C-N	5.43	127.74	122.09
1	B	166	ARG	N-CA-C	5.43	119.53	113.02
1	C	777	LEU	CA-C-O	5.42	124.79	118.77
1	C	864	MET	N-CA-CB	5.42	119.25	110.42
1	B	721	ARG	N-CA-CB	5.41	119.24	110.42
1	C	31	PRO	N-CA-CB	5.41	108.32	103.08
1	D	964	GLN	N-CA-C	-5.41	105.47	111.36
1	D	48	SER	N-CA-C	5.40	117.54	108.73
1	B	351	ILE	N-CA-C	5.40	115.09	106.88
1	A	504	ALA	CA-C-N	-5.40	111.22	122.07
1	A	504	ALA	C-N-CA	-5.40	111.22	122.07
1	D	1017	GLN	N-CA-C	5.40	117.42	108.13
1	A	847	LYS	CA-C-N	-5.40	115.02	122.30
1	A	847	LYS	C-N-CA	-5.40	115.02	122.30
1	B	668	VAL	O-C-N	5.40	127.25	121.10
1	C	252	ASP	CA-CB-CG	5.40	118.00	112.60
1	B	986	ILE	CA-C-N	-5.39	115.56	123.00
1	B	986	ILE	C-N-CA	-5.39	115.56	123.00
1	C	453	VAL	CA-C-N	-5.39	115.43	121.85
1	C	453	VAL	C-N-CA	-5.39	115.43	121.85
1	D	870	VAL	N-CA-C	5.39	116.74	108.71
1	A	89	ASN	CA-C-N	-5.39	111.98	120.60
1	A	89	ASN	C-N-CA	-5.39	111.98	120.60
1	A	396	PRO	N-CA-C	5.39	121.02	113.53
1	B	853	ARG	CA-C-N	-5.39	113.39	123.03
1	B	853	ARG	C-N-CA	-5.39	113.39	123.03
1	A	224	ASP	CA-CB-CG	5.38	117.98	112.60
1	A	799	THR	CB-CA-C	-5.38	102.67	110.96
1	C	987	ASP	CA-CB-CG	-5.38	107.22	112.60
1	D	508	GLU	N-CA-CB	5.38	119.36	110.69
1	A	583	ASN	CA-CB-CG	5.38	117.98	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	753	ASN	CA-CB-CG	5.38	117.98	112.60
1	B	323	ILE	N-CA-CB	5.38	117.46	110.57
1	C	84	VAL	N-CA-CB	-5.38	102.45	111.38
1	D	140	ARG	CA-C-N	-5.38	115.64	123.06
1	D	140	ARG	C-N-CA	-5.38	115.64	123.06
1	D	480	PRO	CA-C-N	5.38	129.20	120.60
1	D	480	PRO	C-N-CA	5.38	129.20	120.60
1	A	661	LYS	O-C-N	5.37	126.29	121.35
1	B	111	PRO	C-N-CD	5.37	132.42	120.60
1	B	257	THR	CA-C-O	5.37	125.94	120.24
1	D	425	ARG	NE-CZ-NH1	5.37	126.87	121.50
1	A	226	HIS	CB-CA-C	-5.37	98.48	109.38
1	C	22	THR	N-CA-C	-5.37	105.47	112.23
1	B	490	GLY	CA-C-N	5.37	131.79	121.54
1	B	490	GLY	C-N-CA	5.37	131.79	121.54
1	A	356	ARG	NE-CZ-NH1	5.37	126.87	121.50
1	C	69	VAL	CA-C-N	5.37	126.55	119.84
1	C	69	VAL	C-N-CA	5.37	126.55	119.84
1	B	781	ARG	N-CA-C	5.36	117.41	108.99
1	B	453	VAL	CA-C-N	-5.36	115.41	122.16
1	B	453	VAL	C-N-CA	-5.36	115.41	122.16
1	C	249	GLU	N-CA-C	5.36	118.22	109.59
1	C	612	THR	N-CA-C	-5.35	103.33	110.07
1	D	590	GLY	N-CA-C	5.35	121.06	114.69
1	D	777	LEU	CA-C-O	5.35	124.71	118.77
1	D	326	GLU	N-CA-CB	5.35	120.86	111.55
1	B	706	THR	CB-CA-C	-5.34	102.22	112.43
1	C	842	TRP	N-CA-C	-5.34	100.99	109.76
1	A	4	THR	N-CA-C	-5.34	106.63	112.72
1	D	878	HIS	CA-C-N	5.34	125.64	119.92
1	D	878	HIS	C-N-CA	5.34	125.64	119.92
1	B	359	HIS	N-CA-C	5.34	118.13	109.06
1	D	172	ASP	CA-CB-CG	-5.34	107.26	112.60
1	A	352	ARG	CB-CA-C	-5.33	103.46	111.73
1	C	841	ALA	CA-C-N	-5.33	114.71	122.65
1	C	841	ALA	C-N-CA	-5.33	114.71	122.65
1	D	319	ASP	N-CA-CB	5.33	119.05	110.42
1	B	542	MET	N-CA-C	5.32	116.98	108.41
1	C	579	ASP	N-CA-C	5.32	117.70	110.35
1	A	612	THR	CA-C-O	5.32	125.57	119.61
1	C	668	VAL	C-N-CD	-5.32	103.18	125.00
1	B	469	ASP	CA-CB-CG	-5.31	107.29	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	378	LEU	O-C-N	5.31	127.75	122.12
1	D	852	SER	N-CA-C	5.31	117.05	108.34
1	B	793	ILE	CB-CA-C	-5.31	104.97	111.92
1	A	279	ILE	N-CA-CB	5.31	119.99	111.23
1	A	664	ALA	O-C-N	5.31	129.65	122.59
1	D	220	THR	N-CA-C	-5.30	99.13	108.20
1	C	598	ASP	CA-CB-CG	5.30	117.90	112.60
1	B	877	PRO	N-CA-CB	5.30	107.77	103.32
1	B	82	ASP	CA-CB-CG	5.29	117.89	112.60
1	B	272	ALA	N-CA-CB	5.29	116.66	111.10
1	A	866	ILE	N-CA-C	5.29	116.91	108.87
1	C	447	ASP	N-CA-C	5.29	119.70	112.88
1	B	302	SER	N-CA-C	-5.29	100.88	108.60
1	C	939	CYS	N-CA-CB	5.29	118.58	110.49
1	B	402	CYS	CA-CB-SG	-5.28	102.25	114.40
1	D	134	LEU	N-CA-C	5.28	119.71	113.16
1	B	95	TYR	CA-CB-CG	-5.28	104.39	113.90
1	A	462	SER	N-CA-C	-5.28	105.12	112.30
1	C	27	LEU	N-CA-C	5.28	117.63	110.35
1	C	614	HIS	N-CA-C	-5.28	104.06	110.13
1	D	559	TYR	CB-CA-C	-5.27	104.95	110.17
1	D	788	PRO	O-C-N	5.27	129.28	122.85
1	C	553	TRP	CA-CB-CG	-5.27	103.58	113.60
1	B	344	LEU	O-C-N	5.27	129.38	123.27
1	A	621	LYS	O-C-N	-5.27	116.61	122.09
1	B	556	PHE	CA-C-N	-5.27	112.31	120.31
1	B	556	PHE	C-N-CA	-5.27	112.31	120.31
1	D	553	TRP	N-CA-CB	5.26	117.78	109.94
1	C	193	ASP	CA-C-O	5.26	125.85	119.38
1	C	542	MET	N-CA-C	5.26	116.82	108.67
1	B	738	PRO	N-CA-CB	5.26	107.72	103.36
1	D	826	THR	N-CA-C	5.25	116.98	108.26
1	A	551	LYS	N-CA-C	-5.25	104.81	111.11
1	B	62	TRP	N-CA-CB	-5.25	102.32	110.57
1	B	363	HIS	CA-CB-CG	-5.25	108.55	113.80
1	A	770	ILE	CB-CA-C	-5.25	105.93	111.23
1	D	1022	GLN	N-CA-C	5.25	117.63	108.76
1	C	802	ASP	CA-C-N	5.25	125.30	119.32
1	C	802	ASP	C-N-CA	5.25	125.30	119.32
1	B	584	PRO	N-CA-CB	5.24	108.80	102.72
1	D	656	VAL	N-CA-C	5.24	116.21	108.45
1	B	681	GLU	N-CA-CB	5.24	118.96	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	297	ASN	CA-C-O	-5.24	116.44	120.48
1	A	80	GLU	N-CA-C	-5.24	106.67	113.16
1	B	464	HIS	CA-CB-CG	-5.24	108.56	113.80
1	C	521	LYS	CB-CA-C	5.23	119.48	110.79
1	D	31	PRO	CB-CA-C	-5.23	106.25	111.17
1	A	140	ARG	N-CA-CB	-5.23	102.80	110.85
1	D	351	ILE	N-CA-CB	-5.23	105.86	111.46
1	A	675	GLN	CA-C-N	-5.23	116.20	122.16
1	A	675	GLN	C-N-CA	-5.23	116.20	122.16
1	A	742	THR	N-CA-C	5.23	117.36	109.41
1	B	121	GLY	CA-C-N	-5.23	115.69	123.11
1	B	121	GLY	C-N-CA	-5.23	115.69	123.11
1	C	350	LEU	CB-CA-C	-5.23	103.81	111.23
1	C	5	ASP	CA-C-O	5.23	124.80	119.05
1	A	648	ASP	N-CA-C	5.22	118.68	112.72
1	D	964	GLN	CA-C-N	-5.22	113.49	120.54
1	D	964	GLN	C-N-CA	-5.22	113.49	120.54
1	A	272	ALA	N-CA-C	5.22	112.92	108.22
1	B	257	THR	CA-C-N	-5.22	116.36	123.10
1	B	257	THR	C-N-CA	-5.22	116.36	123.10
1	D	874	SER	N-CA-C	5.22	117.37	111.11
1	A	360	HIS	C-N-CD	-5.22	103.61	125.00
1	A	493	THR	CA-CB-CG2	-5.22	101.63	110.50
1	B	9	VAL	CA-C-N	5.22	127.33	120.60
1	B	9	VAL	C-N-CA	5.22	127.33	120.60
1	C	221	GLN	N-CA-C	5.22	115.94	108.74
1	D	996	ASP	N-CA-CB	5.22	118.38	110.14
1	C	126	THR	CA-CB-CG2	-5.21	101.64	110.50
1	C	822	LEU	N-CA-CB	5.21	117.75	109.51
1	D	701	VAL	N-CA-C	5.21	116.81	108.89
1	D	211	ASP	N-CA-C	5.21	118.17	110.46
1	D	258	VAL	CA-C-O	-5.21	114.97	120.39
1	A	520	ILE	N-CA-CB	5.21	116.98	110.47
1	C	435	ALA	CB-CA-C	-5.21	102.48	110.81
1	C	837	THR	O-C-N	-5.21	117.10	123.30
1	A	512	PHE	CB-CA-C	-5.20	101.54	108.87
1	B	239	VAL	CA-C-N	-5.20	115.55	122.72
1	B	239	VAL	C-N-CA	-5.20	115.55	122.72
1	B	317	THR	CA-CB-OG1	-5.20	101.80	109.60
1	B	854	LYS	N-CA-C	5.20	117.76	109.81
1	C	184	LEU	CA-C-N	-5.20	115.47	122.95
1	C	184	LEU	C-N-CA	-5.20	115.47	122.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	SER	CB-CA-C	5.19	119.22	109.71
1	D	6	SER	O-C-N	5.19	129.31	122.97
1	D	989	PHE	CA-CB-CG	-5.19	108.61	113.80
1	A	58	TRP	N-CA-CB	-5.19	101.87	111.52
1	A	662	PRO	N-CA-CB	5.19	107.67	103.36
1	A	937	LEU	CA-C-O	-5.19	116.05	121.55
1	D	968	MET	N-CA-C	5.19	116.62	111.07
1	B	384	PHE	CA-C-N	5.18	131.37	122.09
1	B	384	PHE	C-N-CA	5.18	131.37	122.09
1	C	650	GLU	O-C-N	5.18	129.59	123.27
1	B	430	PRO	N-CA-CB	5.18	108.99	103.39
1	B	613	PRO	CB-CA-C	-5.17	104.99	111.56
1	D	554	GLN	N-CA-C	5.17	117.59	111.33
1	B	199	ASP	CA-CB-CG	5.17	117.77	112.60
1	B	485	GLN	O-C-N	5.17	129.27	123.27
1	C	440	VAL	CB-CA-C	-5.17	105.15	111.92
1	B	648	ASP	CA-C-N	-5.17	113.63	121.53
1	B	648	ASP	C-N-CA	-5.17	113.63	121.53
1	D	957	PHE	CB-CA-C	-5.17	101.05	111.17
1	C	448	ARG	N-CA-C	5.16	119.05	112.34
1	D	835	LEU	N-CA-C	5.16	116.94	108.52
1	A	704	ASN	N-CA-C	5.16	118.16	109.95
1	D	505	ARG	CD-NE-CZ	-5.16	117.17	124.40
1	D	674	PRO	CB-CA-C	-5.16	103.05	111.56
1	D	453	VAL	CA-C-N	-5.16	115.66	122.16
1	D	453	VAL	C-N-CA	-5.16	115.66	122.16
1	B	1018	LEU	N-CA-CB	-5.16	101.98	111.37
1	B	304	GLU	N-CA-C	-5.15	107.12	113.41
1	B	167	LEU	CA-C-N	5.15	125.39	119.83
1	B	167	LEU	C-N-CA	5.15	125.39	119.83
1	A	958	ASN	CA-C-O	-5.15	115.22	120.89
1	D	748	CYS	N-CA-CB	5.15	120.35	111.13
1	D	78	LEU	CA-C-N	5.15	124.94	119.28
1	D	78	LEU	C-N-CA	5.15	124.94	119.28
1	D	190	ARG	CB-CA-C	5.15	119.60	110.85
1	A	231	PHE	CA-CB-CG	-5.15	108.65	113.80
1	B	310	ARG	N-CA-C	-5.14	101.49	109.72
1	C	13	ARG	N-CA-CB	-5.14	102.02	110.14
1	C	579	ASP	CA-C-N	5.14	127.42	120.38
1	C	579	ASP	C-N-CA	5.14	127.42	120.38
1	A	737	ILE	CA-C-N	5.14	125.54	119.99
1	A	737	ILE	C-N-CA	5.14	125.54	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	777	LEU	CA-C-O	5.14	124.47	118.77
1	D	339	ASN	N-CA-C	5.13	118.71	111.52
1	A	310	ARG	CA-C-N	-5.13	115.87	123.05
1	A	310	ARG	C-N-CA	-5.13	115.87	123.05
1	A	319	ASP	CB-CA-C	5.13	119.02	111.17
1	A	280	ASP	CA-CB-CG	5.13	117.73	112.60
1	A	612	THR	N-CA-C	-5.13	102.18	109.62
1	C	767	GLN	N-CA-C	5.12	116.31	108.42
1	B	315	LEU	CA-C-N	-5.12	114.28	122.53
1	B	315	LEU	C-N-CA	-5.12	114.28	122.53
1	C	784	PHE	CA-CB-CG	-5.12	108.68	113.80
1	B	247	CYS	CA-CB-SG	-5.12	102.62	114.40
1	D	816	TYR	N-CA-C	5.12	118.62	112.38
1	D	233	ASP	CA-CB-CG	5.12	117.72	112.60
1	C	82	ASP	N-CA-CB	5.11	118.39	110.46
1	B	75	GLU	CA-C-N	-5.11	112.95	121.94
1	B	75	GLU	C-N-CA	-5.11	112.95	121.94
1	C	273	PRO	CB-CA-C	-5.11	103.19	110.75
1	C	111	PRO	O-C-N	5.11	127.49	121.46
1	C	142	ILE	N-CA-CB	-5.11	104.06	111.52
1	A	429	ASP	O-C-N	5.11	127.91	121.12
1	C	409	VAL	CA-CB-CG1	5.11	119.08	110.40
1	A	721	ARG	N-CA-CB	5.11	118.58	110.16
1	B	211	ASP	CA-CB-CG	-5.11	107.50	112.60
1	B	513	PRO	CB-CA-C	-5.10	105.08	111.56
1	B	748	CYS	N-CA-CB	5.10	119.02	110.85
1	C	347	LYS	N-CA-C	-5.10	102.29	110.10
1	B	906	TYR	O-C-N	5.10	124.81	121.14
1	C	282	ARG	NE-CZ-NH2	5.10	123.79	119.20
1	C	351	ILE	CB-CA-C	-5.10	105.11	111.08
1	D	272	ALA	O-C-N	5.09	127.18	121.32
1	A	26	ARG	N-CA-C	5.09	117.54	109.24
1	A	838	THR	N-CA-C	5.09	117.89	109.85
1	B	672	VAL	CA-C-N	-5.09	114.76	122.29
1	B	672	VAL	C-N-CA	-5.09	114.76	122.29
1	C	365	GLN	CA-C-N	-5.09	116.39	122.90
1	C	365	GLN	C-N-CA	-5.09	116.39	122.90
1	D	221	GLN	CA-CB-CG	-5.09	103.92	114.10
1	B	679	LEU	N-CA-C	5.09	118.11	109.76
1	A	113	PHE	N-CA-C	5.08	118.09	109.76
1	B	118	ASN	N-CA-C	5.08	118.36	108.21
1	C	45	ASP	CA-CB-CG	-5.08	107.52	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	533	LEU	N-CA-C	5.08	116.67	108.34
1	B	44	THR	CA-C-N	-5.08	115.28	122.34
1	B	44	THR	C-N-CA	-5.08	115.28	122.34
1	C	502	MET	O-C-N	-5.07	117.26	123.30
1	C	485	GLN	N-CA-CB	5.07	120.60	111.37
1	A	167	LEU	CB-CA-C	5.07	116.67	108.91
1	A	879	PRO	CB-CA-C	-5.07	105.12	111.56
1	C	512	PHE	CA-C-O	5.07	126.75	120.87
1	C	478	VAL	N-CA-C	5.07	115.30	110.53
1	D	433	LEU	CA-C-O	5.07	123.79	119.13
1	B	331	GLY	O-C-N	-5.06	116.12	122.70
1	D	150	PHE	N-CA-C	5.06	116.22	108.42
1	D	216	HIS	CA-CB-CG	-5.06	108.74	113.80
1	C	450	HIS	CA-C-O	-5.06	116.00	119.29
1	B	987	ASP	N-CA-C	5.06	117.22	109.07
1	C	280	ASP	CA-CB-CG	5.06	117.66	112.60
1	C	735	HIS	CB-CA-C	5.06	120.70	110.38
1	A	64	PRO	CB-CA-C	-5.05	103.82	112.26
1	C	100	TYR	CA-CB-CG	-5.05	104.80	113.90
1	C	642	TYR	N-CA-C	-5.05	102.22	110.20
1	D	534	ILE	N-CA-C	5.05	115.25	107.77
1	C	399	TYR	N-CA-C	5.05	116.47	111.07
1	A	993	ILE	N-CA-CB	5.05	119.56	111.23
1	B	769	TRP	CB-CA-C	-5.05	99.39	109.33
1	D	154	CYS	N-CA-CB	5.05	119.00	110.77
1	B	483	PRO	CB-CA-C	-5.04	104.77	111.23
1	A	638	VAL	N-CA-C	5.04	115.11	107.80
1	B	300	LEU	CA-C-O	5.04	126.72	120.92
1	D	416	GLU	N-CA-CB	5.04	118.42	110.71
1	B	134	LEU	N-CA-C	5.04	119.42	113.12
1	B	104	THR	CA-C-N	-5.04	113.39	120.39
1	B	104	THR	C-N-CA	-5.04	113.39	120.39
1	B	740	LEU	N-CA-C	5.04	116.62	108.41
1	C	736	ALA	N-CA-C	-5.04	102.12	109.63
1	C	986	ILE	CB-CG1-CD1	-5.04	103.22	113.80
1	C	429	ASP	O-C-N	5.04	126.95	121.36
1	C	674	PRO	CA-C-N	-5.04	114.68	122.08
1	C	674	PRO	C-N-CA	-5.04	114.68	122.08
1	D	967	LEU	O-C-N	5.04	127.90	122.11
1	C	534	ILE	CA-C-N	-5.03	114.42	121.72
1	C	534	ILE	C-N-CA	-5.03	114.42	121.72
1	D	210	ARG	N-CA-CB	5.03	119.00	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	409	VAL	N-CA-C	5.03	115.82	108.53
1	A	63	PHE	CA-C-O	5.03	124.83	119.50
1	D	548	GLY	N-CA-C	-5.03	108.39	114.92
1	B	292	ARG	N-CA-CB	5.02	118.66	110.77
1	A	927	THR	CB-CA-C	5.02	115.92	110.15
1	C	920	LEU	CA-C-N	5.02	124.95	119.78
1	C	920	LEU	C-N-CA	5.02	124.95	119.78
1	C	392	TYR	CA-C-N	-5.02	114.74	119.76
1	C	392	TYR	C-N-CA	-5.02	114.74	119.76
1	D	246	MET	N-CA-C	5.02	117.03	109.41
1	A	103	VAL	CB-CA-C	-5.01	103.07	111.29
1	B	519	SER	N-CA-C	-5.01	102.63	110.10
1	A	48	SER	N-CA-C	5.01	116.89	108.73
1	A	85	VAL	N-CA-C	5.01	116.48	108.87
1	B	618	THR	N-CA-C	5.01	117.85	111.69
1	C	571	VAL	N-CA-C	5.00	115.69	108.48
1	C	715	SER	N-CA-CB	-5.00	103.98	110.88
1	B	835	LEU	N-CA-C	5.00	116.75	108.20
1	C	142	ILE	N-CA-C	5.00	115.32	108.12
1	D	567	VAL	CB-CA-C	-5.00	104.73	111.63

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	166	ARG	CA
1	A	187	MET	CA
1	A	903[A]	GLN	CA
1	A	903[B]	GLN	CA
1	B	118	ASN	CA
1	C	291	LEU	CA
1	C	503	TYR	CA
1	C	735	HIS	CA
1	C	980	GLU	CA
1	D	52[A]	ARG	CA
1	D	52[B]	ARG	CA
1	D	938	ARG	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	352	ARG	Mainchain

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	8238	0	7824	673	0
1	B	8238	0	7824	743	0
1	C	8238	0	7824	718	0
1	D	8238	0	7823	658	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	211	0	0	13	0
3	B	202	0	0	12	0
3	C	220	0	0	24	0
3	D	212	0	0	13	0
All	All	33805	0	31295	2736	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 43.

All (2736) 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:A:173:LEU:HB3	1:A:177:LEU:HD21	1.21	1.17
1:A:427:THR:HA	1:A:436:MET:HE1	1.24	1.15
1:B:734:SER:HB3	1:B:860:GLY:HA3	1.24	1.12
1:C:427:THR:HA	1:C:436:MET:HE1	1.17	1.11
1:A:777:LEU:HD21	1:A:889:ALA:HB2	1.28	1.10
1:B:427:THR:HA	1:B:436:MET:HE1	1.12	1.10
1:A:7:LEU:HD21	1:A:74:LEU:HD21	1.32	1.09
1:A:436:MET:HE3	1:A:467:ASN:HD22	1.15	1.08
1:D:650:GLU:HB3	1:D:670:LEU:HD12	1.21	1.07
1:D:427:THR:HA	1:D:436:MET:HE1	1.07	1.06
1:A:944:LEU:HD12	1:A:945:ASN:H	1.20	1.04
1:C:362:LEU:HD21	1:C:576:ILE:HD12	1.39	1.03
1:C:237:ARG:HB3	1:C:237:ARG:HH11	1.21	1.03
1:D:499:ILE:HG22	1:D:501:PRO:HD3	1.39	1.03
1:C:734:SER:HB3	1:C:860:GLY:HA3	1.39	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:746:ASP:HA	1:D:760:ARG:HG3	1.34	1.02
1:D:559:TYR:HB2	1:D:562:LEU:HD12	1.39	1.02
1:C:436:MET:HE3	1:C:467:ASN:HD22	1.21	1.00
1:B:673:ALA:HB1	1:B:674:PRO:HD2	1.44	0.99
1:B:858:ILE:HD13	1:B:864:MET:HB3	1.42	0.99
1:C:693:GLN:HG2	1:C:721:ARG:HD3	1.44	0.99
1:D:830:LEU:HD21	1:D:835:LEU:HB2	1.43	0.98
1:B:650:GLU:HB3	1:B:670:LEU:HD12	1.43	0.98
1:B:7:LEU:HD23	1:B:74:LEU:HD11	1.44	0.98
1:C:777:LEU:HD21	1:C:889:ALA:HB2	1.42	0.97
1:A:928:PRO:HB2	1:A:973:ARG:HH12	1.26	0.97
1:D:597:ASN:HD22	1:D:599:ARG:H	1.13	0.96
1:D:597:ASN:ND2	1:D:599:ARG:H	1.64	0.96
1:B:830:LEU:HD21	1:B:835:LEU:HB2	1.47	0.96
1:D:984:LEU:HD21	1:D:986:ILE:HD11	1.44	0.95
1:A:746:ASP:HA	1:A:760:ARG:HG3	1.44	0.95
1:B:595:THR:HG23	1:B:596:PRO:HA	1.50	0.93
1:C:568:TRP:HE1	1:C:604:ASN:ND2	1.66	0.93
1:B:367:MET:HB3	1:B:372:MET:HE3	1.49	0.93
1:D:673:ALA:HB1	1:D:674:PRO:HD2	1.51	0.93
1:D:251:ARG:HH11	1:D:251:ARG:HG3	1.31	0.93
1:A:360:HIS:ND1	1:A:361:PRO:HD2	1.84	0.92
1:B:730:LEU:HD12	1:B:730:LEU:H	1.32	0.92
1:D:230:ARG:HH11	1:D:230:ARG:HG3	1.34	0.92
1:B:246:MET:HE2	1:B:287:ASP:HB3	1.51	0.92
1:C:581:ASN:HD22	1:C:583:ASN:ND2	1.66	0.92
1:B:427:THR:HA	1:B:436:MET:CE	2.00	0.92
1:C:26:ARG:HD2	1:C:169:SER:HA	1.51	0.91
1:B:559:TYR:HB2	1:B:562:LEU:HD12	1.50	0.91
1:A:851:ILE:HD12	1:B:726:LEU:HD13	1.50	0.91
1:B:118:ASN:HB2	1:B:191:TRP:HD1	1.32	0.91
1:C:237:ARG:HB3	1:C:237:ARG:NH1	1.84	0.91
1:A:26:ARG:HH11	1:A:169:SER:HB3	1.37	0.90
1:A:255:ARG:HG3	1:A:255:ARG:HH11	1.35	0.90
1:C:928:PRO:HB2	1:C:973:ARG:HH11	1.33	0.90
1:D:352:ARG:HB2	1:D:385:ASN:HB2	1.53	0.90
1:B:43:ARG:HG2	1:B:43:ARG:HH11	1.36	0.90
1:B:830:LEU:CD2	1:B:835:LEU:HB2	2.02	0.90
1:C:427:THR:HA	1:C:436:MET:CE	2.02	0.90
1:C:1004:SER:HB3	1:C:1006:GLU:OE2	1.71	0.89
1:B:778:THR:HG22	1:B:779:PRO:HD2	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:VAL:HG13	1:A:240:LEU:HD11	1.54	0.89
1:A:427:THR:HA	1:A:436:MET:CE	2.03	0.89
1:B:89:ASN:ND2	1:B:205:MET:HB3	1.87	0.89
1:A:65:ALA:HB1	1:A:66:PRO:HD2	1.55	0.88
1:A:944:LEU:HD12	1:A:945:ASN:N	1.86	0.88
1:B:786:ARG:HD3	1:B:880:ALA:HB1	1.55	0.88
1:D:114:VAL:HG13	1:D:115:PRO:HD2	1.56	0.88
1:C:734:SER:HB3	1:C:860:GLY:CA	2.03	0.88
1:C:928:PRO:HB2	1:C:973:ARG:NH1	1.87	0.88
1:B:282:ARG:HH12	1:C:419:GLY:HA2	1.38	0.88
1:D:427:THR:HA	1:D:436:MET:CE	2.01	0.87
1:C:776:LEU:C	1:C:777:LEU:HD23	1.99	0.87
1:C:653[A]:HIS:CE1	1:C:667:GLU:HG2	2.09	0.87
1:A:433:LEU:HB3	1:A:434:PRO:HD3	1.57	0.87
1:D:830:LEU:CD2	1:D:835:LEU:HB2	2.05	0.86
1:D:360:HIS:CG	1:D:361:PRO:HD2	2.10	0.86
1:A:930:VAL:HA	1:A:973:ARG:HD3	1.55	0.86
1:D:377:LEU:HD22	1:D:708:TRP:HA	1.57	0.86
1:A:38:ASN:HD22	1:A:41:GLU:H	1.22	0.86
1:C:730:LEU:H	1:C:730:LEU:HD12	1.40	0.86
1:B:360:HIS:ND1	1:B:361:PRO:HD2	1.90	0.86
1:C:856:TYR:HD2	1:C:864:MET:HE1	1.41	0.86
1:B:444:VAL:O	1:B:448:ARG:HB3	1.77	0.85
1:A:740:LEU:HD12	1:A:741:THR:H	1.41	0.85
1:B:734:SER:CB	1:B:860:GLY:HA3	2.06	0.85
1:B:842:TRP:CZ3	1:B:852:SER:HB2	2.11	0.85
1:D:105:TYR:CE2	1:D:199:ASP:HB2	2.12	0.85
1:B:589:GLY:HA3	1:B:599:ARG:HA	1.58	0.84
1:C:362:LEU:CD2	1:C:576:ILE:HD12	2.07	0.84
1:D:102:ASN:ND2	1:D:201:ASP:HB2	1.90	0.84
1:A:63:PHE:HB3	1:A:64:PRO:HD2	1.59	0.84
1:A:7:LEU:CD2	1:A:74:LEU:HD21	2.06	0.84
1:B:427:THR:CA	1:B:436:MET:HE1	2.04	0.84
1:D:650:GLU:HB3	1:D:670:LEU:CD1	2.08	0.84
1:A:930:VAL:HA	1:A:973:ARG:CD	2.08	0.84
1:C:433:LEU:HB3	1:C:434:PRO:HD3	1.58	0.84
1:A:134:LEU:H	1:A:134:LEU:HD22	1.43	0.84
1:C:420:MET:HE2	1:C:426:LEU:HG	1.60	0.84
1:C:360:HIS:ND1	1:C:361:PRO:HD2	1.93	0.84
1:D:240:LEU:HD23	1:D:293:LEU:HD12	1.59	0.84
1:D:360:HIS:ND1	1:D:361:PRO:HD2	1.93	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:693:GLN:HG2	1:B:721:ARG:HD3	1.60	0.83
1:A:777:LEU:HD21	1:A:889:ALA:CB	2.08	0.83
1:C:597:ASN:HD22	1:C:599:ARG:H	1.25	0.83
1:D:559:TYR:HB2	1:D:562:LEU:CD1	2.08	0.83
1:A:38:ASN:ND2	1:A:41:GLU:H	1.76	0.83
1:D:202:MET:HE3	1:D:357:HIS:CD2	2.14	0.83
1:C:356:ARG:HH22	1:C:367:MET:HE2	1.44	0.82
1:A:746:ASP:CA	1:A:760:ARG:HG3	2.08	0.82
1:B:693:GLN:HG2	1:B:721:ARG:CD	2.08	0.82
1:C:902:PRO:HD2	1:C:903[B]:GLN:HG3	1.60	0.82
1:D:533:LEU:HD12	1:D:534:ILE:N	1.94	0.82
1:C:102:ASN:ND2	1:C:201:ASP:HB2	1.94	0.82
1:C:255:ARG:HH11	1:C:255:ARG:HG2	1.45	0.82
1:B:230:ARG:HH11	1:B:230:ARG:HG3	1.45	0.82
1:D:255:ARG:HG2	1:D:255:ARG:HH11	1.43	0.82
1:D:856:TYR:HB3	1:D:864:MET:HE2	1.61	0.82
1:C:668:VAL:CG1	1:C:669:PRO:HD2	2.09	0.82
1:D:603:MET:HE1	1:D:930:VAL:CG1	2.09	0.82
1:A:377:LEU:HD22	1:A:708:TRP:HA	1.62	0.82
1:A:658:LEU:HD22	1:A:688:PRO:HG2	1.59	0.82
1:B:118:ASN:HB2	1:B:191:TRP:CD1	2.15	0.82
1:B:30:HIS:HB2	1:B:31:PRO:HD2	1.62	0.81
1:B:141:ILE:HD13	1:B:143:PHE:CZ	2.16	0.81
1:C:9:VAL:O	1:C:12:GLN:HB3	1.81	0.81
1:C:568:TRP:HE1	1:C:604:ASN:HD22	1.26	0.81
1:A:650:GLU:HB3	1:A:670:LEU:HD12	1.61	0.81
1:A:878:HIS:CD2	1:A:1010:SER:HB3	2.16	0.81
1:A:436:MET:CE	1:A:467:ASN:HD22	1.93	0.80
1:C:125:LEU:HG	1:C:126:THR:N	1.95	0.80
1:C:777:LEU:HD21	1:C:889:ALA:CB	2.10	0.80
1:A:9:VAL:O	1:A:12:GLN:HB3	1.80	0.80
1:A:635:THR:HG21	1:A:679:LEU:HD13	1.64	0.80
1:B:658:LEU:HG	1:B:661:LYS:NZ	1.96	0.80
1:D:525:SER:HB2	3:D:4202:HOH:O	1.81	0.80
1:A:7:LEU:CD1	1:A:69:VAL:HG12	2.11	0.80
1:B:685:LEU:HB3	1:B:686:PRO:HD2	1.62	0.80
1:C:135:GLN:HE21	1:C:135:GLN:HA	1.44	0.80
1:C:347:LYS:NZ	1:C:675:GLN:HG3	1.97	0.80
1:C:942:ARG:HA	1:C:953:GLY:O	1.82	0.80
1:B:662:PRO:O	1:B:663:LEU:HD23	1.81	0.80
1:D:984:LEU:CD2	1:D:986:ILE:HD11	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:LEU:HB2	1:A:161:TYR:HB3	1.62	0.80
1:B:840:HIS:HB2	1:B:842:TRP:CZ3	2.16	0.80
1:B:856:TYR:HB3	1:B:864:MET:CE	2.13	0.80
1:B:928:PRO:HB2	1:B:973:ARG:HH11	1.46	0.80
1:C:685:LEU:HD23	1:C:686:PRO:HD3	1.62	0.80
1:A:856:TYR:HB3	1:A:864:MET:CE	2.12	0.79
1:A:202:MET:HE2	1:A:365:GLN:NE2	1.96	0.79
1:D:77:ASP:C	1:D:78:LEU:HD23	2.08	0.79
1:B:299:LYS:HB3	1:B:307:ASN:ND2	1.96	0.79
1:D:322:LEU:HD22	1:D:323:ILE:H	1.46	0.79
1:A:673:ALA:HB1	1:A:674:PRO:HD2	1.64	0.79
1:D:654:TRP:NE1	1:D:666:GLY:HA3	1.97	0.79
1:A:73:TRP:CZ2	1:A:122:CYS:HB3	2.17	0.79
1:B:835:LEU:C	1:B:836:ILE:HD13	2.07	0.79
1:A:367:MET:HB3	1:A:372:MET:CE	2.12	0.79
1:B:246:MET:HE2	1:B:287:ASP:CB	2.13	0.79
1:D:282:ARG:HH11	1:D:282:ARG:HG3	1.47	0.79
1:A:427:THR:CA	1:A:436:MET:HE1	2.09	0.79
1:D:237:ARG:CB	1:D:237:ARG:HH11	1.95	0.79
1:A:599:ARG:NH1	1:A:600:GLN:HE22	1.81	0.78
1:A:696:LEU:HD12	1:A:697:THR:N	1.97	0.78
1:C:100:TYR:HB2	1:C:203:TRP:CE3	2.17	0.78
1:A:202:MET:HA	1:A:573:GLN:HE22	1.47	0.78
1:C:105:TYR:HB3	1:C:106:PRO:HD2	1.65	0.78
1:B:73:TRP:CZ2	1:B:122:CYS:HB3	2.17	0.78
1:D:237:ARG:HH11	1:D:237:ARG:HB2	1.47	0.78
1:B:225:PHE:HB3	1:B:244:VAL:HG13	1.65	0.78
1:C:856:TYR:CD2	1:C:864:MET:HE1	2.17	0.78
1:B:102:ASN:ND2	1:B:201:ASP:HB2	1.99	0.78
1:D:890:GLN:NE2	1:D:890:GLN:H	1.81	0.78
1:B:786:ARG:HA	1:B:964:GLN:OE1	1.84	0.78
1:C:53:SER:O	1:C:54:LEU:HD23	1.84	0.78
1:C:945:ASN:OD1	1:C:950:GLN:HB2	1.83	0.78
1:D:52[B]:ARG:HG3	1:D:133:TRP:CH2	2.19	0.78
1:D:102:ASN:HD22	1:D:201:ASP:HB2	1.49	0.78
1:A:52[B]:ARG:HH22	1:A:130:ASP:HB2	1.47	0.78
1:A:928:PRO:HB2	1:A:973:ARG:NH1	1.99	0.77
1:C:167:LEU:HD21	1:C:393:PRO:HG2	1.66	0.77
1:C:258:VAL:HG23	1:C:291:LEU:HD11	1.66	0.77
1:A:777:LEU:CD2	1:A:889:ALA:HB2	2.11	0.77
1:D:568:TRP:HE1	1:D:604:ASN:HD22	1.31	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:577:LYS:HD3	1:C:585:TRP:CZ2	2.19	0.77
1:C:673:ALA:HB1	1:C:674:PRO:HD2	1.66	0.77
1:A:683:PRO:O	1:A:684:GLU:C	2.24	0.77
1:A:789:LEU:HD11	1:A:993:ILE:HG22	1.67	0.77
1:C:581:ASN:HD22	1:C:583:ASN:HD22	1.31	0.77
1:C:764:PHE:CD2	1:C:781:ARG:HB3	2.19	0.77
1:B:89:ASN:HD22	1:B:205:MET:HB3	1.50	0.77
1:B:433:LEU:HB2	1:B:467:ASN:OD1	1.84	0.77
1:B:422:PRO:CG	1:C:279:ILE:HD11	2.13	0.77
1:D:5:ASP:OD2	1:D:157:ARG:HA	1.84	0.77
1:B:597:ASN:HD22	1:B:599:ARG:H	1.33	0.77
1:D:114:VAL:CG1	1:D:115:PRO:HD2	2.15	0.77
1:A:878:HIS:HB3	1:A:1009:LEU:O	1.85	0.77
1:A:950:GLN:OE1	1:A:952:ARG:HD3	1.85	0.77
1:B:656:VAL:HG12	1:B:694:LEU:HD11	1.67	0.77
1:C:581:ASN:ND2	1:C:583:ASN:ND2	2.32	0.77
1:C:210:ARG:HD3	3:C:4036:HOH:O	1.84	0.76
1:C:559:TYR:HB2	1:C:562:LEU:HD12	1.64	0.76
1:C:446:ARG:HG2	1:C:447:ASP:OD1	1.85	0.76
1:B:375:ASP:O	1:B:379:MET:HE3	1.83	0.76
1:B:748:CYS:C	1:B:749:ILE:HD12	2.10	0.76
1:D:777:LEU:HD21	1:D:889:ALA:HB2	1.67	0.76
1:A:655:MET:HE1	1:A:662:PRO:HB3	1.68	0.76
1:B:420:MET:HE2	1:B:426:LEU:HG	1.66	0.76
1:C:53:SER:C	1:C:54:LEU:HD23	2.09	0.76
1:B:668:VAL:HG13	1:B:669:PRO:HD2	1.68	0.76
1:C:167:LEU:HB3	1:C:168:PRO:HD2	1.67	0.76
1:C:436:MET:HE3	1:C:467:ASN:ND2	2.00	0.76
1:A:598:ASP:O	1:A:601:PHE:HB2	1.85	0.76
1:B:423:MET:HB2	1:C:282:ARG:HG3	1.66	0.76
1:B:457:SER:HA	1:B:485:GLN:O	1.84	0.76
1:B:458:LEU:HB2	1:B:486:TYR:HB2	1.67	0.76
1:C:258:VAL:CG2	1:C:291:LEU:HD11	2.16	0.76
1:B:797:GLU:O	1:B:801:ILE:HD12	1.86	0.75
1:C:356:ARG:NH2	1:C:367:MET:HE2	1.99	0.75
1:C:749:ILE:O	1:C:755:ARG:HG3	1.86	0.75
1:C:778:THR:HB	1:C:887:GLN:HB3	1.68	0.75
1:D:588:TYR:CD2	1:D:603:MET:HE2	2.21	0.75
1:A:740:LEU:HD12	1:A:741:THR:N	2.01	0.75
1:C:420:MET:HE3	1:C:425:ARG:HB3	1.68	0.75
1:C:930:VAL:HA	1:C:973:ARG:HG2	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:ARG:HG2	1:B:43:ARG:NH1	1.99	0.75
1:A:634:GLN:HB3	1:A:685:LEU:HD11	1.66	0.75
1:C:135:GLN:HA	1:C:135:GLN:NE2	1.96	0.75
1:C:797:GLU:O	1:C:801:ILE:HD12	1.85	0.75
1:D:835:LEU:CD1	1:D:857:ARG:HB2	2.16	0.75
1:B:433:LEU:HD12	1:B:433:LEU:O	1.86	0.75
1:B:758:PHE:CE2	1:B:765:LEU:HB2	2.21	0.75
1:B:251:ARG:H	1:B:254:LEU:HD12	1.51	0.75
1:C:128:ASN:HA	1:C:180:GLY:O	1.87	0.75
1:D:1004:SER:HB3	1:D:1006:GLU:OE2	1.86	0.75
1:A:511:PRO:HA	1:A:516:PRO:HB3	1.69	0.74
1:A:778:THR:HG23	1:A:779:PRO:HD2	1.69	0.74
1:A:769:TRP:HE1	1:A:774:LYS:HD2	1.52	0.74
1:B:395:HIS:ND1	1:B:396:PRO:HD2	2.01	0.74
1:A:769:TRP:NE1	1:A:774:LYS:HD2	2.02	0.74
1:A:166:ARG:HG3	1:A:392:TYR:HB2	1.69	0.74
1:B:577:LYS:HD3	1:B:585:TRP:CZ2	2.22	0.74
1:C:499:ILE:HB	1:C:533:LEU:HB2	1.69	0.74
1:B:3:ILE:HG23	1:B:4:THR:H	1.51	0.74
1:B:246:MET:O	1:B:246:MET:HE3	1.87	0.74
1:C:77:ASP:O	1:C:78:LEU:HD23	1.87	0.74
1:D:685:LEU:HB3	1:D:686:PRO:HD2	1.67	0.74
1:A:100:TYR:CE2	1:A:602:CYS:HB3	2.22	0.74
1:D:166:ARG:HD3	3:D:4035:HOH:O	1.86	0.74
1:C:375:ASP:O	1:C:379:MET:HG3	1.86	0.74
1:A:678:GLN:C	1:A:679:LEU:HD23	2.13	0.74
1:B:740:LEU:HD12	1:B:748:CYS:O	1.88	0.74
1:C:662:PRO:C	1:C:663:LEU:HD23	2.13	0.74
1:D:835:LEU:C	1:D:836:ILE:HD13	2.12	0.74
1:D:890:GLN:NE2	1:D:890:GLN:N	2.36	0.74
1:C:395:HIS:ND1	1:C:396:PRO:HD2	2.02	0.74
1:A:637:GLU:HB2	1:A:679:LEU:HD21	1.69	0.73
1:D:11:LEU:HD21	1:D:187:MET:HE2	1.68	0.73
1:D:403:ASP:OD1	1:D:451:PRO:HD2	1.88	0.73
1:A:763:GLY:HA3	1:A:822:LEU:CD2	2.17	0.73
1:C:416:GLU:HG3	1:C:460:ASN:O	1.88	0.73
1:C:581:ASN:ND2	1:C:583:ASN:HD22	1.83	0.73
1:D:655:MET:HG3	1:D:656:VAL:N	1.99	0.73
1:C:217:LYS:HG2	1:C:218:PRO:HD2	1.68	0.73
1:A:41:GLU:HG2	1:A:46:ARG:NH1	2.03	0.73
1:A:420:MET:HE2	1:A:426:LEU:HD11	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:LEU:HD22	1:A:616:ALA:HB1	1.68	0.73
1:C:347:LYS:HZ2	1:C:675:GLN:HG3	1.54	0.73
1:C:777:LEU:CD2	1:C:889:ALA:HB2	2.17	0.73
1:B:796:SER:HB2	1:B:802:ASP:HB3	1.69	0.73
1:A:224:ASP:HB3	1:A:245:GLN:HG3	1.69	0.73
1:A:287:ASP:CG	1:D:425:ARG:HH22	1.96	0.73
1:B:579:ASP:OD1	1:B:583:ASN:HB2	1.89	0.73
1:B:367:MET:HB3	1:B:372:MET:CE	2.19	0.73
1:D:658:LEU:CG	1:D:661:LYS:HZ2	2.02	0.73
1:A:770:ILE:HD12	1:A:775:GLN:NE2	2.02	0.72
1:B:1004:SER:HB2	1:B:1006:GLU:OE2	1.89	0.72
1:C:342:LEU:O	1:C:343:LEU:HD23	1.89	0.72
1:D:26:ARG:HD3	1:D:169:SER:HB3	1.69	0.72
1:B:668:VAL:CG1	1:B:669:PRO:HD2	2.19	0.72
1:B:777:LEU:HD11	1:B:889:ALA:HA	1.69	0.72
1:B:942:ARG:HA	1:B:953:GLY:O	1.89	0.72
1:C:114:VAL:HG13	1:C:115:PRO:HD2	1.69	0.72
1:C:148:SER:HB3	1:C:190:ARG:O	1.89	0.72
1:A:646:HIS:O	1:A:648:ASP:N	2.22	0.72
1:A:5:ASP:OD2	1:A:157:ARG:HA	1.90	0.72
1:B:6:SER:OG	1:B:9:VAL:HB	1.88	0.72
1:B:696:LEU:HB2	1:B:722:LEU:HD11	1.71	0.72
1:C:873:ALA:O	1:C:876:THR:HG22	1.90	0.72
1:B:114:VAL:CG1	1:B:191:TRP:HB2	2.20	0.72
1:C:836:ILE:HD13	1:C:836:ILE:N	2.05	0.72
1:D:52[B]:ARG:HG3	1:D:133:TRP:HH2	1.53	0.72
1:C:356:ARG:HD2	1:C:379:MET:HE1	1.71	0.72
1:D:71:GLU:O	1:D:72:SER:C	2.32	0.72
1:D:531:ARG:O	1:D:561:ARG:NH1	2.22	0.72
1:C:134:LEU:N	1:C:134:LEU:HD23	2.04	0.72
1:B:127:PHE:HE2	1:B:184:LEU:HG	1.55	0.72
1:C:43:ARG:HG2	1:C:43:ARG:HH11	1.53	0.72
1:D:38:ASN:ND2	1:D:41:GLU:H	1.88	0.72
1:B:230:ARG:HG3	1:B:230:ARG:NH1	2.03	0.71
1:B:255:ARG:HG2	1:B:255:ARG:HH11	1.54	0.71
1:B:422:PRO:HG3	1:C:279:ILE:HD11	1.71	0.71
1:C:894:ARG:NH2	1:C:921:PRO:HD3	2.05	0.71
1:D:30:HIS:HB2	1:D:31:PRO:HD2	1.71	0.71
1:A:856:TYR:HD2	1:A:864:MET:HE1	1.53	0.71
1:C:255:ARG:HG2	1:C:255:ARG:NH1	2.01	0.71
1:A:708:TRP:CE3	1:A:709:SER:HB3	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:849:LEU:N	1:B:849:LEU:HD23	2.06	0.71
1:C:737:ILE:HD12	1:C:738:PRO:O	1.89	0.71
1:D:46:ARG:HB3	1:D:47:PRO:HD2	1.71	0.71
1:D:933:SER:O	1:D:934:GLU:C	2.31	0.71
1:A:708:TRP:CZ3	1:A:709:SER:HB3	2.25	0.71
1:B:464:HIS:HB2	1:B:489:GLY:HA3	1.71	0.71
1:B:836:ILE:HD13	1:B:836:ILE:N	2.03	0.71
1:B:858:ILE:CD1	1:B:864:MET:HB3	2.18	0.71
1:C:100:TYR:HB2	1:C:203:TRP:CD2	2.25	0.71
1:C:767:GLN:HG3	1:C:768:MET:N	2.04	0.71
1:D:658:LEU:HG	1:D:661:LYS:HZ2	1.55	0.71
1:A:383:ASN:ND2	1:A:625:GLN:HA	2.06	0.71
1:A:570:TRP:CD1	1:A:571:VAL:HG22	2.25	0.71
1:A:650:GLU:HA	1:A:701:VAL:O	1.90	0.71
1:A:230:ARG:HB3	1:A:230:ARG:HH11	1.55	0.71
1:B:654:TRP:CE2	1:B:666:GLY:HA3	2.26	0.71
1:D:251:ARG:HG3	1:D:251:ARG:NH1	2.03	0.71
1:C:888:LEU:O	1:C:981:GLY:HA3	1.91	0.71
1:A:647:SER:OG	1:A:672:VAL:HG23	1.91	0.71
1:A:742:THR:HG22	1:A:743:SER:H	1.55	0.71
1:B:651:LEU:CD1	1:B:703:PRO:HG3	2.21	0.71
1:B:655:MET:HG3	1:B:656:VAL:N	1.95	0.71
1:A:93:HIS:HB3	1:A:95:TYR:HE1	1.56	0.70
1:A:878:HIS:NE2	1:A:1010:SER:HB3	2.06	0.70
1:A:776:LEU:C	1:A:777:LEU:HD23	2.17	0.70
1:D:568:TRP:HE1	1:D:604:ASN:ND2	1.87	0.70
1:B:152:LEU:O	1:B:159:VAL:HG23	1.90	0.70
1:B:282:ARG:HH12	1:C:419:GLY:CA	2.05	0.70
1:A:734:SER:HB2	1:A:860:GLY:HA3	1.73	0.70
1:C:620:ALA:O	1:C:624:GLN:HG3	1.91	0.70
1:C:856:TYR:HB3	1:C:864:MET:CE	2.21	0.70
1:D:836:ILE:HD13	1:D:836:ILE:N	2.07	0.70
1:A:152:LEU:HG	1:A:153:TRP:N	2.05	0.70
1:A:748:CYS:C	1:A:749:ILE:HD12	2.17	0.70
1:A:242:ALA:O	1:A:290:THR:HA	1.92	0.70
1:C:989:PHE:CE1	1:C:1014:TYR:HB3	2.26	0.70
1:D:655:MET:HE1	1:D:662:PRO:HB3	1.73	0.70
1:D:734:SER:HB2	1:D:860:GLY:HA3	1.73	0.70
1:D:499:ILE:HG22	1:D:501:PRO:CD	2.19	0.69
1:D:859:ASP:OD1	1:D:861:SER:HB2	1.92	0.69
1:A:11:LEU:N	1:A:11:LEU:HD23	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1020:TRP:HD1	1:A:1021:CYS:N	1.89	0.69
1:C:272:ALA:HB1	1:C:273:PRO:HD2	1.75	0.69
1:A:360:HIS:CG	1:A:361:PRO:HD2	2.26	0.69
1:A:473:ARG:O	1:A:473:ARG:HD3	1.92	0.69
1:A:763:GLY:HA3	1:A:822:LEU:HD21	1.75	0.69
1:B:553:TRP:O	1:B:557:ARG:HG3	1.92	0.69
1:D:827:ALA:CB	1:D:836:ILE:HD12	2.22	0.69
1:D:403:ASP:CG	1:D:451:PRO:HD2	2.17	0.69
1:D:835:LEU:HD12	1:D:857:ARG:HB2	1.74	0.69
1:A:134:LEU:HD22	1:A:134:LEU:N	2.07	0.69
1:A:770:ILE:HD12	1:A:775:GLN:CD	2.17	0.69
1:B:383:ASN:ND2	1:B:621:LYS:HG3	2.08	0.69
1:D:62:TRP:CD1	1:D:95:TYR:HB3	2.28	0.69
1:A:991:MET:HG2	1:A:992:GLY:N	2.07	0.69
1:B:576:ILE:HD13	1:B:584:PRO:HB3	1.75	0.69
1:C:850:PHE:HD2	1:C:872:VAL:HG13	1.57	0.69
1:B:166:ARG:HG3	1:B:392:TYR:HB2	1.75	0.69
1:B:355:ASN:OD1	1:B:388:ARG:HD3	1.92	0.69
1:C:12:GLN:HG3	1:C:13:ARG:N	2.08	0.69
1:B:824:GLN:O	1:B:838:THR:HA	1.92	0.69
1:B:844:HIS:C	1:B:845:GLN:HG2	2.18	0.69
1:C:457:SER:HA	1:C:485:GLN:O	1.93	0.69
1:C:682:LEU:HB3	1:C:683:PRO:HD2	1.75	0.69
1:C:1018:LEU:N	1:C:1018:LEU:HD23	2.08	0.69
1:D:746:ASP:CA	1:D:760:ARG:HG3	2.16	0.69
1:A:737:ILE:HG13	1:A:738:PRO:HD2	1.73	0.69
1:C:110:ASN:O	1:C:113:PHE:N	2.26	0.69
1:C:100:TYR:CZ	1:C:602:CYS:HB3	2.27	0.69
1:C:38:ASN:ND2	1:C:41:GLU:H	1.90	0.68
1:C:245:GLN:HB3	1:C:288:ARG:HG2	1.75	0.68
1:C:738:PRO:HA	1:C:751:LEU:HB2	1.74	0.68
1:C:830:LEU:HB2	1:C:833:ALA:O	1.93	0.68
1:A:210:ARG:HD3	3:A:4019:HOH:O	1.93	0.68
1:B:63:PHE:CD1	1:B:69:VAL:HG22	2.28	0.68
1:B:17:GLU:HG2	1:B:114:VAL:HG23	1.74	0.68
1:D:336:ARG:HH21	1:D:338:GLU:CD	2.01	0.68
1:D:657:ALA:O	1:D:694:LEU:HD12	1.94	0.68
1:A:202:MET:CA	1:A:573:GLN:HE22	2.05	0.68
1:B:255:ARG:HG2	1:B:255:ARG:NH1	2.08	0.68
1:C:166:ARG:HG3	1:C:392:TYR:HB2	1.75	0.68
1:D:210:ARG:HD3	3:D:4036:HOH:O	1.91	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:MET:HE2	1:A:426:LEU:CD1	2.24	0.68
1:A:473:ARG:HD3	1:A:473:ARG:C	2.19	0.68
1:A:645:ARG:NH2	1:A:650:GLU:OE1	2.26	0.68
1:A:510:GLN:HB2	1:A:517:LYS:HB2	1.76	0.68
1:B:90:TRP:HE1	1:B:96:ASP:CG	2.01	0.68
1:D:129:VAL:HG23	1:D:182:ASN:HD22	1.56	0.68
1:A:856:TYR:CD2	1:A:864:MET:HE1	2.28	0.68
1:C:531:ARG:O	1:C:561:ARG:NH1	2.27	0.68
1:A:635:THR:CG2	1:A:679:LEU:HD13	2.24	0.68
1:D:166:ARG:HG3	1:D:392:TYR:CG	2.29	0.68
1:D:786:ARG:HA	1:D:964:GLN:OE1	1.94	0.68
1:C:649:ASN:OD1	1:C:703:PRO:HD2	1.94	0.68
1:A:314:GLU:HB3	1:A:322:LEU:HD21	1.75	0.67
1:A:436:MET:HE3	1:A:467:ASN:ND2	2.00	0.67
1:C:356:ARG:HD2	1:C:379:MET:CE	2.24	0.67
1:C:570:TRP:CD1	1:C:571:VAL:HG22	2.29	0.67
1:C:652:LEU:HD11	1:C:698:VAL:HB	1.75	0.67
1:D:187:MET:O	1:D:187:MET:HG3	1.93	0.67
1:A:662:PRO:C	1:A:663:LEU:HD23	2.19	0.67
1:D:24:LEU:HB2	1:D:161:TYR:HB3	1.77	0.67
1:D:654:TRP:HZ3	1:D:656:VAL:HG23	1.59	0.67
1:A:166:ARG:HG3	1:A:392:TYR:CB	2.23	0.67
1:A:304:GLU:C	1:A:305:ILE:HG13	2.18	0.67
1:A:595:THR:HG23	1:A:596:PRO:HA	1.76	0.67
1:B:43:ARG:HD2	1:B:261:TRP:CD2	2.29	0.67
1:A:742:THR:HG22	1:A:743:SER:N	2.08	0.67
1:B:651:LEU:HD13	1:B:703:PRO:HG3	1.75	0.67
1:A:59:ARG:NH2	1:A:81:ALA:O	2.27	0.67
1:B:856:TYR:HB3	1:B:864:MET:HE1	1.76	0.67
1:C:140:ARG:NH1	1:C:170:GLU:OE1	2.27	0.67
1:C:166:ARG:O	1:C:210:ARG:NH2	2.28	0.67
1:C:187:MET:HG3	1:C:187:MET:O	1.95	0.67
1:D:43:ARG:O	1:D:310:ARG:HD3	1.94	0.67
1:A:425:ARG:HH22	1:D:287:ASP:CG	2.02	0.67
1:C:35:SER:OG	1:C:37:ARG:NH1	2.27	0.67
1:B:128:ASN:HA	1:B:180:GLY:O	1.94	0.67
1:B:822:LEU:HD12	1:B:824:GLN:H	1.60	0.67
1:B:928:PRO:HB2	1:B:973:ARG:NH1	2.10	0.67
1:C:80:GLU:OE2	1:C:80:GLU:N	2.28	0.67
1:D:87:PRO:HB3	1:D:210:ARG:O	1.95	0.67
1:D:658:LEU:HD22	1:D:688:PRO:HG2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:776:LEU:C	1:D:777:LEU:HD23	2.19	0.67
1:D:949:HIS:HB2	1:D:951:TRP:CH2	2.30	0.67
1:A:128:ASN:HA	1:A:180:GLY:O	1.95	0.67
1:A:962:TYR:HD2	1:A:966:GLN:HE22	1.42	0.67
1:B:3:ILE:HG23	1:B:4:THR:N	2.10	0.67
1:B:127:PHE:CE2	1:B:184:LEU:HG	2.30	0.67
1:B:425:ARG:NH2	1:C:287:ASP:OD2	2.28	0.67
1:B:738:PRO:HB2	1:B:834:VAL:HG23	1.76	0.67
1:B:824:GLN:OE1	1:B:837:THR:HG21	1.94	0.67
1:A:654:TRP:CZ3	1:A:656:VAL:HG23	2.31	0.66
1:D:73:TRP:CZ2	1:D:122:CYS:HB3	2.29	0.66
1:A:410:VAL:HG22	1:A:455:ILE:HB	1.75	0.66
1:C:342:LEU:C	1:C:343:LEU:HD23	2.20	0.66
1:C:542:MET:HA	1:C:604:ASN:HA	1.77	0.66
1:D:166:ARG:HG3	1:D:392:TYR:HB2	1.77	0.66
1:B:576:ILE:HG23	1:B:577:LYS:N	2.11	0.66
1:D:894:ARG:NH2	1:D:921:PRO:HD3	2.10	0.66
1:A:100:TYR:CZ	1:A:602:CYS:HB3	2.29	0.66
1:A:786:ARG:HG2	1:A:880:ALA:HB1	1.77	0.66
1:B:246:MET:HE3	1:B:246:MET:C	2.20	0.66
1:B:395:HIS:CG	1:B:396:PRO:HD2	2.31	0.66
1:B:587:ALA:HB1	1:B:592:PHE:CE1	2.30	0.66
1:A:928:PRO:O	1:A:973:ARG:NH1	2.29	0.66
1:B:114:VAL:HG13	1:B:191:TRP:HB2	1.76	0.66
1:B:777:LEU:CG	1:B:889:ALA:HA	2.26	0.66
1:C:65:ALA:HB1	1:C:66:PRO:HD2	1.78	0.66
1:A:233:ASP:CG	1:C:233:ASP:HB3	2.21	0.66
1:B:576:ILE:CD1	1:B:584:PRO:HB3	2.25	0.66
1:B:807:VAL:O	1:B:811:LYS:HB2	1.95	0.66
1:C:879:PRO:HD2	1:C:1009:LEU:HB2	1.78	0.66
1:A:645:ARG:HH22	1:A:650:GLU:CD	2.03	0.66
1:A:775:GLN:OE1	1:A:890:GLN:NE2	2.29	0.66
1:A:824:GLN:HG3	1:A:825:CYS:N	2.08	0.66
1:B:577:LYS:HD3	1:B:585:TRP:HZ2	1.61	0.66
1:C:1020:TRP:HD1	1:C:1021:CYS:N	1.92	0.66
1:D:63:PHE:HB3	1:D:64:PRO:HD2	1.78	0.66
1:D:657:ALA:HB2	1:D:662:PRO:HA	1.77	0.66
1:A:693:GLN:HG2	1:A:721:ARG:CD	2.26	0.66
1:B:883:GLY:HA2	1:B:1016:TYR:OH	1.95	0.66
1:C:43:ARG:HG2	1:C:43:ARG:NH1	2.11	0.66
1:C:360:HIS:CE1	1:C:361:PRO:HD2	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:499:ILE:CG2	1:D:501:PRO:HD3	2.21	0.66
1:A:30:HIS:HB2	1:A:31:PRO:CD	2.26	0.66
1:B:15:ASP:HB3	1:B:21:VAL:HG11	1.78	0.66
1:B:211:ASP:N	1:B:211:ASP:OD1	2.28	0.66
1:C:166:ARG:CG	1:C:392:TYR:HB2	2.26	0.66
1:D:202:MET:HA	1:D:573:GLN:HE22	1.60	0.66
1:D:780:LEU:HA	1:D:886:CYS:HB3	1.76	0.66
1:D:875:ASP:OD2	1:D:875:ASP:N	2.27	0.66
1:A:432:TRP:O	1:A:436:MET:HG3	1.94	0.66
1:A:693:GLN:HG2	1:A:721:ARG:HD3	1.76	0.66
1:C:30:HIS:ND1	1:C:31:PRO:O	2.25	0.66
1:A:654:TRP:HZ3	1:A:656:VAL:HG23	1.60	0.65
1:B:237:ARG:NH1	1:B:296:GLU:OE2	2.29	0.65
1:D:36:TRP:NE1	1:D:46:ARG:O	2.28	0.65
1:D:429:ASP:OD1	1:D:431[A]:ARG:HG3	1.96	0.65
1:D:547:GLY:HA2	1:D:908:ASP:O	1.96	0.65
1:A:949:HIS:CD2	1:A:1020:TRP:HE1	2.15	0.65
1:B:537:GLU:HG2	1:B:568:TRP:HE3	1.59	0.65
1:B:866:ILE:HB	1:B:1018:LEU:HB2	1.77	0.65
1:C:906:TYR:HB3	1:C:907:PRO:HD2	1.78	0.65
1:D:360:HIS:CE1	1:D:362:LEU:HB2	2.32	0.65
1:A:637:GLU:HA	1:A:679:LEU:CD2	2.26	0.65
1:B:355:ASN:O	1:B:569:ASP:HB2	1.97	0.65
1:C:161:TYR:OH	1:C:163:GLN:NE2	2.29	0.65
1:D:257:THR:HA	1:D:270:GLY:O	1.96	0.65
1:B:38:ASN:O	1:B:38:ASN:ND2	2.29	0.65
1:B:254:LEU:O	1:B:255:ARG:NH1	2.30	0.65
1:B:750:GLU:OE1	1:B:750:GLU:N	2.28	0.65
1:C:7:LEU:N	1:C:71:GLU:OE2	2.30	0.65
1:C:380:LYS:HE2	3:C:4077:HOH:O	1.97	0.65
1:C:509:ASP:C	1:C:511:PRO:HD3	2.22	0.65
1:C:902:PRO:O	1:C:938:ARG:NH1	2.30	0.65
1:D:668:VAL:HG11	1:D:680:ILE:HD13	1.78	0.65
1:A:255:ARG:HG3	1:A:255:ARG:NH1	2.05	0.65
1:A:440:VAL:HG21	1:A:471:LEU:HD13	1.79	0.65
1:A:851:ILE:HD12	1:B:726:LEU:CD1	2.24	0.65
1:C:900:LEU:HA	1:C:914:CYS:O	1.97	0.65
1:C:420:MET:CE	1:C:425:ARG:HB3	2.27	0.65
1:D:533:LEU:HD12	1:D:533:LEU:C	2.21	0.65
1:A:535:LEU:HD22	1:A:538:TYR:HB3	1.77	0.65
1:B:140:ARG:NH1	1:B:170:GLU:OE1	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:833:ALA:HB1	1:B:858:ILE:O	1.97	0.65
1:C:770:ILE:O	1:C:773:LYS:HD2	1.97	0.65
1:D:245:GLN:HB3	3:D:6016:HOH:O	1.96	0.65
1:B:595:THR:HG23	1:B:596:PRO:CA	2.26	0.65
1:C:668:VAL:HG12	1:C:669:PRO:HD2	1.79	0.65
1:D:166:ARG:HG3	1:D:392:TYR:CB	2.27	0.65
1:A:908:ASP:HB3	1:A:1007:PHE:CD1	2.32	0.65
1:B:141:ILE:HG12	1:B:142:ILE:H	1.62	0.65
1:D:11:LEU:HD21	1:D:187:MET:CE	2.26	0.65
1:A:287:ASP:OD2	1:D:425:ARG:NH2	2.31	0.64
1:C:932:PRO:HG2	1:C:970:THR:O	1.97	0.64
1:B:434:PRO:HB3	1:C:434:PRO:HB3	1.78	0.64
1:C:251:ARG:O	1:C:253:TYR:N	2.30	0.64
1:C:775:GLN:C	1:C:776:LEU:HD23	2.22	0.64
1:D:46:ARG:CB	1:D:47:PRO:HD2	2.25	0.64
1:A:282:ARG:HH11	1:A:282:ARG:HG3	1.62	0.64
1:A:894:ARG:HD3	1:A:919:ASP:OD1	1.97	0.64
1:B:693:GLN:HG2	1:B:721:ARG:HD2	1.79	0.64
1:C:486:TYR:CE2	1:C:488:GLY:HA3	2.32	0.64
1:D:460:ASN:ND2	1:D:461:GLU:HG2	2.12	0.64
1:A:937:LEU:HD21	1:A:956:GLN:HB3	1.80	0.64
1:B:789:LEU:N	1:B:792:ASP:OD2	2.29	0.64
1:C:668:VAL:HG13	1:C:669:PRO:HD2	1.78	0.64
1:D:93:HIS:HB3	1:D:95:TYR:HE1	1.62	0.64
1:C:10:VAL:HG12	1:C:11:LEU:N	2.12	0.64
1:C:367:MET:HE1	1:C:371:THR:HG22	1.79	0.64
1:C:418:HIS:ND1	1:C:461:GLU:HG3	2.12	0.64
1:D:763:GLY:HA3	1:D:822:LEU:HD21	1.80	0.64
1:A:35:SER:OG	1:A:37:ARG:NH1	2.31	0.64
1:B:658:LEU:O	1:B:659:ASP:C	2.40	0.64
1:B:805:ALA:HB3	1:B:808:GLU:HB2	1.80	0.64
1:B:950:GLN:OE1	1:B:952:ARG:NH1	2.31	0.64
1:C:437:SER:O	1:C:441:THR:HG23	1.97	0.64
1:C:833:ALA:HB1	1:C:858:ILE:O	1.97	0.64
1:C:920:LEU:HB3	1:C:921:PRO:HD2	1.78	0.64
1:D:304:GLU:C	1:D:305:ILE:HG13	2.23	0.64
1:A:635:THR:HA	1:A:680:ILE:O	1.98	0.64
1:B:200:GLN:OE1	1:B:200:GLN:N	2.30	0.64
1:B:1020:TRP:HD1	1:B:1021:CYS:N	1.95	0.64
1:C:148:SER:OG	1:C:192:SER:HB3	1.97	0.64
1:C:835:LEU:C	1:C:836:ILE:HD13	2.22	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:850:PHE:CD2	1:C:872:VAL:HG13	2.33	0.64
1:D:350:LEU:N	3:D:4120:HOH:O	2.29	0.64
1:A:202:MET:CB	1:A:573:GLN:HE22	2.11	0.64
1:C:764:PHE:CE2	1:C:781:ARG:HB3	2.32	0.64
1:A:62:TRP:CZ2	1:A:119:PRO:HB3	2.33	0.64
1:A:425:ARG:NH2	1:D:287:ASP:OD2	2.31	0.64
1:A:7:LEU:N	1:A:71:GLU:OE2	2.32	0.63
1:A:380:LYS:HE2	3:A:4042:HOH:O	1.98	0.63
1:A:6:SER:HB2	1:A:71:GLU:OE2	1.98	0.63
1:A:618:THR:HG22	1:A:912:ALA:HB1	1.79	0.63
1:C:167:LEU:HD21	1:C:393:PRO:CG	2.27	0.63
1:D:655:MET:CE	1:D:662:PRO:HB3	2.27	0.63
1:A:153:TRP:HB2	1:A:185:ALA:HB3	1.80	0.63
1:A:240:LEU:CD2	1:A:260:LEU:HD22	2.28	0.63
1:B:385:ASN:HB3	1:B:408:TYR:CD1	2.33	0.63
1:B:778:THR:CG2	1:B:779:PRO:HD2	2.26	0.63
1:C:588:TYR:O	1:C:591:ASP:HB2	1.98	0.63
1:A:678:GLN:O	1:A:679:LEU:HD23	1.98	0.63
1:C:499:ILE:HD11	1:C:529:GLU:OE1	1.99	0.63
1:C:777:LEU:HD23	1:C:777:LEU:N	2.11	0.63
1:C:870:VAL:HG12	1:C:871:GLU:N	2.14	0.63
1:D:377:LEU:CD2	1:D:708:TRP:HA	2.29	0.63
1:B:100:TYR:HB2	1:B:203:TRP:CE3	2.33	0.63
1:B:701:VAL:O	1:B:703:PRO:HD3	1.97	0.63
1:C:167:LEU:CD2	1:C:393:PRO:HB2	2.29	0.63
1:A:789:LEU:CD1	1:A:993:ILE:HG22	2.29	0.63
1:A:823:LEU:HD22	1:B:728:VAL:HG12	1.80	0.63
1:B:842:TRP:HZ3	1:B:852:SER:HB2	1.61	0.63
1:C:645:ARG:NH2	1:C:650:GLU:OE1	2.32	0.63
1:A:38:ASN:ND2	1:A:41:GLU:HG3	2.14	0.63
1:A:749:ILE:HD12	1:A:749:ILE:N	2.14	0.63
1:A:166:ARG:HD3	3:A:4018:HOH:O	1.98	0.63
1:B:374:GLN:O	1:B:378:LEU:HD12	1.99	0.63
1:B:473:ARG:O	1:B:473:ARG:HD3	1.98	0.63
1:B:673:ALA:HB1	1:B:674:PRO:CD	2.26	0.63
1:C:43:ARG:NH2	1:C:264:GLU:OE2	2.32	0.63
1:C:603:MET:HE1	1:C:930:VAL:HB	1.79	0.63
1:D:965:GLN:HE21	1:D:969:GLU:CD	2.07	0.63
1:B:282:ARG:NH1	1:C:418:HIS:O	2.28	0.63
1:B:658:LEU:HG	1:B:661:LYS:HZ1	1.62	0.63
1:A:367:MET:HB3	1:A:372:MET:HE3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:MET:HB2	1:A:503:TYR:CD1	2.34	0.62
1:A:902:PRO:O	1:A:938:ARG:NH1	2.32	0.62
1:B:499:ILE:HB	1:B:533:LEU:HB2	1.80	0.62
1:C:433:LEU:HB3	1:C:434:PRO:CD	2.29	0.62
1:A:377:LEU:CD2	1:A:708:TRP:HA	2.29	0.62
1:A:945:ASN:OD1	1:A:950:GLN:HB2	1.99	0.62
1:B:383:ASN:HD22	1:B:621:LYS:HG3	1.63	0.62
1:C:166:ARG:HG3	1:C:392:TYR:CG	2.33	0.62
1:C:431[B]:ARG:NH2	3:C:7516:HOH:O	2.32	0.62
1:C:502:MET:HA	1:C:537:GLU:O	2.00	0.62
1:D:52[A]:ARG:NH2	1:D:128:ASN:O	2.30	0.62
1:B:204:ARG:HD3	1:B:204:ARG:N	2.13	0.62
1:C:200:GLN:HG2	1:C:391:HIS:HB2	1.81	0.62
1:D:827:ALA:HB2	1:D:836:ILE:HD12	1.81	0.62
1:A:7:LEU:HD11	1:A:69:VAL:HG12	1.80	0.62
1:A:305:ILE:HD11	1:A:645:ARG:HB3	1.81	0.62
1:B:65:ALA:HB1	1:B:66:PRO:HD2	1.82	0.62
1:B:559:TYR:HB2	1:B:562:LEU:CD1	2.28	0.62
1:C:920:LEU:CB	1:C:921:PRO:HD2	2.28	0.62
1:D:38:ASN:HD22	1:D:41:GLU:H	1.45	0.62
1:D:100:TYR:HB3	1:D:589:GLY:HA2	1.80	0.62
1:D:673:ALA:O	1:D:674:PRO:C	2.41	0.62
1:A:38:ASN:HD21	1:A:40:GLU:HB2	1.65	0.62
1:C:367:MET:HE1	1:C:371:THR:CG2	2.28	0.62
1:D:42:ALA:O	1:D:310:ARG:NH1	2.33	0.62
1:D:904:GLU:HG2	1:D:909:ARG:HH22	1.64	0.62
1:B:35:SER:OG	1:B:37:ARG:NH1	2.32	0.62
1:B:424:ASN:OD1	1:C:279:ILE:HD12	2.00	0.62
1:C:246:MET:O	1:C:246:MET:HE3	2.00	0.62
1:D:38:ASN:HD21	1:D:40:GLU:HB2	1.63	0.62
1:D:103:VAL:HG22	1:D:418:HIS:CE1	2.34	0.62
1:D:467:ASN:O	1:D:471:LEU:HG	1.99	0.62
1:A:91:GLN:OE1	1:A:205:MET:HB3	2.00	0.62
1:B:782:ASP:HB2	1:B:842:TRP:CZ2	2.34	0.62
1:C:167:LEU:HD21	1:C:393:PRO:CB	2.30	0.62
1:A:403:ASP:OD1	1:A:451:PRO:HD2	2.00	0.62
1:A:663:LEU:HD23	1:A:663:LEU:N	2.13	0.62
1:D:274:PHE:HB3	1:D:286:ALA:O	2.00	0.62
1:B:579:ASP:CG	1:B:583:ASN:HB2	2.24	0.62
1:C:833:ALA:CB	1:C:859:ASP:HA	2.30	0.62
1:D:693:GLN:HB3	1:D:721:ARG:HD3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:655:MET:CE	1:A:662:PRO:HB3	2.30	0.62
1:A:737:ILE:HD12	1:A:832:ASP:C	2.25	0.62
1:A:928:PRO:CB	1:A:973:ARG:HH12	2.06	0.62
1:B:778:THR:HG22	1:B:779:PRO:CD	2.28	0.62
1:C:662:PRO:O	1:C:663:LEU:HD23	1.99	0.62
1:C:776:LEU:O	1:C:777:LEU:HD23	1.99	0.62
1:D:375:ASP:O	1:D:379:MET:HG3	1.99	0.61
1:D:437:SER:O	1:D:441:THR:HG23	1.99	0.61
1:C:989:PHE:HE1	1:C:1014:TYR:HB3	1.62	0.61
1:D:654:TRP:CZ3	1:D:656:VAL:HG23	2.35	0.61
1:D:919:ASP:O	1:D:920:LEU:HD23	2.00	0.61
1:A:14:ARG:HA	1:A:16:TRP:CZ3	2.35	0.61
1:C:894:ARG:HD3	1:C:919:ASP:OD1	2.01	0.61
1:D:770:ILE:HD13	1:D:775:GLN:CD	2.25	0.61
1:D:1020:TRP:HD1	1:D:1021:CYS:N	1.98	0.61
1:A:102:ASN:C	1:A:102:ASN:HD22	2.07	0.61
1:A:143:PHE:O	1:A:168:PRO:HA	2.01	0.61
1:A:403:ASP:CG	1:A:451:PRO:HD2	2.25	0.61
1:A:613:PRO:HB3	1:A:617:LEU:HD23	1.83	0.61
1:A:668:VAL:HG12	1:A:669:PRO:HD2	1.83	0.61
1:C:22:THR:O	1:C:163:GLN:HG3	1.99	0.61
1:C:769:TRP:HA	1:C:773:LYS:O	1.99	0.61
1:B:537:GLU:HG2	1:B:568:TRP:CE3	2.36	0.61
1:C:141:ILE:HB	1:C:173:LEU:HD11	1.83	0.61
1:D:745:MET:HB2	1:D:746:ASP:OD2	2.01	0.61
1:A:30:HIS:HB2	1:A:31:PRO:HD2	1.83	0.61
1:A:874:SER:HB3	1:B:724:GLU:OE1	2.00	0.61
1:B:373:VAL:O	1:B:377:LEU:HG	2.00	0.61
1:B:506:VAL:HA	1:B:520:ILE:HG12	1.81	0.61
1:D:196:TYR:O	1:D:417:THR:HG22	2.01	0.61
1:D:777:LEU:CD2	1:D:889:ALA:HB2	2.30	0.61
1:D:794:GLY:HA2	1:D:998:SER:O	2.00	0.61
1:A:801:ILE:O	1:A:803:PRO:HD3	2.00	0.61
1:B:129:VAL:HG12	1:B:134:LEU:HD11	1.81	0.61
1:B:141:ILE:HD13	1:B:143:PHE:CE1	2.35	0.61
1:B:542:MET:HB2	1:B:604:ASN:OD1	2.01	0.61
1:D:88:SER:HA	1:D:366:VAL:HG21	1.83	0.61
1:B:776:LEU:HB3	1:B:778:THR:O	2.00	0.61
1:B:908:ASP:HB3	1:B:1007:PHE:CD1	2.36	0.61
1:D:306:PRO:O	1:D:307:ASN:C	2.36	0.61
1:A:50:GLN:N	1:A:50:GLN:NE2	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:894:ARG:NH2	1:A:921:PRO:HD3	2.15	0.61
1:A:965:GLN:O	1:A:969:GLU:HG3	2.01	0.61
1:C:357:HIS:HD2	1:C:392:TYR:OH	1.83	0.61
1:D:255:ARG:HG2	1:D:255:ARG:NH1	2.11	0.61
1:D:479:ASP:N	1:D:480:PRO:HD3	2.12	0.61
1:D:606:LEU:O	1:D:614:HIS:HB2	2.00	0.61
1:A:844:HIS:C	1:A:845:GLN:HG2	2.24	0.61
1:B:422:PRO:HD3	1:C:284:GLY:O	2.01	0.61
1:B:649:ASN:O	1:B:702:GLN:HG2	2.01	0.61
1:C:73:TRP:CZ2	1:C:185:ALA:HB1	2.35	0.61
1:C:655:MET:HE1	1:C:662:PRO:HB3	1.83	0.61
1:A:52[B]:ARG:HG3	1:A:133:TRP:CH2	2.36	0.60
1:A:762:SER:OG	1:A:763:GLY:N	2.33	0.60
1:B:777:LEU:CD1	1:B:889:ALA:HA	2.29	0.60
1:C:246:MET:HE2	1:C:287:ASP:HB3	1.81	0.60
1:C:557:ARG:HD2	3:C:4018:HOH:O	2.01	0.60
1:D:878:HIS:HB3	1:D:1009:LEU:O	2.01	0.60
1:A:369:GLU:O	1:A:373:VAL:HG23	2.01	0.60
1:A:487:GLU:CD	1:A:502:MET:HE3	2.26	0.60
1:A:595:THR:CG2	1:A:596:PRO:HA	2.31	0.60
1:B:964:GLN:O	1:B:967:LEU:HB2	2.00	0.60
1:C:776:LEU:HD23	1:C:776:LEU:N	2.16	0.60
1:D:55:ASN:HD22	1:D:87:PRO:HD3	1.65	0.60
1:D:238:ALA:HB1	1:D:332:PHE:CE2	2.37	0.60
1:B:429:ASP:OD2	1:B:431[A]:ARG:HD3	2.02	0.60
1:B:658:LEU:O	1:B:661:LYS:HE3	2.02	0.60
1:A:257:THR:OG1	1:A:271:THR:HG23	2.02	0.60
1:A:696:LEU:HB2	1:A:722:LEU:HD11	1.82	0.60
1:B:589:GLY:HA3	1:B:599:ARG:CA	2.31	0.60
1:B:929:TYR:O	1:B:930:VAL:C	2.43	0.60
1:C:928:PRO:O	1:C:973:ARG:NH1	2.34	0.60
1:A:502:MET:HB2	1:A:503:TYR:CE1	2.36	0.60
1:B:36:TRP:NE1	1:B:46:ARG:O	2.28	0.60
1:B:299:LYS:C	1:B:307:ASN:HD22	2.10	0.60
1:D:133:TRP:C	1:D:134:LEU:HD23	2.26	0.60
1:D:322:LEU:HD22	1:D:323:ILE:N	2.15	0.60
1:D:424:ASN:ND2	1:D:464:HIS:O	2.33	0.60
1:D:658:LEU:CD2	1:D:661:LYS:HZ2	2.14	0.60
1:A:930:VAL:HG22	1:A:973:ARG:CD	2.30	0.60
1:B:217:LYS:HG2	1:B:218:PRO:HD2	1.83	0.60
1:B:397:LEU:O	1:B:398:TRP:C	2.45	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:881:ARG:C	1:C:882:ILE:HG13	2.26	0.60
1:D:62:TRP:HB2	1:D:95:TYR:CD2	2.37	0.60
1:D:89:ASN:O	1:D:92:MET:HB2	2.01	0.60
1:A:544:ASN:HB3	1:A:789:LEU:HD22	1.83	0.60
1:B:650:GLU:HG3	1:B:700:VAL:CG1	2.32	0.60
1:D:38:ASN:ND2	1:D:41:GLU:HG2	2.17	0.60
1:A:540:HIS:C	1:A:542:MET:H	2.09	0.60
1:A:737:ILE:CG1	1:A:738:PRO:HD2	2.30	0.60
1:B:78:LEU:O	1:B:81:ALA:N	2.30	0.60
1:B:949:HIS:HB2	1:B:951:TRP:CH2	2.37	0.60
1:C:129:VAL:HG12	1:C:134:LEU:HD21	1.84	0.60
1:C:397:LEU:O	1:C:398:TRP:C	2.45	0.60
1:C:559:TYR:CB	1:C:562:LEU:HD12	2.31	0.60
1:A:542:MET:HA	1:A:604:ASN:HA	1.83	0.60
1:A:753:ASN:OD1	1:A:753:ASN:N	2.28	0.60
1:B:127:PHE:O	1:B:182:ASN:N	2.34	0.60
1:C:3:ILE:O	1:C:6:SER:HB3	2.02	0.60
1:C:153:TRP:HA	1:C:157:ARG:O	2.02	0.60
1:C:949:HIS:HB2	1:C:951:TRP:CH2	2.36	0.60
1:A:637:GLU:CB	1:A:679:LEU:HD21	2.32	0.59
1:B:217:LYS:HZ3	1:B:324:GLU:CD	2.10	0.59
1:D:129:VAL:HG23	1:D:182:ASN:ND2	2.16	0.59
1:D:540:HIS:CE1	1:D:542:MET:HB2	2.37	0.59
1:D:581:ASN:HD22	1:D:583:ASN:ND2	1.99	0.59
1:B:138:GLN:HG2	1:B:139:THR:N	2.16	0.59
1:B:897:TRP:HB3	1:B:944:LEU:HB2	1.84	0.59
1:C:78:LEU:HB3	1:C:80:GLU:OE2	2.02	0.59
1:C:133:TRP:CE3	1:C:216:HIS:HB2	2.36	0.59
1:D:856:TYR:HB3	1:D:864:MET:CE	2.30	0.59
1:A:701:VAL:O	1:A:703:PRO:HD3	2.02	0.59
1:D:100:TYR:HB2	1:D:203:TRP:CD2	2.37	0.59
1:D:138:GLN:HG2	1:D:138:GLN:O	1.99	0.59
1:D:504:ALA:HB3	1:D:535:LEU:HD21	1.83	0.59
1:C:200:GLN:OE1	1:C:200:GLN:N	2.35	0.59
1:C:432:TRP:O	1:C:433:LEU:C	2.42	0.59
1:C:767:GLN:NE2	1:C:774:LYS:HG2	2.17	0.59
1:D:881:ARG:HD3	1:D:987:ASP:OD1	2.02	0.59
1:A:217:LYS:HB3	1:A:218:PRO:HD2	1.83	0.59
1:A:777:LEU:HD23	1:A:777:LEU:N	2.17	0.59
1:A:917:ARG:NH2	1:A:943:GLU:OE1	2.35	0.59
1:B:377:LEU:N	1:B:377:LEU:HD23	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:542:MET:HE3	1:C:601:PHE:HA	1.84	0.59
1:C:1011:ALA:HB3	1:C:1014:TYR:CZ	2.37	0.59
1:D:153:TRP:HB2	1:D:185:ALA:HB3	1.84	0.59
1:A:80:GLU:H	1:A:80:GLU:CD	2.11	0.59
1:B:100:TYR:HB2	1:B:203:TRP:CD2	2.37	0.59
1:B:152:LEU:C	1:B:159:VAL:HG23	2.28	0.59
1:B:372:MET:O	1:B:375:ASP:HB2	2.03	0.59
1:B:662:PRO:C	1:B:663:LEU:HD23	2.27	0.59
1:C:124:SER:HA	1:C:184:LEU:O	2.03	0.59
1:C:161:TYR:HE2	1:C:163:GLN:HE21	1.45	0.59
1:A:254:LEU:O	1:A:255:ARG:HG3	2.03	0.59
1:A:367:MET:HB3	1:A:372:MET:HE2	1.83	0.59
1:A:429:ASP:OD1	1:A:431[B]:ARG:HG3	2.03	0.59
1:B:746:ASP:OD2	1:B:757:GLN:NE2	2.30	0.59
1:C:763:GLY:HA3	1:C:822:LEU:HD13	1.85	0.59
1:A:138:GLN:O	1:A:216:HIS:HA	2.02	0.59
1:A:505:ARG:HB2	1:A:508:GLU:O	2.03	0.59
1:A:619:GLU:HG2	1:A:909:ARG:HG2	1.83	0.59
1:B:217:LYS:NZ	1:B:324:GLU:OE1	2.35	0.59
1:B:256:VAL:O	1:B:271:THR:HA	2.03	0.59
1:D:651:LEU:HD12	1:D:668:VAL:O	2.02	0.59
1:D:801:ILE:HG23	1:D:808:GLU:CD	2.27	0.59
1:B:300:LEU:N	1:B:307:ASN:HD22	2.00	0.59
1:B:634:GLN:O	1:B:682:LEU:HB2	2.02	0.59
1:C:167:LEU:HB3	1:C:168:PRO:CD	2.33	0.59
1:C:881:ARG:HD3	1:C:987:ASP:OD1	2.02	0.59
1:A:626:PHE:O	1:A:641:GLU:HB2	2.02	0.58
1:B:134:LEU:O	1:B:135:GLN:C	2.43	0.58
1:B:573:GLN:HB2	1:B:602:CYS:O	2.03	0.58
1:C:100:TYR:CE1	1:C:602:CYS:HB3	2.37	0.58
1:D:658:LEU:HG	1:D:661:LYS:NZ	2.18	0.58
1:B:141:ILE:HG23	1:B:143:PHE:HE1	1.67	0.58
1:B:314:GLU:HB3	1:B:322:LEU:HD21	1.86	0.58
1:B:786:ARG:CD	1:B:880:ALA:HB1	2.31	0.58
1:C:372:MET:HE1	1:C:397:LEU:HB3	1.85	0.58
1:D:7:LEU:HG	1:D:74:LEU:HD11	1.84	0.58
1:D:52[A]:ARG:HG2	1:D:52[A]:ARG:HH11	1.68	0.58
1:A:246:MET:HE1	1:A:248:GLY:O	2.03	0.58
1:B:51:LEU:HD12	1:B:214:LEU:O	2.02	0.58
1:C:427:THR:CA	1:C:436:MET:HE1	2.12	0.58
1:D:38:ASN:HB3	1:D:41:GLU:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:352:ARG:CB	1:D:385:ASN:HB2	2.29	0.58
1:A:261:TRP:HZ3	1:A:264:GLU:O	1.86	0.58
1:B:37:ARG:HG2	1:B:50:GLN:NE2	2.17	0.58
1:B:145:GLY:HA3	1:B:210:ARG:HG3	1.85	0.58
1:B:203:TRP:HB2	1:B:205:MET:HE3	1.86	0.58
1:B:739[A]:HIS:CD2	1:B:740:LEU:H	2.21	0.58
1:C:400:THR:O	1:C:403:ASP:HB2	2.03	0.58
1:D:672:VAL:HG13	1:D:678:GLN:HB2	1.85	0.58
1:A:930:VAL:HG22	1:A:973:ARG:HD3	1.84	0.58
1:B:570:TRP:CD1	1:B:571:VAL:HG13	2.38	0.58
1:B:698:VAL:O	1:B:717:TRP:HB2	2.04	0.58
1:C:38:ASN:HD21	1:C:41:GLU:H	1.50	0.58
1:D:868:VAL:HG12	1:D:869:ASP:N	2.18	0.58
1:A:246:MET:HB3	1:A:274:PHE:CZ	2.38	0.58
1:A:906:TYR:CZ	1:A:937:LEU:HB2	2.38	0.58
1:B:217:LYS:HE2	1:B:326:GLU:OE2	2.04	0.58
1:C:579:ASP:OD1	1:C:583:ASN:N	2.33	0.58
1:D:78:LEU:HD23	1:D:78:LEU:N	2.15	0.58
1:D:635:THR:HA	1:D:680:ILE:O	2.04	0.58
1:D:749:ILE:O	1:D:755:ARG:HG3	2.04	0.58
1:D:890:GLN:H	1:D:890:GLN:CD	2.11	0.58
1:A:230:ARG:HH11	1:A:230:ARG:CB	2.17	0.58
1:A:433:LEU:O	1:A:433:LEU:HD12	2.03	0.58
1:B:385:ASN:HB3	1:B:408:TYR:HD1	1.67	0.58
1:C:721:ARG:HG3	1:C:721:ARG:HH11	1.69	0.58
1:D:100:TYR:HD2	1:D:589:GLY:HA3	1.68	0.58
1:D:867:THR:HB	3:D:4146:HOH:O	2.02	0.58
1:B:272:ALA:HB1	1:B:273:PRO:HD2	1.85	0.58
1:B:416:GLU:HA	1:B:460:ASN:O	2.04	0.58
1:C:505:ARG:HG2	1:C:996:ASP:OD2	2.02	0.58
1:C:537:GLU:HA	1:C:566:PHE:O	2.03	0.58
1:C:896:ASN:HA	1:C:918:TRP:O	2.03	0.58
1:D:331:GLY:HA3	1:D:451:PRO:HB3	1.85	0.58
1:D:649:ASN:O	1:D:702:GLN:HG3	2.03	0.58
1:D:654:TRP:HE3	1:D:655:MET:N	2.02	0.58
1:D:777:LEU:HD21	1:D:889:ALA:CB	2.33	0.58
1:A:433:LEU:HB3	1:A:434:PRO:CD	2.33	0.58
1:A:599:ARG:NH1	1:A:600:GLN:NE2	2.52	0.58
1:A:599:ARG:HH12	1:A:600:GLN:HE22	1.50	0.58
1:B:536:CYS:O	1:B:566:PHE:HB2	2.04	0.58
1:B:658:LEU:C	1:B:661:LYS:HE3	2.29	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:355:ASN:OD1	1:C:388:ARG:HD3	2.03	0.58
1:B:286:ALA:HB1	3:B:4439:HOH:O	2.03	0.58
1:C:10:VAL:O	1:C:11:LEU:C	2.43	0.58
1:C:27:LEU:HD12	1:C:170:GLU:HB3	1.85	0.58
1:C:421:VAL:O	1:C:425:ARG:HD2	2.04	0.58
1:C:746:ASP:HA	1:C:760:ARG:HG2	1.86	0.58
1:D:656:VAL:HG12	1:D:694:LEU:HD11	1.85	0.58
1:A:502:MET:HA	1:A:537:GLU:O	2.04	0.57
1:A:949:HIS:HD2	1:A:1020:TRP:HE1	1.51	0.57
1:B:91:GLN:HB3	1:B:98:PRO:HG3	1.86	0.57
1:B:398:TRP:HA	1:B:401:LEU:HD12	1.86	0.57
1:C:486:TYR:CZ	1:C:488:GLY:HA3	2.38	0.57
1:C:804:ASN:O	1:C:809[A]:ARG:NH1	2.30	0.57
1:D:78:LEU:HB3	1:D:80:GLU:OE2	2.04	0.57
1:A:882:ILE:O	1:A:882:ILE:HG22	2.04	0.57
1:D:603:MET:HE1	1:D:930:VAL:HG11	1.84	0.57
1:A:3:ILE:HD12	1:A:3:ILE:O	2.04	0.57
1:A:53:SER:C	1:A:54:LEU:HD23	2.29	0.57
1:A:69:VAL:HG13	1:A:70:PRO:HD2	1.86	0.57
1:A:490:GLY:N	3:A:4007:HOH:O	2.31	0.57
1:B:225:PHE:HA	1:B:243:GLU:O	2.04	0.57
1:B:840:HIS:ND1	1:B:840:HIS:N	2.50	0.57
1:C:43:ARG:HD2	1:C:261:TRP:CD2	2.39	0.57
1:C:726:LEU:HD12	1:D:848:THR:HG22	1.86	0.57
1:A:579:ASP:C	1:A:581:ASN:H	2.13	0.57
1:A:637:GLU:HA	1:A:679:LEU:HD21	1.84	0.57
1:C:347:LYS:HE3	1:C:643:LEU:O	2.03	0.57
1:C:510:GLN:O	1:C:517:LYS:N	2.31	0.57
1:D:446:ARG:HG2	1:D:447:ASP:OD1	2.04	0.57
1:A:7:LEU:HD13	1:A:69:VAL:HG12	1.86	0.57
1:A:767:GLN:HG3	1:A:768:MET:N	2.19	0.57
1:B:929:TYR:O	1:B:931:PHE:N	2.37	0.57
1:D:903[B]:GLN:HE22	1:D:913:ALA:HA	1.68	0.57
1:A:136:GLU:O	1:A:216:HIS:HE1	1.88	0.57
1:A:202:MET:O	1:A:204:ARG:HD3	2.05	0.57
1:A:375:ASP:O	1:A:379:MET:HG3	2.04	0.57
1:B:30:HIS:HB2	1:B:31:PRO:CD	2.34	0.57
1:B:237:ARG:HB2	1:B:237:ARG:HH11	1.69	0.57
1:C:897:TRP:HB2	1:C:943:GLU:O	2.04	0.57
1:D:141:ILE:HG13	1:D:213:SER:O	2.04	0.57
1:A:672:VAL:HG13	1:A:678:GLN:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:VAL:HG13	1:B:191:TRP:CB	2.34	0.57
1:B:138:GLN:N	1:B:217:LYS:O	2.38	0.57
1:C:198:GLU:OE2	1:C:439:ARG:NH1	2.35	0.57
1:C:746:ASP:CA	1:C:760:ARG:HG2	2.35	0.57
1:D:444:VAL:O	1:D:448:ARG:HB3	2.04	0.57
1:B:777:LEU:HD21	1:B:889:ALA:CB	2.35	0.57
1:C:775:GLN:OE1	1:C:890:GLN:NE2	2.38	0.57
1:C:948:PRO:O	1:C:1022:GLN:HA	2.04	0.57
1:D:511:PRO:HA	1:D:516:PRO:HB3	1.86	0.57
1:D:673:ALA:HB1	1:D:674:PRO:CD	2.32	0.57
1:B:391:HIS:HA	1:B:412:GLU:OE1	2.05	0.57
1:C:36:TRP:CD1	1:C:41:GLU:HB3	2.39	0.57
1:C:258:VAL:N	1:C:270:GLY:O	2.29	0.57
1:C:608:PHE:O	1:C:611:ARG:N	2.32	0.57
1:D:894:ARG:HD3	1:D:919:ASP:OD1	2.04	0.57
1:A:392:TYR:HB2	1:A:393:PRO:HD2	1.86	0.57
1:A:599:ARG:HD2	1:A:600:GLN:OE1	2.05	0.57
1:C:167:LEU:HD21	1:C:393:PRO:HB2	1.86	0.57
1:C:234:ASP:O	1:C:235:PHE:HB2	2.04	0.57
1:C:622:HIS:HD2	1:C:625:GLN:OE1	1.87	0.57
1:A:599:ARG:HB2	1:A:600:GLN:OE1	2.05	0.56
1:A:750:GLU:HB3	1:A:755:ARG:HG3	1.86	0.56
1:C:751:LEU:HD23	1:C:751:LEU:C	2.30	0.56
1:D:653[B]:HIS:HD2	1:D:667:GLU:HG3	1.69	0.56
1:A:433:LEU:HD12	1:A:433:LEU:C	2.30	0.56
1:B:73:TRP:CE2	1:B:122:CYS:HB3	2.40	0.56
1:B:945:ASN:OD1	1:B:950:GLN:HB2	2.04	0.56
1:D:749:ILE:N	1:D:749:ILE:HD12	2.20	0.56
1:A:237:ARG:HH11	1:A:237:ARG:HB2	1.70	0.56
1:A:737:ILE:HG13	1:A:738:PRO:CD	2.36	0.56
1:A:894:ARG:CZ	1:A:921:PRO:HD3	2.36	0.56
1:B:80:GLU:N	1:B:80:GLU:OE2	2.39	0.56
1:B:230:ARG:HH11	1:B:230:ARG:CG	2.17	0.56
1:B:399:TYR:HB3	1:B:450:HIS:CD2	2.39	0.56
1:B:422:PRO:HG3	1:C:279:ILE:CD1	2.35	0.56
1:B:505:ARG:HG2	1:B:996:ASP:OD2	2.04	0.56
1:D:7:LEU:O	1:D:11:LEU:HB2	2.06	0.56
1:D:230:ARG:HH11	1:D:230:ARG:CG	2.12	0.56
1:D:257:THR:OG1	1:D:316:HIS:HE1	1.89	0.56
1:D:393:PRO:HD2	1:D:414:ASN:HB2	1.86	0.56
1:D:767:GLN:HG3	1:D:768:MET:N	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:876:THR:OG1	1:D:877:PRO:HD2	2.05	0.56
1:A:60:PHE:HA	1:A:122:CYS:O	2.06	0.56
1:A:649:ASN:OD1	1:A:703:PRO:HD2	2.05	0.56
1:B:141:ILE:HB	1:B:173:LEU:HD12	1.87	0.56
1:B:1019:VAL:O	1:B:1019:VAL:HG12	2.03	0.56
1:C:246:MET:HE2	1:C:287:ASP:CB	2.35	0.56
1:A:282:ARG:HB2	1:D:422:PRO:HA	1.87	0.56
1:A:693:GLN:NE2	1:A:721:ARG:HH11	2.03	0.56
1:B:251:ARG:H	1:B:254:LEU:CD1	2.18	0.56
1:B:888:LEU:N	1:B:982:THR:O	2.27	0.56
1:C:573:GLN:HB2	1:C:602:CYS:O	2.05	0.56
1:C:833:ALA:HB2	1:C:859:ASP:HA	1.87	0.56
1:D:110:ASN:O	1:D:113:PHE:HB2	2.06	0.56
1:D:522:LYS:O	1:D:522:LYS:HG2	2.05	0.56
1:B:38:ASN:ND2	1:B:41:GLU:H	2.03	0.56
1:B:733:ALA:O	1:B:734:SER:C	2.48	0.56
1:C:44:THR:O	1:C:45:ASP:C	2.46	0.56
1:C:721:ARG:HH11	1:C:721:ARG:CG	2.19	0.56
1:D:316:HIS:HD2	1:D:317:THR:O	1.88	0.56
1:D:836:ILE:HG22	1:D:837:THR:N	2.20	0.56
1:D:906:TYR:O	1:D:907:PRO:C	2.49	0.56
1:A:200:GLN:OE1	1:A:200:GLN:N	2.34	0.56
1:A:930:VAL:HA	1:A:973:ARG:HD2	1.86	0.56
1:A:1020:TRP:CD1	1:A:1021:CYS:N	2.73	0.56
1:C:577:LYS:HD3	1:C:585:TRP:CH2	2.41	0.56
1:A:65:ALA:HB1	1:A:66:PRO:CD	2.32	0.56
1:A:84:VAL:HG13	1:A:85:VAL:N	2.20	0.56
1:A:358:GLU:HB3	1:A:367:MET:HG2	1.88	0.56
1:A:422:PRO:HG2	1:D:285:TYR:CZ	2.40	0.56
1:A:987:ASP:OD2	1:A:990:HIS:HD2	1.88	0.56
1:D:777:LEU:HD23	1:D:777:LEU:N	2.21	0.56
1:A:90:TRP:CD1	1:A:95:TYR:HB2	2.41	0.56
1:A:426:LEU:HD22	1:A:432:TRP:CE2	2.41	0.56
1:A:437:SER:HA	1:A:471:LEU:HD21	1.88	0.56
1:C:256:VAL:O	1:C:271:THR:HA	2.06	0.56
1:C:807:VAL:HG13	1:C:808:GLU:N	2.21	0.56
1:D:645:ARG:HH22	1:D:650:GLU:CD	2.14	0.56
1:D:895:VAL:O	1:D:919:ASP:HA	2.06	0.56
1:A:693:GLN:CG	1:A:721:ARG:HD3	2.35	0.56
1:B:375:ASP:C	1:B:379:MET:HE3	2.30	0.56
1:B:630:ARG:HB3	1:B:630:ARG:CZ	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:ARG:HD3	3:C:4139:HOH:O	2.04	0.56
1:D:42:ALA:O	1:D:43:ARG:C	2.47	0.56
1:A:421:VAL:HG13	1:D:282:ARG:O	2.06	0.55
1:A:693:GLN:HG3	1:A:724:GLU:HG3	1.87	0.55
1:B:309:TYR:HB2	1:B:330:VAL:HG12	1.88	0.55
1:B:533:LEU:C	1:B:533:LEU:HD12	2.30	0.55
1:B:767:GLN:HG3	1:B:768:MET:N	2.18	0.55
1:B:822:LEU:HD12	1:B:823:LEU:H	1.71	0.55
1:B:979:GLU:O	1:B:980:GLU:C	2.49	0.55
1:C:721:ARG:HE	1:D:874:SER:CB	2.18	0.55
1:C:836:ILE:HG22	1:C:837:THR:N	2.20	0.55
1:D:416:GLU:OE1	1:D:418:HIS:HB2	2.06	0.55
1:A:128:ASN:HD22	1:A:180:GLY:C	2.14	0.55
1:B:213:SER:O	1:B:214:LEU:HD23	2.06	0.55
1:B:357:HIS:HD2	1:B:392:TYR:OH	1.89	0.55
1:B:367:MET:CE	1:B:372:MET:HG2	2.36	0.55
1:B:658:LEU:HG	1:B:661:LYS:HZ2	1.69	0.55
1:B:856:TYR:HB3	1:B:864:MET:HE2	1.88	0.55
1:C:354:VAL:HG22	1:C:355:ASN:N	2.21	0.55
1:D:254:LEU:C	1:D:255:ARG:HG2	2.31	0.55
1:D:344:LEU:HG	1:D:345:ASN:N	2.19	0.55
1:D:693:GLN:HB2	1:D:695:TRP:HE1	1.71	0.55
1:B:38:ASN:HD21	1:B:41:GLU:H	1.54	0.55
1:B:433:LEU:HD12	1:B:433:LEU:C	2.29	0.55
1:B:710:GLU:HA	1:B:710:GLU:OE2	2.05	0.55
1:D:13:ARG:O	1:D:14:ARG:C	2.47	0.55
1:D:75:GLU:OE1	1:D:75:GLU:HA	2.06	0.55
1:D:769:TRP:HE1	1:D:774:LYS:HE2	1.71	0.55
1:A:202:MET:HA	1:A:573:GLN:NE2	2.18	0.55
1:A:377:LEU:HD22	1:A:708:TRP:CA	2.36	0.55
1:A:559:TYR:HB2	1:A:562:LEU:HD12	1.88	0.55
1:A:907:PRO:HD3	1:A:939:CYS:SG	2.45	0.55
1:B:200:GLN:CB	1:B:202:MET:HG2	2.36	0.55
1:B:385:ASN:O	1:B:408:TYR:N	2.28	0.55
1:B:910:LEU:C	1:B:910:LEU:HD12	2.32	0.55
1:C:597:ASN:ND2	1:C:599:ARG:H	2.00	0.55
1:D:344:LEU:HD23	1:D:644:PHE:CZ	2.41	0.55
1:D:578:TYR:HA	1:D:583:ASN:O	2.07	0.55
1:D:763:GLY:HA3	1:D:822:LEU:CD2	2.37	0.55
1:A:427:THR:O	1:A:467:ASN:HB2	2.07	0.55
1:B:429:ASP:CG	1:B:431[A]:ARG:HD3	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:510:GLN:HB2	1:B:517:LYS:HB2	1.87	0.55
1:C:166:ARG:HG3	1:C:392:TYR:CB	2.36	0.55
1:C:382:ASN:O	1:C:621:LYS:HA	2.06	0.55
1:C:420:MET:HE2	1:C:426:LEU:CG	2.33	0.55
1:C:568:TRP:NE1	1:C:604:ASN:HD22	1.99	0.55
1:A:379:MET:HB3	1:A:384:PHE:HB2	1.88	0.55
1:B:600:GLN:C	1:B:602:CYS:H	2.15	0.55
1:C:1020:TRP:CD1	1:C:1021:CYS:N	2.74	0.55
1:D:142:ILE:O	1:D:212:VAL:HA	2.06	0.55
1:D:305:ILE:HD11	1:D:645:ARG:HB3	1.88	0.55
1:D:512:PHE:HE1	1:D:517:LYS:HG3	1.71	0.55
1:D:949:HIS:HD2	1:D:1020:TRP:HE1	1.53	0.55
1:D:984:LEU:HD21	1:D:986:ILE:CD1	2.27	0.55
1:A:52[B]:ARG:NH2	1:A:130:ASP:HB2	2.21	0.55
1:A:352:ARG:O	1:A:385:ASN:HB2	2.07	0.55
1:A:590:GLY:HA2	1:A:594:ASP:CG	2.32	0.55
1:B:100:TYR:CZ	1:B:602:CYS:HB3	2.42	0.55
1:B:227:VAL:HG11	1:B:330:VAL:CG2	2.36	0.55
1:B:258:VAL:HA	1:B:312:VAL:O	2.07	0.55
1:B:974:HIS:O	1:B:975:LEU:HD23	2.07	0.55
1:C:27:LEU:HD12	1:C:170:GLU:CB	2.37	0.55
1:C:523:TRP:O	1:C:526:LEU:HB2	2.07	0.55
1:C:629:PHE:N	1:C:629:PHE:CD1	2.75	0.55
1:D:344:LEU:HD23	1:D:644:PHE:CE1	2.42	0.55
1:D:878:HIS:CD2	1:D:1010:SER:HB3	2.41	0.55
1:A:381:GLN:NE2	1:A:708:TRP:O	2.40	0.55
1:B:102:ASN:C	1:B:102:ASN:HD22	2.15	0.55
1:C:376:ILE:HG22	1:C:377:LEU:N	2.21	0.55
1:C:393:PRO:HD3	1:C:412:GLU:O	2.07	0.55
1:D:95:TYR:N	1:D:95:TYR:CD1	2.75	0.55
1:D:432:TRP:O	1:D:436:MET:HG3	2.06	0.55
1:D:457:SER:HA	1:D:485:GLN:O	2.07	0.55
1:D:656:VAL:CG1	1:D:694:LEU:HD11	2.37	0.55
1:D:69:VAL:CG1	1:D:70:PRO:HD2	2.37	0.55
1:D:333:ARG:HA	1:D:345:ASN:OD1	2.06	0.55
1:A:282:ARG:NH1	1:D:420:MET:O	2.39	0.55
1:B:674:PRO:C	1:B:675:GLN:HG2	2.32	0.55
1:C:11:LEU:HD11	1:C:187:MET:HE1	1.87	0.55
1:C:23:GLN:O	1:C:24:LEU:HD13	2.07	0.55
1:C:29:ALA:HB3	1:C:445:GLN:OE1	2.06	0.55
1:C:742:THR:HG22	1:C:743:SER:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:PRO:HA	1:A:516:PRO:CB	2.37	0.54
1:B:212:VAL:HG12	1:B:213:SER:N	2.19	0.54
1:A:762:SER:O	1:A:822:LEU:HD23	2.08	0.54
1:B:51:LEU:HD13	1:B:215:LEU:HB2	1.89	0.54
1:B:141:ILE:HG23	1:B:143:PHE:CE1	2.42	0.54
1:C:432:TRP:N	1:C:432:TRP:CD1	2.71	0.54
1:C:438:GLU:O	1:C:442:ARG:HG3	2.08	0.54
1:D:416:GLU:OE1	1:D:461:GLU:HG3	2.06	0.54
1:D:598:ASP:C	1:D:599:ARG:HG3	2.33	0.54
1:D:782:ASP:HA	1:D:884:LEU:HD23	1.88	0.54
1:A:274:PHE:HB3	1:A:286:ALA:O	2.08	0.54
1:A:890:GLN:O	1:A:891:VAL:HG23	2.07	0.54
1:C:568:TRP:NE1	1:C:604:ASN:ND2	2.46	0.54
1:D:155:ASN:ND2	1:D:182:ASN:OD1	2.29	0.54
1:D:334:GLU:CD	1:D:336:ARG:HD3	2.33	0.54
1:D:528:GLY:O	1:D:530:THR:HG23	2.06	0.54
1:D:852:SER:HB2	1:D:870:VAL:HG22	1.89	0.54
1:D:949:HIS:CD2	1:D:1020:TRP:HE1	2.24	0.54
1:B:424:ASN:HB3	1:C:285:TYR:OH	2.07	0.54
1:C:240:LEU:HG	1:C:241:GLU:N	2.21	0.54
1:A:7:LEU:HD21	1:A:74:LEU:CD2	2.23	0.54
1:A:925:MET:HA	1:A:925:MET:HE3	1.89	0.54
1:B:840:HIS:HB2	1:B:842:TRP:CH2	2.43	0.54
1:C:256:VAL:HG12	1:C:257:THR:N	2.21	0.54
1:C:876:THR:HA	3:C:4521:HOH:O	2.07	0.54
1:C:881:ARG:HG3	1:C:882:ILE:N	2.15	0.54
1:A:63:PHE:CB	1:A:64:PRO:HD2	2.26	0.54
1:B:143:PHE:HB3	3:B:4101:HOH:O	2.07	0.54
1:B:751:LEU:HD23	1:B:751:LEU:O	2.07	0.54
1:B:777:LEU:HD21	1:B:889:ALA:HA	1.88	0.54
1:C:995:GLY:O	1:C:997:ASP:N	2.41	0.54
1:D:202:MET:HE3	1:D:357:HIS:HD2	1.66	0.54
1:D:246:MET:HG2	1:D:274:PHE:CZ	2.43	0.54
1:D:603:MET:HE1	1:D:930:VAL:HG12	1.85	0.54
1:D:893:GLU:O	1:D:921:PRO:HA	2.07	0.54
1:D:904:GLU:HG2	1:D:909:ARG:NH2	2.22	0.54
1:A:570:TRP:HD1	1:A:571:VAL:HG22	1.69	0.54
1:B:493:THR:HG23	3:B:4020:HOH:O	2.08	0.54
1:B:897:TRP:CB	1:B:944:LEU:HB2	2.38	0.54
1:C:589:GLY:C	1:C:591:ASP:H	2.16	0.54
1:C:685:LEU:O	1:C:687:GLN:HG3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:802:ASP:O	1:C:808:GLU:HG3	2.07	0.54
1:A:100:TYR:HB2	1:A:203:TRP:CE3	2.43	0.54
1:A:652:LEU:HD12	1:A:699:ARG:O	2.07	0.54
1:B:100:TYR:CE1	1:B:602:CYS:HB3	2.41	0.54
1:B:200:GLN:HB3	1:B:202:MET:HG2	1.90	0.54
1:B:429:ASP:OD1	1:B:431[B]:ARG:HG3	2.08	0.54
1:B:655:MET:O	1:B:696:LEU:HD12	2.08	0.54
1:B:670:LEU:HD11	1:B:700:VAL:HG22	1.90	0.54
1:B:774:LYS:HB2	1:B:774:LYS:NZ	2.23	0.54
1:C:478:VAL:HG12	1:C:479:ASP:N	2.21	0.54
1:D:742:THR:HG22	1:D:743:SER:N	2.22	0.54
1:A:93:HIS:HB3	1:A:95:TYR:CE1	2.39	0.54
1:A:198:GLU:HB3	3:A:4060:HOH:O	2.07	0.54
1:A:228:ALA:O	1:A:240:LEU:HD12	2.08	0.54
1:B:114:VAL:HG12	1:B:115:PRO:N	2.23	0.54
1:B:822:LEU:HD12	1:B:823:LEU:N	2.23	0.54
1:B:894:ARG:CZ	1:B:921:PRO:HD3	2.38	0.54
1:B:916:ASP:HB3	1:B:918:TRP:CZ2	2.42	0.54
1:C:748:CYS:SG	1:C:757:GLN:HG3	2.48	0.54
1:D:696:LEU:HD12	1:D:697:THR:N	2.23	0.54
1:D:762:SER:C	1:D:822:LEU:HD23	2.33	0.54
1:D:763:GLY:CA	1:D:822:LEU:HD21	2.37	0.54
1:A:138:GLN:OE1	1:A:140:ARG:NH2	2.39	0.54
1:B:949:HIS:CD2	1:B:1020:TRP:HE1	2.26	0.54
1:B:955:PHE:HB2	1:B:987:ASP:O	2.06	0.54
1:C:168:PRO:O	1:C:442:ARG:NH2	2.38	0.54
1:C:768:MET:HE2	1:C:770:ILE:HG13	1.89	0.54
1:C:789:LEU:HG	1:C:792:ASP:OD2	2.08	0.54
1:B:58:TRP:CE3	1:B:123:TYR:HB3	2.43	0.53
1:C:801:ILE:O	1:C:803:PRO:HD3	2.08	0.53
1:D:23:GLN:HB3	1:D:26:ARG:HH21	1.73	0.53
1:D:737:ILE:HG13	1:D:738:PRO:N	2.20	0.53
1:A:930:VAL:HG22	1:A:973:ARG:NE	2.23	0.53
1:B:769:TRP:NE1	1:B:774:LYS:HG3	2.23	0.53
1:C:658:LEU:HD12	1:C:659:ASP:N	2.23	0.53
1:C:856:TYR:HB3	1:C:864:MET:HE1	1.90	0.53
1:D:573:GLN:HB2	1:D:602:CYS:O	2.08	0.53
1:D:639:THR:OG1	1:D:677:LYS:HE2	2.09	0.53
1:D:745:MET:O	1:D:760:ARG:N	2.38	0.53
1:D:890:GLN:N	1:D:890:GLN:HE21	2.06	0.53
1:A:224:ASP:HB3	1:A:245:GLN:CG	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ARG:O	1:B:124:SER:N	2.39	0.53
1:B:434:PRO:O	1:B:435:ALA:C	2.50	0.53
1:B:440:VAL:CG1	1:B:475:ILE:HD11	2.38	0.53
1:B:868:VAL:HG12	1:B:869:ASP:N	2.23	0.53
1:C:463:GLY:HA2	3:C:7509:HOH:O	2.08	0.53
1:D:238:ALA:HB2	1:D:298:PRO:HG3	1.90	0.53
1:D:597:ASN:HD22	1:D:599:ARG:N	1.95	0.53
1:D:737:ILE:HG13	1:D:738:PRO:CD	2.38	0.53
1:D:757:GLN:HG2	1:D:758:PHE:N	2.22	0.53
1:B:80:GLU:H	1:B:80:GLU:CD	2.16	0.53
1:B:592:PHE:N	1:B:592:PHE:CD1	2.76	0.53
1:C:58:TRP:CE3	1:C:123:TYR:HB3	2.43	0.53
1:C:734:SER:HB3	1:C:860:GLY:N	2.23	0.53
1:C:949:HIS:CD2	1:C:1020:TRP:HE1	2.26	0.53
1:D:937:LEU:HA	1:D:958:ASN:HB3	1.89	0.53
1:A:52[B]:ARG:HG3	1:A:133:TRP:HH2	1.73	0.53
1:A:257:THR:HA	1:A:270:GLY:O	2.08	0.53
1:C:590:GLY:HA2	1:C:594:ASP:O	2.09	0.53
1:C:995:GLY:O	1:C:996:ASP:C	2.50	0.53
1:D:524:LEU:O	1:D:561:ARG:NH2	2.41	0.53
1:D:683:PRO:O	1:D:685:LEU:HG	2.08	0.53
1:A:38:ASN:HD22	1:A:41:GLU:HG3	1.73	0.53
1:A:240:LEU:HD23	1:A:260:LEU:HD22	1.89	0.53
1:A:962:TYR:HD2	1:A:966:GLN:NE2	2.06	0.53
1:B:598:ASP:C	1:B:599:ARG:HG3	2.34	0.53
1:C:254:LEU:O	1:C:255:ARG:NH1	2.42	0.53
1:C:694:LEU:HD12	1:C:695:TRP:H	1.74	0.53
1:C:770:ILE:HD11	1:C:1022:GLN:HG2	1.90	0.53
1:C:930:VAL:O	1:C:932:PRO:HD3	2.08	0.53
1:D:71:GLU:O	1:D:73:TRP:N	2.41	0.53
1:D:655:MET:HE3	1:D:664:ALA:O	2.08	0.53
1:D:906:TYR:HB3	1:D:907:PRO:HD2	1.90	0.53
1:A:227:VAL:CG1	1:A:240:LEU:HD11	2.33	0.53
1:A:856:TYR:HB3	1:A:864:MET:HE3	1.90	0.53
1:B:143:PHE:CD1	1:B:143:PHE:N	2.76	0.53
1:B:660:GLY:O	1:B:662:PRO:HD3	2.09	0.53
1:B:906:TYR:HB3	1:B:907:PRO:HD2	1.90	0.53
1:C:11:LEU:HD21	1:C:187:MET:CE	2.39	0.53
1:D:475:ILE:O	1:D:476:LYS:C	2.49	0.53
1:D:946:TYR:CE2	1:D:982:THR:HG21	2.43	0.53
1:A:607:VAL:HG23	1:A:608:PHE:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:696:LEU:HD12	1:A:696:LEU:C	2.34	0.53
1:A:891:VAL:O	1:A:891:VAL:HG12	2.09	0.53
1:B:683:PRO:O	1:B:684:GLU:C	2.51	0.53
1:C:429:ASP:OD1	1:C:431[A]:ARG:HG3	2.09	0.53
1:C:658:LEU:O	1:C:661:LYS:HE3	2.09	0.53
1:A:507:ASP:OD1	1:A:521:LYS:HE2	2.08	0.53
1:A:822:LEU:HD11	1:A:824:GLN:C	2.34	0.53
1:B:739[A]:HIS:CD2	1:B:740:LEU:N	2.77	0.53
1:C:436:MET:CE	1:C:467:ASN:HD22	2.09	0.53
1:D:429:ASP:OD1	1:D:431[B]:ARG:HG3	2.09	0.53
1:D:654:TRP:CE3	1:D:655:MET:N	2.77	0.53
1:A:734:SER:HB2	1:A:860:GLY:CA	2.38	0.53
1:B:221:GLN:O	1:B:221:GLN:HG2	1.95	0.53
1:B:254:LEU:C	1:B:255:ARG:HH11	2.16	0.53
1:C:261:TRP:HA	1:C:267:VAL:HG23	1.91	0.53
1:C:598:ASP:C	1:C:599:ARG:HG2	2.34	0.53
1:D:30:HIS:HB2	1:D:31:PRO:CD	2.38	0.53
1:D:356:ARG:HD2	1:D:379:MET:CE	2.39	0.53
1:D:501:PRO:HD2	1:D:533:LEU:HD13	1.90	0.53
1:A:173:LEU:O	1:A:174:SER:C	2.51	0.52
1:A:416:GLU:OE1	1:A:418:HIS:HB2	2.09	0.52
1:B:30:HIS:CE1	1:B:33:PHE:CD1	2.97	0.52
1:B:275:GLY:HA2	1:B:286:ALA:HA	1.92	0.52
1:B:486:TYR:CE2	1:B:488:GLY:HA3	2.44	0.52
1:B:897:TRP:CZ3	1:B:925:MET:HE1	2.44	0.52
1:C:241:GLU:HG3	1:C:292:ARG:HG2	1.91	0.52
1:C:673:ALA:HB1	1:C:674:PRO:CD	2.36	0.52
1:C:835:LEU:HD12	1:C:836:ILE:N	2.24	0.52
1:D:99:ILE:O	1:D:204:ARG:N	2.41	0.52
1:D:161:TYR:OH	1:D:163:GLN:NE2	2.33	0.52
1:A:126:THR:HA	1:A:182:ASN:O	2.10	0.52
1:B:375:ASP:HB3	1:B:379:MET:HE1	1.91	0.52
1:B:866:ILE:O	1:B:1018:LEU:N	2.32	0.52
1:B:1020:TRP:CD1	1:B:1021:CYS:N	2.77	0.52
1:C:59:ARG:NH2	1:C:81:ALA:O	2.42	0.52
1:D:127:PHE:HE1	1:D:129:VAL:HG22	1.73	0.52
1:D:373:VAL:O	1:D:374:GLN:C	2.49	0.52
1:D:878:HIS:NE2	1:D:1010:SER:HB3	2.24	0.52
1:A:53:SER:O	1:A:54:LEU:HD23	2.10	0.52
1:A:889:ALA:O	1:A:890:GLN:C	2.51	0.52
1:C:176:PHE:N	1:C:176:PHE:CD1	2.76	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:ASP:O	1:D:78:LEU:HD23	2.10	0.52
1:D:473:ARG:O	1:D:473:ARG:HD3	2.10	0.52
1:D:948:PRO:HG2	1:D:949:HIS:CE1	2.44	0.52
1:A:38:ASN:ND2	1:A:41:GLU:N	2.54	0.52
1:A:502:MET:HB3	1:A:537:GLU:HB2	1.91	0.52
1:A:548:GLY:O	1:A:551:LYS:HB2	2.09	0.52
1:A:666:GLY:C	1:A:667:GLU:HG2	2.33	0.52
1:B:839:ALA:HA	1:B:852:SER:O	2.09	0.52
1:C:652:LEU:HB2	1:C:670:LEU:HD21	1.91	0.52
1:C:734:SER:CB	1:C:860:GLY:HA3	2.27	0.52
1:A:389:CYS:HB3	1:A:394:ASN:ND2	2.24	0.52
1:B:425:ARG:HH22	1:C:287:ASP:CG	2.17	0.52
1:B:497:ASP:O	1:B:531:ARG:HG2	2.09	0.52
1:B:784:PHE:HA	1:B:881:ARG:O	2.09	0.52
1:C:533:LEU:C	1:C:533:LEU:HD12	2.34	0.52
1:C:878:HIS:ND1	3:C:4074:HOH:O	2.30	0.52
1:D:62:TRP:CG	1:D:95:TYR:HB3	2.44	0.52
1:D:486:TYR:CZ	1:D:488:GLY:HA3	2.44	0.52
1:D:746:ASP:HA	1:D:760:ARG:CG	2.24	0.52
1:A:6:SER:OG	1:A:8:ALA:HB3	2.10	0.52
1:A:786:ARG:HH11	1:A:990:HIS:CE1	2.28	0.52
1:B:78:LEU:O	1:B:80:GLU:N	2.42	0.52
1:B:422:PRO:HG2	1:B:424:ASN:HB3	1.89	0.52
1:C:353:GLY:HA2	1:C:386:ALA:O	2.09	0.52
1:C:373:VAL:HG12	1:C:377:LEU:HD11	1.90	0.52
1:D:114:VAL:CG1	1:D:191:TRP:HB2	2.39	0.52
1:D:415:ILE:HG12	1:D:439:ARG:HD2	1.91	0.52
1:D:464:HIS:HB2	1:D:489:GLY:HA3	1.91	0.52
1:D:959:ILE:HG23	1:D:959:ILE:O	2.09	0.52
1:A:58:TRP:N	1:A:84:VAL:O	2.42	0.52
1:B:578:TYR:HA	1:B:583:ASN:O	2.09	0.52
3:C:4115:HOH:O	1:D:525:SER:HA	2.10	0.52
1:D:237:ARG:HH11	1:D:237:ARG:CG	2.22	0.52
1:D:486:TYR:CE2	1:D:488:GLY:HA3	2.44	0.52
1:A:18:ASN:OD1	1:A:20:GLY:N	2.40	0.52
1:A:128:ASN:HD22	1:A:181:GLU:N	2.06	0.52
1:A:237:ARG:HH11	1:A:237:ARG:CB	2.23	0.52
1:A:652:LEU:O	1:A:667:GLU:HA	2.10	0.52
1:B:685:LEU:HB3	1:B:686:PRO:CD	2.36	0.52
1:B:737:ILE:C	1:B:751:LEU:HD12	2.34	0.52
1:C:373:VAL:O	1:C:377:LEU:HG	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:395:HIS:CG	1:C:396:PRO:HD2	2.44	0.52
1:C:858:ILE:HA	1:C:863:GLN:O	2.09	0.52
1:D:23:GLN:O	1:D:24:LEU:HD13	2.10	0.52
1:D:650:GLU:HA	1:D:701:VAL:O	2.10	0.52
1:D:826:THR:O	1:D:826:THR:OG1	2.27	0.52
1:B:11:LEU:HD21	1:B:187:MET:CE	2.40	0.52
1:B:759:ASN:OD1	1:B:761:GLN:N	2.29	0.52
1:B:808:GLU:OE1	1:B:808:GLU:HA	2.03	0.52
1:C:7:LEU:HB2	1:C:71:GLU:CD	2.34	0.52
1:C:133:TRP:HA	1:C:216:HIS:CE1	2.45	0.52
1:C:319:ASP:OD1	1:C:321:THR:OG1	2.27	0.52
1:A:417:THR:O	1:A:418:HIS:C	2.49	0.52
1:B:29:ALA:HB3	1:B:445:GLN:HG3	1.92	0.52
1:B:399:TYR:HB2	1:B:450:HIS:NE2	2.25	0.52
1:B:848:THR:C	1:B:849:LEU:HD23	2.35	0.52
1:C:166:ARG:O	1:C:167:LEU:HD23	2.10	0.52
1:C:255:ARG:HH11	1:C:255:ARG:CG	2.20	0.52
1:C:960:SER:HA	3:C:4030:HOH:O	2.10	0.52
1:D:41:GLU:OE2	1:D:46:ARG:NH1	2.43	0.52
1:D:499:ILE:O	1:D:533:LEU:HD13	2.11	0.52
1:D:512:PHE:CE1	1:D:517:LYS:HG3	2.44	0.52
1:A:383:ASN:HD22	1:A:625:GLN:HA	1.74	0.51
1:B:41:GLU:HA	1:B:46:ARG:HB2	1.92	0.51
1:B:856:TYR:N	1:B:856:TYR:CD1	2.78	0.51
1:C:3:ILE:C	1:C:5:ASP:H	2.19	0.51
1:C:84:VAL:HG22	1:C:93:HIS:ND1	2.25	0.51
1:C:258:VAL:CB	1:C:291:LEU:HD11	2.40	0.51
1:C:375:ASP:O	1:C:376:ILE:C	2.52	0.51
1:C:497:ASP:O	1:C:531:ARG:HG2	2.10	0.51
1:C:925:MET:HA	1:C:925:MET:HE3	1.91	0.51
1:D:86:VAL:HA	1:D:87:PRO:C	2.34	0.51
1:D:230:ARG:O	1:D:238:ALA:HA	2.09	0.51
1:D:360:HIS:HE1	1:D:362:LEU:HB2	1.72	0.51
1:D:655:MET:HA	1:D:665:SER:HA	1.92	0.51
1:A:948:PRO:O	1:A:1022:GLN:HA	2.10	0.51
1:A:989:PHE:N	1:A:989:PHE:CD1	2.79	0.51
1:B:234:ASP:O	1:B:235:PHE:HB2	2.10	0.51
1:B:916:ASP:HB3	1:B:918:TRP:CE2	2.44	0.51
1:C:99:ILE:CG2	1:C:101:THR:HG22	2.40	0.51
1:C:645:ARG:HH22	1:C:650:GLU:CD	2.18	0.51
1:D:666:GLY:O	1:D:667:GLU:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:685:LEU:CB	1:D:686:PRO:HD2	2.37	0.51
1:A:12:GLN:HG3	1:A:13:ARG:N	2.26	0.51
1:A:991:MET:HG2	1:A:992:GLY:H	1.73	0.51
1:B:823:LEU:HD11	1:B:841:ALA:HB2	1.91	0.51
1:C:77:ASP:C	1:C:78:LEU:HD23	2.36	0.51
1:D:55:ASN:OD1	1:D:211:ASP:HB3	2.11	0.51
1:D:399:TYR:CE1	1:D:446:ARG:NH2	2.79	0.51
1:D:966:GLN:NE2	1:D:979:GLU:OE2	2.44	0.51
1:A:124:SER:HA	1:A:184:LEU:O	2.11	0.51
1:B:35:SER:O	1:B:50:GLN:NE2	2.42	0.51
1:B:141:ILE:HG12	1:B:142:ILE:N	2.25	0.51
1:B:458:LEU:HD11	1:B:472:TYR:HB2	1.93	0.51
1:D:72:SER:O	1:D:75:GLU:N	2.42	0.51
1:D:588:TYR:O	1:D:589:GLY:C	2.52	0.51
1:A:11:LEU:HD11	1:A:187:MET:HE1	1.91	0.51
1:A:24:LEU:O	1:A:25:ASN:HB2	2.08	0.51
1:A:636:ILE:N	1:A:680:ILE:O	2.35	0.51
1:A:1020:TRP:HD1	1:A:1021:CYS:H	1.56	0.51
1:B:521:LYS:HD3	1:B:559:TYR:CZ	2.45	0.51
1:B:567:VAL:HG12	1:B:568:TRP:N	2.25	0.51
1:C:883:GLY:HA2	1:C:1016:TYR:OH	2.10	0.51
1:A:11:LEU:HD23	1:A:11:LEU:H	1.76	0.51
1:A:106:PRO:HG3	1:A:204:ARG:HG3	1.93	0.51
1:A:416:GLU:OE1	1:A:461:GLU:OE2	2.29	0.51
1:B:650:GLU:CB	1:B:670:LEU:HD12	2.28	0.51
1:C:102:ASN:HD22	1:C:102:ASN:C	2.19	0.51
1:C:515:VAL:HG23	1:C:515:VAL:O	2.10	0.51
1:C:649:ASN:O	1:C:702:GLN:HG3	2.10	0.51
1:D:878:HIS:HB3	1:D:879:PRO:HD2	1.92	0.51
1:B:4:THR:C	1:B:9:VAL:HG11	2.35	0.51
1:C:733:ALA:O	1:C:734:SER:C	2.54	0.51
1:C:1009:LEU:N	1:C:1009:LEU:HD23	2.25	0.51
1:D:472:TYR:O	1:D:476:LYS:HG2	2.10	0.51
1:D:577:LYS:O	1:D:584:PRO:HA	2.10	0.51
1:D:920:LEU:HB3	1:D:921:PRO:HD2	1.93	0.51
1:A:41:GLU:HG2	1:A:46:ARG:HH11	1.76	0.51
1:A:585:TRP:CE3	1:A:974:HIS:CE1	2.99	0.51
1:A:858:ILE:HG12	1:A:864:MET:HB3	1.92	0.51
1:B:956:GLN:O	1:B:987:ASP:N	2.29	0.51
1:C:261:TRP:CD1	1:C:261:TRP:N	2.79	0.51
1:C:505:ARG:HB3	3:C:4226:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:741:THR:O	1:C:741:THR:HG22	2.09	0.51
1:D:636:ILE:N	1:D:680:ILE:O	2.37	0.51
1:D:645:ARG:NH2	1:D:650:GLU:OE1	2.43	0.51
1:B:11:LEU:N	1:B:11:LEU:HD23	2.25	0.51
1:B:36:TRP:CD1	1:B:41:GLU:HB3	2.46	0.51
1:B:851:ILE:O	1:B:870:VAL:HA	2.11	0.51
1:C:499:ILE:HB	1:C:533:LEU:CB	2.40	0.51
1:C:585:TRP:CE3	1:C:974:HIS:CE1	2.98	0.51
1:C:701:VAL:HG12	1:C:702:GLN:N	2.26	0.51
1:D:37:ARG:HD3	1:D:50:GLN:NE2	2.26	0.51
1:A:50:GLN:NE2	1:A:50:GLN:H	2.08	0.51
1:A:233:ASP:OD2	1:C:233:ASP:HB3	2.11	0.51
1:A:234:ASP:OD1	1:A:236:SER:OG	2.28	0.51
1:A:613:PRO:HB3	1:A:617:LEU:CD2	2.40	0.51
1:B:143:PHE:O	1:B:168:PRO:HA	2.11	0.51
1:B:399:TYR:O	1:B:400:THR:C	2.53	0.51
1:B:427:THR:O	1:B:467:ASN:HB2	2.11	0.51
1:B:894:ARG:NH1	1:B:921:PRO:HD3	2.26	0.51
1:C:43:ARG:HD2	1:C:261:TRP:CE2	2.46	0.51
1:D:568:TRP:NE1	1:D:604:ASN:HD22	2.05	0.51
1:A:394:ASN:O	1:A:395:HIS:C	2.52	0.50
1:B:217:LYS:HG2	1:B:218:PRO:CD	2.42	0.50
1:C:610:ASP:OD2	1:C:610:ASP:N	2.41	0.50
1:C:963:SER:OG	1:C:979:GLU:OE2	2.28	0.50
1:D:200:GLN:OE1	1:D:200:GLN:N	2.43	0.50
1:A:80:GLU:OE2	1:A:80:GLU:N	2.30	0.50
1:A:426:LEU:HD22	1:A:432:TRP:NE1	2.26	0.50
1:A:613:PRO:CB	1:A:617:LEU:HD23	2.40	0.50
1:B:58:TRP:HE3	1:B:123:TYR:HB3	1.76	0.50
1:B:411:ASP:OD2	1:B:447:ASP:OD2	2.29	0.50
1:B:788:PRO:HD3	1:B:968:MET:HG3	1.91	0.50
1:C:229:THR:HA	1:C:239:VAL:O	2.10	0.50
1:C:420:MET:HE3	1:C:425:ARG:CB	2.38	0.50
1:D:130:ASP:OD2	1:D:132:SER:OG	2.29	0.50
1:A:411:ASP:OD2	1:A:447:ASP:OD2	2.29	0.50
1:A:436:MET:O	1:A:437:SER:C	2.52	0.50
1:A:746:ASP:HA	1:A:760:ARG:CG	2.29	0.50
1:B:733:ALA:O	1:B:734:SER:O	2.30	0.50
1:C:111:PRO:HG3	1:C:196:TYR:CE2	2.46	0.50
1:C:143:PHE:O	1:C:168:PRO:HA	2.11	0.50
1:C:232:ASN:O	1:C:233:ASP:C	2.53	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:VAL:HB	1:C:291:LEU:CD1	2.41	0.50
1:C:347:LYS:HZ1	1:C:675:GLN:HG3	1.73	0.50
1:C:568:TRP:CD1	1:C:568:TRP:C	2.89	0.50
1:C:689:GLU:O	1:C:690:SER:C	2.54	0.50
1:D:536:CYS:C	1:D:537:GLU:HG3	2.36	0.50
1:D:758:PHE:HZ	1:D:864:MET:HE1	1.77	0.50
1:A:959:ILE:HA	3:A:4028:HOH:O	2.11	0.50
1:B:548:GLY:O	1:B:549:PHE:C	2.54	0.50
1:B:577:LYS:HB3	1:B:585:TRP:CE2	2.46	0.50
1:C:506:VAL:HA	1:C:520:ILE:HG12	1.93	0.50
1:A:655:MET:HE1	1:A:662:PRO:CB	2.39	0.50
1:A:719:GLN:HE22	1:A:915:PHE:H	1.59	0.50
1:A:821:ALA:O	1:A:840:HIS:HA	2.10	0.50
1:A:847:LYS:HD2	1:A:848:THR:N	2.27	0.50
1:A:887:GLN:HB2	1:A:983:TRP:CD2	2.47	0.50
1:B:399:TYR:CB	1:B:450:HIS:CD2	2.95	0.50
1:B:638:VAL:O	1:B:677:LYS:HA	2.11	0.50
1:C:499:ILE:HD11	1:C:529:GLU:CD	2.35	0.50
1:D:3:ILE:HD12	1:D:3:ILE:O	2.12	0.50
1:D:225:PHE:HA	1:D:243:GLU:O	2.11	0.50
1:A:18:ASN:OD1	1:A:19:PRO:HD2	2.12	0.50
1:A:797:GLU:O	1:A:800:ARG:O	2.29	0.50
1:B:118:ASN:CB	1:B:191:TRP:HD1	2.14	0.50
1:B:619:GLU:HA	1:B:912:ALA:HB2	1.94	0.50
1:B:701:VAL:CG1	1:B:702:GLN:N	2.73	0.50
1:B:959:ILE:HG23	1:B:959:ILE:O	2.12	0.50
1:C:649:ASN:ND2	1:C:702:GLN:HG2	2.26	0.50
1:A:36:TRP:CE2	1:A:42:ALA:HA	2.46	0.50
1:A:38:ASN:O	1:A:39:SER:C	2.54	0.50
1:A:202:MET:HB3	1:A:573:GLN:HE22	1.76	0.50
1:A:629:PHE:CD1	1:A:629:PHE:N	2.79	0.50
1:A:652:LEU:N	1:A:668:VAL:O	2.36	0.50
1:A:658:LEU:N	1:A:661:LYS:O	2.38	0.50
1:B:163:GLN:OE1	1:B:193:ASP:OD1	2.30	0.50
1:B:571:VAL:HG11	1:B:611:ARG:CZ	2.41	0.50
1:C:21:VAL:HG13	1:C:24:LEU:HD13	1.94	0.50
1:C:103:VAL:HG12	1:C:104:THR:N	2.27	0.50
1:D:16:TRP:O	1:D:193:ASP:N	2.44	0.50
1:A:647:SER:OG	1:A:672:VAL:O	2.30	0.50
1:A:856:TYR:N	1:A:856:TYR:CD1	2.79	0.50
1:B:645:ARG:NH2	1:B:650:GLU:OE2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:696:LEU:HD12	1:B:697:THR:N	2.27	0.50
1:C:386:ALA:HB2	1:C:408:TYR:HB2	1.94	0.50
1:C:726:LEU:HD11	1:D:873:ALA:HB2	1.93	0.50
1:C:856:TYR:HD2	1:C:864:MET:CE	2.21	0.50
1:C:966:GLN:NE2	1:C:979:GLU:OE2	2.31	0.50
1:D:33:PHE:HA	1:D:326:GLU:OE1	2.11	0.50
1:D:588:TYR:HB2	1:D:602:CYS:SG	2.52	0.50
1:A:217:LYS:NZ	1:A:324:GLU:OE2	2.44	0.50
1:A:682:LEU:HB3	1:A:683:PRO:HD2	1.93	0.50
1:A:808:GLU:OE1	1:A:808:GLU:HA	2.11	0.50
1:C:513:PRO:O	1:C:514:ALA:HB3	2.11	0.50
1:D:234:ASP:O	1:D:235:PHE:HB2	2.11	0.50
1:D:822:LEU:HD12	1:D:824:GLN:N	2.27	0.50
1:A:90:TRP:NE1	1:A:96:ASP:OD1	2.45	0.49
1:A:524:LEU:HD22	1:A:561:ARG:HB3	1.94	0.49
1:A:726:LEU:CD1	1:B:873:ALA:HB2	2.42	0.49
1:A:995:GLY:O	1:A:997:ASP:N	2.45	0.49
1:B:382:ASN:O	1:B:383:ASN:HB2	2.12	0.49
1:B:653[B]:HIS:HD2	1:B:666:GLY:O	1.96	0.49
1:B:769:TRP:N	1:B:769:TRP:CE3	2.80	0.49
1:C:134:LEU:N	1:C:134:LEU:CD2	2.75	0.49
1:C:416:GLU:OE1	1:C:418:HIS:HB2	2.12	0.49
1:C:842:TRP:N	1:C:842:TRP:CE3	2.80	0.49
1:D:79:PRO:HD2	1:D:80:GLU:OE2	2.11	0.49
1:D:130:ASP:O	1:D:131:GLU:C	2.53	0.49
1:D:581:ASN:HD22	1:D:583:ASN:HD21	1.59	0.49
1:D:670:LEU:HA	1:D:678:GLN:OE1	2.11	0.49
1:D:808:GLU:OE1	1:D:808:GLU:HA	2.10	0.49
1:A:89:ASN:O	1:A:92:MET:HB2	2.12	0.49
1:A:856:TYR:HD2	1:A:864:MET:CE	2.21	0.49
1:B:577:LYS:HB3	1:B:585:TRP:CZ2	2.47	0.49
1:B:588:TYR:O	1:B:589:GLY:C	2.53	0.49
1:B:649:ASN:O	1:B:702:GLN:HA	2.12	0.49
1:B:696:LEU:HD12	1:B:697:THR:H	1.77	0.49
1:C:502:MET:CB	1:C:537:GLU:HG3	2.42	0.49
1:C:746:ASP:N	1:C:760:ARG:HG2	2.27	0.49
1:C:867:THR:O	1:C:867:THR:HG22	2.12	0.49
1:D:85:VAL:C	1:D:86:VAL:HG23	2.37	0.49
1:D:360:HIS:CE1	1:D:361:PRO:HD2	2.47	0.49
1:D:540:HIS:HE1	1:D:542:MET:HB2	1.76	0.49
1:D:716:ALA:O	1:D:717:TRP:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:784:PHE:CD1	1:D:850:PHE:CE1	3.00	0.49
1:A:141:ILE:HG23	1:A:141:ILE:O	2.11	0.49
1:A:360:HIS:CE1	1:A:361:PRO:HD2	2.46	0.49
1:A:718:GLN:HG3	1:A:719:GLN:N	2.27	0.49
1:B:166:ARG:CG	1:B:392:TYR:HB2	2.40	0.49
1:B:240:LEU:HD23	1:B:240:LEU:C	2.36	0.49
1:B:351:ILE:O	1:B:351:ILE:HG22	2.11	0.49
1:B:768:MET:HE2	1:B:770:ILE:HD13	1.93	0.49
1:B:906:TYR:CD2	1:B:937:LEU:HD22	2.47	0.49
1:C:579:ASP:OD1	1:C:583:ASN:HB2	2.12	0.49
1:C:835:LEU:C	1:C:835:LEU:HD12	2.37	0.49
1:D:870:VAL:HG12	1:D:871:GLU:N	2.27	0.49
1:A:634:GLN:OE1	1:A:685:LEU:HD12	2.13	0.49
1:A:890:GLN:OE1	1:A:949:HIS:HE1	1.94	0.49
1:B:14:ARG:HG2	1:B:16:TRP:CZ2	2.47	0.49
1:B:15:ASP:HB3	1:B:21:VAL:CG1	2.43	0.49
1:B:141:ILE:HB	1:B:173:LEU:CD1	2.43	0.49
1:B:176:PHE:CD1	1:B:176:PHE:N	2.79	0.49
1:B:474:TRP:CZ2	1:B:478:VAL:HG21	2.47	0.49
1:B:622:HIS:HD2	1:B:625:GLN:OE1	1.95	0.49
1:C:78:LEU:O	1:C:79:PRO:C	2.55	0.49
1:C:78:LEU:O	1:C:81:ALA:HB3	2.12	0.49
1:C:344:LEU:O	1:C:345:ASN:C	2.54	0.49
1:A:556:PHE:CD1	1:A:564:GLY:HA2	2.47	0.49
1:A:876:THR:O	1:A:877:PRO:C	2.55	0.49
1:A:878:HIS:HD2	1:A:1008:GLN:HB3	1.77	0.49
1:B:7:LEU:N	1:B:71:GLU:OE2	2.46	0.49
1:C:399:TYR:CD1	1:C:399:TYR:N	2.80	0.49
1:C:858:ILE:HG12	1:C:864:MET:HB3	1.95	0.49
1:D:63:PHE:HB3	1:D:64:PRO:CD	2.42	0.49
1:D:73:TRP:CE2	1:D:122:CYS:HB3	2.47	0.49
1:A:878:HIS:HB2	3:A:4054:HOH:O	2.12	0.49
1:B:73:TRP:CH2	1:B:187:MET:HB3	2.47	0.49
1:A:44:THR:O	1:A:45:ASP:C	2.54	0.49
1:B:133:TRP:N	1:B:133:TRP:CD1	2.78	0.49
1:C:856:TYR:N	1:C:856:TYR:CD1	2.79	0.49
1:D:86:VAL:HG13	1:D:87:PRO:HA	1.93	0.49
1:D:416:GLU:CD	1:D:461:GLU:HG3	2.37	0.49
1:D:696:LEU:HD12	1:D:696:LEU:C	2.37	0.49
1:D:786:ARG:O	1:D:788:PRO:HD3	2.13	0.49
1:A:367:MET:HE1	1:A:371:THR:HG21	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:859:ASP:OD1	1:C:861:SER:OG	2.27	0.49
1:A:26:ARG:NH1	1:A:169:SER:HB3	2.18	0.49
1:A:208:ILE:HG22	1:A:208:ILE:O	2.12	0.49
1:A:446:ARG:HG2	1:A:447:ASP:OD1	2.13	0.49
1:A:479:ASP:OD1	1:A:481:SER:HB3	2.13	0.49
1:A:737:ILE:HA	1:A:738:PRO:HD3	1.76	0.49
1:B:305:ILE:O	1:B:305:ILE:HG22	2.13	0.49
1:B:423:MET:CB	1:C:282:ARG:HG3	2.41	0.49
1:B:730:LEU:H	1:B:730:LEU:CD1	2.00	0.49
1:B:894:ARG:HD2	1:B:919:ASP:OD1	2.13	0.49
1:C:84:VAL:HG13	1:C:85:VAL:N	2.27	0.49
1:C:339:ASN:HB3	3:C:4161:HOH:O	2.13	0.49
1:C:503:TYR:OH	1:C:537:GLU:OE1	2.28	0.49
1:C:652:LEU:O	1:C:667:GLU:HA	2.13	0.49
1:C:728:VAL:HG23	1:C:728:VAL:O	2.12	0.49
1:C:961:ARG:HG3	1:C:961:ARG:NH1	2.27	0.49
1:D:261:TRP:N	1:D:261:TRP:CD1	2.80	0.49
1:A:568:TRP:CD2	1:A:569:ASP:HB3	2.48	0.49
1:B:153:TRP:HA	1:B:157:ARG:O	2.13	0.49
1:B:510:GLN:HB3	1:B:512:PHE:CZ	2.46	0.49
1:B:788:PRO:CD	1:B:968:MET:HG3	2.43	0.49
1:C:127:PHE:N	1:C:127:PHE:CD2	2.80	0.49
1:C:261:TRP:CH2	1:C:266:GLN:HG3	2.47	0.49
1:C:455:ILE:HG22	1:C:456:TRP:N	2.27	0.49
1:C:869:ASP:CG	1:C:1015:HIS:HD1	2.20	0.49
1:D:100:TYR:O	1:D:597:ASN:HB2	2.13	0.49
1:D:211:ASP:N	1:D:211:ASP:OD1	2.45	0.49
1:D:238:ALA:HB1	1:D:332:PHE:HE2	1.77	0.49
1:D:357:HIS:HD2	1:D:392:TYR:OH	1.96	0.49
1:D:513:PRO:O	1:D:514:ALA:HB3	2.12	0.49
1:D:936:GLY:O	1:D:937:LEU:C	2.55	0.49
1:A:134:LEU:H	1:A:134:LEU:CD2	2.21	0.48
1:A:282:ARG:HG3	1:D:420:MET:O	2.13	0.48
1:A:512:PHE:HE1	1:A:517:LYS:HE2	1.78	0.48
1:A:881:ARG:NH1	1:A:987:ASP:OD2	2.40	0.48
1:B:777:LEU:CD2	1:B:889:ALA:HA	2.43	0.48
1:B:932:PRO:HG2	1:B:970:THR:O	2.13	0.48
1:B:959:ILE:HD12	1:B:984:LEU:HD13	1.95	0.48
1:C:65:ALA:HB1	1:C:66:PRO:CD	2.43	0.48
1:A:62:TRP:HZ2	1:A:119:PRO:HB3	1.78	0.48
1:A:995:GLY:H	1:A:1002:SER:HB2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:SER:C	1:B:214:LEU:HD23	2.37	0.48
1:B:282:ARG:NH1	1:C:419:GLY:HA2	2.19	0.48
1:B:397:LEU:O	1:B:400:THR:N	2.46	0.48
1:C:242:ALA:O	1:C:291:LEU:N	2.46	0.48
1:C:387:VAL:HG11	1:C:398:TRP:HZ2	1.79	0.48
1:C:689:GLU:O	1:C:690:SER:O	2.31	0.48
1:D:62:TRP:HB2	1:D:95:TYR:HD2	1.78	0.48
1:D:118:ASN:O	1:D:119:PRO:C	2.55	0.48
1:A:360:HIS:HA	1:A:361:PRO:HD3	1.57	0.48
1:A:683:PRO:O	1:A:685:LEU:N	2.46	0.48
1:A:822:LEU:HD11	1:A:824:GLN:O	2.14	0.48
1:A:897:TRP:CE2	1:A:918:TRP:HD1	2.30	0.48
1:B:126:THR:HA	1:B:182:ASN:O	2.13	0.48
1:C:685:LEU:CD2	1:C:686:PRO:HD3	2.38	0.48
1:D:309:TYR:N	1:D:309:TYR:CD1	2.81	0.48
1:D:697:THR:HG22	1:D:698:VAL:N	2.26	0.48
1:A:360:HIS:CE1	1:A:362:LEU:HB2	2.48	0.48
1:A:769:TRP:HA	1:A:773:LYS:O	2.12	0.48
1:B:581:ASN:ND2	1:B:583:ASN:ND2	2.61	0.48
1:B:645:ARG:HH22	1:B:650:GLU:CD	2.21	0.48
1:C:58:TRP:HE3	1:C:123:TYR:HB3	1.78	0.48
1:C:141:ILE:HD13	1:C:143:PHE:CZ	2.48	0.48
1:C:429:ASP:OD1	1:C:431[B]:ARG:HG3	2.13	0.48
1:D:853:ARG:NH1	1:D:871:GLU:OE2	2.47	0.48
1:D:937:LEU:HG	1:D:938:ARG:N	2.28	0.48
1:D:949:HIS:HB2	1:D:951:TRP:CZ3	2.48	0.48
1:A:525:SER:O	1:A:526:LEU:C	2.54	0.48
1:A:786:ARG:HG2	1:A:880:ALA:CB	2.41	0.48
1:B:3:ILE:C	1:B:5:ASP:H	2.20	0.48
1:B:454:ILE:HG13	1:B:455:ILE:HG13	1.95	0.48
1:B:609:ALA:O	1:B:611:ARG:NH1	2.44	0.48
1:B:807:VAL:HA	1:B:810:TRP:CE3	2.49	0.48
1:B:838:THR:HG21	3:B:4178:HOH:O	2.14	0.48
1:C:229:THR:HG22	1:C:240:LEU:HA	1.95	0.48
1:C:730:LEU:H	1:C:730:LEU:CD1	2.15	0.48
1:D:8:ALA:O	1:D:12:GLN:HB3	2.14	0.48
1:D:368:ASP:O	1:D:372:MET:HG3	2.12	0.48
1:D:638:VAL:HG23	1:D:678:GLN:O	2.13	0.48
1:D:769:TRP:NE1	1:D:774:LYS:HE2	2.28	0.48
1:A:434:PRO:O	1:A:437:SER:HB3	2.14	0.48
1:A:823:LEU:CD2	1:B:728:VAL:HG12	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:995:GLY:O	1:A:996:ASP:C	2.56	0.48
1:B:92:MET:O	1:B:93:HIS:HD2	1.97	0.48
1:B:441:THR:HG22	1:B:474:TRP:CH2	2.48	0.48
1:B:652:LEU:HD12	1:B:652:LEU:C	2.37	0.48
1:B:721:ARG:HH11	1:B:721:ARG:HB2	1.79	0.48
1:C:876:THR:O	1:C:877:PRO:C	2.54	0.48
1:C:929:TYR:HB3	3:C:4108:HOH:O	2.12	0.48
1:C:944:LEU:O	1:C:950:GLN:HA	2.13	0.48
1:D:105:TYR:CZ	1:D:199:ASP:HB2	2.48	0.48
1:D:143:PHE:O	1:D:168:PRO:HA	2.14	0.48
1:D:446:ARG:HG2	1:D:446:ARG:O	2.11	0.48
1:D:937:LEU:HG	1:D:938:ARG:H	1.76	0.48
1:D:1023:LYS:HE3	1:D:1023:LYS:C	2.39	0.48
1:A:549:PHE:CE2	1:A:620:ALA:HA	2.49	0.48
1:A:592:PHE:HB2	1:A:594:ASP:OD1	2.14	0.48
1:B:255:ARG:HB2	1:B:316:HIS:NE2	2.29	0.48
1:B:908:ASP:OD1	1:B:993:ILE:HG12	2.13	0.48
1:C:133:TRP:N	1:C:133:TRP:CD1	2.80	0.48
1:C:287:ASP:N	1:C:287:ASP:OD1	2.33	0.48
1:C:292:ARG:HG3	1:C:292:ARG:NH1	2.27	0.48
1:C:420:MET:HE3	1:C:420:MET:HB3	1.63	0.48
1:C:652:LEU:CB	1:C:670:LEU:HD21	2.43	0.48
1:C:869:ASP:OD1	1:C:1015:HIS:ND1	2.42	0.48
1:C:965:GLN:O	1:C:966:GLN:C	2.55	0.48
1:D:867:THR:O	1:D:867:THR:HG22	2.13	0.48
1:A:241:GLU:HG3	1:A:292:ARG:HG3	1.96	0.48
1:A:823:LEU:HD12	1:A:839:ALA:HB1	1.95	0.48
1:B:62:TRP:CD1	1:B:95:TYR:HB3	2.48	0.48
1:B:91:GLN:HE21	1:B:190:ARG:NH1	2.10	0.48
1:B:409:VAL:HG23	1:B:452:SER:HB2	1.95	0.48
1:B:721:ARG:HH11	1:B:721:ARG:CB	2.27	0.48
1:B:872:VAL:HG23	1:B:1012:GLY:O	2.13	0.48
1:C:144:ASP:HB3	3:C:4082:HOH:O	2.13	0.48
1:C:190:ARG:HG3	1:C:206:SER:OG	2.13	0.48
1:C:510:GLN:N	1:C:511:PRO:HD3	2.28	0.48
1:C:767:GLN:CG	1:C:768:MET:N	2.75	0.48
1:D:141:ILE:O	1:D:170:GLU:HA	2.13	0.48
1:D:356:ARG:HD2	1:D:379:MET:HE1	1.96	0.48
1:D:757:GLN:O	1:D:765:LEU:HD12	2.14	0.48
1:D:972:HIS:HB2	1:D:974:HIS:CE1	2.49	0.48
1:A:100:TYR:HB2	1:A:203:TRP:CD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:ARG:HD2	1:B:169:SER:HA	1.96	0.48
1:C:88:SER:HA	1:C:366:VAL:HG21	1.95	0.48
1:C:864:MET:HG3	1:C:1020:TRP:HB3	1.96	0.48
1:A:90:TRP:HE1	1:A:96:ASP:CG	2.21	0.48
1:A:577:LYS:O	1:A:584:PRO:HA	2.13	0.48
1:A:588:TYR:CD2	1:A:603:MET:HE2	2.49	0.48
1:A:897:TRP:CE2	1:A:918:TRP:CD1	3.02	0.48
1:B:9:VAL:CG1	1:B:10:VAL:N	2.77	0.48
1:B:210:ARG:NH1	1:B:358:GLU:OE1	2.47	0.48
1:B:349:LEU:O	1:B:563:GLN:HB3	2.14	0.48
1:C:881:ARG:HD3	1:C:987:ASP:CG	2.39	0.48
1:D:144:ASP:HB2	1:D:211:ASP:H	1.79	0.48
1:D:352:ARG:HB2	1:D:385:ASN:CB	2.35	0.48
1:D:356:ARG:HH22	1:D:367:MET:HE2	1.77	0.48
1:D:637:GLU:HB2	1:D:679:LEU:HD21	1.95	0.48
1:A:456:TRP:O	1:A:484:VAL:HA	2.14	0.47
1:A:897:TRP:HA	1:A:943:GLU:O	2.14	0.47
1:B:30:HIS:ND1	1:B:33:PHE:CD1	2.82	0.47
1:B:105:TYR:CE2	1:B:196:TYR:HA	2.49	0.47
1:B:651:LEU:O	1:B:701:VAL:N	2.32	0.47
1:B:906:TYR:CZ	1:B:937:LEU:HB3	2.49	0.47
1:C:86:VAL:HG13	1:C:87:PRO:HA	1.96	0.47
1:D:638:VAL:CG2	1:D:678:GLN:HB3	2.44	0.47
1:D:889:ALA:HB3	1:D:890:GLN:HE22	1.79	0.47
1:D:965:GLN:O	1:D:966:GLN:C	2.54	0.47
1:A:695:TRP:CE2	1:A:721:ARG:HG3	2.49	0.47
1:A:742:THR:CG2	1:A:743:SER:H	2.26	0.47
1:C:230:ARG:HH21	1:C:241:GLU:CD	2.21	0.47
1:C:657:ALA:O	1:C:694:LEU:HD12	2.13	0.47
1:C:859:ASP:CG	1:C:861:SER:HG	2.20	0.47
1:D:610:ASP:OD2	1:D:612:THR:HG23	2.14	0.47
1:D:657:ALA:HB1	1:D:661:LYS:C	2.39	0.47
1:D:740:LEU:HA	1:D:748:CYS:O	2.14	0.47
1:D:906:TYR:OH	1:D:935:ASN:HA	2.13	0.47
1:A:285:TYR:HB2	1:A:288:ARG:HB2	1.95	0.47
1:A:440:VAL:CG1	1:A:475:ILE:HD11	2.44	0.47
1:A:573:GLN:HB2	1:A:602:CYS:O	2.14	0.47
1:A:763:GLY:HA3	1:A:822:LEU:HD23	1.93	0.47
1:A:906:TYR:CE2	1:A:937:LEU:HB2	2.48	0.47
1:C:619:GLU:HA	1:C:912:ALA:HB2	1.97	0.47
1:C:894:ARG:CZ	1:C:921:PRO:HD3	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:ASN:ND2	1:D:87:PRO:HD3	2.28	0.47
1:D:153:TRP:HA	1:D:157:ARG:O	2.13	0.47
1:D:460:ASN:O	1:D:461:GLU:C	2.57	0.47
1:D:515:VAL:N	1:D:516:PRO:HD3	2.29	0.47
1:D:658:LEU:HD23	1:D:661:LYS:HZ2	1.79	0.47
1:D:749:ILE:O	1:D:755:ARG:HA	2.14	0.47
1:D:1020:TRP:CD1	1:D:1021:CYS:N	2.79	0.47
1:B:51:LEU:CD1	1:B:215:LEU:HB2	2.44	0.47
1:B:153:TRP:HA	1:B:159:VAL:HG23	1.96	0.47
1:B:429:ASP:OD1	1:B:431[A]:ARG:HD3	2.15	0.47
1:B:576:ILE:HD11	1:B:584:PRO:CB	2.44	0.47
1:B:881:ARG:C	1:B:882:ILE:HG13	2.40	0.47
1:B:902:PRO:O	1:B:938:ARG:NH1	2.44	0.47
1:C:84:VAL:HG13	1:C:85:VAL:O	2.14	0.47
1:C:100:TYR:CB	1:C:203:TRP:CE3	2.96	0.47
1:C:506:VAL:HG22	1:C:520:ILE:HD11	1.97	0.47
1:C:592:PHE:C	1:C:594:ASP:H	2.22	0.47
1:C:610:ASP:O	1:C:611:ARG:HB2	2.15	0.47
1:C:653[A]:HIS:ND1	1:C:667:GLU:HG2	2.28	0.47
1:C:668:VAL:O	1:C:669:PRO:C	2.52	0.47
1:D:127:PHE:HE1	1:D:129:VAL:CG2	2.28	0.47
1:D:282:ARG:HH11	1:D:282:ARG:CG	2.19	0.47
1:D:742:THR:CG2	1:D:743:SER:N	2.78	0.47
1:D:943:GLU:HG2	1:D:944:LEU:N	2.27	0.47
1:A:316:HIS:HB2	1:A:321:THR:O	2.14	0.47
1:A:928:PRO:CB	1:A:973:ARG:NH1	2.72	0.47
1:A:1017:GLN:O	1:A:1018:LEU:HD23	2.15	0.47
1:B:4:THR:O	1:B:9:VAL:HG11	2.13	0.47
1:B:80:GLU:N	1:B:80:GLU:CD	2.72	0.47
1:B:278:ILE:HD12	1:B:278:ILE:N	2.29	0.47
1:B:559:TYR:N	1:B:559:TYR:CD1	2.80	0.47
1:B:567:VAL:CG1	1:B:568:TRP:N	2.78	0.47
1:B:904:GLU:HB2	1:B:936:GLY:HA2	1.97	0.47
1:C:99:ILE:HG22	1:C:101:THR:HG22	1.97	0.47
1:C:146:VAL:O	1:C:165:SER:HA	2.14	0.47
1:C:791:ASN:N	3:C:4072:HOH:O	2.40	0.47
1:D:331:GLY:HA3	1:D:451:PRO:CB	2.44	0.47
1:D:749:ILE:HG22	1:D:750:GLU:N	2.29	0.47
1:D:786:ARG:HH21	1:D:792:ASP:CG	2.22	0.47
1:A:100:TYR:CD2	1:A:602:CYS:HB3	2.50	0.47
1:A:354:VAL:HG22	1:A:355:ASN:N	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:897:TRP:NE1	1:A:918:TRP:HD1	2.12	0.47
1:B:98:PRO:HB3	1:B:205:MET:HG2	1.97	0.47
1:B:153:TRP:NE1	1:B:158:TRP:HB2	2.30	0.47
1:B:850:PHE:HD2	1:B:872:VAL:HG13	1.80	0.47
1:B:941:THR:HG22	1:B:955:PHE:CZ	2.49	0.47
1:C:36:TRP:CD1	1:C:41:GLU:CB	2.98	0.47
1:C:309:TYR:N	1:C:309:TYR:CD1	2.83	0.47
1:C:659:ASP:HB2	1:C:661:LYS:HE3	1.96	0.47
1:D:697:THR:CG2	1:D:698:VAL:N	2.78	0.47
1:D:881:ARG:HD2	3:D:4054:HOH:O	2.14	0.47
1:A:66:PRO:HD3	1:A:118:ASN:HB3	1.97	0.47
1:B:201:ASP:HB3	3:B:4001:HOH:O	2.15	0.47
1:B:486:TYR:O	1:B:496:THR:HB	2.15	0.47
1:B:559:TYR:HA	1:B:560:PRO:HD2	1.69	0.47
1:B:842:TRP:CH2	1:B:852:SER:HB2	2.47	0.47
1:B:961:ARG:O	1:B:979:GLU:HG3	2.15	0.47
1:B:983:TRP:HA	1:B:983:TRP:CE3	2.49	0.47
1:C:133:TRP:CZ3	1:C:216:HIS:HB2	2.50	0.47
1:C:228:ALA:C	1:C:229:THR:HG23	2.40	0.47
1:C:234:ASP:OD1	1:C:236:SER:OG	2.29	0.47
1:D:76:CYS:HA	3:D:4520:HOH:O	2.13	0.47
1:D:166:ARG:CG	1:D:392:TYR:HB2	2.43	0.47
1:D:230:ARG:HG3	1:D:230:ARG:NH1	2.12	0.47
1:D:230:ARG:CG	1:D:230:ARG:NH1	2.76	0.47
1:D:352:ARG:HG2	1:D:624:GLN:HB3	1.96	0.47
1:D:433:LEU:N	1:D:434:PRO:HD2	2.29	0.47
1:D:737:ILE:HG13	1:D:738:PRO:HD2	1.97	0.47
1:D:767:GLN:CG	1:D:768:MET:N	2.77	0.47
1:D:955:PHE:N	1:D:955:PHE:CD2	2.83	0.47
1:A:147:ASN:HB2	1:A:209:PHE:CE2	2.50	0.47
1:A:885:ASN:O	1:A:886:CYS:HB3	2.15	0.47
1:A:937:LEU:HA	1:A:958:ASN:HB3	1.97	0.47
1:B:253:TYR:O	1:B:318:ALA:N	2.41	0.47
1:B:281:GLU:HG3	1:C:515:VAL:HG21	1.96	0.47
1:B:768:MET:HE2	1:B:770:ILE:CD1	2.44	0.47
1:C:143:PHE:N	1:C:143:PHE:CD1	2.83	0.47
1:C:250:LEU:HD11	1:C:287:ASP:HA	1.95	0.47
1:C:391:HIS:HA	1:C:412:GLU:OE1	2.14	0.47
1:C:764:PHE:CE2	1:C:781:ARG:CB	2.98	0.47
1:D:619:GLU:HA	1:D:912:ALA:HB2	1.96	0.47
1:D:685:LEU:O	1:D:686:PRO:O	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:814:GLY:O	1:D:815:HIS:C	2.58	0.47
1:A:77:ASP:HA	3:A:4068:HOH:O	2.15	0.47
1:A:597:ASN:ND2	1:A:599:ARG:H	2.13	0.47
1:A:778:THR:HA	1:A:779:PRO:HD3	1.77	0.47
1:B:955:PHE:CD1	1:B:955:PHE:C	2.93	0.47
1:C:105:TYR:CE1	1:C:419:GLY:HA3	2.50	0.47
1:C:111:PRO:HA	1:C:112:PRO:HA	1.58	0.47
1:C:147:ASN:HB2	1:C:209:PHE:CE2	2.50	0.47
1:C:655:MET:HE3	1:C:655:MET:HB2	1.56	0.47
1:C:708:TRP:CE3	1:C:709:SER:HB3	2.49	0.47
1:C:778:THR:HG23	1:C:779:PRO:HD2	1.97	0.47
1:C:1020:TRP:HD1	1:C:1021:CYS:H	1.62	0.47
1:D:636:ILE:O	1:D:680:ILE:N	2.39	0.47
1:B:550:ALA:O	1:B:553:TRP:N	2.48	0.47
1:B:656:VAL:CG1	1:B:694:LEU:HD11	2.42	0.47
1:B:701:VAL:HG12	1:B:702:GLN:N	2.29	0.47
1:C:217:LYS:HG2	1:C:218:PRO:CD	2.43	0.47
1:C:647:SER:OG	1:C:672:VAL:HG23	2.15	0.47
1:C:651:LEU:CD2	1:C:653[A]:HIS:HE1	2.28	0.47
1:D:74:LEU:HD21	1:D:153:TRP:CE2	2.49	0.47
1:D:617:LEU:HD12	1:D:617:LEU:HA	1.72	0.47
1:A:11:LEU:HD21	1:A:187:MET:HE3	1.97	0.46
1:A:869:ASP:CG	1:A:1015:HIS:HD1	2.23	0.46
1:B:13:ARG:NH1	1:C:13:ARG:NH1	2.63	0.46
1:B:153:TRP:CD1	1:B:158:TRP:HA	2.50	0.46
1:C:91:GLN:HG2	1:C:98:PRO:HA	1.96	0.46
1:C:403:ASP:OD2	1:C:450:HIS:ND1	2.47	0.46
1:C:649:ASN:O	1:C:702:GLN:HA	2.15	0.46
1:C:897:TRP:CH2	1:C:918:TRP:HB2	2.50	0.46
1:D:229:THR:HA	1:D:239:VAL:O	2.15	0.46
1:A:223:SER:HB3	1:A:247:CYS:HB2	1.97	0.46
1:A:571:VAL:HG12	1:A:609:ALA:HA	1.96	0.46
1:A:693:GLN:HG2	1:A:721:ARG:HD2	1.95	0.46
1:A:702:GLN:O	1:A:712:GLY:N	2.34	0.46
1:A:991:MET:HE2	1:A:1003:VAL:HG21	1.97	0.46
1:B:282:ARG:HG2	1:C:423:MET:HB2	1.97	0.46
1:B:652:LEU:HA	1:B:699:ARG:O	2.15	0.46
1:B:1014:TYR:HE1	3:B:4057:HOH:O	1.96	0.46
1:C:721:ARG:NH1	1:C:721:ARG:HB2	2.31	0.46
1:C:899:GLY:O	1:C:915:PHE:HA	2.16	0.46
1:C:970:THR:CG2	1:C:975:LEU:HB2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1011:ALA:HB3	1:D:1014:TYR:CZ	2.50	0.46
1:A:354:VAL:CG2	1:A:355:ASN:N	2.79	0.46
1:A:479:ASP:HA	1:A:480:PRO:HD2	1.48	0.46
1:B:550:ALA:O	1:B:551:LYS:C	2.59	0.46
1:B:883:GLY:HA2	1:B:1016:TYR:CZ	2.49	0.46
1:D:52[A]:ARG:HG2	1:D:52[A]:ARG:NH1	2.30	0.46
1:D:99:ILE:O	1:D:203:TRP:HA	2.16	0.46
1:D:455:ILE:HG21	1:D:485:GLN:HG2	1.97	0.46
1:D:474:TRP:CZ2	1:D:478:VAL:HG21	2.50	0.46
1:D:568:TRP:CD2	1:D:569:ASP:HB3	2.50	0.46
1:D:661:LYS:HA	1:D:662:PRO:HD3	1.70	0.46
1:D:751:LEU:C	1:D:751:LEU:HD23	2.40	0.46
1:A:333:ARG:NH1	1:A:453:VAL:O	2.49	0.46
1:A:377:LEU:O	1:A:381:GLN:HB2	2.16	0.46
1:A:671:ASP:N	1:A:678:GLN:OE1	2.44	0.46
1:A:829:THR:C	1:A:830:LEU:HD13	2.40	0.46
1:A:867:THR:O	1:A:867:THR:HG22	2.16	0.46
1:A:927:THR:HA	1:A:928:PRO:HD3	1.47	0.46
1:B:419:GLY:C	1:C:282:ARG:NH1	2.74	0.46
1:B:782:ASP:HB2	1:B:842:TRP:HZ2	1.79	0.46
1:C:66:PRO:HD2	1:C:67:GLU:HG2	1.97	0.46
1:C:743:SER:OG	1:C:744:GLU:N	2.48	0.46
1:D:78:LEU:HB2	1:D:81:ALA:HB2	1.98	0.46
1:A:38:ASN:HD21	1:A:40:GLU:CB	2.29	0.46
1:B:203:TRP:CB	1:B:205:MET:HE3	2.45	0.46
1:B:274:PHE:HB3	1:B:286:ALA:O	2.16	0.46
1:B:721:ARG:CB	1:B:721:ARG:NH1	2.78	0.46
1:B:730:LEU:HD12	1:B:730:LEU:N	2.16	0.46
1:B:740:LEU:HD13	1:B:749:ILE:HD11	1.96	0.46
1:D:355:ASN:OD1	1:D:388:ARG:HD3	2.16	0.46
1:D:979:GLU:O	1:D:980:GLU:C	2.57	0.46
1:A:701:VAL:HG12	1:A:702:GLN:N	2.31	0.46
1:B:598:ASP:O	1:B:599:ARG:C	2.57	0.46
1:B:738:PRO:HA	1:B:751:LEU:HB2	1.97	0.46
1:C:203:TRP:HB2	1:C:205:MET:HE3	1.96	0.46
1:C:721:ARG:CG	1:C:721:ARG:NH1	2.78	0.46
1:C:959:ILE:HG23	1:C:959:ILE:O	2.14	0.46
1:A:526:LEU:O	1:A:527:PRO:C	2.56	0.46
1:B:38:ASN:ND2	1:B:41:GLU:HB2	2.30	0.46
1:B:568:TRP:CD1	1:B:568:TRP:C	2.93	0.46
1:B:646:HIS:NE2	1:B:671:ASP:OD1	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:770:ILE:HG22	1:B:770:ILE:O	2.16	0.46
1:C:333:ARG:NH1	1:C:451:PRO:O	2.43	0.46
1:C:362:LEU:CG	1:C:576:ILE:HD12	2.45	0.46
1:C:486:TYR:O	1:C:496:THR:HB	2.16	0.46
1:C:721:ARG:NH1	1:C:721:ARG:CB	2.79	0.46
1:C:788:PRO:O	1:C:933:SER:HB2	2.16	0.46
1:C:928:PRO:O	1:C:929:TYR:C	2.58	0.46
1:D:73:TRP:CH2	1:D:187:MET:HB3	2.51	0.46
1:D:463:GLY:HA2	3:D:7505:HOH:O	2.16	0.46
1:D:999:TRP:CD2	1:D:999:TRP:N	2.84	0.46
1:A:26:ARG:HD2	1:A:169:SER:HB3	1.97	0.46
1:A:427:THR:HG21	1:A:462:SER:HB3	1.97	0.46
1:A:693:GLN:NE2	1:A:721:ARG:NH1	2.64	0.46
1:A:755:ARG:O	1:A:768:MET:HA	2.16	0.46
1:A:906:TYR:CZ	1:A:937:LEU:CB	2.99	0.46
1:B:390:SER:HA	1:B:391:HIS:HA	1.79	0.46
1:B:538:TYR:O	1:B:539:ALA:HB3	2.15	0.46
1:C:600:GLN:NE2	1:C:790:ASP:OD1	2.49	0.46
1:C:963:SER:HG	1:C:979:GLU:CD	2.24	0.46
1:D:421:VAL:O	1:D:425:ARG:HD2	2.16	0.46
1:A:118:ASN:O	1:A:120:THR:N	2.49	0.46
1:A:125:LEU:O	1:A:183:ARG:HA	2.15	0.46
1:A:209:PHE:H	1:A:209:PHE:HD2	1.61	0.46
1:A:255:ARG:N	1:A:316:HIS:O	2.45	0.46
1:B:777:LEU:HD21	1:B:889:ALA:CA	2.46	0.46
1:C:37:ARG:HH22	1:C:216:HIS:CD2	2.34	0.46
1:C:380:LYS:HE3	1:C:406:GLY:O	2.15	0.46
1:C:906:TYR:HB3	1:C:907:PRO:CD	2.45	0.46
1:C:920:LEU:CB	1:C:921:PRO:CD	2.94	0.46
1:D:352:ARG:HH11	1:D:352:ARG:HD2	1.58	0.46
1:D:420:MET:HE2	1:D:425:ARG:HG2	1.98	0.46
1:A:7:LEU:O	1:A:11:LEU:HG	2.15	0.46
1:A:14:ARG:HG2	1:A:16:TRP:CZ2	2.50	0.46
1:A:111:PRO:HA	1:A:112:PRO:HA	1.55	0.46
1:A:696:LEU:HD12	1:A:697:THR:H	1.77	0.46
1:A:764:PHE:CE2	1:A:840:HIS:CE1	3.04	0.46
1:A:842:TRP:HZ3	1:A:852:SER:HB3	1.81	0.46
1:B:881:ARG:O	1:B:882:ILE:HG13	2.16	0.46
1:C:331:GLY:N	1:C:451:PRO:HG3	2.31	0.46
1:C:418:HIS:CG	1:C:461:GLU:HG3	2.51	0.46
1:C:842:TRP:N	1:C:842:TRP:HE3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:897:TRP:HA	1:D:943:GLU:O	2.16	0.46
1:A:150:PHE:HB3	1:A:188:VAL:HA	1.97	0.45
1:A:424:ASN:HB3	1:D:285:TYR:OH	2.16	0.45
1:A:742:THR:CG2	1:A:743:SER:N	2.78	0.45
1:B:422:PRO:HG2	1:B:424:ASN:CB	2.46	0.45
1:B:429:ASP:OD1	1:B:430:PRO:HD2	2.16	0.45
1:C:80:GLU:CD	1:C:80:GLU:H	2.20	0.45
1:C:225:PHE:HA	1:C:243:GLU:O	2.16	0.45
1:C:299:LYS:HB2	1:C:309:TYR:OH	2.16	0.45
1:D:654:TRP:CE2	1:D:666:GLY:N	2.85	0.45
1:A:737:ILE:CD1	1:A:832:ASP:HA	2.46	0.45
1:A:997:ASP:O	1:A:1002:SER:OG	2.34	0.45
1:B:89:ASN:O	1:B:92:MET:N	2.45	0.45
1:B:256:VAL:HG12	1:B:257:THR:N	2.32	0.45
1:B:292:ARG:CG	1:B:292:ARG:HH11	2.29	0.45
1:B:656:VAL:O	1:B:657:ALA:HB2	2.15	0.45
1:B:970:THR:HG22	1:B:972:HIS:O	2.16	0.45
1:C:433:LEU:HD12	1:C:433:LEU:HA	1.64	0.45
1:D:38:ASN:ND2	1:D:41:GLU:CG	2.79	0.45
1:D:133:TRP:O	1:D:134:LEU:HD23	2.17	0.45
1:D:232:ASN:O	1:D:233:ASP:C	2.57	0.45
1:D:999:TRP:N	1:D:999:TRP:CE3	2.84	0.45
1:A:479:ASP:N	1:A:480:PRO:HD3	2.31	0.45
1:B:416:GLU:OE1	1:B:418:HIS:HB2	2.16	0.45
1:B:777:LEU:HG	1:B:889:ALA:HA	1.98	0.45
1:B:791:ASN:HB2	3:B:4029:HOH:O	2.16	0.45
1:C:316:HIS:HB3	1:C:322:LEU:HD23	1.97	0.45
1:D:95:TYR:H	1:D:95:TYR:HD1	1.63	0.45
1:D:105:TYR:OH	1:D:196:TYR:O	2.28	0.45
1:D:768:MET:HG2	1:D:775:GLN:HB2	1.97	0.45
1:A:24:LEU:HD12	1:A:24:LEU:HA	1.52	0.45
1:B:90:TRP:C	1:B:90:TRP:CD1	2.94	0.45
1:B:352:ARG:CZ	1:B:626:PHE:CE2	2.99	0.45
1:B:421:VAL:O	1:B:425:ARG:NH1	2.39	0.45
1:C:303:ALA:CB	1:C:408:TYR:CZ	3.00	0.45
1:D:129:VAL:CG2	1:D:182:ASN:ND2	2.79	0.45
1:D:824:GLN:O	1:D:838:THR:HA	2.17	0.45
1:A:658:LEU:HD11	1:A:692:GLY:C	2.42	0.45
1:A:767:GLN:CG	1:A:768:MET:H	2.30	0.45
1:A:767:GLN:CG	1:A:768:MET:N	2.79	0.45
1:A:775:GLN:CD	1:A:890:GLN:HE22	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:ASN:HB2	1:C:279:ILE:HD11	1.98	0.45
1:B:486:TYR:CE2	1:B:488:GLY:CA	2.99	0.45
1:B:620:ALA:O	1:B:621:LYS:C	2.58	0.45
1:C:37:ARG:HG2	1:C:50:GLN:NE2	2.30	0.45
1:C:147:ASN:HA	1:C:148:SER:HA	1.73	0.45
1:D:147:ASN:HB2	1:D:209:PHE:CE2	2.51	0.45
1:D:649:ASN:OD1	1:D:703:PRO:HD2	2.17	0.45
1:A:67:GLU:H	1:A:67:GLU:HG2	1.20	0.45
1:A:137:GLY:HA3	1:A:216:HIS:CE1	2.51	0.45
1:A:297:ASN:N	1:A:298:PRO:CD	2.77	0.45
1:A:767:GLN:CD	1:A:774:LYS:HG2	2.42	0.45
1:B:7:LEU:CD2	1:B:74:LEU:HD11	2.31	0.45
1:B:91:GLN:NE2	1:B:190:ARG:CZ	2.79	0.45
1:B:369:GLU:O	1:B:370:GLN:C	2.60	0.45
1:B:587:ALA:HB1	1:B:592:PHE:HE1	1.80	0.45
1:B:661:LYS:HA	1:B:662:PRO:HD2	1.62	0.45
1:B:807:VAL:HA	1:B:810:TRP:HE3	1.81	0.45
1:B:814:GLY:O	1:B:818:ALA:N	2.49	0.45
1:C:258:VAL:HB	1:C:291:LEU:HD11	1.99	0.45
1:C:679:LEU:HD23	1:C:679:LEU:HA	1.81	0.45
1:D:127:PHE:CE1	1:D:129:VAL:HG22	2.51	0.45
1:D:407:LEU:HA	1:D:407:LEU:HD23	1.58	0.45
1:D:599:ARG:HB2	1:D:600:GLN:H	1.43	0.45
1:D:956:GLN:CD	1:D:956:GLN:N	2.74	0.45
1:A:110:ASN:O	1:A:113:PHE:N	2.32	0.45
1:A:260:LEU:HD12	1:A:261:TRP:N	2.32	0.45
1:A:377:LEU:HB3	1:A:381:GLN:HE22	1.82	0.45
1:A:789:LEU:HD11	1:A:993:ILE:CG2	2.41	0.45
1:B:734:SER:HB3	1:B:860:GLY:CA	2.18	0.45
1:B:930:VAL:O	1:B:932:PRO:HD3	2.16	0.45
1:C:570:TRP:CD1	1:C:571:VAL:CG2	2.99	0.45
1:C:600:GLN:HB3	1:C:603:MET:HE2	1.97	0.45
1:C:663:LEU:O	1:C:664:ALA:HB2	2.16	0.45
1:C:694:LEU:HD12	1:C:695:TRP:N	2.32	0.45
1:D:279:ILE:HG21	1:D:279:ILE:HD13	1.74	0.45
1:D:436:MET:HE3	1:D:467:ASN:HD22	1.82	0.45
1:D:455:ILE:CG2	1:D:456:TRP:N	2.78	0.45
1:D:658:LEU:O	1:D:661:LYS:HD2	2.17	0.45
1:D:786:ARG:NH2	1:D:792:ASP:OD1	2.44	0.45
1:D:868:VAL:CG1	1:D:869:ASP:N	2.79	0.45
1:D:988:GLY:C	1:D:989:PHE:CD1	2.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:ASN:HB2	3:A:4055:HOH:O	2.17	0.45
1:A:572:ASP:C	1:A:574:SER:H	2.25	0.45
1:A:814:GLY:HA2	3:A:4138:HOH:O	2.16	0.45
1:A:1023:LYS:HB2	1:A:1023:LYS:HE2	1.58	0.45
1:B:375:ASP:O	1:B:376:ILE:C	2.57	0.45
1:B:408:TYR:HB3	1:B:454:ILE:CD1	2.47	0.45
1:B:789:LEU:H	1:B:789:LEU:HG	1.66	0.45
1:B:850:PHE:HA	1:B:871:GLU:O	2.16	0.45
1:B:858:ILE:HD11	1:B:864:MET:HE3	1.98	0.45
1:C:256:VAL:O	1:C:272:ALA:N	2.41	0.45
1:C:545:SER:HB3	1:C:546:LEU:H	1.50	0.45
1:D:507:ASP:OD1	1:D:521:LYS:HE2	2.17	0.45
1:D:769:TRP:HA	1:D:773:LYS:O	2.17	0.45
1:D:836:ILE:CG2	1:D:837:THR:N	2.78	0.45
1:A:679:LEU:HD23	1:A:679:LEU:N	2.04	0.45
1:A:1005:ALA:C	1:A:1007:PHE:H	2.25	0.45
1:B:967:LEU:HA	1:B:967:LEU:HD23	1.56	0.45
1:C:85:VAL:O	1:C:88:SER:OG	2.33	0.45
1:C:192:SER:O	1:C:195:SER:HB2	2.17	0.45
1:C:195:SER:O	1:C:196:TYR:C	2.58	0.45
1:C:256:VAL:CG1	1:C:257:THR:N	2.80	0.45
1:C:957:PHE:CD1	1:C:957:PHE:C	2.95	0.45
1:D:5:ASP:OD2	1:D:157:ARG:HG3	2.16	0.45
1:D:69:VAL:HG13	1:D:70:PRO:HD2	1.99	0.45
1:D:100:TYR:HB2	1:D:203:TRP:CE2	2.52	0.45
1:D:287:ASP:OD1	1:D:287:ASP:N	2.50	0.45
1:D:387:VAL:O	1:D:409:VAL:HA	2.17	0.45
1:D:455:ILE:HG22	1:D:456:TRP:N	2.31	0.45
1:D:571:VAL:HG11	1:D:611:ARG:NH1	2.32	0.45
1:A:129:VAL:HG23	1:A:182:ASN:HD22	1.82	0.45
1:A:147:ASN:HA	1:A:148:SER:HA	1.73	0.45
1:A:360:HIS:CG	1:A:361:PRO:CD	3.00	0.45
1:A:608:PHE:HD1	1:A:612:THR:O	2.00	0.45
1:A:950:GLN:CD	1:A:952:ARG:HD3	2.42	0.45
1:B:234:ASP:OD1	1:B:236:SER:OG	2.34	0.45
1:B:472:TYR:CD2	1:B:472:TYR:C	2.95	0.45
1:B:694:LEU:O	1:B:721:ARG:HG3	2.17	0.45
1:D:844:HIS:ND1	1:D:845:GLN:HG2	2.31	0.45
1:A:73:TRP:CE2	1:A:122:CYS:HB3	2.50	0.44
1:A:116:THR:HA	3:A:4017:HOH:O	2.17	0.44
1:B:18:ASN:C	1:B:20:GLY:H	2.24	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:LEU:HG	1:B:159:VAL:HG21	1.98	0.44
1:B:581:ASN:HD22	1:B:583:ASN:ND2	2.14	0.44
1:B:651:LEU:HD12	1:B:703:PRO:HG3	1.94	0.44
1:B:782:ASP:OD1	1:B:854:LYS:HE3	2.16	0.44
1:C:69:VAL:HG13	1:C:70:PRO:HD2	1.99	0.44
1:C:120:THR:HG21	1:C:187:MET:SD	2.57	0.44
1:C:427:THR:H	1:C:427:THR:HG23	1.36	0.44
1:D:84:VAL:HG22	1:D:93:HIS:CE1	2.51	0.44
1:D:101:THR:HG23	1:D:204:ARG:NH2	2.32	0.44
1:D:272:ALA:HA	1:D:273:PRO:HD3	1.56	0.44
1:D:658:LEU:HA	1:D:693:GLN:O	2.17	0.44
1:D:902:PRO:HD3	1:D:918:TRP:CH2	2.52	0.44
1:A:504:ALA:O	1:A:552:TYR:OH	2.30	0.44
1:B:166:ARG:HG3	1:B:392:TYR:CB	2.46	0.44
1:B:397:LEU:HD12	1:B:397:LEU:HA	1.55	0.44
1:B:529:GLU:HG2	3:B:4084:HOH:O	2.17	0.44
1:B:746:ASP:CG	1:B:757:GLN:HE21	2.22	0.44
1:B:935:ASN:N	1:B:935:ASN:HD22	2.16	0.44
1:C:209:PHE:O	1:C:366:VAL:HG13	2.17	0.44
1:C:448:ARG:HH21	1:C:478:VAL:HG13	1.82	0.44
1:D:245:GLN:HG2	1:D:288:ARG:HG2	1.99	0.44
1:D:282:ARG:CG	1:D:282:ARG:NH1	2.79	0.44
1:D:928:PRO:HB2	1:D:973:ARG:NH1	2.32	0.44
1:A:949:HIS:HD2	1:A:1022:GLN:HE21	1.64	0.44
1:B:367:MET:HE2	1:B:372:MET:HG2	1.98	0.44
1:B:395:HIS:HA	1:B:396:PRO:HD3	1.75	0.44
1:B:654:TRP:N	1:B:666:GLY:O	2.50	0.44
1:B:736:ALA:C	1:B:737:ILE:HG22	2.41	0.44
1:B:929:TYR:HB3	3:B:4090:HOH:O	2.16	0.44
1:C:43:ARG:NH1	1:C:263:GLY:O	2.51	0.44
1:A:303:ALA:HB2	1:A:408:TYR:CZ	2.52	0.44
1:A:750:GLU:CD	1:A:750:GLU:N	2.75	0.44
1:A:904:GLU:O	1:A:904:GLU:HG2	2.17	0.44
1:B:35:SER:O	1:B:36:TRP:C	2.59	0.44
1:B:225:PHE:CB	1:B:244:VAL:HG13	2.40	0.44
1:B:287:ASP:OD1	1:C:425:ARG:NH2	2.47	0.44
1:B:417:THR:O	1:B:418:HIS:C	2.59	0.44
1:B:588:TYR:HD1	1:B:589:GLY:N	2.14	0.44
1:B:658:LEU:O	1:B:660:GLY:N	2.50	0.44
1:B:822:LEU:HD12	1:B:824:GLN:N	2.30	0.44
1:C:354:VAL:O	1:C:387:VAL:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:TYR:CD1	1:D:602:CYS:HB3	2.53	0.44
1:D:234:ASP:CG	1:D:236:SER:HG	2.24	0.44
1:D:559:TYR:HB2	1:D:562:LEU:CG	2.46	0.44
1:D:856:TYR:N	1:D:856:TYR:CD1	2.84	0.44
1:A:60:PHE:HE1	1:A:121:GLY:HA3	1.83	0.44
1:A:309:TYR:N	1:A:309:TYR:CD1	2.86	0.44
1:A:344:LEU:HG	1:A:345:ASN:N	2.32	0.44
1:A:658:LEU:HD12	1:A:693:GLN:O	2.17	0.44
1:A:843:GLN:HB3	1:A:847:LYS:O	2.17	0.44
1:A:868:VAL:HG12	1:A:869:ASP:N	2.32	0.44
1:B:140:ARG:HB2	1:B:171:PHE:O	2.17	0.44
1:B:282:ARG:O	1:C:421:VAL:HG13	2.17	0.44
1:C:62:TRP:C	1:C:63:PHE:CD1	2.95	0.44
1:C:190:ARG:HD3	1:C:191:TRP:CE2	2.52	0.44
1:C:429:ASP:HA	1:C:430:PRO:HD3	1.79	0.44
1:C:568:TRP:CD2	1:C:569:ASP:HB3	2.53	0.44
1:C:618:THR:HG22	1:C:912:ALA:CB	2.48	0.44
1:C:814:GLY:O	1:C:818:ALA:N	2.39	0.44
1:D:202:MET:O	1:D:204:ARG:HD3	2.18	0.44
1:D:482:ARG:HA	1:D:483:PRO:HD2	1.62	0.44
1:D:961:ARG:HE	1:D:961:ARG:HB3	1.73	0.44
1:A:658:LEU:HD11	1:A:692:GLY:O	2.18	0.44
1:B:658:LEU:HD11	1:B:692:GLY:C	2.43	0.44
1:B:836:ILE:O	1:B:855:THR:HA	2.18	0.44
1:B:890:GLN:C	1:B:891:VAL:HG23	2.42	0.44
1:B:948:PRO:O	1:B:1022:GLN:HA	2.17	0.44
1:C:455:ILE:HG21	1:C:485:GLN:HG2	2.00	0.44
1:C:500:CYS:HA	1:C:534:ILE:O	2.17	0.44
1:C:758:PHE:N	1:C:758:PHE:CD1	2.85	0.44
1:C:889:ALA:O	1:C:890:GLN:C	2.60	0.44
1:D:436:MET:O	1:D:437:SER:C	2.60	0.44
1:D:471:LEU:HA	1:D:471:LEU:HD23	1.57	0.44
1:A:105:TYR:HA	1:A:106:PRO:HD3	1.87	0.44
1:A:134:LEU:N	1:A:134:LEU:CD2	2.77	0.44
1:A:635:THR:OG1	1:A:681:GLU:HG2	2.18	0.44
1:B:229:THR:HA	1:B:239:VAL:O	2.17	0.44
1:B:422:PRO:HD2	1:C:285:TYR:CE2	2.53	0.44
1:B:505:ARG:CD	1:B:508:GLU:HG2	2.48	0.44
1:C:230:ARG:O	1:C:238:ALA:HA	2.18	0.44
1:C:513:PRO:C	1:C:515:VAL:H	2.26	0.44
1:C:967:LEU:HD11	3:C:4016:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:PRO:O	1:D:65:ALA:HB2	2.17	0.44
1:D:238:ALA:CB	1:D:332:PHE:CE2	3.00	0.44
1:D:242:ALA:O	1:D:290:THR:HA	2.17	0.44
1:D:658:LEU:CD2	1:D:661:LYS:NZ	2.80	0.44
1:D:678:GLN:O	1:D:679:LEU:HD23	2.17	0.44
1:A:260:LEU:CD1	1:A:309:TYR:HB3	2.48	0.44
1:A:588:TYR:CD2	1:A:603:MET:CE	3.01	0.44
1:A:663:LEU:O	1:A:664:ALA:HB2	2.18	0.44
1:A:767:GLN:HG3	1:A:768:MET:H	1.83	0.44
1:B:18:ASN:HA	1:B:19:PRO:HD3	1.76	0.44
1:B:93:HIS:HB3	1:B:95:TYR:HE1	1.83	0.44
1:B:258:VAL:HG22	1:B:313:VAL:HG22	2.00	0.44
1:B:420:MET:HE2	1:B:426:LEU:CG	2.43	0.44
1:B:570:TRP:HA	1:B:570:TRP:CE3	2.53	0.44
1:B:600:GLN:O	1:B:602:CYS:N	2.51	0.44
1:B:658:LEU:HD12	1:B:659:ASP:H	1.83	0.44
1:B:925:MET:HB3	3:B:4027:HOH:O	2.18	0.44
1:C:395:HIS:CE1	1:C:396:PRO:HD2	2.53	0.44
1:C:746:ASP:OD2	1:C:757:GLN:NE2	2.45	0.44
1:D:435:ALA:O	1:D:439:ARG:HG3	2.16	0.44
1:D:673:ALA:O	1:D:676:GLY:N	2.45	0.44
1:D:949:HIS:CB	1:D:951:TRP:CH2	3.01	0.44
1:A:113:PHE:O	1:A:196:TYR:OH	2.33	0.44
1:A:260:LEU:HD11	1:A:309:TYR:CB	2.48	0.44
1:B:147:ASN:HA	1:B:148:SER:HA	1.60	0.44
1:B:212:VAL:CG1	1:B:213:SER:N	2.78	0.44
1:B:254:LEU:C	1:B:255:ARG:NH1	2.76	0.44
1:B:749:ILE:O	1:B:755:ARG:HG3	2.17	0.44
1:C:754:LYS:HA	1:C:769:TRP:O	2.18	0.44
1:C:866:ILE:O	1:C:1017:GLN:HA	2.18	0.44
1:A:128:ASN:ND2	1:A:181:GLU:HA	2.33	0.43
1:A:261:TRP:CH2	1:A:266:GLN:HB2	2.53	0.43
1:A:518:TRP:CD1	1:A:526:LEU:HD21	2.53	0.43
1:A:730:LEU:HD22	1:B:823:LEU:HB3	2.00	0.43
1:A:899:GLY:O	1:A:918:TRP:NE1	2.49	0.43
1:B:3:ILE:CG2	1:B:4:THR:N	2.80	0.43
1:B:154:CYS:N	1:B:157:ARG:O	2.42	0.43
1:B:278:ILE:HD12	1:B:278:ILE:H	1.81	0.43
1:B:429:ASP:C	1:B:467:ASN:HD21	2.26	0.43
1:B:529:GLU:C	1:B:530:THR:HG23	2.43	0.43
1:B:749:ILE:O	1:B:755:ARG:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:963:SER:HB3	1:B:983:TRP:CZ2	2.53	0.43
1:C:242:ALA:O	1:C:290:THR:HA	2.18	0.43
1:C:311:ALA:O	1:C:327:ALA:HB1	2.18	0.43
1:C:377:LEU:HG	1:C:377:LEU:H	1.53	0.43
1:C:418:HIS:ND1	3:C:4156:HOH:O	2.35	0.43
1:C:463:GLY:O	1:C:488:GLY:HA3	2.18	0.43
1:D:127:PHE:CE1	1:D:129:VAL:CG2	3.01	0.43
1:D:344:LEU:O	1:D:345:ASN:C	2.58	0.43
1:A:22:THR:HG22	3:A:4063:HOH:O	2.18	0.43
1:A:100:TYR:HB3	1:A:589:GLY:HA2	2.00	0.43
1:A:374:GLN:O	1:A:375:ASP:C	2.61	0.43
1:B:118:ASN:HD21	1:B:189:LEU:HD22	1.82	0.43
1:B:125:LEU:HD23	1:B:127:PHE:CD2	2.53	0.43
1:B:152:LEU:HG	1:B:159:VAL:CG2	2.47	0.43
1:B:606:LEU:HB3	1:B:617:LEU:HD13	2.00	0.43
1:B:617:LEU:HD12	1:B:617:LEU:HA	1.81	0.43
1:B:650:GLU:HG3	1:B:700:VAL:HG13	1.99	0.43
1:B:931:PHE:O	1:B:932:PRO:C	2.59	0.43
1:C:127:PHE:HE2	1:C:184:LEU:HG	1.83	0.43
1:C:129:VAL:CG1	1:C:134:LEU:HD21	2.47	0.43
1:C:432:TRP:O	1:C:436:MET:HG3	2.17	0.43
1:C:434:PRO:O	1:C:435:ALA:C	2.59	0.43
1:C:830:LEU:HD12	1:C:830:LEU:HA	1.86	0.43
1:C:888:LEU:HA	1:C:888:LEU:HD23	1.75	0.43
1:C:995:GLY:C	1:C:997:ASP:N	2.76	0.43
1:D:9:VAL:O	1:D:10:VAL:C	2.57	0.43
1:D:214:LEU:HD23	1:D:214:LEU:HA	1.73	0.43
1:D:460:ASN:ND2	1:D:461:GLU:CG	2.78	0.43
1:B:35:SER:HB2	1:B:217:LYS:HG3	2.00	0.43
1:B:282:ARG:HB2	1:C:423:MET:N	2.33	0.43
1:B:577:LYS:NZ	1:B:591:ASP:O	2.31	0.43
1:C:303:ALA:HB2	1:C:408:TYR:CE2	2.52	0.43
1:C:395:HIS:O	1:C:396:PRO:C	2.59	0.43
1:C:600:GLN:O	1:C:602:CYS:N	2.51	0.43
1:C:701:VAL:CG1	1:C:702:GLN:N	2.81	0.43
1:C:941:THR:HG22	1:C:955:PHE:CZ	2.53	0.43
1:D:588:TYR:CD1	1:D:588:TYR:C	2.96	0.43
1:D:746:ASP:HB3	1:D:757:GLN:HE21	1.84	0.43
1:D:815:HIS:HE1	1:D:877:PRO:O	2.01	0.43
1:D:928:PRO:O	1:D:929:TYR:C	2.60	0.43
1:A:599:ARG:NH1	1:A:600:GLN:OE1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:615:PRO:HG2	1:A:929:TYR:OH	2.19	0.43
1:A:766:SER:O	1:A:767:GLN:HB2	2.19	0.43
1:B:282:ARG:NH1	1:C:419:GLY:CA	2.77	0.43
1:B:398:TRP:HA	1:B:398:TRP:CE3	2.52	0.43
1:B:472:TYR:CD2	1:B:473:ARG:N	2.86	0.43
1:B:629:PHE:HA	1:B:637:GLU:O	2.17	0.43
1:B:845:GLN:C	1:B:847:LYS:H	2.26	0.43
1:B:941:THR:HG22	1:B:955:PHE:CE1	2.53	0.43
1:C:103:VAL:O	1:C:104:THR:C	2.62	0.43
1:C:105:TYR:HB3	1:C:106:PRO:CD	2.42	0.43
1:C:232:ASN:OD1	1:C:237:ARG:N	2.45	0.43
1:C:396:PRO:O	1:C:399:TYR:HD1	2.01	0.43
1:C:600:GLN:C	1:C:602:CYS:H	2.26	0.43
1:C:807:VAL:CG1	1:C:808:GLU:N	2.81	0.43
1:C:899:GLY:HA2	1:C:915:PHE:CD1	2.53	0.43
1:D:37:ARG:CD	1:D:50:GLN:NE2	2.82	0.43
1:D:443:MET:HE3	1:D:456:TRP:CE3	2.53	0.43
1:D:576:ILE:HD13	1:D:576:ILE:HA	1.79	0.43
1:D:708:TRP:CD1	1:D:708:TRP:H	2.36	0.43
1:D:959:ILE:HB	1:D:984:LEU:HD12	1.99	0.43
1:A:200:GLN:HA	1:A:416:GLU:OE2	2.17	0.43
1:A:540:HIS:C	1:A:542:MET:N	2.76	0.43
1:A:995:GLY:H	1:A:1002:SER:CB	2.32	0.43
1:B:227:VAL:HG12	1:B:228:ALA:N	2.32	0.43
1:C:21:VAL:O	1:C:21:VAL:HG12	2.17	0.43
1:C:151:HIS:HB3	1:C:153:TRP:CZ3	2.54	0.43
1:C:272:ALA:HB1	1:C:273:PRO:CD	2.47	0.43
1:D:192:SER:OG	1:D:194:GLY:N	2.51	0.43
1:D:237:ARG:CG	1:D:237:ARG:NH1	2.82	0.43
1:D:289:VAL:HG22	1:D:290:THR:N	2.32	0.43
1:D:653[B]:HIS:NE2	1:D:665:SER:HB2	2.33	0.43
1:A:65:ALA:CB	1:A:66:PRO:CD	2.95	0.43
1:A:297:ASN:N	1:A:298:PRO:HD3	2.34	0.43
1:A:540:HIS:O	1:A:542:MET:N	2.52	0.43
1:A:568:TRP:HE1	1:A:604:ASN:HD22	1.65	0.43
1:A:976:LEU:HA	1:A:976:LEU:HD23	1.75	0.43
1:B:186:VAL:HG12	1:B:188:VAL:HG23	2.00	0.43
1:B:658:LEU:HD22	1:B:688:PRO:HG2	2.01	0.43
1:B:679:LEU:HA	1:B:679:LEU:HD23	1.60	0.43
1:C:741:THR:C	1:C:742:THR:O	2.61	0.43
1:C:870:VAL:CG1	1:C:871:GLU:N	2.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:334:GLU:OE1	1:D:336:ARG:HD3	2.19	0.43
1:D:479:ASP:HA	1:D:480:PRO:HD2	1.41	0.43
1:D:654:TRP:NE1	1:D:666:GLY:CA	2.76	0.43
1:D:802:ASP:O	1:D:808:GLU:HG3	2.19	0.43
1:A:17:GLU:OE2	1:A:114:VAL:N	2.30	0.43
1:A:69:VAL:HA	1:A:70:PRO:HD3	1.74	0.43
1:A:240:LEU:HD22	1:A:260:LEU:HD22	1.99	0.43
1:A:254:LEU:HD23	1:A:254:LEU:HA	1.63	0.43
1:A:282:ARG:HG3	1:A:282:ARG:NH1	2.32	0.43
1:A:556:PHE:CE1	1:A:564:GLY:HA2	2.53	0.43
1:B:40:GLU:OE2	1:B:43:ARG:NE	2.52	0.43
1:B:109:VAL:HG23	3:B:4275:HOH:O	2.18	0.43
1:B:141:ILE:O	1:B:170:GLU:HA	2.19	0.43
1:B:261:TRP:CZ2	1:B:266:GLN:HG3	2.53	0.43
1:B:631:LEU:HG	1:B:632:SER:N	2.27	0.43
1:C:11:LEU:HA	1:C:11:LEU:HD23	1.63	0.43
1:C:16:TRP:HA	1:C:161:TYR:OH	2.19	0.43
1:C:90:TRP:CZ3	1:C:121:GLY:HA3	2.54	0.43
1:C:167:LEU:HD23	1:C:393:PRO:HB2	1.99	0.43
1:C:253:TYR:O	1:C:318:ALA:N	2.52	0.43
1:C:647:SER:HG	1:C:672:VAL:H	1.63	0.43
1:C:685:LEU:HA	1:C:686:PRO:HD3	1.87	0.43
1:C:702:GLN:O	1:C:712:GLY:N	2.51	0.43
1:C:821:ALA:O	1:C:823:LEU:HD23	2.18	0.43
1:C:925:MET:HE2	1:C:925:MET:HB3	1.92	0.43
1:D:350:LEU:HD12	1:D:350:LEU:HA	1.85	0.43
1:D:883:GLY:HA3	1:D:987:ASP:HA	2.01	0.43
1:A:58:TRP:CE3	1:A:123:TYR:HB3	2.54	0.43
1:A:98:PRO:HD2	1:A:592:PHE:HB3	2.01	0.43
1:A:210:ARG:NH1	1:A:358:GLU:OE1	2.52	0.43
1:A:654:TRP:C	1:A:654:TRP:CE3	2.97	0.43
1:A:719:GLN:HE22	1:A:915:PHE:N	2.16	0.43
1:B:416:GLU:HA	1:B:462:SER:OG	2.19	0.43
1:B:937:LEU:C	1:B:938:ARG:HG2	2.44	0.43
1:C:40:GLU:O	1:C:43:ARG:N	2.51	0.43
1:C:45:ASP:C	1:C:46:ARG:O	2.59	0.43
1:C:91:GLN:HG2	1:C:98:PRO:CA	2.49	0.43
1:C:131:GLU:O	1:C:134:LEU:N	2.44	0.43
1:C:227:VAL:HG12	1:C:228:ALA:N	2.33	0.43
1:C:502:MET:HB2	1:C:537:GLU:HG3	2.00	0.43
1:D:654:TRP:CD1	1:D:666:GLY:HA3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:966:GLN:O	1:D:967:LEU:C	2.61	0.43
1:A:10:VAL:C	1:A:12:GLN:H	2.26	0.43
1:A:141:ILE:HG12	1:A:142:ILE:N	2.33	0.43
1:A:546:LEU:HD23	1:A:619:GLU:HB3	2.00	0.43
1:A:749:ILE:N	1:A:749:ILE:CD1	2.81	0.43
1:A:966:GLN:HB2	1:A:979:GLU:OE2	2.18	0.43
1:B:152:LEU:O	1:B:159:VAL:N	2.33	0.43
1:B:630:ARG:HB2	1:B:637:GLU:HB3	1.99	0.43
1:B:906:TYR:HB3	1:B:907:PRO:CD	2.49	0.43
1:C:303:ALA:HB2	1:C:408:TYR:CZ	2.54	0.43
1:C:600:GLN:HG2	1:C:931:PHE:HB2	2.01	0.43
1:C:617:LEU:HA	1:C:617:LEU:HD12	1.71	0.43
1:C:685:LEU:HD23	1:C:685:LEU:HA	1.64	0.43
1:C:778:THR:CG2	1:C:779:PRO:N	2.78	0.43
1:D:10:VAL:O	1:D:12:GLN:N	2.51	0.43
1:D:125:LEU:HG	1:D:126:THR:N	2.34	0.43
1:D:240:LEU:O	1:D:292:ARG:HA	2.19	0.43
1:D:424:ASN:ND2	3:D:7510:HOH:O	2.52	0.43
1:D:778:THR:HB	1:D:887:GLN:HB3	2.00	0.43
1:A:460:ASN:CG	1:A:461:GLU:HG2	2.44	0.43
1:A:529:GLU:C	1:A:530:THR:HG23	2.43	0.43
1:A:762:SER:C	1:A:822:LEU:HD23	2.43	0.43
1:B:30:HIS:CB	1:B:31:PRO:CD	2.97	0.43
1:B:423:MET:HB2	1:C:282:ARG:CG	2.44	0.43
1:B:635:THR:CG2	1:B:636:ILE:N	2.81	0.43
1:B:737:ILE:HG13	1:B:738:PRO:N	2.19	0.43
1:C:434:PRO:HA	1:C:437:SER:HB3	2.01	0.43
1:C:730:LEU:HD12	1:C:730:LEU:N	2.14	0.43
1:C:897:TRP:CZ3	1:C:918:TRP:HB2	2.54	0.43
1:D:77:ASP:OD1	1:D:183:ARG:NH2	2.50	0.43
1:D:380:LYS:HE2	3:D:4077:HOH:O	2.18	0.43
1:D:502:MET:HA	1:D:537:GLU:O	2.19	0.43
1:D:904:GLU:HB2	1:D:936:GLY:HA2	2.00	0.43
1:D:967:LEU:HD23	1:D:967:LEU:HA	1.70	0.43
1:A:3:ILE:HG13	1:A:4:THR:N	2.32	0.42
1:A:51:LEU:O	1:A:51:LEU:HG	2.19	0.42
1:A:62:TRP:HE1	1:A:90:TRP:NE1	2.17	0.42
1:A:278:ILE:CG2	1:A:279:ILE:N	2.78	0.42
1:B:128:ASN:C	1:B:129:VAL:HG23	2.44	0.42
1:B:335:VAL:HG22	1:B:344:LEU:HD12	2.01	0.42
1:B:576:ILE:HD11	1:B:584:PRO:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:652:LEU:CD1	1:B:698:VAL:HB	2.49	0.42
1:C:11:LEU:HD21	1:C:187:MET:HE3	2.01	0.42
1:C:292:ARG:HH11	1:C:292:ARG:CG	2.31	0.42
1:C:339:ASN:O	1:D:527:PRO:HB3	2.19	0.42
1:C:367:MET:HE1	1:C:371:THR:HG21	2.01	0.42
1:C:433:LEU:CB	1:C:434:PRO:HD3	2.40	0.42
1:C:434:PRO:O	1:C:437:SER:HB3	2.19	0.42
1:C:548:GLY:O	1:C:551:LYS:HB2	2.19	0.42
1:C:789:LEU:HA	1:C:933:SER:CB	2.49	0.42
1:D:518:TRP:HB3	1:D:522:LYS:HD3	2.00	0.42
1:D:612:THR:HB	1:D:613:PRO:HD2	2.01	0.42
1:D:952:ARG:NH1	1:D:1021:CYS:SG	2.91	0.42
1:A:252:ASP:OD1	1:A:252:ASP:N	2.52	0.42
1:A:422:PRO:HG2	1:D:285:TYR:CE1	2.54	0.42
1:A:737:ILE:HG13	1:A:738:PRO:N	2.34	0.42
1:B:100:TYR:CB	1:B:203:TRP:CE3	3.02	0.42
1:B:255:ARG:HB2	1:B:316:HIS:CD2	2.54	0.42
1:B:654:TRP:CZ2	1:B:666:GLY:HA3	2.54	0.42
1:C:782:ASP:HB2	1:C:842:TRP:CZ2	2.53	0.42
1:C:815:HIS:HD2	1:C:849:LEU:HD13	1.84	0.42
1:D:378:LEU:HD23	1:D:378:LEU:HA	1.73	0.42
1:D:382:ASN:HA	1:D:621:LYS:HD2	2.01	0.42
1:D:442:ARG:HH11	1:D:442:ARG:HD3	1.72	0.42
1:D:686:PRO:C	1:D:687:GLN:HG3	2.44	0.42
1:A:194:GLY:O	1:A:198:GLU:HG3	2.19	0.42
1:A:278:ILE:HD13	1:A:278:ILE:HA	1.60	0.42
1:A:357:HIS:HD2	1:A:392:TYR:OH	2.02	0.42
1:A:726:LEU:HD12	1:B:873:ALA:HB2	1.99	0.42
1:A:914:CYS:O	1:A:918:TRP:HZ2	2.01	0.42
1:B:79:PRO:N	1:B:80:GLU:OE2	2.53	0.42
1:B:281:GLU:CD	1:C:515:VAL:HG21	2.45	0.42
1:B:304:GLU:O	1:B:305:ILE:HG13	2.19	0.42
1:B:354:VAL:HG22	1:B:355:ASN:N	2.34	0.42
1:B:521:LYS:HD3	1:B:559:TYR:OH	2.20	0.42
1:C:255:ARG:HA	1:C:273:PRO:HA	2.00	0.42
1:C:422:PRO:HG2	1:C:424:ASN:HB2	2.00	0.42
1:C:722:LEU:HA	1:C:722:LEU:HD23	1.66	0.42
1:C:958:ASN:ND2	3:C:4153:HOH:O	2.51	0.42
1:D:38:ASN:ND2	1:D:40:GLU:N	2.67	0.42
1:D:147:ASN:HA	1:D:148:SER:HA	1.71	0.42
1:D:303:ALA:HB1	1:D:406:GLY:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ARG:CG	1:A:141:ILE:N	2.79	0.42
1:A:988:GLY:C	1:A:989:PHE:CD1	2.97	0.42
1:B:24:LEU:HB2	1:B:161:TYR:HB3	1.99	0.42
1:B:38:ASN:ND2	1:B:38:ASN:C	2.77	0.42
1:B:496:THR:O	1:B:531:ARG:NH1	2.49	0.42
1:B:655:MET:HE2	1:B:655:MET:HB2	1.57	0.42
1:C:251:ARG:C	1:C:253:TYR:N	2.76	0.42
1:C:655:MET:O	1:C:655:MET:HG3	2.06	0.42
1:C:708:TRP:CD1	1:C:708:TRP:H	2.34	0.42
1:D:308:LEU:HD23	1:D:330:VAL:O	2.19	0.42
1:D:315:LEU:O	1:D:323:ILE:HB	2.19	0.42
1:D:852:SER:CB	1:D:870:VAL:HG22	2.49	0.42
1:D:925:MET:HE3	1:D:938:ARG:CZ	2.49	0.42
1:A:401:LEU:HA	1:A:401:LEU:HD23	1.79	0.42
1:A:907:PRO:HA	1:A:910:LEU:HD23	2.02	0.42
1:B:347:LYS:HE3	1:B:643:LEU:O	2.20	0.42
1:B:721:ARG:NH1	1:B:721:ARG:HB3	2.34	0.42
1:B:750:GLU:N	1:B:750:GLU:CD	2.78	0.42
1:C:65:ALA:O	1:C:66:PRO:C	2.62	0.42
1:D:52[B]:ARG:CG	1:D:133:TRP:CH2	2.98	0.42
1:D:377:LEU:HD22	1:D:708:TRP:CA	2.40	0.42
1:D:778:THR:HA	1:D:779:PRO:HD2	1.86	0.42
1:D:906:TYR:CB	1:D:907:PRO:HD2	2.50	0.42
1:A:110:ASN:N	1:A:111:PRO:HD3	2.34	0.42
1:A:153:TRP:HD1	1:A:157:ARG:C	2.27	0.42
1:A:217:LYS:HB3	1:A:218:PRO:CD	2.47	0.42
1:A:302:SER:HB2	1:A:304:GLU:H	1.83	0.42
1:A:338:GLU:O	1:A:339:ASN:HB3	2.20	0.42
1:A:487:GLU:OE1	1:A:502:MET:HE3	2.18	0.42
1:A:652:LEU:HD12	1:A:652:LEU:HA	1.49	0.42
1:A:746:ASP:N	1:A:760:ARG:HG3	2.33	0.42
1:A:942:ARG:HA	1:A:953:GLY:O	2.19	0.42
1:B:84:VAL:CG1	1:B:85:VAL:N	2.79	0.42
1:B:317:THR:HG23	1:B:321:THR:O	2.19	0.42
1:B:822:LEU:HD21	1:B:825:CYS:HB2	2.01	0.42
1:B:941:THR:CG2	1:B:955:PHE:CE1	3.02	0.42
1:C:114:VAL:HA	1:C:115:PRO:HD3	1.66	0.42
1:C:424:ASN:HD22	1:C:424:ASN:HA	1.29	0.42
1:C:530:THR:C	1:C:561:ARG:NH1	2.78	0.42
1:C:663:LEU:HD23	1:C:663:LEU:N	2.31	0.42
1:C:782:ASP:OD1	1:C:854:LYS:NZ	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:786:ARG:O	1:C:788:PRO:N	2.53	0.42
1:C:870:VAL:HG12	1:C:871:GLU:H	1.84	0.42
1:C:961:ARG:HD2	1:C:981:GLY:O	2.20	0.42
1:C:986:ILE:HG21	1:C:986:ILE:HD13	1.59	0.42
1:D:217:LYS:NZ	1:D:324:GLU:OE1	2.49	0.42
1:D:652:LEU:HD12	1:D:700:VAL:CG2	2.50	0.42
1:A:343:LEU:HD22	1:A:346:GLY:O	2.19	0.42
1:A:658:LEU:CD2	1:A:688:PRO:HG2	2.39	0.42
1:A:718:GLN:HG2	1:A:720:TRP:CZ2	2.55	0.42
1:A:825:CYS:HA	1:A:837:THR:O	2.20	0.42
1:B:3:ILE:O	1:B:6:SER:OG	2.29	0.42
1:B:72:SER:O	1:B:73:TRP:C	2.63	0.42
1:B:736:ALA:O	1:B:737:ILE:HG22	2.20	0.42
1:B:737:ILE:CG1	1:B:738:PRO:N	2.80	0.42
1:B:994:GLY:HA3	1:B:1003:VAL:HG23	2.01	0.42
1:B:1020:TRP:CD1	1:B:1020:TRP:C	2.97	0.42
1:B:1022:GLN:OE1	1:B:1022:GLN:N	2.51	0.42
1:C:63:PHE:CG	1:C:69:VAL:HG22	2.55	0.42
1:C:203:TRP:CB	1:C:205:MET:HE3	2.50	0.42
1:C:334:GLU:HG3	3:C:4209:HOH:O	2.19	0.42
1:C:415:ILE:HG21	1:C:415:ILE:HD13	1.74	0.42
1:C:787:ALA:O	1:C:788:PRO:C	2.63	0.42
1:D:70:PRO:O	1:D:71:GLU:C	2.62	0.42
1:D:100:TYR:HB2	1:D:203:TRP:CE3	2.55	0.42
1:D:197:LEU:HD12	1:D:439:ARG:NE	2.35	0.42
1:D:208:ILE:O	1:D:208:ILE:HG22	2.20	0.42
1:D:217:LYS:NZ	1:D:324:GLU:CD	2.78	0.42
1:D:377:LEU:HD23	1:D:708:TRP:CB	2.50	0.42
1:D:392:TYR:CD1	1:D:392:TYR:C	2.98	0.42
1:D:551:LYS:O	1:D:552:TYR:C	2.60	0.42
1:D:745:MET:H	1:D:745:MET:HG2	1.28	0.42
1:D:769:TRP:NE1	1:D:774:LYS:HG3	2.34	0.42
1:D:927:THR:HG21	1:D:929:TYR:CZ	2.55	0.42
1:A:166:ARG:HG3	1:A:392:TYR:CG	2.54	0.42
1:A:251:ARG:C	1:A:253:TYR:H	2.28	0.42
1:A:349:LEU:HD23	1:A:349:LEU:HA	1.91	0.42
1:B:395:HIS:ND1	1:B:396:PRO:CD	2.79	0.42
1:C:149:ALA:HA	1:C:162:GLY:O	2.19	0.42
1:C:342:LEU:O	1:C:348:PRO:HA	2.19	0.42
1:C:881:ARG:O	1:C:882:ILE:HG13	2.18	0.42
1:D:27:LEU:HD12	1:D:140:ARG:HD3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:ASP:OD1	1:D:183:ARG:NE	2.50	0.42
1:D:643:LEU:CD2	1:D:675:GLN:NE2	2.82	0.42
1:D:864:MET:HG3	1:D:864:MET:O	2.19	0.42
1:D:942:ARG:HA	1:D:953:GLY:O	2.20	0.42
1:D:955:PHE:CD1	1:D:986:ILE:CG2	3.02	0.42
1:A:217:LYS:NZ	1:A:324:GLU:CD	2.78	0.42
1:A:637:GLU:CA	1:A:679:LEU:HD21	2.48	0.42
1:B:166:ARG:HD2	1:B:166:ARG:HA	1.73	0.42
1:B:316:HIS:HB3	1:B:322:LEU:HD23	2.02	0.42
1:B:382:ASN:O	1:B:621:LYS:HA	2.19	0.42
1:B:805:ALA:O	1:B:806:TRP:C	2.60	0.42
1:B:866:ILE:O	1:B:1017:GLN:HB2	2.19	0.42
1:B:906:TYR:CE2	1:B:937:LEU:HD22	2.54	0.42
1:B:1011:ALA:HB3	1:B:1014:TYR:CZ	2.55	0.42
1:C:63:PHE:HA	1:C:64:PRO:HD3	1.38	0.42
1:C:118:ASN:HA	1:C:119:PRO:HD2	1.41	0.42
1:C:138:GLN:HA	1:C:174:SER:OG	2.19	0.42
1:C:193:ASP:C	1:C:195:SER:H	2.27	0.42
1:C:279:ILE:HG21	1:C:279:ILE:HD13	1.61	0.42
1:C:382:ASN:HA	1:C:621:LYS:HD2	2.01	0.42
1:D:282:ARG:HG3	1:D:282:ARG:NH1	2.24	0.42
1:D:548:GLY:O	1:D:549:PHE:C	2.62	0.42
1:D:694:LEU:HD12	1:D:694:LEU:HA	1.82	0.42
1:A:240:LEU:HD22	1:A:260:LEU:CD2	2.49	0.42
1:A:906:TYR:HB3	1:A:907:PRO:HD2	2.02	0.42
1:B:380:LYS:HE2	3:B:4077:HOH:O	2.19	0.42
1:B:393:PRO:HD2	1:B:414:ASN:HB2	2.02	0.42
1:B:400:THR:O	1:B:403:ASP:HB2	2.20	0.42
1:B:524:LEU:HD22	1:B:561:ARG:CZ	2.50	0.42
1:B:652:LEU:O	1:B:652:LEU:HG	2.19	0.42
1:B:658:LEU:HB3	1:B:661:LYS:HD2	2.02	0.42
1:B:900:LEU:HA	1:B:914:CYS:O	2.19	0.42
1:B:1022:GLN:N	1:B:1022:GLN:CD	2.78	0.42
1:C:193:ASP:C	1:C:195:SER:N	2.77	0.42
1:C:315:LEU:O	1:C:323:ILE:HB	2.20	0.42
1:C:721:ARG:CB	1:C:721:ARG:CZ	2.97	0.42
1:D:300:LEU:HD22	1:D:332:PHE:O	2.20	0.42
1:D:309:TYR:N	1:D:309:TYR:HD1	2.17	0.42
1:D:734:SER:CB	1:D:860:GLY:HA3	2.46	0.42
1:D:955:PHE:CD1	1:D:986:ILE:HG23	2.54	0.42
1:A:43:ARG:NH1	1:A:43:ARG:HG2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:LEU:HA	1:A:214:LEU:HD23	1.41	0.41
1:A:533:LEU:CD1	1:A:533:LEU:C	2.93	0.41
1:A:646:HIS:C	1:A:648:ASP:N	2.78	0.41
1:A:780:LEU:HD12	1:A:886:CYS:HB3	2.02	0.41
1:B:575:LEU:HD23	1:B:575:LEU:HA	1.79	0.41
1:B:659:ASP:C	1:B:661:LYS:HE3	2.45	0.41
1:B:768:MET:CE	1:B:770:ILE:CD1	2.97	0.41
1:B:817:GLN:C	1:B:818:ALA:O	2.60	0.41
1:B:885:ASN:HB2	1:B:984:LEU:O	2.21	0.41
1:C:173:LEU:O	1:C:174:SER:C	2.61	0.41
1:C:526:LEU:HD12	1:C:526:LEU:HA	1.84	0.41
1:C:741:THR:HG22	1:C:742:THR:O	2.20	0.41
1:D:33:PHE:CD1	1:D:217:LYS:HE3	2.55	0.41
1:D:72:SER:O	1:D:73:TRP:C	2.61	0.41
1:D:260:LEU:O	1:D:267:VAL:N	2.44	0.41
1:D:403:ASP:OD1	1:D:452:SER:OG	2.26	0.41
1:D:822:LEU:HD11	1:D:824:GLN:O	2.20	0.41
1:D:824:GLN:CG	1:D:825:CYS:N	2.78	0.41
1:A:167:LEU:HG	1:A:393:PRO:HG2	2.01	0.41
1:A:651:LEU:HD12	1:A:651:LEU:HA	1.92	0.41
1:A:734:SER:CB	1:A:860:GLY:CA	2.97	0.41
1:A:851:ILE:O	1:A:870:VAL:HA	2.20	0.41
1:B:42:ALA:O	1:B:310:ARG:NH1	2.53	0.41
1:B:111:PRO:HA	1:B:112:PRO:HA	1.76	0.41
1:B:118:ASN:O	1:B:120:THR:OG1	2.39	0.41
1:B:173:LEU:O	1:B:175:ALA:N	2.53	0.41
1:B:654:TRP:CE3	1:B:654:TRP:C	2.98	0.41
1:B:787:ALA:HA	1:B:788:PRO:HD3	1.72	0.41
1:C:90:TRP:CD1	1:C:90:TRP:C	2.98	0.41
1:C:322:LEU:HD23	1:C:322:LEU:HA	1.84	0.41
1:C:536:CYS:O	1:C:566:PHE:HB2	2.19	0.41
1:C:679:LEU:C	1:C:680:ILE:HG13	2.44	0.41
1:D:177:LEU:HD23	1:D:177:LEU:HA	1.82	0.41
1:D:427:THR:HG22	1:D:436:MET:SD	2.61	0.41
1:D:608:PHE:CD1	1:D:614:HIS:CD2	3.08	0.41
1:D:652:LEU:HD12	1:D:700:VAL:HG22	2.01	0.41
1:D:759:ASN:HB2	1:D:766:SER:OG	2.19	0.41
1:B:344:LEU:HG	1:B:345:ASN:N	2.34	0.41
1:B:392:TYR:HD1	1:B:393:PRO:O	2.03	0.41
1:B:395:HIS:ND1	1:B:395:HIS:C	2.78	0.41
1:B:458:LEU:HA	1:B:458:LEU:HD23	1.65	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:513:PRO:O	1:B:514:ALA:HB3	2.20	0.41
1:B:555:ALA:O	1:B:556:PHE:C	2.63	0.41
1:B:935:ASN:N	1:B:935:ASN:ND2	2.68	0.41
1:C:207:GLY:O	1:C:209:PHE:N	2.54	0.41
1:C:292:ARG:NH1	1:C:292:ARG:CG	2.82	0.41
1:C:569:ASP:HB2	3:C:5099:HOH:O	2.21	0.41
1:C:766:SER:O	1:C:767:GLN:HB2	2.20	0.41
1:D:38:ASN:ND2	1:D:38:ASN:C	2.77	0.41
1:D:60:PHE:CD2	1:D:60:PHE:C	2.98	0.41
1:D:62:TRP:CZ2	1:D:119:PRO:HB3	2.56	0.41
1:D:252:ASP:OD1	1:D:252:ASP:N	2.51	0.41
1:D:834:VAL:HG12	1:D:835:LEU:N	2.34	0.41
1:A:316:HIS:HB3	1:A:322:LEU:HD23	2.01	0.41
1:A:351:ILE:N	1:A:351:ILE:HD13	2.35	0.41
1:A:358:GLU:HB3	1:A:367:MET:SD	2.61	0.41
1:A:361:PRO:CD	1:A:362:LEU:H	2.33	0.41
1:A:472:TYR:CD2	1:A:472:TYR:C	2.98	0.41
1:B:228:ALA:C	1:B:229:THR:HG23	2.43	0.41
1:B:368:ASP:O	1:B:372:MET:HG3	2.19	0.41
1:B:418:HIS:CE1	1:B:461:GLU:CD	2.98	0.41
1:B:640:SER:OG	1:B:642:TYR:HB2	2.20	0.41
1:B:670:LEU:HD11	1:B:700:VAL:CG2	2.51	0.41
1:B:875:ASP:N	1:B:875:ASP:OD2	2.53	0.41
1:C:217:LYS:CG	1:C:218:PRO:CD	2.99	0.41
1:C:791:ASN:HB3	3:C:4270:HOH:O	2.20	0.41
1:D:7:LEU:HD23	1:D:7:LEU:HA	1.85	0.41
1:D:262:GLN:O	1:D:262:GLN:HG2	2.19	0.41
1:D:654:TRP:HE1	1:D:666:GLY:HA3	1.84	0.41
1:D:904:GLU:OE1	1:D:929:TYR:OH	2.28	0.41
1:A:138:GLN:CG	1:A:139:THR:N	2.78	0.41
1:A:315:LEU:HD12	1:A:315:LEU:HA	1.80	0.41
1:A:579:ASP:C	1:A:581:ASN:N	2.78	0.41
1:B:173:LEU:HD23	1:B:173:LEU:HA	1.77	0.41
1:B:257:THR:O	1:B:313:VAL:HA	2.20	0.41
1:B:316:HIS:CD2	1:B:316:HIS:C	2.98	0.41
1:B:356:ARG:HH22	1:B:367:MET:CE	2.33	0.41
1:B:579:ASP:OD2	1:B:583:ASN:HB2	2.21	0.41
1:B:837:THR:CG2	1:B:838:THR:N	2.78	0.41
1:C:46:ARG:HA	1:C:47:PRO:HD3	1.80	0.41
1:C:335:VAL:C	1:C:336:ARG:HG3	2.46	0.41
1:C:876:THR:C	1:C:877:PRO:O	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:TRP:CD1	1:D:95:TYR:CB	3.02	0.41
1:D:896:ASN:HA	1:D:918:TRP:O	2.21	0.41
1:A:38:ASN:ND2	1:A:40:GLU:N	2.68	0.41
1:A:420:MET:HE2	1:A:426:LEU:CG	2.51	0.41
1:A:599:ARG:HB2	1:A:600:GLN:H	1.30	0.41
1:A:653[B]:HIS:CD2	1:A:666:GLY:O	2.74	0.41
1:A:734:SER:CB	1:A:860:GLY:HA3	2.45	0.41
1:A:896:ASN:HA	1:A:918:TRP:O	2.21	0.41
1:A:917:ARG:HH22	1:A:943:GLU:CD	2.28	0.41
1:B:549:PHE:O	1:B:553:TRP:HD1	2.04	0.41
1:B:608:PHE:O	1:B:611:ARG:N	2.45	0.41
1:B:658:LEU:CG	1:B:661:LYS:NZ	2.78	0.41
1:B:740:LEU:HA	1:B:748:CYS:O	2.20	0.41
1:B:897:TRP:HB2	1:B:943:GLU:O	2.21	0.41
1:C:46:ARG:CB	1:C:47:PRO:CD	2.98	0.41
1:C:152:LEU:N	1:C:160:GLY:O	2.54	0.41
1:C:925:MET:HE3	1:C:925:MET:CA	2.48	0.41
1:D:597:ASN:ND2	1:D:597:ASN:C	2.78	0.41
1:D:706:THR:HG23	1:D:709:SER:OG	2.20	0.41
1:D:763:GLY:CA	1:D:822:LEU:CD2	2.98	0.41
1:D:925:MET:CE	1:D:938:ARG:CZ	2.99	0.41
1:D:956:GLN:HB2	1:D:987:ASP:HB2	2.02	0.41
1:A:524:LEU:HD22	1:A:561:ARG:CB	2.50	0.41
1:A:737:ILE:HD12	1:A:832:ASP:HA	2.03	0.41
1:A:768:MET:HG2	1:A:775:GLN:HG3	2.03	0.41
1:A:995:GLY:C	1:A:997:ASP:N	2.75	0.41
1:B:403:ASP:OD1	1:B:452:SER:OG	2.35	0.41
1:B:486:TYR:CZ	1:B:488:GLY:HA3	2.55	0.41
1:B:590:GLY:HA2	1:B:594:ASP:OD1	2.20	0.41
1:B:682:LEU:HA	1:B:682:LEU:HD23	1.60	0.41
1:B:1009:LEU:N	1:B:1009:LEU:HD23	2.34	0.41
1:C:473:ARG:O	1:C:474:TRP:C	2.58	0.41
1:C:595:THR:HA	1:C:596:PRO:C	2.45	0.41
1:C:638:VAL:O	1:C:677:LYS:HA	2.21	0.41
1:D:27:LEU:HD12	1:D:140:ARG:NH1	2.35	0.41
1:D:429:ASP:HA	1:D:430:PRO:HD3	1.85	0.41
1:D:730:LEU:HA	1:D:731:PRO:HD3	1.95	0.41
1:D:765:LEU:O	1:D:765:LEU:HG	2.19	0.41
1:A:39:SER:O	1:A:40:GLU:C	2.63	0.41
1:A:443:MET:O	1:A:444:VAL:C	2.59	0.41
1:A:533:LEU:C	1:A:533:LEU:HD12	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:668:VAL:CG1	1:A:669:PRO:HD2	2.49	0.41
1:A:775:GLN:O	1:A:889:ALA:N	2.53	0.41
1:A:930:VAL:CA	1:A:973:ARG:HD3	2.37	0.41
1:B:17:GLU:O	1:B:112:PRO:HG2	2.21	0.41
1:B:44:THR:O	1:B:45:ASP:HB3	2.21	0.41
1:B:103:VAL:HG22	1:B:418:HIS:CE1	2.56	0.41
1:B:392:TYR:O	1:B:393:PRO:C	2.63	0.41
1:B:589:GLY:CA	1:B:599:ARG:HA	2.39	0.41
1:B:615:PRO:HG2	1:B:904:GLU:OE1	2.20	0.41
1:B:933:SER:O	1:B:934:GLU:C	2.58	0.41
1:C:63:PHE:HB3	1:C:64:PRO:HD2	2.02	0.41
1:C:342:LEU:HD12	1:C:342:LEU:HA	1.67	0.41
1:C:376:ILE:HD13	1:C:401:LEU:HB3	2.03	0.41
1:C:726:LEU:CD1	1:D:848:THR:HG22	2.50	0.41
1:D:105:TYR:HA	1:D:106:PRO:HD2	1.76	0.41
1:D:173:LEU:O	1:D:174:SER:C	2.64	0.41
1:D:300:LEU:HD23	1:D:332:PHE:HB3	2.02	0.41
1:D:460:ASN:CG	1:D:461:GLU:HG2	2.46	0.41
1:A:13:ARG:NH1	1:D:13:ARG:NH1	2.69	0.41
1:A:153:TRP:CD1	1:A:158:TRP:HA	2.56	0.41
1:A:243:GLU:OE1	1:A:288:ARG:HD3	2.20	0.41
1:A:434:PRO:HB3	1:D:434:PRO:HB3	2.03	0.41
1:A:651:LEU:HD12	1:A:669:PRO:HA	2.03	0.41
1:A:728:VAL:HG13	1:B:851:ILE:HD11	2.02	0.41
1:B:3:ILE:C	1:B:5:ASP:N	2.79	0.41
1:B:142:ILE:HD13	1:B:142:ILE:HG21	1.87	0.41
1:B:292:ARG:CG	1:B:292:ARG:NH1	2.84	0.41
1:B:380:LYS:O	1:B:381:GLN:C	2.62	0.41
1:B:549:PHE:HE1	1:B:567:VAL:CG2	2.34	0.41
1:B:679:LEU:C	1:B:680:ILE:HG13	2.45	0.41
1:B:768:MET:O	1:B:768:MET:HG3	2.18	0.41
1:C:22:THR:OG1	1:C:438:GLU:OE1	2.37	0.41
1:C:35:SER:CB	1:C:37:ARG:NH1	2.84	0.41
1:C:38:ASN:ND2	1:C:38:ASN:C	2.75	0.41
1:C:120:THR:CG2	1:C:187:MET:SD	3.09	0.41
1:C:176:PHE:HE1	3:C:4172:HOH:O	2.04	0.41
1:C:190:ARG:HD3	1:C:191:TRP:CZ2	2.55	0.41
1:C:194:GLY:O	1:C:197:LEU:HB2	2.21	0.41
1:C:202:MET:HE3	1:C:357:HIS:CD2	2.56	0.41
1:C:226:HIS:CD2	1:C:448:ARG:HD2	2.56	0.41
1:C:342:LEU:HB3	1:C:563:GLN:HE22	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:482:ARG:HH11	1:C:482:ARG:HD2	1.60	0.41
1:C:567:VAL:H	1:C:567:VAL:HG23	1.67	0.41
1:C:589:GLY:C	1:C:597:ASN:ND2	2.79	0.41
1:C:592:PHE:C	1:C:594:ASP:N	2.78	0.41
1:C:658:LEU:O	1:C:659:ASP:C	2.64	0.41
1:C:737:ILE:HB	1:C:738:PRO:HD2	2.02	0.41
1:C:952:ARG:CZ	1:C:952:ARG:CB	2.99	0.41
1:C:1022:GLN:CD	1:C:1022:GLN:N	2.79	0.41
1:D:40:GLU:CD	1:D:43:ARG:HH21	2.29	0.41
1:D:56:GLY:O	1:D:85:VAL:HA	2.20	0.41
1:D:200:GLN:HG2	1:D:391:HIS:HB2	2.03	0.41
1:D:272:ALA:HB1	1:D:273:PRO:CD	2.51	0.41
1:D:469:ASP:O	1:D:470:ALA:C	2.64	0.41
1:D:505:ARG:HH11	1:D:505:ARG:HD3	1.56	0.41
1:D:599:ARG:C	1:D:601:PHE:H	2.29	0.41
1:D:870:VAL:CG1	1:D:871:GLU:N	2.84	0.41
1:D:904:GLU:CG	1:D:909:ARG:HH22	2.31	0.41
1:A:90:TRP:CD1	1:A:90:TRP:C	2.99	0.41
1:A:141:ILE:O	1:A:170:GLU:HA	2.21	0.41
1:A:260:LEU:HD11	1:A:309:TYR:HB3	2.01	0.41
1:A:460:ASN:O	1:A:461:GLU:C	2.63	0.41
1:A:782:ASP:OD2	1:A:852:SER:OG	2.29	0.41
1:B:252:ASP:C	1:B:254:LEU:H	2.29	0.41
1:B:455:ILE:HD13	1:B:455:ILE:HG21	1.90	0.41
1:C:455:ILE:CG2	1:C:456:TRP:N	2.80	0.41
1:C:796:SER:HB2	1:C:802:ASP:HB3	2.03	0.41
1:D:209:PHE:CD2	1:D:209:PHE:N	2.80	0.41
1:D:360:HIS:ND1	1:D:362:LEU:N	2.62	0.41
1:D:668:VAL:CG1	1:D:669:PRO:N	2.84	0.41
1:D:844:HIS:C	1:D:846:GLY:N	2.78	0.41
1:A:7:LEU:HD13	1:A:69:VAL:CG1	2.51	0.40
1:A:38:ASN:ND2	1:A:38:ASN:C	2.78	0.40
1:A:390:SER:HA	1:A:391:HIS:HA	1.79	0.40
1:A:769:TRP:HB3	1:A:771:GLY:O	2.21	0.40
1:B:6:SER:O	1:B:7:LEU:C	2.64	0.40
1:B:221:GLN:HE21	1:B:221:GLN:HB3	1.26	0.40
1:B:296:GLU:O	1:B:297:ASN:C	2.64	0.40
1:B:406:GLY:O	1:B:407:LEU:HD23	2.21	0.40
1:B:421:VAL:HA	1:B:422:PRO:HA	1.85	0.40
1:B:476:LYS:HB3	1:B:476:LYS:HE3	1.82	0.40
1:B:888:LEU:O	1:B:981:GLY:HA3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:910:LEU:C	1:B:910:LEU:CD1	2.94	0.40
1:C:658:LEU:HD11	1:C:692:GLY:C	2.46	0.40
1:D:184:LEU:HA	1:D:184:LEU:HD23	1.74	0.40
1:D:298:PRO:N	3:D:4211:HOH:O	2.54	0.40
1:D:589:GLY:C	1:D:597:ASN:ND2	2.79	0.40
1:D:679:LEU:HD23	1:D:679:LEU:HA	1.07	0.40
1:D:932:PRO:HG2	1:D:970:THR:O	2.21	0.40
1:D:988:GLY:C	1:D:989:PHE:CG	2.99	0.40
1:A:34:ALA:O	1:A:35:SER:C	2.60	0.40
1:A:131:GLU:O	1:A:134:LEU:HD23	2.21	0.40
1:A:210:ARG:HD3	1:A:210:ARG:HH11	1.71	0.40
1:A:304:GLU:C	1:A:305:ILE:CG1	2.92	0.40
1:A:378:LEU:HD23	1:A:378:LEU:HA	1.61	0.40
1:A:763:GLY:CA	1:A:822:LEU:HD21	2.49	0.40
1:A:931:PHE:CD2	1:A:931:PHE:C	2.99	0.40
1:B:105:TYR:CE2	1:B:199:ASP:HB2	2.57	0.40
1:B:197:LEU:HD23	1:B:197:LEU:HA	1.65	0.40
1:B:422:PRO:HB2	1:C:280:ASP:OD1	2.21	0.40
1:B:607:VAL:HG12	1:B:613:PRO:HA	2.02	0.40
1:C:510:GLN:HB3	1:C:512:PHE:CZ	2.57	0.40
1:C:589:GLY:C	1:C:591:ASP:N	2.80	0.40
1:C:685:LEU:O	1:C:686:PRO:C	2.64	0.40
1:C:815:HIS:CD2	1:C:849:LEU:HD13	2.56	0.40
1:D:6:SER:HB2	1:D:71:GLU:OE2	2.21	0.40
1:A:30:HIS:CE1	1:A:33:PHE:CD1	3.10	0.40
1:A:152:LEU:CG	1:A:153:TRP:N	2.81	0.40
1:A:898:LEU:HB2	1:A:917:ARG:NH2	2.36	0.40
1:A:1020:TRP:CD1	1:A:1020:TRP:C	2.99	0.40
1:B:433:LEU:O	1:B:437:SER:HB3	2.22	0.40
1:B:572:ASP:C	1:B:574:SER:H	2.29	0.40
1:B:595:THR:CG2	1:B:596:PRO:CA	2.98	0.40
1:B:881:ARG:HD3	1:B:987:ASP:OD2	2.22	0.40
1:C:90:TRP:HE1	1:C:96:ASP:CG	2.29	0.40
1:C:100:TYR:HB2	1:C:203:TRP:CZ3	2.56	0.40
1:C:490:GLY:N	3:C:4010:HOH:O	2.32	0.40
1:C:502:MET:HB3	1:C:537:GLU:HG3	2.02	0.40
1:C:590:GLY:N	1:C:597:ASN:CG	2.79	0.40
1:C:987:ASP:OD2	1:C:990:HIS:HD2	2.05	0.40
1:D:476:LYS:HG2	1:D:476:LYS:H	1.60	0.40
1:D:559:TYR:HA	1:D:560:PRO:HD2	1.89	0.40
1:A:57:GLU:HG2	1:A:83:THR:CG2	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:PHE:N	1:A:127:PHE:CD2	2.90	0.40
1:A:559:TYR:HB2	1:A:562:LEU:CD1	2.52	0.40
1:A:788:PRO:O	1:A:933:SER:HB2	2.21	0.40
1:B:559:TYR:CB	1:B:562:LEU:HD12	2.35	0.40
1:B:599:ARG:HB2	1:B:600:GLN:H	1.20	0.40
1:B:839:ALA:C	1:B:840:HIS:ND1	2.79	0.40
1:B:900:LEU:HD13	1:B:913:ALA:HB3	2.02	0.40
1:C:30:HIS:HE1	3:C:4191:HOH:O	2.04	0.40
1:C:118:ASN:HD21	1:C:189:LEU:CD2	2.34	0.40
1:C:835:LEU:O	1:C:835:LEU:HG	2.21	0.40
1:D:106:PRO:HB2	1:D:191:TRP:CH2	2.56	0.40
1:D:352:ARG:O	1:D:385:ASN:HB2	2.22	0.40
1:D:632:SER:O	1:D:634:GLN:N	2.55	0.40
1:A:513:PRO:C	1:A:515:VAL:H	2.30	0.40
1:A:576:ILE:CG2	1:A:577:LYS:N	2.84	0.40
1:A:600:GLN:C	1:A:602:CYS:N	2.80	0.40
1:A:623:GLN:NE2	1:A:911:THR:OG1	2.54	0.40
1:A:852:SER:OG	1:A:854:LYS:HE3	2.21	0.40
1:A:995:GLY:HA3	3:A:4067:HOH:O	2.22	0.40
1:B:41:GLU:HG3	1:B:46:ARG:NH1	2.37	0.40
1:B:67:GLU:H	1:B:67:GLU:HG2	1.28	0.40
1:B:90:TRP:NE1	1:B:96:ASP:OD1	2.55	0.40
1:B:102:ASN:ND2	1:B:102:ASN:C	2.79	0.40
1:B:240:LEU:HG	1:B:241:GLU:N	2.36	0.40
1:B:251:ARG:O	1:B:254:LEU:HD12	2.22	0.40
1:B:376:ILE:CD1	1:B:401:LEU:HB3	2.51	0.40
1:B:749:ILE:CG2	1:B:750:GLU:N	2.82	0.40
1:C:458:LEU:HD11	1:C:472:TYR:HB2	2.04	0.40
1:C:784:PHE:HA	1:C:881:ARG:O	2.22	0.40
1:C:834:VAL:HG12	1:C:835:LEU:N	2.37	0.40
1:C:864:MET:HE2	1:C:864:MET:HB2	1.42	0.40
1:C:961:ARG:HG3	1:C:961:ARG:HH11	1.85	0.40
1:D:5:ASP:O	1:D:6:SER:C	2.64	0.40
1:D:500:CYS:N	1:D:501:PRO:CD	2.85	0.40
1:D:559:TYR:N	1:D:559:TYR:CD1	2.90	0.40
1:D:651:LEU:HD13	1:D:651:LEU:HA	1.60	0.40
1:D:882:ILE:HB	1:D:989:PHE:HB2	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	1026/1021 (100%)	923 (90%)	86 (8%)	17 (2%)	7	25
1	B	1026/1021 (100%)	917 (89%)	89 (9%)	20 (2%)	6	22
1	C	1026/1021 (100%)	918 (90%)	82 (8%)	26 (2%)	4	16
1	D	1026/1021 (100%)	921 (90%)	85 (8%)	20 (2%)	6	22
All	All	4104/4084 (100%)	3679 (90%)	342 (8%)	83 (2%)	6	21

All (83) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	647	SER
1	A	733	ALA
1	A	734	SER
1	A	1005	ALA
1	B	79	PRO
1	B	164	ASP
1	B	174	SER
1	B	734	SER
1	B	930	VAL
1	C	252	ASP
1	C	425	ARG
1	C	493	THR
1	D	10	VAL
1	D	667	GLU
1	D	686	PRO
1	D	687	GLN
1	D	732	ALA
1	A	119	PRO
1	A	461	GLU
1	A	493	THR
1	B	601	PHE
1	B	659	ASP

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Mol	Chain	Res	Type
1	B	733	ALA
1	B	831	ALA
1	C	46	ARG
1	C	79	PRO
1	C	690	SER
1	C	731	PRO
1	C	733	ALA
1	C	743	SER
1	C	746	ASP
1	D	11	LEU
1	D	461	GLU
1	D	815	HIS
1	A	252	ASP
1	A	541	ALA
1	A	601	PHE
1	B	77	ASP
1	B	95	TYR
1	B	425	ARG
1	C	47	PRO
1	C	119	PRO
1	C	601	PHE
1	C	734	SER
1	C	742	THR
1	C	996	ASP
1	D	174	SER
1	D	273	PRO
1	D	546	LEU
1	A	10	VAL
1	A	79	PRO
1	A	540	HIS
1	A	890	GLN
1	B	398	TRP
1	B	546	LEU
1	B	690	SER
1	C	12	GLN
1	C	81	ALA
1	C	461	GLU
1	D	493	THR
1	D	909	ARG
1	A	599	ARG
1	B	383	ASN
1	B	891	VAL

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Mol	Chain	Res	Type
1	C	208	ILE
1	C	211	ASP
1	C	233	ASP
1	D	14	ARG
1	D	72	SER
1	D	109	VAL
1	D	647	SER
1	A	174	SER
1	A	580	GLU
1	C	77	ASP
1	C	788	PRO
1	C	916	ASP
1	D	669	PRO
1	D	948	PRO
1	B	688	PRO
1	C	376	ILE
1	D	488	GLY
1	B	434	PRO
1	B	119	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	880/873 (101%)	688 (78%)	192 (22%)	1	3
1	B	880/873 (101%)	676 (77%)	204 (23%)	1	3
1	C	880/873 (101%)	680 (77%)	200 (23%)	1	3
1	D	880/873 (101%)	703 (80%)	177 (20%)	1	4
All	All	3520/3492 (101%)	2747 (78%)	773 (22%)	1	3

All (773) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	11	LEU

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Mol	Chain	Res	Type
1	A	12	GLN
1	A	22	THR
1	A	24	LEU
1	A	37	ARG
1	A	38	ASN
1	A	39	SER
1	A	51	LEU
1	A	57	GLU
1	A	67	GLU
1	A	71	GLU
1	A	72	SER
1	A	76	CYS
1	A	80	GLU
1	A	83	THR
1	A	84	VAL
1	A	92	MET
1	A	96	ASP
1	A	114	VAL
1	A	117	GLU
1	A	124	SER
1	A	134	LEU
1	A	135	GLN
1	A	136	GLU
1	A	138	GLN
1	A	140	ARG
1	A	148	SER
1	A	152	LEU
1	A	165	SER
1	A	166	ARG
1	A	169	SER
1	A	177	LEU
1	A	178	ARG
1	A	181	GLU
1	A	186	VAL
1	A	187	MET
1	A	189	LEU
1	A	190	ARG
1	A	202	MET
1	A	206	SER
1	A	210	ARG
1	A	211	ASP
1	A	214	LEU

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Mol	Chain	Res	Type
1	A	217	LYS
1	A	219	THR
1	A	230	ARG
1	A	237	ARG
1	A	245	GLN
1	A	246	MET
1	A	247	CYS
1	A	249	GLU
1	A	250	LEU
1	A	251	ARG
1	A	255	ARG
1	A	259	SER
1	A	260	LEU
1	A	277	GLU
1	A	278	ILE
1	A	279	ILE
1	A	280	ASP
1	A	288	ARG
1	A	302	SER
1	A	310	ARG
1	A	322	LEU
1	A	333	ARG
1	A	344	LEU
1	A	347	LYS
1	A	351	ILE
1	A	362	LEU
1	A	367	MET
1	A	380	LYS
1	A	381	GLN
1	A	385	ASN
1	A	424	ASN
1	A	425	ARG
1	A	433	LEU
1	A	437	SER
1	A	448	ARG
1	A	452	SER
1	A	461	GLU
1	A	473	ARG
1	A	477	SER
1	A	478	VAL
1	A	481	SER
1	A	493	THR

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Mol	Chain	Res	Type
1	A	502	MET
1	A	520	ILE
1	A	521	LYS
1	A	525	SER
1	A	526	LEU
1	A	529	GLU
1	A	533	LEU
1	A	540	HIS
1	A	545	SER
1	A	546	LEU
1	A	551	LYS
1	A	554	GLN
1	A	558	GLN
1	A	571	VAL
1	A	581	ASN
1	A	599	ARG
1	A	600	GLN
1	A	607	VAL
1	A	611	ARG
1	A	630	ARG
1	A	632	SER
1	A	634	GLN
1	A	637	GLU
1	A	645	ARG
1	A	647	SER
1	A	655	MET
1	A	663	LEU
1	A	665	SER
1	A	667	GLU
1	A	668	VAL
1	A	671	ASP
1	A	672	VAL
1	A	675	GLN
1	A	677	LYS
1	A	679	LEU
1	A	681	GLU
1	A	682	LEU
1	A	685	LEU
1	A	694	LEU
1	A	696	LEU
1	A	704	ASN
1	A	721	ARG

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Mol	Chain	Res	Type
1	A	728	VAL
1	A	729	THR
1	A	730	LEU
1	A	737	ILE
1	A	750	GLU
1	A	751	LEU
1	A	753	ASN
1	A	761	GLN
1	A	768	MET
1	A	772	ASP
1	A	773	LYS
1	A	774	LYS
1	A	777	LEU
1	A	778	THR
1	A	781	ARG
1	A	790	ASP
1	A	796	SER
1	A	797	GLU
1	A	799	THR
1	A	801	ILE
1	A	811	LYS
1	A	822	LEU
1	A	823	LEU
1	A	824	GLN
1	A	830	LEU
1	A	835	LEU
1	A	843	GLN
1	A	845	GLN
1	A	847	LYS
1	A	853	ARG
1	A	854	LYS
1	A	856	TYR
1	A	857	ARG
1	A	858	ILE
1	A	859	ASP
1	A	861	SER
1	A	863	GLN
1	A	864	MET
1	A	867	THR
1	A	874	SER
1	A	876	THR
1	A	878	HIS

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Mol	Chain	Res	Type
1	A	885	ASN
1	A	887	GLN
1	A	888	LEU
1	A	894	ARG
1	A	900	LEU
1	A	916	ASP
1	A	923	SER
1	A	925	MET
1	A	931	PHE
1	A	937	LEU
1	A	938	ARG
1	A	950	GLN
1	A	956	GLN
1	A	965	GLN
1	A	966	GLN
1	A	969	GLU
1	A	986	ILE
1	A	1004	SER
1	A	1006	GLU
1	A	1017	GLN
1	A	1018	LEU
1	A	1023	LYS
1	B	3	ILE
1	B	4	THR
1	B	6	SER
1	B	7	LEU
1	B	9	VAL
1	B	11	LEU
1	B	24	LEU
1	B	25	ASN
1	B	37	ARG
1	B	38	ASN
1	B	39	SER
1	B	43	ARG
1	B	48	SER
1	B	49	GLN
1	B	53	SER
1	B	57	GLU
1	B	67	GLU
1	B	71	GLU
1	B	75	GLU
1	B	76	CYS

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Mol	Chain	Res	Type
1	B	80	GLU
1	B	82	ASP
1	B	83	THR
1	B	84	VAL
1	B	90	TRP
1	B	101	THR
1	B	102	ASN
1	B	108	THR
1	B	109	VAL
1	B	115	PRO
1	B	116	THR
1	B	117	GLU
1	B	118	ASN
1	B	123	TYR
1	B	124	SER
1	B	125	LEU
1	B	128	ASN
1	B	132	SER
1	B	134	LEU
1	B	135	GLN
1	B	138	GLN
1	B	141	ILE
1	B	143	PHE
1	B	159	VAL
1	B	181	GLU
1	B	187	MET
1	B	189	LEU
1	B	190	ARG
1	B	198	GLU
1	B	202	MET
1	B	210	ARG
1	B	211	ASP
1	B	213	SER
1	B	214	LEU
1	B	217	LYS
1	B	219	THR
1	B	220	THR
1	B	221	GLN
1	B	223	SER
1	B	226	HIS
1	B	230	ARG
1	B	233	ASP

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Mol	Chain	Res	Type
1	B	237	ARG
1	B	240	LEU
1	B	244	VAL
1	B	246	MET
1	B	247	CYS
1	B	249	GLU
1	B	250	LEU
1	B	252	ASP
1	B	255	ARG
1	B	266	GLN
1	B	267	VAL
1	B	279	ILE
1	B	280	ASP
1	B	292	ARG
1	B	310	ARG
1	B	314	GLU
1	B	322	LEU
1	B	323	ILE
1	B	324	GLU
1	B	330	VAL
1	B	333	ARG
1	B	338	GLU
1	B	347	LYS
1	B	350	LEU
1	B	357	HIS
1	B	362	LEU
1	B	365	GLN
1	B	377	LEU
1	B	380	LYS
1	B	397	LEU
1	B	425	ARG
1	B	445	GLN
1	B	448	ARG
1	B	460	ASN
1	B	472	TYR
1	B	473	ARG
1	B	476	LYS
1	B	507	ASP
1	B	509	ASP
1	B	519	SER
1	B	525	SER
1	B	526	LEU

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Mol	Chain	Res	Type
1	B	529	GLU
1	B	531	ARG
1	B	533	LEU
1	B	542	MET
1	B	545	SER
1	B	546	LEU
1	B	554	GLN
1	B	563	GLN
1	B	576	ILE
1	B	580	GLU
1	B	581	ASN
1	B	588	TYR
1	B	598	ASP
1	B	599	ARG
1	B	600	GLN
1	B	630	ARG
1	B	631	LEU
1	B	638	VAL
1	B	645	ARG
1	B	651	LEU
1	B	652	LEU
1	B	655	MET
1	B	658	LEU
1	B	661	LYS
1	B	663	LEU
1	B	672	VAL
1	B	681	GLU
1	B	684	GLU
1	B	687	GLN
1	B	690	SER
1	B	698	VAL
1	B	719	GLN
1	B	728	VAL
1	B	729	THR
1	B	730	LEU
1	B	734	SER
1	B	737	ILE
1	B	745	MET
1	B	750	GLU
1	B	751	LEU
1	B	755	ARG
1	B	761	GLN

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Mol	Chain	Res	Type
1	B	765	LEU
1	B	766	SER
1	B	768	MET
1	B	770	ILE
1	B	772	ASP
1	B	773	LYS
1	B	774	LYS
1	B	778	THR
1	B	781	ARG
1	B	789	LEU
1	B	795	VAL
1	B	797	GLU
1	B	799	THR
1	B	800	ARG
1	B	801	ILE
1	B	808	GLU
1	B	817	GLN
1	B	822	LEU
1	B	824	GLN
1	B	829	THR
1	B	830	LEU
1	B	836	ILE
1	B	837	THR
1	B	843	GLN
1	B	845	GLN
1	B	848	THR
1	B	852	SER
1	B	854	LYS
1	B	858	ILE
1	B	864	MET
1	B	866	ILE
1	B	867	THR
1	B	872	VAL
1	B	874	SER
1	B	876	THR
1	B	884	LEU
1	B	900	LEU
1	B	917	ARG
1	B	923	SER
1	B	924	ASP
1	B	934	GLU
1	B	938	ARG

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Mol	Chain	Res	Type
1	B	941	THR
1	B	942	ARG
1	B	944	LEU
1	B	950	GLN
1	B	958	ASN
1	B	965	GLN
1	B	971	SER
1	B	972	HIS
1	B	986	ILE
1	B	991	MET
1	B	998	SER
1	B	1004	SER
1	B	1006	GLU
1	B	1009	LEU
1	B	1018	LEU
1	B	1023	LYS
1	C	3	ILE
1	C	6	SER
1	C	9	VAL
1	C	10	VAL
1	C	24	LEU
1	C	27	LEU
1	C	35	SER
1	C	38	ASN
1	C	39	SER
1	C	49	GLN
1	C	55	ASN
1	C	67	GLU
1	C	71	GLU
1	C	72	SER
1	C	80	GLU
1	C	82	ASP
1	C	84	VAL
1	C	85	VAL
1	C	99	ILE
1	C	104	THR
1	C	108	THR
1	C	109	VAL
1	C	114	VAL
1	C	116	THR
1	C	125	LEU
1	C	130	ASP

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Mol	Chain	Res	Type
1	C	131	GLU
1	C	134	LEU
1	C	135	GLN
1	C	136	GLU
1	C	138	GLN
1	C	141	ILE
1	C	143	PHE
1	C	148	SER
1	C	159	VAL
1	C	163	GLN
1	C	165	SER
1	C	166	ARG
1	C	173	LEU
1	C	178	ARG
1	C	187	MET
1	C	189	LEU
1	C	192	SER
1	C	195	SER
1	C	197	LEU
1	C	214	LEU
1	C	223	SER
1	C	230	ARG
1	C	236	SER
1	C	237	ARG
1	C	246	MET
1	C	249	GLU
1	C	250	LEU
1	C	251	ARG
1	C	252	ASP
1	C	255	ARG
1	C	259	SER
1	C	264	GLU
1	C	266	GLN
1	C	277	GLU
1	C	282	ARG
1	C	291	LEU
1	C	292	ARG
1	C	296	GLU
1	C	299	LYS
1	C	305	ILE
1	C	322	LEU
1	C	324	GLU

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Mol	Chain	Res	Type
1	C	333	ARG
1	C	338	GLU
1	C	347	LYS
1	C	350	LEU
1	C	352	ARG
1	C	357	HIS
1	C	377	LEU
1	C	380	LYS
1	C	424	ASN
1	C	425	ARG
1	C	426	LEU
1	C	427	THR
1	C	431[A]	ARG
1	C	431[B]	ARG
1	C	437	SER
1	C	461	GLU
1	C	473	ARG
1	C	476	LYS
1	C	478	VAL
1	C	503	TYR
1	C	505	ARG
1	C	508	GLU
1	C	517	LYS
1	C	519	SER
1	C	521	LYS
1	C	526	LEU
1	C	529	GLU
1	C	531	ARG
1	C	533	LEU
1	C	537	GLU
1	C	542	MET
1	C	545	SER
1	C	546	LEU
1	C	554	GLN
1	C	571	VAL
1	C	575	LEU
1	C	580	GLU
1	C	581	ASN
1	C	595	THR
1	C	600	GLN
1	C	604	ASN
1	C	618	THR

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Mol	Chain	Res	Type
1	C	630	ARG
1	C	631	LEU
1	C	645	ARG
1	C	655	MET
1	C	661	LYS
1	C	663	LEU
1	C	670	LEU
1	C	671	ASP
1	C	672	VAL
1	C	675	GLN
1	C	677	LYS
1	C	687	GLN
1	C	690	SER
1	C	698	VAL
1	C	702	GLN
1	C	714	ILE
1	C	719	GLN
1	C	721	ARG
1	C	727	SER
1	C	728	VAL
1	C	730	LEU
1	C	735	HIS
1	C	737	ILE
1	C	742	THR
1	C	743	SER
1	C	744	GLU
1	C	745	MET
1	C	750	GLU
1	C	751	LEU
1	C	760	ARG
1	C	761	GLN
1	C	765	LEU
1	C	768	MET
1	C	772	ASP
1	C	773	LYS
1	C	774	LYS
1	C	776	LEU
1	C	777	LEU
1	C	778	THR
1	C	781	ARG
1	C	789	LEU
1	C	797	GLU

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Mol	Chain	Res	Type
1	C	801	ILE
1	C	811	LYS
1	C	817	GLN
1	C	823	LEU
1	C	824	GLN
1	C	828	ASP
1	C	829	THR
1	C	830	LEU
1	C	836	ILE
1	C	843	GLN
1	C	845	GLN
1	C	847	LYS
1	C	854	LYS
1	C	856	TYR
1	C	857	ARG
1	C	858	ILE
1	C	861	SER
1	C	863	GLN
1	C	864	MET
1	C	866	ILE
1	C	867	THR
1	C	869	ASP
1	C	870	VAL
1	C	871	GLU
1	C	872	VAL
1	C	874	SER
1	C	885	ASN
1	C	891	VAL
1	C	894	ARG
1	C	896	ASN
1	C	910	LEU
1	C	917	ARG
1	C	920	LEU
1	C	923	SER
1	C	925	MET
1	C	934	GLU
1	C	938	ARG
1	C	939	CYS
1	C	950	GLN
1	C	959	ILE
1	C	965	GLN
1	C	973	ARG

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Mol	Chain	Res	Type
1	C	984	LEU
1	C	991	MET
1	C	998	SER
1	C	1006	GLU
1	C	1013	ARG
1	C	1018	LEU
1	D	3	ILE
1	D	4	THR
1	D	11	LEU
1	D	12	GLN
1	D	13	ARG
1	D	24	LEU
1	D	38	ASN
1	D	39	SER
1	D	41	GLU
1	D	52[A]	ARG
1	D	52[B]	ARG
1	D	67	GLU
1	D	71	GLU
1	D	75	GLU
1	D	76	CYS
1	D	80	GLU
1	D	84	VAL
1	D	85	VAL
1	D	116	THR
1	D	117	GLU
1	D	125	LEU
1	D	128	ASN
1	D	134	LEU
1	D	138	GLN
1	D	140	ARG
1	D	157	ARG
1	D	169	SER
1	D	187	MET
1	D	190	ARG
1	D	202	MET
1	D	211	ASP
1	D	213	SER
1	D	219	THR
1	D	227	VAL
1	D	230	ARG
1	D	236	SER

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Mol	Chain	Res	Type
1	D	237	ARG
1	D	240	LEU
1	D	241	GLU
1	D	243	GLU
1	D	244	VAL
1	D	246	MET
1	D	247	CYS
1	D	249	GLU
1	D	252	ASP
1	D	255	ARG
1	D	277	GLU
1	D	278	ILE
1	D	279	ILE
1	D	288	ARG
1	D	289	VAL
1	D	292	ARG
1	D	310	ARG
1	D	314	GLU
1	D	319	ASP
1	D	322	LEU
1	D	333	ARG
1	D	334	GLU
1	D	342	LEU
1	D	344	LEU
1	D	347	LYS
1	D	352	ARG
1	D	378	LEU
1	D	380	LYS
1	D	385	ASN
1	D	423	MET
1	D	424	ASN
1	D	425	ARG
1	D	437	SER
1	D	445	GLN
1	D	448	ARG
1	D	458	LEU
1	D	461	GLU
1	D	473	ARG
1	D	476	LYS
1	D	477	SER
1	D	481	SER
1	D	505	ARG

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Mol	Chain	Res	Type
1	D	519	SER
1	D	521	LYS
1	D	526	LEU
1	D	529	GLU
1	D	533	LEU
1	D	545	SER
1	D	546	LEU
1	D	554	GLN
1	D	571	VAL
1	D	580	GLU
1	D	581	ASN
1	D	594	ASP
1	D	595	THR
1	D	599	ARG
1	D	600	GLN
1	D	630	ARG
1	D	632	SER
1	D	636	ILE
1	D	638	VAL
1	D	639	THR
1	D	645	ARG
1	D	647	SER
1	D	651	LEU
1	D	652	LEU
1	D	655	MET
1	D	661	LYS
1	D	672	VAL
1	D	675	GLN
1	D	680	ILE
1	D	681	GLU
1	D	685	LEU
1	D	690	SER
1	D	696	LEU
1	D	698	VAL
1	D	701	VAL
1	D	702	GLN
1	D	721	ARG
1	D	730	LEU
1	D	737	ILE
1	D	743	SER
1	D	745	MET
1	D	750	GLU

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Mol	Chain	Res	Type
1	D	755	ARG
1	D	760	ARG
1	D	761	GLN
1	D	765	LEU
1	D	766	SER
1	D	768	MET
1	D	770	ILE
1	D	772	ASP
1	D	773	LYS
1	D	774	LYS
1	D	777	LEU
1	D	778	THR
1	D	797	GLU
1	D	799	THR
1	D	804	ASN
1	D	819	GLU
1	D	822	LEU
1	D	823	LEU
1	D	824	GLN
1	D	826	THR
1	D	829	THR
1	D	830	LEU
1	D	836	ILE
1	D	845	GLN
1	D	850	PHE
1	D	853	ARG
1	D	854	LYS
1	D	858	ILE
1	D	867	THR
1	D	874	SER
1	D	875	ASP
1	D	876	THR
1	D	885	ASN
1	D	888	LEU
1	D	890	GLN
1	D	894	ARG
1	D	904	GLU
1	D	910	LEU
1	D	923	SER
1	D	925	MET
1	D	934	GLU
1	D	938	ARG

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Mol	Chain	Res	Type
1	D	950	GLN
1	D	952	ARG
1	D	956	GLN
1	D	959	ILE
1	D	961	ARG
1	D	968	MET
1	D	971	SER
1	D	986	ILE
1	D	991	MET
1	D	993	ILE
1	D	998	SER
1	D	1002	SER
1	D	1006	GLU
1	D	1017	GLN
1	D	1023	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (111) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	50	GLN
1	A	102	ASN
1	A	128	ASN
1	A	216	HIS
1	A	221	GLN
1	A	226	HIS
1	A	357	HIS
1	A	365	GLN
1	A	381	GLN
1	A	385	ASN
1	A	424	ASN
1	A	467	ASN
1	A	554	GLN
1	A	573	GLN
1	A	581	ASN
1	A	597	ASN
1	A	622	HIS
1	A	623	GLN
1	A	675	GLN
1	A	693	GLN
1	A	719	GLN
1	A	863	GLN

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Mol	Chain	Res	Type
1	A	878	HIS
1	A	887	GLN
1	A	949	HIS
1	A	965	GLN
1	A	990	HIS
1	A	1017	GLN
1	B	38	ASN
1	B	89	ASN
1	B	102	ASN
1	B	163	GLN
1	B	216	HIS
1	B	221	GLN
1	B	226	HIS
1	B	297	ASN
1	B	307	ASN
1	B	316	HIS
1	B	357	HIS
1	B	391	HIS
1	B	445	GLN
1	B	581	ASN
1	B	583	ASN
1	B	597	ASN
1	B	600	GLN
1	B	622	HIS
1	B	624	GLN
1	B	675	GLN
1	B	878	HIS
1	B	949	HIS
1	B	965	GLN
1	C	18	ASN
1	C	38	ASN
1	C	50	GLN
1	C	102	ASN
1	C	135	GLN
1	C	138	GLN
1	C	163	GLN
1	C	216	HIS
1	C	221	GLN
1	C	226	HIS
1	C	266	GLN
1	C	316	HIS
1	C	357	HIS

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Mol	Chain	Res	Type
1	C	424	ASN
1	C	460	ASN
1	C	467	ASN
1	C	554	GLN
1	C	563	GLN
1	C	583	ASN
1	C	597	ASN
1	C	604	ASN
1	C	622	HIS
1	C	704	ASN
1	C	817	GLN
1	C	863	GLN
1	C	950	GLN
1	C	965	GLN
1	C	990	HIS
1	C	1017	GLN
1	D	38	ASN
1	D	50	GLN
1	D	102	ASN
1	D	216	HIS
1	D	297	ASN
1	D	316	HIS
1	D	357	HIS
1	D	394	ASN
1	D	424	ASN
1	D	445	GLN
1	D	467	ASN
1	D	485	GLN
1	D	554	GLN
1	D	573	GLN
1	D	581	ASN
1	D	583	ASN
1	D	597	ASN
1	D	604	ASN
1	D	614	HIS
1	D	622	HIS
1	D	623	GLN
1	D	675	GLN
1	D	693	GLN
1	D	757	GLN
1	D	791	ASN
1	D	804	ASN

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Mol	Chain	Res	Type
1	D	845	GLN
1	D	890	GLN
1	D	949	HIS
1	D	965	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 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	1021/1021 (100%)	-0.90	1 (0%) 92 90	2, 25, 64, 100	26 (2%)
1	B	1021/1021 (100%)	-0.78	0 100 100	4, 30, 70, 100	26 (2%)
1	C	1021/1021 (100%)	-0.86	0 100 100	6, 27, 63, 100	26 (2%)
1	D	1021/1021 (100%)	-0.91	0 100 100	3, 25, 64, 100	26 (2%)
All	All	4084/4084 (100%)	-0.87	1 (0%) 100 100	2, 27, 66, 100	104 (2%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	733	ALA	2.3

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
2	MG	B	3002	1/1	0.95	0.06	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	D	3001	1/1	0.96	0.04	40,40,40,40	0
2	MG	A	3001	1/1	0.97	0.05	28,28,28,28	0
2	MG	C	3002	1/1	0.97	0.04	31,31,31,31	0
2	MG	B	3001	1/1	0.97	0.04	20,20,20,20	0
2	MG	A	3002	1/1	0.98	0.07	31,31,31,31	0
2	MG	C	3001	1/1	0.99	0.02	15,15,15,15	0
2	MG	D	3002	1/1	0.99	0.05	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.