wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 02:02 PM BST

PDB ID	:	4CKD
EMDB ID:	:	EMD-2548
Title	:	Model of complex between the E.coli enzyme beta-galactosidase and four single chain Fv antibody domains scFv13R4.
Authors	:	Vinothkumar, K.R.; McMullan, G.; Henderson, R.
Deposited on	:	2014-01-03
Resolution	:	13.00 Å(reported)
Based on PDB ID	:	1F4A

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

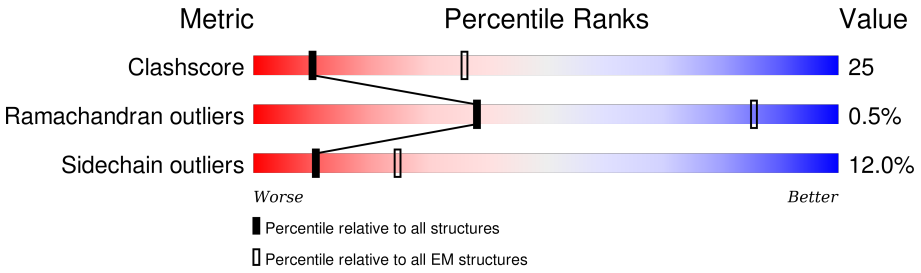
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 13.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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%

Mol	Chain	Length	Quality of chain
1	A	1024	48% 38% 11% •
1	B	1024	49% 38% 11% •
1	C	1024	48% 39% 10% •
1	D	1024	48% 39% 11% •
2	H	114	75% 25% •
2	I	114	73% 26% •
2	J	114	75% 25% •
2	K	114	76% 23% •
3	L	107	83% 16% •

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Mol	Chain	Length	Quality of chain
3	M	107	83% 16%
3	N	107	81% 18%
3	O	107	81% 18%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 39832 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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					AltConf	Trace
1	A	1021	Total	C	N	O	S	7	0
			8238	5209	1466	1525	38		
1	B	1021	Total	C	N	O	S	7	0
			8238	5209	1466	1525	38		
1	C	1021	Total	C	N	O	S	7	0
			8238	5209	1466	1525	38		
1	D	1021	Total	C	N	O	S	7	0
			8238	5209	1466	1525	38		

- Molecule 2 is a protein called SCFV13R4 ANTIBODY FV HEAVY CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	114	Total	C	N	O	S	0	0
			902	567	144	188	3		
2	I	114	Total	C	N	O	S	0	0
			902	567	144	188	3		
2	J	114	Total	C	N	O	S	0	0
			902	567	144	188	3		
2	K	114	Total	C	N	O	S	0	0
			902	567	144	188	3		

- Molecule 3 is a protein called SCFV13R4 ANTIBODY FV LIGHT CHAIN.

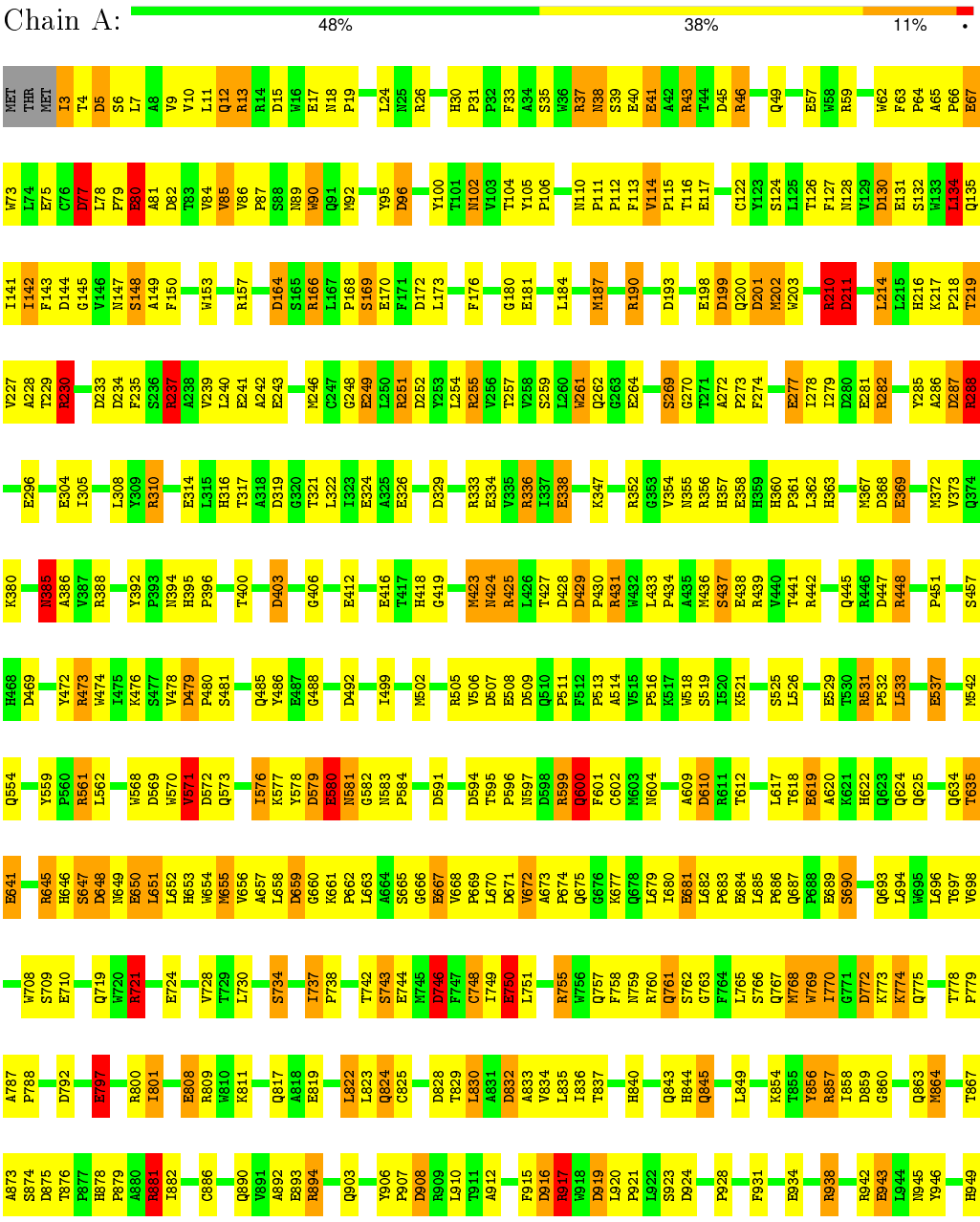
Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	107	Total	C	N	O	S	0	0
			818	511	137	167	3		
3	M	107	Total	C	N	O	S	0	0
			818	511	137	167	3		
3	N	107	Total	C	N	O	S	0	0
			818	511	137	167	3		
3	O	107	Total	C	N	O	S	0	0
			818	511	137	167	3		

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

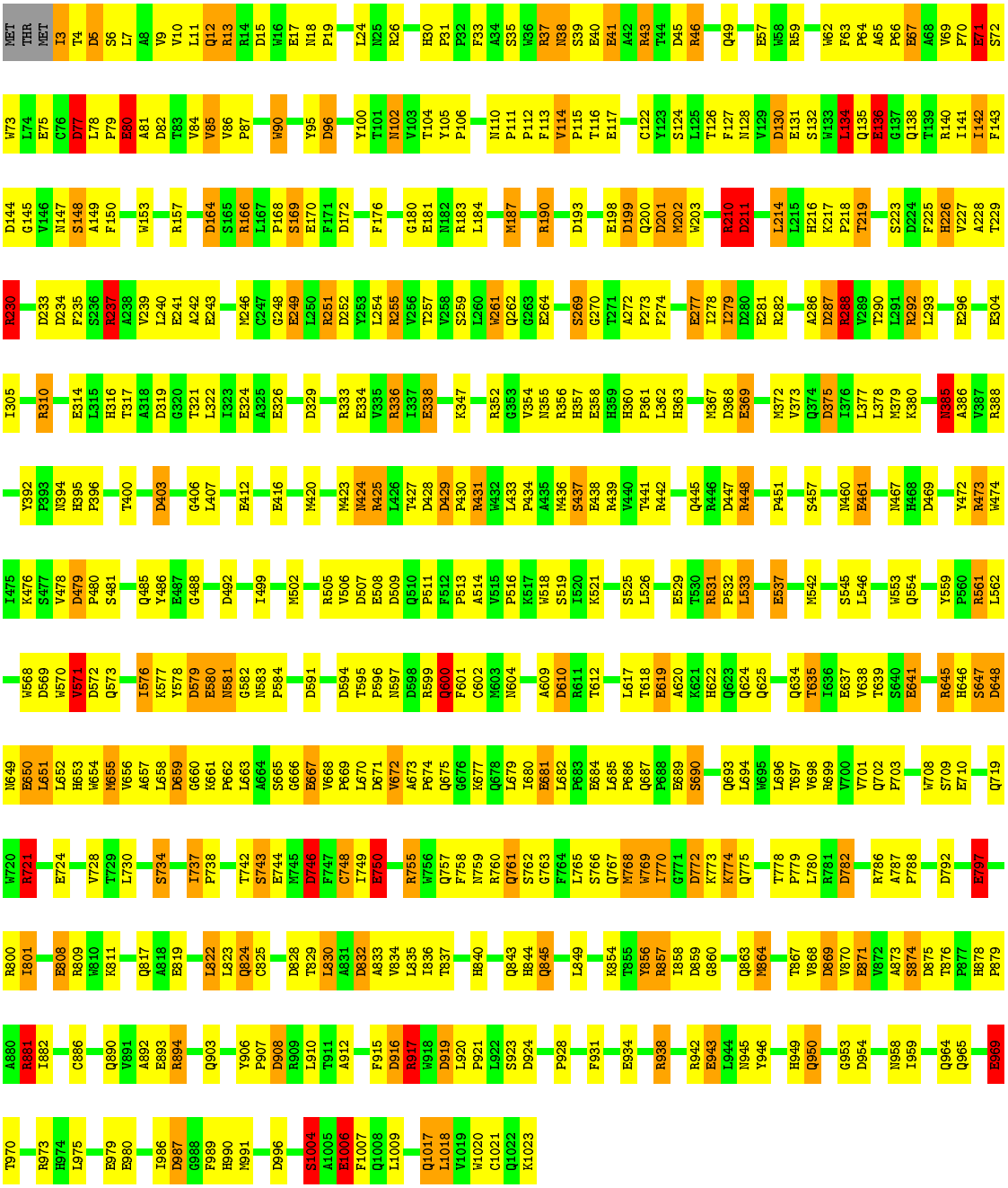
- Molecule 1: BETA-GALACTOSIDASE

Chain A:



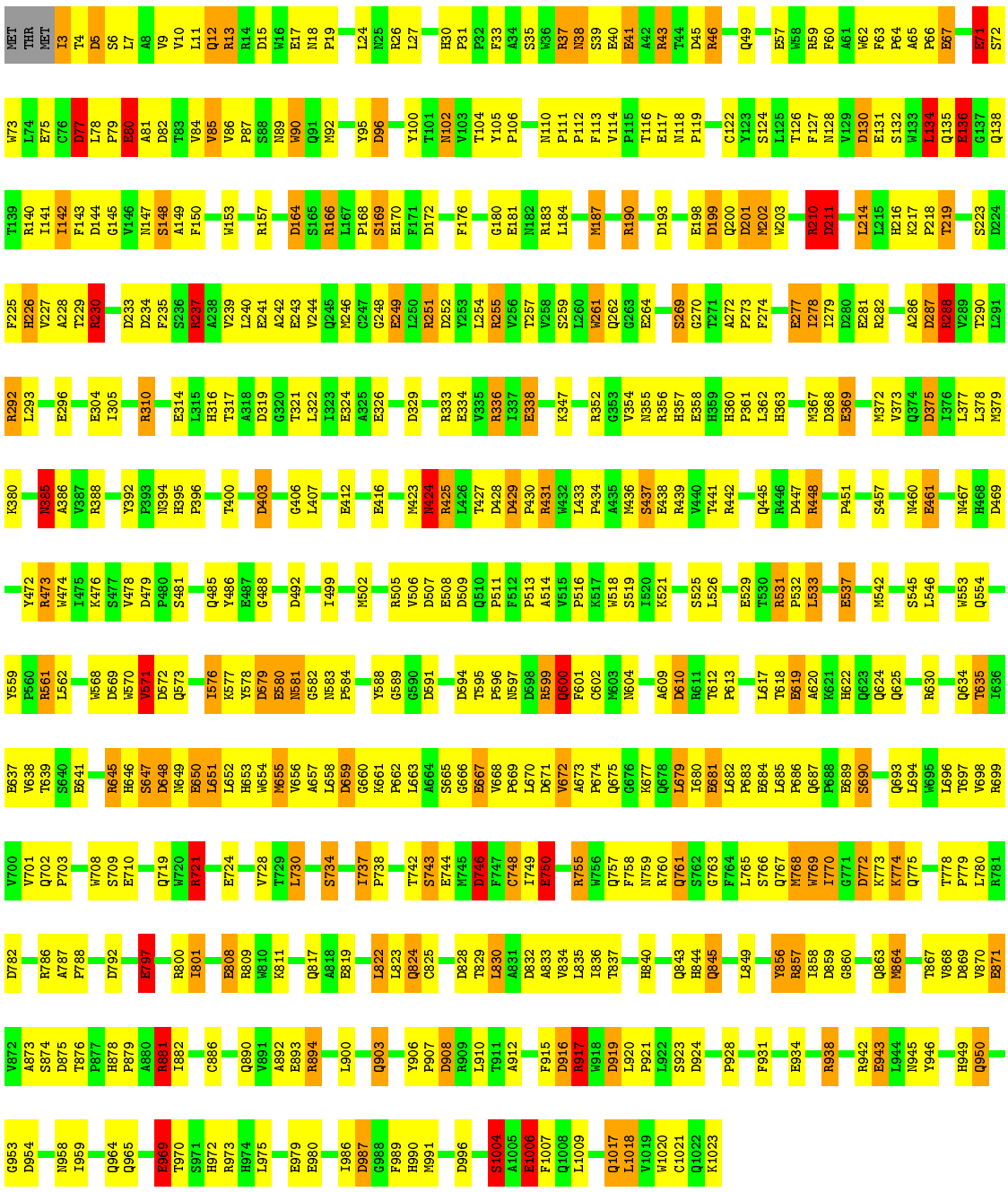
- Molecule 1: BETA-GALACTOSIDASE

Chain B:



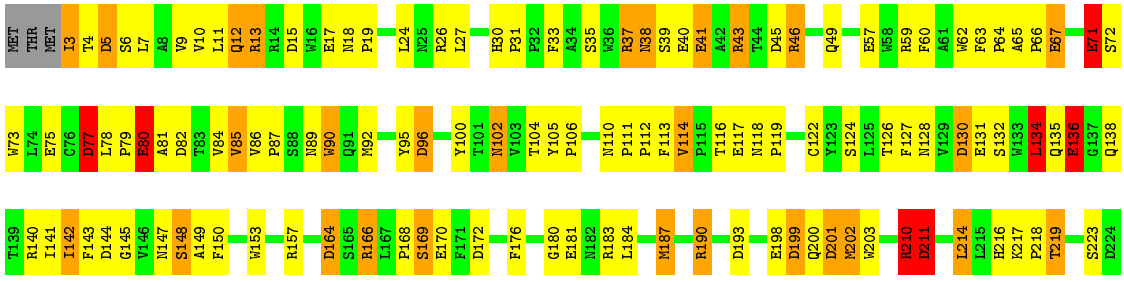
- Molecule 1: BETA-GALACTOSIDASE

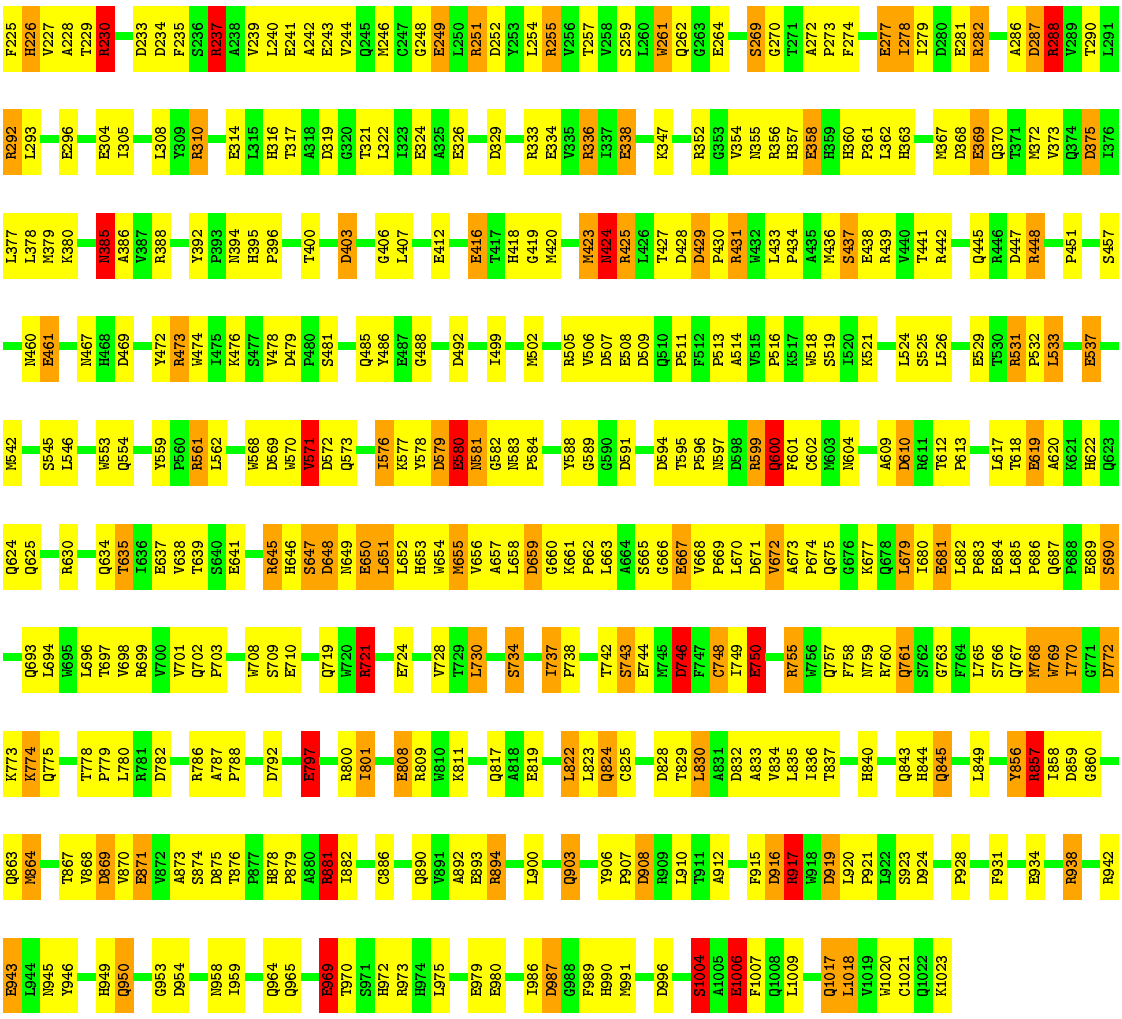
Chain C:



• Molecule 1: BETA-GALACTOSIDASE

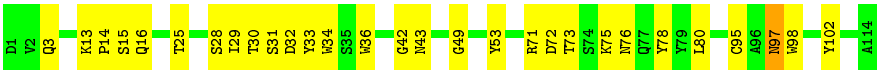
Chain D:





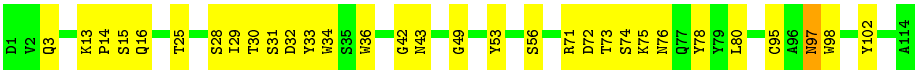
• Molecule 2: SCFV13R4 ANTIBODY FV HEAVY CHAIN

Chain H:



• Molecule 2: SCFV13R4 ANTIBODY FV HEAVY CHAIN

Chain I:

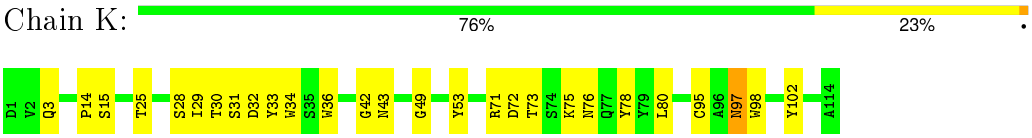


• Molecule 2: SCFV13R4 ANTIBODY FV HEAVY CHAIN

Chain J:

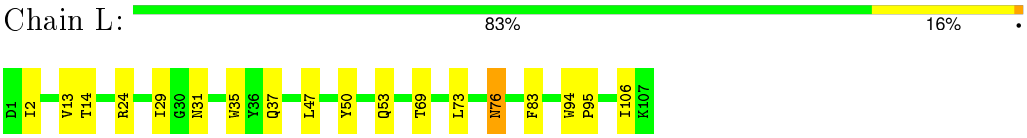
• Molecule 2: SCFV13R4 ANTIBODY FV HEAVY CHAIN

Chain K:



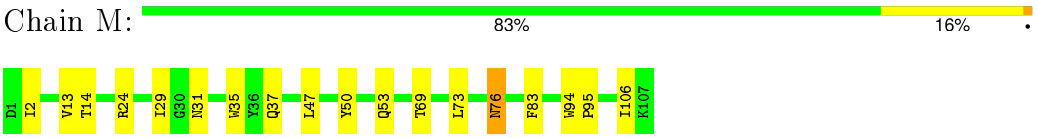
• Molecule 3: SCFV13R4 ANTIBODY FV LIGHT CHAIN

Chain L:



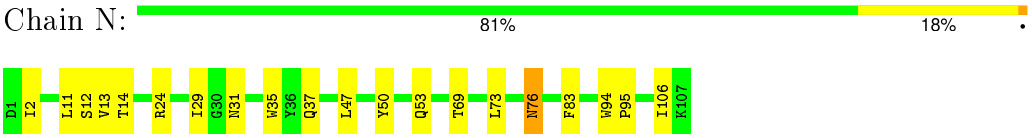
• Molecule 3: SCFV13R4 ANTIBODY FV LIGHT CHAIN

Chain M:



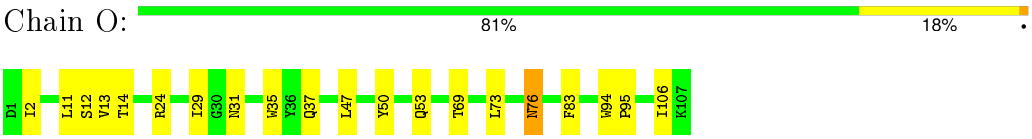
• Molecule 3: SCFV13R4 ANTIBODY FV LIGHT CHAIN

Chain N:



• Molecule 3: SCFV13R4 ANTIBODY FV LIGHT CHAIN

Chain O:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	DONE INSIDE FREALIGN	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	67	Depositor
Minimum defocus (nm)	2678	Depositor
Maximum defocus (nm)	4027	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II (4K X 4K)	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	A	1.08	52/8515 (0.6%)	1.61	174/11615 (1.5%)
1	B	1.08	52/8515 (0.6%)	1.61	175/11615 (1.5%)
1	C	1.08	52/8515 (0.6%)	1.61	173/11615 (1.5%)
1	D	1.08	53/8515 (0.6%)	1.61	180/11615 (1.5%)
2	H	0.31	0/925	0.65	0/1263
2	I	0.31	0/925	0.65	0/1263
2	J	0.31	0/925	0.65	0/1263
2	K	0.31	0/925	0.65	0/1263
3	L	0.32	0/837	0.58	0/1133
3	M	0.32	0/837	0.58	0/1133
3	N	0.32	0/837	0.58	0/1133
3	O	0.32	0/837	0.59	0/1133
All	All	1.00	209/41108 (0.5%)	1.49	702/56044 (1.3%)

All (209) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	75	GLU	CD-OE2	9.50	1.36	1.25
1	A	75	GLU	CD-OE2	9.50	1.36	1.25
1	D	75	GLU	CD-OE2	9.48	1.36	1.25
1	C	75	GLU	CD-OE2	9.41	1.36	1.25
1	B	710	GLU	CD-OE1	7.65	1.34	1.25
1	C	710	GLU	CD-OE1	7.63	1.34	1.25
1	A	710	GLU	CD-OE1	7.60	1.34	1.25
1	D	710	GLU	CD-OE1	7.59	1.33	1.25
1	C	181	GLU	CD-OE1	7.51	1.33	1.25
1	B	136	GLU	CD-OE1	7.48	1.33	1.25
1	D	136	GLU	CD-OE1	7.46	1.33	1.25
1	D	264	GLU	CD-OE2	7.46	1.33	1.25
1	D	508	GLU	CD-OE2	7.46	1.33	1.25
1	B	181	GLU	CD-OE1	7.45	1.33	1.25
1	A	181	GLU	CD-OE1	7.45	1.33	1.25
1	D	181	GLU	CD-OE1	7.45	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	508	GLU	CD-OE2	7.42	1.33	1.25
1	C	40	GLU	CD-OE2	7.38	1.33	1.25
1	A	264	GLU	CD-OE2	7.38	1.33	1.25
1	C	264	GLU	CD-OE2	7.38	1.33	1.25
1	C	136	GLU	CD-OE1	7.37	1.33	1.25
1	B	508	GLU	CD-OE2	7.37	1.33	1.25
1	A	681	GLU	CD-OE2	7.37	1.33	1.25
1	B	681	GLU	CD-OE2	7.36	1.33	1.25
1	A	136	GLU	CD-OE1	7.36	1.33	1.25
1	D	40	GLU	CD-OE2	7.35	1.33	1.25
1	B	40	GLU	CD-OE2	7.34	1.33	1.25
1	A	40	GLU	CD-OE2	7.33	1.33	1.25
1	B	314	GLU	CD-OE1	7.33	1.33	1.25
1	C	681	GLU	CD-OE2	7.33	1.33	1.25
1	C	943	GLU	CD-OE1	7.33	1.33	1.25
1	B	264	GLU	CD-OE2	7.32	1.33	1.25
1	D	681	GLU	CD-OE2	7.32	1.33	1.25
1	C	508	GLU	CD-OE2	7.32	1.33	1.25
1	A	943	GLU	CD-OE1	7.29	1.33	1.25
1	B	943	GLU	CD-OE1	7.23	1.33	1.25
1	C	314	GLU	CD-OE1	7.23	1.33	1.25
1	D	314	GLU	CD-OE1	7.22	1.33	1.25
1	A	314	GLU	CD-OE1	7.22	1.33	1.25
1	D	943	GLU	CD-OE1	7.21	1.33	1.25
1	C	369	GLU	CD-OE1	7.17	1.33	1.25
1	D	369	GLU	CD-OE1	7.07	1.33	1.25
1	A	797	GLU	CD-OE2	7.07	1.33	1.25
1	A	369	GLU	CD-OE1	7.05	1.33	1.25
1	B	369	GLU	CD-OE1	7.04	1.33	1.25
1	B	797	GLU	CD-OE2	7.01	1.33	1.25
1	D	797	GLU	CD-OE2	7.00	1.33	1.25
1	C	797	GLU	CD-OE2	6.97	1.33	1.25
1	C	979	GLU	CD-OE2	6.94	1.33	1.25
1	A	979	GLU	CD-OE2	6.92	1.33	1.25
1	A	650	GLU	CD-OE1	6.88	1.33	1.25
1	D	979	GLU	CD-OE2	6.88	1.33	1.25
1	D	650	GLU	CD-OE1	6.87	1.33	1.25
1	B	650	GLU	CD-OE1	6.85	1.33	1.25
1	C	750	GLU	CD-OE2	6.85	1.33	1.25
1	C	650	GLU	CD-OE1	6.83	1.33	1.25
1	D	969	GLU	CD-OE2	6.81	1.33	1.25
1	B	969	GLU	CD-OE2	6.81	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	979	GLU	CD-OE2	6.80	1.33	1.25
1	C	969	GLU	CD-OE2	6.79	1.33	1.25
1	A	326	GLU	CD-OE2	6.78	1.33	1.25
1	B	724	GLU	CD-OE2	6.77	1.33	1.25
1	A	750	GLU	CD-OE2	6.76	1.33	1.25
1	B	326	GLU	CD-OE2	6.76	1.33	1.25
1	A	198	GLU	CD-OE2	6.76	1.33	1.25
1	D	326	GLU	CD-OE2	6.75	1.33	1.25
1	D	724	GLU	CD-OE2	6.75	1.33	1.25
1	A	969	GLU	CD-OE2	6.75	1.33	1.25
1	A	724	GLU	CD-OE2	6.74	1.33	1.25
1	B	750	GLU	CD-OE2	6.74	1.33	1.25
1	C	326	GLU	CD-OE2	6.73	1.33	1.25
1	C	724	GLU	CD-OE2	6.72	1.33	1.25
1	C	198	GLU	CD-OE2	6.71	1.33	1.25
1	D	198	GLU	CD-OE2	6.68	1.32	1.25
1	B	198	GLU	CD-OE2	6.67	1.32	1.25
1	A	241	GLU	CD-OE2	6.67	1.32	1.25
1	D	241	GLU	CD-OE2	6.65	1.32	1.25
1	B	241	GLU	CD-OE2	6.63	1.32	1.25
1	C	241	GLU	CD-OE2	6.62	1.32	1.25
1	D	750	GLU	CD-OE2	6.62	1.32	1.25
1	C	338	GLU	CD-OE2	6.61	1.32	1.25
1	A	338	GLU	CD-OE2	6.49	1.32	1.25
1	D	338	GLU	CD-OE2	6.49	1.32	1.25
1	B	338	GLU	CD-OE2	6.43	1.32	1.25
1	A	438	GLU	CD-OE2	6.40	1.32	1.25
1	A	461	GLU	CD-OE2	6.39	1.32	1.25
1	B	461	GLU	CD-OE2	6.38	1.32	1.25
1	D	461	GLU	CD-OE2	6.38	1.32	1.25
1	C	438	GLU	CD-OE2	6.37	1.32	1.25
1	B	438	GLU	CD-OE2	6.37	1.32	1.25
1	C	461	GLU	CD-OE2	6.37	1.32	1.25
1	D	438	GLU	CD-OE2	6.34	1.32	1.25
1	B	296	GLU	CD-OE2	6.33	1.32	1.25
1	A	296	GLU	CD-OE2	6.32	1.32	1.25
1	D	296	GLU	CD-OE2	6.31	1.32	1.25
1	C	744	GLU	CD-OE2	6.24	1.32	1.25
1	A	249	GLU	CD-OE1	6.23	1.32	1.25
1	A	744	GLU	CD-OE2	6.22	1.32	1.25
1	B	808	GLU	CD-OE2	6.22	1.32	1.25
1	C	296	GLU	CD-OE2	6.20	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	808	GLU	CD-OE2	6.20	1.32	1.25
1	D	537	GLU	CD-OE2	6.19	1.32	1.25
1	D	249	GLU	CD-OE1	6.19	1.32	1.25
1	B	637	GLU	CD-OE2	6.18	1.32	1.25
1	C	249	GLU	CD-OE1	6.18	1.32	1.25
1	C	537	GLU	CD-OE2	6.18	1.32	1.25
1	A	537	GLU	CD-OE2	6.18	1.32	1.25
1	B	744	GLU	CD-OE2	6.17	1.32	1.25
1	B	537	GLU	CD-OE2	6.16	1.32	1.25
1	C	57	GLU	CD-OE2	6.16	1.32	1.25
1	D	744	GLU	CD-OE2	6.16	1.32	1.25
1	B	249	GLU	CD-OE1	6.15	1.32	1.25
1	D	637	GLU	CD-OE2	6.15	1.32	1.25
1	A	637	GLU	CD-OE2	6.14	1.32	1.25
1	C	637	GLU	CD-OE2	6.13	1.32	1.25
1	A	808	GLU	CD-OE2	6.11	1.32	1.25
1	D	57	GLU	CD-OE2	6.11	1.32	1.25
1	D	808	GLU	CD-OE2	6.10	1.32	1.25
1	A	57	GLU	CD-OE2	6.09	1.32	1.25
1	D	667	GLU	CD-OE2	6.08	1.32	1.25
1	B	57	GLU	CD-OE2	6.07	1.32	1.25
1	A	667	GLU	CD-OE2	6.07	1.32	1.25
1	B	667	GLU	CD-OE2	6.05	1.32	1.25
1	C	667	GLU	CD-OE2	6.03	1.32	1.25
1	D	641	GLU	CD-OE2	6.03	1.32	1.25
1	D	281	GLU	CD-OE2	6.03	1.32	1.25
1	A	641	GLU	CD-OE2	6.01	1.32	1.25
1	A	281	GLU	CD-OE2	6.01	1.32	1.25
1	D	80	GLU	CD-OE1	5.99	1.32	1.25
1	A	80	GLU	CD-OE1	5.99	1.32	1.25
1	B	80	GLU	CD-OE1	5.98	1.32	1.25
1	B	641	GLU	CD-OE2	5.97	1.32	1.25
1	C	281	GLU	CD-OE2	5.97	1.32	1.25
1	C	80	GLU	CD-OE1	5.96	1.32	1.25
1	B	281	GLU	CD-OE2	5.93	1.32	1.25
1	C	871	GLU	CD-OE1	5.91	1.32	1.25
1	C	641	GLU	CD-OE2	5.90	1.32	1.25
1	A	41	GLU	CD-OE2	5.90	1.32	1.25
1	A	871	GLU	CD-OE1	5.89	1.32	1.25
1	D	871	GLU	CD-OE1	5.88	1.32	1.25
1	C	41	GLU	CD-OE2	5.87	1.32	1.25
1	D	41	GLU	CD-OE2	5.84	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	871	GLU	CD-OE1	5.83	1.32	1.25
1	B	41	GLU	CD-OE2	5.82	1.32	1.25
1	B	334	GLU	CD-OE2	5.77	1.32	1.25
1	A	334	GLU	CD-OE2	5.76	1.31	1.25
1	D	334	GLU	CD-OE2	5.73	1.31	1.25
1	C	334	GLU	CD-OE2	5.67	1.31	1.25
1	A	71	GLU	CD-OE2	5.53	1.31	1.25
1	B	619	GLU	CD-OE1	5.50	1.31	1.25
1	C	71	GLU	CD-OE2	5.47	1.31	1.25
1	B	1006	GLU	CD-OE2	5.46	1.31	1.25
1	B	71	GLU	CD-OE2	5.46	1.31	1.25
1	D	1006	GLU	CD-OE2	5.44	1.31	1.25
1	D	71	GLU	CD-OE2	5.43	1.31	1.25
1	A	1006	GLU	CD-OE2	5.41	1.31	1.25
1	B	131	GLU	CD-OE2	5.40	1.31	1.25
1	D	980	GLU	CD-OE2	5.40	1.31	1.25
1	A	619	GLU	CD-OE1	5.40	1.31	1.25
1	D	619	GLU	CD-OE1	5.40	1.31	1.25
1	C	1006	GLU	CD-OE2	5.39	1.31	1.25
1	D	131	GLU	CD-OE2	5.38	1.31	1.25
1	B	412	GLU	CD-OE1	5.37	1.31	1.25
1	C	412	GLU	CD-OE1	5.37	1.31	1.25
1	A	980	GLU	CD-OE2	5.35	1.31	1.25
1	C	980	GLU	CD-OE2	5.35	1.31	1.25
1	D	580	GLU	CD-OE2	5.35	1.31	1.25
1	C	131	GLU	CD-OE2	5.34	1.31	1.25
1	B	277	GLU	CD-OE2	5.34	1.31	1.25
1	C	619	GLU	CD-OE1	5.34	1.31	1.25
1	A	277	GLU	CD-OE2	5.32	1.31	1.25
1	C	17	GLU	CD-OE2	5.32	1.31	1.25
1	D	117	GLU	CD-OE2	5.32	1.31	1.25
1	C	689	GLU	CD-OE1	5.31	1.31	1.25
1	A	17	GLU	CD-OE2	5.31	1.31	1.25
1	B	689	GLU	CD-OE1	5.31	1.31	1.25
1	C	819	GLU	CD-OE2	5.30	1.31	1.25
1	B	934	GLU	CD-OE2	5.30	1.31	1.25
1	A	580	GLU	CD-OE2	5.29	1.31	1.25
1	C	580	GLU	CD-OE2	5.28	1.31	1.25
1	C	893	GLU	CD-OE1	5.28	1.31	1.25
1	B	17	GLU	CD-OE2	5.28	1.31	1.25
1	D	17	GLU	CD-OE2	5.28	1.31	1.25
1	A	934	GLU	CD-OE2	5.28	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	131	GLU	CD-OE2	5.28	1.31	1.25
1	A	117	GLU	CD-OE2	5.27	1.31	1.25
1	D	412	GLU	CD-OE1	5.27	1.31	1.25
1	D	689	GLU	CD-OE1	5.27	1.31	1.25
1	A	893	GLU	CD-OE1	5.27	1.31	1.25
1	A	412	GLU	CD-OE1	5.26	1.31	1.25
1	C	117	GLU	CD-OE2	5.26	1.31	1.25
1	D	277	GLU	CD-OE2	5.26	1.31	1.25
1	B	980	GLU	CD-OE2	5.26	1.31	1.25
1	C	277	GLU	CD-OE2	5.26	1.31	1.25
1	C	684	GLU	CD-OE2	5.25	1.31	1.25
1	A	684	GLU	CD-OE2	5.24	1.31	1.25
1	D	684	GLU	CD-OE2	5.22	1.31	1.25
1	D	934	GLU	CD-OE2	5.22	1.31	1.25
1	B	580	GLU	CD-OE2	5.21	1.31	1.25
1	A	819	GLU	CD-OE2	5.21	1.31	1.25
1	B	893	GLU	CD-OE1	5.21	1.31	1.25
1	B	819	GLU	CD-OE2	5.19	1.31	1.25
1	C	934	GLU	CD-OE2	5.19	1.31	1.25
1	D	893	GLU	CD-OE1	5.17	1.31	1.25
1	B	117	GLU	CD-OE2	5.16	1.31	1.25
1	A	689	GLU	CD-OE1	5.15	1.31	1.25
1	D	819	GLU	CD-OE2	5.14	1.31	1.25
1	B	684	GLU	CD-OE2	5.12	1.31	1.25
1	D	358	GLU	CD-OE2	5.03	1.31	1.25

All (702) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	809[A]	ARG	NE-CZ-NH1	11.67	126.14	120.30
1	B	809[B]	ARG	NE-CZ-NH1	11.67	126.14	120.30
1	D	809[A]	ARG	NE-CZ-NH1	11.59	126.09	120.30
1	D	809[B]	ARG	NE-CZ-NH1	11.59	126.09	120.30
1	A	809[A]	ARG	NE-CZ-NH1	11.58	126.09	120.30
1	A	809[B]	ARG	NE-CZ-NH1	11.58	126.09	120.30
1	C	809[A]	ARG	NE-CZ-NH1	11.48	126.04	120.30
1	C	809[B]	ARG	NE-CZ-NH1	11.48	126.04	120.30
1	A	881	ARG	NE-CZ-NH1	11.12	125.86	120.30
1	C	881	ARG	NE-CZ-NH2	-11.03	114.78	120.30
1	A	881	ARG	NE-CZ-NH2	-11.02	114.79	120.30
1	D	881	ARG	NE-CZ-NH1	11.02	125.81	120.30
1	C	881	ARG	NE-CZ-NH1	10.98	125.79	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	881	ARG	NE-CZ-NH2	-10.96	114.82	120.30
1	B	881	ARG	NE-CZ-NH1	10.94	125.77	120.30
1	B	881	ARG	NE-CZ-NH2	-10.85	114.87	120.30
1	A	531	ARG	NE-CZ-NH1	10.77	125.68	120.30
1	B	531	ARG	NE-CZ-NH1	10.74	125.67	120.30
1	D	531	ARG	NE-CZ-NH1	10.67	125.64	120.30
1	C	531	ARG	NE-CZ-NH1	10.66	125.63	120.30
1	B	385	ASN	CB-CA-C	-10.46	89.47	110.40
1	D	385	ASN	CB-CA-C	-10.45	89.51	110.40
1	C	385	ASN	CB-CA-C	-10.44	89.52	110.40
1	A	385	ASN	CB-CA-C	-10.42	89.56	110.40
1	C	507	ASP	CB-CG-OD2	-10.40	108.94	118.30
1	D	507	ASP	CB-CG-OD2	-10.35	108.98	118.30
1	A	507	ASP	CB-CG-OD2	-10.31	109.02	118.30
1	B	507	ASP	CB-CG-OD2	-10.28	109.05	118.30
1	C	356	ARG	NE-CZ-NH1	9.82	125.21	120.30
1	C	13	ARG	NE-CZ-NH2	-9.76	115.42	120.30
1	D	13	ARG	NE-CZ-NH2	-9.75	115.43	120.30
1	A	356	ARG	NE-CZ-NH1	9.73	125.16	120.30
1	A	13	ARG	NE-CZ-NH2	-9.72	115.44	120.30
1	D	237	ARG	NE-CZ-NH1	9.68	125.14	120.30
1	B	356	ARG	NE-CZ-NH1	9.67	125.14	120.30
1	D	356	ARG	NE-CZ-NH1	9.65	125.12	120.30
1	B	237	ARG	NE-CZ-NH1	9.62	125.11	120.30
1	A	237	ARG	NE-CZ-NH1	9.59	125.10	120.30
1	A	591	ASP	CB-CG-OD2	-9.58	109.68	118.30
1	D	591	ASP	CB-CG-OD2	-9.58	109.68	118.30
1	B	13	ARG	NE-CZ-NH2	-9.55	115.53	120.30
1	C	591	ASP	CB-CG-OD2	-9.54	109.72	118.30
1	C	237	ARG	NE-CZ-NH1	9.51	125.06	120.30
1	D	439	ARG	NE-CZ-NH1	9.51	125.06	120.30
1	B	439	ARG	NE-CZ-NH1	9.48	125.04	120.30
1	B	591	ASP	CB-CG-OD2	-9.45	109.80	118.30
1	C	439	ARG	NE-CZ-NH1	9.43	125.02	120.30
1	A	439	ARG	NE-CZ-NH1	9.37	124.98	120.30
1	C	249	GLU	N-CA-CB	9.24	127.24	110.60
1	B	249	GLU	N-CA-CB	9.24	127.24	110.60
1	D	249	GLU	N-CA-CB	9.23	127.22	110.60
1	A	249	GLU	N-CA-CB	9.23	127.21	110.60
1	A	509	ASP	CB-CG-OD2	-9.18	110.04	118.30
1	D	509	ASP	CB-CG-OD2	-9.14	110.08	118.30
1	B	509	ASP	CB-CG-OD2	-9.13	110.09	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	509	ASP	CB-CG-OD2	-9.12	110.09	118.30
1	A	424	ASN	CB-CA-C	-9.11	92.17	110.40
1	B	424	ASN	CB-CA-C	-9.11	92.18	110.40
1	D	424	ASN	CB-CA-C	-9.11	92.19	110.40
1	C	424	ASN	CB-CA-C	-9.09	92.23	110.40
1	C	938	ARG	NE-CZ-NH2	-8.91	115.84	120.30
1	B	938	ARG	NE-CZ-NH2	-8.85	115.88	120.30
1	C	429	ASP	CB-CG-OD1	8.79	126.21	118.30
1	D	429	ASP	CB-CG-OD1	8.76	126.19	118.30
1	A	938	ARG	NE-CZ-NH2	-8.76	115.92	120.30
1	B	429	ASP	CB-CG-OD1	8.75	126.18	118.30
1	D	938	ARG	NE-CZ-NH2	-8.75	115.93	120.30
1	A	429	ASP	CB-CG-OD1	8.75	126.17	118.30
1	B	210	ARG	NE-CZ-NH1	8.75	124.67	120.30
1	A	210	ARG	NE-CZ-NH1	8.67	124.64	120.30
1	D	210	ARG	NE-CZ-NH1	8.57	124.59	120.30
1	C	210	ARG	NE-CZ-NH1	8.57	124.58	120.30
1	C	509	ASP	CB-CG-OD1	8.48	125.93	118.30
1	D	509	ASP	CB-CG-OD1	8.46	125.91	118.30
1	A	509	ASP	CB-CG-OD1	8.44	125.89	118.30
1	B	509	ASP	CB-CG-OD1	8.42	125.88	118.30
1	C	233	ASP	CB-CG-OD1	8.23	125.70	118.30
1	B	233	ASP	CB-CG-OD1	8.22	125.70	118.30
1	A	233	ASP	CB-CG-OD1	8.22	125.69	118.30
1	D	233	ASP	CB-CG-OD1	8.18	125.66	118.30
1	A	226	HIS	CB-CA-C	-8.16	94.08	110.40
1	D	287	ASP	CB-CG-OD2	-8.16	110.96	118.30
1	B	226	HIS	CB-CA-C	-8.15	94.09	110.40
1	B	130	ASP	CB-CG-OD2	-8.15	110.96	118.30
1	D	226	HIS	CB-CA-C	-8.15	94.09	110.40
1	C	226	HIS	CB-CA-C	-8.14	94.12	110.40
1	C	130	ASP	CB-CG-OD2	-8.12	110.99	118.30
1	B	287	ASP	CB-CG-OD2	-8.11	111.00	118.30
1	D	130	ASP	CB-CG-OD2	-8.11	111.00	118.30
1	C	287	ASP	CB-CG-OD2	-8.10	111.01	118.30
1	A	130	ASP	CB-CG-OD2	-8.10	111.01	118.30
1	A	287	ASP	CB-CG-OD2	-8.07	111.04	118.30
1	D	479	ASP	CB-CG-OD2	-8.07	111.04	118.30
1	C	479	ASP	CB-CG-OD2	-8.04	111.06	118.30
1	B	479	ASP	CB-CG-OD2	-8.03	111.07	118.30
1	D	211	ASP	CB-CG-OD1	7.98	125.48	118.30
1	B	211	ASP	CB-CG-OD1	7.98	125.48	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	479	ASP	CB-CG-OD2	-7.97	111.13	118.30
1	B	828	ASP	CB-CG-OD1	-7.95	111.15	118.30
1	D	828	ASP	CB-CG-OD1	-7.94	111.16	118.30
1	A	211	ASP	CB-CG-OD1	7.94	125.44	118.30
1	C	211	ASP	CB-CG-OD1	7.93	125.44	118.30
1	B	792	ASP	CB-CG-OD2	-7.92	111.17	118.30
1	D	792	ASP	CB-CG-OD2	-7.90	111.19	118.30
1	C	828	ASP	CB-CG-OD1	-7.89	111.20	118.30
1	A	828	ASP	CB-CG-OD1	-7.87	111.22	118.30
1	A	792	ASP	CB-CG-OD2	-7.87	111.22	118.30
1	D	13	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	C	792	ASP	CB-CG-OD2	-7.83	111.25	118.30
1	C	13	ARG	NE-CZ-NH1	7.82	124.21	120.30
1	D	288	ARG	NE-CZ-NH1	-7.81	116.39	120.30
1	D	310	ARG	NE-CZ-NH1	7.79	124.19	120.30
1	A	13	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	C	385	ASN	N-CA-CB	-7.78	96.60	110.60
1	A	385	ASN	N-CA-CB	-7.77	96.62	110.60
1	D	385	ASN	N-CA-CB	-7.76	96.63	110.60
1	B	385	ASN	N-CA-CB	-7.75	96.65	110.60
1	A	648	ASP	CB-CG-OD2	-7.74	111.33	118.30
1	B	648	ASP	CB-CG-OD2	-7.72	111.35	118.30
1	A	659	ASP	CB-CG-OD2	-7.72	111.35	118.30
1	C	310	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	A	310	ARG	NE-CZ-NH1	7.71	124.15	120.30
1	A	288	ARG	NE-CZ-NH1	-7.70	116.45	120.30
1	D	648	ASP	CB-CG-OD2	-7.70	111.37	118.30
1	B	659	ASP	CB-CG-OD2	-7.69	111.38	118.30
1	C	648	ASP	CB-CG-OD2	-7.68	111.39	118.30
1	A	832	ASP	CB-CG-OD1	7.68	125.21	118.30
1	C	288	ARG	NE-CZ-NH1	-7.67	116.47	120.30
1	C	479	ASP	CB-CG-OD1	7.66	125.20	118.30
1	C	659	ASP	CB-CG-OD2	-7.66	111.41	118.30
1	C	832	ASP	CB-CG-OD2	-7.66	111.41	118.30
1	D	832	ASP	CB-CG-OD1	7.66	125.19	118.30
1	A	832	ASP	CB-CG-OD2	-7.65	111.41	118.30
1	B	13	ARG	NE-CZ-NH1	7.65	124.12	120.30
1	B	310	ARG	NE-CZ-NH1	7.65	124.12	120.30
1	D	659	ASP	CB-CG-OD2	-7.62	111.44	118.30
1	C	832	ASP	CB-CG-OD1	7.62	125.16	118.30
1	A	479	ASP	CB-CG-OD1	7.61	125.15	118.30
1	B	479	ASP	CB-CG-OD1	7.61	125.15	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	832	ASP	CB-CG-OD1	7.60	125.14	118.30
1	D	479	ASP	CB-CG-OD1	7.59	125.13	118.30
1	B	832	ASP	CB-CG-OD2	-7.58	111.47	118.30
1	D	832	ASP	CB-CG-OD2	-7.58	111.48	118.30
1	B	288	ARG	NE-CZ-NH1	-7.57	116.51	120.30
1	B	639	THR	CA-CB-CG2	-7.51	101.89	112.40
1	C	252	ASP	CB-CG-OD2	-7.49	111.56	118.30
1	C	639	THR	CA-CB-CG2	-7.46	101.96	112.40
1	A	639	THR	CA-CB-CG2	-7.45	101.97	112.40
1	D	639	THR	CA-CB-CG2	-7.45	101.98	112.40
1	A	252	ASP	CB-CG-OD2	-7.42	111.62	118.30
1	B	199	ASP	CB-CG-OD2	-7.40	111.64	118.30
1	D	252	ASP	CB-CG-OD2	-7.39	111.65	118.30
1	D	431[A]	ARG	NE-CZ-NH1	7.39	123.99	120.30
1	D	431[B]	ARG	NE-CZ-NH1	7.39	123.99	120.30
1	D	211	ASP	CB-CG-OD2	-7.38	111.66	118.30
1	A	199	ASP	CB-CG-OD2	-7.38	111.66	118.30
1	C	199	ASP	CB-CG-OD2	-7.37	111.67	118.30
1	C	431[A]	ARG	NE-CZ-NH1	7.37	123.99	120.30
1	C	431[B]	ARG	NE-CZ-NH1	7.37	123.99	120.30
1	B	252	ASP	CB-CG-OD2	-7.36	111.67	118.30
1	C	211	ASP	CB-CG-OD2	-7.36	111.67	118.30
1	B	211	ASP	CB-CG-OD2	-7.36	111.68	118.30
1	D	1004	SER	N-CA-CB	7.36	121.54	110.50
1	A	1004	SER	N-CA-CB	7.35	121.53	110.50
1	B	431[A]	ARG	NE-CZ-NH1	7.35	123.97	120.30
1	B	431[B]	ARG	NE-CZ-NH1	7.35	123.97	120.30
1	C	1004	SER	N-CA-CB	7.34	121.52	110.50
1	A	431[A]	ARG	NE-CZ-NH1	7.33	123.97	120.30
1	A	431[B]	ARG	NE-CZ-NH1	7.33	123.97	120.30
1	B	403	ASP	CB-CG-OD1	7.33	124.90	118.30
1	D	199	ASP	CB-CG-OD2	-7.33	111.70	118.30
1	B	448	ARG	NE-CZ-NH2	-7.33	116.64	120.30
1	A	211	ASP	CB-CG-OD2	-7.32	111.71	118.30
1	D	403	ASP	CB-CG-OD1	7.32	124.89	118.30
1	B	1004	SER	N-CA-CB	7.31	121.46	110.50
1	C	403	ASP	CB-CG-OD1	7.31	124.88	118.30
1	A	403	ASP	CB-CG-OD1	7.30	124.87	118.30
1	C	448	ARG	NE-CZ-NH2	-7.29	116.65	120.30
1	B	336	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	A	96	ASP	CB-CG-OD2	-7.25	111.78	118.30
1	C	924	ASP	CB-CG-OD1	7.24	124.81	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	448	ARG	NE-CZ-NH2	-7.23	116.69	120.30
1	C	924	ASP	CB-CG-OD2	-7.22	111.81	118.30
1	A	924	ASP	CB-CG-OD2	-7.21	111.81	118.30
1	D	448	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	D	96	ASP	CB-CG-OD2	-7.21	111.81	118.30
1	B	924	ASP	CB-CG-OD2	-7.20	111.82	118.30
1	B	96	ASP	CB-CG-OD2	-7.19	111.83	118.30
1	A	924	ASP	CB-CG-OD1	7.19	124.77	118.30
1	D	924	ASP	CB-CG-OD1	7.18	124.77	118.30
1	B	126	THR	CA-CB-CG2	-7.18	102.35	112.40
1	C	96	ASP	CB-CG-OD2	-7.18	111.84	118.30
1	D	924	ASP	CB-CG-OD2	-7.17	111.85	118.30
1	A	648	ASP	CB-CG-OD1	7.17	124.75	118.30
1	B	648	ASP	CB-CG-OD1	7.16	124.75	118.30
1	C	126	THR	CA-CB-CG2	-7.16	102.38	112.40
1	C	648	ASP	CB-CG-OD1	7.16	124.74	118.30
1	D	126	THR	CA-CB-CG2	-7.15	102.39	112.40
1	C	252	ASP	CB-CG-OD1	7.14	124.73	118.30
1	C	356	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	B	924	ASP	CB-CG-OD1	7.14	124.72	118.30
1	A	126	THR	CA-CB-CG2	-7.13	102.42	112.40
1	D	648	ASP	CB-CG-OD1	7.13	124.71	118.30
1	A	336	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	C	336	ARG	NE-CZ-NH1	7.11	123.86	120.30
1	D	336	ARG	NE-CZ-NH1	7.11	123.86	120.30
1	C	553	TRP	CA-CB-CG	-7.09	100.23	113.70
1	B	553	TRP	CA-CB-CG	-7.08	100.24	113.70
1	A	553	TRP	CA-CB-CG	-7.08	100.24	113.70
1	D	553	TRP	CA-CB-CG	-7.07	100.27	113.70
1	A	746	ASP	CB-CG-OD2	-7.06	111.94	118.30
1	B	746	ASP	CB-CG-OD2	-7.06	111.95	118.30
1	A	252	ASP	CB-CG-OD1	7.02	124.62	118.30
1	D	746	ASP	CB-CG-OD2	-7.02	111.98	118.30
1	D	252	ASP	CB-CG-OD1	7.01	124.61	118.30
1	C	400	THR	CA-CB-CG2	-6.99	102.62	112.40
1	A	400	THR	CA-CB-CG2	-6.98	102.62	112.40
1	C	746	ASP	CB-CG-OD2	-6.98	112.02	118.30
1	D	356	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	B	252	ASP	CB-CG-OD1	6.98	124.58	118.30
1	D	400	THR	CA-CB-CG2	-6.98	102.63	112.40
1	D	859	ASP	CB-CG-OD1	6.98	124.58	118.30
1	B	859	ASP	CB-CG-OD1	6.97	124.57	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	233	ASP	CB-CG-OD2	-6.96	112.04	118.30
1	B	233	ASP	CB-CG-OD2	-6.95	112.04	118.30
1	D	233	ASP	CB-CG-OD2	-6.94	112.05	118.30
1	A	591	ASP	CB-CG-OD1	6.94	124.54	118.30
1	B	859	ASP	CB-CG-OD2	-6.94	112.06	118.30
1	C	96	ASP	CB-CG-OD1	6.94	124.54	118.30
1	A	233	ASP	CB-CG-OD2	-6.93	112.06	118.30
1	C	591	ASP	CB-CG-OD1	6.93	124.54	118.30
1	B	400	THR	CA-CB-CG2	-6.93	102.70	112.40
1	A	287	ASP	CB-CG-OD1	6.92	124.53	118.30
1	D	429	ASP	CB-CG-OD2	-6.91	112.08	118.30
1	A	859	ASP	CB-CG-OD1	6.91	124.52	118.30
1	A	429	ASP	CB-CG-OD2	-6.90	112.09	118.30
1	B	403	ASP	CB-CG-OD2	-6.90	112.09	118.30
1	C	859	ASP	CB-CG-OD2	-6.90	112.09	118.30
1	D	287	ASP	CB-CG-OD1	6.90	124.51	118.30
1	A	569	ASP	CB-CG-OD1	-6.90	112.09	118.30
1	B	287	ASP	CB-CG-OD1	6.90	124.51	118.30
1	C	287	ASP	CB-CG-OD1	6.90	124.51	118.30
1	A	859	ASP	CB-CG-OD2	-6.89	112.10	118.30
1	C	429	ASP	CB-CG-OD2	-6.89	112.10	118.30
1	C	859	ASP	CB-CG-OD1	6.89	124.50	118.30
1	A	96	ASP	CB-CG-OD1	6.88	124.49	118.30
1	B	356	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	C	569	ASP	CB-CG-OD1	-6.88	112.11	118.30
1	B	429	ASP	CB-CG-OD2	-6.87	112.11	118.30
1	D	569	ASP	CB-CG-OD1	-6.87	112.12	118.30
1	D	591	ASP	CB-CG-OD1	6.87	124.48	118.30
1	D	859	ASP	CB-CG-OD2	-6.86	112.12	118.30
1	C	881	ARG	CD-NE-CZ	6.84	133.18	123.60
1	B	881	ARG	CD-NE-CZ	6.84	133.17	123.60
1	A	403	ASP	CB-CG-OD2	-6.83	112.15	118.30
1	B	96	ASP	CB-CG-OD1	6.83	124.45	118.30
1	D	96	ASP	CB-CG-OD1	6.83	124.45	118.30
1	B	569	ASP	CB-CG-OD1	-6.83	112.16	118.30
1	B	591	ASP	CB-CG-OD1	6.82	124.44	118.30
1	C	403	ASP	CB-CG-OD2	-6.82	112.16	118.30
1	D	403	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	D	881	ARG	CD-NE-CZ	6.81	133.13	123.60
1	A	356	ARG	NE-CZ-NH2	-6.77	116.91	120.30
1	A	881	ARG	CD-NE-CZ	6.77	133.08	123.60
1	C	375	ASP	CB-CG-OD2	-6.67	112.29	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	375	ASP	CB-CG-OD2	-6.67	112.30	118.30
1	C	659	ASP	CB-CG-OD1	6.67	124.30	118.30
1	C	571	VAL	CB-CA-C	-6.66	98.75	111.40
1	D	571	VAL	CB-CA-C	-6.65	98.76	111.40
1	C	507	ASP	CB-CG-OD1	6.65	124.28	118.30
1	A	571	VAL	CB-CA-C	-6.63	98.80	111.40
1	A	659	ASP	CB-CG-OD1	6.62	124.26	118.30
1	D	659	ASP	CB-CG-OD1	6.62	124.26	118.30
1	B	659	ASP	CB-CG-OD1	6.62	124.25	118.30
1	B	375	ASP	CB-CG-OD2	-6.62	112.34	118.30
1	B	571	VAL	CB-CA-C	-6.61	98.84	111.40
1	B	166	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	C	672	VAL	CB-CA-C	-6.59	98.87	111.40
1	B	424	ASN	N-CA-CB	-6.59	98.74	110.60
1	D	424	ASN	N-CA-CB	-6.59	98.74	110.60
1	D	672	VAL	CB-CA-C	-6.59	98.88	111.40
1	A	424	ASN	N-CA-CB	-6.58	98.76	110.60
1	B	672	VAL	CB-CA-C	-6.57	98.91	111.40
1	A	672	VAL	CB-CA-C	-6.57	98.93	111.40
1	A	375	ASP	CB-CG-OD2	-6.56	112.39	118.30
1	C	424	ASN	N-CA-CB	-6.56	98.80	110.60
1	D	507	ASP	CB-CG-OD1	6.55	124.19	118.30
1	D	166	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	A	507	ASP	CB-CG-OD1	6.51	124.16	118.30
1	D	919	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	A	15	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	C	919	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	A	166	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	B	507	ASP	CB-CG-OD1	6.47	124.12	118.30
1	D	15	ASP	CB-CG-OD2	-6.46	112.49	118.30
1	B	15	ASP	CB-CG-OD2	-6.46	112.49	118.30
1	A	15	ASP	CB-CG-OD1	6.45	124.11	118.30
1	D	15	ASP	CB-CG-OD1	6.45	124.11	118.30
1	C	875	ASP	CB-CG-OD1	-6.44	112.51	118.30
1	C	15	ASP	CB-CG-OD2	-6.43	112.51	118.30
1	C	5	ASP	CB-CG-OD1	6.42	124.08	118.30
1	A	875	ASP	CB-CG-OD1	-6.42	112.53	118.30
1	A	919	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	B	15	ASP	CB-CG-OD1	6.40	124.06	118.30
1	C	15	ASP	CB-CG-OD1	6.40	124.06	118.30
1	B	5	ASP	CB-CG-OD1	6.40	124.06	118.30
1	D	938	ARG	N-CA-CB	6.40	122.11	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	600	GLN	N-CA-CB	6.40	122.11	110.60
1	B	600	GLN	N-CA-CB	6.39	122.11	110.60
1	B	875	ASP	CB-CG-OD1	-6.39	112.55	118.30
1	A	600	GLN	N-CA-CB	6.39	122.10	110.60
1	C	166	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	D	875	ASP	CB-CG-OD1	-6.39	112.55	118.30
1	B	919	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	A	5	ASP	CB-CG-OD1	6.38	124.04	118.30
1	B	938	ARG	N-CA-CB	6.37	122.07	110.60
1	D	5	ASP	CB-CG-OD1	6.37	124.03	118.30
1	A	319	ASP	CB-CG-OD1	-6.37	112.57	118.30
1	B	750	GLU	N-CA-CB	6.37	122.06	110.60
1	D	750	GLU	N-CA-CB	6.37	122.06	110.60
1	B	319	ASP	CB-CG-OD1	-6.36	112.58	118.30
1	A	938	ARG	N-CA-CB	6.36	122.05	110.60
1	D	600	GLN	N-CA-CB	6.36	122.05	110.60
1	C	938	ARG	N-CA-CB	6.36	122.04	110.60
1	A	782	ASP	CB-CG-OD1	6.35	124.02	118.30
1	C	319	ASP	CB-CG-OD1	-6.35	112.58	118.30
1	D	319	ASP	CB-CG-OD1	-6.34	112.59	118.30
1	C	750	GLU	N-CA-CB	6.34	122.01	110.60
1	A	750	GLU	N-CA-CB	6.33	121.99	110.60
1	B	439	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	C	782	ASP	CB-CG-OD1	6.30	123.97	118.30
1	B	782	ASP	CB-CG-OD1	6.29	123.96	118.30
1	A	428	ASP	CB-CG-OD2	-6.28	112.65	118.30
1	D	782	ASP	CB-CG-OD1	6.28	123.95	118.30
1	D	651	LEU	CB-CA-C	-6.27	98.29	110.20
1	D	428	ASP	CB-CG-OD2	-6.26	112.66	118.30
1	C	439	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	B	651	LEU	CB-CA-C	-6.25	98.32	110.20
1	A	651	LEU	CB-CA-C	-6.24	98.34	110.20
1	A	439	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	C	938	ARG	CG-CD-NE	-6.24	98.70	111.80
1	C	651	LEU	CB-CA-C	-6.24	98.35	110.20
1	A	908	ASP	CB-CG-OD1	6.23	123.91	118.30
1	D	439	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	D	572	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	A	938	ARG	CG-CD-NE	-6.22	98.74	111.80
1	D	938	ARG	CG-CD-NE	-6.22	98.74	111.80
1	C	908	ASP	CB-CG-OD1	6.21	123.89	118.30
1	B	938	ARG	CG-CD-NE	-6.21	98.76	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	954	ASP	CB-CG-OD1	6.20	123.88	118.30
1	B	431[A]	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	B	431[B]	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	B	908	ASP	CB-CG-OD1	6.20	123.88	118.30
1	C	572	ASP	CB-CG-OD2	-6.19	112.72	118.30
1	A	572	ASP	CB-CG-OD2	-6.19	112.73	118.30
1	A	431[A]	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	A	431[B]	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	C	428	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	C	954	ASP	CB-CG-OD1	6.16	123.84	118.30
1	B	772	ASP	CB-CG-OD2	-6.15	112.77	118.30
1	A	172	ASP	CB-CG-OD2	-6.15	112.77	118.30
1	B	572	ASP	CB-CG-OD2	-6.14	112.77	118.30
1	D	431[A]	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	D	431[B]	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	D	954	ASP	CB-CG-OD1	6.13	123.82	118.30
1	A	772	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	B	172	ASP	CB-CG-OD2	-6.12	112.80	118.30
1	B	428	ASP	CB-CG-OD2	-6.12	112.80	118.30
1	D	772	ASP	CB-CG-OD2	-6.11	112.80	118.30
1	D	908	ASP	CB-CG-OD1	6.11	123.80	118.30
1	D	172	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	C	431[A]	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	C	431[B]	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	A	569	ASP	CB-CG-OD2	6.09	123.78	118.30
1	C	172	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	A	954	ASP	CB-CG-OD1	6.07	123.76	118.30
1	D	336	ARG	CB-CA-C	-6.07	98.27	110.40
1	C	336	ARG	CB-CA-C	-6.06	98.28	110.40
1	C	772	ASP	CB-CG-OD2	-6.05	112.86	118.30
1	A	336	ARG	CB-CA-C	-6.04	98.31	110.40
1	B	336	ARG	CB-CA-C	-6.04	98.33	110.40
1	C	679	LEU	CA-CB-CG	-6.03	101.42	115.30
1	A	679	LEU	CA-CB-CG	-6.01	101.47	115.30
1	B	679	LEU	CA-CB-CG	-6.00	101.50	115.30
1	B	569	ASP	CB-CG-OD2	6.00	123.70	118.30
1	D	569	ASP	CB-CG-OD2	5.99	123.69	118.30
1	D	679	LEU	CA-CB-CG	-5.99	101.52	115.30
1	B	136	GLU	CB-CA-C	-5.98	98.45	110.40
1	C	142	ILE	CB-CA-C	-5.98	99.65	111.60
1	A	136	GLU	CB-CA-C	-5.97	98.45	110.40
1	B	142	ILE	CB-CA-C	-5.97	99.67	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	45	ASP	CB-CG-OD2	-5.96	112.93	118.30
1	A	142	ILE	CB-CA-C	-5.96	99.68	111.60
1	B	45	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	D	45	ASP	CB-CG-OD2	-5.95	112.94	118.30
1	D	142	ILE	CB-CA-C	-5.95	99.70	111.60
1	C	136	GLU	CB-CA-C	-5.95	98.50	110.40
1	C	569	ASP	CB-CG-OD2	5.95	123.66	118.30
1	C	908	ASP	CB-CG-OD2	-5.95	112.95	118.30
1	C	5	ASP	CB-CG-OD2	-5.95	112.95	118.30
1	A	908	ASP	CB-CG-OD2	-5.94	112.95	118.30
1	C	199	ASP	CB-CG-OD1	5.94	123.64	118.30
1	D	908	ASP	CB-CG-OD2	-5.94	112.96	118.30
1	D	136	GLU	CB-CA-C	-5.93	98.53	110.40
1	C	45	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	B	908	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	B	43	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	D	5	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	B	5	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	B	1018	LEU	CB-CA-C	-5.89	99.02	110.20
1	D	769	TRP	CB-CA-C	-5.88	98.64	110.40
1	D	1018	LEU	CB-CA-C	-5.88	99.03	110.20
1	A	769	TRP	CB-CA-C	-5.88	98.65	110.40
1	C	769	TRP	CB-CA-C	-5.88	98.65	110.40
1	C	43	ARG	NE-CZ-NH1	5.87	123.24	120.30
1	A	199	ASP	CB-CG-OD1	5.87	123.58	118.30
1	A	1018	LEU	CB-CA-C	-5.87	99.05	110.20
1	B	199	ASP	CB-CG-OD1	5.87	123.58	118.30
1	D	199	ASP	CB-CG-OD1	5.87	123.58	118.30
1	A	5	ASP	CB-CG-OD2	-5.86	113.02	118.30
1	C	82	ASP	CB-CG-OD1	-5.86	113.03	118.30
1	C	423	MET	C-N-CA	5.85	136.33	121.70
1	C	1018	LEU	CB-CA-C	-5.85	99.09	110.20
1	B	769	TRP	CB-CA-C	-5.85	98.71	110.40
1	B	954	ASP	CB-CG-OD2	-5.83	113.06	118.30
1	C	77	ASP	CB-CG-OD2	-5.83	113.06	118.30
1	B	82	ASP	CB-CG-OD1	-5.82	113.06	118.30
1	C	77	ASP	CB-CG-OD1	5.81	123.53	118.30
1	D	77	ASP	CB-CG-OD2	-5.81	113.07	118.30
1	C	130	ASP	CB-CG-OD1	5.80	123.52	118.30
1	C	987	ASP	CB-CG-OD1	5.80	123.52	118.30
1	A	82	ASP	CB-CG-OD1	-5.80	113.08	118.30
1	B	134	LEU	N-CA-CB	5.80	122.00	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	144	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	A	423	MET	C-N-CA	5.80	136.19	121.70
1	B	423	MET	C-N-CA	5.80	136.19	121.70
1	C	134	LEU	N-CA-CB	5.80	121.99	110.40
1	D	423	MET	C-N-CA	5.80	136.19	121.70
1	B	368	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	B	610	ASP	CB-CG-OD1	-5.79	113.09	118.30
1	D	82	ASP	CB-CG-OD1	-5.79	113.09	118.30
1	B	144	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	D	144	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	D	134	LEU	N-CA-CB	5.79	121.97	110.40
1	D	77	ASP	CB-CG-OD1	5.78	123.51	118.30
1	A	77	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	A	610	ASP	CB-CG-OD1	-5.78	113.10	118.30
1	D	130	ASP	CB-CG-OD1	5.77	123.50	118.30
1	A	134	LEU	N-CA-CB	5.77	121.94	110.40
1	A	130	ASP	CB-CG-OD1	5.77	123.49	118.30
1	D	239	VAL	CA-CB-CG2	-5.76	102.25	110.90
1	D	368	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	D	954	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	A	77	ASP	CB-CG-OD1	5.76	123.49	118.30
1	C	610	ASP	CB-CG-OD1	-5.76	113.11	118.30
1	B	77	ASP	CB-CG-OD2	-5.76	113.12	118.30
1	C	144	ASP	CB-CG-OD2	-5.75	113.13	118.30
1	C	239	VAL	CA-CB-CG2	-5.74	102.28	110.90
1	C	954	ASP	CB-CG-OD2	-5.74	113.13	118.30
1	B	792	ASP	CB-CG-OD1	5.74	123.47	118.30
1	D	610	ASP	CB-CG-OD1	-5.74	113.13	118.30
1	C	368	ASP	CB-CG-OD2	-5.74	113.14	118.30
1	D	43	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	A	239	VAL	CA-CB-CG2	-5.73	102.30	110.90
1	B	130	ASP	CB-CG-OD1	5.73	123.46	118.30
1	A	987	ASP	CB-CG-OD1	5.73	123.45	118.30
1	B	230	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	B	77	ASP	CB-CG-OD1	5.72	123.45	118.30
1	D	144	ASP	CB-CG-OD1	5.72	123.45	118.30
1	A	954	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	B	239	VAL	CA-CB-CG2	-5.71	102.33	110.90
1	C	792	ASP	CB-CG-OD1	5.70	123.43	118.30
1	D	792	ASP	CB-CG-OD1	5.70	123.43	118.30
1	A	144	ASP	CB-CG-OD1	5.70	123.43	118.30
1	A	164	ASP	CB-CG-OD2	-5.70	113.17	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	164	ASP	CB-CG-OD1	5.70	123.43	118.30
1	B	635	THR	CA-CB-CG2	-5.70	104.43	112.40
1	A	792	ASP	CB-CG-OD1	5.69	123.42	118.30
1	B	987	ASP	CB-CG-OD1	5.69	123.42	118.30
1	A	368	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	A	164	ASP	CB-CG-OD1	5.68	123.42	118.30
1	D	987	ASP	CB-CG-OD1	5.68	123.41	118.30
1	B	144	ASP	CB-CG-OD1	5.68	123.41	118.30
1	A	469	ASP	CB-CG-OD1	5.67	123.41	118.30
1	A	635	THR	CA-CB-CG2	-5.67	104.47	112.40
1	B	772	ASP	CB-CG-OD1	5.66	123.40	118.30
1	C	469	ASP	CB-CG-OD1	5.66	123.40	118.30
1	D	635	THR	CA-CB-CG2	-5.65	104.49	112.40
1	A	45	ASP	CB-CG-OD1	5.65	123.39	118.30
1	C	164	ASP	CB-CG-OD2	-5.65	113.22	118.30
1	D	164	ASP	CB-CG-OD1	5.64	123.38	118.30
1	A	43	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	594	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	D	45	ASP	CB-CG-OD1	5.64	123.37	118.30
1	D	772	ASP	CB-CG-OD1	5.64	123.37	118.30
1	B	288	ARG	CD-NE-CZ	-5.63	115.71	123.60
1	B	469	ASP	CB-CG-OD1	5.63	123.37	118.30
1	C	635	THR	CA-CB-CG2	-5.63	104.51	112.40
1	B	164	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	B	45	ASP	CB-CG-OD1	5.63	123.36	118.30
1	C	144	ASP	CB-CG-OD1	5.63	123.36	118.30
1	C	288	ARG	CD-NE-CZ	-5.63	115.72	123.60
1	D	230	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	A	292	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	C	230	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	D	292	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	A	288	ARG	CD-NE-CZ	-5.62	115.74	123.60
1	D	469	ASP	CB-CG-OD1	5.62	123.36	118.30
1	C	916	ASP	CB-CG-OD1	5.61	123.35	118.30
1	C	292	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	D	164	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	B	210	ARG	N-CA-CB	5.60	120.69	110.60
1	D	210	ARG	N-CA-CB	5.60	120.68	110.60
1	B	594	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	A	210	ARG	N-CA-CB	5.59	120.66	110.60
1	D	288	ARG	CD-NE-CZ	-5.59	115.78	123.60
1	B	292	ARG	NE-CZ-NH1	5.59	123.09	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	772	ASP	CB-CG-OD1	5.58	123.32	118.30
1	D	594	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	C	594	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	C	164	ASP	CB-CG-OD1	5.58	123.32	118.30
1	A	492	ASP	CB-CG-OD2	-5.57	113.28	118.30
1	C	210	ARG	N-CA-CB	5.57	120.63	110.60
1	A	230	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	C	45	ASP	CB-CG-OD1	5.57	123.31	118.30
1	A	292	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	C	772	ASP	CB-CG-OD1	5.56	123.31	118.30
1	B	916	ASP	CB-CG-OD1	5.56	123.31	118.30
1	D	916	ASP	CB-CG-OD1	5.55	123.30	118.30
1	B	492	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	D	561	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	C	492	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	B	828	ASP	CB-CG-OD2	5.51	123.26	118.30
1	C	987	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	A	916	ASP	CB-CG-OD1	5.50	123.25	118.30
1	B	292	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	828	ASP	CB-CG-OD2	5.49	123.25	118.30
1	A	917	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	D	292	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	D	492	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	B	987	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	C	829	THR	CA-CB-CG2	-5.49	104.72	112.40
1	C	292	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	D	828	ASP	CB-CG-OD2	5.47	123.23	118.30
1	C	828	ASP	CB-CG-OD2	5.46	123.22	118.30
1	D	987	ASP	CB-CG-OD2	-5.46	113.38	118.30
1	A	987	ASP	CB-CG-OD2	-5.46	113.38	118.30
1	B	561	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	B	829	THR	CA-CB-CG2	-5.46	104.76	112.40
1	A	561	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	D	829	THR	CA-CB-CG2	-5.45	104.78	112.40
1	A	447	ASP	CB-CG-OD2	-5.45	113.40	118.30
1	A	829	THR	CA-CB-CG2	-5.44	104.78	112.40
1	D	863	GLN	CB-CA-C	-5.43	99.53	110.40
1	C	447	ASP	CB-CG-OD2	-5.43	113.41	118.30
1	D	671	ASP	CB-CG-OD1	5.43	123.19	118.30
1	C	863	GLN	CB-CA-C	-5.43	99.54	110.40
1	B	863	GLN	CB-CA-C	-5.42	99.57	110.40
1	D	447	ASP	CB-CG-OD2	-5.42	113.43	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	219	THR	CA-CB-CG2	-5.41	104.83	112.40
1	D	319	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	506	VAL	CA-CB-CG1	-5.40	102.81	110.90
1	A	863	GLN	CB-CA-C	-5.40	99.61	110.40
1	C	671	ASP	CB-CG-OD1	5.38	123.14	118.30
1	D	506	VAL	CA-CB-CG1	-5.38	102.83	110.90
1	C	561	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	671	ASP	CB-CG-OD1	5.38	123.14	118.30
1	B	447	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	D	579	ASP	CB-CG-OD1	5.37	123.14	118.30
1	B	506	VAL	CA-CB-CG1	-5.36	102.86	110.90
1	A	219	THR	CA-CB-CG2	-5.35	104.91	112.40
1	C	319	ASP	CB-CG-OD2	5.35	123.12	118.30
1	B	671	ASP	CB-CG-OD1	5.35	123.12	118.30
1	D	219	THR	CA-CB-CG2	-5.35	104.91	112.40
1	B	917	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	A	748	CYS	N-CA-CB	5.35	120.22	110.60
1	C	579	ASP	CB-CG-OD1	5.34	123.11	118.30
1	C	506	VAL	CA-CB-CG1	-5.34	102.89	110.90
1	B	782	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	C	748	CYS	N-CA-CB	5.33	120.19	110.60
1	D	748	CYS	N-CA-CB	5.33	120.19	110.60
1	B	748	CYS	N-CA-CB	5.33	120.19	110.60
1	B	980	GLU	N-CA-CB	5.32	120.18	110.60
1	B	219	THR	CA-CB-CG2	-5.32	104.95	112.40
1	A	319	ASP	CB-CG-OD2	5.32	123.09	118.30
1	C	782	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	A	782	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	C	980	GLU	N-CA-CB	5.30	120.14	110.60
1	B	386	ALA	N-CA-CB	-5.30	102.68	110.10
1	B	261	TRP	CB-CA-C	-5.29	99.82	110.40
1	A	980	GLU	N-CA-CB	5.29	120.11	110.60
1	B	319	ASP	CB-CG-OD2	5.28	123.05	118.30
1	D	386	ALA	N-CA-CB	-5.28	102.70	110.10
1	D	782	ASP	CB-CG-OD2	-5.28	113.54	118.30
1	A	386	ALA	N-CA-CB	-5.28	102.71	110.10
1	D	261	TRP	CB-CA-C	-5.28	99.85	110.40
1	D	980	GLU	N-CA-CB	5.27	120.09	110.60
1	A	261	TRP	CB-CA-C	-5.26	99.87	110.40
1	C	386	ALA	N-CA-CB	-5.26	102.73	110.10
1	C	261	TRP	CB-CA-C	-5.25	99.90	110.40
1	C	916	ASP	CB-CG-OD2	-5.24	113.58	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	917	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	B	579	ASP	CB-CG-OD1	5.24	123.01	118.30
1	D	572	ASP	CB-CG-OD1	5.23	123.01	118.30
1	D	917	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	A	579	ASP	CB-CG-OD1	5.22	123.00	118.30
1	A	269	SER	N-CA-CB	5.22	118.33	110.50
1	C	671	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	B	710	GLU	CB-CA-C	-5.22	99.97	110.40
1	C	201	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	D	201	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	D	916	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	B	269	SER	N-CA-CB	5.21	118.31	110.50
1	A	710	GLU	CB-CA-C	-5.20	100.00	110.40
1	B	916	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	D	269	SER	N-CA-CB	5.20	118.29	110.50
1	D	710	GLU	CB-CA-C	-5.19	100.02	110.40
1	A	201	ASP	CB-CG-OD2	-5.18	113.63	118.30
1	C	329	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	C	710	GLU	CB-CA-C	-5.18	100.04	110.40
1	B	104	THR	CA-CB-CG2	-5.18	105.15	112.40
1	D	46	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	329	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	D	671	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	D	248	GLY	C-N-CA	-5.17	108.77	121.70
1	A	518	TRP	CB-CA-C	-5.17	100.06	110.40
1	A	104	THR	CA-CB-CG2	-5.17	105.17	112.40
1	A	572	ASP	CB-CG-OD1	5.17	122.95	118.30
1	B	201	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	B	329	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	D	518	TRP	CB-CA-C	-5.16	100.08	110.40
1	B	903[A]	GLN	N-CA-CB	5.16	119.89	110.60
1	B	903[B]	GLN	N-CA-CB	5.16	119.89	110.60
1	C	518	TRP	CB-CA-C	-5.16	100.08	110.40
1	D	104	THR	CA-CB-CG2	-5.16	105.18	112.40
1	D	610	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	248	GLY	C-N-CA	-5.16	108.81	121.70
1	C	104	THR	CA-CB-CG2	-5.16	105.18	112.40
1	C	269	SER	N-CA-CB	5.16	118.23	110.50
1	D	46	ARG	C-N-CD	-5.16	109.26	120.60
1	D	329	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	C	46	ARG	C-N-CD	-5.15	109.26	120.60
1	B	864	MET	N-CA-CB	5.15	119.87	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	572	ASP	CB-CG-OD1	5.15	122.94	118.30
1	A	46	ARG	C-N-CD	-5.15	109.28	120.60
1	B	572	ASP	CB-CG-OD1	5.15	122.93	118.30
1	A	903[A]	GLN	N-CA-CB	5.15	119.86	110.60
1	A	903[B]	GLN	N-CA-CB	5.15	119.86	110.60
1	C	248	GLY	C-N-CA	-5.14	108.84	121.70
1	C	903[A]	GLN	N-CA-CB	5.14	119.86	110.60
1	C	903[B]	GLN	N-CA-CB	5.14	119.86	110.60
1	B	248	GLY	C-N-CA	-5.14	108.84	121.70
1	D	864	MET	N-CA-CB	5.14	119.85	110.60
1	B	193	ASP	CB-CG-OD2	-5.14	113.68	118.30
1	A	864	MET	N-CA-CB	5.14	119.85	110.60
1	D	651	LEU	CB-CG-CD2	-5.14	102.27	111.00
1	C	864	MET	N-CA-CB	5.13	119.84	110.60
1	A	671	ASP	CB-CG-OD2	-5.13	113.68	118.30
1	A	916	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	B	46	ARG	C-N-CD	-5.12	109.34	120.60
1	D	903[A]	GLN	N-CA-CB	5.12	119.81	110.60
1	D	903[B]	GLN	N-CA-CB	5.12	119.81	110.60
1	A	610	ASP	CB-CG-OD2	5.12	122.91	118.30
1	C	193	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	D	599	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	B	518	TRP	CB-CA-C	-5.11	100.18	110.40
1	B	651	LEU	CB-CG-CD2	-5.11	102.32	111.00
1	C	651	LEU	CB-CG-CD2	-5.11	102.32	111.00
1	A	599	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	C	599	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	B	671	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	A	651	LEU	CB-CG-CD2	-5.10	102.34	111.00
1	D	237	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	C	919	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	193	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	D	310	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	A	919	ASP	CB-CG-OD1	5.07	122.87	118.30
1	B	237	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	D	193	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	C	610	ASP	CB-CG-OD2	5.06	122.85	118.30
1	D	363	HIS	CA-CB-CG	-5.05	105.01	113.60
1	C	363	HIS	CA-CB-CG	-5.05	105.02	113.60
1	D	721	ARG	N-CA-CB	5.05	119.69	110.60
1	A	869	ASP	CB-CG-OD1	-5.04	113.76	118.30
1	B	721	ARG	N-CA-CB	5.04	119.67	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	919	ASP	CB-CG-OD1	5.04	122.84	118.30
1	C	721	ARG	N-CA-CB	5.04	119.67	110.60
1	D	869	ASP	CB-CG-OD1	-5.04	113.77	118.30
1	A	363	HIS	CA-CB-CG	-5.04	105.04	113.60
1	D	420	MET	CG-SD-CE	-5.03	92.16	100.20
1	A	721	ARG	N-CA-CB	5.03	119.64	110.60
1	C	310	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	B	919	ASP	CB-CG-OD1	5.02	122.82	118.30
1	B	869	ASP	CB-CG-OD1	-5.02	113.78	118.30
1	B	363	HIS	CA-CB-CG	-5.01	105.08	113.60
1	B	610	ASP	CB-CG-OD2	5.01	122.81	118.30
1	B	420	MET	CG-SD-CE	-5.01	92.19	100.20
1	B	46	ARG	NE-CZ-NH1	5.01	122.80	120.30
1	D	114	VAL	CA-CB-CG1	5.01	118.41	110.90
1	D	857	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	A	428	ASP	CB-CG-OD1	5.00	122.80	118.30
1	D	416	GLU	N-CA-CB	5.00	119.60	110.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8238	0	7821	477	0
1	B	8238	0	7822	458	0
1	C	8238	0	7821	460	0
1	D	8238	0	7821	471	0
2	H	902	0	838	111	0
2	I	902	0	838	110	0
2	J	902	0	839	108	0
2	K	902	0	839	109	0
3	L	818	0	780	12	0
3	M	818	0	780	12	0
3	N	818	0	780	13	0
3	O	818	0	780	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	39832	0	37759	1937	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 25.

All (1937) 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:C:584:PRO:CB	2:H:30:THR:HG22	1.48	1.42
1:A:584:PRO:CB	2:J:30:THR:HG22	1.50	1.40
1:B:609:ALA:CB	2:K:53:TYR:OH	1.70	1.40
1:B:584:PRO:CB	2:K:30:THR:HG22	1.50	1.38
1:D:584:PRO:CB	2:I:30:THR:HG22	1.50	1.38
1:A:362:LEU:HD22	2:J:31:SER:C	1.44	1.37
1:B:583:ASN:CG	2:K:73:THR:H	1.29	1.36
1:D:362:LEU:HD22	2:I:31:SER:C	1.43	1.35
1:C:584:PRO:CA	2:H:30:THR:HG22	1.57	1.34
1:C:583:ASN:OD1	2:H:73:THR:N	1.58	1.33
1:D:583:ASN:CG	2:I:73:THR:H	1.30	1.33
1:A:583:ASN:CG	2:J:73:THR:H	1.28	1.32
1:C:609:ALA:CB	2:H:53:TYR:OH	1.79	1.31
1:B:583:ASN:OD1	2:K:73:THR:N	1.63	1.29
1:A:576:ILE:CG2	2:J:30:THR:HB	1.62	1.28
1:D:576:ILE:CG2	2:I:30:THR:HB	1.62	1.28
1:D:578:TYR:CD2	2:I:28:SER:OG	1.82	1.27
1:A:584:PRO:CA	2:J:30:THR:HG22	1.64	1.27
1:C:609:ALA:HB3	2:H:53:TYR:OH	1.11	1.26
1:A:578:TYR:CD2	2:J:28:SER:OG	1.82	1.26
1:B:584:PRO:CA	2:K:30:THR:HG22	1.64	1.25
1:B:362:LEU:HD22	2:K:31:SER:C	1.56	1.25
1:D:584:PRO:CA	2:I:30:THR:HG22	1.65	1.24
1:A:583:ASN:OD1	2:J:72:ASP:CA	1.85	1.24
1:D:583:ASN:OD1	2:I:73:THR:N	1.71	1.24
1:C:578:TYR:CG	2:H:28:SER:OG	1.91	1.23
1:A:579:ASP:OD1	2:J:73:THR:OG1	1.58	1.22
1:B:609:ALA:HB3	2:K:53:TYR:OH	1.04	1.22
1:D:583:ASN:OD1	2:I:72:ASP:CA	1.87	1.22
1:A:583:ASN:OD1	2:J:73:THR:N	1.71	1.21
1:D:579:ASP:OD1	2:I:73:THR:OG1	1.60	1.20
1:D:584:PRO:HG2	2:I:71:ARG:NH1	1.57	1.19
1:A:584:PRO:HG2	2:J:71:ARG:NH1	1.56	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:362:LEU:HD22	2:H:31:SER:C	1.61	1.19
1:C:579:ASP:OD1	2:H:73:THR:OG1	1.59	1.18
1:B:578:TYR:CG	2:K:28:SER:OG	1.96	1.18
1:B:584:PRO:HB3	2:K:30:THR:HG22	1.17	1.16
1:D:427:THR:HA	1:D:436:MET:HE1	1.23	1.16
1:C:584:PRO:CA	2:H:30:THR:CG2	2.24	1.15
1:C:578:TYR:CD2	2:H:28:SER:OG	1.99	1.15
1:B:578:TYR:CD2	2:K:28:SER:OG	1.97	1.15
1:C:427:THR:HA	1:C:436:MET:HE1	1.23	1.15
1:B:584:PRO:HG2	2:K:71:ARG:NH1	1.62	1.15
1:D:578:TYR:CG	2:I:28:SER:OG	1.92	1.15
1:B:576:ILE:CG2	2:K:30:THR:HB	1.76	1.14
1:B:579:ASP:OD1	2:K:73:THR:OG1	1.64	1.14
1:C:584:PRO:HG2	2:H:71:ARG:NH1	1.60	1.14
1:C:584:PRO:HA	2:H:30:THR:CG2	1.77	1.13
1:B:609:ALA:HB3	2:K:53:TYR:CZ	1.81	1.13
1:C:584:PRO:HB3	2:H:30:THR:HG22	1.23	1.12
1:A:583:ASN:OD1	2:J:72:ASP:HA	1.47	1.11
1:A:578:TYR:CG	2:J:28:SER:OG	1.91	1.11
1:A:584:PRO:HA	2:J:30:THR:CG2	1.81	1.10
1:B:609:ALA:CA	2:K:53:TYR:OH	1.98	1.10
1:C:583:ASN:CG	2:H:73:THR:N	2.03	1.10
1:A:584:PRO:HB3	2:J:30:THR:HG22	1.13	1.10
1:A:581:ASN:HB2	2:J:72:ASP:OD1	1.49	1.10
1:A:610:ASP:N	2:J:53:TYR:HE1	1.49	1.10
1:D:581:ASN:HB2	2:I:72:ASP:OD1	1.52	1.10
1:D:610:ASP:N	2:I:53:TYR:CE1	2.20	1.10
1:D:584:PRO:HA	2:I:30:THR:CG2	1.82	1.09
1:C:576:ILE:CG2	2:H:30:THR:HB	1.82	1.09
1:A:610:ASP:N	2:J:53:TYR:CE1	2.20	1.09
1:D:610:ASP:N	2:I:53:TYR:HE1	1.50	1.09
1:C:584:PRO:HA	2:H:30:THR:HG21	1.34	1.08
1:B:584:PRO:HA	2:K:30:THR:CG2	1.83	1.08
1:C:609:ALA:HB3	2:H:53:TYR:CZ	1.87	1.08
1:D:583:ASN:OD1	2:I:72:ASP:HA	1.48	1.08
1:A:427:THR:HA	1:A:436:MET:HE1	1.29	1.07
1:B:427:THR:HA	1:B:436:MET:HE1	1.31	1.07
1:B:584:PRO:CA	2:K:30:THR:CG2	2.31	1.07
1:B:746:ASP:HA	1:B:760:ARG:HG3	1.34	1.07
1:C:582:GLY:O	2:H:29:ILE:CG2	2.02	1.07
1:B:584:PRO:HB3	2:K:30:THR:CG2	1.84	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:746:ASP:HA	1:A:760:ARG:HG3	1.34	1.07
1:B:583:ASN:OD1	2:K:72:ASP:CA	2.04	1.06
1:C:584:PRO:HB3	2:H:30:THR:CG2	1.85	1.06
1:D:584:PRO:HB3	2:I:30:THR:CG2	1.85	1.06
1:A:362:LEU:CD2	2:J:31:SER:C	2.24	1.05
1:D:362:LEU:CD2	2:I:31:SER:HA	1.86	1.05
1:C:576:ILE:CD1	2:H:53:TYR:HB2	1.86	1.05
1:A:584:PRO:HB3	2:J:30:THR:CG2	1.86	1.05
1:B:610:ASP:N	2:K:53:TYR:CE1	2.25	1.05
1:A:584:PRO:CA	2:J:30:THR:CG2	2.34	1.05
1:D:584:PRO:HB3	2:I:30:THR:HG22	1.12	1.05
1:D:746:ASP:HA	1:D:760:ARG:HG3	1.34	1.05
1:C:746:ASP:HA	1:C:760:ARG:HG3	1.34	1.05
1:C:610:ASP:N	2:H:53:TYR:HE1	1.53	1.04
1:C:583:ASN:OD1	2:H:72:ASP:CA	2.06	1.04
1:A:362:LEU:CD2	2:J:31:SER:HA	1.86	1.04
1:D:362:LEU:CD2	2:I:31:SER:C	2.24	1.04
1:B:610:ASP:N	2:K:53:TYR:HE1	1.54	1.04
1:C:609:ALA:CA	2:H:53:TYR:OH	2.04	1.03
1:C:610:ASP:N	2:H:53:TYR:CE1	2.26	1.03
1:C:582:GLY:O	2:H:29:ILE:HG22	1.59	1.03
1:D:583:ASN:CG	2:I:73:THR:N	2.09	1.03
1:D:584:PRO:CA	2:I:30:THR:CG2	2.35	1.03
1:C:584:PRO:CB	2:H:30:THR:CG2	2.37	1.03
1:C:576:ILE:HG21	2:H:30:THR:O	1.58	1.02
1:C:693:GLN:HG2	1:C:721:ARG:HD3	1.39	1.02
1:D:693:GLN:HG2	1:D:721:ARG:HD3	1.39	1.02
1:B:576:ILE:CD1	2:K:53:TYR:HB2	1.90	1.01
1:C:610:ASP:CA	2:H:53:TYR:HE1	1.73	1.00
1:B:362:LEU:CD2	2:K:31:SER:HA	1.90	1.00
1:B:693:GLN:HG2	1:B:721:ARG:HD3	1.39	1.00
1:A:693:GLN:HG2	1:A:721:ARG:HD3	1.39	1.00
1:B:584:PRO:HA	2:K:30:THR:HG21	1.40	1.00
1:A:583:ASN:CG	2:J:73:THR:N	2.07	0.99
1:A:584:PRO:HA	2:J:30:THR:HG21	1.45	0.99
1:A:582:GLY:O	2:J:29:ILE:CG2	2.10	0.99
1:B:582:GLY:O	2:K:29:ILE:CG2	2.11	0.99
1:B:610:ASP:CA	2:K:53:TYR:HE1	1.76	0.98
1:D:576:ILE:CD1	2:I:53:TYR:HB2	1.93	0.98
1:D:597:ASN:HD22	1:D:599:ARG:H	1.11	0.98
1:B:434:PRO:HB3	1:C:434:PRO:HB3	1.44	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:597:ASN:HD22	1:C:599:ARG:H	1.11	0.97
1:C:362:LEU:CD2	2:H:31:SER:HA	1.94	0.97
1:A:576:ILE:CD1	2:J:53:TYR:HB2	1.93	0.96
1:D:582:GLY:O	2:I:29:ILE:CG2	2.12	0.96
1:A:610:ASP:CA	2:J:53:TYR:HE1	1.79	0.96
1:B:362:LEU:CD2	2:K:31:SER:C	2.34	0.96
1:A:583:ASN:OD1	2:J:72:ASP:C	2.03	0.96
1:D:362:LEU:CD2	2:I:31:SER:CA	2.44	0.96
1:B:576:ILE:HG21	2:K:30:THR:O	1.65	0.95
1:A:576:ILE:HG21	2:J:30:THR:O	1.65	0.95
1:B:597:ASN:HD22	1:B:599:ARG:H	1.11	0.95
1:A:362:LEU:CD2	2:J:31:SER:CA	2.45	0.95
1:D:584:PRO:HA	2:I:30:THR:HG21	1.45	0.95
1:A:597:ASN:HD22	1:A:599:ARG:H	1.11	0.94
1:B:583:ASN:OD1	2:K:72:ASP:HA	1.66	0.94
1:C:597:ASN:ND2	1:C:599:ARG:H	1.65	0.94
1:D:576:ILE:HG21	2:I:30:THR:O	1.66	0.94
1:D:597:ASN:ND2	1:D:599:ARG:H	1.65	0.94
1:D:38:ASN:ND2	1:D:41:GLU:H	1.66	0.94
1:C:38:ASN:ND2	1:C:41:GLU:H	1.66	0.94
1:D:583:ASN:OD1	2:I:72:ASP:C	2.05	0.94
1:A:581:ASN:O	2:J:75:LYS:N	1.97	0.93
1:D:610:ASP:CA	2:I:53:TYR:HE1	1.79	0.93
1:B:38:ASN:ND2	1:B:41:GLU:H	1.66	0.93
1:C:583:ASN:OD1	2:H:72:ASP:C	2.07	0.93
1:A:38:ASN:ND2	1:A:41:GLU:H	1.66	0.93
1:B:597:ASN:ND2	1:B:599:ARG:H	1.65	0.93
1:B:583:ASN:CG	2:K:73:THR:N	2.10	0.93
1:C:362:LEU:CD2	2:H:31:SER:C	2.36	0.92
1:C:427:THR:HA	1:C:436:MET:CE	1.99	0.92
1:A:427:THR:HA	1:A:436:MET:CE	1.99	0.92
1:A:597:ASN:ND2	1:A:599:ARG:H	1.65	0.92
1:D:427:THR:HA	1:D:436:MET:CE	1.99	0.92
1:B:427:THR:HA	1:B:436:MET:CE	1.99	0.92
1:B:582:GLY:O	2:K:29:ILE:HG22	1.70	0.91
1:D:362:LEU:HD22	2:I:31:SER:O	1.70	0.91
1:A:584:PRO:CB	2:J:30:THR:CG2	2.43	0.91
1:C:609:ALA:HB3	2:H:53:TYR:HH	1.11	0.91
1:C:255:ARG:HG2	1:C:255:ARG:HH11	1.34	0.91
1:A:582:GLY:O	2:J:29:ILE:HG21	1.71	0.91
1:B:255:ARG:HH11	1:B:255:ARG:HG2	1.34	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:255:ARG:HH11	1:D:255:ARG:HG2	1.34	0.90
1:A:255:ARG:HH11	1:A:255:ARG:HG2	1.34	0.90
1:A:362:LEU:HD22	2:J:31:SER:O	1.70	0.90
1:C:584:PRO:HB3	2:H:30:THR:CB	2.02	0.90
1:C:610:ASP:CA	2:H:53:TYR:CE1	2.55	0.89
1:D:610:ASP:CA	2:I:53:TYR:CE1	2.56	0.89
1:C:581:ASN:HB2	2:H:72:ASP:OD1	1.71	0.89
1:C:362:LEU:HD22	2:H:31:SER:O	1.72	0.89
1:B:581:ASN:HB2	2:K:72:ASP:OD1	1.71	0.88
1:B:584:PRO:CB	2:K:30:THR:CG2	2.40	0.88
1:B:610:ASP:CA	2:K:53:TYR:CE1	2.55	0.88
1:B:583:ASN:OD1	2:K:72:ASP:C	2.10	0.88
1:A:610:ASP:CA	2:J:53:TYR:CE1	2.56	0.87
1:A:734:SER:HB3	1:A:860:GLY:HA3	1.57	0.86
1:B:734:SER:HB3	1:B:860:GLY:HA3	1.57	0.86
1:B:362:LEU:HD22	2:K:31:SER:O	1.75	0.86
1:D:581:ASN:O	2:I:75:LYS:N	1.97	0.86
1:B:362:LEU:CD2	2:K:31:SER:CA	2.52	0.86
1:C:583:ASN:OD1	2:H:72:ASP:HA	1.72	0.86
1:C:734:SER:HB3	1:C:860:GLY:HA3	1.57	0.86
1:D:734:SER:HB3	1:D:860:GLY:HA3	1.57	0.86
1:D:576:ILE:HG21	2:I:30:THR:HB	1.57	0.85
1:A:584:PRO:HG2	2:J:71:ARG:CZ	2.06	0.85
1:C:582:GLY:O	2:H:29:ILE:HG21	1.76	0.85
1:C:856:TYR:HB3	1:C:864:MET:CE	2.07	0.85
1:C:673:ALA:HB1	1:C:674:PRO:HD2	1.58	0.85
1:D:856:TYR:HB3	1:D:864:MET:CE	2.07	0.85
1:D:673:ALA:HB1	1:D:674:PRO:HD2	1.58	0.85
1:A:576:ILE:CG2	2:J:30:THR:O	2.25	0.85
1:D:584:PRO:CG	2:I:71:ARG:NH1	2.40	0.85
1:D:582:GLY:O	2:I:29:ILE:HG21	1.74	0.85
1:D:576:ILE:HG23	2:I:30:THR:HB	1.59	0.85
1:C:576:ILE:CG2	2:H:30:THR:O	2.25	0.84
1:D:362:LEU:HD22	2:I:31:SER:CA	2.03	0.84
1:A:362:LEU:HD13	2:J:32:ASP:HA	1.60	0.84
1:A:584:PRO:CG	2:J:71:ARG:NH1	2.39	0.84
1:D:362:LEU:HD13	2:I:32:ASP:HA	1.59	0.84
1:B:673:ALA:HB1	1:B:674:PRO:HD2	1.58	0.84
1:D:584:PRO:HG2	2:I:71:ARG:CZ	2.06	0.84
1:A:673:ALA:HB1	1:A:674:PRO:HD2	1.58	0.84
1:A:362:LEU:HD22	2:J:31:SER:CA	2.04	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:576:ILE:HG21	2:J:30:THR:HB	1.58	0.84
1:A:576:ILE:CG2	2:J:30:THR:CB	2.53	0.83
1:B:584:PRO:HB3	2:K:30:THR:CB	2.09	0.83
1:C:576:ILE:HD11	2:H:53:TYR:HB2	1.60	0.83
1:D:576:ILE:CG2	2:I:30:THR:O	2.26	0.83
1:C:362:LEU:CD2	2:H:31:SER:CA	2.56	0.83
1:D:583:ASN:CB	2:I:73:THR:H	1.82	0.83
1:A:734:SER:CB	1:A:860:GLY:HA3	2.09	0.83
1:D:734:SER:CB	1:D:860:GLY:HA3	2.08	0.83
1:A:856:TYR:HB3	1:A:864:MET:CE	2.07	0.83
1:B:856:TYR:HB3	1:B:864:MET:CE	2.07	0.83
1:C:734:SER:CB	1:C:860:GLY:HA3	2.09	0.83
1:B:734:SER:CB	1:B:860:GLY:HA3	2.08	0.83
1:A:576:ILE:HG22	2:J:30:THR:HB	1.60	0.82
1:B:654:TRP:NE1	1:B:666:GLY:HA3	1.94	0.82
1:A:576:ILE:HG23	2:J:30:THR:HB	1.58	0.82
1:A:654:TRP:NE1	1:A:666:GLY:HA3	1.94	0.82
1:C:654:TRP:NE1	1:C:666:GLY:HA3	1.94	0.82
1:D:654:TRP:NE1	1:D:666:GLY:HA3	1.94	0.82
1:A:582:GLY:O	2:J:29:ILE:HG22	1.76	0.82
1:C:949:HIS:CD2	1:C:1020:TRP:HE1	1.98	0.82
1:D:949:HIS:CD2	1:D:1020:TRP:HE1	1.98	0.82
1:D:576:ILE:CG2	2:I:30:THR:CB	2.53	0.82
1:B:949:HIS:CD2	1:B:1020:TRP:HE1	1.98	0.81
1:A:949:HIS:CD2	1:A:1020:TRP:HE1	1.98	0.81
1:D:582:GLY:O	2:I:29:ILE:HG22	1.78	0.81
1:D:576:ILE:HG22	2:I:30:THR:HB	1.60	0.81
1:D:609:ALA:C	2:I:53:TYR:CE1	2.54	0.81
1:D:830:LEU:CD2	1:D:835:LEU:HB2	2.11	0.81
1:A:583:ASN:CB	2:J:73:THR:H	1.79	0.81
1:C:830:LEU:CD2	1:C:835:LEU:HB2	2.11	0.81
1:D:578:TYR:CE2	2:I:28:SER:OG	2.34	0.81
1:B:582:GLY:O	2:K:29:ILE:HG21	1.80	0.80
1:C:360:HIS:ND1	1:C:361:PRO:HD2	1.97	0.80
1:A:360:HIS:ND1	1:A:361:PRO:HD2	1.97	0.80
1:A:609:ALA:C	2:J:53:TYR:CE1	2.54	0.80
1:B:360:HIS:ND1	1:B:361:PRO:HD2	1.97	0.80
1:B:134:LEU:HD12	1:B:134:LEU:N	1.97	0.80
1:A:578:TYR:CE2	2:J:28:SER:OG	2.34	0.79
1:D:360:HIS:ND1	1:D:361:PRO:HD2	1.97	0.79
1:B:576:ILE:CG2	2:K:30:THR:O	2.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:830:LEU:CD2	1:B:835:LEU:HB2	2.11	0.79
1:A:134:LEU:HD12	1:A:134:LEU:N	1.97	0.79
1:C:576:ILE:HD12	2:H:53:TYR:HB2	1.63	0.79
1:C:584:PRO:CG	2:H:71:ARG:NH1	2.45	0.79
1:A:830:LEU:CD2	1:A:835:LEU:HB2	2.11	0.79
1:D:77:ASP:O	1:D:78:LEU:HD23	1.83	0.79
1:C:134:LEU:N	1:C:134:LEU:HD12	1.97	0.79
1:C:581:ASN:O	2:H:75:LYS:N	2.09	0.79
1:D:134:LEU:HD12	1:D:134:LEU:N	1.97	0.79
1:C:77:ASP:O	1:C:78:LEU:HD23	1.83	0.79
1:A:920:LEU:HB3	1:A:921:PRO:HD2	1.65	0.79
1:B:920:LEU:HB3	1:B:921:PRO:HD2	1.66	0.78
1:B:362:LEU:HD22	2:K:31:SER:CA	2.11	0.78
1:C:578:TYR:CD1	2:H:28:SER:OG	2.35	0.78
1:B:576:ILE:HG21	2:K:30:THR:HB	1.64	0.78
1:C:610:ASP:HA	2:H:53:TYR:HE1	1.49	0.78
1:C:746:ASP:CA	1:C:760:ARG:HG3	2.14	0.77
1:D:746:ASP:CA	1:D:760:ARG:HG3	2.14	0.77
1:B:77:ASP:O	1:B:78:LEU:HD23	1.83	0.77
1:C:928:PRO:HB2	1:C:973:ARG:NH1	1.99	0.77
1:A:77:ASP:O	1:A:78:LEU:HD23	1.83	0.77
1:D:928:PRO:HB2	1:D:973:ARG:NH1	1.99	0.77
1:B:609:ALA:HB3	2:K:53:TYR:HH	0.94	0.77
1:B:576:ILE:HD12	2:K:53:TYR:HB2	1.65	0.77
2:I:29:ILE:HD11	2:I:78:TYR:HB3	1.67	0.77
2:H:29:ILE:HD11	2:H:78:TYR:HB3	1.67	0.77
1:A:578:TYR:CD2	2:J:28:SER:CB	2.67	0.77
1:B:928:PRO:HB2	1:B:973:ARG:NH1	1.99	0.77
1:A:362:LEU:HD23	2:J:31:SER:HA	1.67	0.77
1:D:578:TYR:CD2	2:I:28:SER:CB	2.68	0.77
1:C:920:LEU:HB3	1:C:921:PRO:HD2	1.65	0.77
1:A:928:PRO:HB2	1:A:973:ARG:NH1	1.99	0.77
1:B:1004:SER:HB2	1:B:1006:GLU:OE2	1.85	0.77
2:J:29:ILE:HD11	2:J:78:TYR:HB3	1.67	0.76
1:B:610:ASP:HA	2:K:53:TYR:HE1	1.48	0.76
1:D:920:LEU:HB3	1:D:921:PRO:HD2	1.65	0.76
1:A:1004:SER:HB2	1:A:1006:GLU:OE2	1.85	0.76
2:K:29:ILE:HD11	2:K:78:TYR:HB3	1.67	0.76
1:B:436:MET:HE1	1:B:467:ASN:HD22	1.51	0.76
1:B:685:LEU:HB3	1:B:686:PRO:HD2	1.68	0.76
1:B:584:PRO:CG	2:K:71:ARG:NH1	2.45	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:581:ASN:O	2:K:75:LYS:N	2.07	0.76
1:B:9:VAL:O	1:B:12:GLN:HB3	1.85	0.76
1:A:9:VAL:O	1:A:12:GLN:HB3	1.85	0.76
1:A:609:ALA:C	2:J:53:TYR:HE1	1.88	0.76
1:B:576:ILE:HD11	2:K:53:TYR:HB2	1.68	0.76
1:A:685:LEU:HB3	1:A:686:PRO:HD2	1.68	0.76
1:B:362:LEU:HD13	2:K:32:ASP:HA	1.68	0.75
1:D:9:VAL:O	1:D:12:GLN:HB3	1.85	0.75
1:C:11:LEU:HD21	1:C:187:MET:CE	2.15	0.75
1:D:11:LEU:HD21	1:D:187:MET:CE	2.15	0.75
1:C:685:LEU:HB3	1:C:686:PRO:HD2	1.68	0.75
1:A:11:LEU:HD21	1:A:187:MET:CE	2.15	0.75
1:D:685:LEU:HB3	1:D:686:PRO:HD2	1.68	0.75
1:C:9:VAL:O	1:C:12:GLN:HB3	1.85	0.75
1:B:11:LEU:HD21	1:B:187:MET:CE	2.15	0.75
1:A:610:ASP:HA	2:J:53:TYR:HE1	1.51	0.75
1:C:1004:SER:HB2	1:C:1006:GLU:OE2	1.85	0.75
1:D:1004:SER:HB2	1:D:1006:GLU:OE2	1.85	0.75
1:A:949:HIS:HD2	1:A:1020:TRP:HE1	1.35	0.75
1:D:584:PRO:HB3	2:I:30:THR:CB	2.17	0.75
1:D:362:LEU:HD23	2:I:31:SER:HA	1.67	0.75
1:D:609:ALA:C	2:I:53:TYR:HE1	1.87	0.75
1:A:436:MET:HE1	1:A:467:ASN:HD22	1.52	0.75
1:B:949:HIS:HD2	1:B:1020:TRP:HE1	1.35	0.75
1:C:362:LEU:HD22	2:H:31:SER:CA	2.17	0.74
1:B:584:PRO:HG2	2:K:71:ARG:CZ	2.17	0.74
1:D:38:ASN:HD22	1:D:41:GLU:H	1.35	0.74
1:C:38:ASN:HD22	1:C:41:GLU:H	1.35	0.74
1:B:609:ALA:CB	2:K:53:TYR:HH	1.76	0.74
1:B:377:LEU:HD22	1:B:708:TRP:HA	1.69	0.74
1:A:377:LEU:HD22	1:A:708:TRP:HA	1.68	0.74
1:B:609:ALA:CB	2:K:53:TYR:CZ	2.57	0.74
1:A:584:PRO:HB3	2:J:30:THR:CB	2.17	0.74
1:D:610:ASP:HA	2:I:53:TYR:HE1	1.51	0.74
1:D:377:LEU:HD22	1:D:708:TRP:HA	1.68	0.74
1:C:377:LEU:HD22	1:C:708:TRP:HA	1.69	0.73
1:C:237:ARG:HH11	1:C:237:ARG:HB3	1.53	0.73
1:A:576:ILE:HD12	2:J:53:TYR:HB2	1.70	0.73
1:A:746:ASP:CA	1:A:760:ARG:HG3	2.14	0.73
1:B:579:ASP:OD1	1:B:583:ASN:HB2	1.89	0.73
1:A:38:ASN:HD22	1:A:41:GLU:H	1.35	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:652:LEU:HD11	1:D:698:VAL:HB	1.71	0.73
1:A:778:THR:HG23	1:A:779:PRO:HD2	1.70	0.73
1:C:652:LEU:HD11	1:C:698:VAL:HB	1.71	0.73
1:A:237:ARG:HH11	1:A:237:ARG:HB3	1.54	0.73
1:B:237:ARG:HB3	1:B:237:ARG:HH11	1.54	0.73
1:D:237:ARG:HH11	1:D:237:ARG:HB3	1.54	0.73
1:B:746:ASP:CA	1:B:760:ARG:HG3	2.14	0.73
1:B:38:ASN:HD22	1:B:41:GLU:H	1.35	0.73
1:B:778:THR:HG23	1:B:779:PRO:HD2	1.70	0.73
1:A:579:ASP:OD1	1:A:583:ASN:HB2	1.89	0.73
1:C:237:ARG:HH11	1:C:237:ARG:CB	2.02	0.72
1:A:434:PRO:HB3	1:D:434:PRO:HB3	1.71	0.72
1:D:237:ARG:HH11	1:D:237:ARG:CB	2.02	0.72
1:D:655:MET:HG3	1:D:656:VAL:N	2.03	0.72
1:A:559:TYR:HB2	1:A:562:LEU:HD12	1.71	0.72
1:C:576:ILE:HG21	2:H:30:THR:HB	1.70	0.72
1:A:436:MET:CE	1:A:467:ASN:HD22	2.03	0.72
1:B:436:MET:CE	1:B:467:ASN:HD22	2.03	0.72
1:A:655:MET:HG3	1:A:656:VAL:N	2.03	0.72
1:B:559:TYR:HB2	1:B:562:LEU:HD12	1.71	0.72
1:C:3:ILE:HG13	1:C:4:THR:N	2.04	0.72
1:C:11:LEU:HD21	1:C:187:MET:HE3	1.70	0.72
1:A:237:ARG:HH11	1:A:237:ARG:CB	2.02	0.72
1:D:3:ILE:HG13	1:D:4:THR:N	2.04	0.72
1:C:655:MET:HG3	1:C:656:VAL:N	2.03	0.72
1:B:578:TYR:CD1	2:K:28:SER:OG	2.42	0.72
1:D:778:THR:HG23	1:D:779:PRO:HD2	1.70	0.72
1:B:655:MET:HG3	1:B:656:VAL:N	2.03	0.72
1:C:436:MET:CE	1:C:467:ASN:HD22	2.03	0.72
1:C:778:THR:HG23	1:C:779:PRO:HD2	1.70	0.72
1:A:3:ILE:HG13	1:A:4:THR:N	2.04	0.72
1:C:576:ILE:HG23	2:H:30:THR:HB	1.71	0.72
1:D:436:MET:CE	1:D:467:ASN:HD22	2.03	0.72
1:B:237:ARG:CB	1:B:237:ARG:HH11	2.03	0.72
1:A:652:LEU:HD11	1:A:698:VAL:HB	1.71	0.72
1:B:652:LEU:HD11	1:B:698:VAL:HB	1.71	0.72
1:B:3:ILE:HG13	1:B:4:THR:N	2.04	0.72
1:A:577:LYS:O	2:J:30:THR:HG21	1.89	0.71
1:C:949:HIS:HD2	1:C:1020:TRP:HE1	1.35	0.71
1:C:578:TYR:CD2	2:H:28:SER:CB	2.72	0.71
1:A:581:ASN:O	2:J:72:ASP:O	2.07	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:856:TYR:CD2	1:A:864:MET:HE1	2.26	0.71
1:C:579:ASP:OD1	1:C:583:ASN:HB2	1.89	0.71
1:B:609:ALA:N	2:K:53:TYR:OH	2.24	0.71
1:B:856:TYR:CD2	1:B:864:MET:HE1	2.26	0.71
1:D:577:LYS:O	2:I:30:THR:HG21	1.90	0.71
1:D:579:ASP:OD1	1:D:583:ASN:HB2	1.89	0.71
1:C:559:TYR:HB2	1:C:562:LEU:HD12	1.71	0.71
1:D:576:ILE:HD12	2:I:53:TYR:HB2	1.70	0.71
1:D:949:HIS:HD2	1:D:1020:TRP:HE1	1.35	0.71
1:D:559:TYR:HB2	1:D:562:LEU:HD12	1.71	0.71
1:B:928:PRO:HB2	1:B:973:ARG:HH11	1.55	0.71
1:A:928:PRO:HB2	1:A:973:ARG:HH11	1.55	0.71
1:B:650:GLU:HB3	1:B:670:LEU:HD12	1.73	0.71
1:B:576:ILE:HG23	2:K:30:THR:HB	1.70	0.71
1:A:650:GLU:HB3	1:A:670:LEU:HD12	1.73	0.71
1:C:362:LEU:HD13	2:H:32:ASP:HA	1.73	0.70
1:A:576:ILE:HD11	2:J:53:TYR:HB2	1.73	0.70
1:C:928:PRO:HB2	1:C:973:ARG:HH11	1.55	0.70
1:D:581:ASN:O	2:I:72:ASP:O	2.10	0.70
1:D:928:PRO:HB2	1:D:973:ARG:HH11	1.55	0.70
1:B:578:TYR:CD2	2:K:28:SER:CB	2.75	0.70
1:B:609:ALA:C	2:K:53:TYR:CE1	2.64	0.70
1:C:584:PRO:HG2	2:H:71:ARG:CZ	2.22	0.69
1:C:584:PRO:N	2:H:30:THR:HG22	2.06	0.69
1:A:856:TYR:HD2	1:A:864:MET:HE1	1.57	0.69
1:B:856:TYR:HD2	1:B:864:MET:HE1	1.57	0.69
1:A:578:TYR:CD1	2:J:28:SER:OG	2.46	0.69
1:A:11:LEU:HD21	1:A:187:MET:HE3	1.73	0.69
1:C:650:GLU:HB3	1:C:670:LEU:HD12	1.73	0.69
1:D:650:GLU:HB3	1:D:670:LEU:HD12	1.73	0.69
1:C:255:ARG:HG2	1:C:255:ARG:NH1	2.07	0.69
1:A:836:ILE:N	1:A:836:ILE:HD13	2.07	0.69
1:A:1020:TRP:HD1	1:A:1021:CYS:N	1.91	0.68
1:D:255:ARG:HG2	1:D:255:ARG:NH1	2.07	0.68
1:B:1020:TRP:HD1	1:B:1021:CYS:N	1.92	0.68
1:C:609:ALA:N	2:H:53:TYR:OH	2.26	0.68
1:B:836:ILE:HD13	1:B:836:ILE:N	2.07	0.68
1:D:11:LEU:HD21	1:D:187:MET:HE3	1.75	0.68
1:D:836:ILE:N	1:D:836:ILE:HD13	2.07	0.68
1:A:35:SER:OG	1:A:37:ARG:NH1	2.27	0.68
1:C:1020:TRP:HD1	1:C:1021:CYS:N	1.91	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1020:TRP:HD1	1:D:1021:CYS:N	1.91	0.68
1:C:836:ILE:N	1:C:836:ILE:HD13	2.07	0.68
1:B:35:SER:OG	1:B:37:ARG:NH1	2.27	0.68
1:D:578:TYR:CD1	2:I:28:SER:OG	2.46	0.67
1:A:581:ASN:CB	2:J:72:ASP:OD1	2.37	0.67
1:C:63:PHE:HB3	1:C:64:PRO:HD2	1.75	0.67
1:B:63:PHE:HB3	1:B:64:PRO:HD2	1.75	0.67
1:A:59:ARG:NH2	1:A:81:ALA:O	2.28	0.67
1:D:35:SER:OG	1:D:37:ARG:NH1	2.27	0.67
1:B:59:ARG:NH2	1:B:81:ALA:O	2.28	0.67
1:D:63:PHE:HB3	1:D:64:PRO:HD2	1.75	0.67
1:C:35:SER:OG	1:C:37:ARG:NH1	2.27	0.67
1:D:610:ASP:HA	2:I:53:TYR:CE1	2.28	0.67
1:D:436:MET:HE1	1:D:467:ASN:HD22	1.59	0.67
1:C:59:ARG:NH2	1:C:81:ALA:O	2.28	0.67
1:D:361:PRO:HG3	2:I:53:TYR:CE1	2.30	0.67
1:D:576:ILE:HD11	2:I:53:TYR:HB2	1.74	0.67
1:C:436:MET:HE1	1:C:467:ASN:HD22	1.59	0.67
1:C:856:TYR:CD2	1:C:864:MET:HE1	2.30	0.67
1:D:59:ARG:NH2	1:D:81:ALA:O	2.28	0.67
1:A:63:PHE:HB3	1:A:64:PRO:HD2	1.75	0.67
1:A:211:ASP:N	1:A:211:ASP:OD1	2.27	0.67
1:D:965:GLN:O	1:D:969:GLU:HG3	1.94	0.67
1:B:11:LEU:HD21	1:B:187:MET:HE3	1.75	0.67
1:C:965:GLN:O	1:C:969:GLU:HG3	1.94	0.67
1:A:375:ASP:O	1:A:379:MET:HG3	1.95	0.67
1:B:211:ASP:OD1	1:B:211:ASP:N	2.27	0.67
1:B:375:ASP:O	1:B:379:MET:HG3	1.95	0.67
1:A:965:GLN:O	1:A:969:GLU:HG3	1.94	0.67
1:C:856:TYR:HB3	1:C:864:MET:HE1	1.77	0.66
1:D:856:TYR:HB3	1:D:864:MET:HE1	1.77	0.66
1:A:581:ASN:O	2:J:72:ASP:C	2.33	0.66
1:D:7:LEU:N	1:D:71:GLU:OE2	2.28	0.66
1:C:7:LEU:N	1:C:71:GLU:OE2	2.28	0.66
1:B:965:GLN:O	1:B:969:GLU:HG3	1.94	0.66
1:D:65:ALA:HB1	1:D:66:PRO:HD2	1.77	0.66
1:A:30:HIS:HB2	1:A:31:PRO:HD2	1.77	0.66
1:B:7:LEU:N	1:B:71:GLU:OE2	2.28	0.66
1:A:7:LEU:N	1:A:71:GLU:OE2	2.28	0.66
1:A:824:GLN:HG3	1:A:825:CYS:N	2.10	0.66
1:C:65:ALA:HB1	1:C:66:PRO:HD2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:856:TYR:CD2	1:D:864:MET:HE1	2.31	0.66
1:B:30:HIS:HB2	1:B:31:PRO:HD2	1.76	0.66
1:B:824:GLN:HG3	1:B:825:CYS:N	2.11	0.66
1:A:610:ASP:HA	2:J:53:TYR:CE1	2.28	0.66
1:C:30:HIS:HB2	1:C:31:PRO:HD2	1.77	0.66
1:B:610:ASP:HA	2:K:53:TYR:CE1	2.28	0.65
1:D:30:HIS:HB2	1:D:31:PRO:HD2	1.77	0.65
1:B:609:ALA:C	2:K:53:TYR:HE1	1.98	0.65
1:D:375:ASP:O	1:D:379:MET:HG3	1.95	0.65
1:A:742:THR:HG22	1:A:743:SER:N	2.12	0.65
1:B:742:THR:HG22	1:B:743:SER:N	2.12	0.65
1:C:609:ALA:C	2:H:53:TYR:CE1	2.69	0.65
1:C:375:ASP:O	1:C:379:MET:HG3	1.95	0.65
1:B:775:GLN:OE1	1:B:890:GLN:NE2	2.30	0.65
1:A:287:ASP:CG	1:D:425:ARG:HH22	2.00	0.65
1:B:856:TYR:HB3	1:B:864:MET:HE1	1.78	0.65
1:A:775:GLN:OE1	1:A:890:GLN:NE2	2.30	0.65
1:B:65:ALA:HB1	1:B:66:PRO:HD2	1.77	0.65
1:A:65:ALA:HB1	1:A:66:PRO:HD2	1.77	0.65
1:A:361:PRO:HG3	2:J:53:TYR:CE1	2.31	0.65
1:C:499:ILE:HB	1:C:533:LEU:HB2	1.79	0.65
1:A:583:ASN:CG	2:J:72:ASP:HA	2.16	0.64
1:A:856:TYR:HB3	1:A:864:MET:HE1	1.78	0.64
1:D:499:ILE:HB	1:D:533:LEU:HB2	1.79	0.64
1:C:824:GLN:HG3	1:C:825:CYS:N	2.11	0.64
1:C:578:TYR:HA	2:H:30:THR:HG21	1.78	0.64
1:C:610:ASP:HA	2:H:53:TYR:CE1	2.30	0.64
1:D:581:ASN:O	2:I:72:ASP:C	2.35	0.64
1:D:824:GLN:HG3	1:D:825:CYS:N	2.11	0.64
1:A:499:ILE:HB	1:A:533:LEU:HB2	1.79	0.64
1:A:255:ARG:HG2	1:A:255:ARG:NH1	2.07	0.64
1:B:499:ILE:HB	1:B:533:LEU:HB2	1.79	0.64
1:D:583:ASN:CG	2:I:72:ASP:HA	2.18	0.64
1:C:775:GLN:OE1	1:C:890:GLN:NE2	2.30	0.64
1:C:610:ASP:HB3	2:H:53:TYR:CE1	2.32	0.64
1:D:797:GLU:O	1:D:801:ILE:HD12	1.98	0.64
1:B:255:ARG:NH1	1:B:255:ARG:HG2	2.07	0.63
1:A:797:GLU:O	1:A:801:ILE:HD12	1.98	0.63
1:B:797:GLU:O	1:B:801:ILE:HD12	1.98	0.63
1:D:775:GLN:OE1	1:D:890:GLN:NE2	2.30	0.63
1:C:797:GLU:O	1:C:801:ILE:HD12	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:835:LEU:C	1:D:836:ILE:HD13	2.19	0.63
1:C:835:LEU:C	1:C:836:ILE:HD13	2.19	0.63
1:C:856:TYR:HD2	1:C:864:MET:HE1	1.62	0.63
1:D:578:TYR:HA	2:I:30:THR:HG21	1.81	0.63
1:C:746:ASP:HA	1:C:760:ARG:CG	2.22	0.63
1:D:742:THR:HG22	1:D:743:SER:N	2.12	0.63
1:C:742:THR:HG22	1:C:743:SER:N	2.12	0.63
1:D:746:ASP:HA	1:D:760:ARG:CG	2.22	0.63
1:B:835:LEU:C	1:B:836:ILE:HD13	2.19	0.63
1:A:287:ASP:OD2	1:D:425:ARG:NH2	2.31	0.63
1:B:576:ILE:HG13	2:K:53:TYR:CD2	2.34	0.63
1:A:835:LEU:C	1:A:836:ILE:HD13	2.19	0.63
1:C:166:ARG:HG3	1:C:392:TYR:HB2	1.81	0.63
1:D:166:ARG:HG3	1:D:392:TYR:HB2	1.81	0.62
1:D:906:TYR:HB3	1:D:907:PRO:HD2	1.80	0.62
1:D:211:ASP:OD1	1:D:211:ASP:N	2.27	0.62
1:A:578:TYR:HA	2:J:30:THR:HG21	1.80	0.62
1:D:856:TYR:HD2	1:D:864:MET:HE1	1.64	0.62
1:B:66:PRO:HD2	1:B:67:GLU:HG2	1.81	0.62
1:C:906:TYR:HB3	1:C:907:PRO:HD2	1.81	0.62
1:C:211:ASP:N	1:C:211:ASP:OD1	2.27	0.62
1:C:576:ILE:HD11	2:H:53:TYR:CB	2.29	0.62
1:A:66:PRO:HD2	1:A:67:GLU:HG2	1.81	0.62
1:A:649:ASN:OD1	1:A:703:PRO:HD2	1.99	0.62
1:B:166:ARG:HG3	1:B:392:TYR:HB2	1.81	0.62
1:A:166:ARG:HG3	1:A:392:TYR:HB2	1.81	0.62
1:B:649:ASN:OD1	1:B:703:PRO:HD2	1.99	0.62
1:D:272:ALA:HB1	1:D:273:PRO:HD2	1.80	0.62
1:A:610:ASP:N	2:J:53:TYR:CZ	2.67	0.62
1:C:272:ALA:HB1	1:C:273:PRO:HD2	1.81	0.62
1:C:649:ASN:OD1	1:C:703:PRO:HD2	1.99	0.62
1:B:362:LEU:HD23	2:K:31:SER:HA	1.78	0.62
1:D:610:ASP:N	2:I:53:TYR:CZ	2.67	0.62
1:D:649:ASN:OD1	1:D:703:PRO:HD2	1.99	0.62
1:D:100:TYR:HB2	1:D:203:TRP:CD2	2.35	0.62
1:D:576:ILE:HG13	2:I:53:TYR:CD2	2.35	0.61
1:C:100:TYR:HB2	1:C:203:TRP:CD2	2.34	0.61
1:A:906:TYR:HB3	1:A:907:PRO:HD2	1.80	0.61
1:D:595:THR:HG23	1:D:596:PRO:HA	1.82	0.61
1:B:140:ARG:NH1	1:B:170:GLU:OE1	2.31	0.61
1:B:578:TYR:HA	2:K:30:THR:HG21	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:822:LEU:HD12	1:A:824:GLN:N	2.16	0.61
2:J:33:TYR:HB2	2:J:98:TRP:HB2	1.83	0.61
1:B:272:ALA:HB1	1:B:273:PRO:HD2	1.81	0.61
2:K:33:TYR:HB2	2:K:98:TRP:HB2	1.83	0.61
1:C:609:ALA:CB	2:H:53:TYR:CZ	2.64	0.61
1:B:928:PRO:O	1:B:973:ARG:NH1	2.34	0.61
1:B:822:LEU:HD12	1:B:824:GLN:N	2.16	0.61
1:C:595:THR:HG23	1:C:596:PRO:HA	1.83	0.61
1:B:576:ILE:CG2	2:K:30:THR:CB	2.67	0.61
1:D:610:ASP:OD1	1:D:612:THR:HG23	2.01	0.61
1:A:928:PRO:O	1:A:973:ARG:NH1	2.34	0.61
1:A:272:ALA:HB1	1:A:273:PRO:HD2	1.81	0.61
1:B:906:TYR:HB3	1:B:907:PRO:HD2	1.81	0.61
1:C:822:LEU:HD12	1:C:824:GLN:N	2.16	0.61
1:D:822:LEU:HD12	1:D:824:GLN:N	2.16	0.61
1:B:100:TYR:HB2	1:B:203:TRP:CD2	2.34	0.61
1:A:227:VAL:HG13	1:A:240:LEU:HD11	1.83	0.61
1:A:140:ARG:NH1	1:A:170:GLU:OE1	2.31	0.61
1:C:610:ASP:OD1	1:C:612:THR:HG23	2.01	0.61
1:D:581:ASN:CB	2:I:72:ASP:OD1	2.40	0.61
1:A:100:TYR:HB2	1:A:203:TRP:CD2	2.35	0.61
1:D:651:LEU:HD12	1:D:669:PRO:HA	1.83	0.61
1:C:651:LEU:HD12	1:C:669:PRO:HA	1.83	0.61
1:B:227:VAL:HG13	1:B:240:LEU:HD11	1.83	0.61
1:C:584:PRO:CG	2:H:30:THR:HG22	2.28	0.61
1:D:66:PRO:HD2	1:D:67:GLU:HG2	1.81	0.61
1:A:822:LEU:HD11	1:A:824:GLN:O	2.01	0.61
1:C:102:ASN:ND2	1:C:201:ASP:HB2	2.16	0.61
1:A:610:ASP:OD1	1:A:612:THR:HG23	2.01	0.61
1:C:66:PRO:HD2	1:C:67:GLU:HG2	1.81	0.61
1:D:102:ASN:ND2	1:D:201:ASP:HB2	2.16	0.61
1:A:576:ILE:HG13	2:J:53:TYR:CD2	2.35	0.60
1:B:610:ASP:OD1	1:B:612:THR:HG23	2.01	0.60
1:B:822:LEU:HD11	1:B:824:GLN:O	2.01	0.60
1:C:928:PRO:O	1:C:973:ARG:NH1	2.33	0.60
1:D:928:PRO:O	1:D:973:ARG:NH1	2.34	0.60
1:D:778:THR:CG2	1:D:779:PRO:HD2	2.30	0.60
1:C:778:THR:CG2	1:C:779:PRO:HD2	2.30	0.60
1:D:767:GLN:HG3	1:D:768:MET:N	2.15	0.60
1:C:227:VAL:HG13	1:C:240:LEU:HD11	1.83	0.60
2:I:34:TRP:HB3	2:I:78:TYR:CZ	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:870:VAL:HG12	1:D:871:GLU:N	2.16	0.60
1:A:282:ARG:HD3	1:D:418:HIS:O	2.01	0.60
1:D:227:VAL:HG13	1:D:240:LEU:HD11	1.83	0.60
2:H:34:TRP:HB3	2:H:78:TYR:CZ	2.36	0.60
2:K:34:TRP:HB3	2:K:78:TYR:CZ	2.36	0.60
1:A:778:THR:CG2	1:A:779:PRO:HD2	2.30	0.60
1:B:651:LEU:HD12	1:B:669:PRO:HA	1.83	0.60
1:C:767:GLN:HG3	1:C:768:MET:N	2.15	0.60
1:C:576:ILE:CG2	2:H:30:THR:CB	2.71	0.60
2:J:34:TRP:HB3	2:J:78:TYR:CZ	2.36	0.60
1:B:830:LEU:HD21	1:B:835:LEU:HB2	1.84	0.60
1:A:830:LEU:HD21	1:A:835:LEU:HB2	1.84	0.60
1:B:778:THR:CG2	1:B:779:PRO:HD2	2.30	0.60
1:A:767:GLN:HG3	1:A:768:MET:N	2.15	0.60
1:B:767:GLN:HG3	1:B:768:MET:N	2.15	0.60
1:C:581:ASN:O	2:H:72:ASP:O	2.18	0.60
1:C:610:ASP:HB3	2:H:53:TYR:CD1	2.36	0.60
1:B:734:SER:HB3	1:B:860:GLY:CA	2.30	0.60
1:C:822:LEU:HD11	1:C:824:GLN:O	2.01	0.60
1:A:505:ARG:HG2	1:A:996:ASP:OD2	2.02	0.60
1:B:505:ARG:HG2	1:B:996:ASP:OD2	2.02	0.60
1:C:870:VAL:HG12	1:C:871:GLU:N	2.16	0.60
1:D:576:ILE:HG21	2:I:30:THR:CB	2.28	0.60
1:A:651:LEU:HD12	1:A:669:PRO:HA	1.83	0.60
1:C:701:VAL:HG12	1:C:702:GLN:N	2.17	0.60
1:D:822:LEU:HD11	1:D:824:GLN:O	2.01	0.60
1:A:870:VAL:HG12	1:A:871:GLU:N	2.16	0.60
1:C:610:ASP:N	2:H:53:TYR:CZ	2.70	0.59
1:B:701:VAL:HG12	1:B:702:GLN:N	2.17	0.59
1:B:595:THR:HG23	1:B:596:PRO:HA	1.82	0.59
1:D:505:ARG:HG2	1:D:996:ASP:OD2	2.02	0.59
1:B:102:ASN:ND2	1:B:201:ASP:HB2	2.16	0.59
1:A:734:SER:HB3	1:A:860:GLY:CA	2.30	0.59
1:A:696:LEU:HD12	1:A:697:THR:N	2.17	0.59
1:B:696:LEU:HD12	1:B:697:THR:N	2.17	0.59
1:A:701:VAL:HG12	1:A:702:GLN:N	2.17	0.59
1:D:701:VAL:HG12	1:D:702:GLN:N	2.17	0.59
1:B:870:VAL:HG12	1:B:871:GLU:N	2.16	0.59
1:C:505:ARG:HG2	1:C:996:ASP:OD2	2.02	0.59
1:A:128:ASN:HA	1:A:180:GLY:O	2.02	0.59
1:B:128:ASN:HA	1:B:180:GLY:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:ASN:ND2	1:A:201:ASP:HB2	2.16	0.59
1:C:362:LEU:HD23	2:H:31:SER:HA	1.83	0.59
1:C:511:PRO:HA	1:C:516:PRO:HB3	1.84	0.59
1:D:140:ARG:NH1	1:D:170:GLU:OE1	2.31	0.59
1:A:511:PRO:HA	1:A:516:PRO:HB3	1.84	0.59
2:H:33:TYR:HB2	2:H:98:TRP:HB2	1.83	0.59
1:A:595:THR:HG23	1:A:596:PRO:HA	1.82	0.59
1:D:511:PRO:HA	1:D:516:PRO:HB3	1.84	0.59
2:I:33:TYR:HB2	2:I:98:TRP:HB2	1.83	0.59
1:C:696:LEU:HD12	1:C:697:THR:N	2.18	0.59
1:C:140:ARG:NH1	1:C:170:GLU:OE1	2.31	0.59
1:C:576:ILE:HG13	2:H:53:TYR:CD2	2.36	0.59
1:D:696:LEU:HD12	1:D:697:THR:N	2.18	0.59
1:A:282:ARG:HH12	1:D:419:GLY:C	2.06	0.59
1:B:511:PRO:HA	1:B:516:PRO:HB3	1.84	0.59
1:C:609:ALA:C	2:H:53:TYR:HE1	2.04	0.59
1:B:610:ASP:N	2:K:53:TYR:CZ	2.69	0.59
1:C:336:ARG:NH2	1:C:338:GLU:OE1	2.36	0.59
1:D:336:ARG:NH2	1:D:338:GLU:OE1	2.36	0.59
1:C:610:ASP:CB	2:H:53:TYR:CE1	2.85	0.59
1:A:579:ASP:CG	2:J:73:THR:OG1	2.38	0.59
1:C:737:ILE:HG13	1:C:738:PRO:N	2.17	0.59
1:D:533:LEU:HD12	1:D:533:LEU:C	2.24	0.58
1:A:578:TYR:CE2	2:J:28:SER:CB	2.87	0.58
1:B:609:ALA:C	2:K:53:TYR:OH	2.40	0.58
1:D:737:ILE:HG13	1:D:738:PRO:N	2.17	0.58
1:D:734:SER:HB3	1:D:860:GLY:CA	2.30	0.58
1:A:336:ARG:NH2	1:A:338:GLU:OE1	2.36	0.58
1:C:128:ASN:HA	1:C:180:GLY:O	2.02	0.58
1:B:759:ASN:OD1	1:B:761:GLN:N	2.35	0.58
1:A:759:ASN:OD1	1:A:761:GLN:N	2.35	0.58
1:D:128:ASN:HA	1:D:180:GLY:O	2.02	0.58
1:B:583:ASN:CB	2:K:73:THR:H	1.97	0.58
1:C:533:LEU:HD12	1:C:533:LEU:C	2.24	0.58
1:B:336:ARG:NH2	1:B:338:GLU:OE1	2.36	0.58
1:C:734:SER:HB3	1:C:860:GLY:CA	2.30	0.58
1:B:533:LEU:HD12	1:B:533:LEU:C	2.24	0.58
1:A:62:TRP:CD1	1:A:95:TYR:HB3	2.39	0.58
1:B:62:TRP:CD1	1:B:95:TYR:HB3	2.39	0.58
1:B:581:ASN:O	2:K:72:ASP:O	2.22	0.58
1:A:533:LEU:HD12	1:A:533:LEU:C	2.24	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:769:TRP:NE1	1:A:774:LYS:HG3	2.19	0.58
1:A:737:ILE:HG13	1:A:738:PRO:N	2.17	0.58
1:B:737:ILE:HG13	1:B:738:PRO:N	2.17	0.58
1:B:769:TRP:NE1	1:B:774:LYS:HG3	2.19	0.58
1:A:6:SER:HB2	1:A:71:GLU:OE2	2.03	0.58
1:C:584:PRO:HB3	2:H:30:THR:CA	2.33	0.58
1:B:361:PRO:HG3	2:K:53:TYR:CE1	2.38	0.58
1:C:62:TRP:CD1	1:C:95:TYR:HB3	2.39	0.58
1:D:62:TRP:CD1	1:D:95:TYR:HB3	2.39	0.58
1:B:6:SER:HB2	1:B:71:GLU:OE2	2.04	0.57
1:D:429:ASP:OD1	1:D:430:PRO:HD2	2.04	0.57
1:C:429:ASP:OD1	1:C:430:PRO:HD2	2.04	0.57
1:C:473:ARG:HD3	1:C:473:ARG:O	2.04	0.57
1:D:473:ARG:O	1:D:473:ARG:HD3	2.04	0.57
1:C:26:ARG:HD2	1:C:169:SER:HA	1.87	0.57
1:A:473:ARG:O	1:A:473:ARG:HD3	2.04	0.57
1:C:769:TRP:NE1	1:C:774:LYS:HG3	2.19	0.57
1:D:26:ARG:HD2	1:D:169:SER:HA	1.87	0.57
1:A:576:ILE:HG21	2:J:30:THR:CB	2.28	0.57
1:B:584:PRO:CG	2:K:30:THR:HG22	2.31	0.57
1:B:584:PRO:N	2:K:30:THR:HG22	2.16	0.57
1:D:834:VAL:HG12	1:D:835:LEU:N	2.19	0.57
1:C:6:SER:HB2	1:C:71:GLU:OE2	2.04	0.57
1:A:460:ASN:ND2	1:A:461:GLU:HG2	2.20	0.57
1:B:460:ASN:ND2	1:B:461:GLU:HG2	2.20	0.57
1:B:473:ARG:HD3	1:B:473:ARG:O	2.04	0.57
1:D:578:TYR:CE2	2:I:28:SER:CB	2.87	0.57
1:D:6:SER:HB2	1:D:71:GLU:OE2	2.04	0.57
1:D:769:TRP:NE1	1:D:774:LYS:HG3	2.19	0.57
1:B:576:ILE:HD11	2:K:53:TYR:CB	2.35	0.57
1:C:581:ASN:O	2:H:72:ASP:C	2.43	0.57
1:B:360:HIS:CE1	1:B:362:LEU:HB2	2.40	0.57
1:B:610:ASP:HB3	2:K:53:TYR:CE1	2.39	0.57
1:C:834:VAL:HG12	1:C:835:LEU:N	2.19	0.57
1:D:460:ASN:ND2	1:D:461:GLU:HG2	2.20	0.57
1:B:429:ASP:OD1	1:B:430:PRO:HD2	2.04	0.57
1:B:26:ARG:HD2	1:B:169:SER:HA	1.87	0.57
1:D:618:THR:HG22	1:D:912:ALA:HB1	1.86	0.57
1:A:360:HIS:CE1	1:A:362:LEU:HB2	2.40	0.57
3:N:94:TRP:CD2	3:N:95:PRO:HA	2.40	0.57
1:C:460:ASN:ND2	1:C:461:GLU:HG2	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:ARG:HD2	1:A:169:SER:HA	1.87	0.57
1:B:316:HIS:HD2	1:B:317:THR:O	1.87	0.57
1:A:583:ASN:OD1	2:J:72:ASP:N	2.36	0.56
1:B:577:LYS:O	2:K:30:THR:HG21	2.05	0.56
1:A:429:ASP:OD1	1:A:431[B]:ARG:HG3	2.05	0.56
1:A:429:ASP:OD1	1:A:430:PRO:HD2	2.05	0.56
1:C:618:THR:HG22	1:C:912:ALA:HB1	1.86	0.56
3:O:94:TRP:CD2	3:O:95:PRO:HA	2.40	0.56
1:A:316:HIS:HD2	1:A:317:THR:O	1.87	0.56
1:C:584:PRO:HB3	2:H:30:THR:HA	1.87	0.56
1:B:834:VAL:HG12	1:B:835:LEU:N	2.19	0.56
1:B:429:ASP:OD1	1:B:431[B]:ARG:HG3	2.05	0.56
1:A:419:GLY:C	1:D:282:ARG:HH12	2.08	0.56
1:C:830:LEU:HD21	1:C:835:LEU:HB2	1.84	0.56
1:A:834:VAL:HG12	1:A:835:LEU:N	2.19	0.56
1:D:134:LEU:H	1:D:134:LEU:HD12	1.69	0.56
1:A:763:GLY:HA3	1:A:822:LEU:HD21	1.87	0.56
1:B:763:GLY:HA3	1:B:822:LEU:HD21	1.87	0.56
1:D:457:SER:HA	1:D:485:GLN:O	2.05	0.56
1:D:830:LEU:HD21	1:D:835:LEU:HB2	1.84	0.56
1:C:457:SER:HA	1:C:485:GLN:O	2.05	0.56
1:C:316:HIS:HD2	1:C:317:THR:O	1.87	0.56
1:C:577:LYS:O	2:H:30:THR:HG21	2.06	0.56
1:C:134:LEU:H	1:C:134:LEU:HD12	1.69	0.56
1:B:618:THR:HG22	1:B:912:ALA:HB1	1.86	0.56
1:D:316:HIS:HD2	1:D:317:THR:O	1.87	0.56
1:A:577:LYS:O	1:A:584:PRO:HA	2.06	0.56
1:B:576:ILE:CG1	2:K:53:TYR:HD2	2.19	0.56
1:A:763:GLY:HA3	1:A:822:LEU:CD2	2.36	0.56
1:B:763:GLY:HA3	1:B:822:LEU:CD2	2.36	0.56
1:C:759:ASN:OD1	1:C:761:GLN:N	2.35	0.56
1:A:618:THR:HG22	1:A:912:ALA:HB1	1.86	0.56
1:C:360:HIS:CE1	1:C:361:PRO:HD2	2.41	0.56
1:B:581:ASN:O	2:K:72:ASP:C	2.43	0.56
1:D:360:HIS:CE1	1:D:361:PRO:HD2	2.41	0.56
1:C:763:GLY:HA3	1:C:822:LEU:HD21	1.87	0.56
1:D:429:ASP:OD1	1:D:431[B]:ARG:HG3	2.05	0.56
1:A:531:ARG:O	1:A:561:ARG:NH1	2.39	0.56
1:C:18:ASN:OD1	1:C:19:PRO:HD2	2.06	0.56
3:O:2:ILE:HD13	3:O:29:ILE:HG22	1.88	0.56
1:D:18:ASN:OD1	1:D:19:PRO:HD2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:531:ARG:O	1:B:561:ARG:NH1	2.39	0.56
1:C:577:LYS:O	1:C:584:PRO:HA	2.06	0.56
1:B:577:LYS:O	1:B:584:PRO:HA	2.06	0.56
1:A:134:LEU:HD12	1:A:134:LEU:H	1.69	0.56
1:C:429:ASP:OD1	1:C:431[B]:ARG:HG3	2.05	0.56
1:D:759:ASN:OD1	1:D:761:GLN:N	2.35	0.56
1:D:577:LYS:O	1:D:584:PRO:HA	2.06	0.56
1:A:833:ALA:HB1	1:A:858:ILE:O	2.06	0.56
1:B:833:ALA:HB1	1:B:858:ILE:O	2.06	0.56
1:A:1020:TRP:CD1	1:A:1021:CYS:N	2.74	0.56
1:D:763:GLY:HA3	1:D:822:LEU:HD21	1.87	0.56
3:N:2:ILE:HD13	3:N:29:ILE:HG22	1.88	0.56
1:C:360:HIS:CE1	1:C:362:LEU:HB2	2.40	0.55
1:D:360:HIS:CE1	1:D:362:LEU:HB2	2.40	0.55
1:B:134:LEU:H	1:B:134:LEU:HD12	1.69	0.55
1:D:304:GLU:C	1:D:305:ILE:HG13	2.26	0.55
1:B:18:ASN:OD1	1:B:19:PRO:HD2	2.06	0.55
1:B:360:HIS:CE1	1:B:361:PRO:HD2	2.40	0.55
3:L:94:TRP:CD2	3:L:95:PRO:HA	2.40	0.55
1:A:360:HIS:CE1	1:A:361:PRO:HD2	2.40	0.55
1:B:576:ILE:HG22	2:K:30:THR:HB	1.77	0.55
1:B:1020:TRP:CD1	1:B:1021:CYS:N	2.74	0.55
3:M:94:TRP:CD2	3:M:95:PRO:HA	2.40	0.55
1:B:610:ASP:HB3	2:K:53:TYR:CD1	2.42	0.55
1:B:304:GLU:C	1:B:305:ILE:HG13	2.26	0.55
1:B:425:ARG:NH2	1:C:287:ASP:OD2	2.39	0.55
1:D:362:LEU:CD2	2:I:32:ASP:N	2.70	0.55
1:C:304:GLU:C	1:C:305:ILE:HG13	2.26	0.55
1:C:763:GLY:HA3	1:C:822:LEU:CD2	2.36	0.55
1:A:18:ASN:OD1	1:A:19:PRO:HD2	2.06	0.55
3:L:2:ILE:HD13	3:L:29:ILE:HG22	1.88	0.55
3:M:2:ILE:HD13	3:M:29:ILE:HG22	1.88	0.55
1:C:609:ALA:C	2:H:53:TYR:OH	2.45	0.55
1:A:304:GLU:C	1:A:305:ILE:HG13	2.26	0.55
1:C:395:HIS:ND1	1:C:396:PRO:HD2	2.22	0.55
1:D:395:HIS:ND1	1:D:396:PRO:HD2	2.22	0.55
1:C:531:ARG:O	1:C:561:ARG:NH1	2.39	0.55
1:D:531:ARG:O	1:D:561:ARG:NH1	2.39	0.55
3:O:37:GLN:HB2	3:O:47:LEU:HD11	1.89	0.55
1:A:576:ILE:HG13	2:J:53:TYR:HD2	1.72	0.55
1:D:763:GLY:HA3	1:D:822:LEU:CD2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:TYR:HB2	1:B:203:TRP:CE3	2.42	0.55
1:B:457:SER:HA	1:B:485:GLN:O	2.06	0.55
3:N:37:GLN:HB2	3:N:47:LEU:HD11	1.89	0.55
1:A:457:SER:HA	1:A:485:GLN:O	2.06	0.55
1:B:610:ASP:CB	2:K:53:TYR:CE1	2.90	0.55
1:A:100:TYR:HB2	1:A:203:TRP:CE3	2.42	0.55
1:A:38:ASN:ND2	1:A:41:GLU:N	2.48	0.55
1:A:786:ARG:HA	1:A:964:GLN:OE1	2.07	0.55
1:B:786:ARG:HA	1:B:964:GLN:OE1	2.07	0.55
1:D:583:ASN:OD1	2:I:72:ASP:N	2.40	0.55
1:B:38:ASN:ND2	1:B:41:GLU:N	2.48	0.55
1:C:100:TYR:HB2	1:C:203:TRP:CE3	2.42	0.55
1:D:100:TYR:HB2	1:D:203:TRP:CE3	2.42	0.54
1:A:395:HIS:ND1	1:A:396:PRO:HD2	2.22	0.54
1:A:425:ARG:HH22	1:D:287:ASP:CG	2.11	0.54
1:B:942:ARG:HA	1:B:953:GLY:O	2.07	0.54
1:B:746:ASP:HA	1:B:760:ARG:CG	2.22	0.54
1:C:833:ALA:HB1	1:C:858:ILE:O	2.06	0.54
1:D:833:ALA:HB1	1:D:858:ILE:O	2.06	0.54
1:A:942:ARG:HA	1:A:953:GLY:O	2.07	0.54
1:C:166:ARG:HG3	1:C:392:TYR:CB	2.38	0.54
1:D:166:ARG:HG3	1:D:392:TYR:CB	2.38	0.54
1:C:749:ILE:O	1:C:755:ARG:HG3	2.07	0.54
1:A:576:ILE:HG21	2:J:30:THR:C	2.27	0.54
1:B:668:VAL:HG13	1:B:669:PRO:HD2	1.89	0.54
1:A:418:HIS:O	1:D:282:ARG:HD3	2.08	0.54
1:D:749:ILE:O	1:D:755:ARG:HG3	2.08	0.54
1:C:110:ASN:O	1:C:113:PHE:N	2.39	0.54
1:B:395:HIS:ND1	1:B:396:PRO:HD2	2.22	0.54
1:A:597:ASN:HD22	1:A:599:ARG:N	1.94	0.54
1:D:38:ASN:HD21	1:D:41:GLU:H	1.53	0.54
1:B:30:HIS:HB2	1:B:31:PRO:CD	2.38	0.54
1:C:362:LEU:HD21	2:H:31:SER:HA	1.88	0.54
1:A:746:ASP:HA	1:A:760:ARG:CG	2.22	0.54
1:A:668:VAL:HG13	1:A:669:PRO:HD2	1.89	0.54
1:A:30:HIS:HB2	1:A:31:PRO:CD	2.38	0.54
1:D:110:ASN:O	1:D:113:PHE:N	2.39	0.54
1:D:576:ILE:HG21	2:I:30:THR:C	2.28	0.54
1:C:597:ASN:HD22	1:C:599:ARG:N	1.94	0.54
1:C:942:ARG:HA	1:C:953:GLY:O	2.07	0.54
1:C:786:ARG:HA	1:C:964:GLN:OE1	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:37:GLN:HB2	3:M:47:LEU:HD11	1.89	0.54
1:A:362:LEU:HD21	2:J:30:THR:O	2.08	0.54
1:B:597:ASN:HD22	1:B:599:ARG:N	1.94	0.54
1:C:1020:TRP:CD1	1:C:1021:CYS:N	2.74	0.54
1:D:1020:TRP:CD1	1:D:1021:CYS:N	2.74	0.54
1:D:668:VAL:HG13	1:D:669:PRO:HD2	1.89	0.54
1:D:786:ARG:HA	1:D:964:GLN:OE1	2.07	0.54
1:A:362:LEU:HD21	2:J:31:SER:CA	2.38	0.54
1:D:597:ASN:HD22	1:D:599:ARG:N	1.94	0.54
1:C:38:ASN:HD21	1:C:41:GLU:H	1.53	0.54
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.89	0.54
1:C:584:PRO:HG2	2:H:71:ARG:HH12	1.63	0.53
1:A:576:ILE:HD11	2:J:53:TYR:CB	2.37	0.53
1:C:668:VAL:HG13	1:C:669:PRO:HD2	1.89	0.53
1:D:645:ARG:HH22	1:D:650:GLU:CD	2.11	0.53
1:D:942:ARG:HA	1:D:953:GLY:O	2.07	0.53
1:D:362:LEU:HD21	2:I:30:THR:O	2.07	0.53
1:D:576:ILE:CG1	2:I:53:TYR:HD2	2.21	0.53
1:C:79:PRO:N	1:C:80:GLU:OE1	2.41	0.53
1:C:645:ARG:HH22	1:C:650:GLU:CD	2.11	0.53
1:B:166:ARG:HG3	1:B:392:TYR:CB	2.38	0.53
1:A:166:ARG:HG3	1:A:392:TYR:CB	2.38	0.53
1:C:576:ILE:CG1	2:H:53:TYR:HD2	2.20	0.53
1:D:79:PRO:N	1:D:80:GLU:OE1	2.41	0.53
1:B:79:PRO:N	1:B:80:GLU:OE1	2.41	0.53
1:A:79:PRO:N	1:A:80:GLU:OE1	2.41	0.53
1:D:894:ARG:NH1	1:D:919:ASP:OD1	2.34	0.53
1:C:584:PRO:N	2:H:30:THR:CG2	2.69	0.53
1:C:1017:GLN:O	1:C:1018:LEU:HD23	2.09	0.53
1:D:1017:GLN:O	1:D:1018:LEU:HD23	2.09	0.53
1:D:576:ILE:HD11	2:I:53:TYR:CB	2.38	0.53
1:B:894:ARG:NH1	1:B:919:ASP:OD1	2.34	0.53
1:C:416:GLU:OE2	1:C:461:GLU:HG3	2.09	0.53
1:A:749:ILE:O	1:A:755:ARG:HG3	2.07	0.53
1:C:654:TRP:CE2	1:C:666:GLY:HA3	2.44	0.53
1:C:894:ARG:NH1	1:C:919:ASP:OD1	2.34	0.53
1:B:749:ILE:O	1:B:755:ARG:HG3	2.08	0.53
1:A:576:ILE:CG1	2:J:53:TYR:HD2	2.22	0.53
1:A:894:ARG:NH1	1:A:919:ASP:OD1	2.34	0.53
1:D:357:HIS:HD2	1:D:392:TYR:OH	1.91	0.53
1:D:416:GLU:OE2	1:D:461:GLU:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1017:GLN:O	1:B:1018:LEU:HD23	2.09	0.53
1:D:654:TRP:CE2	1:D:666:GLY:HA3	2.44	0.53
1:D:696:LEU:HD12	1:D:697:THR:H	1.74	0.53
1:C:357:HIS:HD2	1:C:392:TYR:OH	1.92	0.53
1:A:416:GLU:OE2	1:A:461:GLU:HG3	2.09	0.53
1:B:416:GLU:OE2	1:B:461:GLU:HG3	2.09	0.53
1:C:355:ASN:OD1	1:C:388:ARG:HD3	2.09	0.53
1:A:1017:GLN:O	1:A:1018:LEU:HD23	2.09	0.53
1:B:959:ILE:HG23	1:B:959:ILE:O	2.09	0.53
1:D:355:ASN:OD1	1:D:388:ARG:HD3	2.09	0.53
1:B:357:HIS:HD2	1:B:392:TYR:OH	1.91	0.52
1:A:959:ILE:O	1:A:959:ILE:HG23	2.09	0.52
1:C:696:LEU:HD12	1:C:697:THR:H	1.74	0.52
1:C:742:THR:HG22	1:C:743:SER:H	1.74	0.52
1:A:357:HIS:HD2	1:A:392:TYR:OH	1.92	0.52
1:B:251:ARG:HG2	1:B:251:ARG:NH1	2.25	0.52
1:D:576:ILE:HG13	2:I:53:TYR:HD2	1.72	0.52
1:A:251:ARG:NH1	1:A:251:ARG:HG2	2.25	0.52
1:D:959:ILE:O	1:D:959:ILE:HG23	2.09	0.52
1:D:6:SER:OG	1:D:9:VAL:HB	2.09	0.52
1:C:6:SER:OG	1:C:9:VAL:HB	2.09	0.52
1:C:959:ILE:HG23	1:C:959:ILE:O	2.09	0.52
1:D:742:THR:HG22	1:D:743:SER:H	1.74	0.52
1:A:355:ASN:OD1	1:A:388:ARG:HD3	2.09	0.52
1:B:110:ASN:O	1:B:113:PHE:N	2.39	0.52
1:B:654:TRP:CE2	1:B:666:GLY:HA3	2.44	0.52
1:B:645:ARG:HH22	1:B:650:GLU:CD	2.11	0.52
1:B:749:ILE:HD12	1:B:749:ILE:N	2.25	0.52
1:B:355:ASN:OD1	1:B:388:ARG:HD3	2.09	0.52
1:D:584:PRO:CB	2:I:30:THR:CG2	2.43	0.52
1:A:654:TRP:CE2	1:A:666:GLY:HA3	2.44	0.52
1:A:696:LEU:HD12	1:A:697:THR:H	1.74	0.52
1:A:749:ILE:N	1:A:749:ILE:HD12	2.25	0.52
1:A:110:ASN:O	1:A:113:PHE:N	2.39	0.52
1:A:808:GLU:HA	1:A:808:GLU:OE1	2.10	0.52
1:D:579:ASP:CG	2:I:73:THR:OG1	2.41	0.52
1:C:920:LEU:HB3	1:C:921:PRO:CD	2.39	0.52
1:D:920:LEU:HB3	1:D:921:PRO:CD	2.39	0.52
1:A:6:SER:OG	1:A:9:VAL:HB	2.09	0.52
1:A:425:ARG:NH2	1:D:287:ASP:OD2	2.43	0.52
2:K:42:GLY:O	2:K:43:ASN:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:878:HIS:HB3	1:C:1009:LEU:O	2.10	0.52
1:B:6:SER:OG	1:B:9:VAL:HB	2.09	0.52
2:J:42:GLY:O	2:J:43:ASN:HB2	2.10	0.52
1:A:362:LEU:CD2	2:J:32:ASP:N	2.71	0.51
1:D:878:HIS:HB3	1:D:1009:LEU:O	2.10	0.51
1:B:808:GLU:HA	1:B:808:GLU:OE1	2.10	0.51
1:A:645:ARG:HH22	1:A:650:GLU:CD	2.11	0.51
1:A:742:THR:HG22	1:A:743:SER:H	1.74	0.51
1:B:362:LEU:HD21	2:K:30:THR:O	2.10	0.51
1:A:254:LEU:O	1:A:255:ARG:NH1	2.44	0.51
1:B:742:THR:HG22	1:B:743:SER:H	1.74	0.51
1:A:26:ARG:CD	1:A:169:SER:HB3	2.41	0.51
1:A:576:ILE:HG21	2:J:30:THR:CA	2.41	0.51
1:B:576:ILE:HG13	2:K:53:TYR:HD2	1.73	0.51
1:B:254:LEU:O	1:B:255:ARG:NH1	2.44	0.51
1:B:894:ARG:HD3	1:B:919:ASP:OD1	2.11	0.51
1:D:906:TYR:HB3	1:D:907:PRO:CD	2.41	0.51
1:D:26:ARG:CD	1:D:169:SER:HB3	2.41	0.51
1:B:26:ARG:CD	1:B:169:SER:HB3	2.41	0.51
1:A:878:HIS:HB3	1:A:1009:LEU:O	2.10	0.51
1:A:894:ARG:HD3	1:A:919:ASP:OD1	2.11	0.51
1:C:30:HIS:HB2	1:C:31:PRO:CD	2.38	0.51
1:D:30:HIS:HB2	1:D:31:PRO:CD	2.38	0.51
1:C:26:ARG:CD	1:C:169:SER:HB3	2.41	0.51
3:O:2:ILE:HD13	3:O:29:ILE:CG2	2.41	0.51
1:B:425:ARG:HH22	1:C:287:ASP:CG	2.14	0.51
1:B:578:TYR:CE2	2:K:28:SER:CB	2.94	0.51
1:C:254:LEU:O	1:C:255:ARG:NH1	2.44	0.51
1:D:254:LEU:O	1:D:255:ARG:NH1	2.44	0.51
1:B:130:ASP:OD2	1:B:132:SER:OG	2.28	0.51
1:A:130:ASP:OD2	1:A:132:SER:OG	2.28	0.51
1:C:578:TYR:CE2	2:H:28:SER:CB	2.94	0.51
1:B:584:PRO:HB3	2:K:30:THR:CA	2.41	0.51
3:N:2:ILE:HD13	3:N:29:ILE:CG2	2.41	0.51
1:C:906:TYR:HB3	1:C:907:PRO:CD	2.41	0.51
1:B:878:HIS:HB3	1:B:1009:LEU:O	2.10	0.51
1:D:230:ARG:CG	1:D:230:ARG:HH11	2.24	0.51
1:A:610:ASP:HB3	2:J:53:TYR:CD1	2.46	0.51
1:B:576:ILE:HG21	2:K:30:THR:CB	2.38	0.51
1:A:836:ILE:HG22	1:A:837:THR:N	2.26	0.51
1:D:531:ARG:HB3	1:D:532:PRO:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:749:ILE:N	1:C:749:ILE:HD12	2.25	0.51
2:I:42:GLY:O	2:I:43:ASN:HB2	2.10	0.51
1:B:148:SER:HB3	1:B:190:ARG:O	2.10	0.51
2:H:42:GLY:O	2:H:43:ASN:HB2	2.10	0.51
1:C:230:ARG:CG	1:C:230:ARG:HH11	2.24	0.51
1:C:808:GLU:OE1	1:C:808:GLU:HA	2.10	0.51
1:D:808:GLU:HA	1:D:808:GLU:OE1	2.10	0.51
1:D:576:ILE:HD11	2:I:53:TYR:O	2.11	0.51
1:C:894:ARG:HD3	1:C:919:ASP:OD1	2.11	0.51
1:D:148:SER:HB3	1:D:190:ARG:O	2.10	0.51
1:C:148:SER:HB3	1:C:190:ARG:O	2.10	0.51
1:C:251:ARG:NH1	1:C:251:ARG:HG2	2.25	0.51
1:D:251:ARG:NH1	1:D:251:ARG:HG2	2.25	0.51
1:B:836:ILE:HG22	1:B:837:THR:N	2.26	0.50
1:D:894:ARG:HD3	1:D:919:ASP:OD1	2.11	0.50
1:D:749:ILE:N	1:D:749:ILE:HD12	2.25	0.50
1:C:130:ASP:OD2	1:C:132:SER:OG	2.28	0.50
1:B:542:MET:HA	1:B:604:ASN:HA	1.92	0.50
1:D:130:ASP:OD2	1:D:132:SER:OG	2.28	0.50
1:A:576:ILE:HD11	2:J:53:TYR:O	2.11	0.50
1:D:578:TYR:CE2	2:I:28:SER:HB3	2.47	0.50
1:A:65:ALA:HB1	1:A:66:PRO:CD	2.41	0.50
1:C:822:LEU:HD12	1:C:824:GLN:H	1.76	0.50
1:A:906:TYR:HB3	1:A:907:PRO:CD	2.41	0.50
1:A:542:MET:HA	1:A:604:ASN:HA	1.92	0.50
1:A:770:ILE:HG22	1:A:770:ILE:O	2.10	0.50
1:B:65:ALA:HB1	1:B:66:PRO:CD	2.41	0.50
1:A:73:TRP:CZ2	1:A:122:CYS:HB3	2.47	0.50
1:A:148:SER:HB3	1:A:190:ARG:O	2.10	0.50
1:D:542:MET:HA	1:D:604:ASN:HA	1.92	0.50
1:A:584:PRO:HB3	2:J:30:THR:HA	1.92	0.50
1:D:38:ASN:ND2	1:D:41:GLU:N	2.48	0.50
1:C:38:ASN:ND2	1:C:41:GLU:N	2.48	0.50
1:D:822:LEU:HD12	1:D:824:GLN:H	1.76	0.50
1:C:542:MET:HA	1:C:604:ASN:HA	1.92	0.50
1:B:770:ILE:HG22	1:B:770:ILE:O	2.10	0.50
1:B:906:TYR:HB3	1:B:907:PRO:CD	2.41	0.50
1:B:73:TRP:CZ2	1:B:122:CYS:HB3	2.47	0.50
1:C:362:LEU:HD21	2:H:31:SER:CA	2.41	0.50
1:A:609:ALA:C	2:J:53:TYR:CZ	2.80	0.50
1:D:360:HIS:CG	1:D:361:PRO:HD2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:920:LEU:HB3	1:A:921:PRO:CD	2.39	0.50
1:D:767:GLN:CG	1:D:768:MET:N	2.75	0.50
1:C:531:ARG:HB3	1:C:532:PRO:HD2	1.92	0.50
1:A:580:GLU:O	2:J:74:SER:HB2	2.11	0.50
3:M:76:ASN:HD22	3:M:76:ASN:C	2.15	0.50
1:C:360:HIS:CG	1:C:361:PRO:HD2	2.47	0.50
1:C:767:GLN:CG	1:C:768:MET:N	2.75	0.50
1:C:579:ASP:CG	2:H:73:THR:OG1	2.45	0.50
1:A:584:PRO:HB3	2:J:30:THR:CA	2.42	0.50
1:B:433:LEU:O	1:B:437:SER:HB3	2.12	0.50
1:A:100:TYR:CZ	1:A:602:CYS:HB3	2.47	0.50
1:B:38:ASN:HD21	1:B:41:GLU:H	1.53	0.50
1:B:920:LEU:HB3	1:B:921:PRO:CD	2.39	0.50
1:A:433:LEU:O	1:A:437:SER:HB3	2.12	0.50
1:B:100:TYR:CZ	1:B:602:CYS:HB3	2.47	0.50
3:O:76:ASN:C	3:O:76:ASN:HD22	2.15	0.50
1:C:576:ILE:HG21	2:H:30:THR:C	2.31	0.50
1:C:361:PRO:HG3	2:H:53:TYR:CE1	2.47	0.50
1:A:578:TYR:CE2	2:J:28:SER:HB3	2.47	0.50
1:A:763:GLY:CA	1:A:822:LEU:HD21	2.42	0.50
1:B:763:GLY:CA	1:B:822:LEU:HD21	2.42	0.50
1:C:73:TRP:CZ2	1:C:122:CYS:HB3	2.47	0.50
1:B:662:PRO:C	1:B:663:LEU:HD23	2.32	0.50
1:D:73:TRP:CZ2	1:D:122:CYS:HB3	2.47	0.50
3:L:76:ASN:C	3:L:76:ASN:HD22	2.15	0.50
1:B:584:PRO:HB3	2:K:30:THR:HA	1.94	0.49
1:D:362:LEU:HD21	2:I:31:SER:CA	2.38	0.49
1:A:38:ASN:HD21	1:A:41:GLU:H	1.53	0.49
1:A:822:LEU:HD12	1:A:824:GLN:H	1.76	0.49
1:B:822:LEU:HD12	1:B:824:GLN:H	1.76	0.49
2:I:33:TYR:HB2	2:I:98:TRP:CB	2.42	0.49
1:A:662:PRO:C	1:A:663:LEU:HD23	2.32	0.49
1:B:638:VAL:O	1:B:677:LYS:HA	2.12	0.49
1:B:360:HIS:CG	1:B:361:PRO:HD2	2.47	0.49
1:D:708:TRP:CE3	1:D:709:SER:HB3	2.48	0.49
1:A:282:ARG:CG	1:D:423:MET:HB2	2.42	0.49
2:H:33:TYR:HB2	2:H:98:TRP:CB	2.42	0.49
1:B:531:ARG:HB3	1:B:532:PRO:HD2	1.92	0.49
1:A:638:VAL:O	1:A:677:LYS:HA	2.12	0.49
1:A:360:HIS:CG	1:A:361:PRO:HD2	2.47	0.49
1:C:708:TRP:CE3	1:C:709:SER:HB3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:652:LEU:HD12	1:D:699:ARG:O	2.12	0.49
1:B:696:LEU:HD12	1:B:697:THR:H	1.74	0.49
1:C:763:GLY:CA	1:C:822:LEU:HD21	2.42	0.49
1:C:100:TYR:CZ	1:C:602:CYS:HB3	2.47	0.49
1:A:95:TYR:N	1:A:95:TYR:CD1	2.79	0.49
3:N:76:ASN:HD22	3:N:76:ASN:C	2.15	0.49
1:B:230:ARG:HH11	1:B:230:ARG:CG	2.24	0.49
1:C:836:ILE:HG22	1:C:837:THR:N	2.26	0.49
1:B:708:TRP:CE3	1:B:709:SER:HB3	2.47	0.49
1:C:652:LEU:HD12	1:C:699:ARG:O	2.12	0.49
1:D:763:GLY:CA	1:D:822:LEU:HD21	2.42	0.49
1:B:95:TYR:CD1	1:B:95:TYR:N	2.79	0.49
3:L:2:ILE:HD13	3:L:29:ILE:CG2	2.41	0.49
3:M:2:ILE:HD13	3:M:29:ILE:CG2	2.41	0.49
1:D:638:VAL:O	1:D:677:LYS:HA	2.12	0.49
1:A:230:ARG:CG	1:A:230:ARG:HH11	2.24	0.49
1:C:882:ILE:HG22	1:C:882:ILE:O	2.12	0.49
1:D:100:TYR:CZ	1:D:602:CYS:HB3	2.47	0.49
1:B:767:GLN:CG	1:B:768:MET:N	2.75	0.49
1:A:531:ARG:HB3	1:A:532:PRO:HD2	1.92	0.49
1:C:638:VAL:O	1:C:677:LYS:HA	2.12	0.49
1:D:882:ILE:O	1:D:882:ILE:HG22	2.12	0.49
1:C:578:TYR:CE2	2:H:28:SER:HB3	2.46	0.49
1:D:576:ILE:HG21	2:I:30:THR:CA	2.41	0.49
1:D:576:ILE:CG1	2:I:53:TYR:HB2	2.42	0.49
1:D:836:ILE:HG22	1:D:837:THR:N	2.26	0.49
1:A:708:TRP:CE3	1:A:709:SER:HB3	2.48	0.49
1:C:662:PRO:C	1:C:663:LEU:HD23	2.32	0.49
1:C:770:ILE:HG22	1:C:770:ILE:O	2.10	0.49
1:D:770:ILE:HG22	1:D:770:ILE:O	2.10	0.49
1:D:584:PRO:HB3	2:I:30:THR:CA	2.43	0.49
1:D:436:MET:HE3	1:D:467:ASN:HD22	1.75	0.49
1:C:436:MET:HE3	1:C:467:ASN:HD22	1.75	0.49
2:J:33:TYR:HB2	2:J:98:TRP:CB	2.42	0.49
1:D:105:TYR:CE2	1:D:199:ASP:HB2	2.48	0.49
1:A:576:ILE:CG1	2:J:53:TYR:HB2	2.41	0.49
1:D:610:ASP:HB3	2:I:53:TYR:CD1	2.47	0.49
1:D:595:THR:HG23	1:D:596:PRO:CA	2.43	0.49
1:C:595:THR:HG23	1:C:596:PRO:CA	2.43	0.49
1:A:767:GLN:CG	1:A:768:MET:N	2.75	0.49
1:A:153:TRP:HA	1:A:157:ARG:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:662:PRO:C	1:D:663:LEU:HD23	2.32	0.49
1:B:143:PHE:CD1	1:B:143:PHE:N	2.81	0.49
1:B:12:GLN:HG3	1:B:13:ARG:N	2.27	0.49
2:K:33:TYR:HB2	2:K:98:TRP:CB	2.42	0.49
1:C:105:TYR:CE2	1:C:199:ASP:HB2	2.48	0.49
1:B:90:TRP:HE1	1:B:96:ASP:CG	2.16	0.49
1:A:143:PHE:CD1	1:A:143:PHE:N	2.81	0.49
1:B:153:TRP:HA	1:B:157:ARG:O	2.13	0.49
1:D:90:TRP:HE1	1:D:96:ASP:CG	2.16	0.49
1:D:584:PRO:HB3	2:I:30:THR:HA	1.94	0.49
1:B:835:LEU:CD1	1:B:857:ARG:HB2	2.43	0.49
1:A:30:HIS:ND1	1:A:31:PRO:O	2.40	0.49
1:A:90:TRP:HE1	1:A:96:ASP:CG	2.16	0.49
1:C:433:LEU:O	1:C:437:SER:HB3	2.12	0.48
1:A:835:LEU:CD1	1:A:857:ARG:HB2	2.43	0.48
1:A:830:LEU:HD22	1:A:835:LEU:HB2	1.95	0.48
1:B:652:LEU:HD12	1:B:699:ARG:O	2.12	0.48
1:B:882:ILE:O	1:B:882:ILE:HG22	2.12	0.48
1:C:610:ASP:N	2:H:53:TYR:OH	2.46	0.48
1:D:835:LEU:CD1	1:D:857:ARG:HB2	2.43	0.48
1:A:12:GLN:HG3	1:A:13:ARG:N	2.27	0.48
1:A:652:LEU:HD12	1:A:699:ARG:O	2.12	0.48
1:C:30:HIS:ND1	1:C:31:PRO:O	2.40	0.48
1:B:595:THR:HG23	1:B:596:PRO:CA	2.43	0.48
1:C:90:TRP:HE1	1:C:96:ASP:CG	2.16	0.48
1:A:646:HIS:O	1:A:648:ASP:N	2.46	0.48
1:A:882:ILE:O	1:A:882:ILE:HG22	2.12	0.48
1:D:12:GLN:HG3	1:D:13:ARG:N	2.27	0.48
1:D:433:LEU:O	1:D:437:SER:HB3	2.12	0.48
1:B:668:VAL:CG1	1:B:669:PRO:HD2	2.43	0.48
1:C:65:ALA:HB1	1:C:66:PRO:CD	2.41	0.48
1:A:595:THR:HG23	1:A:596:PRO:CA	2.43	0.48
1:B:105:TYR:CE2	1:B:199:ASP:HB2	2.48	0.48
1:B:646:HIS:O	1:B:648:ASP:N	2.46	0.48
1:C:12:GLN:HG3	1:C:13:ARG:N	2.27	0.48
1:A:668:VAL:CG1	1:A:669:PRO:HD2	2.44	0.48
1:D:30:HIS:ND1	1:D:31:PRO:O	2.40	0.48
1:C:100:TYR:CE1	1:C:602:CYS:HB3	2.49	0.48
1:B:100:TYR:CE1	1:B:602:CYS:HB3	2.49	0.48
1:D:95:TYR:N	1:D:95:TYR:CD1	2.79	0.48
1:C:26:ARG:HD3	1:C:169:SER:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:ARG:HD3	1:D:169:SER:HB3	1.96	0.48
1:A:423:MET:HB2	1:D:282:ARG:CG	2.43	0.48
1:A:100:TYR:CE1	1:A:602:CYS:HB3	2.49	0.48
1:C:835:LEU:CD1	1:C:857:ARG:HB2	2.43	0.48
1:D:65:ALA:HB1	1:D:66:PRO:CD	2.41	0.48
1:B:30:HIS:ND1	1:B:31:PRO:O	2.40	0.48
1:D:100:TYR:CE1	1:D:602:CYS:HB3	2.49	0.48
1:A:105:TYR:CE2	1:A:199:ASP:HB2	2.48	0.48
1:A:610:ASP:HB3	2:J:53:TYR:CE1	2.49	0.48
1:B:610:ASP:N	2:K:53:TYR:OH	2.46	0.48
1:B:26:ARG:HD3	1:B:169:SER:HB3	1.96	0.48
1:B:257:THR:OG1	1:B:316:HIS:HE1	1.97	0.48
1:A:257:THR:OG1	1:A:316:HIS:HE1	1.97	0.48
1:D:153:TRP:HA	1:D:157:ARG:O	2.13	0.48
1:C:651:LEU:HD23	1:C:653[A]:HIS:HE1	1.79	0.48
1:D:272:ALA:HB1	1:D:273:PRO:CD	2.43	0.48
1:C:95:TYR:N	1:C:95:TYR:CD1	2.79	0.48
1:A:26:ARG:HD3	1:A:169:SER:HB3	1.96	0.48
1:B:578:TYR:CE2	2:K:28:SER:HB3	2.49	0.48
1:B:362:LEU:HD21	2:K:31:SER:CA	2.41	0.48
1:A:651:LEU:HD23	1:A:653[A]:HIS:HE1	1.79	0.48
1:C:646:HIS:O	1:C:648:ASP:N	2.46	0.48
1:B:513:PRO:O	1:B:514:ALA:HB3	2.14	0.48
1:C:513:PRO:O	1:C:514:ALA:HB3	2.14	0.48
1:C:153:TRP:HA	1:C:157:ARG:O	2.13	0.48
1:A:610:ASP:CB	2:J:53:TYR:CE1	2.97	0.48
1:B:305:ILE:HD11	1:B:645:ARG:HB3	1.96	0.48
1:C:272:ALA:HB1	1:C:273:PRO:CD	2.43	0.48
1:A:970:THR:CG2	1:A:975:LEU:HB2	2.44	0.48
1:C:609:ALA:CB	2:H:53:TYR:HH	1.92	0.48
1:C:599:ARG:HD2	1:C:600:GLN:OE1	2.14	0.48
1:D:830:LEU:HD22	1:D:835:LEU:HB2	1.95	0.48
1:D:651:LEU:HD23	1:D:653[A]:HIS:HE1	1.79	0.48
1:B:651:LEU:HD23	1:B:653[A]:HIS:HE1	1.79	0.48
1:A:660:GLY:O	1:A:662:PRO:HD3	2.13	0.48
1:D:646:HIS:O	1:D:648:ASP:N	2.47	0.48
1:A:513:PRO:O	1:A:514:ALA:HB3	2.14	0.48
1:B:970:THR:CG2	1:B:975:LEU:HB2	2.44	0.48
1:D:513:PRO:O	1:D:514:ALA:HB3	2.14	0.48
1:B:609:ALA:C	2:K:53:TYR:CZ	2.88	0.47
1:D:599:ARG:HD2	1:D:600:GLN:OE1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:573:GLN:HB2	1:A:602:CYS:O	2.14	0.47
1:A:305:ILE:HD11	1:A:645:ARG:HB3	1.96	0.47
1:D:660:GLY:O	1:D:662:PRO:HD3	2.13	0.47
1:D:210:ARG:NH1	1:D:358:GLU:OE1	2.47	0.47
1:C:210:ARG:NH1	1:C:358:GLU:OE1	2.47	0.47
1:D:610:ASP:HB3	2:I:53:TYR:CE1	2.49	0.47
1:C:830:LEU:HD22	1:C:835:LEU:HB2	1.95	0.47
1:D:305:ILE:HD11	1:D:645:ARG:HB3	1.96	0.47
1:B:568:TRP:HE1	1:B:604:ASN:HD22	1.62	0.47
1:C:780:LEU:HA	1:C:886:CYS:HB3	1.97	0.47
2:K:28:SER:HA	2:K:76:ASN:HD21	1.79	0.47
1:C:305:ILE:HD11	1:C:645:ARG:HB3	1.96	0.47
1:B:573:GLN:HB2	1:B:602:CYS:O	2.14	0.47
1:B:660:GLY:O	1:B:662:PRO:HD3	2.13	0.47
1:B:210:ARG:NH1	1:B:358:GLU:OE1	2.47	0.47
1:D:580:GLU:O	2:I:74:SER:HB2	2.13	0.47
1:A:210:ARG:NH1	1:A:358:GLU:OE1	2.47	0.47
1:A:568:TRP:HE1	1:A:604:ASN:HD22	1.62	0.47
2:J:28:SER:HA	2:J:76:ASN:HD21	1.79	0.47
1:C:660:GLY:O	1:C:662:PRO:HD3	2.13	0.47
1:C:970:THR:CG2	1:C:975:LEU:HB2	2.44	0.47
1:D:780:LEU:HA	1:D:886:CYS:HB3	1.97	0.47
1:C:143:PHE:N	1:C:143:PHE:CD1	2.81	0.47
1:D:578:TYR:CA	2:I:30:THR:HG21	2.44	0.47
1:D:668:VAL:CG1	1:D:669:PRO:HD2	2.44	0.47
1:C:668:VAL:CG1	1:C:669:PRO:HD2	2.44	0.47
1:B:701:VAL:CG1	1:B:702:GLN:N	2.78	0.47
1:D:573:GLN:HB2	1:D:602:CYS:O	2.14	0.47
1:C:147:ASN:HA	1:C:148:SER:HA	1.66	0.47
1:D:143:PHE:CD1	1:D:143:PHE:N	2.81	0.47
1:A:576:ILE:HG22	2:J:30:THR:CB	2.34	0.47
1:A:578:TYR:CA	2:J:30:THR:HG21	2.43	0.47
2:J:29:ILE:H	2:J:76:ASN:HD21	1.63	0.47
2:K:29:ILE:H	2:K:76:ASN:HD21	1.63	0.47
2:I:28:SER:HA	2:I:76:ASN:HD21	1.79	0.47
1:A:701:VAL:CG1	1:A:702:GLN:N	2.77	0.47
1:C:701:VAL:CG1	1:C:702:GLN:N	2.77	0.47
1:D:701:VAL:CG1	1:D:702:GLN:N	2.77	0.47
1:C:573:GLN:HB2	1:C:602:CYS:O	2.14	0.47
1:C:257:THR:OG1	1:C:316:HIS:HE1	1.97	0.47
1:D:251:ARG:HH11	1:D:251:ARG:HG2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:970:THR:CG2	1:D:975:LEU:HB2	2.44	0.47
1:C:292:ARG:C	1:C:293:LEU:HD23	2.35	0.47
1:A:635:THR:OG1	1:A:681:GLU:HG3	2.15	0.47
2:H:28:SER:HA	2:H:76:ASN:HD21	1.79	0.47
1:D:610:ASP:CB	2:I:53:TYR:CE1	2.97	0.47
1:B:742:THR:CG2	1:B:743:SER:N	2.77	0.47
1:A:282:ARG:NH1	1:D:419:GLY:C	2.68	0.47
1:A:423:MET:HB2	1:D:282:ARG:HG2	1.97	0.47
1:D:257:THR:OG1	1:D:316:HIS:HE1	1.97	0.47
1:C:251:ARG:HG2	1:C:251:ARG:HH11	1.79	0.47
1:C:568:TRP:HE1	1:C:604:ASN:HD22	1.62	0.47
1:D:292:ARG:C	1:D:293:LEU:HD23	2.35	0.47
1:D:635:THR:OG1	1:D:681:GLU:HG3	2.15	0.47
1:A:292:ARG:C	1:A:293:LEU:HD23	2.35	0.47
1:B:292:ARG:C	1:B:293:LEU:HD23	2.35	0.47
1:D:127:PHE:HE1	1:D:184:LEU:HG	1.80	0.47
1:B:80:GLU:N	1:B:80:GLU:OE1	2.29	0.47
1:D:568:TRP:HE1	1:D:604:ASN:HD22	1.62	0.47
1:C:127:PHE:HE1	1:C:184:LEU:HG	1.80	0.47
1:B:635:THR:OG1	1:B:681:GLU:HG3	2.15	0.47
1:C:635:THR:OG1	1:C:681:GLU:HG3	2.15	0.47
1:C:630:ARG:HE	1:C:630:ARG:HB3	1.31	0.47
1:A:80:GLU:N	1:A:80:GLU:OE1	2.29	0.47
1:A:742:THR:CG2	1:A:743:SER:N	2.77	0.47
1:B:441:THR:HG22	1:B:474:TRP:CH2	2.50	0.47
1:A:441:THR:HG22	1:A:474:TRP:CH2	2.50	0.47
1:A:599:ARG:HD2	1:A:600:GLN:OE1	2.14	0.46
1:D:134:LEU:N	1:D:134:LEU:CD1	2.73	0.46
1:C:202:MET:HE3	1:C:357:HIS:CD2	2.50	0.46
1:B:251:ARG:HH11	1:B:251:ARG:HG2	1.79	0.46
1:B:780:LEU:HA	1:B:886:CYS:HB3	1.97	0.46
1:A:780:LEU:HA	1:A:886:CYS:HB3	1.97	0.46
1:B:599:ARG:HD2	1:B:600:GLN:OE1	2.14	0.46
1:A:13:ARG:NH1	1:D:13:ARG:NH1	2.63	0.46
1:B:620:ALA:O	1:B:624:GLN:HG3	2.16	0.46
1:C:261:TRP:CD1	1:C:261:TRP:N	2.83	0.46
1:C:134:LEU:N	1:C:134:LEU:CD1	2.73	0.46
1:B:63:PHE:HB3	1:B:64:PRO:CD	2.45	0.46
1:B:945:ASN:OD1	1:B:950:GLN:HB2	2.16	0.46
1:D:261:TRP:N	1:D:261:TRP:CD1	2.83	0.46
1:A:234:ASP:O	1:A:235:PHE:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:945:ASN:OD1	1:C:950:GLN:HB2	2.16	0.46
1:B:234:ASP:O	1:B:235:PHE:HB2	2.15	0.46
1:A:945:ASN:OD1	1:A:950:GLN:HB2	2.16	0.46
1:C:369:GLU:O	1:C:373:VAL:HG23	2.16	0.46
1:D:584:PRO:N	2:I:30:THR:HG22	2.28	0.46
1:B:230:ARG:CG	1:B:230:ARG:NH1	2.79	0.46
1:D:111:PRO:HA	1:D:112:PRO:HA	1.56	0.46
1:D:945:ASN:OD1	1:D:950:GLN:HB2	2.16	0.46
1:A:620:ALA:O	1:A:624:GLN:HG3	2.16	0.46
1:D:369:GLU:O	1:D:373:VAL:HG23	2.16	0.46
1:C:620:ALA:O	1:C:624:GLN:HG3	2.16	0.46
1:D:620:ALA:O	1:D:624:GLN:HG3	2.16	0.46
1:D:630:ARG:HB3	1:D:630:ARG:HE	1.31	0.46
1:C:849:LEU:N	1:C:849:LEU:HD23	2.30	0.46
1:D:849:LEU:HD23	1:D:849:LEU:N	2.30	0.46
1:B:894:ARG:NH2	1:B:921:PRO:HD3	2.31	0.46
1:A:251:ARG:HG2	1:A:251:ARG:HH11	1.79	0.46
1:B:878:HIS:HA	1:B:879:PRO:HD3	1.69	0.46
1:A:230:ARG:NH1	1:A:230:ARG:CG	2.79	0.46
1:A:403:ASP:CG	1:A:451:PRO:HD2	2.36	0.46
1:B:403:ASP:CG	1:B:451:PRO:HD2	2.36	0.46
1:C:658:LEU:O	1:C:659:ASP:C	2.54	0.46
1:C:581:ASN:CB	2:H:72:ASP:OD1	2.55	0.46
1:B:734:SER:HB2	1:B:860:GLY:HA3	1.95	0.46
1:A:894:ARG:NH2	1:A:921:PRO:HD3	2.31	0.46
1:A:166:ARG:HG3	1:A:392:TYR:CG	2.51	0.46
1:D:227:VAL:HG12	1:D:228:ALA:N	2.30	0.46
1:A:73:TRP:CE2	1:A:122:CYS:HB3	2.50	0.46
1:D:658:LEU:O	1:D:659:ASP:C	2.54	0.46
1:C:873:ALA:O	1:C:876:THR:HG22	2.16	0.46
1:D:873:ALA:O	1:D:876:THR:HG22	2.16	0.46
1:B:254:LEU:C	1:B:255:ARG:HG2	2.36	0.46
1:D:834:VAL:CG1	1:D:835:LEU:N	2.79	0.46
1:A:3:ILE:HD12	1:A:3:ILE:O	2.16	0.46
1:B:651:LEU:HD12	1:B:651:LEU:HA	1.46	0.46
1:B:166:ARG:HG3	1:B:392:TYR:CG	2.51	0.46
1:B:272:ALA:HB1	1:B:273:PRO:CD	2.43	0.46
1:A:282:ARG:HG2	1:D:423:MET:HB2	1.97	0.46
1:A:147:ASN:HA	1:A:148:SER:HA	1.65	0.46
1:B:73:TRP:CE2	1:B:122:CYS:HB3	2.51	0.46
1:A:141:ILE:CG1	1:A:142:ILE:N	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:ILE:CG1	1:B:142:ILE:N	2.79	0.46
1:C:84:VAL:HG13	1:C:85:VAL:N	2.31	0.46
1:D:84:VAL:HG13	1:D:85:VAL:N	2.31	0.46
1:D:403:ASP:CG	1:D:451:PRO:HD2	2.36	0.46
1:A:127:PHE:HE1	1:A:184:LEU:HG	1.80	0.46
1:C:403:ASP:CG	1:C:451:PRO:HD2	2.36	0.46
2:I:29:ILE:H	2:I:76:ASN:HD21	1.63	0.46
1:C:834:VAL:CG1	1:C:835:LEU:N	2.79	0.46
1:A:272:ALA:HB1	1:A:273:PRO:CD	2.43	0.46
1:B:316:HIS:HB2	1:B:321:THR:O	2.16	0.46
1:A:316:HIS:HB2	1:A:321:THR:O	2.16	0.46
1:A:878:HIS:HA	1:A:879:PRO:HD3	1.69	0.46
1:D:147:ASN:HA	1:D:148:SER:HA	1.65	0.46
1:C:111:PRO:HA	1:C:112:PRO:HA	1.57	0.46
1:B:127:PHE:HE1	1:B:184:LEU:HG	1.80	0.46
2:H:29:ILE:H	2:H:76:ASN:HD21	1.63	0.46
1:D:610:ASP:N	2:I:53:TYR:OH	2.49	0.46
1:B:834:VAL:CG1	1:B:835:LEU:N	2.79	0.46
1:C:227:VAL:HG12	1:C:228:ALA:N	2.31	0.46
1:B:429:ASP:OD1	1:B:431[A]:ARG:HG3	2.16	0.46
1:A:419:GLY:C	1:D:282:ARG:NH1	2.68	0.46
1:D:531:ARG:CB	1:D:532:PRO:HD2	2.46	0.46
1:C:73:TRP:CE2	1:C:122:CYS:HB3	2.51	0.46
1:A:230:ARG:HH11	1:A:230:ARG:HG2	1.81	0.46
1:B:881:ARG:HD3	1:B:987:ASP:CG	2.36	0.46
1:A:254:LEU:C	1:A:255:ARG:HG2	2.36	0.45
1:B:3:ILE:HD12	1:B:3:ILE:O	2.16	0.45
1:A:227:VAL:HG12	1:A:228:ALA:N	2.31	0.45
1:D:870:VAL:CG1	1:D:871:GLU:N	2.79	0.45
1:A:429:ASP:OD1	1:A:431[A]:ARG:HG3	2.16	0.45
1:D:73:TRP:CE2	1:D:122:CYS:HB3	2.51	0.45
1:A:261:TRP:N	1:A:261:TRP:CD1	2.83	0.45
1:A:610:ASP:N	2:J:53:TYR:OH	2.49	0.45
1:C:38:ASN:ND2	1:C:41:GLU:HG3	2.31	0.45
1:A:734:SER:HB2	1:A:860:GLY:HA3	1.95	0.45
1:A:11:LEU:CD2	1:A:187:MET:HE3	2.45	0.45
1:A:67:GLU:H	1:A:67:GLU:HG2	1.15	0.45
1:C:870:VAL:CG1	1:C:871:GLU:N	2.79	0.45
1:D:230:ARG:HG2	1:D:230:ARG:HH11	1.81	0.45
1:B:230:ARG:HG2	1:B:230:ARG:HH11	1.81	0.45
1:B:873:ALA:O	1:B:876:THR:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:881:ARG:HD3	1:A:987:ASP:CG	2.36	0.45
1:C:234:ASP:O	1:C:235:PHE:HB2	2.15	0.45
1:C:242:ALA:O	1:C:290:THR:HA	2.16	0.45
1:A:369:GLU:OE1	3:N:53:GLN:NE2	2.49	0.45
1:B:261:TRP:N	1:B:261:TRP:CD1	2.83	0.45
1:C:226:HIS:CD2	1:C:226:HIS:N	2.83	0.45
1:A:873:ALA:O	1:A:876:THR:HG22	2.16	0.45
1:D:38:ASN:ND2	1:D:41:GLU:HG3	2.32	0.45
1:A:856:TYR:HD2	1:A:864:MET:CE	2.27	0.45
1:A:834:VAL:CG1	1:A:835:LEU:N	2.79	0.45
1:C:531:ARG:CB	1:C:532:PRO:HD2	2.46	0.45
1:C:230:ARG:HG2	1:C:230:ARG:HH11	1.81	0.45
1:D:234:ASP:O	1:D:235:PHE:HB2	2.15	0.45
1:B:908:ASP:HB3	1:B:1007:PHE:CD2	2.51	0.45
1:B:369:GLU:O	1:B:373:VAL:HG23	2.16	0.45
1:C:908:ASP:HB3	1:C:1007:PHE:CD2	2.52	0.45
1:C:254:LEU:C	1:C:255:ARG:HG2	2.36	0.45
1:D:254:LEU:C	1:D:255:ARG:HG2	2.36	0.45
1:A:701:VAL:O	1:A:703:PRO:HD3	2.16	0.45
1:B:227:VAL:HG12	1:B:228:ALA:N	2.31	0.45
1:C:316:HIS:HB2	1:C:321:THR:O	2.16	0.45
1:D:316:HIS:HB2	1:D:321:THR:O	2.16	0.45
1:A:369:GLU:O	1:A:373:VAL:HG23	2.16	0.45
1:D:908:ASP:HB3	1:D:1007:PHE:CD2	2.52	0.45
1:D:242:ALA:O	1:D:290:THR:HA	2.17	0.45
1:D:202:MET:HE3	1:D:357:HIS:CD2	2.52	0.45
1:A:531:ARG:CB	1:A:532:PRO:HD2	2.46	0.45
1:B:531:ARG:CB	1:B:532:PRO:HD2	2.46	0.45
1:A:1018:LEU:HD23	1:A:1018:LEU:HA	1.53	0.45
1:D:694:LEU:HD12	1:D:694:LEU:HA	1.82	0.45
1:D:441:THR:HG22	1:D:474:TRP:CH2	2.51	0.45
1:B:287:ASP:OD2	1:C:425:ARG:NH2	2.50	0.45
1:C:881:ARG:HD3	1:C:987:ASP:CG	2.36	0.45
1:A:352:ARG:O	1:A:385:ASN:HB2	2.17	0.45
1:D:881:ARG:HD3	1:D:987:ASP:CG	2.36	0.45
1:C:441:THR:HG22	1:C:474:TRP:CH2	2.50	0.45
1:B:352:ARG:O	1:B:385:ASN:HB2	2.17	0.45
1:D:226:HIS:CD2	1:D:226:HIS:N	2.83	0.45
1:D:734:SER:HB2	1:D:860:GLY:HA3	1.95	0.45
1:B:77:ASP:C	1:B:78:LEU:HD23	2.37	0.45
1:C:166:ARG:HG3	1:C:392:TYR:CG	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:369:GLU:OE1	3:M:53:GLN:NE2	2.50	0.45
1:A:908:ASP:HB3	1:A:1007:PHE:CD2	2.52	0.45
1:B:915:PHE:O	1:B:916:ASP:HB2	2.17	0.45
1:C:576:ILE:HG13	2:H:53:TYR:HD2	1.78	0.45
1:C:599:ARG:HB2	1:C:600:GLN:H	1.53	0.45
1:A:77:ASP:C	1:A:78:LEU:HD23	2.37	0.45
1:D:3:ILE:O	1:D:3:ILE:HD12	2.16	0.45
1:B:701:VAL:O	1:B:703:PRO:HD3	2.16	0.45
1:D:166:ARG:HG3	1:D:392:TYR:CG	2.51	0.45
1:D:429:ASP:OD1	1:D:431[A]:ARG:HG3	2.16	0.45
1:A:84:VAL:HG13	1:A:85:VAL:N	2.31	0.45
1:C:694:LEU:HA	1:C:694:LEU:HD12	1.82	0.45
1:B:597:ASN:ND2	1:B:599:ARG:N	2.48	0.45
1:C:734:SER:HB2	1:C:860:GLY:HA3	1.95	0.45
1:D:856:TYR:HD2	1:D:864:MET:CE	2.27	0.45
1:B:856:TYR:HD2	1:B:864:MET:CE	2.27	0.45
1:A:685:LEU:CB	1:A:686:PRO:HD2	2.38	0.45
1:C:11:LEU:CD2	1:C:187:MET:HE3	2.42	0.45
1:A:651:LEU:HA	1:A:651:LEU:HD12	1.46	0.45
1:B:67:GLU:H	1:B:67:GLU:HG2	1.15	0.45
1:C:742:THR:CG2	1:C:743:SER:N	2.77	0.45
1:C:429:ASP:OD1	1:C:431[A]:ARG:HG3	2.16	0.45
1:B:168:PRO:O	1:B:442:ARG:NH2	2.48	0.45
1:A:915:PHE:O	1:A:916:ASP:HB2	2.17	0.45
1:A:214:LEU:HD23	1:A:214:LEU:HA	1.61	0.45
1:D:352:ARG:O	1:D:385:ASN:HB2	2.17	0.45
1:C:576:ILE:HG21	2:H:30:THR:CB	2.43	0.45
1:C:362:LEU:HD21	2:H:30:THR:O	2.17	0.45
1:C:856:TYR:HD2	1:C:864:MET:CE	2.27	0.45
1:C:3:ILE:HD12	1:C:3:ILE:O	2.16	0.45
1:D:742:THR:CG2	1:D:743:SER:N	2.77	0.45
1:A:43:ARG:HD2	1:A:261:TRP:CD2	2.52	0.45
1:B:84:VAL:HG13	1:B:85:VAL:N	2.31	0.45
3:L:24:ARG:HA	3:L:69:THR:O	2.17	0.45
1:C:352:ARG:O	1:C:385:ASN:HB2	2.17	0.45
3:M:24:ARG:HA	3:M:69:THR:O	2.17	0.45
1:A:757:GLN:HG2	1:A:758:PHE:N	2.31	0.45
1:B:658:LEU:O	1:B:659:ASP:C	2.54	0.45
1:C:578:TYR:CA	2:H:30:THR:HG21	2.47	0.45
1:C:894:ARG:NH2	1:C:921:PRO:HD3	2.31	0.45
1:D:894:ARG:NH2	1:D:921:PRO:HD3	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:HIS:HA	1:B:396:PRO:HD3	1.83	0.45
1:A:168:PRO:O	1:A:442:ARG:NH2	2.48	0.45
1:C:143:PHE:O	1:C:168:PRO:HA	2.17	0.45
1:D:143:PHE:O	1:D:168:PRO:HA	2.17	0.45
1:B:43:ARG:HD2	1:B:261:TRP:CD2	2.52	0.45
1:B:114:VAL:HA	1:B:115:PRO:HD3	1.77	0.45
1:C:576:ILE:HG22	2:H:30:THR:HB	1.85	0.44
1:B:576:ILE:HG21	2:K:30:THR:C	2.34	0.44
1:D:599:ARG:HB2	1:D:600:GLN:H	1.54	0.44
1:B:685:LEU:CB	1:B:686:PRO:HD2	2.38	0.44
1:B:757:GLN:HG2	1:B:758:PHE:N	2.31	0.44
1:C:86:VAL:HG13	1:C:87:PRO:HA	1.99	0.44
1:D:86:VAL:HG13	1:D:87:PRO:HA	1.99	0.44
1:A:30:HIS:CE1	1:A:33:PHE:CD2	3.06	0.44
1:A:881:ARG:HD3	1:A:987:ASP:OD2	2.18	0.44
2:H:36:TRP:CE2	2:H:80:LEU:HB2	2.53	0.44
1:A:658:LEU:O	1:A:659:ASP:C	2.54	0.44
3:O:24:ARG:HA	3:O:69:THR:O	2.17	0.44
2:J:36:TRP:CE2	2:J:80:LEU:HB2	2.52	0.44
2:I:36:TRP:CE2	2:I:80:LEU:HB2	2.53	0.44
1:B:38:ASN:ND2	1:B:41:GLU:HG3	2.32	0.44
1:B:30:HIS:CE1	1:B:33:PHE:CD2	3.06	0.44
1:B:202:MET:HE3	1:B:357:HIS:CD2	2.52	0.44
1:A:737:ILE:HA	1:A:738:PRO:HD3	1.78	0.44
1:C:395:HIS:HA	1:C:396:PRO:HD3	1.83	0.44
1:B:881:ARG:HD3	1:B:987:ASP:OD2	2.17	0.44
1:C:441:THR:HG22	1:C:474:TRP:CZ3	2.52	0.44
2:K:36:TRP:CE2	2:K:80:LEU:HB2	2.52	0.44
1:B:242:ALA:O	1:B:290:THR:HA	2.16	0.44
1:B:362:LEU:HD21	2:K:31:SER:HA	1.90	0.44
1:C:685:LEU:HA	1:C:686:PRO:HD3	1.84	0.44
1:D:708:TRP:CD1	1:D:708:TRP:N	2.85	0.44
1:C:708:TRP:CD1	1:C:708:TRP:N	2.85	0.44
1:A:870:VAL:CG1	1:A:871:GLU:N	2.79	0.44
1:B:870:VAL:CG1	1:B:871:GLU:N	2.79	0.44
1:C:369:GLU:OE1	3:L:53:GLN:NE2	2.51	0.44
1:D:441:THR:HG22	1:D:474:TRP:CZ3	2.53	0.44
1:A:226:HIS:N	1:A:226:HIS:CD2	2.83	0.44
1:D:378:LEU:HD23	1:D:378:LEU:HA	1.75	0.44
1:B:226:HIS:CD2	1:B:226:HIS:N	2.83	0.44
1:A:360:HIS:HA	1:A:361:PRO:HD3	1.88	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ASN:ND2	1:A:41:GLU:HG3	2.32	0.44
1:D:78:LEU:HB3	1:D:80:GLU:OE1	2.18	0.44
1:B:650:GLU:HA	1:B:701:VAL:O	2.17	0.44
1:D:645:ARG:NH2	1:D:650:GLU:OE2	2.51	0.44
1:D:701:VAL:O	1:D:703:PRO:HD3	2.16	0.44
1:A:786:ARG:HH11	1:A:990:HIS:CE1	2.36	0.44
1:A:395:HIS:HA	1:A:396:PRO:HD3	1.83	0.44
1:B:147:ASN:HA	1:B:148:SER:HA	1.65	0.44
1:C:141:ILE:CG1	1:C:142:ILE:N	2.79	0.44
3:N:24:ARG:HA	3:N:69:THR:O	2.17	0.44
1:D:141:ILE:CG1	1:D:142:ILE:N	2.79	0.44
1:B:584:PRO:HG2	2:K:71:ARG:HH12	1.66	0.44
1:D:685:LEU:HA	1:D:686:PRO:HD3	1.84	0.44
1:B:645:ARG:NH2	1:B:650:GLU:OE2	2.51	0.44
1:A:645:ARG:NH2	1:A:650:GLU:OE2	2.51	0.44
1:C:645:ARG:NH2	1:C:650:GLU:OE2	2.51	0.44
1:C:645:ARG:NH2	1:C:650:GLU:OE1	2.46	0.44
1:D:650:GLU:HA	1:D:701:VAL:O	2.17	0.44
1:D:63:PHE:N	1:D:63:PHE:CD1	2.86	0.44
1:D:43:ARG:HD2	1:D:261:TRP:CD2	2.52	0.44
1:A:242:ALA:O	1:A:290:THR:HA	2.16	0.44
1:C:915:PHE:O	1:C:916:ASP:HB2	2.17	0.44
1:B:433:LEU:HB3	1:B:434:PRO:HD3	1.99	0.44
1:C:78:LEU:HB3	1:C:80:GLU:OE1	2.18	0.44
1:C:701:VAL:O	1:C:703:PRO:HD3	2.16	0.44
1:C:63:PHE:N	1:C:63:PHE:CD1	2.86	0.44
1:D:30:HIS:CE1	1:D:33:PHE:CD2	3.06	0.44
1:C:395:HIS:CG	1:C:396:PRO:HD2	2.53	0.44
1:D:395:HIS:CG	1:D:396:PRO:HD2	2.53	0.44
1:C:43:ARG:HD2	1:C:261:TRP:CD2	2.52	0.44
1:A:114:VAL:HA	1:A:115:PRO:HD3	1.77	0.44
1:C:679:LEU:HD23	1:C:679:LEU:HA	1.13	0.44
1:A:989:PHE:CD1	1:A:989:PHE:N	2.86	0.44
1:D:679:LEU:HA	1:D:679:LEU:HD23	1.13	0.44
1:B:989:PHE:N	1:B:989:PHE:CD1	2.86	0.44
1:B:134:LEU:CD1	1:B:134:LEU:N	2.73	0.44
1:A:650:GLU:HA	1:A:701:VAL:O	2.17	0.44
1:C:650:GLU:HA	1:C:701:VAL:O	2.17	0.44
1:C:30:HIS:CE1	1:C:33:PHE:CD2	3.06	0.44
1:B:742:THR:CG2	1:B:743:SER:H	2.31	0.44
1:D:429:ASP:HA	1:D:430:PRO:HD3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:429:ASP:HA	1:C:430:PRO:HD3	1.82	0.44
1:A:395:HIS:CG	1:A:396:PRO:HD2	2.53	0.44
1:B:1018:LEU:HD23	1:B:1018:LEU:HA	1.53	0.44
1:C:168:PRO:O	1:C:442:ARG:NH2	2.48	0.44
1:D:915:PHE:O	1:D:916:ASP:HB2	2.17	0.44
1:D:424:ASN:HD22	1:D:424:ASN:HA	1.40	0.44
1:B:581:ASN:CB	2:K:72:ASP:OD1	2.56	0.44
1:D:612:THR:HG21	2:I:56:SER:HB3	2.00	0.44
1:A:597:ASN:ND2	1:A:599:ARG:N	2.49	0.44
1:C:79:PRO:HB2	1:C:80:GLU:HG3	2.00	0.44
1:A:78:LEU:HB3	1:A:80:GLU:OE1	2.18	0.44
1:A:742:THR:CG2	1:A:743:SER:H	2.31	0.44
1:B:786:ARG:HH11	1:B:990:HIS:CE1	2.36	0.44
1:B:395:HIS:CG	1:B:396:PRO:HD2	2.53	0.44
1:D:1018:LEU:HA	1:D:1018:LEU:HD23	1.53	0.44
1:D:168:PRO:O	1:D:442:ARG:NH2	2.48	0.44
1:B:214:LEU:HA	1:B:214:LEU:HD23	1.61	0.44
1:D:79:PRO:HB2	1:D:80:GLU:HG3	2.00	0.43
1:A:433:LEU:HB3	1:A:434:PRO:HD3	2.00	0.43
1:D:433:LEU:HB3	1:D:434:PRO:HD3	2.00	0.43
2:I:97:ASN:ND2	2:I:102:TYR:H	2.16	0.43
1:C:757:GLN:HG2	1:C:758:PHE:N	2.31	0.43
1:D:757:GLN:HG2	1:D:758:PHE:N	2.31	0.43
2:H:97:ASN:ND2	2:H:102:TYR:H	2.16	0.43
1:C:378:LEU:HA	1:C:378:LEU:HD23	1.75	0.43
1:B:288:ARG:HD3	1:B:288:ARG:HH11	1.48	0.43
1:C:433:LEU:HB3	1:C:434:PRO:HD3	2.00	0.43
1:D:3:ILE:C	1:D:5:ASP:H	2.22	0.43
1:C:63:PHE:HB3	1:C:64:PRO:CD	2.45	0.43
1:D:822:LEU:HD13	1:D:822:LEU:HA	1.79	0.43
1:C:748:CYS:C	1:C:749:ILE:HD12	2.39	0.43
1:D:230:ARG:NH1	1:D:230:ARG:CG	2.79	0.43
1:A:143:PHE:O	1:A:168:PRO:HA	2.17	0.43
1:B:145:GLY:HA3	1:B:210:ARG:HG3	2.00	0.43
1:A:441:THR:HG22	1:A:474:TRP:CZ3	2.52	0.43
1:B:86:VAL:HG13	1:B:87:PRO:HA	1.99	0.43
1:A:657:ALA:O	1:A:694:LEU:HD12	2.18	0.43
1:B:657:ALA:O	1:B:694:LEU:HD12	2.18	0.43
1:A:86:VAL:HG13	1:A:87:PRO:HA	1.99	0.43
1:C:584:PRO:HB3	2:H:30:THR:HB	1.92	0.43
1:B:78:LEU:HB3	1:B:80:GLU:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:822:LEU:HA	1:C:822:LEU:HD13	1.79	0.43
1:B:737:ILE:HA	1:B:738:PRO:HD3	1.78	0.43
1:D:748:CYS:C	1:D:749:ILE:HD12	2.39	0.43
1:B:441:THR:HG22	1:B:474:TRP:CZ3	2.52	0.43
1:C:881:ARG:HD3	1:C:987:ASP:OD2	2.17	0.43
1:B:787:ALA:HA	1:B:788:PRO:HD3	1.66	0.43
1:D:787:ALA:HA	1:D:788:PRO:HD3	1.66	0.43
1:C:730:LEU:H	1:C:730:LEU:HG	1.41	0.43
1:C:424:ASN:HA	1:C:424:ASN:HD22	1.40	0.43
1:A:840:HIS:N	1:A:840:HIS:ND1	2.67	0.43
1:C:3:ILE:C	1:C:5:ASP:H	2.22	0.43
1:D:63:PHE:HB3	1:D:64:PRO:CD	2.45	0.43
1:C:1018:LEU:HD23	1:C:1018:LEU:HA	1.53	0.43
1:C:230:ARG:CG	1:C:230:ARG:NH1	2.79	0.43
1:A:145:GLY:HA3	1:A:210:ARG:HG3	2.01	0.43
1:C:217:LYS:HB3	1:C:218:PRO:HD2	2.00	0.43
1:C:136:GLU:O	1:C:216:HIS:HE1	2.01	0.43
1:A:288:ARG:HH11	1:A:288:ARG:HD3	1.48	0.43
1:D:576:ILE:HG22	2:I:30:THR:CB	2.34	0.43
1:C:786:ARG:HH11	1:C:990:HIS:CE1	2.36	0.43
1:D:786:ARG:HH11	1:D:990:HIS:CE1	2.36	0.43
1:C:354:VAL:HG22	1:C:355:ASN:N	2.34	0.43
1:B:143:PHE:O	1:B:168:PRO:HA	2.17	0.43
1:D:657:ALA:O	1:D:694:LEU:HD12	2.18	0.43
1:C:657:ALA:O	1:C:694:LEU:HD12	2.18	0.43
1:A:285:TYR:OH	1:D:424:ASN:HB3	2.19	0.43
1:D:136:GLU:O	1:D:216:HIS:HE1	2.01	0.43
1:B:840:HIS:ND1	1:B:840:HIS:N	2.67	0.43
1:A:134:LEU:N	1:A:134:LEU:CD1	2.73	0.43
1:D:354:VAL:HG22	1:D:355:ASN:N	2.34	0.43
1:D:881:ARG:HD3	1:D:987:ASP:OD2	2.18	0.43
1:B:225:PHE:HA	1:B:243:GLU:O	2.19	0.43
1:C:634:GLN:NE2	1:C:682:LEU:O	2.51	0.43
1:D:217:LYS:HB3	1:D:218:PRO:HD2	2.00	0.43
1:D:634:GLN:NE2	1:D:682:LEU:O	2.52	0.43
1:A:362:LEU:HD13	2:J:32:ASP:CA	2.39	0.43
1:A:227:VAL:CG1	1:A:240:LEU:HD11	2.48	0.43
1:B:136:GLU:O	1:B:216:HIS:HE1	2.01	0.43
1:C:787:ALA:HA	1:C:788:PRO:HD3	1.66	0.43
2:J:97:ASN:ND2	2:J:102:TYR:H	2.16	0.43
1:A:225:PHE:HA	1:A:243:GLU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:362:LEU:HD13	2:I:32:ASP:CA	2.38	0.43
1:D:612:THR:HG21	2:I:56:SER:CB	2.48	0.43
1:B:251:ARG:HH11	1:B:251:ARG:CG	2.32	0.43
1:B:354:VAL:HG22	1:B:355:ASN:N	2.34	0.43
2:K:97:ASN:ND2	2:K:102:TYR:H	2.16	0.43
1:C:989:PHE:CD1	1:C:989:PHE:N	2.86	0.43
1:A:721:ARG:HE	1:B:874:SER:CB	2.32	0.43
1:B:79:PRO:HB2	1:B:80:GLU:HG3	2.00	0.43
1:B:227:VAL:CG1	1:B:240:LEU:HD11	2.48	0.43
1:B:257:THR:HA	1:B:270:GLY:O	2.19	0.43
1:A:257:THR:HA	1:A:270:GLY:O	2.19	0.43
1:C:18:ASN:HA	1:C:19:PRO:HD3	1.56	0.43
1:A:251:ARG:CG	1:A:251:ARG:HH11	2.32	0.43
1:B:369:GLU:OE1	3:O:53:GLN:NE2	2.51	0.43
1:B:634:GLN:NE2	1:B:682:LEU:O	2.51	0.43
1:D:989:PHE:CD1	1:D:989:PHE:N	2.86	0.43
1:A:136:GLU:O	1:A:216:HIS:HE1	2.01	0.43
1:B:708:TRP:CD1	1:B:708:TRP:N	2.85	0.43
1:A:748:CYS:C	1:A:749:ILE:HD12	2.39	0.43
1:B:105:TYR:HA	1:B:106:PRO:HD3	1.91	0.43
1:A:217:LYS:HB3	1:A:218:PRO:HD2	2.00	0.43
1:A:634:GLN:NE2	1:A:682:LEU:O	2.51	0.43
1:D:730:LEU:HG	1:D:730:LEU:H	1.41	0.43
1:D:308:LEU:HA	1:D:308:LEU:HD23	1.80	0.43
1:A:612:THR:HG21	2:J:56:SER:CB	2.49	0.42
1:B:576:ILE:HD11	2:K:53:TYR:O	2.19	0.42
1:A:79:PRO:HB2	1:A:80:GLU:HG3	2.00	0.42
1:A:187:MET:HG3	1:A:187:MET:O	2.19	0.42
1:B:187:MET:O	1:B:187:MET:HG3	2.19	0.42
1:B:822:LEU:HD12	1:B:823:LEU:N	2.34	0.42
1:D:18:ASN:HA	1:D:19:PRO:HD3	1.56	0.42
1:A:354:VAL:HG22	1:A:355:ASN:N	2.34	0.42
1:B:635:THR:HA	1:B:680:ILE:O	2.19	0.42
1:A:622:HIS:HD2	1:A:625:GLN:OE1	2.02	0.42
1:B:63:PHE:CD1	1:B:63:PHE:N	2.86	0.42
1:A:822:LEU:HD12	1:A:823:LEU:N	2.34	0.42
1:C:257:THR:HA	1:C:270:GLY:O	2.19	0.42
1:D:257:THR:HA	1:D:270:GLY:O	2.19	0.42
1:B:748:CYS:C	1:B:749:ILE:HD12	2.39	0.42
1:C:682:LEU:HA	1:C:683:PRO:HD3	1.91	0.42
1:B:622:HIS:HD2	1:B:625:GLN:OE1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:GLN:OE1	1:C:200:GLN:N	2.44	0.42
1:A:176:PHE:CD1	1:A:176:PHE:N	2.87	0.42
1:C:578:TYR:CD2	2:H:28:SER:HB3	2.54	0.42
1:A:584:PRO:N	2:J:30:THR:HG22	2.27	0.42
1:B:360:HIS:HE1	1:B:362:LEU:HB2	1.84	0.42
1:A:599:ARG:HB2	1:A:600:GLN:H	1.54	0.42
1:A:708:TRP:N	1:A:708:TRP:CD1	2.85	0.42
1:A:282:ARG:NH1	1:D:418:HIS:O	2.52	0.42
1:B:18:ASN:HA	1:B:19:PRO:HD3	1.56	0.42
1:A:635:THR:HA	1:A:680:ILE:O	2.19	0.42
1:A:787:ALA:HA	1:A:788:PRO:HD3	1.66	0.42
1:A:570:TRP:CD1	1:A:571:VAL:HG22	2.54	0.42
1:A:910:LEU:HD12	1:A:910:LEU:C	2.39	0.42
1:B:176:PHE:N	1:B:176:PHE:CD1	2.87	0.42
1:B:183:ARG:HD3	1:B:183:ARG:HH11	1.55	0.42
1:B:910:LEU:C	1:B:910:LEU:HD12	2.39	0.42
1:A:63:PHE:N	1:A:63:PHE:CD1	2.86	0.42
1:C:67:GLU:HG2	1:C:67:GLU:H	1.15	0.42
1:D:227:VAL:CG1	1:D:228:ALA:N	2.83	0.42
1:C:251:ARG:CG	1:C:251:ARG:HH11	2.32	0.42
1:A:105:TYR:HA	1:A:106:PRO:HD3	1.91	0.42
1:D:145:GLY:HA3	1:D:210:ARG:HG3	2.00	0.42
1:A:124:SER:HA	1:A:184:LEU:O	2.20	0.42
1:B:217:LYS:HB3	1:B:218:PRO:HD2	2.01	0.42
1:D:622:HIS:HD2	1:D:625:GLN:OE1	2.02	0.42
1:B:111:PRO:HA	1:B:112:PRO:HA	1.56	0.42
1:C:472:TYR:O	1:C:476:LYS:HG2	2.20	0.42
1:C:609:ALA:C	2:H:53:TYR:CZ	2.93	0.42
1:A:858:ILE:HG12	1:A:864:MET:HB3	2.02	0.42
1:A:685:LEU:HA	1:A:686:PRO:HD3	1.84	0.42
1:C:11:LEU:N	1:C:11:LEU:HD23	2.35	0.42
1:C:227:VAL:CG1	1:C:228:ALA:N	2.83	0.42
1:B:429:ASP:HA	1:B:430:PRO:HD3	1.82	0.42
1:D:251:ARG:CG	1:D:251:ARG:HH11	2.32	0.42
1:D:105:TYR:HB3	1:D:106:PRO:HD2	2.01	0.42
1:D:472:TYR:O	1:D:476:LYS:HG2	2.20	0.42
1:B:570:TRP:CD1	1:B:571:VAL:HG22	2.54	0.42
1:A:367:MET:HB3	1:A:372:MET:CE	2.50	0.42
1:C:622:HIS:HD2	1:C:625:GLN:OE1	2.02	0.42
1:B:262:GLN:HG2	1:B:262:GLN:O	2.19	0.42
1:C:583:ASN:CG	2:H:72:ASP:HA	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:576:ILE:HD13	1:D:584:PRO:HB2	2.02	0.42
1:C:858:ILE:HG12	1:C:864:MET:HB3	2.02	0.42
1:B:858:ILE:HG12	1:B:864:MET:HB3	2.02	0.42
1:B:7:LEU:HD23	1:B:7:LEU:HA	1.85	0.42
1:D:11:LEU:N	1:D:11:LEU:HD23	2.35	0.42
1:B:702:GLN:HA	1:B:703:PRO:HD3	1.82	0.42
1:D:67:GLU:HG2	1:D:67:GLU:H	1.15	0.42
1:C:227:VAL:CG1	1:C:240:LEU:HD11	2.48	0.42
1:D:227:VAL:CG1	1:D:240:LEU:HD11	2.48	0.42
1:D:878:HIS:HA	1:D:879:PRO:HD3	1.69	0.42
1:C:145:GLY:HA3	1:C:210:ARG:HG3	2.01	0.42
1:D:635:THR:HA	1:D:680:ILE:O	2.19	0.42
1:C:635:THR:HA	1:C:680:ILE:O	2.19	0.42
1:B:124:SER:HA	1:B:184:LEU:O	2.20	0.42
1:D:570:TRP:CD1	1:D:571:VAL:HG22	2.54	0.42
1:A:111:PRO:HA	1:A:112:PRO:HA	1.56	0.42
1:D:176:PHE:N	1:D:176:PHE:CD1	2.87	0.42
1:D:910:LEU:HD12	1:D:910:LEU:C	2.39	0.42
1:D:200:GLN:N	1:D:200:GLN:OE1	2.44	0.42
1:A:262:GLN:O	1:A:262:GLN:HG2	2.19	0.42
1:C:183:ARG:HD3	1:C:183:ARG:HH11	1.55	0.42
1:C:576:ILE:HD13	1:C:584:PRO:HB2	2.02	0.42
1:D:856:TYR:CD1	1:D:856:TYR:N	2.88	0.42
1:D:80:GLU:N	1:D:80:GLU:OE1	2.29	0.42
1:C:187:MET:O	1:C:187:MET:HG3	2.19	0.42
1:D:187:MET:HG3	1:D:187:MET:O	2.19	0.42
1:B:3:ILE:C	1:B:5:ASP:H	2.22	0.42
1:D:682:LEU:HA	1:D:683:PRO:HD3	1.91	0.42
1:C:570:TRP:CD1	1:C:571:VAL:HG22	2.54	0.42
1:B:274:PHE:HB3	1:B:286:ALA:O	2.20	0.42
1:C:367:MET:HB3	1:C:372:MET:CE	2.50	0.42
1:B:407:LEU:HD23	1:B:407:LEU:HA	1.86	0.42
1:C:176:PHE:CD1	1:C:176:PHE:N	2.87	0.42
1:A:360:HIS:HE1	1:A:362:LEU:HB2	1.84	0.42
1:C:856:TYR:CD1	1:C:856:TYR:N	2.88	0.42
1:A:3:ILE:C	1:A:5:ASP:H	2.22	0.42
1:A:429:ASP:HA	1:A:430:PRO:HD3	1.82	0.42
1:C:878:HIS:HA	1:C:879:PRO:HD3	1.69	0.42
1:C:105:TYR:HB3	1:C:106:PRO:HD2	2.01	0.42
1:C:474:TRP:CZ2	1:C:478:VAL:HG21	2.55	0.42
1:D:118:ASN:HA	1:D:119:PRO:HD2	1.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:PHE:HB3	1:A:286:ALA:O	2.20	0.42
1:B:367:MET:HB3	1:B:372:MET:CE	2.50	0.42
1:D:367:MET:HB3	1:D:372:MET:CE	2.50	0.42
1:D:183:ARG:HD3	1:D:183:ARG:HH11	1.56	0.42
1:C:910:LEU:HD12	1:C:910:LEU:C	2.39	0.42
1:D:858:ILE:HG12	1:D:864:MET:HB3	2.02	0.42
1:B:685:LEU:HA	1:B:686:PRO:HD3	1.84	0.42
1:B:645:ARG:NH2	1:B:650:GLU:OE1	2.46	0.42
1:B:822:LEU:HD13	1:B:822:LEU:HA	1.78	0.42
1:C:822:LEU:HD12	1:C:823:LEU:N	2.34	0.42
1:B:227:VAL:CG1	1:B:228:ALA:N	2.83	0.42
1:C:26:ARG:HD2	1:C:169:SER:HB3	2.02	0.42
1:D:26:ARG:HD2	1:D:169:SER:HB3	2.02	0.42
1:D:441:THR:O	1:D:445:GLN:HG3	2.20	0.42
1:D:474:TRP:CZ2	1:D:478:VAL:HG21	2.55	0.42
1:C:441:THR:O	1:C:445:GLN:HG3	2.20	0.42
1:D:225:PHE:HA	1:D:243:GLU:O	2.19	0.42
1:C:214:LEU:HA	1:C:214:LEU:HD23	1.61	0.42
1:B:378:LEU:HD23	1:B:378:LEU:HA	1.75	0.42
1:A:576:ILE:HD13	1:A:584:PRO:HB2	2.02	0.42
1:B:576:ILE:HD13	1:B:584:PRO:HB2	2.02	0.42
1:D:581:ASN:O	2:I:73:THR:N	2.50	0.42
1:D:77:ASP:C	1:D:78:LEU:HD23	2.37	0.42
1:C:77:ASP:C	1:C:78:LEU:HD23	2.37	0.42
1:A:652:LEU:O	1:A:667:GLU:HA	2.20	0.42
1:D:822:LEU:HD12	1:D:823:LEU:N	2.34	0.42
1:A:227:VAL:CG1	1:A:228:ALA:N	2.83	0.42
1:C:118:ASN:HA	1:C:119:PRO:HD2	1.61	0.42
1:C:225:PHE:HA	1:C:243:GLU:O	2.19	0.42
1:C:80:GLU:OE1	1:C:80:GLU:N	2.29	0.41
1:B:78:LEU:HA	1:B:79:PRO:HD2	1.58	0.41
1:B:11:LEU:N	1:B:11:LEU:HD23	2.35	0.41
1:D:652:LEU:O	1:D:667:GLU:HA	2.20	0.41
1:B:652:LEU:O	1:B:667:GLU:HA	2.21	0.41
1:D:124:SER:HA	1:D:184:LEU:O	2.20	0.41
1:D:840:HIS:ND1	1:D:840:HIS:N	2.67	0.41
1:A:617:LEU:HA	1:A:617:LEU:HD12	1.82	0.41
1:D:214:LEU:HD23	1:D:214:LEU:HA	1.61	0.41
1:A:200:GLN:N	1:A:200:GLN:OE1	2.44	0.41
1:C:652:LEU:O	1:C:667:GLU:HA	2.20	0.41
1:A:26:ARG:HD2	1:A:169:SER:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:ILE:HG12	1:B:142:ILE:N	2.35	0.41
1:C:141:ILE:HG12	1:C:142:ILE:N	2.35	0.41
1:D:141:ILE:HG12	1:D:142:ILE:N	2.35	0.41
1:B:892:ALA:HB3	1:B:946:TYR:CE1	2.55	0.41
3:L:83:PHE:CE2	3:L:106:ILE:HB	2.55	0.41
1:A:362:LEU:HD22	2:J:32:ASP:N	2.19	0.41
1:A:11:LEU:HD23	1:A:11:LEU:N	2.35	0.41
1:A:237:ARG:HH11	1:A:237:ARG:HB2	1.85	0.41
1:D:649:ASN:O	1:D:702:GLN:HG3	2.20	0.41
1:B:26:ARG:HD2	1:B:169:SER:HB3	2.02	0.41
2:J:49:GLY:HA2	3:N:94:TRP:CH2	2.56	0.41
1:B:105:TYR:HB3	1:B:106:PRO:HD2	2.01	0.41
1:C:124:SER:HA	1:C:184:LEU:O	2.20	0.41
1:B:441:THR:O	1:B:445:GLN:HG3	2.20	0.41
1:A:441:THR:O	1:A:445:GLN:HG3	2.20	0.41
1:A:141:ILE:HG12	1:A:142:ILE:N	2.35	0.41
1:A:892:ALA:HB3	1:A:946:TYR:CE1	2.55	0.41
3:L:35:TRP:CD2	3:L:73:LEU:HB2	2.55	0.41
3:M:83:PHE:CE2	3:M:106:ILE:HB	2.55	0.41
3:O:31:ASN:O	3:O:50:TYR:HA	2.20	0.41
3:O:35:TRP:CD2	3:O:73:LEU:HB2	2.55	0.41
3:N:31:ASN:O	3:N:50:TYR:HA	2.20	0.41
3:M:35:TRP:CD2	3:M:73:LEU:HB2	2.55	0.41
1:C:840:HIS:ND1	1:C:840:HIS:N	2.67	0.41
1:A:849:LEU:HD23	1:A:849:LEU:N	2.30	0.41
1:A:856:TYR:N	1:A:856:TYR:CD1	2.88	0.41
1:B:80:GLU:CD	1:B:80:GLU:H	2.01	0.41
1:D:906:TYR:CB	1:D:907:PRO:CD	2.99	0.41
1:A:782:ASP:OD1	1:A:854:LYS:NZ	2.52	0.41
1:C:149:ALA:O	1:C:150:PHE:HB3	2.21	0.41
3:N:35:TRP:CD2	3:N:73:LEU:HB2	2.55	0.41
1:A:7:LEU:HA	1:A:7:LEU:HD23	1.85	0.41
1:B:649:ASN:O	1:B:702:GLN:HG3	2.20	0.41
2:K:49:GLY:HA2	3:O:94:TRP:CH2	2.56	0.41
1:A:105:TYR:HB3	1:A:106:PRO:HD2	2.01	0.41
3:L:13:VAL:HG22	3:L:14:THR:N	2.35	0.41
1:B:782:ASP:OD1	1:B:854:LYS:NZ	2.52	0.41
1:C:274:PHE:HB3	1:C:286:ALA:O	2.20	0.41
1:B:578:TYR:CA	2:K:30:THR:HG21	2.48	0.41
2:K:78:TYR:OH	2:K:95:CYS:HB2	2.21	0.41
1:D:609:ALA:C	2:I:53:TYR:CZ	2.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:949:HIS:CD2	1:B:1020:TRP:NE1	2.79	0.41
1:A:949:HIS:CD2	1:A:1020:TRP:NE1	2.79	0.41
1:A:835:LEU:HD12	1:A:857:ARG:HB2	2.03	0.41
1:A:645:ARG:NH2	1:A:650:GLU:OE1	2.46	0.41
1:A:649:ASN:O	1:A:702:GLN:HG3	2.20	0.41
1:C:649:ASN:O	1:C:702:GLN:HG3	2.21	0.41
1:A:63:PHE:HB3	1:A:64:PRO:CD	2.45	0.41
1:C:742:THR:CG2	1:C:743:SER:H	2.31	0.41
1:D:370:GLN:CB	2:I:98:TRP:HH2	2.33	0.41
2:H:49:GLY:HA2	3:L:94:TRP:CH2	2.56	0.41
2:I:49:GLY:HA2	3:M:94:TRP:CH2	2.56	0.41
1:A:474:TRP:CZ2	1:A:478:VAL:HG21	2.55	0.41
1:C:588:TYR:O	1:C:589:GLY:C	2.59	0.41
3:L:31:ASN:O	3:L:50:TYR:HA	2.20	0.41
1:D:588:TYR:O	1:D:589:GLY:C	2.59	0.41
3:N:13:VAL:HG22	3:N:14:THR:N	2.35	0.41
3:O:13:VAL:HG22	3:O:14:THR:N	2.35	0.41
1:A:479:ASP:HA	1:A:480:PRO:HD2	1.73	0.41
1:D:274:PHE:HB3	1:D:286:ALA:O	2.20	0.41
1:A:308:LEU:HA	1:A:308:LEU:HD23	1.80	0.41
1:B:200:GLN:OE1	1:B:200:GLN:N	2.45	0.41
1:D:407:LEU:HD23	1:D:407:LEU:HA	1.86	0.41
1:D:612:THR:HA	1:D:613:PRO:HD3	1.90	0.41
1:B:599:ARG:HB2	1:B:600:GLN:H	1.54	0.41
1:B:856:TYR:CD1	1:B:856:TYR:N	2.88	0.41
1:B:835:LEU:HD12	1:B:857:ARG:HB2	2.03	0.41
1:B:778:THR:HG22	1:B:779:PRO:N	2.35	0.41
1:C:906:TYR:CB	1:C:907:PRO:CD	2.99	0.41
1:B:619:GLU:HA	1:B:912:ALA:HB2	2.03	0.41
1:A:619:GLU:HA	1:A:912:ALA:HB2	2.03	0.41
1:C:970:THR:HG22	1:C:972:HIS:O	2.21	0.41
1:B:868:VAL:HG12	1:B:869:ASP:N	2.36	0.41
3:M:13:VAL:HG22	3:M:14:THR:N	2.36	0.41
1:A:868:VAL:HG12	1:A:869:ASP:N	2.36	0.41
1:D:149:ALA:O	1:D:150:PHE:HB3	2.21	0.41
1:C:578:TYR:HA	1:C:583:ASN:O	2.20	0.41
2:I:78:TYR:OH	2:I:95:CYS:HB2	2.21	0.41
1:A:78:LEU:HA	1:A:79:PRO:HD2	1.58	0.41
1:D:655:MET:O	1:D:696:LEU:HD12	2.21	0.41
1:C:655:MET:O	1:C:696:LEU:HD12	2.21	0.41
1:D:619:GLU:HA	1:D:912:ALA:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:970:THR:HG22	1:D:972:HIS:O	2.21	0.41
1:B:352:ARG:NH2	1:B:641:GLU:OE1	2.54	0.41
1:B:479:ASP:HA	1:B:480:PRO:HD2	1.73	0.41
3:N:11:LEU:HD23	3:N:12:SER:N	2.36	0.41
3:M:31:ASN:O	3:M:50:TYR:HA	2.20	0.41
1:A:380:LYS:HE3	1:A:406:GLY:O	2.21	0.41
1:D:892:ALA:HB3	1:D:946:TYR:CE1	2.56	0.41
1:B:380:LYS:HE3	1:B:406:GLY:O	2.21	0.41
1:D:900:LEU:HA	1:D:900:LEU:HD23	1.83	0.41
1:C:900:LEU:HA	1:C:900:LEU:HD23	1.83	0.41
1:C:578:TYR:CE2	2:H:28:SER:OG	2.51	0.41
2:H:78:TYR:OH	2:H:95:CYS:HB2	2.21	0.41
1:C:612:THR:HA	1:C:613:PRO:HD3	1.90	0.41
1:A:612:THR:HG21	2:J:56:SER:HB3	2.02	0.41
2:J:78:TYR:OH	2:J:95:CYS:HB2	2.21	0.41
1:A:578:TYR:HA	1:A:583:ASN:O	2.20	0.41
1:D:578:TYR:HA	1:D:583:ASN:O	2.20	0.41
1:D:41:GLU:HG2	1:D:46:ARG:NH1	2.35	0.41
1:C:41:GLU:HG2	1:C:46:ARG:NH1	2.35	0.41
1:A:41:GLU:HG2	1:A:46:ARG:NH1	2.35	0.41
1:A:778:THR:HG22	1:A:779:PRO:N	2.35	0.41
1:B:655:MET:O	1:B:696:LEU:HD12	2.21	0.41
1:D:742:THR:CG2	1:D:743:SER:H	2.32	0.41
1:A:202:MET:HE3	1:A:357:HIS:CD2	2.55	0.41
1:C:619:GLU:HA	1:C:912:ALA:HB2	2.03	0.41
1:D:127:PHE:CE1	1:D:184:LEU:HG	2.56	0.41
1:C:127:PHE:CE1	1:C:184:LEU:HG	2.56	0.41
1:B:474:TRP:CZ2	1:B:478:VAL:HG21	2.55	0.41
1:B:287:ASP:CG	1:C:425:ARG:HH22	2.23	0.41
1:A:352:ARG:NH2	1:A:641:GLU:OE1	2.54	0.41
1:C:892:ALA:HB3	1:C:946:TYR:CE1	2.56	0.41
3:O:83:PHE:CE2	3:O:106:ILE:HB	2.55	0.41
1:B:149:ALA:O	1:B:150:PHE:HB3	2.21	0.41
1:A:917:ARG:NH2	1:A:943:GLU:OE2	2.54	0.41
2:K:14:PRO:O	2:K:15:SER:HB3	2.21	0.41
3:O:11:LEU:HD23	3:O:12:SER:N	2.36	0.41
1:B:917:ARG:NH2	1:B:943:GLU:OE2	2.54	0.41
1:A:378:LEU:HD23	1:A:378:LEU:HA	1.75	0.41
1:A:832:ASP:OD1	1:A:832:ASP:N	2.50	0.41
1:C:262:GLN:O	1:C:262:GLN:HG2	2.19	0.41
1:D:617:LEU:HA	1:D:617:LEU:HD12	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:360:HIS:HE1	1:C:362:LEU:HB2	1.84	0.41
1:C:581:ASN:HD22	1:C:583:ASN:ND2	2.19	0.41
1:B:578:TYR:HA	1:B:583:ASN:O	2.20	0.41
1:B:584:PRO:N	2:K:30:THR:CG2	2.79	0.41
1:B:576:ILE:CG1	2:K:53:TYR:HB2	2.48	0.41
1:D:581:ASN:HD22	1:D:583:ASN:ND2	2.19	0.41
1:B:41:GLU:HG2	1:B:46:ARG:NH1	2.35	0.41
1:A:655:MET:O	1:A:696:LEU:HD12	2.21	0.41
1:A:702:GLN:HA	1:A:703:PRO:HD3	1.82	0.41
1:B:63:PHE:HA	1:B:64:PRO:HD3	1.81	0.41
1:A:149:ALA:O	1:A:150:PHE:HB3	2.21	0.41
1:B:472:TYR:O	1:B:476:LYS:HG2	2.20	0.41
3:N:83:PHE:CE2	3:N:106:ILE:HB	2.55	0.41
1:D:262:GLN:O	1:D:262:GLN:HG2	2.19	0.41
1:D:27:LEU:HA	1:D:27:LEU:HD23	1.92	0.41
1:B:849:LEU:N	1:B:849:LEU:HD23	2.30	0.41
1:C:617:LEU:HD12	1:C:617:LEU:HA	1.83	0.41
1:B:279:ILE:HG21	1:B:279:ILE:HD12	1.91	0.41
1:C:27:LEU:HD23	1:C:27:LEU:HA	1.92	0.41
1:C:380:LYS:HE3	1:C:406:GLY:O	2.21	0.41
1:B:69:VAL:HG13	1:B:70:PRO:HD2	2.03	0.40
1:D:380:LYS:HE3	1:D:406:GLY:O	2.21	0.40
1:B:844:HIS:ND1	1:B:845:GLN:HG2	2.36	0.40
1:D:486:TYR:CE2	1:D:488:GLY:HA3	2.56	0.40
1:C:89:ASN:O	1:C:92:MET:HB2	2.22	0.40
1:B:486:TYR:CE2	1:B:488:GLY:HA3	2.56	0.40
2:J:14:PRO:O	2:J:15:SER:HB3	2.21	0.40
1:D:278:ILE:HD13	1:D:278:ILE:N	2.37	0.40
1:B:832:ASP:N	1:B:832:ASP:OD1	2.49	0.40
1:C:278:ILE:N	1:C:278:ILE:HD13	2.37	0.40
1:C:917:ARG:NH2	1:C:943:GLU:OE2	2.54	0.40
1:D:949:HIS:CD2	1:D:1020:TRP:NE1	2.79	0.40
1:A:1020:TRP:HD1	1:A:1021:CYS:H	1.68	0.40
1:B:237:ARG:CB	1:B:237:ARG:NH1	2.79	0.40
1:D:65:ALA:CB	1:D:66:PRO:CD	3.00	0.40
1:A:762:SER:C	1:A:822:LEU:HD23	2.42	0.40
1:B:762:SER:C	1:B:822:LEU:HD23	2.42	0.40
1:A:229:THR:HG22	1:A:240:LEU:HD12	2.04	0.40
1:C:229:THR:HG22	1:C:240:LEU:HD12	2.03	0.40
1:A:69:VAL:HG13	1:A:70:PRO:HD2	2.03	0.40
1:D:917:ARG:NH2	1:D:943:GLU:OE2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:3:GLN:HB2	2:J:25:THR:OG1	2.22	0.40
1:D:844:HIS:ND1	1:D:845:GLN:HG2	2.36	0.40
1:C:868:VAL:HG12	1:C:869:ASP:N	2.36	0.40
2:K:3:GLN:HB2	2:K:25:THR:OG1	2.22	0.40
1:D:868:VAL:HG12	1:D:869:ASP:N	2.36	0.40
1:D:89:ASN:O	1:D:92:MET:HB2	2.22	0.40
1:A:472:TYR:O	1:A:476:LYS:HG2	2.20	0.40
1:C:502:MET:HA	1:C:537:GLU:O	2.22	0.40
1:A:486:TYR:CE2	1:A:488:GLY:HA3	2.56	0.40
1:B:617:LEU:HD12	1:B:617:LEU:HA	1.82	0.40
1:A:581:ASN:HD22	1:A:583:ASN:ND2	2.19	0.40
1:C:949:HIS:CD2	1:C:1020:TRP:NE1	2.78	0.40
1:C:651:LEU:HD12	1:C:651:LEU:HA	1.46	0.40
1:C:65:ALA:CB	1:C:66:PRO:CD	3.00	0.40
1:A:282:ARG:HG3	1:D:423:MET:HB2	2.03	0.40
1:D:524:LEU:O	1:D:561:ARG:NH2	2.50	0.40
1:A:694:LEU:HD12	1:A:694:LEU:HA	1.81	0.40
1:C:844:HIS:ND1	1:C:845:GLN:HG2	2.36	0.40
1:C:486:TYR:CE2	1:C:488:GLY:HA3	2.56	0.40
2:H:14:PRO:O	2:H:15:SER:HB3	2.21	0.40
2:I:14:PRO:O	2:I:15:SER:HB3	2.21	0.40
1:D:502:MET:HA	1:D:537:GLU:O	2.22	0.40
1:C:407:LEU:HD23	1:C:407:LEU:HA	1.87	0.40
1:B:581:ASN:HD22	1:B:583:ASN:ND2	2.19	0.40
1:D:360:HIS:HE1	1:D:362:LEU:HB2	1.84	0.40
1:A:100:TYR:O	1:A:597:ASN:HB2	2.22	0.40
1:A:237:ARG:NH1	1:A:237:ARG:CB	2.79	0.40
1:A:272:ALA:HA	1:A:273:PRO:HD3	1.88	0.40
1:B:229:THR:HG22	1:B:240:LEU:HD12	2.04	0.40
1:C:60:PHE:HA	1:C:122:CYS:O	2.22	0.40
1:D:60:PHE:HA	1:D:122:CYS:O	2.22	0.40
1:D:244:VAL:O	1:D:288:ARG:HA	2.22	0.40
1:C:244:VAL:O	1:C:288:ARG:HA	2.22	0.40
1:A:502:MET:HA	1:A:537:GLU:O	2.22	0.40
1:A:844:HIS:ND1	1:A:845:GLN:HG2	2.36	0.40
2:H:3:GLN:HB2	2:H:25:THR:OG1	2.22	0.40
1:A:173:LEU:HA	1:A:173:LEU:HD23	1.80	0.40
1:A:751:LEU:HD23	1:A:751:LEU:O	2.22	0.40
2:I:3:GLN:HB2	2:I:25:THR:OG1	2.22	0.40
1:D:778:THR:HG22	1:D:779:PRO:N	2.35	0.40
1:C:778:THR:HG22	1:C:779:PRO:N	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:PHE:CB	1:A:64:PRO:CD	2.98	0.40
1:D:229:THR:HG22	1:D:240:LEU:HD12	2.04	0.40
1:B:694:LEU:HD12	1:B:694:LEU:HA	1.82	0.40
1:A:682:LEU:HA	1:A:683:PRO:HD3	1.91	0.40
1:A:89:ASN:O	1:A:92:MET:HB2	2.21	0.40
2:H:13:LYS:O	2:H:16:GLN:HG2	2.22	0.40
1:B:502:MET:HA	1:B:537:GLU:O	2.22	0.40
2:I:13:LYS:O	2:I:16:GLN:HG2	2.22	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 PDB entries followed by that with respect to all EM entries.

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	1026/1024 (100%)	954 (93%)	66 (6%)	6 (1%)	30	74
1	B	1026/1024 (100%)	953 (93%)	67 (6%)	6 (1%)	30	74
1	C	1026/1024 (100%)	953 (93%)	67 (6%)	6 (1%)	30	74
1	D	1026/1024 (100%)	953 (93%)	67 (6%)	6 (1%)	30	74
2	H	112/114 (98%)	109 (97%)	3 (3%)	0	100	100
2	I	112/114 (98%)	109 (97%)	3 (3%)	0	100	100
2	J	112/114 (98%)	109 (97%)	3 (3%)	0	100	100
2	K	112/114 (98%)	109 (97%)	3 (3%)	0	100	100
3	L	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
3	M	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
3	N	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
3	O	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
All	All	4972/4980 (100%)	4657 (94%)	291 (6%)	24 (0%)	38	77

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	647	SER
1	B	647	SER
1	C	647	SER
1	D	647	SER
1	A	77	ASP
1	A	601	PHE
1	B	77	ASP
1	B	601	PHE
1	C	77	ASP
1	C	601	PHE
1	D	77	ASP
1	D	601	PHE
1	A	164	ASP
1	B	164	ASP
1	C	164	ASP
1	D	164	ASP
1	A	690	SER
1	B	690	SER
1	C	690	SER
1	D	690	SER
1	A	10	VAL
1	B	10	VAL
1	C	10	VAL
1	D	10	VAL

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 PDB entries followed by that with respect to all EM entries.

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	880/876 (100%)	754 (86%)	126 (14%)	4 25
1	B	880/876 (100%)	754 (86%)	126 (14%)	4 25
1	C	880/876 (100%)	754 (86%)	126 (14%)	4 25
1	D	880/876 (100%)	754 (86%)	126 (14%)	4 25
2	H	102/102 (100%)	101 (99%)	1 (1%)	82 92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	I	102/102 (100%)	101 (99%)	1 (1%)	82 92
2	J	102/102 (100%)	101 (99%)	1 (1%)	82 92
2	K	102/102 (100%)	101 (99%)	1 (1%)	82 92
3	L	94/94 (100%)	93 (99%)	1 (1%)	80 91
3	M	94/94 (100%)	93 (99%)	1 (1%)	80 91
3	N	94/94 (100%)	93 (99%)	1 (1%)	80 91
3	O	94/94 (100%)	93 (99%)	1 (1%)	80 91
All	All	4304/4288 (100%)	3792 (88%)	512 (12%)	11 31

All (512) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	12	GLN
1	A	24	LEU
1	A	37	ARG
1	A	38	ASN
1	A	39	SER
1	A	49	GLN
1	A	67	GLU
1	A	71	GLU
1	A	72	SER
1	A	80	GLU
1	A	85	VAL
1	A	90	TRP
1	A	102	ASN
1	A	114	VAL
1	A	116	THR
1	A	134	LEU
1	A	135	GLN
1	A	136	GLU
1	A	138	GLN
1	A	148	SER
1	A	169	SER
1	A	187	MET
1	A	190	ARG
1	A	202	MET
1	A	210	ARG
1	A	211	ASP
1	A	214	LEU

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Mol	Chain	Res	Type
1	A	219	THR
1	A	223	SER
1	A	230	ARG
1	A	237	ARG
1	A	246	MET
1	A	249	GLU
1	A	251	ARG
1	A	255	ARG
1	A	259	SER
1	A	269	SER
1	A	277	GLU
1	A	278	ILE
1	A	279	ILE
1	A	282	ARG
1	A	288	ARG
1	A	310	ARG
1	A	322	LEU
1	A	324	GLU
1	A	333	ARG
1	A	347	LYS
1	A	385	ASN
1	A	394	ASN
1	A	424	ASN
1	A	425	ARG
1	A	437	SER
1	A	448	ARG
1	A	473	ARG
1	A	481	SER
1	A	519	SER
1	A	521	LYS
1	A	525	SER
1	A	526	LEU
1	A	529	GLU
1	A	533	LEU
1	A	545	SER
1	A	546	LEU
1	A	554	GLN
1	A	571	VAL
1	A	576	ILE
1	A	580	GLU
1	A	581	ASN
1	A	600	GLN

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Mol	Chain	Res	Type
1	A	645	ARG
1	A	647	SER
1	A	655	MET
1	A	661	LYS
1	A	665	SER
1	A	672	VAL
1	A	675	GLN
1	A	687	GLN
1	A	690	SER
1	A	719	GLN
1	A	721	ARG
1	A	728	VAL
1	A	730	LEU
1	A	734	SER
1	A	737	ILE
1	A	743	SER
1	A	746	ASP
1	A	750	GLU
1	A	755	ARG
1	A	761	GLN
1	A	765	LEU
1	A	766	SER
1	A	768	MET
1	A	770	ILE
1	A	772	ASP
1	A	773	LYS
1	A	774	LYS
1	A	797	GLU
1	A	800	ARG
1	A	801	ILE
1	A	811	LYS
1	A	817	GLN
1	A	822	LEU
1	A	824	GLN
1	A	830	LEU
1	A	843	GLN
1	A	845	GLN
1	A	856	TYR
1	A	857	ARG
1	A	867	THR
1	A	874	SER
1	A	881	ARG

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Mol	Chain	Res	Type
1	A	894	ARG
1	A	917	ARG
1	A	923	SER
1	A	931	PHE
1	A	938	ARG
1	A	950	GLN
1	A	958	ASN
1	A	969	GLU
1	A	986	ILE
1	A	991	MET
1	A	1004	SER
1	A	1006	GLU
1	A	1017	GLN
1	A	1023	LYS
1	B	3	ILE
1	B	12	GLN
1	B	24	LEU
1	B	37	ARG
1	B	38	ASN
1	B	39	SER
1	B	49	GLN
1	B	67	GLU
1	B	71	GLU
1	B	72	SER
1	B	80	GLU
1	B	85	VAL
1	B	90	TRP
1	B	102	ASN
1	B	114	VAL
1	B	116	THR
1	B	134	LEU
1	B	135	GLN
1	B	136	GLU
1	B	138	GLN
1	B	148	SER
1	B	169	SER
1	B	187	MET
1	B	190	ARG
1	B	202	MET
1	B	210	ARG
1	B	211	ASP
1	B	214	LEU

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Mol	Chain	Res	Type
1	B	219	THR
1	B	223	SER
1	B	230	ARG
1	B	237	ARG
1	B	246	MET
1	B	249	GLU
1	B	251	ARG
1	B	255	ARG
1	B	259	SER
1	B	269	SER
1	B	277	GLU
1	B	278	ILE
1	B	279	ILE
1	B	282	ARG
1	B	288	ARG
1	B	310	ARG
1	B	322	LEU
1	B	324	GLU
1	B	333	ARG
1	B	347	LYS
1	B	385	ASN
1	B	394	ASN
1	B	424	ASN
1	B	425	ARG
1	B	437	SER
1	B	448	ARG
1	B	473	ARG
1	B	481	SER
1	B	519	SER
1	B	521	LYS
1	B	525	SER
1	B	526	LEU
1	B	529	GLU
1	B	533	LEU
1	B	545	SER
1	B	546	LEU
1	B	554	GLN
1	B	571	VAL
1	B	576	ILE
1	B	580	GLU
1	B	581	ASN
1	B	600	GLN

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Mol	Chain	Res	Type
1	B	645	ARG
1	B	647	SER
1	B	655	MET
1	B	661	LYS
1	B	665	SER
1	B	672	VAL
1	B	675	GLN
1	B	687	GLN
1	B	690	SER
1	B	719	GLN
1	B	721	ARG
1	B	728	VAL
1	B	730	LEU
1	B	734	SER
1	B	737	ILE
1	B	743	SER
1	B	746	ASP
1	B	750	GLU
1	B	755	ARG
1	B	761	GLN
1	B	765	LEU
1	B	766	SER
1	B	768	MET
1	B	770	ILE
1	B	772	ASP
1	B	773	LYS
1	B	774	LYS
1	B	797	GLU
1	B	800	ARG
1	B	801	ILE
1	B	811	LYS
1	B	817	GLN
1	B	822	LEU
1	B	824	GLN
1	B	830	LEU
1	B	843	GLN
1	B	845	GLN
1	B	856	TYR
1	B	857	ARG
1	B	867	THR
1	B	874	SER
1	B	881	ARG

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Mol	Chain	Res	Type
1	B	894	ARG
1	B	917	ARG
1	B	923	SER
1	B	931	PHE
1	B	938	ARG
1	B	950	GLN
1	B	958	ASN
1	B	969	GLU
1	B	986	ILE
1	B	991	MET
1	B	1004	SER
1	B	1006	GLU
1	B	1017	GLN
1	B	1023	LYS
1	C	3	ILE
1	C	12	GLN
1	C	24	LEU
1	C	37	ARG
1	C	38	ASN
1	C	39	SER
1	C	49	GLN
1	C	67	GLU
1	C	71	GLU
1	C	72	SER
1	C	80	GLU
1	C	85	VAL
1	C	90	TRP
1	C	102	ASN
1	C	114	VAL
1	C	116	THR
1	C	134	LEU
1	C	135	GLN
1	C	136	GLU
1	C	138	GLN
1	C	148	SER
1	C	169	SER
1	C	187	MET
1	C	190	ARG
1	C	202	MET
1	C	210	ARG
1	C	211	ASP
1	C	214	LEU

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Mol	Chain	Res	Type
1	C	219	THR
1	C	223	SER
1	C	230	ARG
1	C	237	ARG
1	C	246	MET
1	C	249	GLU
1	C	251	ARG
1	C	255	ARG
1	C	259	SER
1	C	269	SER
1	C	277	GLU
1	C	278	ILE
1	C	279	ILE
1	C	282	ARG
1	C	288	ARG
1	C	310	ARG
1	C	322	LEU
1	C	324	GLU
1	C	333	ARG
1	C	347	LYS
1	C	385	ASN
1	C	394	ASN
1	C	424	ASN
1	C	425	ARG
1	C	437	SER
1	C	448	ARG
1	C	473	ARG
1	C	481	SER
1	C	519	SER
1	C	521	LYS
1	C	525	SER
1	C	526	LEU
1	C	529	GLU
1	C	533	LEU
1	C	545	SER
1	C	546	LEU
1	C	554	GLN
1	C	571	VAL
1	C	576	ILE
1	C	580	GLU
1	C	581	ASN
1	C	600	GLN

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Mol	Chain	Res	Type
1	C	645	ARG
1	C	647	SER
1	C	655	MET
1	C	661	LYS
1	C	665	SER
1	C	672	VAL
1	C	675	GLN
1	C	687	GLN
1	C	690	SER
1	C	719	GLN
1	C	721	ARG
1	C	728	VAL
1	C	730	LEU
1	C	734	SER
1	C	737	ILE
1	C	743	SER
1	C	746	ASP
1	C	750	GLU
1	C	755	ARG
1	C	761	GLN
1	C	765	LEU
1	C	766	SER
1	C	768	MET
1	C	770	ILE
1	C	772	ASP
1	C	773	LYS
1	C	774	LYS
1	C	797	GLU
1	C	800	ARG
1	C	801	ILE
1	C	811	LYS
1	C	817	GLN
1	C	822	LEU
1	C	824	GLN
1	C	830	LEU
1	C	843	GLN
1	C	845	GLN
1	C	856	TYR
1	C	857	ARG
1	C	867	THR
1	C	874	SER
1	C	881	ARG

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Mol	Chain	Res	Type
1	C	894	ARG
1	C	917	ARG
1	C	923	SER
1	C	931	PHE
1	C	938	ARG
1	C	950	GLN
1	C	958	ASN
1	C	969	GLU
1	C	986	ILE
1	C	991	MET
1	C	1004	SER
1	C	1006	GLU
1	C	1017	GLN
1	C	1023	LYS
1	D	3	ILE
1	D	12	GLN
1	D	24	LEU
1	D	37	ARG
1	D	38	ASN
1	D	39	SER
1	D	49	GLN
1	D	67	GLU
1	D	71	GLU
1	D	72	SER
1	D	80	GLU
1	D	85	VAL
1	D	90	TRP
1	D	102	ASN
1	D	114	VAL
1	D	116	THR
1	D	134	LEU
1	D	135	GLN
1	D	136	GLU
1	D	138	GLN
1	D	148	SER
1	D	169	SER
1	D	187	MET
1	D	190	ARG
1	D	202	MET
1	D	210	ARG
1	D	211	ASP
1	D	214	LEU

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Mol	Chain	Res	Type
1	D	219	THR
1	D	223	SER
1	D	230	ARG
1	D	237	ARG
1	D	246	MET
1	D	249	GLU
1	D	251	ARG
1	D	255	ARG
1	D	259	SER
1	D	269	SER
1	D	277	GLU
1	D	278	ILE
1	D	279	ILE
1	D	282	ARG
1	D	288	ARG
1	D	310	ARG
1	D	322	LEU
1	D	324	GLU
1	D	333	ARG
1	D	347	LYS
1	D	385	ASN
1	D	394	ASN
1	D	424	ASN
1	D	425	ARG
1	D	437	SER
1	D	448	ARG
1	D	473	ARG
1	D	481	SER
1	D	519	SER
1	D	521	LYS
1	D	525	SER
1	D	526	LEU
1	D	529	GLU
1	D	533	LEU
1	D	545	SER
1	D	546	LEU
1	D	554	GLN
1	D	571	VAL
1	D	576	ILE
1	D	580	GLU
1	D	581	ASN
1	D	600	GLN

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Mol	Chain	Res	Type
1	D	645	ARG
1	D	647	SER
1	D	655	MET
1	D	661	LYS
1	D	665	SER
1	D	672	VAL
1	D	675	GLN
1	D	687	GLN
1	D	690	SER
1	D	719	GLN
1	D	721	ARG
1	D	728	VAL
1	D	730	LEU
1	D	734	SER
1	D	737	ILE
1	D	743	SER
1	D	746	ASP
1	D	750	GLU
1	D	755	ARG
1	D	761	GLN
1	D	765	LEU
1	D	766	SER
1	D	768	MET
1	D	770	ILE
1	D	772	ASP
1	D	773	LYS
1	D	774	LYS
1	D	797	GLU
1	D	800	ARG
1	D	801	ILE
1	D	811	LYS
1	D	817	GLN
1	D	822	LEU
1	D	824	GLN
1	D	830	LEU
1	D	843	GLN
1	D	845	GLN
1	D	856	TYR
1	D	857	ARG
1	D	867	THR
1	D	874	SER
1	D	881	ARG

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Mol	Chain	Res	Type
1	D	894	ARG
1	D	917	ARG
1	D	923	SER
1	D	931	PHE
1	D	938	ARG
1	D	950	GLN
1	D	958	ASN
1	D	969	GLU
1	D	986	ILE
1	D	991	MET
1	D	1004	SER
1	D	1006	GLU
1	D	1017	GLN
1	D	1023	LYS
2	H	97	ASN
2	I	97	ASN
2	J	97	ASN
2	K	97	ASN
3	L	76	ASN
3	M	76	ASN
3	N	76	ASN
3	O	76	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (115) 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	163	GLN
1	A	216	HIS
1	A	226	HIS
1	A	316	HIS
1	A	357	HIS
1	A	385	ASN
1	A	394	ASN
1	A	424	ASN
1	A	467	ASN
1	A	554	GLN
1	A	581	ASN
1	A	597	ASN

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Mol	Chain	Res	Type
1	A	604	ASN
1	A	622	HIS
1	A	634	GLN
1	A	817	GLN
1	A	890	GLN
1	A	949	HIS
1	A	990	HIS
1	A	1017	GLN
1	B	38	ASN
1	B	50	GLN
1	B	102	ASN
1	B	128	ASN
1	B	163	GLN
1	B	216	HIS
1	B	226	HIS
1	B	316	HIS
1	B	357	HIS
1	B	385	ASN
1	B	394	ASN
1	B	424	ASN
1	B	467	ASN
1	B	554	GLN
1	B	581	ASN
1	B	597	ASN
1	B	604	ASN
1	B	622	HIS
1	B	634	GLN
1	B	817	GLN
1	B	890	GLN
1	B	949	HIS
1	B	990	HIS
1	B	1017	GLN
1	C	38	ASN
1	C	50	GLN
1	C	102	ASN
1	C	128	ASN
1	C	216	HIS
1	C	226	HIS
1	C	316	HIS
1	C	357	HIS
1	C	385	ASN
1	C	394	ASN

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Mol	Chain	Res	Type
1	C	424	ASN
1	C	467	ASN
1	C	554	GLN
1	C	581	ASN
1	C	597	ASN
1	C	604	ASN
1	C	622	HIS
1	C	634	GLN
1	C	817	GLN
1	C	890	GLN
1	C	949	HIS
1	C	990	HIS
1	C	1017	GLN
1	D	38	ASN
1	D	50	GLN
1	D	102	ASN
1	D	128	ASN
1	D	216	HIS
1	D	226	HIS
1	D	316	HIS
1	D	357	HIS
1	D	385	ASN
1	D	394	ASN
1	D	424	ASN
1	D	467	ASN
1	D	554	GLN
1	D	581	ASN
1	D	597	ASN
1	D	604	ASN
1	D	622	HIS
1	D	634	GLN
1	D	817	GLN
1	D	890	GLN
1	D	949	HIS
1	D	990	HIS
1	D	1017	GLN
2	H	5	GLN
2	H	76	ASN
2	H	77	GLN
2	H	97	ASN
2	I	5	GLN
2	I	76	ASN

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Mol	Chain	Res	Type
2	I	77	GLN
2	I	97	ASN
2	J	5	GLN
2	J	76	ASN
2	J	77	GLN
2	J	97	ASN
2	K	5	GLN
2	K	76	ASN
2	K	77	GLN
2	K	97	ASN
3	L	53	GLN
3	L	76	ASN
3	M	76	ASN
3	N	76	ASN
3	O	76	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.