Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:21 PM GMT

PDB ID	:	1F4H
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

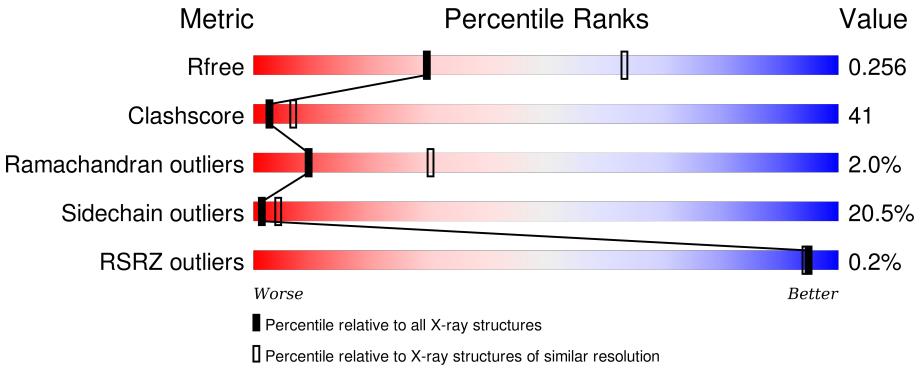
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	34% 45% 18% ·
1	B	1021	30% 48% 19% ·
1	C	1021	32% 47% 18% ·
1	D	1021	35% 43% 18% ·

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	A	3002	-	-	-	X
2	MG	D	3002	-	-	-	X

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 (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is water.

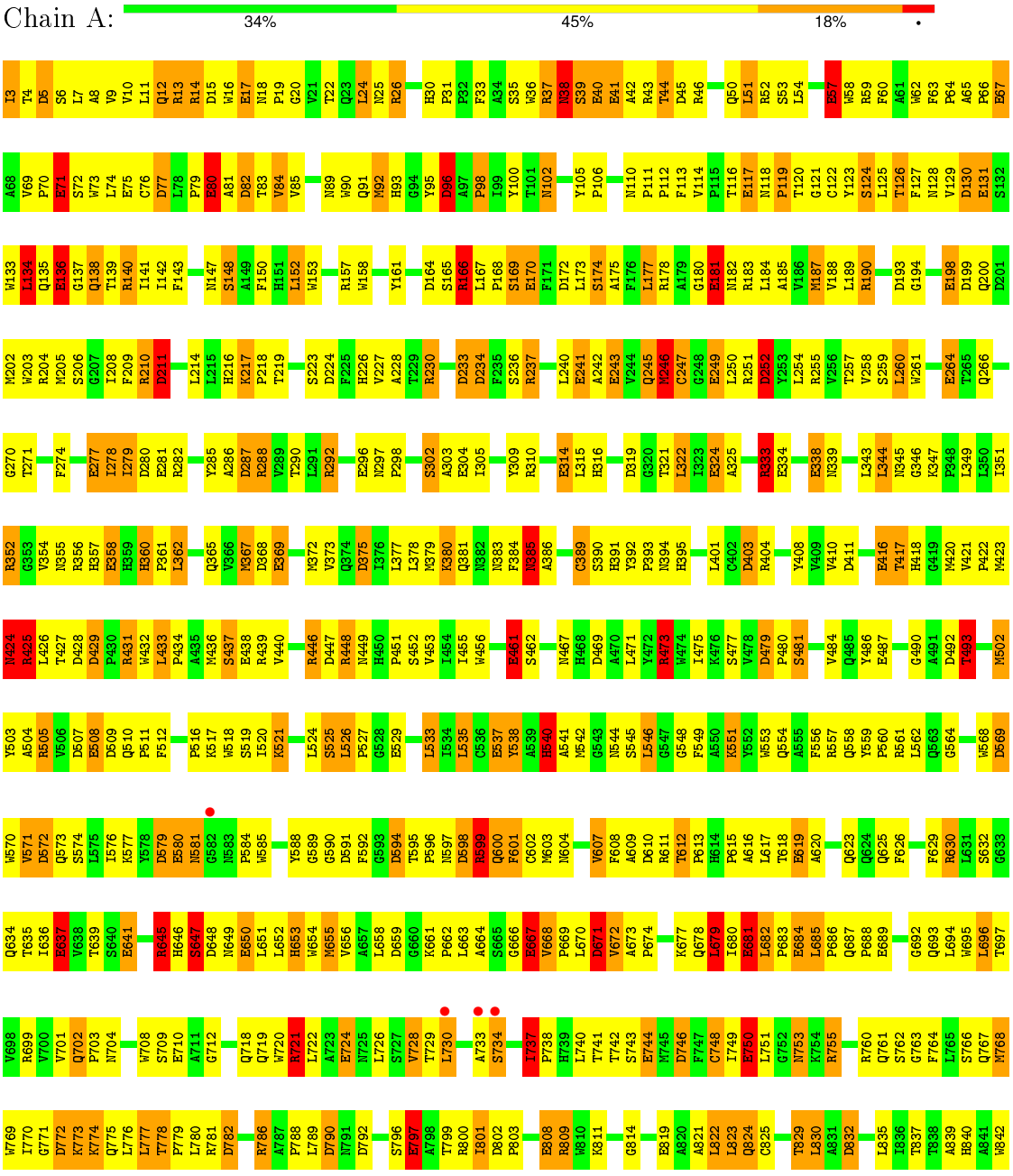
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	211	Total	O	0	0
			211	211		
3	B	202	Total	O	0	0
			202	202		
3	C	220	Total	O	0	0
			220	220		
3	D	212	Total	O	0	0
			212	212		

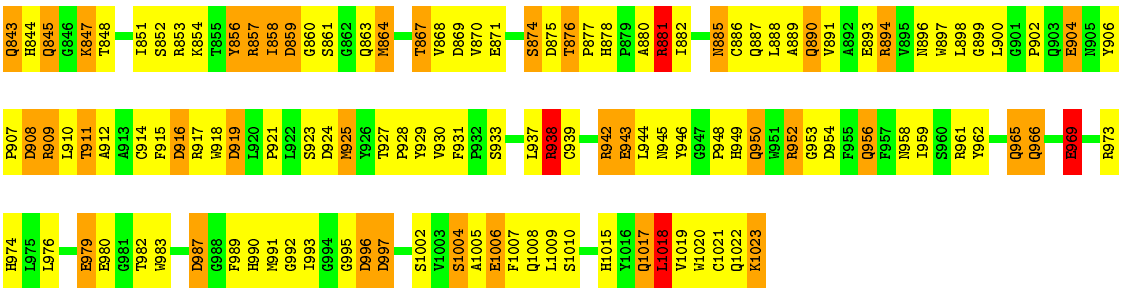
3 Residue-property plots (i)

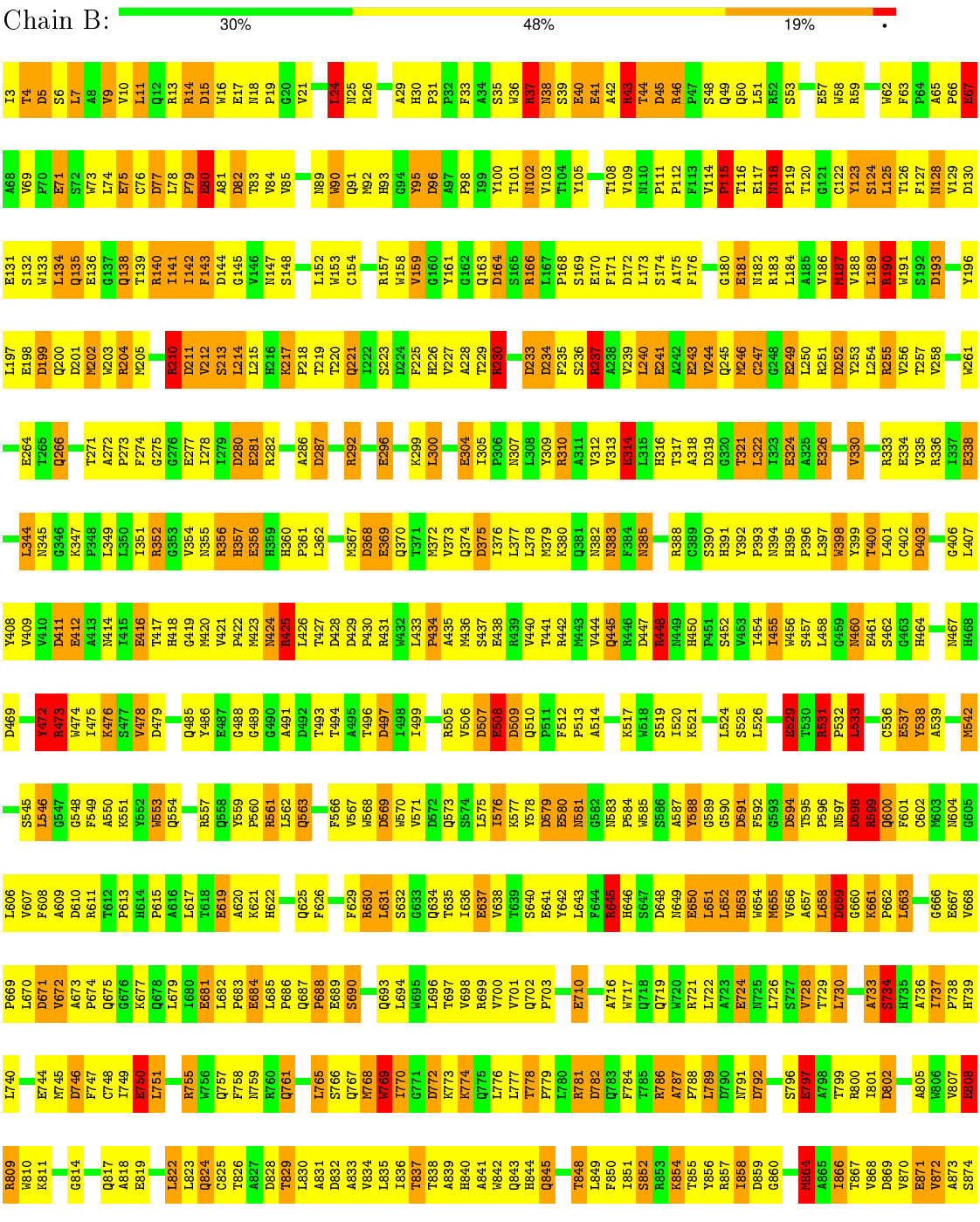
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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

Chain A:

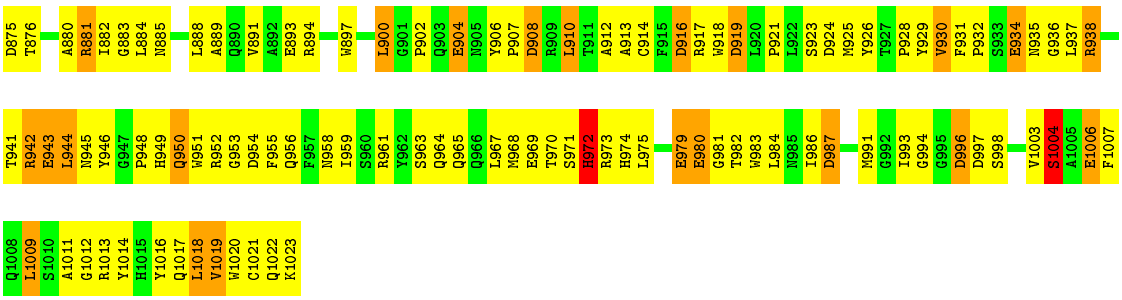






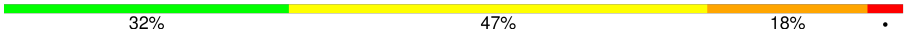
• Molecule 1: BETA-GALACTOSIDASE

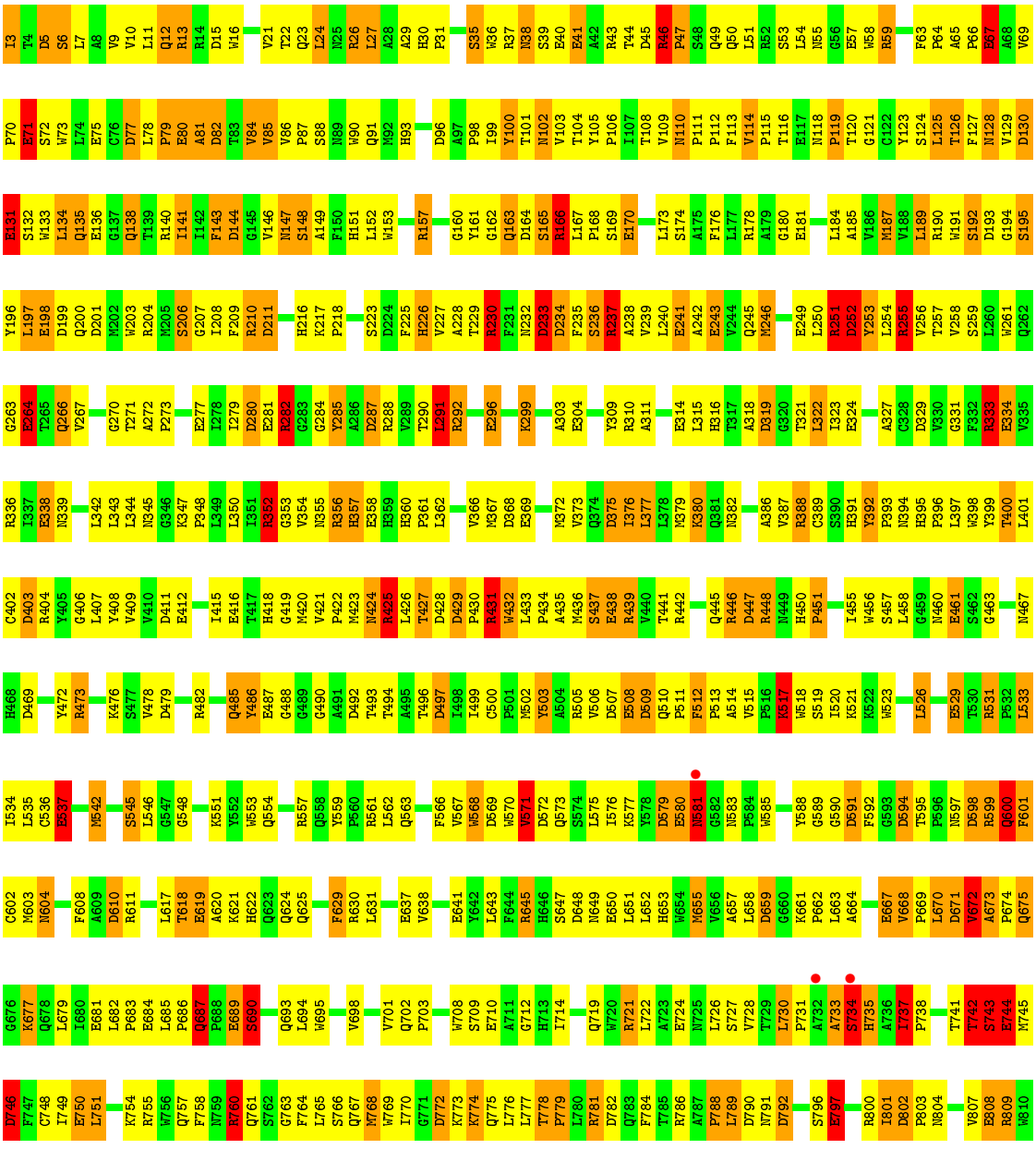
Chain B:

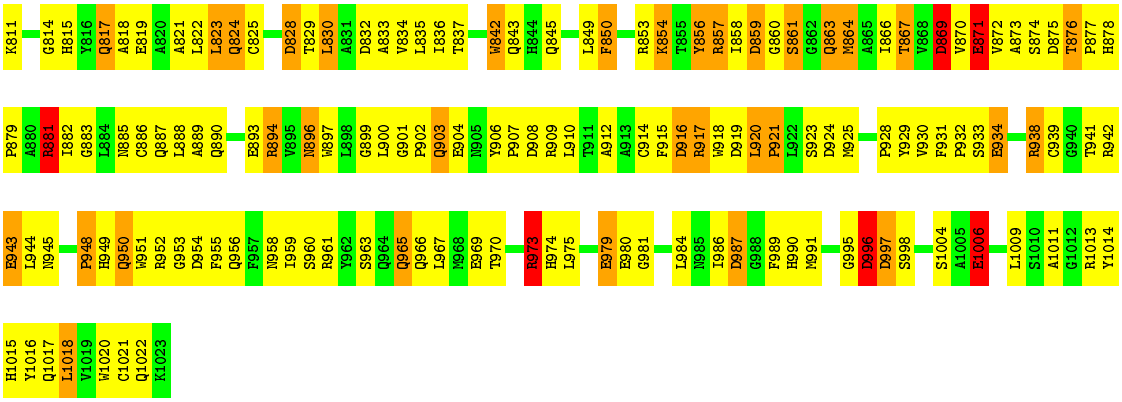


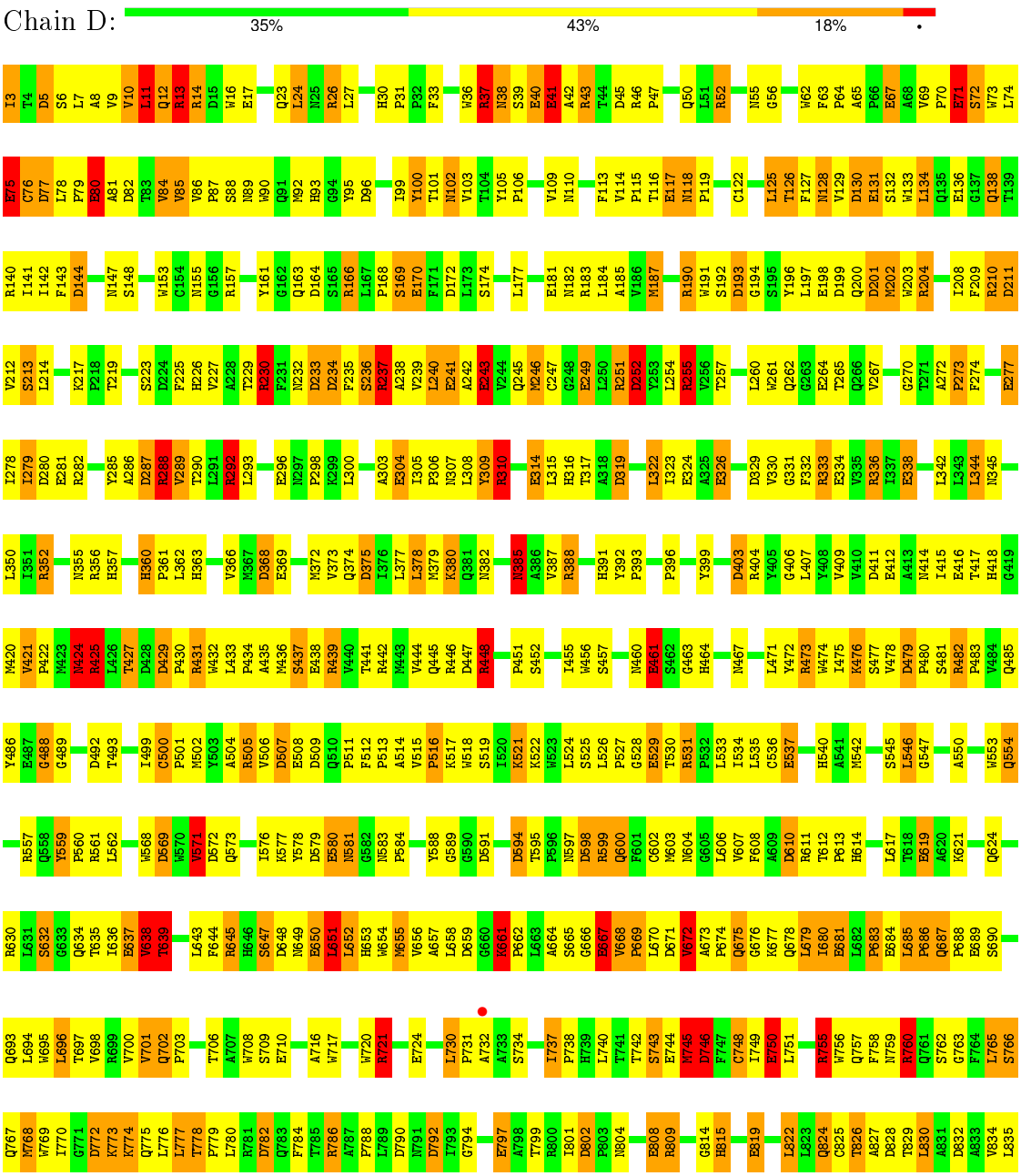
• Molecule 1: BETA-GALACTOSIDASE

Chain C:



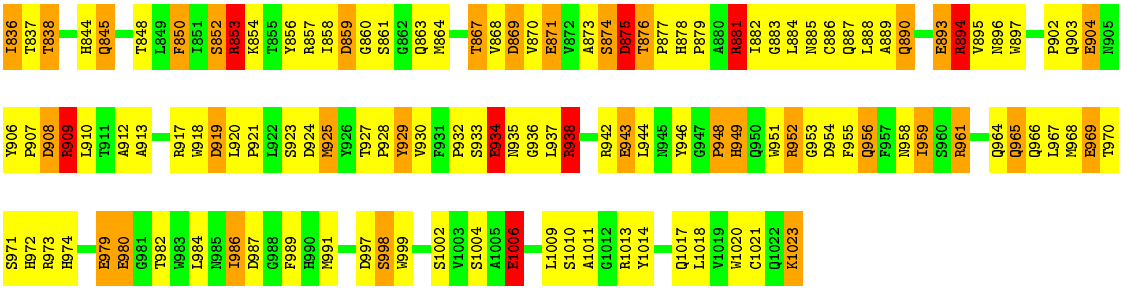






• Molecule 1: BETA-GALACTOSIDASE

Chain D:


I836 T837 T838 H844 Q845 T848 L849 F850 I851 S852 R853 K854 T855 Y856 R857 I858 D859 G860 S861 G862 Q863 M864 T867 V868 D869 V870 E871 V872 A873 S874 D875 T876 P877 H878 P879 A880 R881 I882 G883 L884 N885 C886 Q887 L888 A889 Q890 E893 R894 V895 N896 W897 P902 Q903 E904 N905
Y906 P907 D908 R909 L910 T911 A912 A913 R917 W918 D919 L920 P921 L922 S923 D924 M925 Y926 T927 P928 Y929 V930 F931 P932 S933 E934 N935 G936 L937 R938 R942 E943 L944 N945 Y946 G947 P948 H949 Q950 W951 R952 G953 D954 F955 Q956 F957 N958 I959 S960 R961 Q964 Q965 Q966 L967 M968 E969 T970
S971 H972 R973 H974 E979 E980 G981 T982 W983 L984 N985 I986 D987 G988 F989 H990 M991 D997 S998 W999 S1002 V1003 S1004 A1005 E1006 L1009 S1010 A1011 G1012 R1013 Y1014 Q1017 L1018 V1019 W1020 C1021 Q1022 K1023

4 Data and refinement statistics (i)

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 24.97 – 2.82	Depositor EDS
% Data completeness (in resolution range)	88.0 (25.00-2.80) 80.5 (24.97-2.82)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 2.80Å)	Xtriage
Refinement program	TNT V. 5-E	Depositor
R, R_{free}	0.137 , 0.279 0.125 , 0.256	Depositor DCC
R_{free} test set	1590 reflections (1.53%)	DCC
Wilson B-factor (Å^2)	40.7	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 133.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 105768 reflections	Xtriage
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

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	1.11	56/8515 (0.7%)	1.72	186/11615 (1.6%)
1	B	1.09	53/8515 (0.6%)	1.69	174/11615 (1.5%)
1	C	1.08	49/8515 (0.6%)	1.69	187/11615 (1.6%)
1	D	1.10	54/8515 (0.6%)	1.70	183/11615 (1.6%)
All	All	1.09	212/34060 (0.6%)	1.70	730/46460 (1.6%)

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	2	0
1	B	1	0
1	C	4	1
1	D	1	0
All	All	8	1

All (212) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	249	GLU	CD-OE2	8.77	1.35	1.25
1	B	241	GLU	CD-OE2	8.07	1.34	1.25
1	C	508	GLU	CD-OE2	8.02	1.34	1.25
1	D	181	GLU	CD-OE2	7.94	1.34	1.25
1	A	198	GLU	CD-OE2	7.86	1.34	1.25
1	A	358	GLU	CD-OE2	7.77	1.34	1.25
1	A	487	GLU	CD-OE2	7.74	1.34	1.25
1	D	75	GLU	CD-OE2	7.71	1.34	1.25
1	B	75	GLU	CD-OE2	7.61	1.34	1.25
1	C	243	GLU	CD-OE2	7.61	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	281	GLU	CD-OE2	7.55	1.33	1.25
1	D	797	GLU	CD-OE2	7.54	1.33	1.25
1	D	314	GLU	CD-OE2	7.51	1.33	1.25
1	C	296	GLU	CD-OE2	7.48	1.33	1.25
1	D	619	GLU	CD-OE2	7.48	1.33	1.25
1	D	40	GLU	CD-OE2	7.45	1.33	1.25
1	C	75	GLU	CD-OE2	7.38	1.33	1.25
1	C	710	GLU	CD-OE2	7.30	1.33	1.25
1	C	744	GLU	CD-OE2	7.30	1.33	1.25
1	B	181	GLU	CD-OE2	7.30	1.33	1.25
1	D	537	GLU	CD-OE2	7.28	1.33	1.25
1	B	508	GLU	CD-OE2	7.27	1.33	1.25
1	D	724	GLU	CD-OE2	7.26	1.33	1.25
1	A	241	GLU	CD-OE2	7.26	1.33	1.25
1	A	281	GLU	CD-OE2	7.19	1.33	1.25
1	D	170	GLU	CD-OE2	7.16	1.33	1.25
1	B	650	GLU	CD-OE2	7.16	1.33	1.25
1	B	40	GLU	CD-OE2	7.08	1.33	1.25
1	C	314	GLU	CD-OE2	7.08	1.33	1.25
1	A	750	GLU	CD-OE2	7.06	1.33	1.25
1	C	338	GLU	CD-OE2	7.04	1.33	1.25
1	B	264	GLU	CD-OE2	6.99	1.33	1.25
1	C	667	GLU	CD-OE2	6.98	1.33	1.25
1	B	67	GLU	CD-OE2	6.96	1.33	1.25
1	B	797	GLU	CD-OE2	6.95	1.33	1.25
1	B	136	GLU	CD-OE2	6.95	1.33	1.25
1	D	338	GLU	CD-OE2	6.95	1.33	1.25
1	B	416	GLU	CD-OE2	6.92	1.33	1.25
1	C	904	GLU	CD-OE2	6.83	1.33	1.25
1	A	681	GLU	CD-OE2	6.77	1.33	1.25
1	A	943	GLU	CD-OE2	6.76	1.33	1.25
1	C	637	GLU	CD-OE2	6.73	1.33	1.25
1	D	969	GLU	CD-OE2	6.71	1.33	1.25
1	A	979	GLU	CD-OE2	6.69	1.33	1.25
1	D	667	GLU	CD-OE2	6.69	1.33	1.25
1	A	75	GLU	CD-OE2	6.69	1.33	1.25
1	D	71	GLU	CD-OE2	6.69	1.33	1.25
1	B	744	GLU	CD-OE2	6.67	1.32	1.25
1	D	681	GLU	CD-OE2	6.64	1.32	1.25
1	B	57	GLU	CD-OE2	6.63	1.32	1.25
1	C	681	GLU	CD-OE2	6.62	1.32	1.25
1	D	1006	GLU	CD-OE2	6.60	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1006	GLU	CD-OE2	6.58	1.32	1.25
1	A	529	GLU	CD-OE2	6.58	1.32	1.25
1	D	710	GLU	CD-OE2	6.57	1.32	1.25
1	D	264	GLU	CD-OE2	6.57	1.32	1.25
1	B	369	GLU	CD-OE2	6.54	1.32	1.25
1	C	358	GLU	CD-OE2	6.52	1.32	1.25
1	D	744	GLU	CD-OE2	6.52	1.32	1.25
1	D	243	GLU	CD-OE2	6.52	1.32	1.25
1	A	871	GLU	CD-OE2	6.50	1.32	1.25
1	B	619	GLU	CD-OE2	6.50	1.32	1.25
1	C	641	GLU	CD-OE2	6.45	1.32	1.25
1	C	934	GLU	CD-OE2	6.45	1.32	1.25
1	C	281	GLU	CD-OE2	6.44	1.32	1.25
1	B	667	GLU	CD-OE2	6.43	1.32	1.25
1	B	537	GLU	CD-OE2	6.43	1.32	1.25
1	D	41	GLU	CD-OE2	6.43	1.32	1.25
1	A	80	GLU	CD-OE2	6.41	1.32	1.25
1	B	641	GLU	CD-OE2	6.39	1.32	1.25
1	B	871	GLU	CD-OE2	6.34	1.32	1.25
1	C	438	GLU	CD-OE2	6.33	1.32	1.25
1	A	969	GLU	CD-OE2	6.31	1.32	1.25
1	B	979	GLU	CD-OE2	6.29	1.32	1.25
1	A	508	GLU	CD-OE2	6.27	1.32	1.25
1	D	438	GLU	CD-OE2	6.26	1.32	1.25
1	D	750	GLU	CD-OE2	6.25	1.32	1.25
1	B	681	GLU	CD-OE2	6.23	1.32	1.25
1	A	438	GLU	CD-OE2	6.19	1.32	1.25
1	A	249	GLU	CD-OE2	6.19	1.32	1.25
1	B	80	GLU	CD-OE2	6.18	1.32	1.25
1	C	808	GLU	CD-OE2	6.16	1.32	1.25
1	A	264	GLU	CD-OE2	6.14	1.32	1.25
1	D	979	GLU	CD-OE2	6.13	1.32	1.25
1	B	710	GLU	CD-OE2	6.13	1.32	1.25
1	A	57	GLU	CD-OE2	6.12	1.32	1.25
1	A	724	GLU	CD-OE2	6.11	1.32	1.25
1	C	724	GLU	CD-OE2	6.10	1.32	1.25
1	A	744	GLU	CD-OE2	6.09	1.32	1.25
1	C	57	GLU	CD-OE2	6.08	1.32	1.25
1	B	969	GLU	CD-OE2	6.06	1.32	1.25
1	C	170	GLU	CD-OE2	6.06	1.32	1.25
1	D	241	GLU	CD-OE2	6.05	1.32	1.25
1	C	71	GLU	CD-OE2	6.03	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	198	GLU	CD-OE2	6.01	1.32	1.25
1	C	67	GLU	CD-OE2	5.99	1.32	1.25
1	B	412	GLU	CD-OE2	5.98	1.32	1.25
1	A	667	GLU	CD-OE2	5.97	1.32	1.25
1	B	637	GLU	CD-OE2	5.96	1.32	1.25
1	D	808	GLU	CD-OE2	5.95	1.32	1.25
1	C	181	GLU	CD-OE2	5.94	1.32	1.25
1	B	934	GLU	CD-OE2	5.93	1.32	1.25
1	A	641	GLU	CD-OE2	5.92	1.32	1.25
1	A	797	GLU	CD-OE2	5.92	1.32	1.25
1	B	943	GLU	CD-OE2	5.92	1.32	1.25
1	C	334	GLU	CD-OE2	5.92	1.32	1.25
1	A	710	GLU	CD-OE2	5.91	1.32	1.25
1	D	80	GLU	CD-OE2	5.91	1.32	1.25
1	C	979	GLU	CD-OE2	5.91	1.32	1.25
1	B	334	GLU	CD-OE2	5.90	1.32	1.25
1	B	750	GLU	CD-OE2	5.90	1.32	1.25
1	D	369	GLU	CD-OE2	5.89	1.32	1.25
1	C	487	GLU	CD-OE2	5.87	1.32	1.25
1	D	508	GLU	CD-OE2	5.84	1.32	1.25
1	C	264	GLU	CD-OE2	5.84	1.32	1.25
1	D	17	GLU	CD-OE2	5.84	1.32	1.25
1	C	241	GLU	CD-OE2	5.83	1.32	1.25
1	A	334	GLU	CD-OE2	5.82	1.32	1.25
1	A	40	GLU	CD-OE2	5.82	1.32	1.25
1	D	650	GLU	CD-OE2	5.81	1.32	1.25
1	A	369	GLU	CD-OE2	5.79	1.32	1.25
1	A	904	GLU	CD-OE2	5.79	1.32	1.25
1	B	529	GLU	CD-OE2	5.79	1.32	1.25
1	C	943	GLU	CD-OE2	5.79	1.32	1.25
1	D	296	GLU	CD-OE2	5.78	1.32	1.25
1	B	904	GLU	CD-OE2	5.76	1.31	1.25
1	B	724	GLU	CD-OE2	5.75	1.31	1.25
1	A	170	GLU	CD-OE2	5.72	1.31	1.25
1	C	537	GLU	CD-OE2	5.71	1.31	1.25
1	A	537	GLU	CD-OE2	5.71	1.31	1.25
1	C	41	GLU	CD-OE2	5.71	1.31	1.25
1	C	750	GLU	CD-OE2	5.70	1.31	1.25
1	B	338	GLU	CD-OE2	5.69	1.31	1.25
1	B	358	GLU	CD-OE2	5.68	1.31	1.25
1	C	797	GLU	CD-OE2	5.67	1.31	1.25
1	C	969	GLU	CD-OE2	5.67	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	369	GLU	CD-OE2	5.67	1.31	1.25
1	A	416	GLU	CD-OE2	5.67	1.31	1.25
1	B	41	GLU	CD-OE2	5.66	1.31	1.25
1	B	808	GLU	CD-OE2	5.61	1.31	1.25
1	B	314	GLU	CD-OE2	5.60	1.31	1.25
1	C	304	GLU	CD-OE2	5.60	1.31	1.25
1	A	181	GLU	CD-OE2	5.60	1.31	1.25
1	D	461	GLU	CD-OE2	5.59	1.31	1.25
1	B	243	GLU	CD-OE2	5.57	1.31	1.25
1	A	338	GLU	CD-OE2	5.57	1.31	1.25
1	A	71	GLU	CD-OE2	5.57	1.31	1.25
1	A	314	GLU	CD-OE2	5.56	1.31	1.25
1	D	136	GLU	CD-OE2	5.56	1.31	1.25
1	A	41	GLU	CD-OE2	5.55	1.31	1.25
1	A	296	GLU	CD-OE2	5.55	1.31	1.25
1	B	461	GLU	CD-OE2	5.54	1.31	1.25
1	C	198	GLU	CD-OE2	5.53	1.31	1.25
1	C	136	GLU	CD-OE2	5.53	1.31	1.25
1	A	650	GLU	CD-OE2	5.46	1.31	1.25
1	D	461	GLU	CD-OE1	-5.39	1.19	1.25
1	D	304	GLU	CD-OE1	-5.39	1.19	1.25
1	D	943	GLU	CD-OE2	5.39	1.31	1.25
1	A	117	GLU	CD-OE2	5.39	1.31	1.25
1	A	17	GLU	CD-OE2	5.38	1.31	1.25
1	D	131	GLU	CD-OE2	5.37	1.31	1.25
1	D	529	GLU	CD-OE2	5.37	1.31	1.25
1	D	819	GLU	CD-OE2	5.35	1.31	1.25
1	C	277	GLU	CD-OE2	5.35	1.31	1.25
1	A	637	GLU	CD-OE2	5.34	1.31	1.25
1	D	980	GLU	CD-OE2	5.33	1.31	1.25
1	D	689	GLU	CD-OE2	5.31	1.31	1.25
1	A	131	GLU	CD-OE2	5.30	1.31	1.25
1	B	438	GLU	CD-OE2	5.30	1.31	1.25
1	C	580	GLU	CD-OE2	5.29	1.31	1.25
1	A	980	GLU	CD-OE2	5.29	1.31	1.25
1	B	689	GLU	CD-OE2	5.29	1.31	1.25
1	D	117	GLU	CD-OE2	5.28	1.31	1.25
1	C	131	GLU	CD-OE2	5.27	1.31	1.25
1	C	684	GLU	CD-OE2	5.27	1.31	1.25
1	C	980	GLU	CD-OE2	5.27	1.31	1.25
1	D	893	GLU	CD-OE2	5.26	1.31	1.25
1	C	893	GLU	CD-OE2	5.26	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	819	GLU	CD-OE2	5.26	1.31	1.25
1	B	980	GLU	CD-OE2	5.26	1.31	1.25
1	C	689	GLU	CD-OE2	5.26	1.31	1.25
1	B	277	GLU	CD-OE2	5.25	1.31	1.25
1	D	684	GLU	CD-OE2	5.25	1.31	1.25
1	A	684	GLU	CD-OE2	5.25	1.31	1.25
1	D	580	GLU	CD-OE2	5.24	1.31	1.25
1	C	619	GLU	CD-OE2	5.23	1.31	1.25
1	B	131	GLU	CD-OE2	5.22	1.31	1.25
1	B	819	GLU	CD-OE2	5.22	1.31	1.25
1	B	893	GLU	CD-OE2	5.22	1.31	1.25
1	A	136	GLU	CD-OE2	5.21	1.31	1.25
1	B	326	GLU	CD-OE2	5.21	1.31	1.25
1	A	689	GLU	CD-OE2	5.21	1.31	1.25
1	A	893	GLU	CD-OE2	5.20	1.31	1.25
1	B	684	GLU	CD-OE2	5.20	1.31	1.25
1	C	819	GLU	CD-OE2	5.20	1.31	1.25
1	A	580	GLU	CD-OE2	5.19	1.31	1.25
1	B	304	GLU	CD-OE2	5.18	1.31	1.25
1	D	67	GLU	CD-OE2	5.18	1.31	1.25
1	D	277	GLU	CD-OE2	5.18	1.31	1.25
1	A	324	GLU	CD-OE2	5.17	1.31	1.25
1	B	580	GLU	CD-OE2	5.17	1.31	1.25
1	A	277	GLU	CD-OE2	5.17	1.31	1.25
1	D	934	GLU	CD-OE2	5.16	1.31	1.25
1	B	296	GLU	CD-OE2	5.15	1.31	1.25
1	C	871	GLU	CD-OE2	5.15	1.31	1.25
1	A	808	GLU	CD-OE2	5.14	1.31	1.25
1	A	243	GLU	CD-OE2	5.14	1.31	1.25
1	D	871	GLU	CD-OE2	5.11	1.31	1.25
1	D	281	GLU	CD-OE2	5.05	1.31	1.25
1	D	412	GLU	CD-OE2	5.04	1.31	1.25
1	D	637	GLU	CD-OE2	5.03	1.31	1.25
1	A	619	GLU	CD-OE2	5.02	1.31	1.25

All (730) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	251	ARG	NE-CZ-NH2	-13.90	113.35	120.30
1	D	210	ARG	NE-CZ-NH1	13.54	127.07	120.30
1	D	425	ARG	NE-CZ-NH1	13.14	126.87	120.30
1	D	668	VAL	C-N-CD	-13.14	91.69	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	356	ARG	NE-CZ-NH1	13.13	126.87	120.30
1	A	557	ARG	NE-CZ-NH2	-12.49	114.05	120.30
1	B	507	ASP	CB-CG-OD2	-12.47	107.08	118.30
1	B	908	ASP	CB-CG-OD2	-12.45	107.09	118.30
1	B	809[A]	ARG	NE-CZ-NH1	12.29	126.44	120.30
1	B	809[B]	ARG	NE-CZ-NH1	12.29	126.44	120.30
1	C	809[A]	ARG	NE-CZ-NH1	11.93	126.27	120.30
1	C	809[B]	ARG	NE-CZ-NH1	11.93	126.27	120.30
1	D	251	ARG	NE-CZ-NH1	11.82	126.21	120.30
1	A	424	ASN	CB-CA-C	-11.55	87.29	110.40
1	D	509	ASP	CB-CG-OD2	-11.52	107.93	118.30
1	B	356	ARG	NE-CZ-NH1	11.45	126.02	120.30
1	A	287	ASP	CB-CG-OD1	11.23	128.41	118.30
1	B	385	ASN	CB-CA-C	-10.82	88.75	110.40
1	D	938	ARG	N-CA-CB	10.69	129.84	110.60
1	D	792	ASP	CB-CG-OD2	-10.67	108.70	118.30
1	A	385	ASN	CB-CA-C	-10.62	89.17	110.40
1	B	356	ARG	NE-CZ-NH2	-10.61	115.00	120.30
1	A	199	ASP	CB-CG-OD2	-10.57	108.79	118.30
1	A	881	ARG	NE-CZ-NH1	10.55	125.58	120.30
1	A	938	ARG	NE-CZ-NH2	-10.30	115.15	120.30
1	C	659	ASP	CB-CG-OD1	10.21	127.48	118.30
1	C	659	ASP	CB-CG-OD2	-10.17	109.14	118.30
1	B	479	ASP	CB-CG-OD2	-10.14	109.18	118.30
1	A	310	ARG	NE-CZ-NH2	-10.12	115.24	120.30
1	B	237	ARG	NE-CZ-NH1	10.12	125.36	120.30
1	A	356	ARG	NE-CZ-NH2	-10.12	115.24	120.30
1	A	881	ARG	NE-CZ-NH2	-10.09	115.25	120.30
1	C	46	ARG	C-N-CD	-10.03	98.53	120.60
1	D	385	ASN	N-CA-CB	-10.01	92.58	110.60
1	D	507	ASP	CB-CG-OD2	-9.93	109.37	118.30
1	A	287	ASP	CB-CG-OD2	-9.84	109.45	118.30
1	C	210	ARG	NE-CZ-NH1	9.81	125.21	120.30
1	D	909	ARG	NE-CZ-NH1	9.73	125.17	120.30
1	B	507	ASP	CB-CG-OD1	9.73	127.06	118.30
1	B	46	ARG	NE-CZ-NH2	-9.65	115.47	120.30
1	C	144	ASP	CB-CG-OD2	-9.56	109.69	118.30
1	A	509	ASP	CB-CG-OD2	-9.53	109.72	118.30
1	A	952	ARG	NE-CZ-NH1	9.51	125.06	120.30
1	A	428	ASP	CB-CG-OD2	-9.49	109.76	118.30
1	B	473	ARG	NE-CZ-NH1	9.39	125.00	120.30
1	D	287	ASP	CB-CG-OD2	-9.39	109.85	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	425	ARG	NE-CZ-NH1	9.38	124.99	120.30
1	A	782	ASP	CB-CG-OD1	9.32	126.69	118.30
1	B	908	ASP	CB-CG-OD1	9.26	126.64	118.30
1	B	996	ASP	CB-CG-OD2	-9.25	109.98	118.30
1	A	645	ARG	NE-CZ-NH2	-9.09	115.76	120.30
1	C	429	ASP	CB-CG-OD1	9.06	126.45	118.30
1	A	809[A]	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	A	809[B]	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	D	792	ASP	CB-CG-OD1	9.00	126.40	118.30
1	A	446	ARG	NE-CZ-NH2	-8.97	115.81	120.30
1	C	26	ARG	NE-CZ-NH1	8.87	124.74	120.30
1	A	429	ASP	CB-CG-OD2	-8.80	110.38	118.30
1	A	659	ASP	CB-CG-OD2	-8.79	110.38	118.30
1	B	46	ARG	NE-CZ-NH1	8.79	124.70	120.30
1	D	531	ARG	NE-CZ-NH1	8.74	124.67	120.30
1	D	572	ASP	CB-CG-OD2	-8.73	110.44	118.30
1	D	492	ASP	CB-CG-OD2	-8.68	110.49	118.30
1	B	881	ARG	NE-CZ-NH1	8.67	124.64	120.30
1	A	319	ASP	CB-CG-OD2	-8.66	110.50	118.30
1	D	881	ARG	NE-CZ-NH2	-8.63	115.99	120.30
1	A	310	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	C	973	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	B	782	ASP	CB-CG-OD2	-8.58	110.58	118.30
1	D	875	ASP	CB-CG-OD2	-8.55	110.60	118.30
1	A	448	ARG	NE-CZ-NH1	8.55	124.58	120.30
1	C	431[A]	ARG	NE-CZ-NH1	8.51	124.56	120.30
1	C	431[B]	ARG	NE-CZ-NH1	8.51	124.56	120.30
1	D	648	ASP	CB-CG-OD2	-8.51	110.64	118.30
1	C	997	ASP	CB-CG-OD2	-8.49	110.66	118.30
1	C	447	ASP	CB-CG-OD2	-8.43	110.72	118.30
1	C	672	VAL	CB-CA-C	-8.38	95.47	111.40
1	C	599	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	A	792	ASP	CB-CG-OD2	-8.34	110.79	118.30
1	C	402	CYS	CA-CB-SG	-8.33	99.01	114.00
1	A	908	ASP	CB-CG-OD1	8.28	125.75	118.30
1	D	172	ASP	CB-CG-OD2	-8.28	110.85	118.30
1	A	591	ASP	CB-CG-OD2	-8.28	110.85	118.30
1	B	716	ALA	CB-CA-C	-8.27	97.70	110.10
1	D	579	ASP	CB-CG-OD1	8.24	125.72	118.30
1	A	671	ASP	CB-CG-OD1	8.22	125.70	118.30
1	A	13	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	D	26	ARG	NE-CZ-NH1	8.21	124.41	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	671	ASP	CB-CG-OD1	8.17	125.66	118.30
1	D	924	ASP	CB-CG-OD1	8.16	125.65	118.30
1	D	431[A]	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	D	431[B]	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	C	211	ASP	CB-CG-OD2	-8.12	110.99	118.30
1	B	164	ASP	N-CA-CB	8.10	125.19	110.60
1	A	233	ASP	CB-CG-OD2	-8.07	111.03	118.30
1	C	916	ASP	CB-CG-OD2	-8.06	111.04	118.30
1	B	442	ARG	NE-CZ-NH2	-8.05	116.27	120.30
1	B	469	ASP	CB-CG-OD2	-8.04	111.06	118.30
1	C	403	ASP	CB-CG-OD2	-8.04	111.06	118.30
1	C	917	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	A	448	ARG	NE-CZ-NH2	-8.01	116.30	120.30
1	C	403	ASP	CB-CG-OD1	8.00	125.50	118.30
1	A	572	ASP	CB-CG-OD1	7.98	125.48	118.30
1	A	252	ASP	CB-CG-OD1	7.97	125.47	118.30
1	C	26	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	B	591	ASP	CB-CG-OD2	-7.94	111.16	118.30
1	A	952	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	C	572	ASP	CB-CG-OD2	-7.92	111.17	118.30
1	A	13	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	C	668	VAL	C-N-CD	-7.92	103.18	120.60
1	D	210	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	D	859	ASP	CB-CG-OD1	7.91	125.42	118.30
1	A	569	ASP	CB-CG-OD2	-7.89	111.20	118.30
1	A	492	ASP	CB-CG-OD2	-7.88	111.21	118.30
1	A	479	ASP	CB-CG-OD2	-7.87	111.22	118.30
1	A	792	ASP	CB-CG-OD1	7.85	125.37	118.30
1	D	579	ASP	CB-CG-OD2	-7.83	111.25	118.30
1	B	212	VAL	CA-CB-CG1	-7.78	99.23	110.90
1	B	1004	SER	N-CA-CB	7.77	122.15	110.50
1	A	193	ASP	CB-CG-OD1	7.74	125.27	118.30
1	D	924	ASP	CB-CG-OD2	-7.74	111.34	118.30
1	C	429	ASP	CB-CG-OD2	-7.73	111.35	118.30
1	A	360	HIS	C-N-CD	-7.72	103.61	120.60
1	D	233	ASP	CB-CG-OD1	7.72	125.25	118.30
1	A	987	ASP	CB-CG-OD1	7.71	125.24	118.30
1	D	828	ASP	CB-CG-OD2	-7.71	111.36	118.30
1	A	252	ASP	CB-CG-OD2	-7.71	111.36	118.30
1	A	493	THR	CA-CB-CG2	-7.69	101.63	112.40
1	C	126	THR	CA-CB-CG2	-7.69	101.64	112.40
1	B	411	ASP	CB-CG-OD1	7.68	125.21	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	96	ASP	CB-CG-OD2	-7.68	111.39	118.30
1	A	671	ASP	CB-CA-C	7.67	125.75	110.40
1	C	144	ASP	CB-CG-OD1	7.67	125.20	118.30
1	D	610	ASP	CB-CG-OD2	-7.67	111.40	118.30
1	B	411	ASP	CB-CG-OD2	-7.66	111.41	118.30
1	C	237	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	D	388	ARG	NE-CZ-NH1	7.65	124.13	120.30
1	C	509	ASP	CB-CG-OD2	-7.62	111.44	118.30
1	A	721	ARG	NE-CZ-NH1	7.61	124.10	120.30
1	D	448	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	D	651	LEU	CB-CA-C	-7.59	95.78	110.20
1	A	659	ASP	CB-CG-OD1	7.58	125.13	118.30
1	A	790	ASP	CB-CG-OD2	-7.58	111.48	118.30
1	A	403	ASP	CB-CG-OD1	7.57	125.12	118.30
1	D	917	ARG	NE-CZ-NH2	-7.57	116.51	120.30
1	C	750	GLU	N-CA-CB	7.56	124.20	110.60
1	D	659	ASP	CB-CG-OD2	-7.56	111.50	118.30
1	D	509	ASP	CB-CG-OD1	7.55	125.10	118.30
1	A	857	ARG	NE-CZ-NH1	7.55	124.08	120.30
1	A	385	ASN	N-CA-CB	-7.55	97.01	110.60
1	B	671	ASP	CB-CG-OD2	-7.54	111.51	118.30
1	D	45	ASP	CB-CG-OD2	-7.54	111.51	118.30
1	C	802	ASP	CB-CG-OD1	7.53	125.08	118.30
1	C	15	ASP	CB-CG-OD2	-7.52	111.53	118.30
1	D	594	ASP	CB-CG-OD2	-7.49	111.56	118.30
1	D	45	ASP	CB-CG-OD1	7.48	125.03	118.30
1	D	881	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	C	591	ASP	CB-CG-OD1	7.46	125.02	118.30
1	B	954	ASP	CB-CG-OD2	-7.46	111.59	118.30
1	D	750	GLU	N-CA-CB	7.45	124.01	110.60
1	D	782	ASP	CB-CG-OD2	-7.45	111.60	118.30
1	C	486	TYR	CB-CG-CD1	-7.43	116.54	121.00
1	A	938	ARG	N-CA-CB	7.42	123.96	110.60
1	A	908	ASP	CB-CG-OD2	-7.41	111.63	118.30
1	A	375	ASP	CB-CG-OD2	-7.41	111.64	118.30
1	D	610	ASP	CB-CG-OD1	7.38	124.94	118.30
1	D	329	ASP	CB-CG-OD2	-7.37	111.67	118.30
1	B	287	ASP	CB-CG-OD2	-7.36	111.67	118.30
1	C	164	ASP	CB-CG-OD2	-7.36	111.68	118.30
1	D	336	ARG	NE-CZ-NH1	7.35	123.98	120.30
1	A	909	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	C	579	ASP	CB-CG-OD1	7.33	124.90	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	375	ASP	CB-CG-OD2	-7.33	111.70	118.30
1	A	924	ASP	CB-CG-OD2	-7.33	111.70	118.30
1	B	497	ASP	CB-CG-OD1	7.33	124.89	118.30
1	B	491	ALA	N-CA-CB	7.32	120.35	110.10
1	B	352	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	D	507	ASP	CB-CG-OD1	7.31	124.88	118.30
1	B	648	ASP	CB-CG-OD2	-7.31	111.72	118.30
1	C	591	ASP	CB-CG-OD2	-7.31	111.72	118.30
1	B	140	ARG	NE-CZ-NH2	-7.29	116.65	120.30
1	C	5	ASP	CB-CG-OD1	7.28	124.85	118.30
1	C	503	TYR	CB-CG-CD1	7.28	125.37	121.00
1	D	929	TYR	CB-CG-CD1	7.28	125.37	121.00
1	C	211	ASP	CB-CG-OD1	7.27	124.85	118.30
1	B	591	ASP	CB-CG-OD1	7.27	124.84	118.30
1	D	292	ARG	NE-CZ-NH2	-7.27	116.67	120.30
1	C	1006	GLU	CG-CD-OE2	-7.26	103.77	118.30
1	D	919	ASP	CB-CG-OD2	-7.25	111.78	118.30
1	C	233	ASP	CB-CG-OD1	7.24	124.81	118.30
1	A	403	ASP	CB-CG-OD2	-7.23	111.80	118.30
1	C	997	ASP	CB-CG-OD1	7.21	124.79	118.30
1	D	233	ASP	CB-CG-OD2	-7.20	111.82	118.30
1	C	329	ASP	CB-CG-OD2	-7.18	111.84	118.30
1	D	572	ASP	CB-CG-OD1	7.17	124.75	118.30
1	A	557	ARG	NE-CZ-NH1	7.17	123.88	120.30
1	B	15	ASP	CB-CG-OD2	-7.16	111.86	118.30
1	D	360	HIS	C-N-CD	-7.16	104.85	120.60
1	B	497	ASP	CB-CG-OD2	-7.16	111.86	118.30
1	A	82	ASP	CB-CG-OD2	-7.14	111.87	118.30
1	A	509	ASP	CB-CG-OD1	7.14	124.72	118.30
1	B	400	THR	CA-CB-CG2	-7.13	102.42	112.40
1	B	832	ASP	CB-CG-OD2	-7.12	111.89	118.30
1	C	291	LEU	CB-CA-C	7.12	123.72	110.20
1	A	553	TRP	CA-CB-CG	-7.11	100.19	113.70
1	B	199	ASP	CB-CG-OD1	7.11	124.70	118.30
1	A	479	ASP	CB-CG-OD1	7.11	124.70	118.30
1	A	594	ASP	CB-CG-OD1	7.08	124.68	118.30
1	B	598	ASP	CB-CG-OD1	7.08	124.68	118.30
1	D	96	ASP	CB-CG-OD2	-7.06	111.95	118.30
1	C	130	ASP	CB-CG-OD2	-7.05	111.95	118.30
1	D	571	VAL	CB-CA-C	-7.05	98.00	111.40
1	C	792	ASP	CB-CG-OD2	-7.05	111.96	118.30
1	A	292	ARG	NE-CZ-NH2	-7.05	116.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	721	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	A	679	LEU	CA-CB-CG	-7.03	99.12	115.30
1	B	919	ASP	CB-CG-OD2	-7.03	111.97	118.30
1	A	166	ARG	N-CA-CB	7.02	123.24	110.60
1	D	403	ASP	CB-CG-OD1	7.01	124.61	118.30
1	A	987	ASP	CB-CG-OD2	-7.00	112.00	118.30
1	D	746	ASP	CB-CG-OD2	-7.00	112.00	118.30
1	A	15	ASP	CB-CG-OD2	-7.00	112.00	118.30
1	A	630	ARG	NE-CZ-NH2	-6.99	116.80	120.30
1	A	233	ASP	CB-CG-OD1	6.98	124.58	118.30
1	C	282	ARG	NE-CZ-NH2	6.98	123.79	120.30
1	A	737	ILE	CB-CA-C	6.97	125.55	111.60
1	B	610	ASP	CB-CG-OD2	-6.97	112.02	118.30
1	D	594	ASP	CB-CG-OD1	6.97	124.57	118.30
1	C	46	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	C	973	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	D	482	ARG	C-N-CD	-6.96	105.30	120.60
1	C	333	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	C	924	ASP	CB-CG-OD2	-6.93	112.06	118.30
1	D	591	ASP	CB-CG-OD2	-6.93	112.06	118.30
1	C	82	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	B	479	ASP	CB-CG-OD1	6.92	124.53	118.30
1	D	671	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	B	166	ARG	NE-CZ-NH2	-6.91	116.84	120.30
1	D	77	ASP	CB-CG-OD1	6.91	124.52	118.30
1	A	746	ASP	CB-CG-OD2	-6.91	112.08	118.30
1	A	368	ASP	CB-CG-OD2	-6.90	112.09	118.30
1	D	745	MET	CB-CA-C	-6.90	96.59	110.40
1	A	572	ASP	CB-CG-OD2	-6.89	112.09	118.30
1	D	287	ASP	CB-CG-OD1	6.89	124.50	118.30
1	A	790	ASP	CB-CG-OD1	6.89	124.50	118.30
1	D	13	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	C	15	ASP	CB-CG-OD1	6.86	124.47	118.30
1	A	172	ASP	CB-CG-OD2	-6.86	112.13	118.30
1	D	424	ASN	CB-CA-C	-6.85	96.70	110.40
1	C	492	ASP	CB-CG-OD2	-6.84	112.14	118.30
1	D	280	ASP	CB-CG-OD2	-6.84	112.14	118.30
1	B	43	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	D	411	ASP	CB-CG-OD1	6.84	124.45	118.30
1	C	157	ARG	NE-CZ-NH1	6.83	123.71	120.30
1	C	568	TRP	CA-CB-CG	-6.82	100.73	113.70
1	A	938	ARG	NE-CZ-NH1	6.82	123.71	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	252	ASP	CB-CG-OD1	6.82	124.44	118.30
1	A	211	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	C	579	ASP	CB-CG-OD2	-6.79	112.19	118.30
1	D	853	ARG	NE-CZ-NH1	6.77	123.68	120.30
1	A	190	ARG	NE-CZ-NH1	6.75	123.68	120.30
1	A	911	THR	CA-CB-CG2	-6.75	102.95	112.40
1	D	875	ASP	CB-CG-OD1	6.71	124.34	118.30
1	D	607	VAL	CA-CB-CG1	-6.70	100.84	110.90
1	D	832	ASP	CB-CG-OD2	-6.70	112.27	118.30
1	D	782	ASP	CB-CG-OD1	6.68	124.31	118.30
1	C	251	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	D	802	ASP	CB-CG-OD2	-6.67	112.30	118.30
1	A	82	ASP	CB-CG-OD1	6.67	124.30	118.30
1	D	166	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	D	786	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	A	352	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	B	987	ASP	CB-CG-OD2	-6.65	112.31	118.30
1	A	919	ASP	CB-CG-OD2	-6.65	112.32	118.30
1	A	859	ASP	CB-CG-OD1	6.64	124.28	118.30
1	D	118	ASN	N-CA-CB	-6.63	98.67	110.60
1	B	375	ASP	CB-CG-OD2	-6.63	112.33	118.30
1	D	671	ASP	CB-CG-OD1	6.63	124.27	118.30
1	D	403	ASP	CB-CG-OD2	-6.61	112.35	118.30
1	A	859	ASP	CB-CG-OD2	-6.60	112.36	118.30
1	D	292	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	B	509	ASP	CB-CG-OD2	-6.57	112.39	118.30
1	A	187	MET	N-CA-CB	6.56	122.41	110.60
1	D	429	ASP	CB-CG-OD1	6.56	124.20	118.30
1	B	118	ASN	CB-CA-C	6.55	123.50	110.40
1	B	448	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	C	828	ASP	CB-CG-OD2	-6.55	112.41	118.30
1	D	431[A]	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	D	431[B]	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	A	942	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	C	368	ASP	CB-CG-OD2	-6.54	112.42	118.30
1	C	336	ARG	NE-CZ-NH1	6.53	123.57	120.30
1	B	402	CYS	CA-CB-SG	-6.53	102.25	114.00
1	D	5	ASP	CB-CG-OD2	-6.53	112.42	118.30
1	C	5	ASP	CB-CG-OD2	-6.53	112.43	118.30
1	C	110	ASN	N-CA-CB	6.52	122.34	110.60
1	A	594	ASP	CB-CG-OD2	-6.52	112.43	118.30
1	C	1006	GLU	CG-CD-OE1	6.52	131.34	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	857	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	A	249	GLU	CG-CD-OE2	-6.50	105.30	118.30
1	A	386	ALA	N-CA-CB	-6.50	101.00	110.10
1	C	760	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	A	386	ALA	CB-CA-C	-6.48	100.38	110.10
1	C	832	ASP	CB-CG-OD2	-6.46	112.48	118.30
1	C	439	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	D	265	THR	N-CA-CB	-6.46	98.02	110.30
1	C	916	ASP	CB-CG-OD1	6.46	124.11	118.30
1	D	557	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	C	252	ASP	CB-CG-OD2	-6.45	112.50	118.30
1	A	875	ASP	CB-CG-OD2	-6.44	112.50	118.30
1	B	77	ASP	CB-CG-OD1	6.44	124.09	118.30
1	D	226	HIS	CB-CA-C	-6.43	97.54	110.40
1	C	226	HIS	CB-CA-C	-6.42	97.55	110.40
1	C	233	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	B	37	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	D	43	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	C	432	TRP	CA-CB-CG	-6.39	101.56	113.70
1	A	38	ASN	N-CA-CB	6.38	122.09	110.60
1	B	802	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	C	404	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	D	929	TYR	CB-CG-CD2	-6.38	117.17	121.00
1	C	494	THR	CA-CB-CG2	-6.38	103.47	112.40
1	D	790	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	B	472	TYR	CB-CG-CD1	-6.38	117.17	121.00
1	B	142	ILE	CB-CA-C	-6.38	98.85	111.60
1	D	908	ASP	CB-CG-OD2	-6.37	112.57	118.30
1	C	908	ASP	CB-CG-OD2	-6.36	112.58	118.30
1	C	310	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	D	230	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	D	859	ASP	CB-CG-OD2	-6.34	112.59	118.30
1	B	183	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	C	869	ASP	CB-CG-OD2	-6.33	112.60	118.30
1	D	809[A]	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	D	809[B]	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	A	598	ASP	CB-CG-OD2	-6.33	112.60	118.30
1	B	287	ASP	CB-CG-OD1	6.33	124.00	118.30
1	B	252	ASP	CB-CG-OD1	6.32	123.99	118.30
1	B	247	CYS	CA-CB-SG	-6.32	102.62	114.00
1	A	175	ALA	CB-CA-C	-6.32	100.63	110.10
1	A	319	ASP	CB-CG-OD1	6.31	123.98	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	875	ASP	CB-CG-OD1	6.31	123.98	118.30
1	D	591	ASP	CB-CG-OD1	6.31	123.97	118.30
1	B	368	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	A	164	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	A	504	ALA	CB-CA-C	6.30	119.55	110.10
1	C	446	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	C	629	PHE	CB-CA-C	-6.28	97.83	110.40
1	D	760	ARG	N-CA-CB	6.28	121.90	110.60
1	C	737	ILE	N-CA-CB	6.28	125.23	110.80
1	D	5	ASP	CB-CG-OD1	6.28	123.95	118.30
1	C	287	ASP	CB-CG-OD2	-6.27	112.65	118.30
1	A	44	THR	CA-CB-CG2	-6.27	103.62	112.40
1	C	517	LYS	CB-CA-C	6.27	122.94	110.40
1	A	533	LEU	CB-CG-CD1	6.26	121.65	111.00
1	B	531	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	C	598	ASP	CB-CG-OD2	-6.25	112.67	118.30
1	B	234	ASP	CB-CG-OD2	-6.25	112.67	118.30
1	D	954	ASP	CB-CG-OD2	-6.25	112.68	118.30
1	C	980	GLU	N-CA-CB	6.25	121.84	110.60
1	C	600	GLN	N-CA-CB	6.24	121.82	110.60
1	A	130	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	D	869	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	B	750	GLU	N-CA-CB	6.21	121.78	110.60
1	C	857	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	D	368	ASP	CB-CG-OD2	-6.19	112.73	118.30
1	A	234	ASP	CB-CG-OD2	-6.19	112.73	118.30
1	A	446	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	D	13	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	A	77	ASP	CB-CG-OD2	-6.16	112.75	118.30
1	B	164	ASP	CB-CG-OD1	6.16	123.84	118.30
1	A	954	ASP	CB-CG-OD1	6.15	123.84	118.30
1	D	130	ASP	CB-CG-OD2	-6.15	112.77	118.30
1	D	863	GLN	N-CA-CB	-6.15	99.53	110.60
1	B	954	ASP	CB-CG-OD1	6.15	123.83	118.30
1	C	204	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	B	130	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	C	832	ASP	CB-CG-OD1	6.13	123.82	118.30
1	C	473	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	772	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	C	744	GLU	CB-CA-C	6.12	122.64	110.40
1	D	144	ASP	CB-CG-OD2	-6.12	112.80	118.30
1	D	492	ASP	CB-CG-OD1	6.11	123.80	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	187	MET	N-CA-CB	6.11	121.59	110.60
1	B	786	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	D	997	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	B	553	TRP	CA-CB-CG	-6.09	102.13	113.70
1	B	746	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	D	310	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	D	755	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	A	193	ASP	CB-CG-OD2	-6.07	112.83	118.30
1	C	431[A]	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	C	431[B]	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	C	673	ALA	CB-CA-C	6.07	119.21	110.10
1	B	249	GLU	CA-C-N	-6.07	103.84	117.20
1	D	288	ARG	NE-CZ-NH1	-6.07	117.27	120.30
1	C	512	PHE	C-N-CD	-6.07	107.25	120.60
1	B	561	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	C	571	VAL	CB-CA-C	-6.06	99.88	111.40
1	C	486	TYR	CB-CG-CD2	6.06	124.64	121.00
1	C	147	ASN	N-CA-CB	-6.05	99.70	110.60
1	A	389	CYS	CA-CB-SG	-6.05	103.11	114.00
1	D	550	ALA	N-CA-CB	6.05	118.57	110.10
1	A	954	ASP	CB-CG-OD2	-6.04	112.86	118.30
1	A	832	ASP	CB-CG-OD2	-6.04	112.87	118.30
1	B	140	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	B	579	ASP	CB-CG-OD2	-6.03	112.87	118.30
1	C	518	TRP	CB-CA-C	-6.03	98.34	110.40
1	D	838	THR	CA-CB-CG2	-6.03	103.96	112.40
1	D	917	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	A	5	ASP	CB-CG-OD2	-6.02	112.89	118.30
1	C	204	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	B	237	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	A	469	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	B	599	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	C	859	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	A	249	GLU	OE1-CD-OE2	6.00	130.50	123.30
1	C	671	ASP	CB-CG-OD1	6.00	123.70	118.30
1	A	473	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	B	832	ASP	CB-CG-OD1	6.00	123.69	118.30
1	A	687	GLN	CB-CA-C	5.99	122.39	110.40
1	C	572	ASP	CB-CG-OD1	5.99	123.69	118.30
1	B	772	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	B	5	ASP	CB-CG-OD1	5.99	123.69	118.30
1	A	591	ASP	CB-CG-OD1	5.99	123.69	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	996	ASP	CB-CG-OD2	-5.97	112.92	118.30
1	D	439	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	B	859	ASP	CB-CG-OD2	-5.97	112.93	118.30
1	D	772	ASP	CB-CG-OD2	-5.97	112.93	118.30
1	A	505	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	C	428	ASP	CB-CG-OD2	-5.96	112.93	118.30
1	A	226	HIS	CB-CA-C	-5.96	98.48	110.40
1	A	786	ARG	NE-CZ-NH2	-5.95	117.32	120.30
1	C	404	ARG	NE-CZ-NH2	-5.95	117.32	120.30
1	C	199	ASP	CB-CG-OD2	-5.95	112.94	118.30
1	D	639	THR	CA-CB-CG2	-5.95	104.07	112.40
1	D	252	ASP	CB-CG-OD2	-5.95	112.95	118.30
1	D	598	ASP	CB-CG-OD1	5.95	123.65	118.30
1	C	772	ASP	CB-CG-OD2	-5.94	112.95	118.30
1	B	538	TYR	CB-CG-CD1	-5.94	117.43	121.00
1	B	672	VAL	CB-CA-C	-5.94	100.11	111.40
1	D	249	GLU	CA-C-N	-5.93	104.14	117.20
1	B	859	ASP	CB-CG-OD1	5.93	123.64	118.30
1	D	237	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	C	996	ASP	CB-CG-OD1	5.93	123.63	118.30
1	C	802	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	C	881	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	D	429	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	C	509	ASP	CB-CG-OD1	5.91	123.62	118.30
1	D	96	ASP	CB-CG-OD1	5.90	123.61	118.30
1	A	96	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	B	24	LEU	CB-CG-CD1	5.90	121.03	111.00
1	B	782	ASP	CB-CG-OD1	5.90	123.61	118.30
1	D	569	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	C	166	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	C	96	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	C	746	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	C	392	TYR	CB-CG-CD2	-5.88	117.47	121.00
1	A	325	ALA	N-CA-CB	5.88	118.33	110.10
1	D	679	LEU	CA-CB-CG	-5.87	101.81	115.30
1	C	291	LEU	N-CA-CB	5.87	122.13	110.40
1	A	246	MET	CG-SD-CE	-5.86	90.82	100.20
1	B	455	ILE	CB-CA-C	-5.85	99.89	111.60
1	D	553	TRP	CA-CB-CG	-5.85	102.58	113.70
1	B	230	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	A	166	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	C	164	ASP	CB-CG-OD1	5.85	123.56	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	319	ASP	CB-CG-OD2	-5.85	113.04	118.30
1	D	404	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	368	ASP	CB-CG-OD1	5.84	123.56	118.30
1	B	996	ASP	CB-CG-OD1	5.84	123.56	118.30
1	C	497	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	A	190	ARG	N-CA-CB	5.83	121.09	110.60
1	A	996	ASP	CB-CG-OD1	5.82	123.54	118.30
1	C	319	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	D	952	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	C	389	CYS	CA-CB-SG	-5.81	103.54	114.00
1	D	648	ASP	CB-CG-OD1	5.81	123.53	118.30
1	D	638	VAL	CB-CA-C	-5.81	100.37	111.40
1	C	285	TYR	CB-CG-CD2	5.80	124.48	121.00
1	B	509	ASP	CB-CG-OD1	5.80	123.52	118.30
1	C	817	GLN	N-CA-CB	5.79	121.01	110.60
1	B	598	ASP	N-CA-CB	5.78	121.01	110.60
1	D	164	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	C	13	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	B	924	ASP	CB-CG-OD2	-5.76	113.12	118.30
1	B	448	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	A	164	ASP	CB-CG-OD1	5.75	123.48	118.30
1	A	429	ASP	CB-CG-OD1	5.75	123.48	118.30
1	B	210	ARG	N-CA-CB	5.75	120.96	110.60
1	C	469	ASP	CB-CG-OD1	5.75	123.47	118.30
1	B	924	ASP	CB-CG-OD1	5.75	123.47	118.30
1	A	610	ASP	CB-CG-OD1	5.74	123.47	118.30
1	B	857	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	D	506	VAL	CA-CB-CG1	-5.74	102.29	110.90
1	B	428	ASP	CB-CG-OD2	-5.74	113.14	118.30
1	D	427	THR	CA-CB-CG2	-5.73	104.38	112.40
1	D	598	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	B	659	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	D	363	HIS	CA-CB-CG	-5.72	103.87	113.60
1	D	954	ASP	CB-CG-OD1	5.72	123.45	118.30
1	D	1006	GLU	CB-CA-C	-5.71	98.99	110.40
1	B	792	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	D	326	GLU	N-CA-CB	5.70	120.86	110.60
1	C	594	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	B	230	ARG	CB-CA-C	-5.69	99.02	110.40
1	A	916	ASP	CB-CG-OD1	5.69	123.42	118.30
1	B	403	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	C	451	PRO	N-CA-CB	5.68	110.12	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	206	SER	N-CA-CB	5.68	119.02	110.50
1	C	388	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	C	876	THR	CA-CB-CG2	5.66	120.33	112.40
1	D	255	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	B	45	ASP	CB-CG-OD1	5.65	123.39	118.30
1	A	997	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	A	26	ARG	CD-NE-CZ	-5.63	115.72	123.60
1	B	234	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	292	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	D	828	ASP	CB-CG-OD1	5.61	123.35	118.30
1	C	734	SER	C-N-CA	-5.60	107.70	121.70
1	B	648	ASP	CB-CG-OD1	5.59	123.33	118.30
1	B	538	TYR	CB-CG-CD2	5.59	124.36	121.00
1	A	772	ASP	CB-CG-OD1	5.58	123.32	118.30
1	B	45	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	D	790	ASP	CB-CG-OD1	5.58	123.32	118.30
1	D	439	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	B	344	LEU	N-CA-CB	5.58	121.55	110.40
1	A	782	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	A	424	ASN	N-CA-CB	-5.57	100.58	110.60
1	A	579	ASP	CB-CG-OD1	5.57	123.31	118.30
1	B	781	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	B	233	ASP	N-CA-CB	5.56	120.61	110.60
1	C	96	ASP	CB-CG-OD1	5.56	123.31	118.30
1	B	193	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	B	5	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	C	485	GLN	N-CA-CB	5.56	120.60	110.60
1	B	249	GLU	O-C-N	5.55	131.59	122.70
1	D	661	LYS	N-CA-CB	5.55	120.60	110.60
1	A	916	ASP	CB-CG-OD2	-5.55	113.31	118.30
1	C	598	ASP	CB-CG-OD1	5.55	123.29	118.30
1	C	875	ASP	CB-CG-OD2	-5.55	113.31	118.30
1	D	421	VAL	CB-CA-C	-5.55	100.86	111.40
1	B	144	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	B	772	ASP	CB-CG-OD1	5.54	123.29	118.30
1	B	249	GLU	N-CA-CB	5.54	120.58	110.60
1	D	952	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	1018	LEU	CB-CA-C	-5.53	99.69	110.20
1	B	130	ASP	CB-CG-OD1	5.53	123.27	118.30
1	B	204	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	C	329	ASP	CB-CG-OD1	5.53	123.27	118.30
1	D	479	ASP	C-N-CD	-5.53	108.44	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1006	GLU	N-CA-CB	5.52	120.54	110.60
1	B	442	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	B	828	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	D	772	ASP	CB-CG-OD1	5.52	123.27	118.30
1	A	431[A]	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	431[B]	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	B	769	TRP	CB-CA-C	-5.51	99.39	110.40
1	D	77	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	A	979	GLU	CB-CA-C	5.50	121.41	110.40
1	C	411	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	A	832	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	423	MET	C-N-CA	5.50	135.44	121.70
1	B	245	GLN	N-CA-CB	5.49	120.48	110.60
1	A	961	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	B	82	ASP	CB-CG-OD1	5.48	123.23	118.30
1	C	100	TYR	CB-CG-CD2	-5.47	117.72	121.00
1	C	954	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	A	560	PRO	CA-N-CD	-5.47	103.85	111.50
1	B	997	ASP	CB-CG-OD1	5.47	123.22	118.30
1	A	439	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	980	GLU	N-CA-CB	5.46	120.43	110.60
1	A	919	ASP	CB-CG-OD1	5.46	123.21	118.30
1	C	409	VAL	CA-CB-CG1	5.46	119.08	110.90
1	C	772	ASP	CB-CG-OD1	5.45	123.20	118.30
1	C	251	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	D	126	THR	CA-CB-CG2	-5.44	104.78	112.40
1	B	645	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	D	319	ASP	CB-CG-OD1	5.44	123.19	118.30
1	B	533	LEU	CB-CA-C	5.44	120.53	110.20
1	B	280	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	A	802	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	D	748	CYS	N-CA-CB	5.42	120.35	110.60
1	A	612	THR	CA-CB-CG2	-5.42	104.82	112.40
1	C	581	ASN	N-CA-CB	5.41	120.34	110.60
1	B	653[A]	HIS	CA-CB-CG	-5.41	104.41	113.60
1	B	653[B]	HIS	CA-CB-CG	-5.41	104.41	113.60
1	B	252	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	C	375	ASP	CB-CG-OD1	5.40	123.16	118.30
1	B	115	PRO	CA-N-CD	-5.40	103.94	111.50
1	B	478	VAL	CA-CB-CG1	-5.38	102.83	110.90
1	A	417	THR	CA-CB-CG2	-5.38	104.87	112.40
1	A	702	GLN	CA-CB-CG	-5.37	101.58	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	630	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	A	211	ASP	CB-CG-OD1	5.37	123.13	118.30
1	C	954	ASP	CB-CG-OD1	5.37	123.13	118.30
1	B	746	ASP	CB-CG-OD1	5.36	123.12	118.30
1	B	569	ASP	CB-CG-OD1	5.35	123.11	118.30
1	B	37	ARG	CB-CA-C	5.35	121.09	110.40
1	D	204	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	B	946	TYR	CB-CG-CD2	-5.34	117.80	121.00
1	A	686	PRO	C-N-CA	-5.33	108.36	121.70
1	B	594	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	A	671	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	C	850	PHE	CB-CA-C	-5.33	99.75	110.40
1	D	37	ARG	CB-CA-C	5.33	121.05	110.40
1	D	411	ASP	CB-CG-OD2	-5.33	113.51	118.30
1	B	864	MET	N-CA-CB	5.33	120.19	110.60
1	D	949	HIS	CA-CB-CG	-5.33	104.55	113.60
1	C	553	TRP	CA-CB-CG	-5.32	103.58	113.70
1	D	375	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	C	987	ASP	CB-CG-OD1	5.32	123.09	118.30
1	A	829	THR	N-CA-CB	5.32	120.41	110.30
1	C	537	GLU	N-CA-CB	5.32	120.18	110.60
1	C	409	VAL	CG1-CB-CG2	-5.32	102.39	110.90
1	C	287	ASP	CB-CG-OD1	5.32	123.08	118.30
1	C	853	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	B	233	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	671	ASP	N-CA-CB	5.31	120.15	110.60
1	B	787	ALA	C-N-CD	-5.31	108.92	120.60
1	C	356	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	333	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	C	352	ARG	N-CA-C	-5.30	96.69	111.00
1	B	916	ASP	CB-CG-OD2	-5.29	113.53	118.30
1	D	659	ASP	CB-CG-OD1	5.29	123.06	118.30
1	D	894	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	D	172	ASP	CB-CG-OD1	5.29	123.06	118.30
1	C	407	LEU	CB-CG-CD2	-5.29	102.02	111.00
1	D	965	GLN	N-CA-CB	5.28	120.11	110.60
1	A	746	ASP	CB-CG-OD1	5.28	123.05	118.30
1	B	44	THR	CA-CB-CG2	-5.28	105.01	112.40
1	A	505	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	B	509	ASP	N-CA-CB	5.27	120.09	110.60
1	B	561	ARG	CD-NE-CZ	5.27	130.98	123.60
1	A	1004	SER	N-CA-CB	5.27	118.41	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	319	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	A	924	ASP	CB-CG-OD1	5.27	123.04	118.30
1	B	199	ASP	CB-CG-OD2	-5.26	113.56	118.30
1	C	210	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	134	LEU	N-CA-CB	5.26	120.92	110.40
1	C	392	TYR	CB-CG-CD1	5.26	124.16	121.00
1	D	190	ARG	N-CA-CB	5.25	120.04	110.60
1	D	832	ASP	CB-CG-OD1	5.24	123.02	118.30
1	A	687	GLN	N-CA-CB	5.24	120.03	110.60
1	D	100	TYR	CA-CB-CG	-5.23	103.46	113.40
1	B	37	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	D	531	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	A	15	ASP	CB-CG-OD1	5.22	123.00	118.30
1	A	404	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	C	903[A]	GLN	N-CA-CB	5.22	120.00	110.60
1	C	903[B]	GLN	N-CA-CB	5.22	120.00	110.60
1	B	190	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	C	170	GLU	N-CA-CB	5.22	120.00	110.60
1	D	227	VAL	CA-CB-CG1	-5.22	103.07	110.90
1	C	610	ASP	CB-CG-OD1	5.22	123.00	118.30
1	C	687	GLN	N-CA-CB	5.21	119.99	110.60
1	D	193	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	258	VAL	O-C-N	5.21	131.04	122.70
1	B	336	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	D	853	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	B	881	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	A	126	THR	CA-CB-CG2	-5.20	105.12	112.40
1	A	96	ASP	CB-CG-OD1	5.20	122.97	118.30
1	C	492	ASP	CB-CG-OD1	5.19	122.97	118.30
1	D	396	PRO	N-CA-CB	5.19	109.53	103.30
1	B	747	PHE	N-CA-C	-5.18	97.01	111.00
1	B	972	HIS	N-CA-CB	5.18	119.93	110.60
1	B	1019	VAL	CA-CB-CG1	-5.18	103.13	110.90
1	B	980	GLU	N-CA-CB	5.18	119.92	110.60
1	C	193	ASP	CB-CG-OD2	-5.17	113.64	118.30
1	C	255	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	C	280	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	B	300	LEU	CA-C-N	-5.17	105.83	117.20
1	B	659	ASP	CB-CG-OD1	5.17	122.95	118.30
1	D	425	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	B	610	ASP	CB-CG-OD1	5.17	122.95	118.30
1	B	96	ASP	CB-CG-OD1	5.16	122.95	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	77	ASP	CB-CG-OD2	-5.15	113.66	118.30
1	C	735	HIS	CB-CA-C	5.15	120.70	110.40
1	D	201	ASP	CB-CG-OD1	5.15	122.93	118.30
1	D	721	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	C	610	ASP	CB-CG-OD2	-5.15	113.67	118.30
1	D	210	ARG	CD-NE-CZ	5.14	130.80	123.60
1	C	130	ASP	CB-CG-OD1	5.14	122.93	118.30
1	A	639	THR	CA-CB-CG2	-5.14	105.21	112.40
1	D	234	ASP	CB-CG-OD2	-5.13	113.68	118.30
1	C	128	ASN	CA-CB-CG	-5.12	102.14	113.40
1	B	494	THR	CA-CB-CG2	-5.12	105.24	112.40
1	C	59	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	C	507	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	A	486	TYR	CB-CG-CD1	-5.11	117.93	121.00
1	C	909	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	A	356	ARG	CD-NE-CZ	5.11	130.75	123.60
1	D	756	TRP	CB-CA-C	-5.11	100.18	110.40
1	D	1018	LEU	CB-CA-C	-5.11	100.49	110.20
1	B	172	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	B	368	ASP	CB-CG-OD1	5.11	122.90	118.30
1	D	908	ASP	CB-CG-OD1	5.11	122.90	118.30
1	D	500	CYS	CA-CB-SG	-5.10	104.82	114.00
1	C	924	ASP	CB-CG-OD1	5.10	122.89	118.30
1	B	916	ASP	CB-CG-OD1	5.10	122.89	118.30
1	C	234	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	A	748	CYS	N-CA-CB	5.09	119.76	110.60
1	A	98	PRO	N-CA-C	-5.08	98.88	112.10
1	C	435	ALA	CB-CA-C	-5.08	102.48	110.10
1	D	223	SER	CB-CA-C	5.07	119.73	110.10
1	B	829	THR	CA-CB-CG2	-5.07	105.31	112.40
1	B	857	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	A	569	ASP	CB-CG-OD1	5.06	122.85	118.30
1	B	321	THR	CA-CB-CG2	-5.06	105.32	112.40
1	B	164	ASP	CB-CG-OD2	-5.05	113.75	118.30
1	B	997	ASP	CB-CG-OD2	-5.05	113.76	118.30
1	D	672	VAL	CB-CA-C	-5.05	101.81	111.40
1	A	598	ASP	CB-CG-OD1	5.04	122.84	118.30
1	C	132	SER	N-CA-CB	5.04	118.06	110.50
1	C	400	THR	CA-CB-CG2	-5.04	105.35	112.40
1	A	428	ASP	CB-CG-OD1	5.04	122.83	118.30
1	B	425	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	D	385	ASN	CB-CA-C	-5.01	100.37	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	826	THR	CA-CB-CG2	-5.01	105.39	112.40
1	C	648	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	D	554	GLN	CB-CA-C	5.01	120.42	110.40
1	A	755	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	C	230	ARG	NE-CZ-NH1	5.01	122.80	120.30
1	B	237	ARG	CD-NE-CZ	5.00	130.60	123.60
1	B	314	GLU	N-CA-CB	5.00	119.61	110.60
1	C	901	GLY	N-CA-C	-5.00	100.59	113.10
1	C	908	ASP	CB-CG-OD1	5.00	122.80	118.30
1	D	894	ARG	NE-CZ-NH2	-5.00	117.80	120.30
1	A	5	ASP	CB-CG-OD1	5.00	122.80	118.30
1	C	842	TRP	N-CA-CB	5.00	119.60	110.60

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	166	ARG	CA
1	A	187	MET	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	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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8238	0	7824	643	0
1	B	8238	0	7824	695	0
1	C	8238	0	7824	667	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	8238	0	7823	632	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	2582	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 41.

All (2582) 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:B:427:THR:HA	1:B:436:MET:HE1	1.26	1.14
1:B:734:SER:HB3	1:B:860:GLY:HA3	1.24	1.12
1:D:427:THR:HA	1:D:436:MET:HE1	1.32	1.11
1:A:777:LEU:HD21	1:A:889:ALA:HB2	1.28	1.10
1:A:7:LEU:HD21	1:A:74:LEU:HD21	1.32	1.09
1:D:650:GLU:HB3	1:D:670:LEU:HD12	1.21	1.07
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:HH11	1:C:237:ARG:HB3	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:367:MET:HB3	1:B:372:MET:HE3	1.48	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: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:HG3	1:D:230:ARG:HH11	1.34	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:830:LEU:CD2	1:B:835:LEU:HB2	2.02	0.90
1:B:43:ARG:HH11	1:B:43:ARG:HG2	1.36	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
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:D:427:THR:HA	1:D:436:MET:CE	2.01	0.88
1:A:944:LEU:HD12	1:A:945:ASN:N	1.86	0.88
1:A:65:ALA:HB1	1:A:66:PRO:HD2	1.55	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD12	1:C:730:LEU:H	1.40	0.86
1:B:360:HIS:ND1	1:B:361:PRO:HD2	1.90	0.86
1:B:444:VAL:O	1:B:448:ARG:HB3	1.77	0.85
1:B:734:SER:CB	1:B:860:GLY:HA3	2.06	0.85
1:A:740:LEU:HD12	1:A:741:THR:H	1.41	0.85
1:D:105:TYR:CE2	1:D:199:ASP:HB2	2.12	0.85
1:B:842:TRP:CZ3	1:B:852:SER:HB2	2.11	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: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:HD22	1:A:134:LEU:H	1.43	0.84
1:D:240:LEU:HD23	1:D:293:LEU:HD12	1.59	0.84
1:C:360:HIS:ND1	1:C:361:PRO:HD2	1.93	0.84
1:D:360:HIS:ND1	1:D:361:PRO:HD2	1.93	0.83
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:C:776:LEU:C	1:C:777:LEU:HD23	1.99	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:HG2	1:C:255:ARG:HH11	1.45	0.82
1:D:255:ARG:HH11	1:D:255:ARG:HG2	1.43	0.82
1:B:230:ARG:HH11	1:B:230:ARG:HG3	1.45	0.82
1:C:668:VAL:CG1	1:C:669:PRO:HD2	2.09	0.82
1:A:377:LEU:HD22	1:A:708:TRP:HA	1.62	0.82
1:B:118:ASN:HB2	1:B:191:TRP:CD1	2.15	0.82
1:A:658:LEU:HD22	1:A:688:PRO:HG2	1.59	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:HIS:HB2	1:B:31:PRO:HD2	1.62	0.81
1:C:568:TRP:HE1	1:C:604:ASN:HD22	1.26	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: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:C:436:MET:HE3	1:C:467:ASN:HD22	1.45	0.81
1:B:655:MET:HG3	1:B:656:VAL:N	1.95	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:D:525:SER:HB2	3:D:4202:HOH:O	1.81	0.80
1:B:658:LEU:HG	1:B:661:LYS:NZ	1.96	0.80
1:A:635:THR:HG21	1:A:679:LEU:HD13	1.64	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:942:ARG:HA	1:C:953:GLY:O	1.82	0.80
1:C:347:LYS:NZ	1:C:675:GLN:HG3	1.97	0.80
1:D:984:LEU:CD2	1:D:986:ILE:HD11	2.12	0.80
1:B:662:PRO:O	1:B:663:LEU:HD23	1.81	0.80
1:B:840:HIS:HB2	1:B:842:TRP:CZ3	2.16	0.80
1:A:24:LEU:HB2	1:A:161:TYR:HB3	1.62	0.80
1:B:856:TYR:HB3	1:B:864:MET:CE	2.13	0.80
1:C:685:LEU:HD23	1:C:686:PRO:HD3	1.62	0.80
1:B:928:PRO:HB2	1:B:973:ARG:HH11	1.46	0.80
1:A:856:TYR:HB3	1:A:864:MET:CE	2.12	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:C:427:THR:HA	1:C:436:MET:HE1	1.64	0.79
1:D:654:TRP:NE1	1:D:666:GLY:HA3	1.97	0.79
1:A:673:ALA:HB1	1:A:674:PRO:HD2	1.64	0.79
1:A:73:TRP:CZ2	1:A:122:CYS:HB3	2.17	0.79
1:D:282:ARG:HG3	1:D:282:ARG:HH11	1.47	0.79
1:A:367:MET:HB3	1:A:372:MET:CE	2.12	0.79
1:D:237:ARG:HH11	1:D:237:ARG:CB	1.95	0.79
1:C:100:TYR:HB2	1:C:203:TRP:CE3	2.17	0.78
1:A:696:LEU:HD12	1:A:697:THR:N	1.97	0.78
1:A:599:ARG:NH1	1:A:600:GLN:HE22	1.81	0.78
1:C:105:TYR:HB3	1:C:106:PRO:HD2	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:MET:HA	1:A:573:GLN:HE22	1.47	0.78
1:D:237:ARG:HH11	1:D:237:ARG:HB2	1.47	0.78
1:B:73:TRP:CZ2	1:B:122:CYS:HB3	2.17	0.78
1:B:225:PHE:HB3	1:B:244:VAL:HG13	1.65	0.78
1:D:890:GLN:NE2	1:D:890:GLN:H	1.81	0.78
1:B:102:ASN:ND2	1:B:201:ASP:HB2	1.99	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:102:ASN:HD22	1:D:201:ASP:HB2	1.49	0.78
1:D:52[B]:ARG:HG3	1:D:133:TRP:CH2	2.19	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
1:C:673:ALA:HB1	1:C:674:PRO:HD2	1.66	0.77
1:C:577:LYS:HD3	1:C:585:TRP:CZ2	2.19	0.77
1:C:581:ASN:HD22	1:C:583:ASN:HD22	1.31	0.77
1:A:789:LEU:HD11	1:A:993:ILE:HG22	1.67	0.77
1:C:764:PHE:CD2	1:C:781:ARG:HB3	2.19	0.77
1:B:433:LEU:HB2	1:B:467:ASN:OD1	1.84	0.77
1:B:89:ASN:HD22	1:B:205:MET:HB3	1.50	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:A:427:THR:HA	1:A:436:MET:HE2	1.65	0.77
1:D:114:VAL:CG1	1:D:115:PRO:HD2	2.15	0.77
1:B:597:ASN:HD22	1:B:599:ARG:H	1.33	0.77
1:A:950:GLN:OE1	1:A:952:ARG:HD3	1.85	0.77
1:C:581:ASN:ND2	1:C:583:ASN:ND2	2.32	0.77
1:B:656:VAL:HG12	1:B:694:LEU:HD11	1.67	0.77
1:A:878:HIS:HB3	1:A:1009:LEU:O	1.85	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:D:777:LEU:HD21	1:D:889:ALA:HB2	1.67	0.76
1:C:167:LEU:HB3	1:C:168:PRO:HD2	1.67	0.76
1:B:668:VAL:HG13	1:B:669:PRO:HD2	1.68	0.76
1:C:258:VAL:CG2	1:C:291:LEU:HD11	2.16	0.76
1:A:598:ASP:O	1:A:601:PHE:HB2	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:749:ILE:O	1:C:755:ARG:HG3	1.86	0.75
1:B:797:GLU:O	1:B:801:ILE:HD12	1.86	0.75
1:C:778:THR:HB	1:C:887:GLN:HB3	1.68	0.75
1:C:930:VAL:HA	1:C:973:ARG:HG2	1.68	0.75
1:A:740:LEU:HD12	1:A:741:THR:N	2.01	0.75
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:D:835:LEU:CD1	1:D:857:ARG:HB2	2.16	0.75
1:C:135:GLN:NE2	1:C:135:GLN:HA	1.96	0.75
1:C:797:GLU:O	1:C:801:ILE:HD12	1.85	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:C:427:THR:HA	1:C:436:MET:HE2	1.69	0.74
1:A:511:PRO:HA	1:A:516:PRO:HB3	1.69	0.74
1:D:77:ASP:C	1:D:78:LEU:HD23	2.08	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: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:A:166:ARG:HG3	1:A:392:TYR:HB2	1.69	0.74
1:B:835:LEU:C	1:B:836:ILE:HD13	2.07	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:B:3:ILE:HG23	1:B:4:THR:H	1.51	0.74
1:D:166:ARG:HD3	3:D:4035:HOH:O	1.86	0.74
1:A:100:TYR:CE2	1:A:602:CYS:HB3	2.22	0.74
1:C:375:ASP:O	1:C:379:MET:HG3	1.86	0.74
1:D:655:MET:HG3	1:D:656:VAL:N	1.99	0.74
1:D:890:GLN:NE2	1:D:890:GLN:N	2.36	0.74
1:B:740:LEU:HD12	1:B:748:CYS:O	1.88	0.74
1:A:420:MET:HE2	1:A:426:LEU:HG	1.70	0.74
1:C:655:MET:HE1	1:C:662:PRO:HB3	1.68	0.74
1:C:395:HIS:ND1	1:C:396:PRO:HD2	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:637:GLU:HB2	1:A:679:LEU:HD21	1.69	0.73
1:D:403:ASP:OD1	1:D:451:PRO:HD2	1.88	0.73
1:C:581:ASN:ND2	1:C:583:ASN:HD22	1.83	0.73
1:C:416:GLU:HG3	1:C:460:ASN:O	1.88	0.73
1:A:763:GLY:HA3	1:A:822:LEU:CD2	2.17	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:546:LEU:HD22	1:A:616:ALA:HB1	1.68	0.73
1:C:777:LEU:CD2	1:C:889:ALA:HB2	2.17	0.73
1:D:658:LEU:CG	1:D:661:LYS:HZ2	2.02	0.73
1:B:796:SER:HB2	1:B:802:ASP:HB3	1.69	0.73
1:B:579:ASP:OD1	1:B:583:ASN:HB2	1.89	0.73
1:A:224:ASP:HB3	1:A:245:GLN:HG3	1.69	0.73
1:B:367:MET:HB3	1:B:372:MET:CE	2.19	0.73
1:A:770:ILE:HD12	1:A:775:GLN:NE2	2.02	0.72
1:D:26:ARG:HD3	1:D:169:SER:HB3	1.69	0.72
1:C:342:LEU:O	1:C:343:LEU:HD23	1.89	0.72
1:B:1004:SER:HB2	1:B:1006:GLU:OE2	1.89	0.72
1:A:367:MET:HB3	1:A:372:MET:HE3	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:D:655:MET:HE1	1:D:662:PRO:HB3	1.71	0.72
1:C:114:VAL:HG13	1:C:115:PRO:HD2	1.69	0.72
1:B:942:ARG:HA	1:B:953:GLY:O	1.89	0.72
1:A:683:PRO:O	1:A:684:GLU:C	2.24	0.72
1:C:148:SER:HB3	1:C:190:ARG:O	1.89	0.72
1:B:427:THR:CA	1:B:436:MET:HE1	2.15	0.72
1:A:646:HIS:O	1:A:648:ASP:N	2.22	0.72
1:B:696:LEU:HB2	1:B:722:LEU:HD11	1.71	0.72
1:D:658:LEU:HG	1:D:661:LYS:HZ2	1.55	0.72
1:B:6:SER:OG	1:B:9:VAL:HB	1.88	0.72
1:B:748:CYS:C	1:B:749:ILE:HD12	2.10	0.72
1:C:873:ALA:O	1:C:876:THR:HG22	1.90	0.72
1:A:5:ASP:OD2	1:A:157:ARG:HA	1.90	0.72
1:B:114:VAL:CG1	1:B:191:TRP:HB2	2.20	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:C:836:ILE:HD13	1:C:836:ILE:N	2.05	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:422:PRO:HG3	1:C:279:ILE:HD11	1.71	0.71
1:B:255:ARG:HG2	1:B:255:ARG:HH11	1.54	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: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
1:D:46:ARG:HB3	1:D:47:PRO:HD2	1.71	0.71
1:C:737:ILE:HD12	1:C:738:PRO:O	1.89	0.71
1:B:849:LEU:N	1:B:849:LEU:HD23	2.06	0.71
1:B:836:ILE:HD13	1:B:836:ILE:N	2.03	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: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:A:650:GLU:HA	1:A:701:VAL:O	1.90	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:D:251:ARG:NH1	1:D:251:ARG:HG3	2.03	0.71
1:C:53:SER:C	1:C:54:LEU:HD23	2.09	0.71
1:B:654:TRP:CE2	1:B:666:GLY:HA3	2.26	0.71
1:A:230:ARG:HB3	1:A:230:ARG:HH11	1.55	0.71
1:A:427:THR:HA	1:A:436:MET:HE1	1.70	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:B:651:LEU:CD1	1:B:703:PRO:HG3	2.21	0.71
1:A:742:THR:HG22	1:A:743:SER:H	1.55	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:D:568:TRP:HE1	1:D:604:ASN:ND2	1.87	0.70
1:B:282:ARG:HH12	1:C:419:GLY:CA	2.05	0.70
1:B:152:LEU:O	1:B:159:VAL:HG23	1.90	0.70
1:C:856:TYR:HB3	1:C:864:MET:CE	2.21	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:D:836:ILE:N	1:D:836:ILE:HD13	2.07	0.70
1:A:152:LEU:HG	1:A:153:TRP:N	2.05	0.70
1:D:835:LEU:C	1:D:836:ILE:HD13	2.12	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:989:PHE:CE1	1:C:1014:TYR:HB3	2.26	0.70
1:A:242:ALA:O	1:A:290:THR:HA	1.92	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:1020:TRP:HD1	1:A:1021:CYS:N	1.89	0.69
1:A:11:LEU:HD23	1:A:11:LEU:N	2.07	0.69
1:C:272:ALA:HB1	1:C:273:PRO:HD2	1.75	0.69
1:D:827:ALA:CB	1:D:836:ILE:HD12	2.22	0.69
1:A:360:HIS:CG	1:A:361:PRO:HD2	2.26	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:A:473:ARG:O	1:A:473:ARG:HD3	1.92	0.69
1:D:835:LEU:HD12	1:D:857:ARG:HB2	1.74	0.69
1:A:134:LEU:N	1:A:134:LEU:HD22	2.07	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:678:GLN:C	1:A:679:LEU:HD23	2.13	0.69
1:B:576:ILE:HD13	1:B:584:PRO:HB3	1.75	0.69
1:C:662:PRO:C	1:C:663:LEU:HD23	2.13	0.69
1:A:991:MET:HG2	1:A:992:GLY:N	2.07	0.69
1:C:850:PHE:HD2	1:C:872:VAL:HG13	1.57	0.69
1:C:12:GLN:HG3	1:C:13:ARG:N	2.08	0.69
1:B:355:ASN:OD1	1:B:388:ARG:HD3	1.92	0.69
1:B:166:ARG:HG3	1:B:392:TYR:HB2	1.75	0.69
1:D:746:ASP:CA	1:D:760:ARG:HG3	2.16	0.69
1:B:824:GLN:O	1:B:838:THR:HA	1.92	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:HD23	1:C:1018:LEU:N	2.08	0.69
1:C:110:ASN:O	1:C:113:PHE:N	2.26	0.69
1:A:737:ILE:HG13	1:A:738:PRO:HD2	1.73	0.69
1:C:100:TYR:CZ	1:C:602:CYS:HB3	2.27	0.69
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:C:245:GLN:HB3	1:C:288:ARG:HG2	1.75	0.68
1:C:38:ASN:ND2	1:C:41:GLU:H	1.90	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:657:ALA:O	1:D:694:LEU:HD12	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:MET:CA	1:A:573:GLN:HE22	2.05	0.68
1:C:166:ARG:HG3	1:C:392:TYR:HB2	1.75	0.68
1:B:255:ARG:NH1	1:B:255:ARG:HG2	2.08	0.68
1:D:210:ARG:HD3	3:D:4036:HOH:O	1.91	0.68
1:A:645:ARG:NH2	1:A:650:GLU:OE1	2.26	0.68
1:A:287:ASP:CG	1:D:425:ARG:HH22	1.96	0.68
1:A:510:GLN:HB2	1:A:517:LYS:HB2	1.76	0.68
1:D:129:VAL:HG23	1:D:182:ASN:HD22	1.56	0.68
1:C:531:ARG:O	1:C:561:ARG:NH1	2.27	0.68
1:D:166:ARG:HG3	1:D:392:TYR:CG	2.29	0.68
1:A:635:THR:CG2	1:A:679:LEU:HD13	2.24	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:C:652:LEU:HD11	1:C:698:VAL:HB	1.75	0.67
1:D:187:MET:HG3	1:D:187:MET:O	1.93	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:D:654:TRP:HZ3	1:D:656:VAL:HG23	1.59	0.67
1:D:24:LEU:HB2	1:D:161:TYR:HB3	1.77	0.67
1:A:166:ARG:HG3	1:A:392:TYR:CB	2.23	0.67
1:D:856:TYR:HB3	1:D:864:MET:HE2	1.76	0.67
1:B:43:ARG:HD2	1:B:261:TRP:CD2	2.29	0.67
1:A:595:THR:HG23	1:A:596:PRO:HA	1.76	0.67
1:D:71:GLU:O	1:D:72:SER:C	2.32	0.67
1:B:651:LEU:HD13	1:B:703:PRO:HG3	1.75	0.67
1:A:742:THR:HG22	1:A:743:SER:N	2.08	0.67
1:C:166:ARG:O	1:C:210:ARG:NH2	2.28	0.67
1:D:43:ARG:O	1:D:310:ARG:HD3	1.94	0.67
1:C:187:MET:O	1:C:187:MET:HG3	1.95	0.67
1:C:140:ARG:NH1	1:C:170:GLU:OE1	2.27	0.67
1:A:59:ARG:NH2	1:A:81:ALA:O	2.27	0.67
1:C:35:SER:OG	1:C:37:ARG:NH1	2.27	0.67
1:B:928:PRO:HB2	1:B:973:ARG:NH1	2.10	0.67
1:D:658:LEU:HD22	1:D:688:PRO:HG2	1.77	0.67
1:C:80:GLU:OE2	1:C:80:GLU:N	2.28	0.67
1:B:822:LEU:HD12	1:B:824:GLN:H	1.60	0.67
1:D:87:PRO:HB3	1:D:210:ARG:O	1.95	0.67
1:D:949:HIS:HB2	1:D:951:TRP:CH2	2.30	0.67
1:B:128:ASN:HA	1:B:180:GLY:O	1.94	0.67
1:A:436:MET:HE3	1:A:467:ASN:HD22	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:ARG:NH2	1:C:287:ASP:OD2	2.28	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:A:962:TYR:HD2	1:A:966:GLN:HE22	1.42	0.67
1:D:933:SER:O	1:D:934:GLU:C	2.31	0.67
1:B:738:PRO:HB2	1:B:834:VAL:HG23	1.76	0.67
1:A:128:ASN:HA	1:A:180:GLY:O	1.95	0.67
1:B:824:GLN:OE1	1:B:837:THR:HG21	1.94	0.67
1:D:73:TRP:CZ2	1:D:122:CYS:HB3	2.29	0.66
1:A:654:TRP:CZ3	1:A:656:VAL:HG23	2.31	0.66
1:D:166:ARG:HG3	1:D:392:TYR:HB2	1.77	0.66
1:C:542:MET:HE3	1:C:601:PHE:HA	1.77	0.66
1:C:542:MET:HA	1:C:604:ASN:HA	1.77	0.66
1:A:410:VAL:HG22	1:A:455:ILE:HB	1.75	0.66
1:A:436:MET:HE1	1:A:467:ASN:HD22	1.58	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: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:786:ARG:HG2	1:A:880:ALA:HB1	1.77	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:D:603:MET:HE1	1:D:930:VAL:CG1	2.26	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:775:GLN:OE1	1:A:890:GLN:NE2	2.29	0.66
1:D:657:ALA:HB2	1:D:662:PRO:HA	1.77	0.66
1:B:577:LYS:HD3	1:B:585:TRP:HZ2	1.61	0.66
1:A:824:GLN:HG3	1:A:825:CYS:N	2.08	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:499:ILE:CG2	1:D:501:PRO:HD3	2.21	0.66
1:C:360:HIS:CE1	1:C:361:PRO:HD2	2.30	0.66
1:A:693:GLN:HG2	1:A:721:ARG:CD	2.26	0.66
1:C:347:LYS:HZ1	1:C:675:GLN:HG3	1.59	0.66
1:C:43:ARG:HG2	1:C:43:ARG:NH1	2.11	0.66
1:B:883:GLY:HA2	1:B:1016:TYR:OH	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:202:MET:HA	1:D:573:GLN:HE22	1.60	0.66
1:C:166:ARG:CG	1:C:392:TYR:HB2	2.26	0.66
1:C:856:TYR:HD2	1:C:864:MET:HE1	1.61	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:D:780:LEU:HA	1:D:886:CYS:HB3	1.76	0.66
1:B:211:ASP:OD1	1:B:211:ASP:N	2.28	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:776:LEU:C	1:A:777:LEU:HD23	2.17	0.65
1:D:36:TRP:NE1	1:D:46:ARG:O	2.28	0.65
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:547:GLY:HA2	1:D:908:ASP:O	1.96	0.65
1:D:429:ASP:OD1	1:D:431[A]:ARG:HG3	1.96	0.65
1:A:949:HIS:CD2	1:A:1020:TRP:HE1	2.15	0.65
1:D:360:HIS:CE1	1:D:362:LEU:HB2	2.32	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:B:856:TYR:HB3	1:B:864:MET:HE1	1.78	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:C:902:PRO:O	1:C:938:ARG:NH1	2.30	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:D:668:VAL:HG11	1:D:680:ILE:HD13	1.78	0.65
1:C:7:LEU:N	1:C:71:GLU:OE2	2.30	0.65
1:B:38:ASN:O	1:B:38:ASN:ND2	2.29	0.65
1:C:380:LYS:HE2	3:C:4077:HOH:O	1.97	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:B:833:ALA:HB1	1:B:858:ILE:O	1.97	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:C:770:ILE:O	1:C:773:LYS:HD2	1.97	0.65
1:A:535:LEU:HD22	1:A:538:TYR:HB3	1.77	0.65
1:D:245:GLN:HB3	3:D:6016:HOH:O	1.96	0.65
1:D:166:ARG:HG3	1:D:392:TYR:CB	2.27	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:403:ASP:CG	1:D:451:PRO:HD2	2.17	0.65
1:C:856:TYR:CD2	1:C:864:MET:HE1	2.32	0.65
1:A:770:ILE:HD12	1:A:775:GLN:CD	2.17	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:908:ASP:HB3	1:A:1007:PHE:CD1	2.32	0.65
1:C:932:PRO:HG2	1:C:970:THR:O	1.97	0.64
1:C:436:MET:HE1	1:C:467:ASN:HB2	1.79	0.64
1:A:287:ASP:OD2	1:D:425:ARG:NH2	2.31	0.64
1:A:748:CYS:C	1:A:749:ILE:HD12	2.17	0.64
1:B:434:PRO:HB3	1:C:434:PRO:HB3	1.78	0.64
1:C:246:MET:HE2	1:C:287:ASP:CB	2.26	0.64
1:D:46:ARG:CB	1:D:47:PRO:HD2	2.25	0.64
1:C:251:ARG:O	1:C:253:TYR:N	2.30	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:A:894:ARG:HD3	1:A:919:ASP:OD1	1.97	0.64
1:A:282:ARG:HG3	1:A:282:ARG:HH11	1.62	0.64
1:D:460:ASN:ND2	1:D:461:GLU:HG2	2.12	0.64
1:C:436:MET:CE	1:C:467:ASN:HD22	2.09	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:B:789:LEU:N	1:B:792:ASP:OD2	2.29	0.64
1:A:937:LEU:HD21	1:A:956:GLN:HB3	1.80	0.64
1:C:418:HIS:ND1	1:C:461:GLU:HG3	2.12	0.64
1:C:10:VAL:HG12	1:C:11:LEU:N	2.12	0.64
1:D:763:GLY:HA3	1:D:822:LEU:HD21	1.80	0.64
1:B:844:HIS:C	1:B:845:GLN:HG2	2.18	0.64
1:C:437:SER:O	1:C:441:THR:HG23	1.97	0.64
1:C:920:LEU:HB3	1:C:921:PRO:HD2	1.78	0.64
1:C:833:ALA:HB1	1:C:858:ILE:O	1.97	0.64
1:B:950:GLN:OE1	1:B:952:ARG:NH1	2.31	0.64
1:A:35:SER:OG	1:A:37:ARG:NH1	2.31	0.64
1:B:805:ALA:HB3	1:B:808:GLU:HB2	1.80	0.64
1:A:635:THR:HA	1:A:680:ILE:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:SER:OG	1:C:192:SER:HB3	1.97	0.64
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:B:200:GLN:N	1:B:200:GLN:OE1	2.30	0.64
1:B:1020:TRP:HD1	1:B:1021:CYS:N	1.95	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:D:776:LEU:C	1:D:777:LEU:HD23	2.19	0.64
1:A:425:ARG:NH2	1:D:287:ASP:OD2	2.31	0.64
1:A:62:TRP:CZ2	1:A:119:PRO:HB3	2.33	0.64
1:D:11:LEU:HD21	1:D:187:MET:HE1	1.79	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:D:655:MET:CE	1:D:662:PRO:HB3	2.27	0.63
1:C:167:LEU:HD21	1:C:393:PRO:CG	2.27	0.63
1:A:618:THR:HG22	1:A:912:ALA:HB1	1.79	0.63
1:B:778:THR:CG2	1:B:779:PRO:HD2	2.26	0.63
1:A:240:LEU:CD2	1:A:260:LEU:HD22	2.28	0.63
1:A:153:TRP:HB2	1:A:185:ALA:HB3	1.80	0.63
1:B:385:ASN:HB3	1:B:408:TYR:CD1	2.33	0.63
1:C:588:TYR:O	1:C:591:ASP:HB2	1.98	0.63
1:C:777:LEU:N	1:C:777:LEU:HD23	2.11	0.63
1:D:377:LEU:CD2	1:D:708:TRP:HA	2.29	0.63
1:A:678:GLN:O	1:A:679:LEU:HD23	1.98	0.63
1:A:856:TYR:HD2	1:A:864:MET:HE1	1.62	0.63
1:C:499:ILE:HD11	1:C:529:GLU:OE1	1.99	0.63
1:B:90:TRP:HE1	1:B:96:ASP:CG	2.01	0.63
1:C:870:VAL:HG12	1:C:871:GLU:N	2.14	0.63
1:B:100:TYR:HB2	1:B:203:TRP:CE3	2.33	0.63
1:C:167:LEU:CD2	1:C:393:PRO:HB2	2.29	0.63
1:B:701:VAL:O	1:B:703:PRO:HD3	1.97	0.63
1:D:336:ARG:HH21	1:D:338:GLU:CD	2.01	0.63
1:B:842:TRP:HZ3	1:B:852:SER:HB2	1.61	0.63
1:A:789:LEU:CD1	1:A:993:ILE:HG22	2.29	0.63
1:C:645:ARG:NH2	1:C:650:GLU:OE1	2.32	0.63
1:A:823:LEU:HD22	1:B:728:VAL:HG12	1.80	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:B:673:ALA:HB1	1:B:674:PRO:CD	2.26	0.63
1:B:473:ARG:HD3	1:B:473:ARG:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ARG:HD3	3:A:4018:HOH:O	1.98	0.63
1:C:43:ARG:NH2	1:C:264:GLU:OE2	2.32	0.63
1:B:374:GLN:O	1:B:378:LEU:HD12	1.99	0.63
1:B:282:ARG:NH1	1:C:418:HIS:O	2.28	0.63
1:A:304:GLU:C	1:A:305:ILE:HG13	2.18	0.63
1:B:658:LEU:HG	1:B:661:LYS:HZ1	1.62	0.63
1:C:433:LEU:HB3	1:C:434:PRO:CD	2.29	0.62
1:B:499:ILE:HB	1:B:533:LEU:HB2	1.80	0.62
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:A:945:ASN:OD1	1:A:950:GLN:HB2	1.99	0.62
1:A:377:LEU:CD2	1:A:708:TRP:HA	2.29	0.62
1:D:52[A]:ARG:NH2	1:D:128:ASN:O	2.30	0.62
1:C:166:ARG:HG3	1:C:392:TYR:CG	2.33	0.62
1:B:383:ASN:HD22	1:B:621:LYS:HG3	1.63	0.62
1:C:502:MET:HA	1:C:537:GLU:O	2.00	0.62
1:C:431[B]:ARG:NH2	3:C:7516:HOH:O	2.32	0.62
1:D:827:ALA:HB2	1:D:836:ILE:HD12	1.81	0.62
1:C:200:GLN:HG2	1:C:391:HIS:HB2	1.81	0.62
1:B:204:ARG:N	1:B:204:ARG:HD3	2.13	0.62
1:A:7:LEU:HD11	1:A:69:VAL:HG12	1.80	0.62
1:D:100:TYR:HB3	1:D:589:GLY:HA2	1.80	0.62
1:D:603:MET:HE1	1:D:930:VAL:HG11	1.80	0.62
1:B:559:TYR:HB2	1:B:562:LEU:CD1	2.28	0.62
1:A:305:ILE:HD11	1:A:645:ARG:HB3	1.81	0.62
1:D:38:ASN:HD22	1:D:41:GLU:H	1.45	0.62
1:C:920:LEU:CB	1:C:921:PRO:HD2	2.28	0.62
1:A:425:ARG:HH22	1:D:287:ASP:CG	2.02	0.62
1:B:65:ALA:HB1	1:B:66:PRO:HD2	1.82	0.62
1:A:38:ASN:HD21	1:A:40:GLU:HB2	1.65	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:424:ASN:OD1	1:C:279:ILE:HD12	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:B:35:SER:OG	1:B:37:ARG:NH1	2.32	0.62
1:D:467:ASN:O	1:D:471:LEU:HG	1.99	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:91:GLN:OE1	1:A:205:MET:HB3	2.00	0.62
1:A:403:ASP:OD1	1:A:451:PRO:HD2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:693:GLN:HB3	1:D:721:ARG:HD3	1.82	0.62
1:C:833:ALA:CB	1:C:859:ASP:HA	2.30	0.62
1:C:776:LEU:O	1:C:777:LEU:HD23	1.99	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:A:655:MET:CE	1:A:662:PRO:HB3	2.30	0.62
1:C:342:LEU:C	1:C:343:LEU:HD23	2.20	0.61
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:A:856:TYR:CD2	1:A:864:MET:HE1	2.34	0.61
1:D:654:TRP:CZ3	1:D:656:VAL:HG23	2.35	0.61
1:C:989:PHE:HE1	1:C:1014:TYR:HB3	1.62	0.61
1:D:919:ASP:O	1:D:920:LEU:HD23	2.00	0.61
1:C:894:ARG:HD3	1:C:919:ASP:OD1	2.01	0.61
1:D:1020:TRP:HD1	1:D:1021:CYS:N	1.98	0.61
1:A:14:ARG:HA	1:A:16:TRP:CZ3	2.35	0.61
1:A:233:ASP:CG	1:C:233:ASP:HB3	2.21	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:A:613:PRO:HB3	1:A:617:LEU:HD23	1.83	0.61
1:A:143:PHE:O	1:A:168:PRO:HA	2.01	0.61
1:A:668:VAL:HG12	1:A:669:PRO:HD2	1.83	0.61
1:D:745:MET:HB2	1:D:746:ASP:OD2	2.01	0.61
1:C:141:ILE:HB	1:C:173:LEU:HD11	1.83	0.61
1:B:537:GLU:HG2	1:B:568:TRP:CE3	2.36	0.61
1:A:645:ARG:HH22	1:A:650:GLU:CD	2.03	0.61
1:D:777:LEU:CD2	1:D:889:ALA:HB2	2.30	0.61
1:A:30:HIS:HB2	1:A:31:PRO:HD2	1.83	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:794:GLY:HA2	1:D:998:SER:O	2.00	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:141:ILE:HD13	1:B:143:PHE:CE1	2.35	0.61
1:A:662:PRO:C	1:A:663:LEU:HD23	2.19	0.61
1:B:129:VAL:HG12	1:B:134:LEU:HD11	1.81	0.61
1:B:542:MET:HB2	1:B:604:ASN:OD1	2.01	0.61
1:A:801:ILE:O	1:A:803:PRO:HD3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:255:ARG:HG2	1:D:255:ARG:NH1	2.11	0.61
1:C:357:HIS:HD2	1:C:392:TYR:OH	1.83	0.61
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: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:50:GLN:N	1:A:50:GLN:NE2	2.48	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: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:D:878:HIS:HB3	1:D:1009:LEU:O	2.01	0.60
1:C:557:ARG:HD2	3:C:4018:HOH:O	2.01	0.60
1:A:595:THR:CG2	1:A:596:PRO:HA	2.31	0.60
1:C:509:ASP:C	1:C:511:PRO:HD3	2.22	0.60
1:A:369:GLU:O	1:A:373:VAL:HG23	2.01	0.60
1:C:776:LEU:HD23	1:C:776:LEU:N	2.16	0.60
1:D:238:ALA:HB1	1:D:332:PHE:CE2	2.37	0.60
1:B:964:GLN:O	1:B:967:LEU:HB2	2.00	0.60
1:D:55:ASN:HD22	1:D:87:PRO:HD3	1.65	0.60
1:B:658:LEU:O	1:B:661:LYS:HE3	2.02	0.60
1:B:429:ASP:OD2	1:B:431[A]:ARG:HD3	2.02	0.60
1:D:533:LEU:HD12	1:D:533:LEU:C	2.21	0.60
1:C:928:PRO:O	1:C:973:ARG:NH1	2.34	0.60
1:B:589:GLY:HA3	1:B:599:ARG:CA	2.31	0.60
1:A:696:LEU:HB2	1:A:722:LEU:HD11	1.82	0.60
1:A:257:THR:OG1	1:A:271:THR:HG23	2.02	0.60
1:D:322:LEU:HD22	1:D:323:ILE:N	2.15	0.60
1:B:36:TRP:NE1	1:B:46:ARG:O	2.28	0.60
1:A:502:MET:HB2	1:A:503:TYR:CE1	2.36	0.60
1:D:424:ASN:ND2	1:D:464:HIS:O	2.33	0.60
1:A:930:VAL:HG22	1:A:973:ARG:CD	2.30	0.60
1:B:246:MET:HE2	1:B:287:ASP:HB2	1.82	0.60
1:D:62:TRP:HB2	1:D:95:TYR:CD2	2.37	0.60
1:B:217:LYS:HG2	1:B:218:PRO:HD2	1.83	0.60
1:D:89:ASN:O	1:D:92:MET:HB2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:650:GLU:HG3	1:B:700:VAL:CG1	2.32	0.60
1:A:544:ASN:HB3	1:A:789:LEU:HD22	1.83	0.60
1:D:38:ASN:ND2	1:D:41:GLU:HG2	2.17	0.60
1:C:559:TYR:CB	1:C:562:LEU:HD12	2.31	0.60
1:C:129:VAL:HG12	1:C:134:LEU:HD21	1.84	0.60
1:A:737:ILE:CG1	1:A:738:PRO:HD2	2.30	0.60
1:B:949:HIS:HB2	1:B:951:TRP:CH2	2.37	0.60
1:B:78:LEU:O	1:B:81:ALA:N	2.30	0.60
1:C:775:GLN:C	1:C:776:LEU:HD23	2.22	0.60
1:B:127:PHE:O	1:B:182:ASN:N	2.34	0.60
1:C:949:HIS:HB2	1:C:951:TRP:CH2	2.36	0.60
1:C:3:ILE:O	1:C:6:SER:HB3	2.02	0.60
1:A:542:MET:HA	1:A:604:ASN:HA	1.83	0.60
1:C:881:ARG:HG3	1:C:882:ILE:N	2.15	0.60
1:C:153:TRP:HA	1:C:157:ARG:O	2.02	0.60
1:A:753:ASN:OD1	1:A:753:ASN:N	2.28	0.60
1:D:856:TYR:HB3	1:D:864:MET:CE	2.30	0.59
1:A:637:GLU:CB	1:A:679:LEU:HD21	2.32	0.59
1:D:129:VAL:HG23	1:D:182:ASN:ND2	2.16	0.59
1:D:581:ASN:HD22	1:D:583:ASN:ND2	1.99	0.59
1:D:540:HIS:CE1	1:D:542:MET:HB2	2.37	0.59
1:C:78:LEU:HB3	1:C:80:GLU:OE2	2.02	0.59
1:A:473:ARG:C	1:A:473:ARG:HD3	2.19	0.59
1:C:133:TRP:CE3	1:C:216:HIS:HB2	2.36	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:D:100:TYR:HB2	1:D:203:TRP:CD2	2.37	0.59
1:A:701:VAL:O	1:A:703:PRO:HD3	2.02	0.59
1:D:504:ALA:HB3	1:D:535:LEU:HD21	1.83	0.59
1:D:138:GLN:HG2	1:D:138:GLN:O	1.99	0.59
1:B:658:LEU:O	1:B:659:ASP:C	2.40	0.59
1:D:658:LEU:CD2	1:D:661:LYS:HZ2	2.15	0.59
1:C:200:GLN:OE1	1:C:200:GLN:N	2.35	0.59
1:C:767:GLN:NE2	1:C:774:LYS:HG2	2.17	0.59
1:B:808:GLU:OE1	1:B:808:GLU:HA	2.03	0.59
1:D:881:ARG:HD3	1:D:987:ASP:OD1	2.02	0.59
1:A:777:LEU:N	1:A:777:LEU:HD23	2.17	0.59
1:C:835:LEU:C	1:C:836:ILE:HD13	2.22	0.59
1:B:377:LEU:N	1:B:377:LEU:HD23	2.16	0.59
1:A:917:ARG:NH2	1:A:943:GLU:OE1	2.35	0.59
1:A:217:LYS:HB3	1:A:218:PRO:HD2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:588:TYR:HD2	1:D:603:MET:HE1	1.67	0.59
1:D:153:TRP:HB2	1:D:185:ALA:HB3	1.84	0.59
1:C:1011:ALA:HB3	1:C:1014:TYR:CZ	2.37	0.59
1:D:588:TYR:CD2	1:D:603:MET:HE1	2.37	0.59
1:B:372:MET:O	1:B:375:ASP:HB2	2.03	0.59
1:B:100:TYR:HB2	1:B:203:TRP:CD2	2.37	0.59
1:C:161:TYR:HE2	1:C:163:GLN:HE21	1.45	0.59
1:C:124:SER:HA	1:C:184:LEU:O	2.03	0.59
1:A:254:LEU:O	1:A:255:ARG:HG3	2.03	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:619:GLU:HG2	1:A:909:ARG:HG2	1.83	0.59
1:D:651:LEU:HD12	1:D:668:VAL:O	2.02	0.59
1:B:217:LYS:NZ	1:B:324:GLU:OE1	2.35	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:B:256:VAL:O	1:B:271:THR:HA	2.03	0.59
1:C:347:LYS:HZ2	1:C:675:GLN:HG3	1.67	0.59
1:B:300:LEU:N	1:B:307:ASN:HD22	2.00	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:B:634:GLN:O	1:B:682:LEU:HB2	2.02	0.59
1:C:100:TYR:CE1	1:C:602:CYS:HB3	2.37	0.58
1:B:573:GLN:HB2	1:B:602:CYS:O	2.03	0.58
1:D:658:LEU:HG	1:D:661:LYS:NZ	2.18	0.58
1:A:626:PHE:O	1:A:641:GLU:HB2	2.02	0.58
1:B:786:ARG:CD	1:B:880:ALA:HB1	2.31	0.58
1:B:141:ILE:HG23	1:B:143:PHE:HE1	1.67	0.58
1:D:52[A]:ARG:HG2	1:D:52[A]:ARG:HH11	1.68	0.58
1:D:7:LEU:HG	1:D:74:LEU:HD11	1.84	0.58
1:B:314:GLU:HB3	1:B:322:LEU:HD21	1.86	0.58
1:D:352:ARG:CB	1:D:385:ASN:HB2	2.29	0.58
1:D:38:ASN:HB3	1:D:41:GLU:HG3	1.85	0.58
1:B:51:LEU:HD12	1:B:214:LEU:O	2.02	0.58
1:D:672:VAL:HG13	1:D:678:GLN:HB2	1.85	0.58
1:A:261:TRP:HZ3	1:A:264:GLU:O	1.86	0.58
1:B:739[A]:HIS:CD2	1:B:740:LEU:H	2.21	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:C:400:THR:O	1:C:403:ASP:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:930:VAL:HG22	1:A:973:ARG:HD3	1.84	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:B:570:TRP:CD1	1:B:571:VAL:HG13	2.38	0.58
1:D:868:VAL:HG12	1:D:869:ASP:N	2.18	0.58
1:C:579:ASP:OD1	1:C:583:ASN:N	2.33	0.58
1:D:78:LEU:N	1:D:78:LEU:HD23	2.15	0.58
1:D:635:THR:HA	1:D:680:ILE:O	2.04	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:D:749:ILE:O	1:D:755:ARG:HG3	2.04	0.58
1:A:246:MET:HB3	1:A:274:PHE:CZ	2.38	0.58
1:D:965:GLN:HE21	1:D:969:GLU:CD	2.07	0.58
1:D:304:GLU:C	1:D:305:ILE:HG13	2.23	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:A:433:LEU:HD12	1:A:433:LEU:O	2.03	0.58
1:C:420:MET:HE2	1:C:425:ARG:HB3	1.85	0.58
1:A:230:ARG:CB	1:A:230:ARG:HH11	2.17	0.58
1:B:385:ASN:HB3	1:B:408:TYR:HD1	1.67	0.58
1:D:867:THR:HB	3:D:4146:HOH:O	2.02	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:D:331:GLY:HA3	1:D:451:PRO:HB3	1.85	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: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:B:272:ALA:HB1	1:B:273:PRO:HD2	1.85	0.58
1:D:649:ASN:O	1:D:702:GLN:HG3	2.03	0.58
1:A:433:LEU:HB3	1:A:434:PRO:CD	2.33	0.58
1:A:599:ARG:HH12	1:A:600:GLN:HE22	1.50	0.58
1:A:599:ARG:NH1	1:A:600:GLN:NE2	2.52	0.58
1:B:536:CYS:O	1:B:566:PHE:HB2	2.04	0.58
1:C:355:ASN:OD1	1:C:388:ARG:HD3	2.03	0.58
1:C:421:VAL:O	1:C:425:ARG:HD2	2.04	0.58
1:D:656:VAL:HG12	1:D:694:LEU:HD11	1.85	0.58
1:C:27:LEU:HD12	1:C:170:GLU:HB3	1.85	0.58
1:B:286:ALA:HB1	3:B:4439:HOH:O	2.03	0.58
1:C:746:ASP:HA	1:C:760:ARG:HG2	1.86	0.58
1:A:949:HIS:HD2	1:A:1020:TRP:HE1	1.51	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:TRP:HA	1:B:401:LEU:HD12	1.86	0.57
1:D:673:ALA:O	1:D:674:PRO:C	2.41	0.57
1:B:91:GLN:HB3	1:B:98:PRO:HG3	1.86	0.57
1:D:78:LEU:HB3	1:D:80:GLU:OE2	2.04	0.57
1:C:486:TYR:CZ	1:C:488:GLY:HA3	2.38	0.57
1:A:502:MET:HA	1:A:537:GLU:O	2.04	0.57
1:C:804:ASN:O	1:C:809[A]:ARG:NH1	2.30	0.57
1:A:882:ILE:O	1:A:882:ILE:HG22	2.04	0.57
1:A:69:VAL:HG13	1:A:70:PRO:HD2	1.86	0.57
1:B:856:TYR:HB3	1:B:864:MET:HE2	1.86	0.57
1:B:840:HIS:ND1	1:B:840:HIS:N	2.50	0.57
1:A:202:MET:HE2	1:A:365:GLN:NE2	2.19	0.57
1:B:225:PHE:HA	1:B:243:GLU:O	2.04	0.57
1:C:43:ARG:HD2	1:C:261:TRP:CD2	2.39	0.57
1:A:3:ILE:HD12	1:A:3:ILE:O	2.04	0.57
1:C:726:LEU:HD12	1:D:848:THR:HG22	1.86	0.57
1:A:490:GLY:N	3:A:4007:HOH:O	2.31	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:767:GLN:HG3	1:A:768:MET:N	2.19	0.57
1:A:7:LEU:HD13	1:A:69:VAL:HG12	1.86	0.57
1:B:579:ASP:CG	1:B:583:ASN:HB2	2.24	0.57
1:D:903[B]:GLN:HE22	1:D:913:ALA:HA	1.68	0.57
1:B:929:TYR:O	1:B:931:PHE:N	2.37	0.57
1:B:30:HIS:HB2	1:B:31:PRO:CD	2.34	0.57
1:A:202:MET:O	1:A:204:ARG:HD3	2.05	0.57
1:B:237:ARG:HB2	1:B:237:ARG:HH11	1.69	0.57
1:A:136:GLU:O	1:A:216:HIS:HE1	1.88	0.57
1:C:897:TRP:HB2	1:C:943:GLU:O	2.04	0.57
1:A:375:ASP:O	1:A:379:MET:HG3	2.04	0.57
1:D:141:ILE:HG13	1:D:213:SER:O	2.04	0.57
1:B:114:VAL:HG13	1:B:191:TRP:CB	2.34	0.57
1:A:672:VAL:HG13	1:A:678:GLN:HB2	1.86	0.57
1:A:737:ILE:HD12	1:A:832:ASP:C	2.25	0.57
1:B:138:GLN:N	1:B:217:LYS:O	2.38	0.57
1:C:746:ASP:CA	1:C:760:ARG:HG2	2.35	0.57
1:C:198:GLU:OE2	1:C:439:ARG:NH1	2.35	0.57
1:D:444:VAL:O	1:D:448:ARG:HB3	2.04	0.57
1:C:775:GLN:OE1	1:C:890:GLN:NE2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:673:ALA:HB1	1:D:674:PRO:CD	2.32	0.57
1:B:777:LEU:HD21	1:B:889:ALA:CB	2.35	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:C:258:VAL:N	1:C:270:GLY:O	2.29	0.57
1:C:246:MET:HE2	1:C:287:ASP:HB3	1.87	0.57
1:C:36:TRP:CD1	1:C:41:GLU:HB3	2.39	0.57
1:D:894:ARG:HD3	1:D:919:ASP:OD1	2.04	0.57
1:B:391:HIS:HA	1:B:412:GLU:OE1	2.05	0.57
1:C:608:PHE:O	1:C:611:ARG:N	2.32	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:A:392:TYR:HB2	1:A:393:PRO:HD2	1.86	0.57
1:A:403:ASP:CG	1:A:451:PRO:HD2	2.25	0.57
1:D:770:ILE:HD13	1:D:775:GLN:CD	2.25	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:750:GLU:HB3	1:A:755:ARG:HG3	1.86	0.56
1:D:653[B]:HIS:HD2	1:D:667:GLU:HG3	1.69	0.56
1:A:599:ARG:HB2	1:A:600:GLN:OE1	2.05	0.56
1:A:102:ASN:C	1:A:102:ASN:HD22	2.07	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:B:399:TYR:HB3	1:B:450:HIS:CD2	2.39	0.56
1:D:230:ARG:CG	1:D:230:ARG:HH11	2.12	0.56
1:B:230:ARG:HH11	1:B:230:ARG:CG	2.17	0.56
1:D:7:LEU:O	1:D:11:LEU:HB2	2.06	0.56
1:B:422:PRO:HG3	1:C:279:ILE:CD1	2.35	0.56
1:A:737:ILE:HG13	1:A:738:PRO:CD	2.36	0.56
1:D:257:THR:OG1	1:D:316:HIS:HE1	1.89	0.56
1:A:894:ARG:CZ	1:A:921:PRO:HD3	2.36	0.56
1:B:80:GLU:OE2	1:B:80:GLU:N	2.39	0.56
1:D:767:GLN:HG3	1:D:768:MET:N	2.19	0.56
1:D:876:THR:OG1	1:D:877:PRO:HD2	2.05	0.56
1:D:393:PRO:HD2	1:D:414:ASN:HB2	1.86	0.56
1:B:505:ARG:HG2	1:B:996:ASP:OD2	2.04	0.56
1:A:844:HIS:C	1:A:845:GLN:HG2	2.24	0.56
1:A:237:ARG:HH11	1:A:237:ARG:HB2	1.70	0.56
1:B:141:ILE:HB	1:B:173:LEU:HD12	1.87	0.56
1:A:649:ASN:OD1	1:A:703:PRO:HD2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:PHE:HA	1:A:122:CYS:O	2.06	0.56
1:B:1019:VAL:HG12	1:B:1019:VAL:O	2.03	0.56
1:C:573:GLN:HB2	1:C:602:CYS:O	2.05	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:C:833:ALA:HB2	1:C:859:ASP:HA	1.87	0.56
1:A:282:ARG:HB2	1:D:422:PRO:HA	1.87	0.56
1:D:110:ASN:O	1:D:113:PHE:HB2	2.06	0.56
1:B:888:LEU:N	1:B:982:THR:O	2.27	0.56
1:D:306:PRO:O	1:D:307:ASN:C	2.36	0.56
1:D:522:LYS:O	1:D:522:LYS:HG2	2.05	0.56
1:C:721:ARG:HH11	1:C:721:ARG:CG	2.19	0.56
1:D:836:ILE:HG22	1:D:837:THR:N	2.20	0.56
1:C:432:TRP:O	1:C:433:LEU:C	2.42	0.56
1:D:316:HIS:HD2	1:D:317:THR:O	1.88	0.56
1:B:38:ASN:ND2	1:B:41:GLU:H	2.03	0.56
1:A:1020:TRP:CD1	1:A:1021:CYS:N	2.73	0.56
1:A:930:VAL:HA	1:A:973:ARG:HD2	1.86	0.56
1:C:577:LYS:HD3	1:C:585:TRP:CH2	2.41	0.56
1:A:200:GLN:N	1:A:200:GLN:OE1	2.34	0.56
1:A:65:ALA:HB1	1:A:66:PRO:CD	2.32	0.56
1:A:358:GLU:HB3	1:A:367:MET:HG2	1.88	0.56
1:D:777:LEU:HD23	1:D:777:LEU:N	2.21	0.56
1:A:987:ASP:OD2	1:A:990:HIS:HD2	1.88	0.56
1:A:422:PRO:HG2	1:D:285:TYR:CZ	2.40	0.56
1:A:84:VAL:HG13	1:A:85:VAL:N	2.20	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:A:90:TRP:CD1	1:A:95:TYR:HB2	2.41	0.56
1:D:895:VAL:O	1:D:919:ASP:HA	2.06	0.56
1:C:807:VAL:HG13	1:C:808:GLU:N	2.21	0.56
1:A:693:GLN:CG	1:A:721:ARG:HD3	2.35	0.56
1:C:356:ARG:HD3	3:C:4139:HOH:O	2.04	0.56
1:B:630:ARG:HB3	1:B:630:ARG:CZ	2.35	0.56
1:C:721:ARG:HE	1:D:874:SER:CB	2.18	0.55
1:A:693:GLN:HG3	1:A:724:GLU:HG3	1.87	0.55
1:A:421:VAL:HG13	1:D:282:ARG:O	2.06	0.55
1:C:836:ILE:HG22	1:C:837:THR:N	2.20	0.55
1:B:822:LEU:HD12	1:B:823:LEU:H	1.71	0.55
1:D:416:GLU:OE1	1:D:418:HIS:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:354:VAL:HG22	1:C:355:ASN:N	2.21	0.55
1:B:929:TYR:O	1:B:930:VAL:C	2.43	0.55
1:B:767:GLN:HG3	1:B:768:MET:N	2.18	0.55
1:B:309:TYR:HB2	1:B:330:VAL:HG12	1.88	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:299:LYS:C	1:B:307:ASN:HD22	2.10	0.55
1:D:693:GLN:HB2	1:D:695:TRP:HE1	1.71	0.55
1:D:133:TRP:C	1:D:134:LEU:HD23	2.26	0.55
1:B:357:HIS:HD2	1:B:392:TYR:OH	1.89	0.55
1:B:213:SER:O	1:B:214:LEU:HD23	2.06	0.55
1:D:344:LEU:HG	1:D:345:ASN:N	2.19	0.55
1:B:397:LEU:O	1:B:398:TRP:C	2.45	0.55
1:D:75:GLU:OE1	1:D:75:GLU:HA	2.06	0.55
1:B:38:ASN:HD21	1:B:41:GLU:H	1.54	0.55
1:C:881:ARG:C	1:C:882:ILE:HG13	2.26	0.55
1:A:946:TYR:HH	1:A:982:THR:HG1	1.53	0.55
1:D:769:TRP:HE1	1:D:774:LYS:HE2	1.71	0.55
1:B:710:GLU:OE2	1:B:710:GLU:HA	2.05	0.55
1:C:597:ASN:ND2	1:C:599:ARG:H	2.00	0.55
1:A:377:LEU:HD22	1:A:708:TRP:CA	2.36	0.55
1:A:202:MET:HA	1:A:573:GLN:NE2	2.18	0.55
1:A:907:PRO:HD3	1:A:939:CYS:SG	2.45	0.55
1:D:763:GLY:HA3	1:D:822:LEU:CD2	2.37	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:A:540:HIS:C	1:A:542:MET:H	2.09	0.55
1:D:578:TYR:HA	1:D:583:ASN:O	2.07	0.55
1:D:344:LEU:HD23	1:D:644:PHE:CZ	2.41	0.55
1:D:737:ILE:HG13	1:D:738:PRO:N	2.20	0.55
1:A:559:TYR:HB2	1:A:562:LEU:HD12	1.88	0.55
1:A:427:THR:O	1:A:467:ASN:HB2	2.07	0.55
1:C:166:ARG:HG3	1:C:392:TYR:CB	2.36	0.55
1:C:397:LEU:O	1:C:398:TRP:C	2.45	0.55
1:B:510:GLN:HB2	1:B:517:LYS:HB2	1.87	0.55
1:C:382:ASN:O	1:C:621:LYS:HA	2.06	0.55
1:D:305:ILE:HD11	1:D:645:ARG:HB3	1.88	0.55
1:D:984:LEU:HD21	1:D:986:ILE:CD1	2.27	0.55
1:C:1020:TRP:CD1	1:C:1021:CYS:N	2.74	0.55
1:D:949:HIS:HD2	1:D:1020:TRP:HE1	1.53	0.55
1:A:379:MET:HB3	1:A:384:PHE:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142:ILE:O	1:D:212:VAL:HA	2.06	0.55
1:D:512:PHE:HE1	1:D:517:LYS:HG3	1.71	0.55
1:B:100:TYR:CZ	1:B:602:CYS:HB3	2.42	0.55
1:A:52[B]:ARG:NH2	1:A:130:ASP:HB2	2.21	0.55
1:C:27:LEU:HD12	1:C:170:GLU:CB	2.37	0.55
1:A:655:MET:HE1	1:A:662:PRO:HB3	1.89	0.55
1:D:878:HIS:CD2	1:D:1010:SER:HB3	2.41	0.55
1:B:258:VAL:HA	1:B:312:VAL:O	2.07	0.55
1:B:227:VAL:HG11	1:B:330:VAL:CG2	2.36	0.55
1:D:344:LEU:HD23	1:D:644:PHE:CE1	2.42	0.55
1:B:974:HIS:O	1:B:975:LEU:HD23	2.07	0.55
1:C:523:TRP:O	1:C:526:LEU:HB2	2.07	0.55
1:A:352:ARG:O	1:A:385:ASN:HB2	2.07	0.55
1:C:629:PHE:CD1	1:C:629:PHE:N	2.75	0.55
1:D:432:TRP:O	1:D:436:MET:HG3	2.06	0.55
1:A:381:GLN:NE2	1:A:708:TRP:O	2.40	0.55
1:D:656:VAL:CG1	1:D:694:LEU:HD11	2.37	0.55
1:C:393:PRO:HD3	1:C:412:GLU:O	2.07	0.55
1:C:376:ILE:HG22	1:C:377:LEU:N	2.21	0.55
1:D:95:TYR:N	1:D:95:TYR:CD1	2.75	0.55
1:D:457:SER:HA	1:D:485:GLN:O	2.07	0.55
1:B:246:MET:HE2	1:B:246:MET:O	2.06	0.55
1:D:333:ARG:HA	1:D:345:ASN:OD1	2.06	0.55
1:D:69:VAL:CG1	1:D:70:PRO:HD2	2.37	0.55
1:A:282:ARG:NH1	1:D:420:MET:O	2.39	0.55
1:A:925:MET:HE3	1:A:925:MET:HA	1.88	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
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:C:432:TRP:N	1:C:432:TRP:CD1	2.71	0.54
1:B:141:ILE:HG23	1:B:143:PHE:CE1	2.42	0.54
1:C:438:GLU:O	1:C:442:ARG:HG3	2.08	0.54
1:A:762:SER:O	1:A:822:LEU:HD23	2.08	0.54
1:D:416:GLU:OE1	1:D:461:GLU:HG3	2.06	0.54
1:B:51:LEU:HD13	1:B:215:LEU:HB2	1.89	0.54
1:D:782:ASP:HA	1:D:884:LEU:HD23	1.88	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:B:152:LEU:C	1:B:159:VAL:HG23	2.28	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:ASN:ND2	1:D:182:ASN:OD1	2.29	0.54
1:D:949:HIS:CD2	1:D:1020:TRP:HE1	2.24	0.54
1:A:274:PHE:HB3	1:A:286:ALA:O	2.08	0.54
1:D:852:SER:HB2	1:D:870:VAL:HG22	1.89	0.54
1:D:528:GLY:O	1:D:530:THR:HG23	2.06	0.54
1:A:80:GLU:H	1:A:80:GLU:CD	2.11	0.54
1:B:662:PRO:C	1:B:663:LEU:HD23	2.27	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: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:D:801:ILE:HG23	1:D:808:GLU:CD	2.27	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:777:LEU:HD21	1:B:889:ALA:HA	1.88	0.54
1:B:751:LEU:HD23	1:B:751:LEU:O	2.07	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:D:246:MET:HG2	1:D:274:PHE:CZ	2.43	0.54
1:C:995:GLY:O	1:C:997:ASP:N	2.41	0.54
1:C:685:LEU:O	1:C:687:GLN:HG3	2.08	0.54
1:A:570:TRP:HD1	1:A:571:VAL:HG22	1.69	0.54
1:B:134:LEU:O	1:B:135:GLN:C	2.43	0.54
1:B:897:TRP:CB	1:B:944:LEU:HB2	2.38	0.54
1:C:802:ASP:O	1:C:808:GLU:HG3	2.07	0.54
1:B:493:THR:HG23	3:B:4020:HOH:O	2.08	0.54
1:B:670:LEU:HD11	1:B:700:VAL:HG22	1.90	0.54
1:B:100:TYR:CE1	1:B:602:CYS:HB3	2.41	0.54
1:B:655:MET:O	1:B:696:LEU:HD12	2.08	0.54
1:A:100:TYR:HB2	1:A:203:TRP:CE3	2.43	0.54
1:B:200:GLN:HB3	1:B:202:MET:HG2	1.90	0.54
1:A:652:LEU:HD12	1:A:699:ARG:O	2.07	0.54
1:B:429:ASP:OD1	1:B:431[B]:ARG:HG3	2.08	0.54
1:B:774:LYS:HB2	1:B:774:LYS:NZ	2.23	0.54
1:D:742:THR:HG22	1:D:743:SER:N	2.22	0.54
1:C:478:VAL:HG12	1:C:479:ASP:N	2.21	0.54
1:B:114:VAL:HG12	1:B:115:PRO:N	2.23	0.54
1:A:228:ALA:O	1:A:240:LEU:HD12	2.08	0.54
1:A:93:HIS:HB3	1:A:95:TYR:CE1	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:822:LEU:HD12	1:B:823:LEU:N	2.23	0.54
1:D:763:GLY:CA	1:D:822:LEU:HD21	2.37	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:A:198:GLU:HB3	3:A:4060:HOH:O	2.07	0.54
1:B:916:ASP:HB3	1:B:918:TRP:CZ2	2.42	0.54
1:B:894:ARG:CZ	1:B:921:PRO:HD3	2.38	0.54
1:C:168:PRO:O	1:C:442:ARG:NH2	2.38	0.54
1:B:949:HIS:CD2	1:B:1020:TRP:HE1	2.26	0.54
1:A:138:GLN:OE1	1:A:140:ARG:NH2	2.39	0.54
1:B:955:PHE:HB2	1:B:987:ASP:O	2.06	0.54
1:C:789:LEU:HG	1:C:792:ASP:OD2	2.08	0.54
1:B:246:MET:HE2	1:B:287:ASP:CB	2.38	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:B:58:TRP:CE3	1:B:123:TYR:HB3	2.43	0.53
1:B:420:MET:HE2	1:B:426:LEU:HG	1.91	0.53
1:D:745:MET:O	1:D:760:ARG:N	2.38	0.53
1:A:930:VAL:HG22	1:A:973:ARG:NE	2.23	0.53
1:D:573:GLN:HB2	1:D:602:CYS:O	2.08	0.53
1:C:420:MET:HE2	1:C:426:LEU:HG	1.90	0.53
1:D:890:GLN:H	1:D:890:GLN:CD	2.11	0.53
1:D:890:GLN:HE21	1:D:890:GLN:N	2.06	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:D:639:THR:OG1	1:D:677:LYS:HE2	2.09	0.53
1:D:757:GLN:HG2	1:D:758:PHE:N	2.22	0.53
1:D:597:ASN:HD22	1:D:599:ARG:N	1.95	0.53
1:D:238:ALA:HB2	1:D:298:PRO:HG3	1.90	0.53
1:A:224:ASP:HB3	1:A:245:GLN:CG	2.37	0.53
1:C:463:GLY:HA2	3:C:7509:HOH:O	2.08	0.53
1:D:737:ILE:HG13	1:D:738:PRO:CD	2.38	0.53
1:B:868:VAL:HG12	1:B:869:ASP:N	2.23	0.53
1:B:59:ARG:O	1:B:124:SER:N	2.39	0.53
1:B:440:VAL:CG1	1:B:475:ILE:HD11	2.38	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:B:592:PHE:CD1	1:B:592:PHE:N	2.76	0.53
1:D:937:LEU:HA	1:D:958:ASN:HB3	1.89	0.53
1:C:58:TRP:CE3	1:C:123:TYR:HB3	2.43	0.53
1:A:53:SER:C	1:A:54:LEU:HD23	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:658:LEU:C	1:B:661:LYS:HE3	2.29	0.53
1:A:856:TYR:HB3	1:A:864:MET:HE3	1.89	0.53
1:A:52[B]:ARG:HG3	1:A:133:TRP:HH2	1.73	0.53
1:D:683:PRO:O	1:D:685:LEU:HG	2.08	0.53
1:D:524:LEU:O	1:D:561:ARG:NH2	2.41	0.53
1:C:856:TYR:HD2	1:C:864:MET:CE	2.21	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:930:VAL:O	1:C:932:PRO:HD3	2.08	0.53
1:A:240:LEU:HD23	1:A:260:LEU:HD22	1.89	0.53
1:A:38:ASN:HD22	1:A:41:GLU:HG3	1.73	0.53
1:C:254:LEU:O	1:C:255:ARG:NH1	2.42	0.53
1:D:71:GLU:O	1:D:73:TRP:N	2.41	0.53
1:C:10:VAL:O	1:C:11:LEU:C	2.43	0.53
1:A:962:TYR:HD2	1:A:966:GLN:NE2	2.06	0.53
1:C:770:ILE:HD11	1:C:1022:GLN:HG2	1.90	0.53
1:D:906:TYR:HB3	1:D:907:PRO:HD2	1.90	0.53
1:C:694:LEU:HD12	1:C:695:TRP:H	1.74	0.53
1:A:227:VAL:CG1	1:A:240:LEU:HD11	2.33	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:C:11:LEU:HD21	1:C:187:MET:CE	2.39	0.53
1:B:906:TYR:HB3	1:B:907:PRO:HD2	1.90	0.53
1:D:946:TYR:CE2	1:D:982:THR:HG21	2.43	0.53
1:A:891:VAL:HG12	1:A:891:VAL:O	2.09	0.53
1:A:856:TYR:HD2	1:A:864:MET:CE	2.21	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:607:VAL:HG23	1:A:608:PHE:O	2.08	0.53
1:D:654:TRP:CE3	1:D:655:MET:N	2.77	0.53
1:B:739[A]:HIS:CD2	1:B:740:LEU:N	2.77	0.53
1:D:429:ASP:OD1	1:D:431[B]:ARG:HG3	2.09	0.53
1:A:507:ASP:OD1	1:A:521:LYS:HE2	2.08	0.53
1:D:501:PRO:HD2	1:D:533:LEU:HD13	1.90	0.53
1:C:261:TRP:HA	1:C:267:VAL:HG23	1.91	0.53
1:D:30:HIS:HB2	1:D:31:PRO:CD	2.38	0.53
1:A:734:SER:HB2	1:A:860:GLY:CA	2.38	0.53
1:D:356:ARG:HD2	1:D:379:MET:CE	2.39	0.53
1:A:579:ASP:C	1:A:581:ASN:H	2.13	0.53
1:B:221:GLN:O	1:B:221:GLN:HG2	1.95	0.53
1:D:99:ILE:O	1:D:204:ARG:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:HIS:CE1	1:B:33:PHE:CD1	2.97	0.52
1:C:673:ALA:HB1	1:C:674:PRO:CD	2.36	0.52
1:B:486:TYR:CE2	1:B:488:GLY:HA3	2.44	0.52
1:D:161:TYR:OH	1:D:163:GLN:NE2	2.33	0.52
1:C:835:LEU:HD12	1:C:836:ILE:N	2.24	0.52
1:B:275:GLY:HA2	1:B:286:ALA:HA	1.92	0.52
1:A:416:GLU:OE1	1:A:418:HIS:HB2	2.09	0.52
1:C:241:GLU:HG3	1:C:292:ARG:HG2	1.91	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: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:D:878:HIS:NE2	1:D:1010:SER:HB3	2.24	0.52
1:A:140:ARG:HG2	1:A:141:ILE:N	2.23	0.52
1:A:126:THR:HA	1:A:182:ASN:O	2.10	0.52
1:D:77:ASP:O	1:D:78:LEU:HD23	2.10	0.52
1:D:948:PRO:HG2	1:D:949:HIS:CE1	2.44	0.52
1:A:53:SER:O	1:A:54:LEU:HD23	2.10	0.52
1:C:176:PHE:N	1:C:176:PHE:CD1	2.76	0.52
1:D:473:ARG:O	1:D:473:ARG:HD3	2.10	0.52
1:C:734:SER:CB	1:C:860:GLY:HA3	2.27	0.52
1:C:652:LEU:HB2	1:C:670:LEU:HD21	1.91	0.52
1:A:38:ASN:ND2	1:A:41:GLU:N	2.54	0.52
1:B:839:ALA:HA	1:B:852:SER:O	2.09	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:D:746:ASP:HA	1:D:760:ARG:CG	2.24	0.52
1:B:497:ASP:O	1:B:531:ARG:HG2	2.09	0.52
1:C:356:ARG:HH22	1:C:367:MET:HE2	1.74	0.52
1:D:62:TRP:CG	1:D:95:TYR:HB3	2.44	0.52
1:B:784:PHE:HA	1:B:881:ARG:O	2.09	0.52
1:D:486:TYR:CZ	1:D:488:GLY:HA3	2.44	0.52
1:C:878:HIS:ND1	3:C:4074:HOH:O	2.30	0.52
1:A:389:CYS:HB3	1:A:394:ASN:ND2	2.24	0.52
1:A:6:SER:OG	1:A:8:ALA:HB3	2.10	0.52
1:D:959:ILE:O	1:D:959:ILE:HG23	2.09	0.52
1:A:420:MET:HE2	1:A:426:LEU:CG	2.37	0.52
1:D:114:VAL:CG1	1:D:191:TRP:HB2	2.39	0.52
1:B:422:PRO:HG2	1:B:424:ASN:HB3	1.89	0.52
1:C:373:VAL:HG12	1:C:377:LEU:HD11	1.90	0.52
1:A:786:ARG:HH11	1:A:990:HIS:CE1	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:464:HIS:HB2	1:D:489:GLY:HA3	1.91	0.52
1:B:78:LEU:O	1:B:80:GLU:N	2.42	0.52
1:C:353:GLY:HA2	1:C:386:ALA:O	2.09	0.52
1:D:415:ILE:HG12	1:D:439:ARG:HD2	1.91	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:B:578:TYR:HA	1:B:583:ASN:O	2.09	0.52
1:C:751:LEU:HD23	1:C:751:LEU:C	2.30	0.52
1:A:58:TRP:N	1:A:84:VAL:O	2.42	0.52
1:D:486:TYR:CE2	1:D:488:GLY:HA3	2.44	0.52
1:D:650:GLU:HA	1:D:701:VAL:O	2.10	0.52
1:A:433:LEU:HD12	1:A:433:LEU:C	2.30	0.52
1:B:685:LEU:HB3	1:B:686:PRO:CD	2.36	0.52
1:C:373:VAL:O	1:C:377:LEU:HG	2.09	0.52
1:C:395:HIS:CG	1:C:396:PRO:HD2	2.44	0.52
1:D:23:GLN:O	1:D:24:LEU:HD13	2.10	0.52
1:C:858:ILE:HA	1:C:863:GLN:O	2.09	0.52
1:A:128:ASN:HD22	1:A:181:GLU:N	2.06	0.52
1:A:652:LEU:O	1:A:667:GLU:HA	2.10	0.52
1:A:138:GLN:HG2	1:A:139:THR:N	2.20	0.52
1:A:237:ARG:HH11	1:A:237:ARG:CB	2.23	0.52
1:A:18:ASN:OD1	1:A:20:GLY:N	2.40	0.52
1:D:826:THR:OG1	1:D:826:THR:O	2.27	0.52
1:B:11:LEU:HD21	1:B:187:MET:CE	2.40	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:B:759:ASN:OD1	1:B:761:GLN:N	2.29	0.52
1:D:499:ILE:O	1:D:533:LEU:HD13	2.11	0.52
1:B:399:TYR:HB2	1:B:450:HIS:NE2	2.25	0.52
1:C:255:ARG:HH11	1:C:255:ARG:CG	2.20	0.52
1:C:166:ARG:O	1:C:167:LEU:HD23	2.10	0.52
1:D:41:GLU:OE2	1:D:46:ARG:NH1	2.43	0.52
1:C:856:TYR:HB3	1:C:864:MET:HE1	1.90	0.52
1:D:512:PHE:CE1	1:D:517:LYS:HG3	2.44	0.52
1:C:960:SER:HA	3:C:4030:HOH:O	2.10	0.52
1:B:29:ALA:HB3	1:B:445:GLN:HG3	1.92	0.52
1:B:856:TYR:CD1	1:B:856:TYR:N	2.78	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:C:258:VAL:CB	1:C:291:LEU:HD11	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:ASN:HD22	1:A:625:GLN:HA	1.74	0.51
1:C:497:ASP:O	1:C:531:ARG:HG2	2.10	0.51
1:B:41:GLU:HA	1:B:46:ARG:HB2	1.92	0.51
1:C:84:VAL:HG22	1:C:93:HIS:ND1	2.25	0.51
1:A:948:PRO:O	1:A:1022:GLN:HA	2.10	0.51
1:D:666:GLY:O	1:D:667:GLU:HG3	2.10	0.51
1:D:685:LEU:CB	1:D:686:PRO:HD2	2.37	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:B:234:ASP:O	1:B:235:PHE:HB2	2.10	0.51
1:A:989:PHE:N	1:A:989:PHE:CD1	2.79	0.51
1:B:733:ALA:O	1:B:734:SER:C	2.48	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:D:55:ASN:OD1	1:D:211:ASP:HB3	2.11	0.51
1:D:966:GLN:NE2	1:D:979:GLU:OE2	2.44	0.51
1:D:399:TYR:CE1	1:D:446:ARG:NH2	2.79	0.51
1:D:906:TYR:O	1:D:907:PRO:C	2.49	0.51
1:C:44:THR:O	1:C:45:ASP:C	2.46	0.51
1:B:141:ILE:HG12	1:B:142:ILE:N	2.25	0.51
1:D:72:SER:O	1:D:75:GLU:N	2.42	0.51
1:B:458:LEU:HD11	1:B:472:TYR:HB2	1.93	0.51
1:B:35:SER:O	1:B:50:GLN:NE2	2.42	0.51
1:A:124:SER:HA	1:A:184:LEU:O	2.11	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:A:636:ILE:N	1:A:680:ILE:O	2.35	0.51
1:A:24:LEU:O	1:A:25:ASN:HB2	2.08	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:B:650:GLU:CB	1:B:670:LEU:HD12	2.28	0.51
1:A:106:PRO:HG3	1:A:204:ARG:HG3	1.93	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:A:416:GLU:OE1	1:A:461:GLU:OE2	2.29	0.51
1:C:515:VAL:O	1:C:515:VAL:HG23	2.10	0.51
1:D:645:ARG:HH22	1:D:650:GLU:CD	2.14	0.51
1:D:920:LEU:HB3	1:D:921:PRO:HD2	1.93	0.51
1:C:1009:LEU:HD23	1:C:1009:LEU:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:513:PRO:O	1:C:514:ALA:HB3	2.11	0.51
1:B:433:LEU:HD12	1:B:433:LEU:C	2.29	0.51
1:D:645:ARG:NH2	1:D:650:GLU:OE1	2.43	0.51
1:A:41:GLU:HG2	1:A:46:ARG:HH11	1.76	0.51
1:D:254:LEU:C	1:D:255:ARG:HG2	2.31	0.51
1:A:858:ILE:HG12	1:A:864:MET:HB3	1.92	0.51
1:C:261:TRP:CD1	1:C:261:TRP:N	2.79	0.51
1:D:42:ALA:O	1:D:43:ARG:C	2.47	0.51
1:D:636:ILE:N	1:D:680:ILE:O	2.37	0.51
1:B:533:LEU:HD12	1:B:533:LEU:C	2.30	0.51
1:C:505:ARG:HB3	3:C:4226:HOH:O	2.11	0.51
1:C:741:THR:HG22	1:C:741:THR:O	2.09	0.51
1:B:956:GLN:O	1:B:987:ASP:N	2.29	0.51
1:A:585:TRP:CE3	1:A:974:HIS:CE1	2.99	0.51
1:B:979:GLU:O	1:B:980:GLU:C	2.49	0.51
1:D:655:MET:HE3	1:D:664:ALA:O	2.10	0.51
1:B:11:LEU:N	1:B:11:LEU:HD23	2.25	0.51
1:C:585:TRP:CE3	1:C:974:HIS:CE1	2.98	0.51
1:C:499:ILE:HB	1:C:533:LEU:CB	2.40	0.51
1:C:701:VAL:HG12	1:C:702:GLN:N	2.26	0.51
1:A:128:ASN:HD22	1:A:180:GLY:C	2.14	0.51
1:B:36:TRP:CD1	1:B:41:GLU:HB3	2.46	0.51
1:D:697:THR:HG22	1:D:698:VAL:N	2.26	0.51
1:D:37:ARG:HD3	1:D:50:GLN:NE2	2.26	0.51
1:B:851:ILE:O	1:B:870:VAL:HA	2.11	0.51
1:B:427:THR:O	1:B:467:ASN:HB2	2.11	0.51
1:A:233:ASP:OD2	1:C:233:ASP:HB3	2.11	0.51
1:C:600:GLN:HB3	1:C:603:MET:HE2	1.93	0.51
1:B:143:PHE:O	1:B:168:PRO:HA	2.11	0.51
1:D:13:ARG:O	1:D:14:ARG:C	2.47	0.51
1:C:43:ARG:HD2	1:C:261:TRP:CE2	2.46	0.51
1:A:613:PRO:HB3	1:A:617:LEU:CD2	2.40	0.51
1:A:50:GLN:H	1:A:50:GLN:NE2	2.08	0.51
1:B:894:ARG:NH1	1:B:921:PRO:HD3	2.26	0.51
1:A:234:ASP:OD1	1:A:236:SER:OG	2.28	0.51
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:D:200:GLN:N	1:D:200:GLN:OE1	2.43	0.50
1:B:959:ILE:HG23	1:B:959:ILE:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:963:SER:OG	1:C:979:GLU:OE2	2.28	0.50
1:B:910:LEU:C	1:B:910:LEU:HD12	2.32	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:429:ASP:CG	1:B:431[A]:ARG:HD3	2.32	0.50
1:A:80:GLU:N	1:A:80:GLU:OE2	2.30	0.50
1:C:229:THR:HA	1:C:239:VAL:O	2.10	0.50
1:B:58:TRP:HE3	1:B:123:TYR:HB3	1.76	0.50
1:D:475:ILE:O	1:D:476:LYS:C	2.49	0.50
1:B:788:PRO:HD3	1:B:968:MET:HG3	1.91	0.50
1:D:130:ASP:OD2	1:D:132:SER:OG	2.29	0.50
1:B:411:ASP:OD2	1:B:447:ASP:OD2	2.29	0.50
1:B:733:ALA:O	1:B:734:SER:O	2.30	0.50
1:A:746:ASP:HA	1:A:760:ARG:CG	2.29	0.50
1:B:600:GLN:C	1:B:602:CYS:H	2.15	0.50
1:C:143:PHE:O	1:C:168:PRO:HA	2.11	0.50
1:C:258:VAL:HB	1:C:291:LEU:CD1	2.41	0.50
1:C:111:PRO:HG3	1:C:196:TYR:CE2	2.46	0.50
1:D:446:ARG:HG2	1:D:446:ARG:O	2.11	0.50
1:A:411:ASP:OD2	1:A:447:ASP:OD2	2.29	0.50
1:D:234:ASP:O	1:D:235:PHE:HB2	2.11	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:959:ILE:HA	3:A:4028:HOH:O	2.11	0.50
1:A:590:GLY:HA2	1:A:594:ASP:CG	2.32	0.50
1:B:399:TYR:CB	1:B:450:HIS:CD2	2.95	0.50
1:B:102:ASN:HD22	1:B:102:ASN:C	2.15	0.50
1:B:638:VAL:O	1:B:677:LYS:HA	2.11	0.50
1:A:887:GLN:HB2	1:A:983:TRP:CD2	2.47	0.50
1:A:719:GLN:HE22	1:A:915:PHE:H	1.59	0.50
1:D:225:PHE:HA	1:D:243:GLU:O	2.11	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:D:3:ILE:O	1:D:3:ILE:HD12	2.12	0.50
1:B:118:ASN:CB	1:B:191:TRP:HD1	2.14	0.50
1:B:701:VAL:CG1	1:B:702:GLN:N	2.73	0.50
1:C:649:ASN:ND2	1:C:702:GLN:HG2	2.26	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:619:GLU:HA	1:B:912:ALA:HB2	1.94	0.50
1:C:925:MET:HE3	1:C:925:MET:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:674:PRO:C	1:B:675:GLN:HG2	2.32	0.50
1:A:658:LEU:N	1:A:661:LYS:O	2.38	0.50
1:A:202:MET:HB3	1:A:573:GLN:HE22	1.76	0.50
1:A:652:LEU:N	1:A:668:VAL:O	2.36	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:36:TRP:CE2	1:A:42:ALA:HA	2.46	0.50
1:B:163:GLN:OE1	1:B:193:ASP:OD1	2.30	0.50
1:A:211:ASP:N	1:A:211:ASP:OD1	2.25	0.50
1:A:629:PHE:CD1	1:A:629:PHE:N	2.79	0.50
1:B:645:ARG:NH2	1:B:650:GLU:OE2	2.42	0.50
1:D:588:TYR:HB2	1:D:602:CYS:SG	2.52	0.50
1:B:696:LEU:HD12	1:B:697:THR:N	2.27	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:C:726:LEU:HD11	1:D:873:ALA:HB2	1.93	0.50
1:C:386:ALA:HB2	1:C:408:TYR:HB2	1.94	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:598:ASP:C	1:D:599:ARG:HG3	2.33	0.50
1:A:682:LEU:HB3	1:A:683:PRO:HD2	1.93	0.50
1:D:822:LEU:HD12	1:D:824:GLN:N	2.27	0.50
1:A:217:LYS:NZ	1:A:324:GLU:OE2	2.44	0.50
1:A:808:GLU:HA	1:A:808:GLU:OE1	2.11	0.50
1:D:670:LEU:HA	1:D:678:GLN:OE1	2.11	0.49
1:C:416:GLU:OE1	1:C:418:HIS:HB2	2.12	0.49
1:D:79:PRO:HD2	1:D:80:GLU:OE2	2.11	0.49
1:C:134:LEU:CD2	1:C:134:LEU:N	2.75	0.49
1:B:653[B]:HIS:HD2	1:B:666:GLY:O	1.96	0.49
1:A:90:TRP:NE1	1:A:96:ASP:OD1	2.45	0.49
1:B:382:ASN:O	1:B:383:ASN:HB2	2.12	0.49
1:D:581:ASN:HD22	1:D:583:ASN:HD21	1.59	0.49
1:D:808:GLU:HA	1:D:808:GLU:OE1	2.10	0.49
1:B:769:TRP:CE3	1:B:769:TRP:N	2.80	0.49
1:C:842:TRP:N	1:C:842:TRP:CE3	2.80	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:A:524:LEU:HD22	1:A:561:ARG:HB3	1.94	0.49
1:D:360:HIS:CE1	1:D:361:PRO:HD2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:696:LEU:HD12	1:B:697:THR:H	1.77	0.49
1:B:577:LYS:HB3	1:B:585:TRP:CZ2	2.47	0.49
1:B:649:ASN:O	1:B:702:GLN:HA	2.12	0.49
1:D:334:GLU:CD	1:D:336:ARG:HD3	2.33	0.49
1:C:502:MET:CB	1:C:537:GLU:HG3	2.42	0.49
1:D:540:HIS:HE1	1:D:542:MET:HB2	1.76	0.49
1:C:746:ASP:N	1:C:760:ARG:HG2	2.27	0.49
1:D:784:PHE:CD1	1:D:850:PHE:CE1	3.00	0.49
1:D:716:ALA:O	1:D:717:TRP:HB3	2.12	0.49
1:C:867:THR:O	1:C:867:THR:HG22	2.12	0.49
1:A:89:ASN:O	1:A:92:MET:HB2	2.12	0.49
1:A:360:HIS:CE1	1:A:361:PRO:HD2	2.46	0.49
1:C:579:ASP:OD1	1:C:583:ASN:HB2	2.12	0.49
1:B:166:ARG:CG	1:B:392:TYR:HB2	2.40	0.49
1:A:141:ILE:O	1:A:141:ILE:HG23	2.11	0.49
1:D:870:VAL:HG12	1:D:871:GLU:N	2.27	0.49
1:B:906:TYR:CD2	1:B:937:LEU:HD22	2.47	0.49
1:A:718:GLN:HG3	1:A:719:GLN:N	2.27	0.49
1:B:351:ILE:O	1:B:351:ILE:HG22	2.11	0.49
1:A:890:GLN:OE1	1:A:949:HIS:HE1	1.94	0.49
1:B:141:ILE:HB	1:B:173:LEU:CD1	2.43	0.49
1:A:634:GLN:OE1	1:A:685:LEU:HD12	2.13	0.49
1:C:78:LEU:O	1:C:81:ALA:HB3	2.12	0.49
1:B:15:ASP:HB3	1:B:21:VAL:CG1	2.43	0.49
1:B:14:ARG:HG2	1:B:16:TRP:CZ2	2.47	0.49
1:B:622:HIS:HD2	1:B:625:GLN:OE1	1.95	0.49
1:B:474:TRP:CZ2	1:B:478:VAL:HG21	2.47	0.49
1:B:176:PHE:N	1:B:176:PHE:CD1	2.79	0.49
1:B:7:LEU:N	1:B:71:GLU:OE2	2.46	0.49
1:A:878:HIS:HD2	1:A:1008:GLN:HB3	1.77	0.49
1:D:73:TRP:CE2	1:D:122:CYS:HB3	2.47	0.49
1:C:399:TYR:N	1:C:399:TYR:CD1	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:A:556:PHE:CD1	1:A:564:GLY:HA2	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:C:589:GLY:C	1:C:591:ASP:H	2.16	0.49
1:C:856:TYR:CD1	1:C:856:TYR:N	2.79	0.49
1:D:86:VAL:HG13	1:D:87:PRO:HA	1.93	0.49
1:D:786:ARG:O	1:D:788:PRO:HD3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:373:VAL:O	1:D:374:GLN:C	2.49	0.49
1:B:133:TRP:CD1	1:B:133:TRP:N	2.78	0.49
1:C:859:ASP:OD1	1:C:861:SER:OG	2.27	0.49
1:D:762:SER:C	1:D:822:LEU:HD23	2.33	0.49
1:B:730:LEU:H	1:B:730:LEU:CD1	2.00	0.49
1:A:26:ARG:NH1	1:A:169:SER:HB3	2.18	0.49
1:C:652:LEU:O	1:C:667:GLU:HA	2.13	0.49
1:B:423:MET:CB	1:C:282:ARG:HG3	2.41	0.49
1:C:961:ARG:HG3	1:C:961:ARG:NH1	2.27	0.49
1:A:737:ILE:HA	1:A:738:PRO:HD3	1.76	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:A:446:ARG:HG2	1:A:447:ASP:OD1	2.13	0.49
1:B:305:ILE:O	1:B:305:ILE:HG22	2.13	0.49
1:A:479:ASP:OD1	1:A:481:SER:HB3	2.13	0.49
1:C:339:ASN:HB3	3:C:4161:HOH:O	2.13	0.49
1:D:261:TRP:CD1	1:D:261:TRP:N	2.80	0.49
1:C:728:VAL:HG23	1:C:728:VAL:O	2.12	0.49
1:A:208:ILE:HG22	1:A:208:ILE:O	2.12	0.49
1:D:100:TYR:O	1:D:597:ASN:HB2	2.13	0.49
1:D:357:HIS:HD2	1:D:392:TYR:OH	1.96	0.49
1:D:238:ALA:HB1	1:D:332:PHE:HE2	1.77	0.49
1:C:261:TRP:CH2	1:C:266:GLN:HG3	2.47	0.49
1:B:153:TRP:HA	1:B:157:ARG:O	2.13	0.49
1:C:455:ILE:HG22	1:C:456:TRP:N	2.27	0.49
1:D:211:ASP:OD1	1:D:211:ASP:N	2.45	0.49
1:A:568:TRP:CD2	1:A:569:ASP:HB3	2.48	0.49
1:C:127:PHE:CD2	1:C:127:PHE:N	2.80	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:D:513:PRO:O	1:D:514:ALA:HB3	2.12	0.49
1:B:434:PRO:O	1:B:435:ALA:C	2.50	0.48
1:A:134:LEU:CD2	1:A:134:LEU:H	2.21	0.48
1:B:777:LEU:CD2	1:B:889:ALA:HA	2.43	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:C:65:ALA:HB1	1:C:66:PRO:CD	2.43	0.48
1:A:282:ARG:HG3	1:D:420:MET:O	2.13	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:B:397:LEU:O	1:B:400:THR:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:ARG:NH1	1:C:419:GLY:HA2	2.19	0.48
1:C:242:ALA:O	1:C:291:LEU:N	2.46	0.48
1:D:62:TRP:HB2	1:D:95:TYR:HD2	1.78	0.48
1:A:62:TRP:HZ2	1:A:119:PRO:HB3	1.78	0.48
1:B:80:GLU:CD	1:B:80:GLU:H	2.16	0.48
1:C:387:VAL:HG11	1:C:398:TRP:HZ2	1.79	0.48
1:A:995:GLY:H	1:A:1002:SER:HB2	1.78	0.48
1:C:689:GLU:O	1:C:690:SER:O	2.31	0.48
1:A:360:HIS:HA	1:A:361:PRO:HD3	1.57	0.48
1:C:685:LEU:CD2	1:C:686:PRO:HD3	2.38	0.48
1:A:683:PRO:O	1:A:685:LEU:N	2.46	0.48
1:C:367:MET:HE2	1:C:372:MET:HG2	1.96	0.48
1:A:822:LEU:HD11	1:A:824:GLN:O	2.14	0.48
1:B:126:THR:HA	1:B:182:ASN:O	2.13	0.48
1:A:897:TRP:CE2	1:A:918:TRP:HD1	2.30	0.48
1:C:995:GLY:O	1:C:996:ASP:C	2.50	0.48
1:D:309:TYR:CD1	1:D:309:TYR:N	2.81	0.48
1:A:769:TRP:HA	1:A:773:LYS:O	2.12	0.48
1:A:360:HIS:CE1	1:A:362:LEU:HB2	2.48	0.48
1:B:598:ASP:C	1:B:599:ARG:HG3	2.34	0.48
1:C:141:ILE:HD13	1:C:143:PHE:CZ	2.48	0.48
1:B:581:ASN:ND2	1:B:583:ASN:ND2	2.61	0.48
1:D:949:HIS:HB2	1:D:951:TRP:CZ3	2.48	0.48
1:C:429:ASP:OD1	1:C:431[B]:ARG:HG3	2.13	0.48
1:D:937:LEU:HG	1:D:938:ARG:N	2.28	0.48
1:D:853:ARG:NH1	1:D:871:GLU:OE2	2.47	0.48
1:C:58:TRP:HE3	1:C:123:TYR:HB3	1.78	0.48
1:D:638:VAL:HG23	1:D:678:GLN:O	2.13	0.48
1:C:730:LEU:CD1	1:C:730:LEU:H	2.15	0.48
1:B:838:THR:HG21	3:B:4178:HOH:O	2.14	0.48
1:A:786:ARG:HG2	1:A:880:ALA:CB	2.41	0.48
1:B:807:VAL:HA	1:B:810:TRP:CE3	2.49	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:D:769:TRP:NE1	1:D:774:LYS:HE2	2.28	0.48
1:C:229:THR:HG22	1:C:240:LEU:HA	1.95	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:C:929:TYR:HB3	3:C:4108:HOH:O	2.12	0.48
1:A:434:PRO:O	1:A:437:SER:HB3	2.14	0.48
1:B:92:MET:O	1:B:93:HIS:HD2	1.97	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105:TYR:CZ	1:D:199:ASP:HB2	2.48	0.48
1:B:721:ARG:HH11	1:B:721:ARG:HB2	1.79	0.48
1:A:696:LEU:C	1:A:696:LEU:HD12	2.34	0.48
1:C:944:LEU:O	1:C:950:GLN:HA	2.13	0.48
1:A:823:LEU:CD2	1:B:728:VAL:HG12	2.44	0.48
1:D:937:LEU:HG	1:D:938:ARG:H	1.76	0.48
1:B:441:THR:HG22	1:B:474:TRP:CH2	2.48	0.48
1:B:683:PRO:O	1:B:684:GLU:C	2.51	0.48
1:D:143:PHE:O	1:D:168:PRO:HA	2.14	0.48
1:C:652:LEU:CB	1:C:670:LEU:HD21	2.43	0.48
1:C:287:ASP:N	1:C:287:ASP:OD1	2.33	0.48
1:B:255:ARG:HB2	1:B:316:HIS:NE2	2.29	0.48
1:C:133:TRP:N	1:C:133:TRP:CD1	2.80	0.48
1:B:737:ILE:HG13	1:B:738:PRO:N	2.19	0.48
1:B:908:ASP:OD1	1:B:993:ILE:HG12	2.13	0.48
1:D:867:THR:HG22	1:D:867:THR:O	2.13	0.48
1:C:292:ARG:HG3	1:C:292:ARG:NH1	2.27	0.48
1:A:592:PHE:HB2	1:A:594:ASP:OD1	2.14	0.48
1:C:869:ASP:OD1	1:C:1015:HIS:ND1	2.42	0.48
1:A:549:PHE:CE2	1:A:620:ALA:HA	2.49	0.48
1:D:757:GLN:O	1:D:765:LEU:HD12	2.14	0.48
1:B:91:GLN:HE21	1:B:190:ARG:NH1	2.10	0.48
1:B:62:TRP:CD1	1:B:95:TYR:HB3	2.48	0.48
1:B:721:ARG:HH11	1:B:721:ARG:CB	2.27	0.48
1:C:598:ASP:C	1:C:599:ARG:HG2	2.34	0.48
1:B:254:LEU:C	1:B:255:ARG:HH11	2.16	0.48
1:C:190:ARG:HG3	1:C:206:SER:OG	2.13	0.48
1:C:767:GLN:CG	1:C:768:MET:N	2.75	0.48
1:A:823:LEU:HD12	1:A:839:ALA:HB1	1.95	0.48
1:C:510:GLN:N	1:C:511:PRO:HD3	2.28	0.48
1:D:141:ILE:O	1:D:170:GLU:HA	2.13	0.48
1:B:409:VAL:HG23	1:B:452:SER:HB2	1.95	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:D:972:HIS:HB2	1:D:974:HIS:CE1	2.49	0.48
1:A:241:GLU:HG3	1:A:292:ARG:HG3	1.96	0.48
1:A:173:LEU:O	1:A:174:SER:C	2.51	0.48
1:A:100:TYR:HB2	1:A:203:TRP:CD2	2.49	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:B:26:ARG:HD2	1:B:169:SER:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:637:GLU:HB2	1:D:679:LEU:HD21	1.95	0.48
1:D:352:ARG:HB2	1:D:385:ASN:CB	2.35	0.48
1:B:9:VAL:CG1	1:B:10:VAL:N	2.77	0.48
1:D:144:ASP:HB2	1:D:211:ASP:H	1.79	0.48
1:A:897:TRP:CE2	1:A:918:TRP:CD1	3.02	0.48
1:B:210:ARG:NH1	1:B:358:GLU:OE1	2.47	0.48
1:A:577:LYS:O	1:A:584:PRO:HA	2.13	0.48
1:B:349:LEU:O	1:B:563:GLN:HB3	2.14	0.48
1:D:638:VAL:CG2	1:D:678:GLN:HB3	2.44	0.47
1:D:588:TYR:O	1:D:589:GLY:C	2.52	0.47
1:B:30:HIS:ND1	1:B:33:PHE:CD1	2.82	0.47
1:D:889:ALA:HB3	1:D:890:GLN:HE22	1.79	0.47
1:B:651:LEU:O	1:B:701:VAL:N	2.32	0.47
1:A:897:TRP:HA	1:A:943:GLU:O	2.14	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:A:456:TRP:O	1:A:484:VAL:HA	2.14	0.47
1:B:105:TYR:CE2	1:B:196:TYR:HA	2.49	0.47
1:A:889:ALA:O	1:A:890:GLN:C	2.51	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:D:906:TYR:OH	1:D:935:ASN:HA	2.13	0.47
1:C:657:ALA:O	1:C:694:LEU:HD12	2.13	0.47
1:D:740:LEU:HA	1:D:748:CYS:O	2.14	0.47
1:D:610:ASP:OD2	1:D:612:THR:HG23	2.14	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:D:153:TRP:HA	1:D:157:ARG:O	2.13	0.47
1:A:763:GLY:HA3	1:A:822:LEU:HD23	1.93	0.47
1:C:894:ARG:CZ	1:C:921:PRO:HD3	2.44	0.47
1:D:55:ASN:ND2	1:D:87:PRO:HD3	2.28	0.47
1:D:1020:TRP:CD1	1:D:1021:CYS:N	2.79	0.47
1:C:7:LEU:HB2	1:C:71:GLU:CD	2.34	0.47
1:A:906:TYR:CE2	1:A:937:LEU:HB2	2.48	0.47
1:D:749:ILE:O	1:D:755:ARG:HA	2.14	0.47
1:D:515:VAL:N	1:D:516:PRO:HD3	2.29	0.47
1:A:285:TYR:HB2	1:A:288:ARG:HB2	1.95	0.47
1:C:619:GLU:HA	1:C:912:ALA:HB2	1.97	0.47
1:C:100:TYR:CB	1:C:203:TRP:CE3	2.96	0.47
1:C:653[A]:HIS:ND1	1:C:667:GLU:HG2	2.28	0.47
1:D:282:ARG:CG	1:D:282:ARG:HH11	2.19	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:576:ILE:HD11	1:B:584:PRO:CB	2.44	0.47
1:C:533:LEU:HD12	1:C:533:LEU:C	2.34	0.47
1:B:153:TRP:HA	1:B:159:VAL:HG23	1.96	0.47
1:D:127:PHE:HE1	1:D:129:VAL:CG2	2.28	0.47
1:B:429:ASP:OD1	1:B:431[A]:ARG:HD3	2.15	0.47
1:B:51:LEU:CD1	1:B:215:LEU:HB2	2.44	0.47
1:C:610:ASP:O	1:C:611:ARG:HB2	2.15	0.47
1:D:742:THR:CG2	1:D:743:SER:N	2.78	0.47
1:C:84:VAL:HG13	1:C:85:VAL:O	2.14	0.47
1:C:506:VAL:HG22	1:C:520:ILE:HD11	1.97	0.47
1:B:902:PRO:O	1:B:938:ARG:NH1	2.44	0.47
1:D:943:GLU:HG2	1:D:944:LEU:N	2.27	0.47
1:A:928:PRO:CB	1:A:973:ARG:NH1	2.72	0.47
1:B:559:TYR:CD1	1:B:559:TYR:N	2.80	0.47
1:A:316:HIS:HB2	1:A:321:THR:O	2.14	0.47
1:B:425:ARG:HH22	1:C:287:ASP:CG	2.17	0.47
1:B:4:THR:O	1:B:9:VAL:HG11	2.13	0.47
1:D:331:GLY:HA3	1:D:451:PRO:CB	2.44	0.47
1:D:403:ASP:OD1	1:D:452:SER:OG	2.26	0.47
1:B:567:VAL:CG1	1:B:568:TRP:N	2.78	0.47
1:D:749:ILE:HG22	1:D:750:GLU:N	2.29	0.47
1:A:417:THR:O	1:A:418:HIS:C	2.49	0.47
1:C:99:ILE:HG22	1:C:101:THR:HG22	1.97	0.47
1:C:791:ASN:N	3:C:4072:HOH:O	2.40	0.47
1:B:904:GLU:HB2	1:B:936:GLY:HA2	1.97	0.47
1:C:146:VAL:O	1:C:165:SER:HA	2.14	0.47
1:A:1017:GLN:O	1:A:1018:LEU:HD23	2.15	0.47
1:B:278:ILE:N	1:B:278:ILE:HD12	2.29	0.47
1:B:98:PRO:HB3	1:B:205:MET:HG2	1.97	0.47
1:A:100:TYR:CD2	1:A:602:CYS:HB3	2.50	0.47
1:B:153:TRP:NE1	1:B:158:TRP:HB2	2.30	0.47
1:C:36:TRP:CD1	1:C:41:GLU:CB	2.98	0.47
1:B:737:ILE:C	1:B:751:LEU:HD12	2.34	0.47
1:D:881:ARG:HD2	3:D:4054:HOH:O	2.14	0.47
1:A:897:TRP:NE1	1:A:918:TRP:HD1	2.12	0.47
1:D:697:THR:CG2	1:D:698:VAL:N	2.78	0.47
1:B:941:THR:HG22	1:B:955:PHE:CZ	2.49	0.47
1:C:659:ASP:HB2	1:C:661:LYS:HE3	1.96	0.47
1:B:850:PHE:HD2	1:B:872:VAL:HG13	1.80	0.47
1:C:309:TYR:CD1	1:C:309:TYR:N	2.83	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:D:758:PHE:HZ	1:D:864:MET:HE1	1.80	0.47
1:D:166:ARG:CG	1:D:392:TYR:HB2	2.43	0.47
1:D:955:PHE:CD2	1:D:955:PHE:N	2.83	0.47
1:D:230:ARG:NH1	1:D:230:ARG:HG3	2.12	0.47
1:D:230:ARG:NH1	1:D:230:ARG:CG	2.76	0.47
1:B:559:TYR:HA	1:B:560:PRO:HD2	1.69	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:A:66:PRO:HD3	1:A:118:ASN:HB3	1.97	0.47
1:B:842:TRP:CH2	1:B:852:SER:HB2	2.47	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:C:778:THR:CG2	1:C:779:PRO:N	2.78	0.47
1:A:822:LEU:HD11	1:A:824:GLN:C	2.34	0.47
1:C:133:TRP:CZ3	1:C:216:HIS:HB2	2.50	0.47
1:A:666:GLY:C	1:A:667:GLU:HG2	2.33	0.47
1:D:767:GLN:CG	1:D:768:MET:N	2.77	0.47
1:C:234:ASP:OD1	1:C:236:SER:OG	2.29	0.47
1:D:737:ILE:HG13	1:D:738:PRO:HD2	1.97	0.47
1:B:961:ARG:O	1:B:979:GLU:HG3	2.15	0.47
1:D:76:CYS:HA	3:D:4520:HOH:O	2.13	0.47
1:B:983:TRP:HA	1:B:983:TRP:CE3	2.49	0.47
1:C:143:PHE:CD1	1:C:143:PHE:N	2.83	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:C:250:LEU:HD11	1:C:287:ASP:HA	1.95	0.47
1:D:685:LEU:O	1:D:686:PRO:O	2.32	0.47
1:C:375:ASP:O	1:C:376:ILE:C	2.52	0.47
1:B:848:THR:C	1:B:849:LEU:HD23	2.35	0.47
1:A:937:LEU:HA	1:A:958:ASN:HB3	1.97	0.47
1:B:281:GLU:HG3	1:C:515:VAL:HG21	1.96	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:B:253:TYR:O	1:B:318:ALA:N	2.41	0.47
1:D:619:GLU:HA	1:D:912:ALA:HB2	1.96	0.47
1:C:105:TYR:CE1	1:C:419:GLY:HA3	2.50	0.47
1:A:597:ASN:ND2	1:A:599:ARG:H	2.13	0.47
1:C:778:THR:HG23	1:C:779:PRO:HD2	1.97	0.47
1:A:778:THR:HA	1:A:779:PRO:HD3	1.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:645:ARG:HH22	1:C:650:GLU:CD	2.18	0.47
1:A:77:ASP:HA	3:A:4068:HOH:O	2.15	0.47
1:C:708:TRP:CE3	1:C:709:SER:HB3	2.49	0.47
1:C:651:LEU:CD2	1:C:653[A]:HIS:HE1	2.28	0.47
1:B:656:VAL:CG1	1:B:694:LEU:HD11	2.42	0.47
1:D:74:LEU:HD21	1:D:153:TRP:CE2	2.49	0.47
1:C:77:ASP:C	1:C:78:LEU:HD23	2.36	0.47
1:C:217:LYS:HG2	1:C:218:PRO:CD	2.43	0.47
1:B:701:VAL:HG12	1:B:702:GLN:N	2.29	0.47
1:B:550:ALA:O	1:B:553:TRP:N	2.48	0.47
1:C:647:SER:OG	1:C:672:VAL:HG23	2.15	0.47
1:D:617:LEU:HA	1:D:617:LEU:HD12	1.72	0.47
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:649:ASN:O	1:C:702:GLN:HA	2.15	0.46
1:C:403:ASP:OD2	1:C:450:HIS:ND1	2.47	0.46
1:C:897:TRP:CH2	1:C:918:TRP:HB2	2.50	0.46
1:C:91:GLN:HG2	1:C:98:PRO:HA	1.96	0.46
1:A:278:ILE:CG2	1:A:279:ILE:N	2.78	0.46
1:D:229:THR:HA	1:D:239:VAL:O	2.15	0.46
1:C:721:ARG:NH1	1:C:721:ARG:HB2	2.31	0.46
1:C:970:THR:CG2	1:C:975:LEU:HB2	2.46	0.46
1:B:282:ARG:HG2	1:C:423:MET:HB2	1.97	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:571:VAL:HG12	1:A:609:ALA:HA	1.96	0.46
1:B:652:LEU:HA	1:B:699:ARG:O	2.15	0.46
1:A:223:SER:HB3	1:A:247:CYS:HB2	1.97	0.46
1:B:1014:TYR:HE1	3:B:4057:HOH:O	1.96	0.46
1:D:1011:ALA:HB3	1:D:1014:TYR:CZ	2.50	0.46
1:C:899:GLY:O	1:C:915:PHE:HA	2.16	0.46
1:D:99:ILE:O	1:D:203:TRP:HA	2.16	0.46
1:C:102:ASN:C	1:C:102:ASN:HD22	2.19	0.46
1:D:661:LYS:HA	1:D:662:PRO:HD3	1.70	0.46
1:D:52[A]:ARG:HG2	1:D:52[A]:ARG:NH1	2.30	0.46
1:D:568:TRP:CD2	1:D:569:ASP:HB3	2.50	0.46
1:D:86:VAL:HA	1:D:87:PRO:C	2.34	0.46
1:B:883:GLY:HA2	1:B:1016:TYR:CZ	2.49	0.46
1:D:455:ILE:HG21	1:D:485:GLN:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:ASP:HA	1:A:480:PRO:HD2	1.48	0.46
1:A:354:VAL:CG2	1:A:355:ASN:N	2.79	0.46
1:D:474:TRP:CZ2	1:D:478:VAL:HG21	2.50	0.46
1:A:927:THR:HA	1:A:928:PRO:HD3	1.47	0.46
1:B:782:ASP:HB2	1:B:842:TRP:HZ2	1.79	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:D:658:LEU:HD23	1:D:661:LYS:HZ2	1.80	0.46
1:D:78:LEU:HB2	1:D:81:ALA:HB2	1.98	0.46
1:B:4:THR:C	1:B:9:VAL:HG11	2.35	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:A:333:ARG:NH1	1:A:453:VAL:O	2.49	0.46
1:A:867:THR:HG22	1:A:867:THR:O	2.16	0.46
1:C:733:ALA:O	1:C:734:SER:C	2.54	0.46
1:B:730:LEU:HD12	1:B:730:LEU:N	2.16	0.46
1:A:38:ASN:HD21	1:A:40:GLU:CB	2.29	0.46
1:B:721:ARG:CB	1:B:721:ARG:NH1	2.78	0.46
1:B:740:LEU:HD13	1:B:749:ILE:HD11	1.96	0.46
1:B:274:PHE:HB3	1:B:286:ALA:O	2.16	0.46
1:D:355:ASN:OD1	1:D:388:ARG:HD3	2.16	0.46
1:C:721:ARG:CG	1:C:721:ARG:NH1	2.78	0.46
1:D:836:ILE:CG2	1:D:837:THR:N	2.78	0.46
1:D:588:TYR:CD2	1:D:603:MET:CE	2.99	0.46
1:A:701:VAL:HG12	1:A:702:GLN:N	2.31	0.46
1:B:738:PRO:HA	1:B:751:LEU:HB2	1.97	0.46
1:D:925:MET:HE3	1:D:938:ARG:CZ	2.45	0.46
1:C:959:ILE:O	1:C:959:ILE:HG23	2.14	0.46
1:C:362:LEU:CG	1:C:576:ILE:HD12	2.45	0.46
1:C:721:ARG:CB	1:C:721:ARG:NH1	2.79	0.46
1:B:375:ASP:HB3	1:B:379:MET:HE3	1.96	0.46
1:B:399:TYR:O	1:B:400:THR:C	2.53	0.46
1:B:246:MET:CE	1:B:287:ASP:HB3	2.45	0.46
1:D:73:TRP:CH2	1:D:187:MET:HB3	2.51	0.46
1:B:38:ASN:ND2	1:B:41:GLU:HB2	2.30	0.46
1:C:486:TYR:O	1:C:496:THR:HB	2.16	0.46
1:B:770:ILE:HG22	1:B:770:ILE:O	2.16	0.46
1:C:788:PRO:O	1:C:933:SER:HB2	2.16	0.46
1:D:463:GLY:HA2	3:D:7505:HOH:O	2.16	0.46
1:C:333:ARG:NH1	1:C:451:PRO:O	2.43	0.46
1:D:999:TRP:N	1:D:999:TRP:CD2	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:646:HIS:NE2	1:B:671:ASP:OD1	2.41	0.46
1:A:755:ARG:O	1:A:768:MET:HA	2.16	0.46
1:A:26:ARG:HD2	1:A:169:SER:HB3	1.97	0.46
1:C:600:GLN:NE2	1:C:790:ASP:OD1	2.49	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:D:421:VAL:O	1:D:425:ARG:HD2	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:A:394:ASN:O	1:A:395:HIS:C	2.52	0.46
1:B:538:TYR:O	1:B:539:ALA:HB3	2.15	0.46
1:D:536:CYS:C	1:D:537:GLU:HG3	2.36	0.46
1:B:367:MET:HE2	1:B:372:MET:HG2	1.97	0.46
1:A:255:ARG:N	1:A:316:HIS:O	2.45	0.46
1:D:352:ARG:HD2	1:D:352:ARG:HH11	1.58	0.46
1:A:118:ASN:O	1:A:120:THR:N	2.49	0.46
1:C:663:LEU:O	1:C:664:ALA:HB2	2.16	0.46
1:B:777:LEU:HD21	1:B:889:ALA:CA	2.46	0.46
1:C:920:LEU:CB	1:C:921:PRO:CD	2.94	0.46
1:C:37:ARG:HH22	1:C:216:HIS:CD2	2.34	0.46
1:C:906:TYR:HB3	1:C:907:PRO:CD	2.45	0.46
1:C:380:LYS:HE3	1:C:406:GLY:O	2.15	0.46
1:A:209:PHE:H	1:A:209:PHE:HD2	1.61	0.46
1:A:125:LEU:O	1:A:183:ARG:HA	2.15	0.46
1:A:7:LEU:O	1:A:11:LEU:HG	2.15	0.46
1:C:232:ASN:O	1:C:233:ASP:C	2.53	0.46
1:C:568:TRP:C	1:C:568:TRP:CD1	2.89	0.46
1:A:436:MET:O	1:A:437:SER:C	2.52	0.46
1:C:420:MET:CE	1:C:426:LEU:HG	2.46	0.46
1:C:418:HIS:CG	1:C:461:GLU:HG3	2.51	0.46
1:A:696:LEU:HD12	1:A:697:THR:H	1.77	0.46
1:A:14:ARG:HG2	1:A:16:TRP:CZ2	2.50	0.46
1:B:881:ARG:O	1:B:882:ILE:HG13	2.16	0.46
1:A:764:PHE:CE2	1:A:840:HIS:CE1	3.04	0.46
1:C:842:TRP:N	1:C:842:TRP:HE3	2.14	0.46
1:C:689:GLU:O	1:C:690:SER:C	2.54	0.46
1:D:897:TRP:HA	1:D:943:GLU:O	2.16	0.46
1:C:331:GLY:N	1:C:451:PRO:HG3	2.31	0.46
1:A:842:TRP:HZ3	1:A:852:SER:HB3	1.81	0.46
1:A:111:PRO:HA	1:A:112:PRO:HA	1.55	0.46
1:A:679:LEU:HD23	1:A:679:LEU:N	2.04	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:654:TRP:CE2	1:D:666:GLY:N	2.85	0.45
1:B:422:PRO:HG2	1:B:424:ASN:CB	2.46	0.45
1:A:742:THR:CG2	1:A:743:SER:N	2.78	0.45
1:B:548:GLY:O	1:B:549:PHE:C	2.54	0.45
1:B:429:ASP:OD1	1:B:430:PRO:HD2	2.16	0.45
1:A:424:ASN:HB3	1:D:285:TYR:OH	2.16	0.45
1:C:299:LYS:HB2	1:C:309:TYR:OH	2.16	0.45
1:A:150:PHE:HB3	1:A:188:VAL:HA	1.97	0.45
1:C:225:PHE:HA	1:C:243:GLU:O	2.16	0.45
1:C:433:LEU:HA	1:C:433:LEU:HD12	1.64	0.45
1:B:89:ASN:O	1:B:92:MET:N	2.45	0.45
1:C:420:MET:HE3	1:C:425:ARG:HB3	1.96	0.45
1:B:656:VAL:O	1:B:657:ALA:HB2	2.15	0.45
1:D:133:TRP:O	1:D:134:LEU:HD23	2.17	0.45
1:C:499:ILE:HD11	1:C:529:GLU:CD	2.35	0.45
1:D:38:ASN:ND2	1:D:41:GLU:CG	2.79	0.45
1:A:737:ILE:CD1	1:A:832:ASP:HA	2.46	0.45
1:B:256:VAL:HG12	1:B:257:THR:N	2.32	0.45
1:B:970:THR:HG22	1:B:972:HIS:O	2.16	0.45
1:A:997:ASP:O	1:A:1002:SER:OG	2.34	0.45
1:D:999:TRP:N	1:D:999:TRP:CE3	2.84	0.45
1:B:292:ARG:HH11	1:B:292:ARG:CG	2.29	0.45
1:B:777:LEU:HG	1:B:889:ALA:HA	1.98	0.45
1:D:95:TYR:HD1	1:D:95:TYR:H	1.63	0.45
1:B:416:GLU:OE1	1:B:418:HIS:HB2	2.16	0.45
1:D:768:MET:HG2	1:D:775:GLN:HB2	1.97	0.45
1:D:455:ILE:CG2	1:D:456:TRP:N	2.78	0.45
1:A:479:ASP:N	1:A:480:PRO:HD3	2.31	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:C:603:MET:HE3	1:C:930:VAL:HB	1.98	0.45
1:A:38:ASN:O	1:A:39:SER:C	2.54	0.45
1:A:24:LEU:HD12	1:A:24:LEU:HA	1.52	0.45
1:A:202:MET:CE	1:A:365:GLN:NE2	2.79	0.45
1:B:421:VAL:O	1:B:425:ARG:NH1	2.39	0.45
1:B:3:ILE:C	1:B:5:ASP:H	2.20	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:C:303:ALA:CB	1:C:408:TYR:CZ	3.00	0.45
1:B:352:ARG:CZ	1:B:626:PHE:CE2	2.99	0.45
1:A:767:GLN:CG	1:A:768:MET:H	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:767:GLN:CG	1:A:768:MET:N	2.79	0.45
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:C:147:ASN:HA	1:C:148:SER:HA	1.73	0.45
1:C:37:ARG:HG2	1:C:50:GLN:NE2	2.30	0.45
1:D:649:ASN:OD1	1:D:703:PRO:HD2	2.17	0.45
1:B:84:VAL:CG1	1:B:85:VAL:N	2.79	0.45
1:D:147:ASN:HB2	1:D:209:PHE:CE2	2.51	0.45
1:B:7:LEU:CD2	1:B:74:LEU:HD11	2.31	0.45
1:D:599:ARG:HB2	1:D:600:GLN:H	1.43	0.45
1:B:91:GLN:NE2	1:B:190:ARG:CZ	2.79	0.45
1:B:661:LYS:HA	1:B:662:PRO:HD2	1.62	0.45
1:C:258:VAL:HB	1:C:291:LEU:HD11	1.99	0.45
1:C:455:ILE:CG2	1:C:456:TRP:N	2.80	0.45
1:D:127:PHE:CE1	1:D:129:VAL:HG22	2.51	0.45
1:B:587:ALA:HB1	1:B:592:PHE:HE1	1.80	0.45
1:B:807:VAL:HA	1:B:810:TRP:HE3	1.81	0.45
1:A:137:GLY:HA3	1:A:216:HIS:CE1	2.51	0.45
1:B:240:LEU:HD23	1:B:240:LEU:C	2.36	0.45
1:B:814:GLY:O	1:B:818:ALA:N	2.49	0.45
1:A:297:ASN:N	1:A:298:PRO:CD	2.77	0.45
1:C:679:LEU:HD23	1:C:679:LEU:HA	1.81	0.45
1:D:407:LEU:HD23	1:D:407:LEU:HA	1.58	0.45
1:A:67:GLU:H	1:A:67:GLU:HG2	1.20	0.45
1:B:734:SER:HB3	1:B:860:GLY:CA	2.18	0.45
1:A:260:LEU:HD12	1:A:261:TRP:N	2.32	0.45
1:B:246:MET:HE1	1:B:287:ASP:HB3	1.99	0.45
1:A:377:LEU:HB3	1:A:381:GLN:HE22	1.82	0.45
1:D:658:LEU:O	1:D:661:LYS:HD2	2.17	0.45
1:A:789:LEU:HD11	1:A:993:ILE:CG2	2.41	0.45
1:D:786:ARG:NH2	1:D:792:ASP:OD1	2.44	0.45
1:C:570:TRP:CD1	1:C:571:VAL:CG2	2.99	0.45
1:D:824:GLN:CG	1:D:825:CYS:N	2.78	0.45
1:D:868:VAL:CG1	1:D:869:ASP:N	2.79	0.45
1:B:930:VAL:O	1:B:932:PRO:HD3	2.16	0.45
1:C:694:LEU:HD12	1:C:695:TRP:N	2.32	0.45
1:D:130:ASP:O	1:D:131:GLU:C	2.53	0.45
1:D:217:LYS:NZ	1:D:324:GLU:OE1	2.49	0.45
1:A:110:ASN:O	1:A:113:PHE:N	2.32	0.45
1:D:279:ILE:HD13	1:D:279:ILE:HG21	1.74	0.45
1:B:588:TYR:O	1:B:589:GLY:C	2.53	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:256:VAL:O	1:C:272:ALA:N	2.41	0.45
1:C:835:LEU:C	1:C:835:LEU:HD12	2.37	0.45
1:D:85:VAL:C	1:D:86:VAL:HG23	2.37	0.45
1:B:789:LEU:H	1:B:789:LEU:HG	1.66	0.45
1:B:408:TYR:HB3	1:B:454:ILE:CD1	2.47	0.45
1:D:769:TRP:HA	1:D:773:LYS:O	2.17	0.45
1:B:850:PHE:HA	1:B:871:GLU:O	2.16	0.45
1:A:449:ASN:HB2	3:A:4055:HOH:O	2.17	0.45
1:A:814:GLY:HA2	3:A:4138:HOH:O	2.16	0.45
1:D:507:ASP:OD1	1:D:521:LYS:HE2	2.17	0.45
1:C:545:SER:HB3	1:C:546:LEU:H	1.50	0.45
1:A:1023:LYS:HB2	1:A:1023:LYS:HE2	1.58	0.45
1:D:100:TYR:HB2	1:D:203:TRP:CE2	2.52	0.45
1:B:967:LEU:HA	1:B:967:LEU:HD23	1.56	0.45
1:C:256:VAL:CG1	1:C:257:THR:N	2.80	0.45
1:D:5:ASP:OD2	1:D:157:ARG:HG3	2.16	0.45
1:C:192:SER:O	1:C:195:SER:HB2	2.17	0.45
1:D:287:ASP:N	1:D:287:ASP:OD1	2.50	0.45
1:D:455:ILE:HG22	1:D:456:TRP:N	2.31	0.45
1:D:69:VAL:HG13	1:D:70:PRO:HD2	1.99	0.45
1:D:387:VAL:O	1:D:409:VAL:HA	2.17	0.45
1:D:571:VAL:HG11	1:D:611:ARG:NH1	2.32	0.45
1:A:360:HIS:CG	1:A:361:PRO:CD	3.00	0.45
1:B:694:LEU:O	1:B:721:ARG:HG3	2.17	0.45
1:A:608:PHE:HD1	1:A:612:THR:O	2.00	0.45
1:A:129:VAL:HG23	1:A:182:ASN:HD22	1.82	0.45
1:B:234:ASP:OD1	1:B:236:SER:OG	2.34	0.45
1:A:147:ASN:HA	1:A:148:SER:HA	1.73	0.45
1:D:844:HIS:ND1	1:D:845:GLN:HG2	2.31	0.45
1:C:344:LEU:O	1:C:345:ASN:C	2.54	0.45
1:D:101:THR:HG23	1:D:204:ARG:NH2	2.32	0.44
1:C:427:THR:HG23	1:C:427:THR:H	1.36	0.44
1:B:782:ASP:OD1	1:B:854:LYS:HE3	2.16	0.44
1:D:658:LEU:HA	1:D:693:GLN:O	2.17	0.44
1:A:73:TRP:CE2	1:A:122:CYS:HB3	2.50	0.44
1:C:54:LEU:N	1:C:54:LEU:HD23	2.31	0.44
1:C:78:LEU:O	1:C:79:PRO:C	2.55	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:152:LEU:HG	1:B:159:VAL:HG21	1.98	0.44
1:D:84:VAL:HG22	1:D:93:HIS:CE1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:THR:HG21	1:C:187:MET:SD	2.57	0.44
1:B:227:VAL:HG12	1:B:228:ALA:N	2.32	0.44
1:C:965:GLN:O	1:C:966:GLN:C	2.55	0.44
1:A:876:THR:O	1:A:877:PRO:C	2.55	0.44
1:C:69:VAL:HG13	1:C:70:PRO:HD2	1.99	0.44
1:D:902:PRO:HD3	1:D:918:TRP:CH2	2.52	0.44
1:A:116:THR:HA	3:A:4017:HOH:O	2.17	0.44
1:D:272:ALA:HA	1:D:273:PRO:HD3	1.56	0.44
1:D:757:GLN:CG	1:D:758:PHE:N	2.80	0.44
1:B:397:LEU:HA	1:B:397:LEU:HD12	1.55	0.44
1:D:282:ARG:CG	1:D:282:ARG:NH1	2.79	0.44
1:C:209:PHE:O	1:C:366:VAL:HG13	2.17	0.44
1:B:166:ARG:HG3	1:B:392:TYR:CB	2.46	0.44
1:D:245:GLN:HG2	1:D:288:ARG:HG2	1.99	0.44
1:C:448:ARG:HH21	1:C:478:VAL:HG13	1.82	0.44
1:D:928:PRO:HB2	1:D:973:ARG:NH1	2.32	0.44
1:B:529:GLU:HG2	3:B:4084:HOH:O	2.17	0.44
1:B:935:ASN:N	1:B:935:ASN:HD22	2.16	0.44
1:A:949:HIS:HD2	1:A:1022:GLN:HE21	1.64	0.44
1:A:436:MET:HE1	1:A:467:ASN:ND2	2.31	0.44
1:B:395:HIS:HA	1:B:396:PRO:HD3	1.75	0.44
1:C:43:ARG:NH1	1:C:263:GLY:O	2.51	0.44
1:B:654:TRP:N	1:B:666:GLY:O	2.50	0.44
1:D:416:GLU:CD	1:D:461:GLU:HG3	2.37	0.44
1:B:929:TYR:HB3	3:B:4090:HOH:O	2.16	0.44
1:D:696:LEU:C	1:D:696:LEU:HD12	2.37	0.44
1:A:44:THR:O	1:A:45:ASP:C	2.54	0.44
1:D:856:TYR:CD1	1:D:856:TYR:N	2.84	0.44
1:D:559:TYR:HB2	1:D:562:LEU:CG	2.46	0.44
1:D:100:TYR:CD1	1:D:602:CYS:HB3	2.53	0.44
1:B:287:ASP:OD1	1:C:425:ARG:NH2	2.47	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:225:PHE:CB	1:B:244:VAL:HG13	2.40	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
1:A:303:ALA:HB2	1:A:408:TYR:CZ	2.52	0.44
1:A:904:GLU:O	1:A:904:GLU:HG2	2.17	0.44
1:D:202:MET:O	1:D:204:ARG:HD3	2.18	0.44
1:C:568:TRP:CD2	1:C:569:ASP:HB3	2.53	0.44
1:A:309:TYR:N	1:A:309:TYR:CD1	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:ARG:O	1:C:421:VAL:HG13	2.17	0.44
1:A:658:LEU:HD12	1:A:693:GLN:O	2.17	0.44
1:B:140:ARG:HB2	1:B:171:PHE:O	2.17	0.44
1:A:60:PHE:HE1	1:A:121:GLY:HA3	1.83	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:A:843:GLN:HB3	1:A:847:LYS:O	2.17	0.44
1:C:618:THR:HG22	1:C:912:ALA:CB	2.48	0.44
1:D:482:ARG:HA	1:D:483:PRO:HD2	1.62	0.44
1:A:344:LEU:HG	1:A:345:ASN:N	2.32	0.44
1:A:868:VAL:HG12	1:A:869:ASP:N	2.32	0.44
1:C:814:GLY:O	1:C:818:ALA:N	2.39	0.44
1:D:961:ARG:HB3	1:D:961:ARG:HE	1.73	0.44
1:B:836:ILE:O	1:B:855:THR:HA	2.18	0.44
1:A:658:LEU:HD11	1:A:692:GLY:O	2.18	0.44
1:C:455:ILE:HG21	1:C:485:GLN:HG2	2.00	0.44
1:D:471:LEU:HA	1:D:471:LEU:HD23	1.57	0.44
1:C:869:ASP:CG	1:C:1015:HIS:HD1	2.20	0.44
1:C:500:CYS:HA	1:C:534:ILE:O	2.17	0.44
1:C:758:PHE:CD1	1:C:758:PHE:N	2.85	0.44
1:B:948:PRO:O	1:B:1022:GLN:HA	2.17	0.44
1:D:678:GLN:O	1:D:679:LEU:HD23	2.17	0.44
1:D:238:ALA:CB	1:D:332:PHE:CE2	3.00	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:D:658:LEU:CD2	1:D:661:LYS:NZ	2.80	0.44
1:A:105:TYR:HA	1:A:106:PRO:HD3	1.87	0.44
1:B:422:PRO:HD2	1:C:285:TYR:CE2	2.53	0.44
1:D:64:PRO:O	1:D:65:ALA:HB2	2.17	0.44
1:D:936:GLY:O	1:D:937:LEU:C	2.55	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:D:242:ALA:O	1:D:290:THR:HA	2.17	0.44
1:B:229:THR:HA	1:B:239:VAL:O	2.17	0.44
1:C:967:LEU:HD11	3:C:4016:HOH:O	2.17	0.44
1:A:767:GLN:HG3	1:A:768:MET:H	1.83	0.44
1:D:202:MET:HE3	1:D:357:HIS:HD2	1.83	0.44
1:D:673:ALA:O	1:D:676:GLY:N	2.45	0.44
1:A:260:LEU:CD1	1:A:309:TYR:HB3	2.48	0.44
1:B:93:HIS:HB3	1:B:95:TYR:HE1	1.83	0.44
1:B:600:GLN:O	1:B:602:CYS:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:658:LEU:HD12	1:B:659:ASP:H	1.83	0.44
1:C:395:HIS:CE1	1:C:396:PRO:HD2	2.53	0.44
1:B:652:LEU:HD12	1:B:652:LEU:C	2.37	0.44
1:D:118:ASN:O	1:D:119:PRO:C	2.55	0.44
1:D:949:HIS:CB	1:D:951:TRP:CH2	3.01	0.44
1:A:663:LEU:O	1:A:664:ALA:HB2	2.18	0.44
1:B:258:VAL:HG22	1:B:313:VAL:HG22	2.00	0.44
1:B:213:SER:C	1:B:214:LEU:HD23	2.37	0.44
1:B:570:TRP:CE3	1:B:570:TRP:HA	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:A:588:TYR:CD2	1:A:603:MET:CE	3.01	0.44
1:B:18:ASN:HA	1:B:19:PRO:HD3	1.76	0.44
1:B:925:MET:HB3	3:B:4027:HOH:O	2.18	0.44
1:A:260:LEU:HD11	1:A:309:TYR:CB	2.48	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:B:212:VAL:CG1	1:B:213:SER:N	2.78	0.44
1:C:866:ILE:O	1:C:1017:GLN:HA	2.18	0.44
1:B:147:ASN:HA	1:B:148:SER:HA	1.60	0.44
1:B:645:ARG:HH22	1:B:650:GLU:CD	2.21	0.43
1:A:261:TRP:CH2	1:A:266:GLN:HB2	2.53	0.43
1:C:418:HIS:ND1	3:C:4156:HOH:O	2.35	0.43
1:C:420:MET:HE1	1:C:426:LEU:CD2	2.48	0.43
1:C:242:ALA:O	1:C:290:THR:HA	2.18	0.43
1:D:11:LEU:HD21	1:D:187:MET:HE2	1.97	0.43
1:B:3:ILE:CG2	1:B:4:THR:N	2.80	0.43
1:C:377:LEU:H	1:C:377:LEU:HG	1.53	0.43
1:B:749:ILE:O	1:B:755:ARG:HA	2.18	0.43
1:B:154:CYS:N	1:B:157:ARG:O	2.42	0.43
1:A:730:LEU:HD22	1:B:823:LEU:HB3	2.00	0.43
1:D:127:PHE:CE1	1:D:129:VAL:CG2	3.01	0.43
1:A:128:ASN:ND2	1:A:181:GLU:HA	2.33	0.43
1:C:463:GLY:O	1:C:488:GLY:HA3	2.18	0.43
1:A:899:GLY:O	1:A:918:TRP:NE1	2.49	0.43
1:D:770:ILE:O	1:D:770:ILE:HG22	2.17	0.43
1:B:278:ILE:H	1:B:278:ILE:HD12	1.81	0.43
1:B:963:SER:HB3	1:B:983:TRP:CZ2	2.53	0.43
1:A:518:TRP:CD1	1:A:526:LEU:HD21	2.53	0.43
1:C:311:ALA:O	1:C:327:ALA:HB1	2.18	0.43
1:B:650:GLU:HG3	1:B:700:VAL:HG13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:ASN:HD21	1:B:189:LEU:HD22	1.82	0.43
1:C:432:TRP:O	1:C:436:MET:HG3	2.17	0.43
1:A:100:TYR:HB3	1:A:589:GLY:HA2	2.00	0.43
1:D:214:LEU:HD23	1:D:214:LEU:HA	1.73	0.43
1:C:246:MET:HE2	1:C:287:ASP:HB2	1.97	0.43
1:C:129:VAL:CG1	1:C:134:LEU:HD21	2.47	0.43
1:B:125:LEU:HD23	1:B:127:PHE:CD2	2.53	0.43
1:C:888:LEU:HA	1:C:888:LEU:HD23	1.75	0.43
1:B:152:LEU:HG	1:B:159:VAL:CG2	2.47	0.43
1:C:830:LEU:HA	1:C:830:LEU:HD12	1.86	0.43
1:D:460:ASN:ND2	1:D:461:GLU:CG	2.78	0.43
1:C:127:PHE:HE2	1:C:184:LEU:HG	1.83	0.43
1:A:525:SER:O	1:A:526:LEU:C	2.54	0.43
1:A:22:THR:HG22	3:A:4063:HOH:O	2.18	0.43
1:B:617:LEU:HD12	1:B:617:LEU:HA	1.81	0.43
1:B:606:LEU:HB3	1:B:617:LEU:HD13	2.00	0.43
1:D:746:ASP:HB3	1:D:757:GLN:HE21	1.84	0.43
1:C:600:GLN:O	1:C:602:CYS:N	2.51	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:876:THR:O	1:C:877:PRO:C	2.54	0.43
1:C:701:VAL:CG1	1:C:702:GLN:N	2.81	0.43
1:B:35:SER:HB2	1:B:217:LYS:HG3	2.00	0.43
1:D:815:HIS:HE1	1:D:877:PRO:O	2.01	0.43
1:C:303:ALA:HB2	1:C:408:TYR:CE2	2.52	0.43
1:A:995:GLY:O	1:A:996:ASP:C	2.56	0.43
1:C:941:THR:HG22	1:C:955:PHE:CZ	2.53	0.43
1:D:1023:LYS:HE3	1:D:1023:LYS:C	2.39	0.43
1:A:766:SER:O	1:A:767:GLN:HB2	2.19	0.43
1:C:232:ASN:OD1	1:C:237:ARG:N	2.45	0.43
1:D:959:ILE:HB	1:D:984:LEU:HD12	1.99	0.43
1:B:398:TRP:HA	1:B:398:TRP:CE3	2.52	0.43
1:C:105:TYR:HB3	1:C:106:PRO:CD	2.42	0.43
1:B:282:ARG:NH1	1:C:419:GLY:CA	2.77	0.43
1:A:599:ARG:NH1	1:A:600:GLN:OE1	2.51	0.43
1:B:472:TYR:CD2	1:B:473:ARG:N	2.86	0.43
1:C:396:PRO:O	1:C:399:TYR:HD1	2.01	0.43
1:C:807:VAL:CG1	1:C:808:GLU:N	2.81	0.43
1:B:629:PHE:HA	1:B:637:GLU:O	2.17	0.43
1:B:941:THR:HG22	1:B:955:PHE:CE1	2.53	0.43
1:D:37:ARG:CD	1:D:50:GLN:NE2	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:899:GLY:HA2	1:C:915:PHE:CD1	2.53	0.43
1:A:615:PRO:HG2	1:A:929:TYR:OH	2.19	0.43
1:D:576:ILE:HA	1:D:576:ILE:HD13	1.79	0.43
1:C:272:ALA:HB1	1:C:273:PRO:CD	2.47	0.43
1:D:653[B]:HIS:NE2	1:D:665:SER:HB2	2.33	0.43
1:D:237:ARG:CG	1:D:237:ARG:NH1	2.82	0.43
1:C:151:HIS:HB3	1:C:153:TRP:CZ3	2.54	0.43
1:A:200:GLN:HA	1:A:416:GLU:OE2	2.17	0.43
1:C:21:VAL:HG12	1:C:21:VAL:O	2.17	0.43
1:A:995:GLY:H	1:A:1002:SER:CB	2.32	0.43
1:D:289:VAL:HG22	1:D:290:THR:N	2.32	0.43
1:D:192:SER:OG	1:D:194:GLY:N	2.51	0.43
1:A:65:ALA:CB	1:A:66:PRO:CD	2.95	0.43
1:C:668:VAL:O	1:C:669:PRO:C	2.52	0.43
1:B:658:LEU:HD22	1:B:688:PRO:HG2	2.01	0.43
1:D:654:TRP:NE1	1:D:666:GLY:CA	2.76	0.43
1:C:870:VAL:CG1	1:C:871:GLU:N	2.80	0.43
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: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:D:802:ASP:O	1:D:808:GLU:HG3	2.19	0.43
1:A:297:ASN:N	1:A:298:PRO:HD3	2.34	0.43
1:B:186:VAL:HG12	1:B:188:VAL:HG23	2.00	0.43
1:B:679:LEU:HD23	1:B:679:LEU:HA	1.60	0.43
1:A:976:LEU:HA	1:A:976:LEU:HD23	1.75	0.43
1:A:69:VAL:HA	1:A:70:PRO:HD3	1.74	0.43
1:B:858:ILE:HD11	1:B:864:MET:HE3	2.00	0.43
1:A:254:LEU:HD23	1:A:254:LEU:HA	1.63	0.43
1:B:261:TRP:CZ2	1:B:266:GLN:HG3	2.53	0.43
1:B:40:GLU:OE2	1:B:43:ARG:NE	2.52	0.43
1:A:240:LEU:HD22	1:A:260:LEU:HD22	1.99	0.43
1:B:141:ILE:O	1:B:170:GLU:HA	2.19	0.43
1:C:685:LEU:HA	1:C:686:PRO:HD3	1.87	0.43
1:C:167:LEU:HD23	1:C:393:PRO:HB2	1.99	0.43
1:A:90:TRP:HE1	1:A:96:ASP:CG	2.21	0.43
1:C:702:GLN:O	1:C:712:GLY:N	2.51	0.43
1:C:11:LEU:HD23	1:C:11:LEU:HA	1.63	0.43
1:C:16:TRP:HA	1:C:161:TYR:OH	2.19	0.43
1:C:253:TYR:O	1:C:318:ALA:N	2.52	0.43
1:A:282:ARG:HG3	1:A:282:ARG:NH1	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:460:ASN:O	1:D:461:GLU:C	2.57	0.43
1:D:350:LEU:HA	1:D:350:LEU:HD12	1.85	0.43
1:D:883:GLY:HA3	1:D:987:ASP:HA	2.01	0.43
1:A:556:PHE:CE1	1:A:564:GLY:HA2	2.53	0.43
1:C:90:TRP:CZ3	1:C:121:GLY:HA3	2.54	0.43
1:B:109:VAL:HG23	3:B:4275:HOH:O	2.18	0.43
1:A:17:GLU:OE2	1:A:114:VAL:N	2.30	0.43
1:B:631:LEU:HG	1:B:632:SER:N	2.27	0.43
1:C:821:ALA:O	1:C:823:LEU:HD23	2.18	0.43
1:A:420:MET:HE2	1:A:426:LEU:CD1	2.49	0.43
1:D:654:TRP:CD1	1:D:666:GLY:HA3	2.53	0.43
1:A:210:ARG:NH1	1:A:358:GLU:OE1	2.52	0.43
1:C:131:GLU:O	1:C:134:LEU:N	2.44	0.43
1:C:40:GLU:O	1:C:43:ARG:N	2.51	0.43
1:C:502:MET:HB2	1:C:537:GLU:HG3	2.00	0.43
1:D:965:GLN:O	1:D:966:GLN:C	2.54	0.43
1:B:416:GLU:HA	1:B:462:SER:OG	2.19	0.43
1:A:58:TRP:CE3	1:A:123:TYR:HB3	2.54	0.43
1:C:227:VAL:HG12	1:C:228:ALA:N	2.33	0.43
1:C:230:ARG:HH21	1:C:241:GLU:CD	2.21	0.43
1:A:98:PRO:HD2	1:A:592:PHE:HB3	2.01	0.43
1:A:719:GLN:HE22	1:A:915:PHE:N	2.16	0.43
1:C:91:GLN:HG2	1:C:98:PRO:CA	2.49	0.43
1:C:600:GLN:HG2	1:C:931:PHE:HB2	2.01	0.43
1:D:240:LEU:O	1:D:292:ARG:HA	2.19	0.43
1:C:685:LEU:HA	1:C:685:LEU:HD23	1.64	0.43
1:D:657:ALA:HB1	1:D:661:LYS:C	2.39	0.43
1:A:546:LEU:HD23	1:A:619:GLU:HB3	2.00	0.43
1:B:152:LEU:O	1:B:159:VAL:N	2.33	0.43
1:C:859:ASP:CG	1:C:861:SER:HG	2.20	0.43
1:A:966:GLN:HB2	1:A:979:GLU:OE2	2.18	0.43
1:A:749:ILE:CD1	1:A:749:ILE:N	2.81	0.43
1:D:424:ASN:ND2	3:D:7510:HOH:O	2.52	0.43
1:A:141:ILE:HG12	1:A:142:ILE: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:D:234:ASP:OD1	1:D:236:SER:OG	2.36	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:778:THR:HB	1:D:887:GLN:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:617:LEU:HA	1:C:617:LEU:HD12	1.71	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: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:D:77:ASP:OD1	1:D:183:ARG:NH2	2.50	0.43
1:D:904:GLU:HB2	1:D:936:GLY:HA2	2.00	0.43
1:B:80:GLU:N	1:B:80:GLU:CD	2.72	0.43
1:C:897:TRP:CZ3	1:C:918:TRP:HB2	2.54	0.43
1:D:502:MET:HA	1:D:537:GLU:O	2.19	0.43
1:D:380:LYS:HE2	3:D:4077:HOH:O	2.18	0.43
1:B:635:THR:CG2	1:B:636:ILE:N	2.81	0.43
1:D:967:LEU:HA	1:D:967:LEU:HD23	1.70	0.43
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:A:367:MET:HB3	1:A:372:MET:HE2	1.96	0.42
1:B:576:ILE:HD11	1:B:584:PRO:HB3	2.00	0.42
1:B:652:LEU:CD1	1:B:698:VAL:HB	2.49	0.42
1:D:952:ARG:NH1	1:D:1021:CYS:SG	2.91	0.42
1:A:3:ILE:HG13	1:A:4:THR:N	2.32	0.42
1:D:518:TRP:HB3	1:D:522:LYS:HD3	2.00	0.42
1:C:292:ARG:CG	1:C:292:ARG:HH11	2.31	0.42
1:B:881:ARG:C	1:B:882:ILE:HG13	2.40	0.42
1:C:789:LEU:HA	1:C:933:SER:CB	2.49	0.42
1:C:339:ASN:O	1:D:527:PRO:HB3	2.19	0.42
1:D:612:THR:HB	1:D:613:PRO:HD2	2.01	0.42
1:B:335:VAL:HG22	1:B:344:LEU:HD12	2.01	0.42
1:C:548:GLY:O	1:C:551:LYS:HB2	2.19	0.42
1:A:51:LEU:HG	1:A:51:LEU:O	2.19	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:A:737:ILE:HG13	1:A:738:PRO:N	2.34	0.42
1:D:786:ARG:HH21	1:D:792:ASP:CG	2.22	0.42
1:A:422:PRO:HG2	1:D:285:TYR:CE1	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: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:378:LEU:HD23	1:D:378:LEU:HA	1.73	0.42
1:A:252:ASP:OD1	1:A:252:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:357:HIS:HD2	1:A:392:TYR:OH	2.02	0.42
1:D:38:ASN:ND2	1:D:40:GLU:N	2.67	0.42
1:B:354:VAL:HG22	1:B:355:ASN:N	2.34	0.42
1:B:79:PRO:N	1:B:80:GLU:OE2	2.53	0.42
1:A:914:CYS:O	1:A:918:TRP:HZ2	2.01	0.42
1:A:194:GLY:O	1:A:198:GLU:HG3	2.19	0.42
1:A:726:LEU:HD12	1:B:873:ALA:HB2	1.99	0.42
1:B:304:GLU:O	1:B:305:ILE:HG13	2.19	0.42
1:A:278:ILE:HA	1:A:278:ILE:HD13	1.60	0.42
1:D:147:ASN:HA	1:D:148:SER:HA	1.71	0.42
1:A:588:TYR:CD2	1:A:603:MET:HE1	2.54	0.42
1:C:958:ASN:ND2	3:C:4153:HOH:O	2.51	0.42
1:D:303:ALA:HB1	1:D:406:GLY:O	2.20	0.42
1:C:422:PRO:HG2	1:C:424:ASN:HB2	2.00	0.42
1:C:722:LEU:HD23	1:C:722:LEU:HA	1.66	0.42
1:D:315:LEU:O	1:D:323:ILE:HB	2.19	0.42
1:B:496:THR:O	1:B:531:ARG:NH1	2.49	0.42
1:C:655:MET:HG3	1:C:655:MET:O	2.06	0.42
1:A:140:ARG:CG	1:A:141:ILE:N	2.79	0.42
1:D:852:SER:CB	1:D:870:VAL:HG22	2.49	0.42
1:B:24:LEU:HB2	1:B:161:TYR:HB3	1.99	0.42
1:D:308:LEU:HD23	1:D:330:VAL:O	2.19	0.42
1:D:377:LEU:HD22	1:D:708:TRP:CA	2.40	0.42
1:B:721:ARG:HB3	1:B:721:ARG:NH1	2.34	0.42
1:D:52[B]:ARG:CG	1:D:133:TRP:CH2	2.98	0.42
1:A:907:PRO:HA	1:A:910:LEU:HD23	2.02	0.42
1:C:881:ARG:HD3	1:C:987:ASP:CG	2.39	0.42
1:C:228:ALA:C	1:C:229:THR:HG23	2.40	0.42
1:D:906:TYR:CB	1:D:907:PRO:HD2	2.50	0.42
1:D:778:THR:HA	1:D:779:PRO:HD2	1.86	0.42
1:B:347:LYS:HE3	1:B:643:LEU:O	2.20	0.42
1:A:401:LEU:HA	1:A:401:LEU:HD23	1.79	0.42
1:A:746:ASP:N	1:A:760:ARG:HG3	2.33	0.42
1:A:302:SER:HB2	1:A:304:GLU:H	1.83	0.42
1:A:680:ILE:O	1:A:680:ILE:HG22	2.15	0.42
1:C:663:LEU:HD23	1:C:663:LEU:N	2.31	0.42
1:C:114:VAL:HA	1:C:115:PRO:HD3	1.66	0.42
1:B:652:LEU:HG	1:B:652:LEU:O	2.19	0.42
1:C:961:ARG:HD2	1:C:981:GLY:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:822:LEU:HD21	1:B:825:CYS:HB2	2.01	0.42
1:C:870:VAL:HG12	1:C:871:GLU:H	1.84	0.42
1:A:652:LEU:HD12	1:A:652:LEU:HA	1.49	0.42
1:A:217:LYS:HB3	1:A:218:PRO:CD	2.47	0.42
1:D:814:GLY:O	1:D:815:HIS:C	2.58	0.42
1:B:941:THR:CG2	1:B:955:PHE:CE1	3.02	0.42
1:C:786:ARG:O	1:C:788:PRO:N	2.53	0.42
1:C:782:ASP:OD1	1:C:854:LYS:NZ	2.50	0.42
1:A:110:ASN:N	1:A:111:PRO:HD3	2.34	0.42
1:C:424:ASN:HD22	1:C:424:ASN:HA	1.29	0.42
1:B:317:THR:HG23	1:B:321:THR:O	2.19	0.42
1:A:338:GLU:O	1:A:339:ASN:HB3	2.20	0.42
1:D:652:LEU:HD12	1:D:700:VAL:CG2	2.50	0.42
1:A:942:ARG:HA	1:A:953:GLY:O	2.19	0.42
1:C:986:ILE:HD13	1:C:986:ILE:HG21	1.59	0.42
1:D:745:MET:HG2	1:D:745:MET:H	1.28	0.42
1:D:100:TYR:HB2	1:D:203:TRP:CE3	2.55	0.42
1:D:377:LEU:HD23	1:D:708:TRP:CB	2.50	0.42
1:A:658:LEU:CD2	1:A:688:PRO:HG2	2.39	0.42
1:B:3:ILE:O	1:B:6:SER:OG	2.29	0.42
1:A:825:CYS:HA	1:A:837:THR:O	2.20	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:D:979:GLU:O	1:D:980:GLU:C	2.57	0.42
1:D:769:TRP:NE1	1:D:774:LYS:HG3	2.34	0.42
1:D:197:LEU:HD12	1:D:439:ARG:NE	2.35	0.42
1:A:718:GLN:HG2	1:A:720:TRP:CZ2	2.55	0.42
1:C:63:PHE:CG	1:C:69:VAL:HG22	2.55	0.42
1:B:1022:GLN:OE1	1:B:1022:GLN:N	2.51	0.42
1:D:927:THR:HG21	1:D:929:TYR:CZ	2.55	0.42
1:A:343:LEU:HD22	1:A:346:GLY:O	2.19	0.42
1:B:994:GLY:HA3	1:B:1003:VAL:HG23	2.01	0.42
1:C:334:GLU:HG3	3:C:4209:HOH:O	2.19	0.42
1:D:208:ILE:HG22	1:D:208:ILE:O	2.20	0.42
1:C:415:ILE:HG21	1:C:415:ILE:HD13	1.74	0.42
1:D:864:MET:O	1:D:864:MET:HG3	2.19	0.42
1:D:955:PHE:CD1	1:D:986:ILE:CG2	3.02	0.42
1:D:77:ASP:OD1	1:D:183:ARG:NE	2.50	0.42
1:B:395:HIS:ND1	1:B:396:PRO:CD	2.79	0.42
1:A:166:ARG:HG3	1:A:392:TYR:CG	2.54	0.42
1:C:342:LEU:O	1:C:348:PRO:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:356:ARG:HD2	1:D:379:MET:HE3	2.01	0.42
1:C:881:ARG:O	1:C:882:ILE:HG13	2.18	0.42
1:B:955:PHE:CD1	1:B:955:PHE:C	2.93	0.42
1:D:643:LEU:CD2	1:D:675:GLN:NE2	2.82	0.42
1:D:27:LEU:HD12	1:D:140:ARG:HD3	2.00	0.42
1:D:942:ARG:HA	1:D:953:GLY:O	2.20	0.42
1:C:149:ALA:HA	1:C:162:GLY:O	2.19	0.42
1:A:349:LEU:HA	1:A:349:LEU:HD23	1.91	0.42
1:A:637:GLU:CA	1:A:679:LEU:HD21	2.48	0.42
1:D:694:LEU:HD12	1:D:694:LEU:HA	1.82	0.42
1:D:282:ARG:HG3	1:D:282:ARG:NH1	2.24	0.42
1:C:279:ILE:HD13	1:C:279:ILE:HG21	1.61	0.42
1:B:316:HIS:HB3	1:B:322:LEU:HD23	2.02	0.42
1:B:749:ILE:CG2	1:B:750:GLU:N	2.82	0.42
1:B:382:ASN:O	1:B:621:LYS:HA	2.19	0.42
1:B:166:ARG:HA	1:B:166:ARG:HD2	1.73	0.42
1:B:866:ILE:O	1:B:1017:GLN:HB2	2.19	0.42
1:C:382:ASN:HA	1:C:621:LYS:HD2	2.01	0.42
1:B:906:TYR:CE2	1:B:937:LEU:HD22	2.54	0.42
1:C:925:MET:HE2	1:C:925:MET:HB3	1.77	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:A:869:ASP:CG	1:A:1015:HIS:HD1	2.23	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:721:ARG:CB	1:C:721:ARG:CZ	2.97	0.42
1:D:955:PHE:CD1	1:D:986:ILE:HG23	2.54	0.42
1:B:400:THR:O	1:B:403:ASP:HB2	2.20	0.42
1:D:300:LEU:HD22	1:D:332:PHE:O	2.20	0.42
1:A:240:LEU:HD22	1:A:260:LEU:CD2	2.49	0.42
1:B:658:LEU:HB3	1:B:661:LYS:HD2	2.02	0.42
1:D:734:SER:CB	1:D:860:GLY:HA3	2.46	0.42
1:B:393:PRO:HD2	1:B:414:ASN:HB2	2.02	0.42
1:C:11:LEU:HD21	1:C:187:MET:HE3	2.02	0.42
1:A:906:TYR:HB3	1:A:907:PRO:HD2	2.02	0.42
1:D:309:TYR:HD1	1:D:309:TYR:N	2.17	0.42
1:D:9:VAL:O	1:D:10:VAL:C	2.57	0.42
1:C:315:LEU:O	1:C:323:ILE:HB	2.20	0.42
1:B:524:LEU:HD22	1:B:561:ARG:CZ	2.50	0.42
1:B:900:LEU:HA	1:B:914:CYS:O	2.19	0.42
1:B:380:LYS:HE2	3:B:4077:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:856:TYR:CD2	1:A:864:MET:CE	3.01	0.41
1:B:550:ALA:O	1:B:551:LYS:C	2.59	0.41
1:D:822:LEU:HD11	1:D:824:GLN:O	2.20	0.41
1:B:768:MET:CE	1:B:770:ILE:CD1	2.97	0.41
1:C:526:LEU:HA	1:C:526:LEU:HD12	1.84	0.41
1:C:741:THR:HG22	1:C:742:THR:O	2.20	0.41
1:B:885:ASN:HB2	1:B:984:LEU:O	2.21	0.41
1:D:33:PHE:CD1	1:D:217:LYS:HE3	2.55	0.41
1:A:780:LEU:HD12	1:A:886:CYS:HB3	2.02	0.41
1:D:260:LEU:O	1:D:267:VAL:N	2.44	0.41
1:A:214:LEU:HD23	1:A:214:LEU:HA	1.41	0.41
1:B:575:LEU:HD23	1:B:575:LEU:HA	1.79	0.41
1:A:43:ARG:NH1	1:A:43:ARG:HG2	2.35	0.41
1:D:427:THR:HG22	1:D:436:MET:SD	2.61	0.41
1:A:851:ILE:O	1:A:870:VAL:HA	2.20	0.41
1:B:111:PRO:HA	1:B:112:PRO:HA	1.76	0.41
1:A:427:THR:CA	1:A:436:MET:HE1	2.47	0.41
1:B:173:LEU:O	1:B:175:ALA:N	2.53	0.41
1:B:419:GLY:C	1:C:282:ARG:NH1	2.74	0.41
1:A:167:LEU:HG	1:A:393:PRO:HG2	2.01	0.41
1:A:734:SER:CB	1:A:860:GLY:CA	2.97	0.41
1:B:455:ILE:HG22	1:B:456:TRP:N	2.35	0.41
1:C:536:CYS:O	1:C:566:PHE:HB2	2.19	0.41
1:A:651:LEU:HA	1:A:651:LEU:HD12	1.92	0.41
1:D:608:PHE:CD1	1:D:614:HIS:CD2	3.08	0.41
1:B:787:ALA:HA	1:B:788:PRO:HD3	1.72	0.41
1:C:322:LEU:HD23	1:C:322:LEU:HA	1.84	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:A:829:THR:C	1:A:830:LEU:HD13	2.40	0.41
1:B:42:ALA:O	1:B:310:ARG:NH1	2.53	0.41
1:D:177:LEU:HA	1:D:177:LEU:HD23	1.82	0.41
1:D:834:VAL:HG12	1:D:835:LEU:N	2.34	0.41
1:C:569:ASP:HB2	3:C:5099:HOH:O	2.21	0.41
1:B:63:PHE:HE1	1:B:122:CYS:HG	1.68	0.41
1:B:458:LEU:HD23	1:B:458:LEU:HA	1.65	0.41
1:C:207:GLY:O	1:C:209:PHE:N	2.54	0.41
1:C:766:SER:O	1:C:767:GLN:HB2	2.20	0.41
1:D:62:TRP:CZ2	1:D:119:PRO:HB3	2.56	0.41
1:B:392:TYR:HD1	1:B:393:PRO:O	2.03	0.41
1:C:292:ARG:CG	1:C:292:ARG:NH1	2.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:935:ASN:N	1:B:935:ASN:ND2	2.68	0.41
1:B:344:LEU:HG	1:B:345:ASN:N	2.34	0.41
1:B:513:PRO:O	1:B:514:ALA:HB3	2.20	0.41
1:D:252:ASP:OD1	1:D:252:ASP:N	2.51	0.41
1:B:670:LEU:HD11	1:B:700:VAL:CG2	2.51	0.41
1:B:368:ASP:O	1:B:372:MET:HG3	2.19	0.41
1:A:361:PRO:CD	1:A:362:LEU:H	2.33	0.41
1:A:316:HIS:HB3	1:A:322:LEU:HD23	2.01	0.41
1:D:654:TRP:HE1	1:D:666:GLY:HA3	1.84	0.41
1:A:358:GLU:HB3	1:A:367:MET:SD	2.61	0.41
1:D:7:LEU:HA	1:D:7:LEU:HD23	1.85	0.41
1:C:217:LYS:CG	1:C:218:PRO:CD	2.99	0.41
1:C:592:PHE:C	1:C:594:ASP:H	2.22	0.41
1:C:791:ASN:HB3	3:C:4270:HOH:O	2.20	0.41
1:D:232:ASN:O	1:D:233:ASP:C	2.57	0.41
1:B:640:SER:OG	1:B:642:TYR:HB2	2.20	0.41
1:D:262:GLN:O	1:D:262:GLN:HG2	2.19	0.41
1:B:875:ASP:N	1:B:875:ASP:OD2	2.53	0.41
1:D:751:LEU:C	1:D:751:LEU:HD23	2.40	0.41
1:A:351:ILE:N	1:A:351:ILE:HD13	2.35	0.41
1:B:356:ARG:HH22	1:B:367:MET:CE	2.33	0.41
1:C:928:PRO:O	1:C:929:TYR:C	2.58	0.41
1:B:173:LEU:HD23	1:B:173:LEU:HA	1.77	0.41
1:B:579:ASP:OD2	1:B:583:ASN:HB2	2.21	0.41
1:B:568:TRP:C	1:B:568:TRP:CD1	2.93	0.41
1:D:62:TRP:CD1	1:D:95:TYR:CB	3.02	0.41
1:B:837:THR:CG2	1:B:838:THR:N	2.78	0.41
1:A:138:GLN:CG	1:A:139:THR:N	2.78	0.41
1:B:257:THR:O	1:B:313:VAL:HA	2.20	0.41
1:D:896:ASN:HA	1:D:918:TRP:O	2.21	0.41
1:A:526:LEU:O	1:A:527:PRO:C	2.56	0.41
1:C:46:ARG:HA	1:C:47:PRO:HD3	1.80	0.41
1:A:315:LEU:HD12	1:A:315:LEU:HA	1.80	0.41
1:B:436:MET:HE1	1:B:467:ASN:HD22	1.86	0.41
1:D:858:ILE:HD11	1:D:864:MET:HE3	2.02	0.41
1:D:603:MET:HE1	1:D:930:VAL:HG12	2.03	0.41
1:A:38:ASN:ND2	1:A:40:GLU:N	2.68	0.41
1:B:598:ASP:O	1:B:599:ARG:C	2.57	0.41
1:B:658:LEU:CG	1:B:661:LYS:NZ	2.78	0.41
1:A:599:ARG:HB2	1:A:600:GLN:H	1.30	0.41
1:B:740:LEU:HA	1:B:748:CYS:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:734:SER:CB	1:A:860:GLY:HA3	2.45	0.41
1:B:549:PHE:O	1:B:553:TRP:HD1	2.04	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:A:653[B]:HIS:CD2	1:A:666:GLY:O	2.74	0.41
1:B:897:TRP:HB2	1:B:943:GLU:O	2.21	0.41
1:D:956:GLN:HB2	1:D:987:ASP:HB2	2.02	0.41
1:A:896:ASN:HA	1:A:918:TRP:O	2.21	0.41
1:B:608:PHE:O	1:B:611:ARG:N	2.45	0.41
1:C:963:SER:HG	1:C:979:GLU:CD	2.24	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:D:706:THR:HG23	1:D:709:SER:OG	2.20	0.41
1:A:768:MET:HG2	1:A:775:GLN:HG3	2.03	0.41
1:D:765:LEU:O	1:D:765:LEU:HG	2.19	0.41
1:B:486:TYR:CZ	1:B:488:GLY:HA3	2.55	0.41
1:A:737:ILE:HD12	1:A:832:ASP:HA	2.03	0.41
1:D:429:ASP:HA	1:D:430:PRO:HD3	1.85	0.41
1:B:682:LEU:HD23	1:B:682:LEU:HA	1.60	0.41
1:A:524:LEU:HD22	1:A:561:ARG:CB	2.50	0.41
1:D:27:LEU:HD12	1:D:140:ARG:NH1	2.35	0.41
1:D:730:LEU:HA	1:D:731:PRO:HD3	1.95	0.41
1:B:590:GLY:HA2	1:B:594:ASP:OD1	2.20	0.41
1:C:638:VAL:O	1:C:677:LYS:HA	2.21	0.41
1:B:1009:LEU:HD23	1:B:1009:LEU:N	2.34	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:D:202:MET:HE3	1:D:357:HIS:CD2	2.56	0.41
1:B:375:ASP:O	1:B:376:ILE:C	2.57	0.41
1:D:300:LEU:HD23	1:D:332:PHE:HB3	2.02	0.41
1:B:17:GLU:O	1:B:112:PRO:HG2	2.21	0.41
1:D:105:TYR:HA	1:D:106:PRO:HD2	1.76	0.41
1:B:589:GLY:CA	1:B:599:ARG:HA	2.39	0.41
1:C:376:ILE:HD13	1:C:401:LEU:HB3	2.03	0.41
1:C:342:LEU:HA	1:C:342:LEU:HD12	1.67	0.41
1:A:668:VAL:CG1	1:A:669:PRO:HD2	2.49	0.41
1:B:103:VAL:HG22	1:B:418:HIS:CE1	2.56	0.41
1:C:726:LEU:CD1	1:D:848:THR:HG22	2.50	0.41
1:B:615:PRO:HG2	1:B:904:GLU:OE1	2.20	0.41
1:C:63:PHE:HB3	1:C:64:PRO:HD2	2.02	0.41
1:C:824:GLN:HG3	1:C:825:CYS:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:THR:O	1:B:45:ASP:HB3	2.21	0.41
1:A:434:PRO:HB3	1:D:434:PRO:HB3	2.03	0.41
1:B:142:ILE:HG21	1:B:142:ILE:HD13	1.87	0.41
1:A:13:ARG:NH1	1:D:13:ARG:NH1	2.69	0.41
1:C:342:LEU:HB3	1:C:563:GLN:HE22	1.86	0.41
1:C:190:ARG:HD3	1:C:191:TRP:CZ2	2.55	0.41
1:C:737:ILE:HB	1:C:738:PRO:HD2	2.02	0.41
1:A:153:TRP:CD1	1:A:158:TRP:HA	2.56	0.41
1:B:549:PHE:HE1	1:B:567:VAL:CG2	2.34	0.41
1:B:620:ALA:O	1:B:621:LYS:C	2.58	0.41
1:A:737:ILE:HD12	1:A:832:ASP:CA	2.51	0.41
1:D:56:GLY:O	1:D:85:VAL:HA	2.20	0.41
1:C:120:THR:CG2	1:C:187:MET:SD	3.09	0.41
1:C:35:SER:CB	1:C:37:ARG:NH1	2.84	0.41
1:D:904:GLU:CG	1:D:909:ARG:HH22	2.31	0.41
1:A:651:LEU:HD12	1:A:669:PRO:HA	2.03	0.41
1:C:3:ILE:C	1:C:5:ASP:H	2.19	0.41
1:B:768:MET:HG3	1:B:768:MET:O	2.18	0.41
1:A:946:TYR:OH	1:A:982:THR:OG1	2.30	0.41
1:D:870:VAL:CG1	1:D:871:GLU:N	2.84	0.41
1:C:226:HIS:CD2	1:C:448:ARG:HD2	2.56	0.41
1:C:176:PHE:HE1	3:C:4172:HOH:O	2.04	0.41
1:A:728:VAL:HG13	1:B:851:ILE:HD11	2.02	0.41
1:D:200:GLN:HG2	1:D:391:HIS:HB2	2.03	0.41
1:A:243:GLU:OE1	1:A:288:ARG:HD3	2.20	0.41
1:B:292:ARG:NH1	1:B:292:ARG:CG	2.84	0.41
1:D:272:ALA:HB1	1:D:273:PRO:CD	2.51	0.41
1:C:194:GLY:O	1:C:197:LEU:HB2	2.21	0.41
1:C:567:VAL:H	1:C:567:VAL:HG23	1.67	0.41
1:C:482:ARG:HH11	1:C:482:ARG:HD2	1.60	0.41
1:C:952:ARG:CZ	1:C:952:ARG:CB	2.99	0.41
1:D:505:ARG:HH11	1:D:505:ARG:HD3	1.56	0.41
1:A:260:LEU:HD11	1:A:309:TYR:HB3	2.01	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:B:455:ILE:HD13	1:B:455:ILE:HG21	1.90	0.41
1:A:141:ILE:O	1:A:170:GLU:HA	2.21	0.41
1:B:417:THR:O	1:B:418:HIS:C	2.59	0.41
1:C:796:SER:HB2	1:C:802:ASP:HB3	2.03	0.41
1:A:782:ASP:OD2	1:A:852:SER:OG	2.29	0.41
1:D:209:PHE:N	1:D:209:PHE:CD2	2.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:769:TRP:HB3	1:A:771:GLY:O	2.21	0.40
1:A:7:LEU:HD13	1:A:69:VAL:CG1	2.51	0.40
1:D:679:LEU:HA	1:D:679:LEU:HD23	1.07	0.40
1:D:298:PRO:N	3:D:4211:HOH:O	2.54	0.40
1:B:421:VAL:HA	1:B:422:PRO:HA	1.85	0.40
1:C:195:SER:O	1:C:196:TYR:C	2.58	0.40
1:B:90:TRP:CD1	1:B:90:TRP:C	2.94	0.40
1:B:888:LEU:O	1:B:981:GLY:HA3	2.20	0.40
1:B:221:GLN:HB3	1:B:221:GLN:HE21	1.26	0.40
1:B:406:GLY:O	1:B:407:LEU:HD23	2.21	0.40
1:D:932:PRO:HG2	1:D:970:THR:O	2.21	0.40
1:A:390:SER:HA	1:A:391:HIS:HA	1.79	0.40
1:D:184:LEU:HA	1:D:184:LEU:HD23	1.74	0.40
1:B:476:LYS:HE3	1:B:476:LYS:HB3	1.82	0.40
1:A:775:GLN:CD	1:A:890:GLN:HE22	2.24	0.40
1:A:131:GLU:O	1:A:134:LEU:HD23	2.21	0.40
1:A:658:LEU:HD11	1:A:692:GLY:C	2.42	0.40
1:A:210:ARG:HD3	1:A:210:ARG:HH11	1.71	0.40
1:B:422:PRO:HB2	1:C:280:ASP:OD1	2.21	0.40
1:D:6:SER:HB2	1:D:71:GLU:OE2	2.21	0.40
1:C:373:VAL:HG12	1:C:373:VAL:O	2.20	0.40
1:A:763:GLY:CA	1:A:822:LEU:HD21	2.49	0.40
1:A:925:MET:HE1	1:A:938:ARG:CZ	2.52	0.40
1:C:510:GLN:HB3	1:C:512:PHE:CZ	2.57	0.40
1:B:105:TYR:CE2	1:B:199:ASP:HB2	2.57	0.40
1:C:815:HIS:CD2	1:C:849:LEU:HD13	2.56	0.40
1:B:607:VAL:HG12	1:B:613:PRO:HA	2.02	0.40
1:A:378:LEU:HA	1:A:378:LEU:HD23	1.61	0.40
1:A:1019:VAL:O	1:A:1019:VAL:HG12	2.20	0.40
1:B:197:LEU:HD23	1:B:197:LEU:HA	1.65	0.40
1:B:433:LEU:O	1:B:437:SER:HB3	2.22	0.40
1:A:767:GLN:CD	1:A:774:LYS:HG2	2.42	0.40
1:D:559:TYR:HA	1:D:560:PRO:HD2	1.89	0.40
1:D:202:MET:CE	1:D:357:HIS:CD2	3.04	0.40
1:B:595:THR:CG2	1:B:596:PRO:CA	2.98	0.40
1:B:118:ASN:O	1:B:120:THR:OG1	2.39	0.40
1:C:100:TYR:HB2	1:C:203:TRP:CZ3	2.56	0.40
1:A:152:LEU:CG	1:A:153:TRP:N	2.81	0.40
1:A:30:HIS:CE1	1:A:33:PHE:CD1	3.10	0.40
1:C:502:MET:HB3	1:C:537:GLU:HG3	2.02	0.40
1:C:987:ASP:OD2	1:C:990:HIS:HD2	2.05	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:956:GLN:N	1:D:956:GLN:CD	2.74	0.40
1:A:898:LEU:HB2	1:A:917:ARG:NH2	2.36	0.40
1:B:881:ARG:HD3	1:B:987:ASP:OD2	2.22	0.40
1:D:476:LYS:H	1:D:476:LYS:HG2	1.60	0.40
1:C:490:GLY:N	3:C:4010:HOH:O	2.32	0.40
1:B:559:TYR:CB	1:B:562:LEU:HD12	2.35	0.40
1:D:352:ARG:O	1:D:385:ASN:HB2	2.22	0.40
1:D:106:PRO:HB2	1:D:191:TRP:CH2	2.56	0.40
1:B:599:ARG:HB2	1:B:600:GLN:H	1.20	0.40
1:C:835:LEU:HG	1:C:835:LEU:O	2.21	0.40
1:C:30:HIS:HE1	3:C:4191:HOH:O	2.04	0.40
1:A:559:TYR:HB2	1:A:562:LEU:CD1	2.52	0.40
1:C:118:ASN:HD21	1:C:189:LEU:CD2	2.34	0.40
1:B:900:LEU:HD13	1:B:913:ALA:HB3	2.02	0.40
1:B:369:GLU:O	1:B:370:GLN:C	2.60	0.40
1:A:57:GLU:HG2	1:A:83:THR:CG2	2.52	0.40
1:D:632:SER:O	1:D:634:GLN:N	2.55	0.40
1:A:788:PRO:O	1:A:933:SER:HB2	2.21	0.40
1:A:127:PHE:N	1:A:127:PHE:CD2	2.90	0.40
1:D:500:CYS:N	1:D:501:PRO:CD	2.85	0.40
1:D:559:TYR:CD1	1:D:559:TYR:N	2.90	0.40
1:B:376:ILE:CD1	1:B:401:LEU:HB3	2.51	0.40
1:B:251:ARG:O	1:B:254:LEU:HD12	2.22	0.40
1:C:834:VAL:HG12	1:C:835:LEU:N	2.37	0.40
1:C:961:ARG:HG3	1:C:961:ARG:HH11	1.85	0.40
1:D:651:LEU:HD13	1:D:651:LEU:HA	1.60	0.40
1:B:41:GLU:HG3	1:B:46:ARG:NH1	2.37	0.40
1:B:90:TRP:NE1	1:B:96:ASP:OD1	2.55	0.40
1:C:784:PHE:HA	1:C:881:ARG:O	2.22	0.40
1:A:995:GLY:HA3	3:A:4067:HOH:O	2.22	0.40
1:A:576:ILE:CG2	1:A:577:LYS:N	2.84	0.40
1:A:852:SER:OG	1:A:854:LYS:HE3	2.21	0.40
1:B:240:LEU:HG	1:B:241:GLU:N	2.36	0.40
1:A:623:GLN:NE2	1:A:911:THR:OG1	2.54	0.40
1:D:882:ILE:HB	1:D:989:PHE:HB2	2.04	0.40
1:A:572:ASP:C	1:A:574:SER:H	2.25	0.40
1:C:458:LEU:HD11	1:C:472:TYR:HB2	2.04	0.40
1:B:67:GLU:HG2	1:B:67:GLU:H	1.28	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1026/1021 (100%)	923 (90%)	86 (8%)	17 (2%)	11 36
1	B	1026/1021 (100%)	917 (89%)	89 (9%)	20 (2%)	10 32
1	C	1026/1021 (100%)	918 (90%)	82 (8%)	26 (2%)	7 24
1	D	1026/1021 (100%)	921 (90%)	85 (8%)	20 (2%)	10 32
All	All	4104/4084 (100%)	3679 (90%)	342 (8%)	83 (2%)	9 30

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 (i)

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%)	700 (80%)	180 (20%)	1 4
1	B	880/873 (101%)	690 (78%)	190 (22%)	1 3
1	C	880/873 (101%)	703 (80%)	177 (20%)	1 4
1	D	880/873 (101%)	709 (81%)	171 (19%)	2 5
All	All	3520/3492 (101%)	2802 (80%)	718 (20%)	1 4

All (718) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	12	GLN

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Mol	Chain	Res	Type
1	A	14	ARG
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	82	ASP
1	A	84	VAL
1	A	92	MET
1	A	96	ASP
1	A	102	ASN
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	187	MET
1	A	189	LEU
1	A	190	ARG
1	A	206	SER
1	A	210	ARG
1	A	211	ASP
1	A	217	LYS
1	A	219	THR
1	A	230	ARG
1	A	237	ARG

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Mol	Chain	Res	Type
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	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	322	LEU
1	A	333	ARG
1	A	344	LEU
1	A	347	LYS
1	A	362	LEU
1	A	367	MET
1	A	380	LYS
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	481	SER
1	A	493	THR
1	A	502	MET
1	A	519	SER
1	A	520	ILE
1	A	521	LYS
1	A	525	SER
1	A	526	LEU
1	A	533	LEU
1	A	535	LEU
1	A	538	TYR

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Mol	Chain	Res	Type
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	637	GLU
1	A	645	ARG
1	A	647	SER
1	A	653[A]	HIS
1	A	653[B]	HIS
1	A	655	MET
1	A	667	GLU
1	A	668	VAL
1	A	671	ASP
1	A	672	VAL
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
1	A	728	VAL
1	A	729	THR
1	A	730	LEU
1	A	737	ILE
1	A	744	GLU
1	A	750	GLU
1	A	751	LEU
1	A	753	ASN
1	A	761	GLN

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Mol	Chain	Res	Type
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	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	881	ARG
1	A	885	ASN
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	938	ARG

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Mol	Chain	Res	Type
1	A	950	GLN
1	A	956	GLN
1	A	965	GLN
1	A	966	GLN
1	A	969	GLU
1	A	1004	SER
1	A	1006	GLU
1	A	1017	GLN
1	A	1018	LEU
1	A	1023	LYS
1	B	4	THR
1	B	7	LEU
1	B	9	VAL
1	B	11	LEU
1	B	14	ARG
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	67	GLU
1	B	71	GLU
1	B	75	GLU
1	B	76	CYS
1	B	80	GLU
1	B	82	ASP
1	B	83	THR
1	B	90	TRP
1	B	101	THR
1	B	102	ASN
1	B	108	THR
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

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Mol	Chain	Res	Type
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
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	280	ASP
1	B	292	ARG
1	B	310	ARG
1	B	314	GLU
1	B	322	LEU
1	B	324	GLU

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Mol	Chain	Res	Type
1	B	330	VAL
1	B	333	ARG
1	B	338	GLU
1	B	357	HIS
1	B	362	LEU
1	B	394	ASN
1	B	424	ASN
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	508	GLU
1	B	509	ASP
1	B	519	SER
1	B	525	SER
1	B	526	LEU
1	B	529	GLU
1	B	531	ARG
1	B	532	PRO
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	645	ARG
1	B	651	LEU
1	B	652	LEU
1	B	655	MET

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Mol	Chain	Res	Type
1	B	658	LEU
1	B	661	LYS
1	B	663	LEU
1	B	672	VAL
1	B	681	GLU
1	B	687	GLN
1	B	690	SER
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
1	B	765	LEU
1	B	766	SER
1	B	768	MET
1	B	769	TRP
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	797	GLU
1	B	799	THR
1	B	800	ARG
1	B	808	GLU
1	B	817	GLN
1	B	822	LEU
1	B	824	GLN
1	B	829	THR
1	B	837	THR
1	B	843	GLN
1	B	845	GLN
1	B	848	THR
1	B	852	SER

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Mol	Chain	Res	Type
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	910	LEU
1	B	917	ARG
1	B	923	SER
1	B	926	TYR
1	B	934	GLU
1	B	938	ARG
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	1013	ARG
1	B	1018	LEU
1	B	1023	LYS
1	C	3	ILE
1	C	6	SER
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

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Mol	Chain	Res	Type
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	102	ASN
1	C	108	THR
1	C	109	VAL
1	C	114	VAL
1	C	116	THR
1	C	125	LEU
1	C	130	ASP
1	C	131	GLU
1	C	134	LEU
1	C	135	GLN
1	C	138	GLN
1	C	141	ILE
1	C	143	PHE
1	C	148	SER
1	C	163	GLN
1	C	165	SER
1	C	166	ARG
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	223	SER
1	C	230	ARG
1	C	236	SER
1	C	237	ARG
1	C	246	MET
1	C	249	GLU
1	C	251	ARG
1	C	252	ASP
1	C	253	TYR
1	C	255	ARG
1	C	259	SER
1	C	264	GLU
1	C	266	GLN

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Mol	Chain	Res	Type
1	C	282	ARG
1	C	291	LEU
1	C	292	ARG
1	C	296	GLU
1	C	299	LYS
1	C	322	LEU
1	C	324	GLU
1	C	333	ARG
1	C	338	GLU
1	C	350	LEU
1	C	352	ARG
1	C	357	HIS
1	C	377	LEU
1	C	380	LYS
1	C	394	ASN
1	C	424	ASN
1	C	425	ARG
1	C	427	THR
1	C	431[A]	ARG
1	C	431[B]	ARG
1	C	437	SER
1	C	448	ARG
1	C	473	ARG
1	C	476	LYS
1	C	503	TYR
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	535	LEU
1	C	537	GLU
1	C	542	MET
1	C	545	SER
1	C	554	GLN
1	C	571	VAL
1	C	575	LEU
1	C	580	GLU
1	C	581	ASN

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Mol	Chain	Res	Type
1	C	595	THR
1	C	600	GLN
1	C	604	ASN
1	C	618	THR
1	C	631	LEU
1	C	645	ARG
1	C	655	MET
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	714	ILE
1	C	719	GLN
1	C	721	ARG
1	C	727	SER
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	774	LYS
1	C	778	THR
1	C	779	PRO
1	C	781	ARG
1	C	789	LEU
1	C	797	GLU
1	C	800	ARG
1	C	801	ILE
1	C	811	LYS
1	C	817	GLN

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Mol	Chain	Res	Type
1	C	823	LEU
1	C	824	GLN
1	C	828	ASP
1	C	829	THR
1	C	830	LEU
1	C	843	GLN
1	C	845	GLN
1	C	854	LYS
1	C	856	TYR
1	C	857	ARG
1	C	861	SER
1	C	863	GLN
1	C	864	MET
1	C	867	THR
1	C	869	ASP
1	C	871	GLU
1	C	874	SER
1	C	881	ARG
1	C	885	ASN
1	C	886	CYS
1	C	894	ARG
1	C	896	ASN
1	C	910	LEU
1	C	917	ARG
1	C	920	LEU
1	C	921	PRO
1	C	923	SER
1	C	934	GLU
1	C	938	ARG
1	C	939	CYS
1	C	948	PRO
1	C	950	GLN
1	C	956	GLN
1	C	965	GLN
1	C	973	ARG
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

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Mol	Chain	Res	Type
1	D	11	LEU
1	D	12	GLN
1	D	13	ARG
1	D	24	LEU
1	D	37	ARG
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	82	ASP
1	D	84	VAL
1	D	85	VAL
1	D	90	TRP
1	D	102	ASN
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	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	230	ARG
1	D	236	SER
1	D	237	ARG
1	D	240	LEU
1	D	241	GLU
1	D	243	GLU
1	D	246	MET
1	D	247	CYS
1	D	249	GLU

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Mol	Chain	Res	Type
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	309	TYR
1	D	310	ARG
1	D	314	GLU
1	D	319	ASP
1	D	322	LEU
1	D	333	ARG
1	D	342	LEU
1	D	344	LEU
1	D	352	ARG
1	D	378	LEU
1	D	380	LYS
1	D	385	ASN
1	D	424	ASN
1	D	425	ARG
1	D	437	SER
1	D	445	GLN
1	D	448	ARG
1	D	473	ARG
1	D	476	LYS
1	D	477	SER
1	D	481	SER
1	D	505	ARG
1	D	516	PRO
1	D	519	SER
1	D	521	LYS
1	D	526	LEU
1	D	529	GLU
1	D	545	SER
1	D	546	LEU
1	D	554	GLN
1	D	559	TYR
1	D	571	VAL
1	D	580	GLU
1	D	581	ASN

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Mol	Chain	Res	Type
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	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	683	PRO
1	D	685	LEU
1	D	687	GLN
1	D	690	SER
1	D	696	LEU
1	D	701	VAL
1	D	702	GLN
1	D	720	TRP
1	D	721	ARG
1	D	730	LEU
1	D	737	ILE
1	D	743	SER
1	D	745	MET
1	D	746	ASP
1	D	750	GLU
1	D	755	ARG
1	D	760	ARG
1	D	765	LEU
1	D	766	SER
1	D	768	MET
1	D	772	ASP
1	D	773	LYS
1	D	774	LYS
1	D	777	LEU

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Mol	Chain	Res	Type
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	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	852	SER
1	D	853	ARG
1	D	854	LYS
1	D	867	THR
1	D	874	SER
1	D	875	ASP
1	D	876	THR
1	D	881	ARG
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
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	998	SER
1	D	1002	SER
1	D	1006	GLU
1	D	1013	ARG

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Mol	Chain	Res	Type
1	D	1017	GLN
1	D	1023	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) 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	226	HIS
1	A	316	HIS
1	A	357	HIS
1	A	365	GLN
1	A	381	GLN
1	A	385	ASN
1	A	394	ASN
1	A	424	ASN
1	A	467	ASN
1	A	510	GLN
1	A	554	GLN
1	A	558	GLN
1	A	573	GLN
1	A	581	ASN
1	A	597	ASN
1	A	614	HIS
1	A	622	HIS
1	A	623	GLN
1	A	693	GLN
1	A	704	ASN
1	A	718	GLN
1	A	863	GLN
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

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Mol	Chain	Res	Type
1	B	163	GLN
1	B	216	HIS
1	B	221	GLN
1	B	226	HIS
1	B	245	GLN
1	B	307	ASN
1	B	316	HIS
1	B	357	HIS
1	B	445	GLN
1	B	583	ASN
1	B	597	ASN
1	B	622	HIS
1	B	624	GLN
1	B	675	GLN
1	B	949	HIS
1	B	965	GLN
1	C	38	ASN
1	C	102	ASN
1	C	135	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
1	C	424	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	624	GLN
1	C	817	GLN
1	C	863	GLN
1	C	949	HIS
1	C	965	GLN
1	C	990	HIS
1	C	1017	GLN
1	D	38	ASN

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Mol	Chain	Res	Type
1	D	102	ASN
1	D	216	HIS
1	D	316	HIS
1	D	357	HIS
1	D	394	ASN
1	D	424	ASN
1	D	510	GLN
1	D	554	GLN
1	D	573	GLN
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	702	GLN
1	D	718	GLN
1	D	757	GLN
1	D	845	GLN
1	D	890	GLN
1	D	949	HIS
1	D	965	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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%)	-1.15	4 (0%) 93 90	2, 26, 68, 100	19 (1%)
1	B	1021/1021 (100%)	-1.04	0 100 100	4, 31, 72, 100	19 (1%)
1	C	1021/1021 (100%)	-1.09	3 (0%) 94 92	6, 28, 65, 100	19 (1%)
1	D	1021/1021 (100%)	-1.13	1 (0%) 95 95	3, 26, 65, 100	19 (1%)
All	All	4084/4084 (100%)	-1.10	8 (0%) 95 94	2, 28, 68, 100	76 (1%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	733	ALA	2.7
1	A	734	SER	2.7
1	D	732	ALA	2.6
1	C	581	ASN	2.3
1	A	730	LEU	2.3
1	C	734	SER	2.1
1	C	732	ALA	2.0
1	A	582	GLY	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	MG	A	3002	1/1	0.99	0.16	4.20	31,31,31,31	0
2	MG	D	3002	1/1	0.99	0.11	2.10	25,25,25,25	0
2	MG	B	3002	1/1	0.97	0.09	0.45	36,36,36,36	0
2	MG	A	3001	1/1	0.96	0.12	0.45	28,28,28,28	0
2	MG	C	3002	1/1	0.98	0.08	-0.74	31,31,31,31	0
2	MG	D	3001	1/1	0.98	0.06	-1.20	40,40,40,40	0
2	MG	B	3001	1/1	0.99	0.04	-1.58	20,20,20,20	0
2	MG	C	3001	1/1	0.99	0.03	-2.49	15,15,15,15	0

6.5 Other polymers

There are no such residues in this entry.