



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 11:14 PM UTC

PDB ID : 4CKD / pdb_00004ckd
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 initial model : 1F4A

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

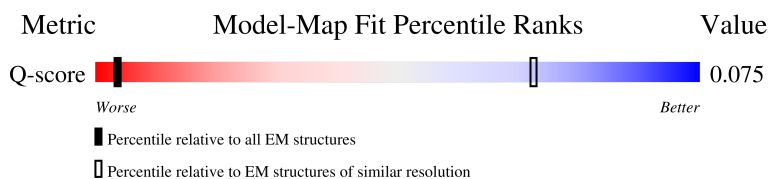
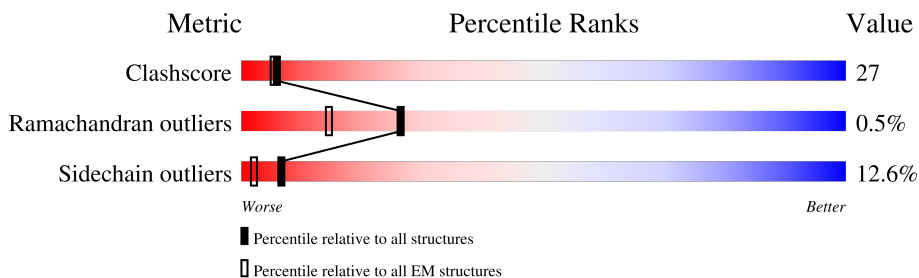
1 Overall quality at a glance i

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	65 (12.50 - 13.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1024	
1	B	1024	
1	C	1024	
1	D	1024	

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Mol	Chain	Length	Quality of chain
2	H	114	
2	I	114	
2	J	114	
2	K	114	
3	L	107	
3	M	107	
3	N	107	
3	O	107	

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		

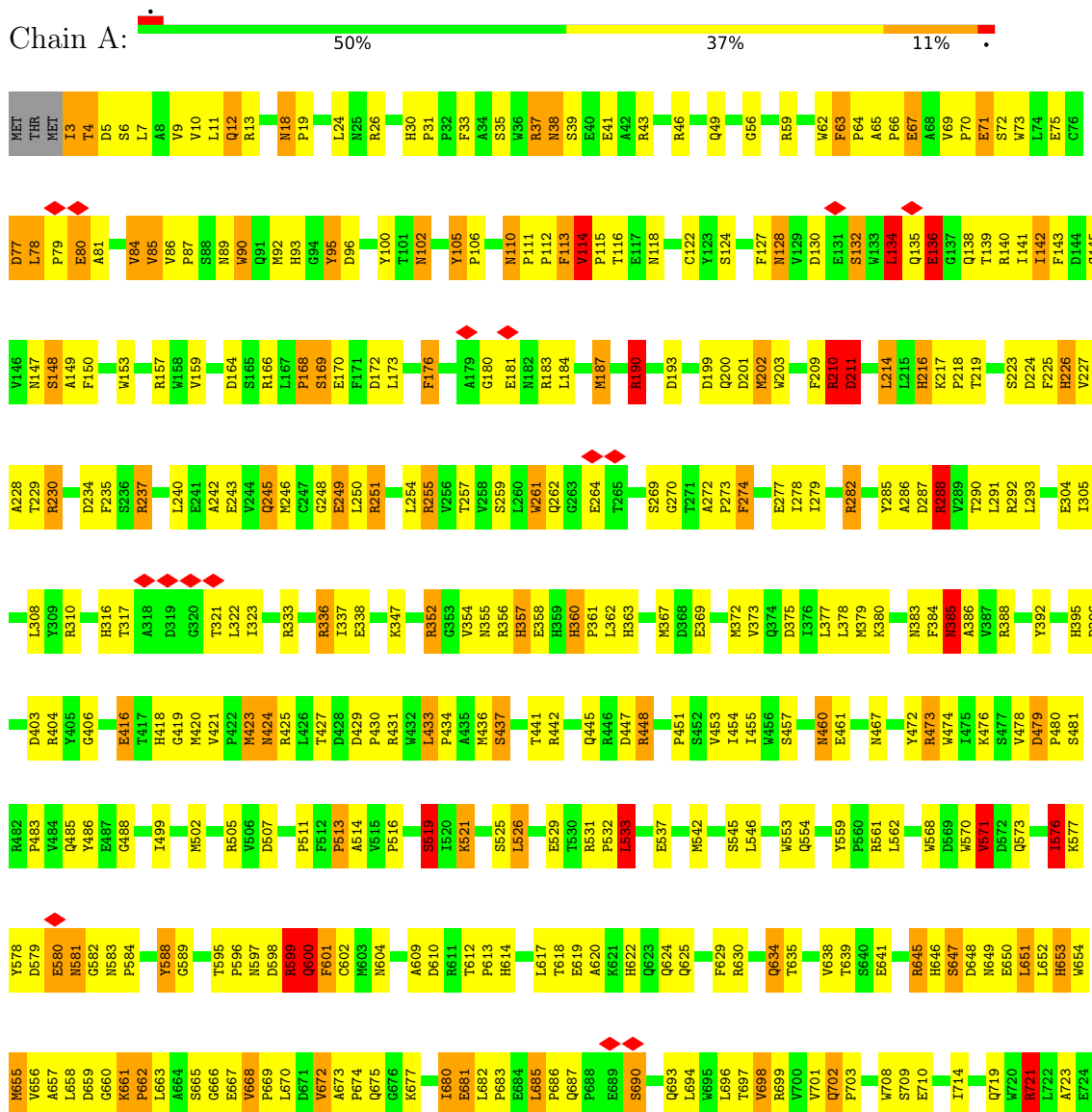
- Molecule 3 is a protein called SCFV13R4 ANTIBODY FV LIGHT CHAIN.

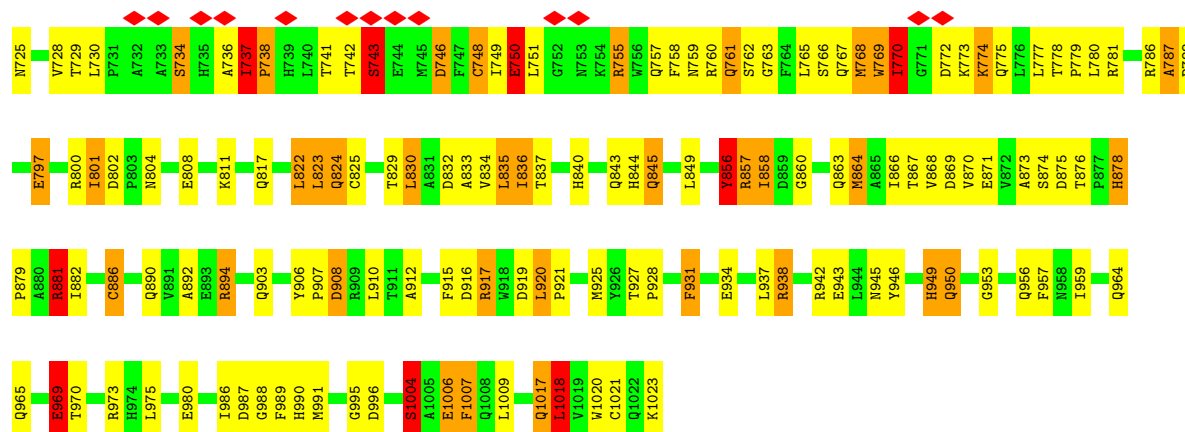
Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	107	Total	C	N	O	S	0	0
			818	511	137	167	3		
3	M	107	Total	C	N	O	S	0	0
			818	511	137	167	3		
3	N	107	Total	C	N	O	S	0	0
			818	511	137	167	3		
3	O	107	Total	C	N	O	S	0	0
			818	511	137	167	3		

3 Residue-property plots

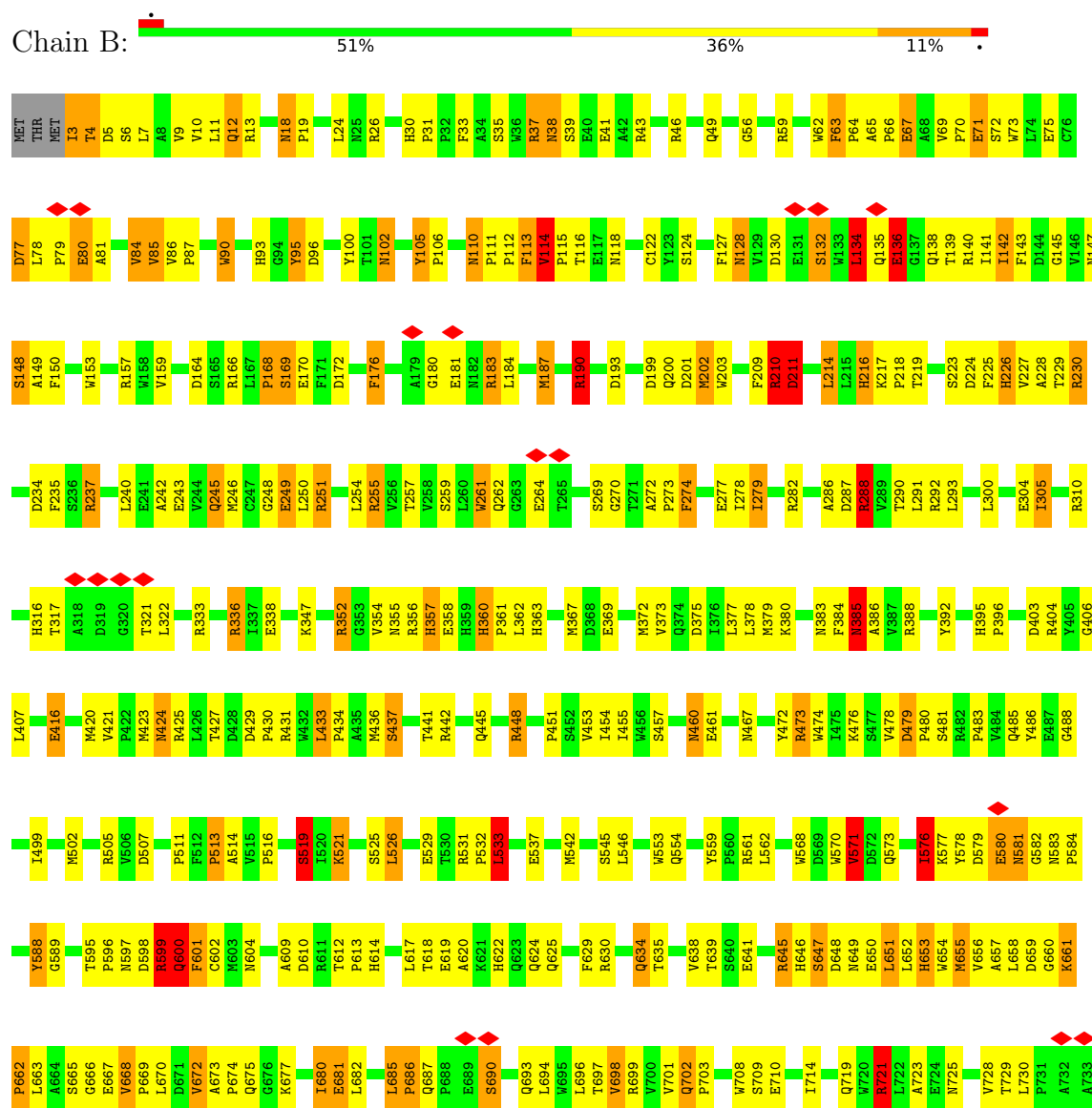
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

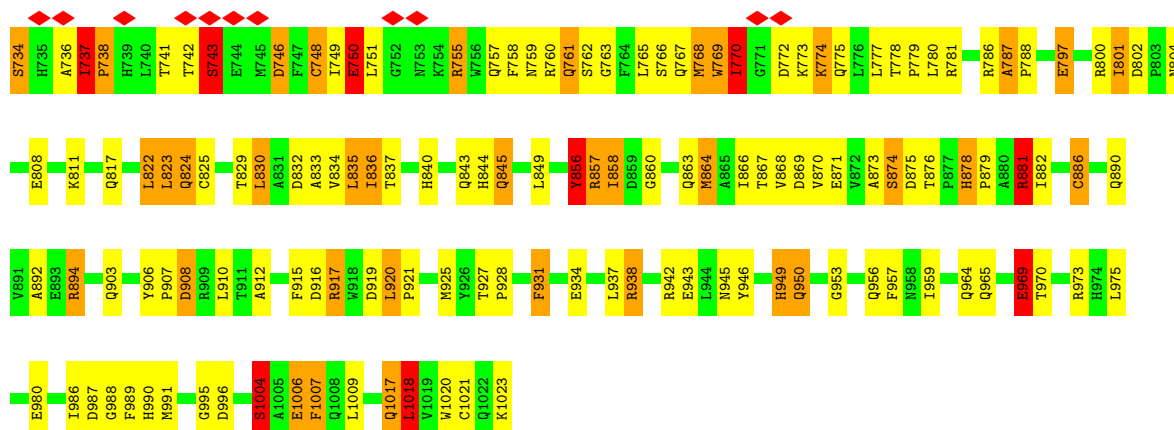
• Molecule 1: BETA-GALACTOSIDASE



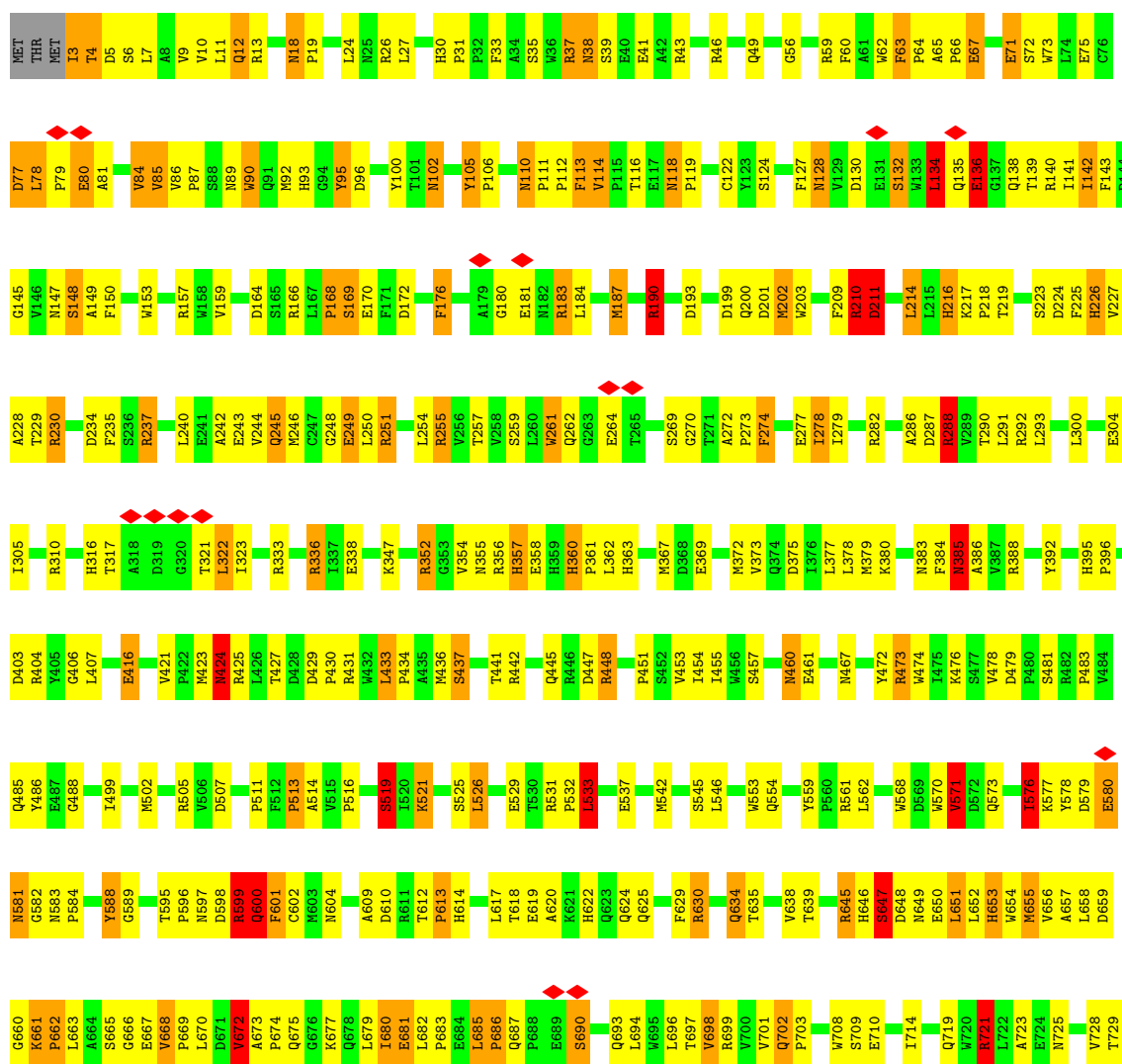


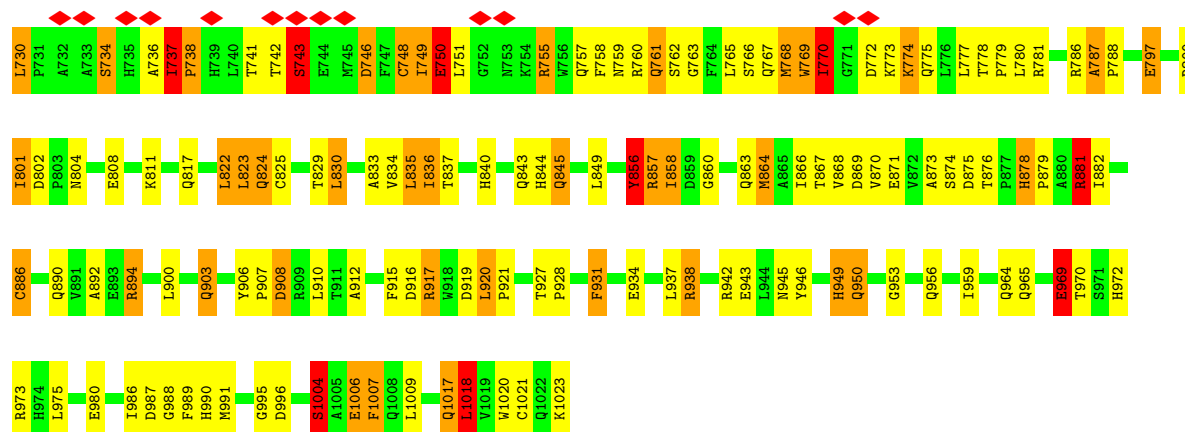
• Molecule 1: BETA-GALACTOSIDASE



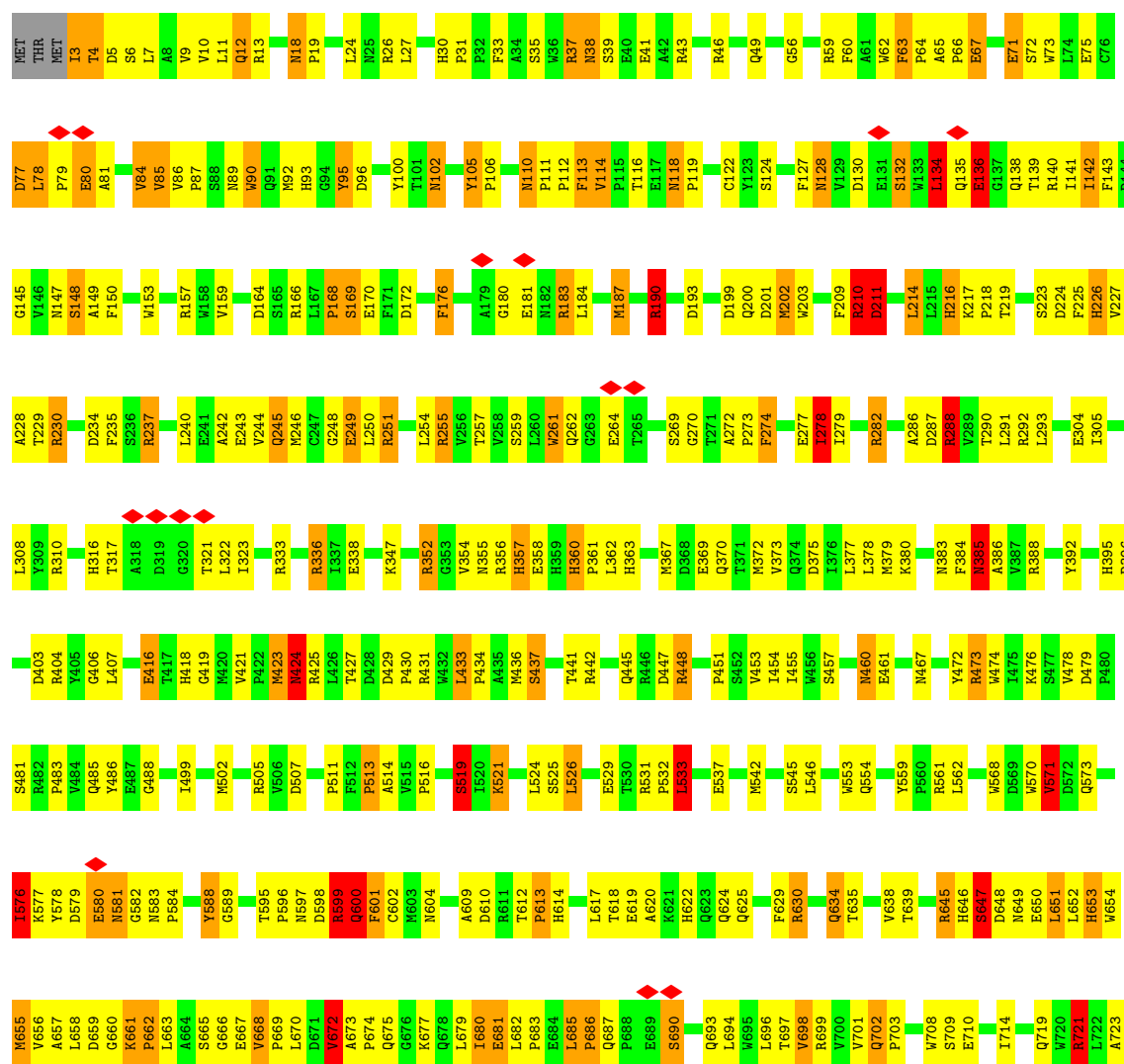


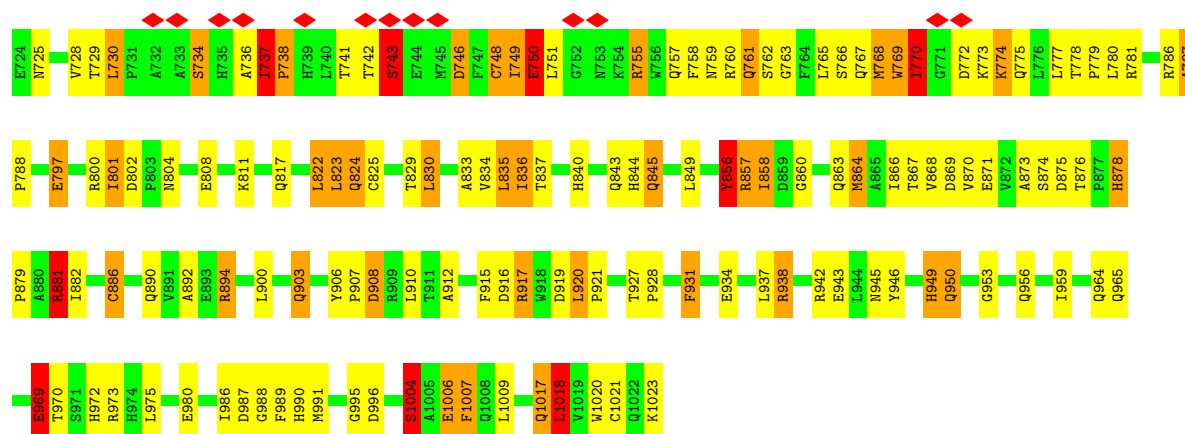
• Molecule 1: BETA-GALACTOSIDASE



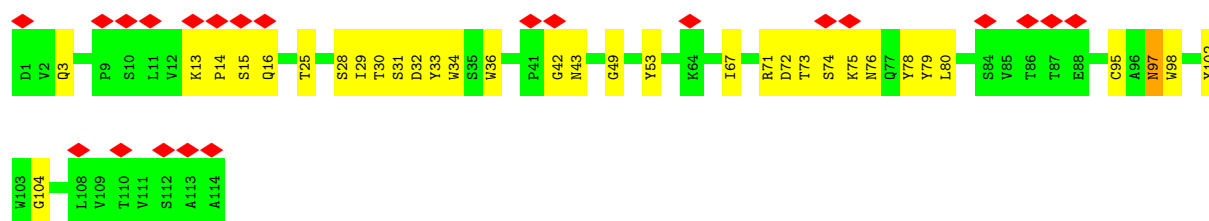


• Molecule 1: BETA-GALACTOSIDASE

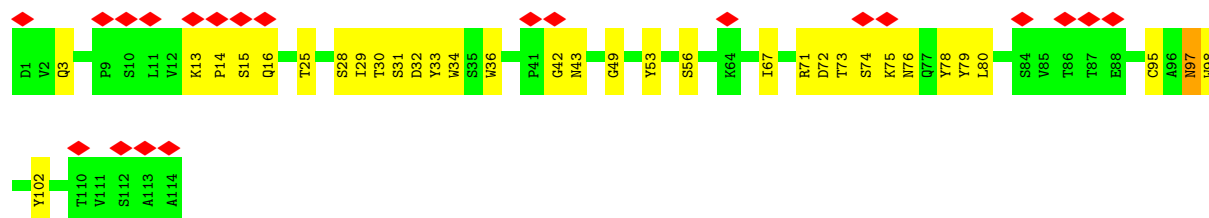




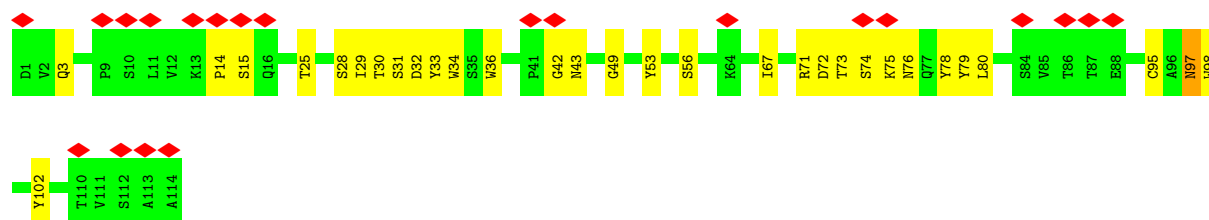
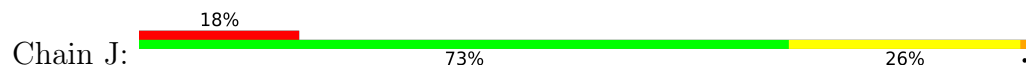
• Molecule 2: SCFV13R4 ANTIBODY FV HEAVY CHAIN



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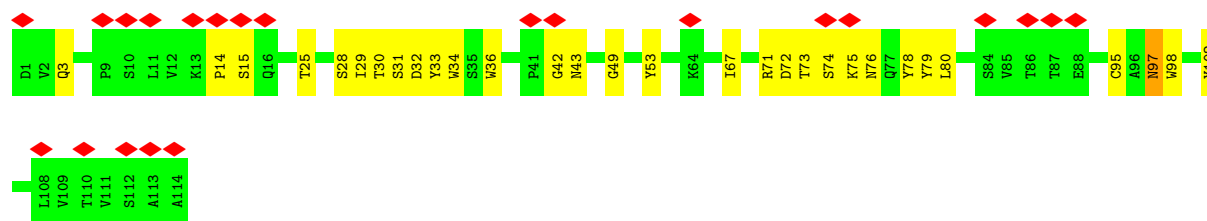


• Molecule 2: SCFV13R4 ANTIBODY FV HEAVY CHAIN

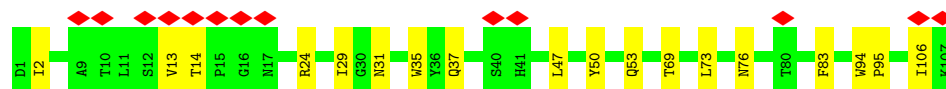
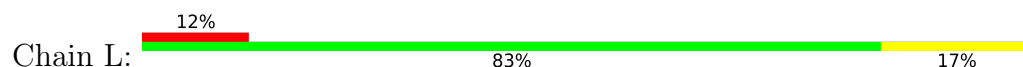


• Molecule 2: SCFV13R4 ANTIBODY FV HEAVY CHAIN

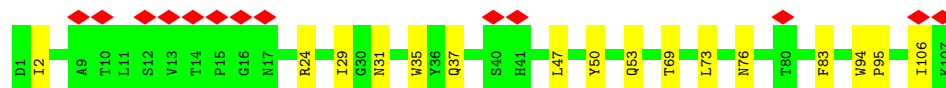
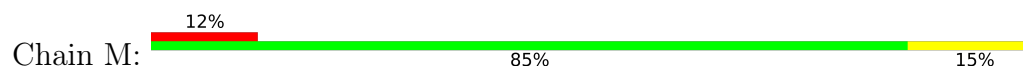




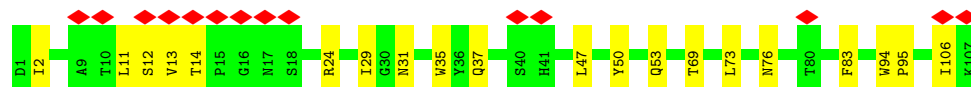
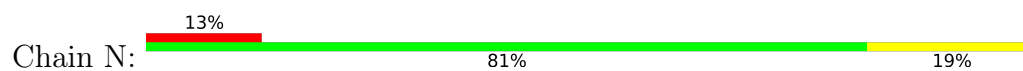
• Molecule 3: SCFV13R4 ANTIBODY FV LIGHT CHAIN



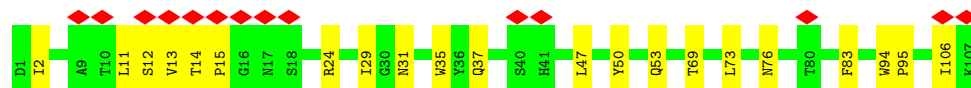
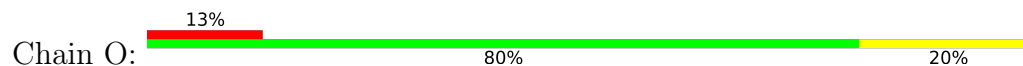
• Molecule 3: SCFV13R4 ANTIBODY FV LIGHT CHAIN



• Molecule 3: SCFV13R4 ANTIBODY FV LIGHT CHAIN



• Molecule 3: SCFV13R4 ANTIBODY FV LIGHT CHAIN



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D2	Depositor
Number of particles used	2965	Depositor
Resolution determination method	Not provided	
CTF correction method	DONE INSIDE FREALIGN	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	67	Depositor
Minimum defocus (nm)	2678	Depositor
Maximum defocus (nm)	4027	Depositor
Magnification	81600	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.322	Depositor
Minimum map value	-0.057	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.046	Depositor
Recommended contour level	0.13	Depositor
Map size ($\text{\AA}$)	300.0, 300.0, 300.0	wwPDB
Map dimensions	100, 100, 100	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	3.0, 3.0, 3.0	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 > 5$	RMSZ	# $ Z > 5$
1	A	1.34	18/8515 (0.2%)	1.82	168/11615 (1.4%)
1	B	1.34	17/8515 (0.2%)	1.82	166/11615 (1.4%)
1	C	1.34	17/8515 (0.2%)	1.82	170/11615 (1.5%)
1	D	1.34	18/8515 (0.2%)	1.82	167/11615 (1.4%)
2	H	0.32	0/925	0.90	3/1263 (0.2%)
2	I	0.32	0/925	0.89	2/1263 (0.2%)
2	J	0.32	0/925	0.89	2/1263 (0.2%)
2	K	0.32	0/925	0.89	2/1263 (0.2%)
3	L	0.31	0/837	0.77	0/1133
3	M	0.31	0/837	0.77	0/1133
3	N	0.31	0/837	0.77	0/1133
3	O	0.31	0/837	0.77	0/1133
All	All	1.23	70/41108 (0.2%)	1.70	680/56044 (1.2%)

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	479	ASP	C-N	-9.15	1.25	1.34
1	B	479	ASP	C-N	-9.15	1.25	1.34
1	A	479	ASP	C-N	-9.13	1.25	1.34
1	C	479	ASP	C-N	-9.03	1.25	1.34
1	A	249	GLU	CA-C	-8.01	1.42	1.52
1	D	249	GLU	CA-C	-8.00	1.42	1.52
1	C	249	GLU	CA-C	-7.98	1.42	1.52
1	B	249	GLU	CA-C	-7.91	1.43	1.52
1	A	521	LYS	C-O	-7.83	1.15	1.24
1	B	521	LYS	C-O	-7.82	1.15	1.24
1	D	521	LYS	C-O	-7.80	1.15	1.24
1	C	521	LYS	C-O	-7.78	1.15	1.24
1	A	668	VAL	C-N	-6.20	1.26	1.33
1	C	835	LEU	N-CA	-6.19	1.39	1.46
1	C	668	VAL	C-N	-6.18	1.26	1.33
1	B	668	VAL	C-N	-6.17	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	835	LEU	N-CA	-6.12	1.39	1.46
1	D	668	VAL	C-N	-6.12	1.26	1.33
1	D	835	LEU	N-CA	-6.10	1.39	1.46
1	B	835	LEU	N-CA	-6.07	1.39	1.46
1	C	118	ASN	N-CA	-5.96	1.41	1.46
1	B	118	ASN	N-CA	-5.95	1.41	1.46
1	C	261	TRP	CA-C	-5.92	1.45	1.52
1	A	118	ASN	N-CA	-5.92	1.41	1.46
1	D	118	ASN	N-CA	-5.88	1.41	1.46
1	A	261	TRP	CA-C	-5.88	1.45	1.52
1	B	261	TRP	CA-C	-5.85	1.45	1.52
1	D	261	TRP	CA-C	-5.80	1.46	1.52
1	A	681	GLU	CA-C	-5.76	1.45	1.52
1	C	681	GLU	CA-C	-5.74	1.45	1.52
1	D	681	GLU	CA-C	-5.72	1.45	1.52
1	B	723	ALA	CA-C	-5.72	1.45	1.52
1	D	723	ALA	CA-C	-5.72	1.45	1.52
1	B	681	GLU	CA-C	-5.71	1.45	1.52
1	A	723	ALA	CA-C	-5.69	1.45	1.52
1	B	75	GLU	CD-OE2	5.66	1.36	1.25
1	A	75	GLU	CD-OE2	5.66	1.36	1.25
1	D	75	GLU	CD-OE2	5.64	1.36	1.25
1	C	723	ALA	CA-C	-5.63	1.45	1.52
1	C	75	GLU	CD-OE2	5.61	1.36	1.25
1	B	113	PHE	CA-C	-5.57	1.45	1.52
1	A	113	PHE	CA-C	-5.55	1.45	1.52
1	C	113	PHE	CA-C	-5.53	1.45	1.52
1	D	113	PHE	CA-C	-5.50	1.45	1.52
1	D	521	LYS	C-N	-5.50	1.26	1.34
1	B	521	LYS	C-N	-5.49	1.26	1.34
1	C	521	LYS	C-N	-5.46	1.26	1.34
1	A	521	LYS	C-N	-5.44	1.26	1.34
1	C	261	TRP	C-N	-5.27	1.26	1.33
1	D	261	TRP	C-N	-5.26	1.26	1.33
1	D	662	PRO	CA-C	-5.26	1.46	1.52
1	B	261	TRP	C-N	-5.25	1.26	1.33
1	C	662	PRO	CA-C	-5.24	1.46	1.52
1	B	662	PRO	CA-C	-5.24	1.46	1.52
1	A	662	PRO	CA-C	-5.22	1.46	1.52
1	A	261	TRP	C-N	-5.19	1.27	1.33
1	D	78	LEU	CA-C	-5.10	1.48	1.52
1	B	738	PRO	N-CA	-5.08	1.41	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	250	LEU	N-CA	-5.08	1.39	1.46
1	A	250	LEU	N-CA	-5.08	1.40	1.46
1	D	738	PRO	N-CA	-5.07	1.41	1.47
1	D	250	LEU	N-CA	-5.07	1.40	1.46
1	A	738	PRO	N-CA	-5.05	1.41	1.47
1	A	337	ILE	CA-CB	-5.04	1.48	1.54
1	A	78	LEU	CA-C	-5.03	1.48	1.52
1	D	749	ILE	N-CA	-5.03	1.40	1.46
1	B	250	LEU	N-CA	-5.03	1.40	1.46
1	C	78	LEU	CA-C	-5.02	1.48	1.52
1	C	738	PRO	N-CA	-5.02	1.41	1.47
1	B	305	ILE	CA-CB	-5.01	1.47	1.54

All (680) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	VAL	N-CA-CB	-14.10	102.10	111.83
1	B	114	VAL	N-CA-CB	-14.09	102.11	111.83
1	C	114	VAL	N-CA-CB	-14.08	102.11	111.83
1	D	114	VAL	N-CA-CB	-14.07	102.12	111.83
1	B	385	ASN	CB-CA-C	-12.07	89.47	109.03
1	D	385	ASN	CB-CA-C	-12.05	89.51	109.03
1	C	385	ASN	CB-CA-C	-12.04	89.52	109.03
1	A	385	ASN	CB-CA-C	-12.02	89.56	109.03
1	C	423	MET	CA-C-N	11.14	136.33	120.28
1	C	423	MET	C-N-CA	11.14	136.33	120.28
1	A	423	MET	CA-C-N	11.05	136.19	120.28
1	A	423	MET	C-N-CA	11.05	136.19	120.28
1	B	423	MET	CA-C-N	11.05	136.19	120.28
1	B	423	MET	C-N-CA	11.05	136.19	120.28
1	D	423	MET	CA-C-N	11.05	136.19	120.28
1	D	423	MET	C-N-CA	11.05	136.19	120.28
1	C	385	ASN	N-CA-CB	-10.52	96.60	110.59
1	A	385	ASN	N-CA-CB	-10.51	96.62	110.59
1	D	385	ASN	N-CA-CB	-10.50	96.63	110.59
1	B	385	ASN	N-CA-CB	-10.48	96.65	110.59
1	C	249	GLU	N-CA-CB	10.35	127.24	110.16
1	B	249	GLU	N-CA-CB	10.35	127.24	110.16
1	D	249	GLU	N-CA-CB	10.34	127.22	110.16
1	A	249	GLU	N-CA-CB	10.34	127.21	110.16
1	A	424	ASN	CB-CA-C	-9.98	92.17	110.63
1	B	424	ASN	CB-CA-C	-9.97	92.18	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	424	ASN	CB-CA-C	-9.97	92.19	110.63
1	C	424	ASN	CB-CA-C	-9.95	92.23	110.63
1	D	248	GLY	CA-C-N	-9.52	108.77	122.19
1	D	248	GLY	C-N-CA	-9.52	108.77	122.19
1	A	248	GLY	CA-C-N	-9.49	108.81	122.19
1	A	248	GLY	C-N-CA	-9.49	108.81	122.19
1	C	248	GLY	CA-C-N	-9.47	108.84	122.19
1	C	248	GLY	C-N-CA	-9.47	108.84	122.19
1	B	248	GLY	CA-C-N	-9.47	108.84	122.19
1	B	248	GLY	C-N-CA	-9.47	108.84	122.19
1	A	224	ASP	CA-CB-CG	8.90	121.50	112.60
1	D	224	ASP	CA-CB-CG	8.88	121.48	112.60
1	C	224	ASP	CA-CB-CG	8.87	121.47	112.60
1	B	224	ASP	CA-CB-CG	8.86	121.46	112.60
1	D	363	HIS	CA-CB-CG	-8.79	105.01	113.80
1	C	363	HIS	CA-CB-CG	-8.78	105.02	113.80
1	A	363	HIS	CA-CB-CG	-8.76	105.04	113.80
1	B	363	HIS	CA-CB-CG	-8.72	105.08	113.80
1	C	931	PHE	CB-CA-C	8.64	118.22	110.44
1	D	931	PHE	CB-CA-C	8.64	118.22	110.44
1	A	931	PHE	CB-CA-C	8.62	118.20	110.44
1	B	931	PHE	CB-CA-C	8.56	118.15	110.44
1	D	903[A]	GLN	N-CA-C	8.11	121.50	110.55
1	D	903[B]	GLN	N-CA-C	8.11	121.50	110.55
1	C	903[A]	GLN	N-CA-C	8.07	121.45	110.55
1	C	903[B]	GLN	N-CA-C	8.07	121.45	110.55
1	A	903[A]	GLN	N-CA-C	8.04	121.41	110.55
1	A	903[B]	GLN	N-CA-C	8.04	121.41	110.55
1	B	903[A]	GLN	N-CA-C	8.03	121.39	110.55
1	B	903[B]	GLN	N-CA-C	8.03	121.39	110.55
1	A	787	ALA	CA-C-N	7.97	129.81	119.84
1	A	787	ALA	C-N-CA	7.97	129.81	119.84
1	C	787	ALA	CA-C-N	7.94	129.77	119.84
1	C	787	ALA	C-N-CA	7.94	129.77	119.84
1	B	787	ALA	CA-C-N	7.90	129.72	119.84
1	B	787	ALA	C-N-CA	7.90	129.72	119.84
1	D	787	ALA	CA-C-N	7.88	129.69	119.84
1	D	787	ALA	C-N-CA	7.88	129.69	119.84
1	C	777	LEU	N-CA-C	-7.88	104.15	114.31
1	D	1004	SER	N-CA-CB	7.87	121.54	109.97
1	A	1004	SER	N-CA-CB	7.86	121.53	109.97
1	A	777	LEU	N-CA-C	-7.86	104.17	114.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1004	SER	N-CA-CB	7.86	121.52	109.97
1	C	672	VAL	CB-CA-C	-7.85	98.87	110.33
1	D	672	VAL	CB-CA-C	-7.84	98.88	110.33
1	D	777	LEU	N-CA-C	-7.84	104.19	114.31
1	B	672	VAL	CB-CA-C	-7.82	98.91	110.33
1	B	1004	SER	N-CA-CB	7.82	121.46	109.97
1	A	672	VAL	CB-CA-C	-7.81	98.93	110.33
1	B	777	LEU	N-CA-C	-7.81	104.23	114.31
1	C	113	PHE	CA-CB-CG	-7.70	106.10	113.80
1	D	113	PHE	CA-CB-CG	-7.66	106.14	113.80
1	B	113	PHE	CA-CB-CG	-7.64	106.16	113.80
1	A	113	PHE	CA-CB-CG	-7.63	106.17	113.80
1	B	18	ASN	CA-C-N	7.61	127.28	119.82
1	B	18	ASN	C-N-CA	7.61	127.28	119.82
1	A	274	PHE	CA-CB-CG	-7.60	106.20	113.80
1	D	274	PHE	CA-CB-CG	-7.59	106.21	113.80
1	C	571	VAL	CB-CA-C	-7.58	98.75	110.95
1	C	18	ASN	CA-C-N	7.58	127.24	119.82
1	C	18	ASN	C-N-CA	7.58	127.24	119.82
1	B	274	PHE	CA-CB-CG	-7.57	106.23	113.80
1	D	571	VAL	CB-CA-C	-7.57	98.76	110.95
1	C	274	PHE	CA-CB-CG	-7.56	106.24	113.80
1	D	18	ASN	CA-C-N	7.56	127.23	119.82
1	D	18	ASN	C-N-CA	7.56	127.23	119.82
1	C	4	THR	N-CA-C	-7.55	103.95	113.02
1	A	18	ASN	CA-C-N	7.55	127.22	119.82
1	A	18	ASN	C-N-CA	7.55	127.22	119.82
1	A	571	VAL	CB-CA-C	-7.55	98.80	110.95
1	B	4	THR	N-CA-C	-7.55	103.97	113.02
1	B	571	VAL	CB-CA-C	-7.52	98.84	110.95
1	D	4	THR	N-CA-C	-7.52	104.00	113.02
1	A	4	THR	N-CA-C	-7.51	104.01	113.02
1	D	424	ASN	N-CA-CB	-7.46	98.74	110.22
1	B	424	ASN	N-CA-CB	-7.46	98.74	110.22
1	A	424	ASN	N-CA-CB	-7.44	98.76	110.22
1	D	211	ASP	N-CA-C	7.43	119.92	110.33
1	B	211	ASP	N-CA-C	7.42	119.90	110.33
1	C	424	ASN	N-CA-CB	-7.42	98.80	110.22
1	A	211	ASP	N-CA-C	7.39	119.86	110.33
1	C	211	ASP	N-CA-C	7.37	119.84	110.33
1	C	433	LEU	CA-C-O	7.36	125.40	118.63
1	B	134	LEU	N-CA-CB	7.35	122.00	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	134	LEU	N-CA-CB	7.34	121.99	110.46
1	D	134	LEU	N-CA-CB	7.33	121.97	110.46
1	A	226	HIS	CB-CA-C	-7.32	94.08	109.38
1	B	226	HIS	CB-CA-C	-7.32	94.09	109.38
1	C	142	ILE	CB-CA-C	-7.32	99.65	110.33
1	D	226	HIS	CB-CA-C	-7.32	94.09	109.38
1	D	433	LEU	CA-C-O	7.31	125.36	118.63
1	A	134	LEU	N-CA-CB	7.31	121.94	110.46
1	B	142	ILE	CB-CA-C	-7.30	99.67	110.33
1	C	226	HIS	CB-CA-C	-7.30	94.12	109.38
1	A	142	ILE	CB-CA-C	-7.30	99.68	110.33
1	B	433	LEU	CA-C-O	7.29	125.34	118.63
1	D	142	ILE	CB-CA-C	-7.28	99.70	110.33
1	A	433	LEU	CA-C-O	7.27	125.32	118.63
1	D	938	ARG	N-CA-CB	7.23	122.11	110.77
1	B	938	ARG	N-CA-CB	7.20	122.07	110.77
1	A	938	ARG	N-CA-CB	7.18	122.05	110.77
1	C	938	ARG	N-CA-CB	7.18	122.04	110.77
1	C	553	TRP	CA-CB-CG	-7.04	100.23	113.60
1	A	553	TRP	CA-CB-CG	-7.03	100.24	113.60
1	B	553	TRP	CA-CB-CG	-7.03	100.24	113.60
1	D	553	TRP	CA-CB-CG	-7.01	100.27	113.60
1	C	614	HIS	N-CA-C	-7.01	100.97	110.36
1	A	614	HIS	N-CA-C	-7.00	100.97	110.36
1	B	614	HIS	N-CA-C	-7.00	100.98	110.36
1	D	614	HIS	N-CA-C	-6.95	101.04	110.36
1	C	600	GLN	N-CA-CB	6.94	122.11	110.32
1	B	600	GLN	N-CA-CB	6.93	122.11	110.32
1	A	600	GLN	N-CA-CB	6.93	122.10	110.32
1	B	823	LEU	N-CA-C	-6.92	104.96	113.41
1	C	823	LEU	N-CA-C	-6.91	104.98	113.41
1	D	823	LEU	N-CA-C	-6.90	104.99	113.41
1	D	600	GLN	N-CA-CB	6.90	122.05	110.32
1	D	863	GLN	CA-C-N	-6.88	113.51	123.00
1	D	863	GLN	C-N-CA	-6.88	113.51	123.00
1	B	980	GLU	N-CA-CB	6.87	120.18	109.94
1	A	823	LEU	N-CA-C	-6.87	105.03	113.41
1	A	863	GLN	CA-C-N	-6.87	113.53	123.00
1	A	863	GLN	C-N-CA	-6.87	113.53	123.00
1	C	863	GLN	CA-C-N	-6.86	113.54	123.00
1	C	863	GLN	C-N-CA	-6.86	113.54	123.00
1	C	980	GLU	N-CA-CB	6.85	120.14	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	980	GLU	N-CA-CB	6.83	120.11	109.94
1	D	980	GLU	N-CA-CB	6.81	120.09	109.94
1	B	863	GLN	CA-C-N	-6.80	113.62	123.00
1	B	863	GLN	C-N-CA	-6.80	113.62	123.00
1	B	209	PHE	CA-CB-CG	-6.78	107.02	113.80
1	A	181	GLU	N-CA-C	6.78	119.74	108.96
1	A	209	PHE	CA-CB-CG	-6.76	107.04	113.80
1	C	209	PHE	CA-CB-CG	-6.75	107.05	113.80
1	A	613	PRO	CB-CA-C	-6.74	102.14	110.98
1	D	804	ASN	CA-CB-CG	-6.74	105.86	112.60
1	D	613	PRO	CB-CA-C	-6.73	102.16	110.98
1	C	181	GLU	N-CA-C	6.73	119.67	108.96
1	D	181	GLU	N-CA-C	6.73	119.66	108.96
1	B	804	ASN	CA-CB-CG	-6.72	105.88	112.60
1	A	804	ASN	CA-CB-CG	-6.72	105.88	112.60
1	A	159	VAL	N-CA-C	6.72	118.05	111.67
1	C	159	VAL	N-CA-C	6.72	118.05	111.67
1	D	159	VAL	N-CA-C	6.71	118.05	111.67
1	C	804	ASN	CA-CB-CG	-6.71	105.89	112.60
1	D	209	PHE	CA-CB-CG	-6.71	107.09	113.80
1	B	181	GLU	N-CA-C	6.71	119.62	108.96
1	C	613	PRO	CB-CA-C	-6.71	102.20	110.98
1	B	613	PRO	CB-CA-C	-6.70	102.21	110.98
1	A	856	TYR	CA-C-N	-6.69	113.36	122.86
1	A	856	TYR	C-N-CA	-6.69	113.36	122.86
1	A	352	ARG	CA-C-N	-6.67	116.23	122.17
1	A	352	ARG	C-N-CA	-6.67	116.23	122.17
1	C	856	TYR	CA-C-N	-6.67	113.39	122.86
1	C	856	TYR	C-N-CA	-6.67	113.39	122.86
1	D	856	TYR	CA-C-N	-6.67	113.39	122.86
1	D	856	TYR	C-N-CA	-6.67	113.39	122.86
1	B	159	VAL	N-CA-C	6.67	118.00	111.67
1	B	856	TYR	CA-C-N	-6.66	113.40	122.86
1	B	856	TYR	C-N-CA	-6.66	113.40	122.86
1	C	352	ARG	CA-C-N	-6.63	116.27	122.17
1	C	352	ARG	C-N-CA	-6.63	116.27	122.17
1	C	1007	PHE	CA-CB-CG	-6.61	107.19	113.80
1	A	1007	PHE	CA-CB-CG	-6.60	107.20	113.80
1	D	1007	PHE	CA-CB-CG	-6.60	107.20	113.80
1	A	949	HIS	CA-CB-CG	-6.59	107.21	113.80
1	B	949	HIS	CA-CB-CG	-6.59	107.21	113.80
1	B	352	ARG	CA-C-N	-6.58	116.31	122.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	352	ARG	C-N-CA	-6.58	116.31	122.17
1	D	352	ARG	CA-C-N	-6.58	116.31	122.17
1	D	352	ARG	C-N-CA	-6.58	116.31	122.17
1	B	1007	PHE	CA-CB-CG	-6.57	107.23	113.80
1	D	949	HIS	CA-CB-CG	-6.57	107.23	113.80
1	B	725	ASN	CA-CB-CG	-6.57	106.03	112.60
1	A	725	ASN	CA-CB-CG	-6.57	106.03	112.60
1	C	949	HIS	CA-CB-CG	-6.57	107.23	113.80
1	A	770	ILE	CA-C-N	-6.57	113.00	120.42
1	A	770	ILE	C-N-CA	-6.57	113.00	120.42
1	B	770	ILE	CA-C-N	-6.56	113.00	120.42
1	B	770	ILE	C-N-CA	-6.56	113.00	120.42
1	C	725	ASN	CA-CB-CG	-6.54	106.06	112.60
1	A	802	ASP	CA-C-N	6.53	126.22	119.82
1	A	802	ASP	C-N-CA	6.53	126.22	119.82
1	C	770	ILE	CA-C-N	-6.52	113.05	120.42
1	C	770	ILE	C-N-CA	-6.52	113.05	120.42
1	D	770	ILE	CA-C-N	-6.51	113.06	120.42
1	D	770	ILE	C-N-CA	-6.51	113.06	120.42
1	D	725	ASN	CA-CB-CG	-6.51	106.09	112.60
1	C	802	ASP	CA-C-N	6.48	126.17	119.82
1	C	802	ASP	C-N-CA	6.48	126.17	119.82
1	B	424	ASN	N-CA-C	6.47	119.16	111.71
1	A	424	ASN	N-CA-C	6.47	119.15	111.71
1	D	424	ASN	N-CA-C	6.45	119.12	111.71
1	C	424	ASN	N-CA-C	6.44	119.12	111.71
1	D	802	ASP	CA-C-N	6.42	126.11	119.82
1	D	802	ASP	C-N-CA	6.42	126.11	119.82
1	B	802	ASP	CA-C-N	6.41	126.10	119.82
1	B	802	ASP	C-N-CA	6.41	126.10	119.82
1	A	105	TYR	CA-C-N	6.40	126.15	119.05
1	A	105	TYR	C-N-CA	6.40	126.15	119.05
1	B	105	TYR	CA-C-N	6.39	126.15	119.05
1	B	105	TYR	C-N-CA	6.39	126.15	119.05
1	C	105	TYR	CA-C-N	6.39	126.14	119.05
1	C	105	TYR	C-N-CA	6.39	126.14	119.05
1	D	105	TYR	CA-C-N	6.38	126.14	119.05
1	D	105	TYR	C-N-CA	6.38	126.14	119.05
1	A	383	ASN	N-CA-C	6.38	122.78	113.40
1	B	383	ASN	N-CA-C	6.37	122.76	113.40
1	C	521	LYS	N-CA-C	-6.36	104.35	111.28
1	B	521	LYS	N-CA-C	-6.35	104.36	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	521	LYS	N-CA-C	-6.33	104.37	111.28
1	A	521	LYS	N-CA-C	-6.33	104.38	111.28
1	C	383	ASN	N-CA-C	6.32	122.69	113.40
1	D	383	ASN	N-CA-C	6.32	122.69	113.40
1	A	629	PHE	CA-CB-CG	-6.29	107.52	113.80
1	C	881	ARG	CD-NE-CZ	6.27	133.18	124.40
1	B	881	ARG	CD-NE-CZ	6.26	133.17	124.40
1	D	881	ARG	CD-NE-CZ	6.24	133.13	124.40
1	C	629	PHE	CA-CB-CG	-6.23	107.57	113.80
1	D	629	PHE	CA-CB-CG	-6.21	107.59	113.80
1	B	629	PHE	CA-CB-CG	-6.21	107.59	113.80
1	B	288	ARG	CD-NE-CZ	-6.20	115.71	124.40
1	A	881	ARG	CD-NE-CZ	6.20	133.08	124.40
1	C	288	ARG	CD-NE-CZ	-6.20	115.72	124.40
1	A	288	ARG	CD-NE-CZ	-6.19	115.74	124.40
1	B	142	ILE	N-CA-C	6.18	117.02	108.12
1	A	588	TYR	N-CA-C	6.17	116.59	108.07
1	A	142	ILE	N-CA-C	6.17	117.00	108.12
1	D	142	ILE	N-CA-C	6.17	117.00	108.12
1	D	288	ARG	CD-NE-CZ	-6.16	115.78	124.40
1	B	588	TYR	N-CA-C	6.15	116.56	108.07
1	C	142	ILE	N-CA-C	6.15	116.98	108.12
1	C	360	HIS	CA-CB-CG	-6.13	107.67	113.80
1	D	588	TYR	N-CA-C	6.13	116.53	108.07
1	A	360	HIS	CA-CB-CG	-6.12	107.68	113.80
1	B	360	HIS	CA-CB-CG	-6.12	107.68	113.80
1	D	360	HIS	CA-CB-CG	-6.11	107.69	113.80
1	B	750	GLU	N-CA-CB	6.11	122.06	111.00
1	C	723	ALA	O-C-N	6.11	129.51	123.46
1	D	750	GLU	N-CA-CB	6.11	122.06	111.00
1	C	588	TYR	N-CA-C	6.10	116.49	108.07
1	C	118	ASN	CA-C-O	6.09	127.28	120.34
1	C	750	GLU	N-CA-CB	6.08	122.01	111.00
1	A	750	GLU	N-CA-CB	6.07	121.99	111.00
1	A	878	HIS	CA-C-N	6.07	125.98	119.85
1	A	878	HIS	C-N-CA	6.07	125.98	119.85
1	B	878	HIS	CA-C-N	6.06	125.97	119.85
1	B	878	HIS	C-N-CA	6.06	125.97	119.85
1	D	723	ALA	O-C-N	6.06	129.46	123.46
1	A	723	ALA	O-C-N	6.06	129.46	123.46
1	B	110	ASN	CA-CB-CG	-6.06	106.54	112.60
1	C	938	ARG	CG-CD-NE	-6.05	98.70	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	139	THR	CA-C-N	-6.04	113.11	122.59
1	C	139	THR	C-N-CA	-6.04	113.11	122.59
1	B	723	ALA	O-C-N	6.04	129.44	123.46
1	B	118	ASN	CA-C-O	6.03	127.22	120.34
1	D	118	ASN	CA-C-O	6.03	127.22	120.34
1	A	938	ARG	CG-CD-NE	-6.03	98.74	112.00
1	D	938	ARG	CG-CD-NE	-6.03	98.74	112.00
1	D	139	THR	CA-C-N	-6.02	113.13	122.59
1	D	139	THR	C-N-CA	-6.02	113.13	122.59
1	C	878	HIS	CA-C-N	6.02	125.93	119.85
1	C	878	HIS	C-N-CA	6.02	125.93	119.85
1	A	110	ASN	CA-CB-CG	-6.02	106.58	112.60
1	B	938	ARG	CG-CD-NE	-6.02	98.76	112.00
1	A	483	PRO	CA-C-N	-6.01	115.34	123.10
1	A	483	PRO	C-N-CA	-6.01	115.34	123.10
1	A	139	THR	CA-C-N	-6.01	113.15	122.59
1	A	139	THR	C-N-CA	-6.01	113.15	122.59
1	A	118	ASN	CA-C-O	6.01	127.19	120.34
1	B	139	THR	CA-C-N	-6.01	113.16	122.59
1	B	139	THR	C-N-CA	-6.01	113.16	122.59
1	D	878	HIS	CA-C-N	6.00	125.91	119.85
1	D	878	HIS	C-N-CA	6.00	125.91	119.85
1	C	110	ASN	CA-CB-CG	-6.00	106.60	112.60
1	B	210	ARG	N-CA-CB	5.99	120.69	111.22
1	D	210	ARG	N-CA-CB	5.99	120.68	111.22
1	A	210	ARG	N-CA-CB	5.98	120.66	111.22
1	D	128	ASN	CA-C-N	-5.98	115.78	123.19
1	D	128	ASN	C-N-CA	-5.98	115.78	123.19
1	A	128	ASN	CA-C-N	-5.97	115.78	123.19
1	A	128	ASN	C-N-CA	-5.97	115.78	123.19
1	B	483	PRO	CA-C-N	-5.97	115.40	123.10
1	B	483	PRO	C-N-CA	-5.97	115.40	123.10
1	D	95	TYR	N-CA-C	5.96	118.27	111.11
1	C	601	PHE	CA-CB-CG	-5.96	107.84	113.80
1	D	110	ASN	CA-CB-CG	-5.96	106.64	112.60
1	D	176	PHE	CA-CB-CG	-5.96	107.84	113.80
1	C	210	ARG	N-CA-CB	5.96	120.63	111.22
1	C	95	TYR	N-CA-C	5.95	118.25	111.11
1	B	128	ASN	CA-C-N	-5.95	115.82	123.19
1	B	128	ASN	C-N-CA	-5.95	115.82	123.19
1	C	176	PHE	CA-CB-CG	-5.94	107.86	113.80
1	D	483	PRO	CA-C-N	-5.94	115.44	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	483	PRO	C-N-CA	-5.94	115.44	123.10
1	B	601	PHE	CA-CB-CG	-5.94	107.86	113.80
1	B	176	PHE	CA-CB-CG	-5.94	107.86	113.80
1	C	483	PRO	CA-C-N	-5.93	115.45	123.10
1	C	483	PRO	C-N-CA	-5.93	115.45	123.10
1	C	128	ASN	CA-C-N	-5.93	115.84	123.19
1	C	128	ASN	C-N-CA	-5.93	115.84	123.19
1	B	95	TYR	N-CA-C	5.92	118.22	111.11
1	B	864	MET	N-CA-CB	5.92	119.87	110.57
1	A	601	PHE	CA-CB-CG	-5.92	107.88	113.80
1	D	601	PHE	CA-CB-CG	-5.92	107.88	113.80
1	D	864	MET	N-CA-CB	5.91	119.85	110.57
1	A	95	TYR	N-CA-C	5.91	118.20	111.11
1	B	448	ARG	N-CA-C	5.91	119.59	112.38
1	A	864	MET	N-CA-CB	5.91	119.85	110.57
1	C	63	PHE	CA-C-N	5.91	126.02	119.87
1	C	63	PHE	C-N-CA	5.91	126.02	119.87
1	C	864	MET	N-CA-CB	5.91	119.84	110.57
1	A	176	PHE	CA-CB-CG	-5.90	107.90	113.80
1	A	598	ASP	N-CA-C	5.89	119.44	112.72
1	C	680	ILE	N-CA-C	5.89	116.48	107.77
1	D	598	ASP	N-CA-C	5.88	119.42	112.72
1	B	598	ASP	N-CA-C	5.88	119.42	112.72
1	B	702	GLN	CA-C-O	5.87	124.47	119.71
1	C	448	ARG	N-CA-C	5.87	119.55	112.38
1	A	448	ARG	N-CA-C	5.87	119.54	112.38
1	A	680	ILE	N-CA-C	5.87	116.46	107.77
1	D	680	ILE	N-CA-C	5.86	116.45	107.77
1	D	448	ARG	N-CA-C	5.86	119.53	112.38
1	A	63	PHE	CA-C-N	5.85	125.96	119.87
1	A	63	PHE	C-N-CA	5.85	125.96	119.87
1	A	384	PHE	CA-C-N	5.84	132.41	122.36
1	A	384	PHE	C-N-CA	5.84	132.41	122.36
1	D	829	THR	N-CA-CB	5.84	119.72	110.55
1	B	680	ILE	N-CA-C	5.84	116.41	107.77
1	A	702	GLN	CA-C-O	5.84	124.44	119.71
1	B	384	PHE	CA-C-N	5.84	132.40	122.36
1	B	384	PHE	C-N-CA	5.84	132.40	122.36
1	D	599	ARG	CB-CA-C	-5.83	109.83	116.54
1	C	598	ASP	N-CA-C	5.83	119.37	112.72
1	D	702	GLN	CA-C-O	5.83	124.43	119.71
1	C	829	THR	N-CA-CB	5.83	119.70	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	63	PHE	CA-C-N	5.82	125.92	119.87
1	B	63	PHE	C-N-CA	5.82	125.92	119.87
1	C	384	PHE	CA-C-N	5.82	132.37	122.36
1	C	384	PHE	C-N-CA	5.82	132.37	122.36
1	D	63	PHE	CA-C-N	5.82	125.92	119.87
1	D	63	PHE	C-N-CA	5.82	125.92	119.87
1	D	384	PHE	CA-C-N	5.82	132.37	122.36
1	D	384	PHE	C-N-CA	5.82	132.37	122.36
1	A	829	THR	N-CA-CB	5.81	119.67	110.55
1	A	599	ARG	CB-CA-C	-5.80	109.87	116.54
1	B	829	THR	N-CA-CB	5.79	119.65	110.55
1	C	702	GLN	CA-C-O	5.77	124.39	119.71
1	D	721	ARG	N-CA-CB	5.77	119.69	110.16
1	C	226	HIS	ND1-CE1-NE2	5.77	114.17	108.40
1	B	599	ARG	CB-CA-C	-5.77	109.91	116.54
1	B	721	ARG	N-CA-CB	5.77	119.67	110.16
1	C	599	ARG	CB-CA-C	-5.77	109.91	116.54
1	C	721	ARG	N-CA-CB	5.76	119.67	110.16
1	A	721	ARG	N-CA-CB	5.75	119.64	110.16
1	B	226	HIS	ND1-CE1-NE2	5.74	114.14	108.40
1	D	424	ASN	CA-CB-CG	-5.74	106.86	112.60
1	D	226	HIS	ND1-CE1-NE2	5.73	114.13	108.40
1	C	460	ASN	CA-CB-CG	5.72	118.33	112.60
1	C	519	SER	N-CA-C	-5.72	101.94	110.23
1	B	424	ASN	CA-CB-CG	-5.72	106.88	112.60
1	C	245	GLN	CB-CG-CD	-5.71	102.89	112.60
1	A	172	ASP	CA-CB-CG	-5.71	106.89	112.60
1	B	172	ASP	CA-CB-CG	-5.71	106.89	112.60
1	D	460	ASN	CA-CB-CG	5.70	118.30	112.60
1	A	460	ASN	CA-CB-CG	5.69	118.29	112.60
1	B	93	HIS	CA-CB-CG	-5.69	108.11	113.80
1	C	93	HIS	CA-CB-CG	-5.69	108.11	113.80
1	B	519	SER	N-CA-C	-5.68	101.99	110.23
1	A	519	SER	N-CA-C	-5.68	101.99	110.23
1	C	424	ASN	CA-CB-CG	-5.68	106.92	112.60
1	C	521	LYS	O-C-N	-5.68	116.10	122.12
1	A	226	HIS	ND1-CE1-NE2	5.68	114.08	108.40
1	C	172	ASP	CA-CB-CG	-5.68	106.92	112.60
1	D	519	SER	N-CA-C	-5.68	101.99	110.23
1	D	142	ILE	N-CA-CB	-5.67	103.24	111.52
1	A	245	GLN	CB-CG-CD	-5.67	102.96	112.60
1	D	245	GLN	CB-CG-CD	-5.66	102.97	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	142	ILE	N-CA-CB	-5.66	103.25	111.52
1	A	424	ASN	CA-CB-CG	-5.66	106.94	112.60
1	B	245	GLN	CB-CG-CD	-5.64	103.00	112.60
1	B	460	ASN	CA-CB-CG	5.64	118.24	112.60
1	A	93	HIS	CA-CB-CG	-5.64	108.16	113.80
1	D	172	ASP	CA-CB-CG	-5.64	106.96	112.60
1	A	142	ILE	N-CA-CB	-5.63	103.30	111.52
1	D	93	HIS	CA-CB-CG	-5.63	108.17	113.80
1	C	142	ILE	N-CA-CB	-5.62	103.32	111.52
2	I	67	ILE	N-CA-C	5.61	117.66	108.97
2	J	67	ILE	N-CA-C	5.61	117.66	108.97
1	A	521	LYS	O-C-N	-5.60	116.18	122.12
2	H	67	ILE	N-CA-C	5.60	117.65	108.97
1	D	128	ASN	N-CA-C	5.60	118.37	109.24
1	B	168	PRO	CB-CA-C	-5.59	103.78	111.21
1	D	168	PRO	CB-CA-C	-5.59	103.78	111.21
1	D	651	LEU	CB-CA-C	-5.59	98.29	109.35
1	C	576	ILE	N-CA-C	5.58	116.62	108.58
1	A	576	ILE	N-CA-C	5.58	116.62	108.58
1	B	576	ILE	N-CA-C	5.58	116.62	108.58
1	C	920	LEU	CA-C-N	5.58	125.34	119.76
1	C	920	LEU	C-N-CA	5.58	125.34	119.76
2	K	67	ILE	N-CA-C	5.57	117.61	108.97
1	C	128	ASN	N-CA-C	5.57	118.32	109.24
1	D	521	LYS	O-C-N	-5.57	116.22	122.12
1	B	651	LEU	CB-CA-C	-5.57	98.32	109.35
1	A	651	LEU	CB-CA-C	-5.56	98.34	109.35
1	B	128	ASN	N-CA-C	5.56	118.31	109.24
1	D	863	GLN	CB-CA-C	-5.56	99.53	109.71
1	A	168	PRO	CB-CA-C	-5.56	103.82	111.21
1	B	521	LYS	O-C-N	-5.56	116.23	122.12
1	C	651	LEU	CB-CA-C	-5.56	98.35	109.35
1	C	863	GLN	CB-CA-C	-5.55	99.54	109.71
1	A	128	ASN	N-CA-C	5.55	118.28	109.24
1	A	226	HIS	ND1-CG-CD2	5.55	111.65	106.10
1	B	863	GLN	CB-CA-C	-5.54	99.57	109.71
1	A	920	LEU	CA-C-N	5.54	125.30	119.76
1	A	920	LEU	C-N-CA	5.54	125.30	119.76
1	B	226	HIS	ND1-CG-CD2	5.54	111.64	106.10
1	B	920	LEU	CA-C-N	5.53	125.29	119.76
1	B	920	LEU	C-N-CA	5.53	125.29	119.76
1	D	576	ILE	N-CA-C	5.53	116.55	108.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	GLY	N-CA-C	5.53	117.50	110.20
1	D	226	HIS	ND1-CG-CD2	5.53	111.63	106.10
1	C	168	PRO	CB-CA-C	-5.53	103.86	111.21
1	A	863	GLN	CB-CA-C	-5.52	99.61	109.71
1	B	56	GLY	N-CA-C	5.52	117.48	110.20
1	C	226	HIS	ND1-CG-CD2	5.51	111.61	106.10
1	B	249	GLU	O-C-N	5.51	129.50	123.22
1	D	920	LEU	CA-C-N	5.50	125.26	119.76
1	D	920	LEU	C-N-CA	5.50	125.26	119.76
1	B	136	GLU	CB-CA-C	-5.50	98.45	111.65
1	A	136	GLU	CB-CA-C	-5.50	98.45	111.65
1	D	336	ARG	CB-CA-C	-5.48	98.27	109.94
1	C	136	GLU	CB-CA-C	-5.48	98.50	111.65
1	C	336	ARG	CB-CA-C	-5.47	98.28	109.94
1	D	136	GLU	CB-CA-C	-5.47	98.53	111.65
1	A	336	ARG	CB-CA-C	-5.46	98.31	109.94
1	B	336	ARG	CB-CA-C	-5.45	98.33	109.94
1	B	702	GLN	CA-CB-CG	-5.45	103.19	114.10
1	C	56	GLY	N-CA-C	5.45	117.40	110.20
1	A	249	GLU	O-C-N	5.44	129.42	123.22
1	D	702	GLN	CA-CB-CG	-5.44	103.23	114.10
1	D	743	SER	CA-C-N	-5.44	110.97	121.58
1	D	743	SER	C-N-CA	-5.44	110.97	121.58
1	D	56	GLY	N-CA-C	5.43	117.37	110.20
1	D	249	GLU	O-C-N	5.43	129.41	123.22
1	A	743	SER	CA-C-N	-5.42	111.00	121.58
1	A	743	SER	C-N-CA	-5.42	111.00	121.58
1	A	702	GLN	CA-CB-CG	-5.42	103.25	114.10
1	D	416	GLU	N-CA-CB	5.42	119.60	110.77
1	C	743	SER	CA-C-N	-5.42	111.01	121.58
1	C	743	SER	C-N-CA	-5.42	111.01	121.58
1	D	190	ARG	CB-CA-C	5.42	119.46	110.90
1	C	702	GLN	CA-CB-CG	-5.41	103.28	114.10
1	D	969	GLU	N-CA-CB	5.41	118.50	110.49
1	B	743	SER	CA-C-N	-5.41	111.03	121.58
1	B	743	SER	C-N-CA	-5.41	111.03	121.58
1	B	190	ARG	CB-CA-C	5.41	119.44	110.90
1	C	513	PRO	CB-CA-C	-5.40	104.49	111.46
1	B	416	GLU	N-CA-CB	5.40	119.57	110.77
1	A	190	ARG	CB-CA-C	5.40	119.43	110.90
1	A	416	GLU	N-CA-CB	5.40	119.57	110.77
1	A	748	CYS	N-CA-CB	5.40	120.22	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	423	MET	N-CA-C	5.39	117.16	111.28
1	D	423	MET	N-CA-C	5.39	117.16	111.28
1	C	249	GLU	O-C-N	5.39	129.37	123.22
1	C	416	GLU	N-CA-CB	5.39	119.55	110.77
1	A	969	GLU	N-CA-CB	5.38	118.45	110.49
1	B	748	CYS	N-CA-CB	5.38	120.19	110.83
1	B	886	CYS	CA-C-N	-5.38	115.52	123.05
1	B	886	CYS	C-N-CA	-5.38	115.52	123.05
1	C	748	CYS	N-CA-CB	5.38	120.19	110.83
1	D	513	PRO	CB-CA-C	-5.38	104.52	111.46
1	D	748	CYS	N-CA-CB	5.38	120.19	110.83
1	A	513	PRO	CB-CA-C	-5.38	104.52	111.46
1	B	969	GLU	N-CA-CB	5.38	118.45	110.49
1	C	969	GLU	N-CA-CB	5.38	118.45	110.49
1	B	386	ALA	N-CA-CB	-5.38	102.68	111.66
1	B	423	MET	N-CA-C	5.38	117.14	111.28
1	D	886	CYS	CA-C-N	-5.37	115.53	123.05
1	D	886	CYS	C-N-CA	-5.37	115.53	123.05
1	A	886	CYS	CA-C-N	-5.36	115.54	123.05
1	A	886	CYS	C-N-CA	-5.36	115.54	123.05
1	B	513	PRO	CB-CA-C	-5.36	104.54	111.46
1	C	423	MET	N-CA-C	5.36	117.13	111.28
1	D	386	ALA	N-CA-CB	-5.36	102.70	111.66
1	A	386	ALA	N-CA-CB	-5.36	102.71	111.66
1	D	421	VAL	CB-CA-C	-5.36	104.75	110.16
1	C	190	ARG	CB-CA-C	5.36	119.37	110.90
1	A	421	VAL	CB-CA-C	-5.36	104.75	110.16
1	C	886	CYS	CA-C-N	-5.35	115.56	123.05
1	C	886	CYS	C-N-CA	-5.35	115.56	123.05
1	C	386	ALA	N-CA-CB	-5.35	102.73	111.66
1	D	980	GLU	N-CA-C	5.34	117.52	111.11
1	C	980	GLU	N-CA-C	5.34	117.52	111.11
1	C	421	VAL	CB-CA-C	-5.33	104.77	110.16
1	A	653[A]	HIS	CA-C-N	-5.33	113.49	123.03
1	A	653[A]	HIS	C-N-CA	-5.33	113.49	123.03
1	A	653[B]	HIS	CA-C-N	-5.33	113.49	123.03
1	A	653[B]	HIS	C-N-CA	-5.33	113.49	123.03
1	A	980	GLU	N-CA-C	5.32	117.50	111.11
1	B	421	VAL	CB-CA-C	-5.32	104.78	110.16
1	A	102	ASN	CA-CB-CG	5.32	117.92	112.60
1	A	634	GLN	CA-C-O	5.32	125.95	119.78
1	B	980	GLU	N-CA-C	5.32	117.49	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	685	LEU	CA-C-O	5.31	124.02	119.66
1	C	781	ARG	N-CA-C	5.31	117.25	109.24
1	C	653[A]	HIS	CA-C-N	-5.30	113.54	123.03
1	C	653[A]	HIS	C-N-CA	-5.30	113.54	123.03
1	C	653[B]	HIS	CA-C-N	-5.30	113.54	123.03
1	C	653[B]	HIS	C-N-CA	-5.30	113.54	123.03
1	B	634	GLN	CA-C-O	5.30	125.93	119.78
1	B	653[A]	HIS	CA-C-N	-5.30	113.54	123.03
1	B	653[A]	HIS	C-N-CA	-5.30	113.54	123.03
1	B	653[B]	HIS	CA-C-N	-5.30	113.54	123.03
1	B	653[B]	HIS	C-N-CA	-5.30	113.54	123.03
1	C	927	THR	CA-C-O	5.30	124.47	119.59
1	B	685	LEU	CA-C-O	5.30	124.00	119.66
1	C	264	GLU	CA-C-O	5.29	124.88	119.05
1	B	102	ASN	CA-CB-CG	5.29	117.89	112.60
1	A	781	ARG	N-CA-C	5.29	117.23	109.24
1	C	634	GLN	CA-C-O	5.29	125.92	119.78
1	D	781	ARG	N-CA-C	5.29	117.23	109.24
1	D	653[A]	HIS	CA-C-N	-5.29	113.56	123.03
1	D	653[A]	HIS	C-N-CA	-5.29	113.56	123.03
1	D	653[B]	HIS	CA-C-N	-5.29	113.56	123.03
1	D	653[B]	HIS	C-N-CA	-5.29	113.56	123.03
1	B	264	GLU	CA-C-O	5.28	124.86	119.05
1	C	102	ASN	CA-CB-CG	5.27	117.87	112.60
1	A	264	GLU	CA-C-O	5.27	124.84	119.05
1	D	102	ASN	CA-CB-CG	5.26	117.86	112.60
1	D	685	LEU	CA-C-O	5.26	123.98	119.66
1	D	264	GLU	CA-C-O	5.26	124.84	119.05
1	B	1018	LEU	CB-CA-C	-5.25	99.02	109.79
1	D	1018	LEU	CB-CA-C	-5.25	99.03	109.79
1	D	404	ARG	N-CA-C	5.25	118.14	111.69
1	A	927	THR	CA-C-O	5.24	124.41	119.59
1	A	1018	LEU	CB-CA-C	-5.24	99.05	109.79
1	C	404	ARG	N-CA-C	5.24	118.13	111.69
1	D	908	ASP	N-CA-C	-5.24	106.75	112.72
1	B	781	ARG	N-CA-C	5.24	117.15	109.24
1	B	927	THR	CA-C-O	5.23	124.40	119.59
1	A	404	ARG	N-CA-C	5.23	118.12	111.69
1	C	1018	LEU	CB-CA-C	-5.22	99.09	109.79
1	A	210	ARG	N-CA-C	-5.22	101.77	109.18
1	B	216	HIS	CA-CB-CG	-5.22	108.58	113.80
1	B	261	TRP	CB-CA-C	-5.22	99.82	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	634	GLN	CA-C-O	5.21	125.83	119.78
1	C	183	ARG	CD-NE-CZ	-5.21	117.11	124.40
1	D	210	ARG	N-CA-C	-5.21	101.78	109.18
1	A	908	ASP	N-CA-C	-5.21	106.78	112.72
1	B	908	ASP	N-CA-C	-5.21	106.79	112.72
1	B	183	ARG	CD-NE-CZ	-5.20	117.11	124.40
1	C	210	ARG	N-CA-C	-5.20	101.79	109.18
1	D	261	TRP	CB-CA-C	-5.20	99.85	109.37
1	C	908	ASP	N-CA-C	-5.20	106.80	112.72
1	B	404	ARG	N-CA-C	5.19	118.08	111.69
1	A	261	TRP	CB-CA-C	-5.19	99.87	109.37
1	B	210	ARG	N-CA-C	-5.19	101.81	109.18
1	C	216	HIS	CA-CB-CG	-5.19	108.61	113.80
1	D	927	THR	CA-C-O	5.18	124.36	119.59
1	C	261	TRP	CB-CA-C	-5.18	99.90	109.37
1	C	685	LEU	CA-C-O	5.16	123.89	119.66
1	D	714	ILE	CB-CA-C	-5.16	103.91	110.98
1	A	714	ILE	CB-CA-C	-5.15	103.92	110.98
1	B	526	LEU	N-CA-C	-5.15	102.69	109.84
1	A	183	ARG	CD-NE-CZ	-5.14	117.20	124.40
1	A	216	HIS	CA-CB-CG	-5.14	108.66	113.80
1	C	526	LEU	N-CA-C	-5.14	102.69	109.84
1	D	183	ARG	CD-NE-CZ	-5.14	117.20	124.40
2	J	79	TYR	N-CA-C	5.14	117.48	109.52
1	A	769	TRP	CB-CA-C	-5.14	98.65	109.38
1	C	769	TRP	CB-CA-C	-5.14	98.65	109.38
1	D	526	LEU	N-CA-C	-5.14	102.70	109.84
1	D	769	TRP	CB-CA-C	-5.14	98.64	109.38
1	B	714	ILE	CB-CA-C	-5.13	103.95	110.98
2	I	79	TYR	N-CA-C	5.13	117.47	109.52
1	C	714	ILE	CB-CA-C	-5.13	103.96	110.98
1	C	875	ASP	N-CA-C	5.12	118.66	112.93
2	K	79	TYR	N-CA-C	5.12	117.45	109.52
2	H	79	TYR	N-CA-C	5.11	117.44	109.52
1	A	875	ASP	N-CA-C	5.11	118.65	112.93
1	B	769	TRP	CB-CA-C	-5.11	98.71	109.38
1	D	216	HIS	CA-CB-CG	-5.11	108.69	113.80
1	D	288	ARG	NE-CZ-NH1	-5.11	116.39	121.50
1	A	453	VAL	CA-C-N	-5.10	116.48	122.14
1	A	453	VAL	C-N-CA	-5.10	116.48	122.14
1	A	526	LEU	N-CA-C	-5.10	102.75	109.84
1	C	132	SER	N-CA-C	5.09	116.83	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	190	ARG	N-CA-CB	5.08	117.44	110.07
1	D	453	VAL	CA-C-N	-5.08	116.50	122.14
1	D	453	VAL	C-N-CA	-5.08	116.50	122.14
1	A	447	ASP	CA-CB-CG	-5.07	107.53	112.60
1	D	875	ASP	N-CA-C	5.07	118.61	112.93
1	B	639	THR	CA-CB-CG2	-5.06	101.89	110.50
1	B	875	ASP	N-CA-C	5.06	118.60	112.93
1	C	729	THR	N-CA-CB	5.06	118.50	110.55
1	D	132	SER	N-CA-C	5.06	116.80	111.28
1	B	190	ARG	N-CA-CB	5.06	117.40	110.07
1	B	193	ASP	CA-CB-CG	-5.06	107.54	112.60
1	B	729	THR	N-CA-CB	5.06	118.49	110.55
1	A	729	THR	N-CA-CB	5.05	118.48	110.55
1	C	447	ASP	CA-CB-CG	-5.05	107.55	112.60
1	A	288	ARG	NE-CZ-NH1	-5.05	116.45	121.50
1	B	787	ALA	O-C-N	5.05	125.75	121.20
1	C	193	ASP	CA-CB-CG	-5.05	107.55	112.60
1	D	729	THR	N-CA-CB	5.05	118.48	110.55
1	B	533	LEU	CB-CA-C	5.05	118.54	110.16
1	A	132	SER	N-CA-C	5.04	116.78	111.28
1	D	533	LEU	CB-CA-C	5.04	118.53	110.16
1	B	710	GLU	CB-CA-C	-5.04	99.97	110.40
1	B	686	PRO	CB-CA-C	-5.04	104.62	111.12
1	D	737	ILE	N-CA-CB	5.04	118.27	111.21
1	B	737	ILE	N-CA-CB	5.04	118.26	111.21
1	C	533	LEU	CB-CA-C	5.04	118.52	110.16
1	D	193	ASP	CA-CB-CG	-5.04	107.56	112.60
1	A	193	ASP	CA-CB-CG	-5.04	107.56	112.60
1	C	737	ILE	N-CA-CB	5.04	118.26	111.21
1	C	288	ARG	NE-CZ-NH1	-5.03	116.47	121.50
1	B	132	SER	N-CA-C	5.03	116.76	111.28
1	C	453	VAL	CA-C-N	-5.03	116.56	122.14
1	C	453	VAL	C-N-CA	-5.03	116.56	122.14
1	A	190	ARG	N-CA-CB	5.03	117.36	110.07
1	A	533	LEU	CB-CA-C	5.03	118.51	110.16
1	D	323	ILE	N-CA-C	-5.03	105.94	110.82
1	A	710	GLU	CB-CA-C	-5.03	100.00	110.40
2	H	104	GLY	N-CA-C	-5.03	104.52	112.66
1	C	639	THR	CA-CB-CG2	-5.02	101.96	110.50
1	D	686	PRO	CB-CA-C	-5.02	104.64	111.12
1	D	787	ALA	O-C-N	5.02	125.72	121.20
1	B	639	THR	CA-C-N	-5.02	115.11	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	639	THR	C-N-CA	-5.02	115.11	122.19
1	C	686	PRO	CB-CA-C	-5.02	104.64	111.12
1	C	639	THR	CA-C-N	-5.02	115.11	122.19
1	C	639	THR	C-N-CA	-5.02	115.11	122.19
1	A	737	ILE	N-CA-CB	5.02	118.23	111.21
1	C	749	ILE	N-CA-CB	5.02	118.33	111.41
1	B	453	VAL	CA-C-N	-5.02	116.57	122.14
1	B	453	VAL	C-N-CA	-5.02	116.57	122.14
1	D	710	GLU	CB-CA-C	-5.02	100.02	110.40
1	A	639	THR	CA-CB-CG2	-5.01	101.97	110.50
1	C	323	ILE	N-CA-C	-5.01	105.96	110.82
1	D	639	THR	CA-CB-CG2	-5.01	101.98	110.50
1	A	927	THR	CA-C-N	5.01	126.11	119.84
1	A	927	THR	C-N-CA	5.01	126.11	119.84
1	A	639	THR	CA-C-N	-5.01	115.12	122.19
1	A	639	THR	C-N-CA	-5.01	115.12	122.19
1	D	447	ASP	CA-CB-CG	-5.01	107.59	112.60
1	A	323	ILE	N-CA-C	-5.01	105.96	110.82
1	C	710	GLU	CB-CA-C	-5.01	100.04	110.40
1	D	278	ILE	CA-C-N	-5.01	116.18	121.84
1	D	278	ILE	C-N-CA	-5.01	116.18	121.84
1	C	300	LEU	N-CA-C	5.00	118.28	110.32
1	C	322	LEU	CB-CA-C	-5.00	102.08	110.29
1	B	300	LEU	N-CA-C	5.00	118.27	110.32

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8238	0	7821	510	0
1	B	8238	0	7822	493	0
1	C	8238	0	7821	489	0
1	D	8238	0	7821	500	0
2	H	902	0	838	112	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	902	0	838	111	0
2	J	902	0	839	109	0
2	K	902	0	839	112	0
3	L	818	0	780	13	0
3	M	818	0	780	12	0
3	N	818	0	780	14	0
3	O	818	0	780	14	0
All	All	39832	0	37759	2066	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 27.

All (2066) 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:362:LEU:HD22	2:J:31:SER:C	1.44	1.42
1:B:583:ASN:CG	2:K:73:THR:H	1.29	1.41
1:D:362:LEU:HD22	2:I:31:SER:C	1.43	1.40
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:D:583:ASN:CG	2:I:73:THR:H	1.30	1.37
1:A:583:ASN:CG	2:J:73:THR:H	1.28	1.37
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:C:609:ALA:CB	2:H:53:TYR:OH	1.79	1.31
1:B:362:LEU:HD22	2:K:31:SER:C	1.56	1.29
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: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:362:LEU:HD22	2:H:31:SER:C	1.61	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:578:TYR:CG	2:K:28:SER:OG	1.96	1.18
1:C:579:ASP:OD1	2:H:73:THR:OG1	1.59	1.18
1:B:584:PRO:HB3	2:K:30:THR:HG22	1.17	1.16
1:C:584:PRO:CA	2:H:30:THR:CG2	2.24	1.15
1:B:578:TYR:CD2	2:K:28:SER:OG	1.97	1.15
1:C:578:TYR:CD2	2:H:28:SER:OG	1.99	1.15
1:B:584:PRO:HG2	2:K:71:ARG:NH1	1.62	1.15
1:C:583:ASN:CG	2:H:73:THR:N	2.03	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:583:ASN:CG	2:J:73:THR:N	2.07	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:A:581:ASN:HB2	2:J:72:ASP:OD1	1.49	1.10
1:A:584:PRO:HB3	2:J:30:THR:HG22	1.13	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:362:LEU:CD2	2:I:31:SER:C	2.24	1.09
1:D:584:PRO:HA	2:I:30:THR:CG2	1.82	1.09
1:A:610:ASP:N	2:J:53:TYR:CE1	2.20	1.09
1:C:576:ILE:CG2	2:H:30:THR:HB	1.82	1.09
1:D:610:ASP:N	2:I:53:TYR:HE1	1.50	1.09
1:A:362:LEU:CD2	2:J:31:SER:C	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:583:ASN:CG	2:I:73:THR:N	2.09	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:A:746:ASP:HA	1:A:760:ARG:HG3	1.34	1.07
1:B:584:PRO:HB3	2:K:30:THR:CG2	1.84	1.07
1:C:582:GLY:O	2:H:29:ILE:CG2	2.02	1.07
1:B:583:ASN:CG	2:K:73:THR:N	2.10	1.06
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:A:427:THR:HA	1:A:436:MET:HE1	1.09	1.06
1:B:427:THR:HA	1:B:436:MET:HE1	1.09	1.06
1:D:584:PRO:HB3	2:I:30:THR:CG2	1.85	1.06
1:C:427:THR:HA	1:C:436:MET:HE1	1.09	1.05
1:D:362:LEU:CD2	2:I:31:SER:HA	1.86	1.05
1:D:427:THR:HA	1:D:436:MET:HE1	1.09	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:C:576:ILE:CD1	2:H:53:TYR:HB2	1.86	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:A:362:LEU:CD2	2:J:31:SER:HA	1.86	1.04
1:C:583:ASN:OD1	2:H:72:ASP:CA	2.06	1.04
1:C:610:ASP:N	2:H:53:TYR:HE1	1.53	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: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:A:583:ASN:OD1	2:J:72:ASP:C	2.03	1.01
1:B:362:LEU:CD2	2:K:31:SER:C	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:610:ASP:CA	2:H:53:TYR:HE1	1.73	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: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:583:ASN:OD1	2:I:72:ASP:C	2.05	0.98
1:C:583:ASN:OD1	2:H:72:ASP:C	2.07	0.98
1:B:434:PRO:HB3	1:C:434:PRO:HB3	1.44	0.98
1:D:597:ASN:HD22	1:D:599:ARG:H	1.11	0.98
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:C:362:LEU:CD2	2:H:31:SER:C	2.36	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: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: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:C:38:ASN:ND2	1:C:41:GLU:H	1.66	0.94
1:D:38:ASN:ND2	1:D:41:GLU:H	1.66	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:B:38:ASN:ND2	1:B:41:GLU:H	1.66	0.93
1:D:610:ASP:CA	2:I:53:TYR:HE1	1.79	0.93
1:A:362:LEU:CD2	2:J:31:SER:CA	2.45	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:OD1	2:K:72:ASP:C	2.10	0.93
1:C:427:THR:HA	1:C: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:584:PRO:CB	2:J:30:THR:CG2	2.43	0.91
1:C:255:ARG:HH11	1:C:255:ARG:HG2	1.34	0.91
1:A:582:GLY:O	2:J:29:ILE:HG21	1.71	0.91
1:B:255:ARG:HG2	1:B:255:ARG:HH11	1.34	0.90
1:C:609:ALA:HB3	2:H:53:TYR:HH	1.27	0.90
1:D:255:ARG:HG2	1:D:255:ARG:HH11	1.34	0.90
1:A:255:ARG:HG2	1:A:255:ARG:HH11	1.34	0.90
1:A:362:LEU:HD22	2:J:31:SER:O	1.70	0.90
1:A:427:THR:HA	1:A:436:MET:CE	1.99	0.90
1:C:584:PRO:HB3	2:H:30:THR:CB	2.02	0.90
1:B:427:THR:HA	1:B:436:MET:CE	1.99	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:A:610:ASP:CA	2:J:53:TYR:CE1	2.56	0.87
1:A:581:ASN:O	2:J:75:LYS:N	1.97	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:D:609:ALA:C	2:I:53:TYR:CE1	2.54	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:673:ALA:HB1	1:C:674:PRO:HD2	1.58	0.85
1:C:856:TYR:HB3	1:C:864:MET:CE	2.07	0.85
1:D:673:ALA:HB1	1:D:674:PRO:HD2	1.58	0.85
1:D:856:TYR:HB3	1:D:864:MET:CE	2.07	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:576:ILE:HG23	2:I:30:THR:HB	1.59	0.85
1:D:582:GLY:O	2:I:29:ILE:HG21	1.74	0.85
1:C:576:ILE:CG2	2:H:30:THR:O	2.25	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:609:ALA:C	2:J:53:TYR:CE1	2.54	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
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: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:D:734:SER:CB	1:D:860:GLY:HA3	2.08	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: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:A:609:ALA:C	2:J:53:TYR:HE1	1.88	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:582:GLY:O	2:K:29:ILE:HG21	1.80	0.80
1:A:360:HIS:ND1	1:A:361:PRO:HD2	1.97	0.80
1:B:134:LEU:N	1:B:134:LEU:HD12	1.97	0.80
1:B:360:HIS:ND1	1:B:361:PRO:HD2	1.97	0.80
1:C:360:HIS:ND1	1:C:361:PRO:HD2	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:D:609:ALA:C	2:I:53:TYR:HE1	1.87	0.79
1:A:134:LEU:N	1:A:134:LEU:HD12	1.97	0.79
1:B:576:ILE:CG2	2:K:30:THR:O	2.30	0.79
1:B:830:LEU:CD2	1:B:835:LEU:HB2	2.11	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:C:134:LEU:HD12	1:C:134:LEU:N	1.97	0.79
1:D:77:ASP:O	1:D:78:LEU:HD23	1.83	0.79
1:C:581:ASN:O	2:H:75:LYS:N	2.09	0.79
1:D:134:LEU:N	1:D:134:LEU:HD12	1.97	0.79
1:A:920:LEU:HB3	1:A:921:PRO:HD2	1.65	0.79
1:C:77:ASP:O	1:C:78:LEU:HD23	1.83	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: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:D:746:ASP:CA	1:D:760:ARG:HG3	2.14	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:576:ILE:HD12	2:K:53:TYR:HB2	1.65	0.77
1:B:609:ALA:HB3	2:K:53:TYR:HH	0.94	0.77
2:I:29:ILE:HD11	2:I: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
2:H:29:ILE:HD11	2:H:78:TYR:HB3	1.67	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:920:LEU:HB3	1:C:921:PRO:HD2	1.65	0.77
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
2:J:29:ILE:HD11	2:J:78:TYR:HB3	1.67	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:685:LEU:HB3	1:B:686:PRO:HD2	1.68	0.76
1:A:9:VAL:O	1:A:12:GLN:HB3	1.85	0.76
1:B:9:VAL:O	1:B:12:GLN:HB3	1.85	0.76
1:B:581:ASN:O	2:K:75:LYS:N	2.07	0.76
1:B:584:PRO:CG	2:K:71:ARG:NH1	2.45	0.76
1:A:685:LEU:HB3	1:A:686:PRO:HD2	1.68	0.76
1:B:576:ILE:HD11	2:K:53:TYR:HB2	1.68	0.76
1:B:362:LEU:HD13	2:K:32:ASP:HA	1.68	0.75
1:C:11:LEU:HD21	1:C:187:MET:CE	2.15	0.75
1:D:9:VAL:O	1:D:12:GLN:HB3	1.85	0.75
1:D:11:LEU:HD21	1:D:187:MET:CE	2.15	0.75
1:A:11:LEU:HD21	1:A:187:MET:CE	2.15	0.75
1:C:685:LEU:HB3	1:C:686:PRO:HD2	1.68	0.75
1:B:11:LEU:HD21	1:B:187:MET:CE	2.15	0.75
1:C:9:VAL:O	1:C:12:GLN:HB3	1.85	0.75
1:D:685:LEU:HB3	1:D:686:PRO:HD2	1.68	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:B:949:HIS:HD2	1:B:1020:TRP:HE1	1.35	0.75
1:D:362:LEU:HD23	2:I:31:SER:HA	1.67	0.75
1:D:584:PRO:HB3	2:I:30:THR:CB	2.17	0.75
1:B:584:PRO:HG2	2:K:71:ARG:CZ	2.17	0.74
1:C:362:LEU:HD22	2:H:31:SER:CA	2.17	0.74
1:D:38:ASN:HD22	1:D:41:GLU:H	1.35	0.74
1:B:609:ALA:C	2:K:53:TYR:CE1	2.64	0.74
1:C:38:ASN:HD22	1:C:41:GLU:H	1.35	0.74
1:B:377:LEU:HD22	1:B:708:TRP:HA	1.69	0.74
1:B:609:ALA:CB	2:K:53:TYR:HH	1.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:ARG:HB3	1:C:237:ARG:HH11	1.53	0.73
1:C:377:LEU:HD22	1:C:708:TRP:HA	1.69	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:A:38:ASN:HD22	1:A:41:GLU:H	1.35	0.73
1:A:237:ARG:HB3	1:A:237:ARG:HH11	1.54	0.73
1:A:778:THR:HG23	1:A:779:PRO:HD2	1.70	0.73
1:B:237:ARG:HB3	1:B:237:ARG:HH11	1.54	0.73
1:B:579:ASP:OD1	1:B:583:ASN:HB2	1.89	0.73
1:C:652:LEU:HD11	1:C:698:VAL:HB	1.71	0.73
1:D:237:ARG:HH11	1:D:237:ARG:HB3	1.54	0.73
1:D:652:LEU:HD11	1:D:698:VAL:HB	1.71	0.73
1:B:38:ASN:HD22	1:B:41:GLU:H	1.35	0.73
1:B:746:ASP:CA	1:B:760:ARG:HG3	2.14	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:A:559:TYR:HB2	1:A:562:LEU:HD12	1.71	0.72
1:D:237:ARG:HH11	1:D:237:ARG:CB	2.02	0.72
1:A:436:MET:CE	1:A:467:ASN:HD22	2.03	0.72
1:A:655:MET:HG3	1:A:656:VAL:N	2.03	0.72
1:B:436:MET:CE	1:B:467:ASN:HD22	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:576:ILE:HG21	2:H:30:THR:HB	1.70	0.72
1:A:237:ARG:HH11	1:A:237:ARG:CB	2.02	0.72
1:B:436:MET:HE3	1:B:467:ASN:HD22	1.53	0.72
1:D:3:ILE:HG13	1:D:4:THR:N	2.04	0.72
1:B:578:TYR:CD1	2:K:28:SER:OG	2.42	0.72
1:B:655:MET:HG3	1:B:656:VAL:N	2.03	0.72
1:D:778:THR:HG23	1:D:779:PRO:HD2	1.70	0.72
1:A:3:ILE:HG13	1:A:4:THR:N	2.04	0.72
1:A:436:MET:HE3	1:A:467:ASN:HD22	1.53	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:652:LEU:HD11	1:A:698:VAL:HB	1.71	0.72
1:B:237:ARG:HH11	1:B:237:ARG:CB	2.03	0.72
1:C:436:MET:HE3	1:C:467:ASN:HD22	1.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:ILE:HG13	1:B:4:THR:N	2.04	0.72
1:B:652:LEU:HD11	1:B:698:VAL:HB	1.71	0.72
1:A:577:LYS:O	2:J:30:THR:HG21	1.89	0.71
1:D:436:MET:HE3	1:D:467:ASN:HD22	1.53	0.71
1:C:949:HIS:HD2	1:C:1020:TRP:HE1	1.35	0.71
1:A:581:ASN:O	2:J:72:ASP:O	2.07	0.71
1:C:578:TYR:CD2	2:H:28:SER:CB	2.72	0.71
1:B:609:ALA:N	2:K:53:TYR:OH	2.24	0.71
1:C:579:ASP:OD1	1:C:583:ASN:HB2	1.89	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:559:TYR:HB2	1:D: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: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:928:PRO:HB2	1:B:973:ARG:HH11	1.55	0.71
1:A:367:MET:HB3	1:A:372:MET:HE2	1.73	0.71
1:A:650:GLU:HB3	1:A:670:LEU:HD12	1.73	0.71
1:B:576:ILE:HG23	2:K:30:THR:HB	1.70	0.71
1:A:581:ASN:O	2:J:72:ASP:C	2.33	0.70
1:B:367:MET:HB3	1:B:372:MET:HE2	1.73	0.70
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:B:609:ALA:C	2:K:53:TYR:HE1	1.98	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:C:609:ALA:C	2:H:53:TYR:CE1	2.69	0.70
1:A:583:ASN:CG	2:J:72:ASP:HA	2.16	0.69
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:287:ASP:CG	1:D:425:ARG:HH22	2.00	0.69
1:C:367:MET:HB3	1:C:372:MET:HE2	1.73	0.69
1:D:367:MET:HB3	1:D:372:MET:HE2	1.73	0.69
1:A:578:TYR:CD1	2:J:28:SER:OG	2.46	0.69
1:C:650:GLU:HB3	1:C:670:LEU:HD12	1.73	0.69
1:D:581:ASN:O	2:I:72:ASP:C	2.35	0.69
1:D:650:GLU:HB3	1:D:670:LEU:HD12	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:836:ILE:HD13	1:A:836:ILE:N	2.07	0.69
1:C:255:ARG:HG2	1:C:255:ARG:NH1	2.07	0.69
1:A:1020:TRP:HD1	1:A:1021:CYS:N	1.91	0.68
1:B:1020:TRP:HD1	1:B:1021:CYS:N	1.92	0.68
1:D:255:ARG:HG2	1:D:255:ARG:NH1	2.07	0.68
1:D:583:ASN:CG	2:I:72:ASP:HA	2.18	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:835:LEU:C	1:D:836:ILE:HD13	2.19	0.68
1:C:835:LEU:C	1:C:836:ILE:HD13	2.19	0.68
1:D:836:ILE:HD13	1:D:836:ILE:N	2.07	0.68
1:A:35:SER:OG	1:A:37:ARG:NH1	2.27	0.68
1:C:836:ILE:HD13	1:C:836:ILE:N	2.07	0.68
1:C:1020:TRP:HD1	1:C:1021:CYS:N	1.91	0.68
1:D:1020:TRP:HD1	1:D:1021:CYS:N	1.91	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:59:ARG:NH2	1:A:81:ALA:O	2.28	0.67
1:A:581:ASN:CB	2:J:72:ASP:OD1	2.37	0.67
1:B:63:PHE:HB3	1:B:64:PRO:HD2	1.75	0.67
1:C:63:PHE:HB3	1:C:64:PRO:HD2	1.75	0.67
1:D:35:SER:OG	1:D:37:ARG:NH1	2.27	0.67
1:A:11:LEU:HD21	1:A:187:MET:HE3	1.75	0.67
1:B:59:ARG:NH2	1:B:81:ALA:O	2.28	0.67
1:C:35:SER:OG	1:C:37:ARG:NH1	2.27	0.67
1:D:63:PHE:HB3	1:D:64:PRO:HD2	1.75	0.67
1:A:835:LEU:C	1:A:836:ILE:HD13	2.19	0.67
1:B:11:LEU:HD21	1:B:187:MET:HE3	1.76	0.67
1:B:835:LEU:C	1:B:836:ILE:HD13	2.19	0.67
1:C:59:ARG:NH2	1:C:81:ALA:O	2.28	0.67
1:D:610:ASP:HA	2:I:53:TYR:CE1	2.28	0.67
1:A:63:PHE:HB3	1:A:64:PRO:HD2	1.75	0.67
1:A:211:ASP:OD1	1:A:211:ASP:N	2.27	0.67
1:D:59:ARG:NH2	1:D: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:D:965:GLN:O	1:D:969:GLU:HG3	1.94	0.67
1:C:965:GLN:O	1:C:969:GLU:HG3	1.94	0.67
1:D:856:TYR:HB3	1:D:864:MET:HE1	1.77	0.67
1:A:375:ASP:O	1:A:379:MET:HG3	1.95	0.67
1:B:211:ASP:N	1:B:211:ASP:OD1	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:856:TYR:HB3	1:C:864:MET:HE1	1.77	0.67
1:A:965:GLN:O	1:A:969:GLU:HG3	1.94	0.67
1:B:375:ASP:O	1:B:379:MET:HG3	1.95	0.67
1:C:11:LEU:HD21	1:C:187:MET:HE3	1.76	0.66
1:D:11:LEU:HD21	1:D:187:MET:HE3	1.75	0.66
1:D:7:LEU:N	1:D:71:GLU:OE2	2.28	0.66
1:A:30:HIS:HB2	1:A:31:PRO:HD2	1.77	0.66
1:B:965:GLN:O	1:B:969:GLU:HG3	1.94	0.66
1:C:7:LEU:N	1:C:71:GLU:OE2	2.28	0.66
1:D:65:ALA:HB1	1:D:66:PRO:HD2	1.77	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:B:7:LEU:N	1:B:71:GLU:OE2	2.28	0.66
1:C:65:ALA:HB1	1:C:66:PRO:HD2	1.77	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:C:655:MET:HG3	1:C:656:VAL:N	2.03	0.65
1:D:30:HIS:HB2	1:D:31:PRO:HD2	1.77	0.65
1:A:742:THR:HG22	1:A:743:SER:N	2.12	0.65
1:C:427:THR:CA	1:C:436:MET:HE1	2.05	0.65
1:D:375:ASP:O	1:D:379:MET:HG3	1.95	0.65
1:D:655:MET:HG3	1:D:656:VAL:N	2.03	0.65
1:A:427:THR:CA	1:A:436:MET:HE1	2.05	0.65
1:B:742:THR:HG22	1:B:743:SER:N	2.12	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:65:ALA:HB1	1:A:66:PRO:HD2	1.77	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:D:427:THR:CA	1:D:436:MET:HE1	2.05	0.65
1:A:361:PRO:HG3	2:J:53:TYR:CE1	2.31	0.65
1:B:427:THR:CA	1:B:436:MET:HE1	2.05	0.65
1:C:499:ILE:HB	1:C:533:LEU:HB2	1.79	0.65
1:B:856:TYR:HB3	1:B:864:MET:HE1	1.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:ILE:HB	1:A:533:LEU:HB2	1.79	0.64
1:A:856:TYR:HB3	1:A:864:MET:HE1	1.77	0.64
1:D:579:ASP:CG	2:I:73:THR:OG1	2.41	0.64
1:D:824:GLN:HG3	1:D:825:CYS:N	2.11	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:A:282:ARG:HH12	1:D:419:GLY:C	2.06	0.64
1:C:775:GLN:OE1	1:C:890:GLN:NE2	2.30	0.64
1:C:609:ALA:C	2:H:53:TYR:HE1	2.04	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:A:579:ASP:CG	2:J:73:THR:OG1	2.38	0.63
1:A:797:GLU:O	1:A:801:ILE:HD12	1.98	0.63
1:B:255:ARG:HG2	1:B:255:ARG:NH1	2.07	0.63
1:B:797:GLU:O	1:B:801:ILE:HD12	1.98	0.63
1:C:797:GLU:O	1:C:801:ILE:HD12	1.98	0.63
1:D:775:GLN:OE1	1:D:890:GLN:NE2	2.30	0.63
1:D:533:LEU:C	1:D:533:LEU:HD12	2.24	0.63
1:B:609:ALA:C	2:K:53:TYR:OH	2.40	0.63
1:A:533:LEU:HD12	1:A:533:LEU:C	2.24	0.63
1:C:533:LEU:C	1:C:533:LEU:HD12	2.24	0.63
1:D:578:TYR:HA	2:I:30:THR:HG21	1.81	0.63
1:A:856:TYR:CD2	1:A:864:MET:HE1	2.34	0.63
1:B:856:TYR:CD2	1:B:864:MET:HE1	2.34	0.63
1:B:533:LEU:C	1:B:533:LEU:HD12	2.24	0.63
1:C:742:THR:HG22	1:C:743:SER:N	2.12	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:A:287:ASP:OD2	1:D:425:ARG:NH2	2.31	0.63
1:D:746:ASP:HA	1:D:760:ARG:CG	2.22	0.63
1:B:576:ILE:HG13	2:K:53:TYR:CD2	2.34	0.63
1:C:166:ARG:HG3	1:C:392:TYR:HB2	1.81	0.63
1:C:856:TYR:CD2	1:C:864:MET:HE1	2.34	0.62
1:D:166:ARG:HG3	1:D:392:TYR:HB2	1.81	0.62
1:D:856:TYR:CD2	1:D:864:MET:HE1	2.34	0.62
1:D:906:TYR:HB3	1:D:907:PRO:HD2	1.80	0.62
1:D:211:ASP:N	1:D:211:ASP:OD1	2.27	0.62
1:A:578:TYR:HA	2:J:30:THR:HG21	1.80	0.62
1:B:66:PRO:HD2	1:B:67:GLU:HG2	1.81	0.62
1:C:211:ASP:OD1	1:C:211:ASP:N	2.27	0.62
1:C:906:TYR:HB3	1:C:907:PRO:HD2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:PRO:HD2	1:A:67:GLU:HG2	1.81	0.62
1:C:576:ILE:HD11	2:H:53:TYR:CB	2.29	0.62
1:A:166:ARG:HG3	1:A:392:TYR:HB2	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: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:100:TYR:HB2	1:D:203:TRP:CD2	2.35	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:A:906:TYR:HB3	1:A:907:PRO:HD2	1.80	0.61
1:C:100:TYR:HB2	1:C:203:TRP:CD2	2.34	0.61
1:D:576:ILE:HG13	2:I:53:TYR:CD2	2.35	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:A:822:LEU:HD12	1:A:824:GLN:N	2.16	0.61
1:B:272:ALA:HB1	1:B:273:PRO:HD2	1.81	0.61
1:B:578:TYR:HA	2:K:30:THR:HG21	1.82	0.61
2:J:33:TYR:HB2	2:J:98:TRP:HB2	1.83	0.61
2:K:33:TYR:HB2	2:K:98:TRP:HB2	1.83	0.61
1:A:419:GLY:C	1:D:282:ARG:HH12	2.08	0.61
1:B:822:LEU:HD12	1:B:824:GLN:N	2.16	0.61
1:B:928:PRO:O	1:B:973:ARG:NH1	2.34	0.61
1:C:595:THR:HG23	1:C:596:PRO:HA	1.83	0.61
1:C:609:ALA:CB	2:H:53:TYR:CZ	2.64	0.61
1:A:272:ALA:HB1	1:A:273:PRO:HD2	1.81	0.61
1:A:928:PRO:O	1:A:973:ARG:NH1	2.34	0.61
1:B:576:ILE:CG2	2:K:30:THR:CB	2.67	0.61
1:B:906:TYR:HB3	1:B:907:PRO:HD2	1.81	0.61
1:D:610:ASP:OD1	1:D:612:THR:HG23	2.01	0.61
1:A:140:ARG:NH1	1:A:170:GLU:OE1	2.31	0.61
1:A:227:VAL:HG13	1:A:240:LEU:HD11	1.83	0.61
1:B:100:TYR:HB2	1:B:203:TRP:CD2	2.34	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:A:100:TYR:HB2	1:A:203:TRP:CD2	2.35	0.61
1:B:227:VAL:HG13	1:B:240:LEU:HD11	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:MET:HE3	1:C:357:HIS:CD2	2.36	0.61
1:C:610:ASP:OD1	1:C:612:THR:HG23	2.01	0.61
1:C:651:LEU:HD12	1:C:669:PRO:HA	1.83	0.61
1:D:581:ASN:CB	2:I:72:ASP:OD1	2.40	0.61
1:D:651:LEU:HD12	1:D:669:PRO:HA	1.83	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:C:304:GLU:C	1:C:305:ILE:HG13	2.26	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:D:202:MET:HE3	1:D:357:HIS:CD2	2.36	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:D:304:GLU:C	1:D:305:ILE:HG13	2.26	0.60
1:A:576:ILE:HG13	2:J:53:TYR:CD2	2.35	0.60
1:B:581:ASN:O	2:K:72:ASP:C	2.43	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:581:ASN:O	2:H:72:ASP:C	2.43	0.60
1:C:928:PRO:O	1:C:973:ARG:NH1	2.33	0.60
1:C:227:VAL:HG13	1:C:240:LEU:HD11	1.83	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:D:778:THR:CG2	1:D:779:PRO:HD2	2.30	0.60
1:D:928:PRO:O	1:D:973:ARG:NH1	2.34	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:I:34:TRP:HB3	2:I: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
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:767:GLN:HG3	1:A:768:MET:N	2.15	0.60
1:A:830:LEU:HD21	1:A:835:LEU:HB2	1.84	0.60
1:B:767:GLN:HG3	1:B:768:MET:N	2.15	0.60
1:B:778:THR:CG2	1:B:779:PRO:HD2	2.30	0.60
1:B:830:LEU:HD21	1:B:835:LEU:HB2	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:734:SER:HB3	1:B:860:GLY:CA	2.30	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:C:822:LEU:HD11	1:C:824:GLN:O	2.01	0.60
1:D:870:VAL:HG12	1:D:871:GLU:N	2.16	0.60
1:A:651:LEU:HD12	1:A:669:PRO:HA	1.83	0.60
1:B:304:GLU:C	1:B:305:ILE:HG13	2.26	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:870:VAL:HG12	1:A:871:GLU:N	2.16	0.60
1:C:609:ALA:C	2:H:53:TYR:OH	2.45	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:B:102:ASN:ND2	1:B:201:ASP:HB2	2.16	0.59
1:B:595:THR:HG23	1:B:596:PRO:HA	1.82	0.59
1:B:701:VAL:HG12	1:B:702:GLN:N	2.17	0.59
1:C:610:ASP:N	2:H:53:TYR:CZ	2.70	0.59
1:D:505:ARG:HG2	1:D:996:ASP:OD2	2.02	0.59
1:A:128:ASN:HA	1:A:180:GLY:O	2.02	0.59
1:A:304:GLU:C	1:A:305:ILE:HG13	2.26	0.59
1:A:696:LEU:HD12	1:A:697:THR:N	2.17	0.59
1:A:701:VAL:HG12	1:A:702:GLN:N	2.17	0.59
1:A:734:SER:HB3	1:A:860:GLY:CA	2.30	0.59
1:B:128:ASN:HA	1:B:180:GLY:O	2.02	0.59
1:B:696:LEU:HD12	1:B:697:THR: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:D:701:VAL:HG12	1:D:702:GLN:N	2.17	0.59
1:A:102:ASN:ND2	1:A:201:ASP:HB2	2.16	0.59
1:B:202:MET:HE3	1:B:357:HIS:CD2	2.36	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:A:511:PRO:HA	1:A:516:PRO:HB3	1.84	0.59
1:A:595:THR:HG23	1:A:596:PRO:HA	1.82	0.59
1:D:140:ARG:NH1	1:D:170:GLU:OE1	2.31	0.59
1:D:511:PRO:HA	1:D:516:PRO:HB3	1.84	0.59
2:H:33:TYR:HB2	2:H:98:TRP:HB2	1.83	0.59
2:I:33:TYR:HB2	2:I:98:TRP:HB2	1.83	0.59
1:A:202:MET:HE3	1:A:357:HIS:CD2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:ARG:HH22	1:D:287:ASP:CG	2.11	0.59
1:C:140:ARG:NH1	1:C:170:GLU:OE1	2.31	0.59
1:C:696:LEU:HD12	1:C:697:THR:N	2.18	0.59
1:B:511:PRO:HA	1:B:516:PRO:HB3	1.84	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:576:ILE:HG21	2:J:30:THR:C	2.27	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:C:737:ILE:HG13	1:C:738:PRO:N	2.17	0.59
1:A:856:TYR:HD2	1:A:864:MET:HE1	1.68	0.58
1:A:578:TYR:CE2	2:J:28:SER:CB	2.87	0.58
1:D:576:ILE:HG21	2:I:30:THR:C	2.28	0.58
1:D:737:ILE:HG13	1:D:738:PRO:N	2.17	0.58
1:A:336:ARG:NH2	1:A:338:GLU:OE1	2.36	0.58
1:A:759:ASN:OD1	1:A:761:GLN:N	2.35	0.58
1:B:759:ASN:OD1	1:B:761:GLN:N	2.35	0.58
1:C:128:ASN:HA	1:C:180:GLY:O	2.02	0.58
1:D:128:ASN:HA	1:D:180:GLY:O	2.02	0.58
1:D:734:SER:HB3	1:D:860:GLY:CA	2.30	0.58
1:B:856:TYR:HD2	1:B:864:MET:HE1	1.68	0.58
1:B:336:ARG:NH2	1:B:338:GLU:OE1	2.36	0.58
1:B:583:ASN:CB	2:K:73:THR:H	1.97	0.58
1:D:645:ARG:HH22	1:D:650:GLU:CD	2.11	0.58
1:D:856:TYR:HD2	1:D:864:MET:HE1	1.68	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:C:645:ARG:HH22	1:C:650:GLU:CD	2.11	0.58
1:C:734:SER:HB3	1:C:860:GLY:CA	2.30	0.58
1:C:856:TYR:HD2	1:C:864:MET:HE1	1.68	0.58
1:A:769:TRP:NE1	1:A:774:LYS:HG3	2.19	0.58
1:B:581:ASN:O	2:K:72:ASP:O	2.22	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: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:C:584:PRO:HB3	2:H:30:THR:CA	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:C:473:ARG:HD3	2.04	0.57
1:D:473:ARG:O	1:D:473:ARG:HD3	2.04	0.57
1:A:473:ARG:O	1:A:473:ARG:HD3	2.04	0.57
1:A:645:ARG:HH22	1:A:650:GLU:CD	2.11	0.57
1:C:26:ARG:HD2	1:C:169:SER:HA	1.87	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:460:ASN:ND2	1:A:461:GLU:HG2	2.20	0.57
1:A:576:ILE:HG21	2:J:30:THR:CB	2.28	0.57
1:B:460:ASN:ND2	1:B:461:GLU:HG2	2.20	0.57
1:B:473:ARG:O	1:B:473:ARG:HD3	2.04	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:C:6:SER:HB2	1:C:71:GLU:OE2	2.04	0.57
1:D:834:VAL:HG12	1:D:835:LEU:N	2.19	0.57
1:D:6:SER:HB2	1:D:71:GLU:OE2	2.04	0.57
1:D:578:TYR:CE2	2:I:28:SER:CB	2.87	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:B:645:ARG:HH22	1:B:650:GLU:CD	2.11	0.57
1:B:26:ARG:HD2	1:B:169:SER:HA	1.87	0.57
1:B:360:HIS:CE1	1:B:362:LEU:HB2	2.40	0.57
1:B:429:ASP:OD1	1:B:430:PRO:HD2	2.04	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:D:618:THR:HG22	1:D:912:ALA:HB1	1.86	0.57
1:A:26:ARG:HD2	1:A:169:SER:HA	1.87	0.57
1:A:360:HIS:CE1	1:A:362:LEU:HB2	2.40	0.57
1:B:316:HIS:HD2	1:B:317:THR:O	1.87	0.57
1:C:460:ASN:ND2	1:C:461:GLU:HG2	2.20	0.57
3:N:94:TRP:CD2	3:N:95:PRO:HA	2.40	0.57
1:A:316:HIS:HD2	1:A:317:THR:O	1.87	0.56
1:A:429:ASP:OD1	1:A:430:PRO:HD2	2.05	0.56
1:A:429:ASP:OD1	1:A:431[B]:ARG:HG3	2.05	0.56
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:429:ASP:OD1	1:B:431[B]:ARG:HG3	2.05	0.56
1:B:834:VAL:HG12	1:B:835:LEU:N	2.19	0.56
1:C:584:PRO:HB3	2:H:30:THR:HA	1.87	0.56
1:A:763:GLY:HA3	1:A:822:LEU:HD21	1.87	0.56
1:A:834:VAL:HG12	1:A:835:LEU:N	2.19	0.56
1:B:763:GLY:HA3	1:B:822:LEU:HD21	1.87	0.56
1:C:830:LEU:HD21	1:C:835:LEU:HB2	1.84	0.56
1:D:134:LEU:HD12	1:D:134:LEU:H	1.69	0.56
1:D:457:SER:HA	1:D:485:GLN:O	2.05	0.56
1:C:316:HIS:HD2	1:C:317:THR:O	1.87	0.56
1:C:457:SER:HA	1:C:485:GLN:O	2.05	0.56
1:D:830:LEU:HD21	1:D:835:LEU:HB2	1.84	0.56
1:B:618:THR:HG22	1:B:912:ALA:HB1	1.86	0.56
1:C:134:LEU:HD12	1:C:134:LEU:H	1.69	0.56
1:C:577:LYS:O	2:H:30:THR:HG21	2.06	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:A:618:THR:HG22	1:A:912:ALA:HB1	1.86	0.56
1:A:763:GLY:HA3	1:A:822:LEU:CD2	2.36	0.56
1:B:576:ILE:CG1	2:K:53:TYR:HD2	2.19	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:C:360:HIS:CE1	1:C:361:PRO:HD2	2.41	0.56
1:D:360:HIS:CE1	1:D:361:PRO:HD2	2.41	0.56
1:A:531:ARG:O	1:A:561:ARG:NH1	2.39	0.56
1:B:425:ARG:HH22	1:C:287:ASP:CG	2.14	0.56
1:B:531:ARG:O	1:B:561:ARG:NH1	2.39	0.56
1:C:18:ASN:OD1	1:C:19:PRO:HD2	2.06	0.56
1:C:763:GLY:HA3	1:C:822:LEU:HD21	1.87	0.56
1:D:18:ASN:OD1	1:D:19:PRO:HD2	2.06	0.56
1:D:429:ASP:OD1	1:D:431[B]:ARG:HG3	2.05	0.56
3:O:2:ILE:HD13	3:O:29:ILE:HG22	1.88	0.56
1:A:134:LEU:HD12	1:A:134:LEU:H	1.69	0.56
1:B:577:LYS:O	1:B:584:PRO:HA	2.06	0.56
1:C:429:ASP:OD1	1:C:431[B]:ARG:HG3	2.05	0.56
1:C:577:LYS:O	1:C:584:PRO:HA	2.06	0.56
1:D:759:ASN:OD1	1:D:761:GLN:N	2.35	0.56
1:A:833:ALA:HB1	1:A:858:ILE:O	2.06	0.56
1:A:1020:TRP:CD1	1:A:1021:CYS:N	2.74	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:833:ALA:HB1	1:B:858:ILE:O	2.06	0.56
1:D:577:LYS:O	1:D:584:PRO:HA	2.06	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:B:18:ASN:OD1	1:B:19:PRO:HD2	2.06	0.55
1:B:134:LEU:HD12	1:B:134:LEU:H	1.69	0.55
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: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:425:ARG:NH2	1:C:287:ASP:OD2	2.39	0.55
1:B:610:ASP:HB3	2:K:53:TYR:CD1	2.42	0.55
1:A:18:ASN:OD1	1:A:19:PRO:HD2	2.06	0.55
1:C:763:GLY:HA3	1:C:822:LEU:CD2	2.36	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:395:HIS:ND1	1:C:396:PRO:HD2	2.22	0.55
1:C:531:ARG:O	1:C:561:ARG:NH1	2.39	0.55
1:D:395:HIS:ND1	1:D:396:PRO:HD2	2.22	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:457:SER:HA	1:A:485:GLN:O	2.06	0.55
1:A:576:ILE:HG13	2:J:53:TYR:HD2	1.72	0.55
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
1:D:763:GLY:HA3	1:D:822:LEU:CD2	2.36	0.55
3:N:37:GLN:HB2	3:N:47:LEU:HD11	1.89	0.55
1:A:38:ASN:ND2	1:A:41:GLU:N	2.48	0.55
1:A:100:TYR:HB2	1:A:203:TRP:CE3	2.42	0.55
1:A:786:ARG:HA	1:A:964:GLN:OE1	2.07	0.55
1:B:610:ASP:CB	2:K:53:TYR:CE1	2.90	0.55
1:B:786:ARG:HA	1:B:964:GLN:OE1	2.07	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:583:ASN:OD1	2:I:72:ASP:N	2.40	0.55
3:M:76:ASN:C	3:M:76:ASN:HD22	2.15	0.55
1:A:395:HIS:ND1	1:A:396:PRO:HD2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:579:ASP:CG	2:H:73:THR:OG1	2.45	0.54
1:D:100:TYR:HB2	1:D:203:TRP:CE3	2.42	0.54
1:A:609:ALA:C	2:J:53:TYR:CZ	2.80	0.54
1:B:942:ARG:HA	1:B:953:GLY:O	2.07	0.54
1:C:576:ILE:HG21	2:H:30:THR:C	2.31	0.54
3:O:76:ASN:C	3:O:76:ASN:HD22	2.15	0.54
1:A:942:ARG:HA	1:A: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
3:L:76:ASN:C	3:L:76:ASN:HD22	2.15	0.54
1:A:662:PRO:C	1:A:663:LEU:HD23	2.32	0.54
1:B:662:PRO:C	1:B:663:LEU:HD23	2.32	0.54
1:C:166:ARG:HG3	1:C:392:TYR:CB	2.38	0.54
1:C:749:ILE:O	1:C:755:ARG:HG3	2.07	0.54
1:D:166:ARG:HG3	1:D:392:TYR:CB	2.38	0.54
1:A:418:HIS:O	1:D:282:ARG:HD3	2.08	0.54
1:B:395:HIS:ND1	1:B:396:PRO:HD2	2.22	0.54
1:B:668:VAL:HG13	1:B:669:PRO:HD2	1.89	0.54
1:C:110:ASN:O	1:C:113:PHE:N	2.39	0.54
1:D:749:ILE:O	1:D:755:ARG:HG3	2.08	0.54
1:A:597:ASN:HD22	1:A:599:ARG:N	1.94	0.54
1:B:30:HIS:HB2	1:B:31:PRO:CD	2.38	0.54
1:D:38:ASN:HD21	1:D:41:GLU:H	1.53	0.54
3:N:76:ASN:HD22	3:N:76:ASN:C	2.15	0.54
1:A:30:HIS:HB2	1:A:31:PRO:CD	2.38	0.54
1:A:668:VAL:HG13	1:A:669:PRO:HD2	1.89	0.54
1:A:746:ASP:HA	1:A:760:ARG:CG	2.22	0.54
1:C:362:LEU:HD21	2:H:31:SER:HA	1.88	0.54
1:C:662:PRO:C	1:C:663:LEU:HD23	2.32	0.54
1:D:110:ASN:O	1:D:113:PHE:N	2.39	0.54
1:C:597:ASN:HD22	1:C:599:ARG:N	1.94	0.54
1:C:786:ARG:HA	1:C:964:GLN:OE1	2.07	0.54
1:C:942:ARG:HA	1:C:953:GLY:O	2.07	0.54
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: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:D:1020:TRP:CD1	1:D:1021:CYS:N	2.74	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:LEU:HD21	2:J:31:SER:CA	2.38	0.54
1:B:90:TRP:HE1	1:B:96:ASP:CG	2.16	0.54
1:C:38:ASN:HD21	1:C:41:GLU:H	1.53	0.54
1:D:597:ASN:HD22	1:D:599:ARG:N	1.94	0.54
1:D:662:PRO:C	1:D:663:LEU:HD23	2.32	0.54
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.89	0.54
1:A:576:ILE:HD11	2:J:53:TYR:CB	2.37	0.53
1:C:584:PRO:HG2	2:H:71:ARG:HH12	1.63	0.53
1:C:668:VAL:HG13	1:C:669:PRO:HD2	1.89	0.53
1:D:90:TRP:HE1	1:D:96:ASP:CG	2.16	0.53
1:D:942:ARG:HA	1:D:953:GLY:O	2.07	0.53
1:A:90:TRP:HE1	1:A:96:ASP:CG	2.16	0.53
1:A:166:ARG:HG3	1:A:392:TYR:CB	2.38	0.53
1:B:80:GLU:H	1:B:80:GLU:CD	2.01	0.53
1:B:166:ARG:HG3	1:B:392:TYR:CB	2.38	0.53
1:C:79:PRO:N	1:C:80:GLU:OE1	2.41	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: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:A:79:PRO:N	1:A:80:GLU:OE1	2.41	0.53
1:B:79:PRO:N	1:B:80:GLU:OE1	2.41	0.53
1:C:90:TRP:HE1	1:C:96:ASP:CG	2.16	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:A:749:ILE:O	1:A:755:ARG:HG3	2.07	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:356:ARG:HH22	1:A:367:MET:HE2	1.74	0.53
1:B:356:ARG:HH22	1:B:367:MET:HE2	1.74	0.53
1:B:749:ILE:O	1:B:755:ARG:HG3	2.08	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:A:80:GLU:H	1:A:80:GLU:CD	2.01	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:B:1017:GLN:O	1:B:1018:LEU:HD23	2.09	0.53
1:D:357:HIS:HD2	1:D:392:TYR:OH	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:416:GLU:OE2	1:D:461:GLU:HG3	2.09	0.53
1:A:416:GLU:OE2	1:A:461:GLU:HG3	2.09	0.53
1:A:1017:GLN:O	1:A:1018:LEU:HD23	2.09	0.53
1:B:416:GLU:OE2	1:B:461:GLU:HG3	2.09	0.53
1:B:959:ILE:HG23	1:B:959:ILE:O	2.09	0.53
1:C:355:ASN:OD1	1:C:388:ARG:HD3	2.09	0.53
1:C:357:HIS:HD2	1:C:392:TYR:OH	1.92	0.53
1:D:355:ASN:OD1	1:D:388:ARG:HD3	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:A:959:ILE:O	1:A:959:ILE:HG23	2.09	0.52
1:B:357:HIS:HD2	1:B:392:TYR:OH	1.91	0.52
1:A:357:HIS:HD2	1:A:392:TYR:OH	1.92	0.52
1:B:251:ARG:NH1	1:B:251:ARG:HG2	2.25	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:251:ARG:HG2	1:A:251:ARG:NH1	2.25	0.52
1:B:609:ALA:C	2:K:53:TYR:CZ	2.88	0.52
1:D:576:ILE:HG13	2:I:53:TYR:HD2	1.72	0.52
1:D:959:ILE:HG23	1:D:959:ILE:O	2.09	0.52
1:C:6:SER:OG	1:C:9:VAL:HB	2.09	0.52
1:C:80:GLU:CD	1:C:80:GLU:H	2.01	0.52
1:C:959:ILE:HG23	1:C:959:ILE:O	2.09	0.52
1:D:6:SER:OG	1:D:9:VAL:HB	2.09	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:D:742:THR:HG22	1:D:743:SER:H	1.74	0.52
1:B:355:ASN:OD1	1:B:388:ARG:HD3	2.09	0.52
1:B:654:TRP:CE2	1:B:666:GLY:HA3	2.44	0.52
1:B:749:ILE:HD12	1:B:749:ILE:N	2.25	0.52
1:D:80:GLU:H	1:D:80:GLU:CD	2.01	0.52
1:A:110:ASN:O	1:A:113:PHE:N	2.39	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:808:GLU:OE1	1:A:808:GLU:HA	2.10	0.52
1:C:356:ARG:HD2	1:C:379:MET:HE1	1.92	0.52
1:D:584:PRO:CB	2:I:30:THR:CG2	2.43	0.52
1:A:6:SER:OG	1:A:9:VAL:HB	2.09	0.52
1:C:920:LEU:HB3	1:C:921:PRO:CD	2.39	0.52
1:D:356:ARG:HD2	1:D:379:MET:HE1	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:920:LEU:HB3	1:D:921:PRO:CD	2.39	0.52
1:A:425:ARG:NH2	1:D:287:ASP:OD2	2.43	0.52
1:C:292:ARG:C	1:C:293:LEU:HD23	2.35	0.52
1:C:878:HIS:HB3	1:C:1009:LEU:O	2.10	0.52
1:D:362:LEU:CD2	2:I:32:ASP:N	2.70	0.52
2:K:42:GLY:O	2:K:43:ASN:HB2	2.10	0.52
1:A:292:ARG:C	1:A:293:LEU:HD23	2.35	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:B:292:ARG:C	1:B:293:LEU:HD23	2.35	0.51
1:B:808:GLU:OE1	1:B:808:GLU:HA	2.10	0.51
1:D:292:ARG:C	1:D:293:LEU:HD23	2.35	0.51
1:D:878:HIS:HB3	1:D:1009:LEU:O	2.10	0.51
1:A:282:ARG:NH1	1:D:419:GLY:C	2.68	0.51
1:A:742:THR:HG22	1:A:743:SER:H	1.74	0.51
1:A:26:ARG:CD	1:A:169:SER:HB3	2.41	0.51
1:A:254:LEU:O	1:A:255:ARG:NH1	2.44	0.51
1:B:362:LEU:HD21	2:K:30:THR:O	2.10	0.51
1:B:742:THR:HG22	1:B:743:SER:H	1.74	0.51
1:A:576:ILE:HG21	2:J:30:THR:CA	2.41	0.51
1:A:878:HIS:HB3	1:A:1009:LEU:O	2.10	0.51
1:B:26:ARG:CD	1:B:169:SER:HB3	2.41	0.51
1:B:254:LEU:O	1:B:255:ARG:NH1	2.44	0.51
1:B:576:ILE:HG13	2:K:53:TYR:HD2	1.73	0.51
1:B:894:ARG:HD3	1:B:919:ASP:OD1	2.11	0.51
1:D:26:ARG:CD	1:D:169:SER:HB3	2.41	0.51
1:D:906:TYR:HB3	1:D:907:PRO:CD	2.41	0.51
1:A:894:ARG:HD3	1:A:919:ASP:OD1	2.11	0.51
1:C:26:ARG:CD	1:C:169:SER:HB3	2.41	0.51
1:C:30:HIS:HB2	1:C:31:PRO:CD	2.38	0.51
1:C:356:ARG:HH22	1:C:367:MET:HE2	1.74	0.51
1:D:30:HIS:HB2	1:D:31:PRO:CD	2.38	0.51
3:O:2:ILE:HD13	3:O:29:ILE:CG2	2.41	0.51
1:A:130:ASP:OD2	1:A:132:SER:OG	2.28	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:D:403:ASP:CG	1:D:451:PRO:HD2	2.36	0.51
1:B:584:PRO:HB3	2:K:30:THR:CA	2.41	0.51
1:C:403:ASP:CG	1:C:451:PRO:HD2	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:578:TYR:CE2	2:H:28:SER:CB	2.94	0.51
1:D:356:ARG:HH22	1:D:367:MET:HE2	1.74	0.51
3:N:2:ILE:HD13	3:N:29:ILE:CG2	2.41	0.51
1:B:403:ASP:CG	1:B:451:PRO:HD2	2.36	0.51
1:B:878:HIS:HB3	1:B:1009:LEU:O	2.10	0.51
1:C:906:TYR:HB3	1:C:907:PRO:CD	2.41	0.51
1:D:230:ARG:HH11	1:D:230:ARG:CG	2.24	0.51
1:A:254:LEU:C	1:A:255:ARG:HG2	2.36	0.51
1:A:403:ASP:CG	1:A:451:PRO:HD2	2.36	0.51
1:A:610:ASP:HB3	2:J:53:TYR:CD1	2.46	0.51
1:A:836:ILE:HG22	1:A:837:THR:N	2.26	0.51
1:B:148:SER:HB3	1:B:190:ARG:O	2.10	0.51
1:B:254:LEU:C	1:B:255:ARG:HG2	2.36	0.51
1:B:576:ILE:HG21	2:K:30:THR:CB	2.38	0.51
1:C:230:ARG:CG	1:C:230:ARG:HH11	2.24	0.51
1:C:658:LEU:O	1:C:659:ASP:C	2.54	0.51
1:C:749:ILE:HD12	1:C:749:ILE:N	2.25	0.51
1:C:808:GLU:OE1	1:C:808:GLU:HA	2.10	0.51
1:D:531:ARG:HB3	1:D:532:PRO:HD2	1.92	0.51
1:D:808:GLU:OE1	1:D:808:GLU:HA	2.10	0.51
2:H:42:GLY:O	2:H:43:ASN:HB2	2.10	0.51
2:I:42:GLY:O	2:I:43:ASN:HB2	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: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:D:251:ARG:HG2	1:D:251:ARG:NH1	2.25	0.51
1:D:576:ILE:HD11	2:I:53:TYR:O	2.11	0.51
1:D:658:LEU:O	1:D:659:ASP:C	2.54	0.51
1:B:542:MET:HA	1:B:604:ASN:HA	1.92	0.50
1:B:836:ILE:HG22	1:B:837:THR:N	2.26	0.50
1:C:130:ASP:OD2	1:C:132:SER:OG	2.28	0.50
1:D:130:ASP:OD2	1:D:132:SER:OG	2.28	0.50
1:D:749:ILE:N	1:D:749:ILE:HD12	2.25	0.50
1:D:894:ARG:HD3	1:D:919:ASP:OD1	2.11	0.50
1:A:65:ALA:HB1	1:A:66:PRO:CD	2.41	0.50
1:A:542:MET:HA	1:A:604:ASN:HA	1.92	0.50
1:A:576:ILE:HD11	2:J:53:TYR:O	2.11	0.50
1:A:770:ILE:O	1:A:770:ILE:HG22	2.10	0.50
1:A:906:TYR:HB3	1:A:907:PRO:CD	2.41	0.50
1:C:822:LEU:HD12	1:C:824:GLN:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:578:TYR:CE2	2:I:28:SER:HB3	2.47	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:A:419:GLY:C	1:D:282:ARG:NH1	2.68	0.50
1:B:65:ALA:HB1	1:B:66:PRO:CD	2.41	0.50
1:B:881:ARG:HD3	1:B:987:ASP:CG	2.36	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:B:356:ARG:HD2	1:B:379:MET:HE1	1.92	0.50
1:B:770:ILE:O	1:B:770:ILE:HG22	2.10	0.50
1:C:38:ASN:ND2	1:C:41:GLU:N	2.48	0.50
1:C:542:MET:HA	1:C:604:ASN:HA	1.92	0.50
1:D:38:ASN:ND2	1:D:41:GLU:N	2.48	0.50
1:D:822:LEU:HD12	1:D:824:GLN:H	1.76	0.50
1:A:356:ARG:HD2	1:A:379:MET:HE1	1.92	0.50
1:A:881:ARG:HD3	1:A:987:ASP:CG	2.36	0.50
1:B:73:TRP:CZ2	1:B:122:CYS:HB3	2.47	0.50
1:B:906:TYR:HB3	1:B:907:PRO:CD	2.41	0.50
1:A:580:GLU:O	2:J:74:SER:HB2	2.11	0.50
1:A:920:LEU:HB3	1:A:921:PRO:CD	2.39	0.50
1:C:362:LEU:HD21	2:H:31:SER:CA	2.41	0.50
1:C:531:ARG:HB3	1:C:532:PRO:HD2	1.92	0.50
1:D:360:HIS:CG	1:D:361:PRO:HD2	2.47	0.50
1:D:767:GLN:CG	1:D:768:MET:N	2.75	0.50
1:C:254:LEU:C	1:C:255:ARG:HG2	2.36	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:D:254:LEU:C	1:D:255:ARG:HG2	2.36	0.50
1:A:100:TYR:CZ	1:A:602:CYS:HB3	2.47	0.50
1:A:433:LEU:O	1:A:437:SER:HB3	2.12	0.50
1:A:584:PRO:HB3	2:J:30:THR:CA	2.42	0.50
1:A:658:LEU:HD23	1:A:661:LYS:HZ3	1.77	0.50
1:B:38:ASN:HD21	1:B:41:GLU:H	1.53	0.50
1:B:100:TYR:CZ	1:B:602:CYS:HB3	2.47	0.50
1:B:433:LEU:O	1:B:437:SER:HB3	2.12	0.50
1:B:920:LEU:HB3	1:B:921:PRO:CD	2.39	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:77:ASP:C	1:B:78:LEU:HD23	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:361:PRO:HG3	2:H:53:TYR:CE1	2.47	0.50
1:C:881:ARG:HD3	1:C:987:ASP:CG	2.36	0.50
1:D:73:TRP:CZ2	1:D:122:CYS:HB3	2.47	0.50
1:D:881:ARG:HD3	1:D:987:ASP:CG	2.36	0.50
1:A:38:ASN:HD21	1:A:41:GLU:H	1.53	0.49
1:A:77:ASP:C	1:A:78:LEU:HD23	2.37	0.49
1:A:822:LEU:HD12	1:A:824:GLN:H	1.76	0.49
1:B:584:PRO:HB3	2:K:30:THR:HA	1.94	0.49
1:B:638:VAL:O	1:B:677:LYS:HA	2.12	0.49
1:B:822:LEU:HD12	1:B:824:GLN:H	1.76	0.49
1:D:362:LEU:HD21	2:I:31:SER:CA	2.38	0.49
2:I:33:TYR:HB2	2:I:98:TRP:CB	2.42	0.49
1:A:282:ARG:CG	1:D:423:MET:HB2	2.42	0.49
1:A:638:VAL:O	1:A:677:LYS:HA	2.12	0.49
1:B:360:HIS:CG	1:B:361:PRO:HD2	2.47	0.49
1:B:531:ARG:HB3	1:B:532:PRO:HD2	1.92	0.49
1:D:708:TRP:CE3	1:D:709:SER:HB3	2.48	0.49
2:H:33:TYR:HB2	2:H:98:TRP:CB	2.42	0.49
1:A:95:TYR:CD1	1:A:95:TYR:N	2.79	0.49
1:A:360:HIS:CG	1:A:361:PRO:HD2	2.47	0.49
1:B:230:ARG:HH11	1:B:230:ARG:CG	2.24	0.49
1:B:696:LEU:HD12	1:B:697:THR:H	1.74	0.49
1:C:100:TYR:CZ	1:C:602:CYS:HB3	2.47	0.49
1:C:708:TRP:CE3	1:C:709:SER:HB3	2.48	0.49
1:C:763:GLY:CA	1:C:822:LEU:HD21	2.42	0.49
1:D:652:LEU:HD12	1:D:699:ARG:O	2.12	0.49
1:A:230:ARG:HH11	1:A:230:ARG:CG	2.24	0.49
1:B:95:TYR:CD1	1:B:95:TYR:N	2.79	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:C:836:ILE:HG22	1:C:837:THR:N	2.26	0.49
1:C:882:ILE:O	1:C:882:ILE:HG22	2.12	0.49
1:D:638:VAL:O	1:D:677:LYS:HA	2.12	0.49
1:D:763:GLY:CA	1:D:822:LEU:HD21	2.42	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:A:531:ARG:HB3	1:A:532:PRO:HD2	1.92	0.49
1:B:130:ASP:OD2	1:B:132:SER:OG	2.28	0.49
1:B:576:ILE:HG21	2:K:30:THR:C	2.34	0.49
1:B:767:GLN:CG	1:B:768:MET:N	2.75	0.49
1:C:638:VAL:O	1:C:677:LYS:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:TYR:CZ	1:D:602:CYS:HB3	2.47	0.49
1:D:882:ILE:O	1:D:882:ILE:HG22	2.12	0.49
1:A:708:TRP:CE3	1:A:709:SER:HB3	2.48	0.49
1:C:578:TYR:CE2	2:H:28:SER:HB3	2.46	0.49
1:C:770:ILE:O	1:C:770:ILE:HG22	2.10	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:770:ILE:O	1:D:770:ILE:HG22	2.10	0.49
1:D:836:ILE:HG22	1:D:837:THR:N	2.26	0.49
1:B:658:LEU:O	1:B:659:ASP:C	2.54	0.49
1:D:105:TYR:CE2	1:D:199:ASP:HB2	2.48	0.49
1:D:584:PRO:HB3	2:I:30:THR:CA	2.43	0.49
2:J:33:TYR:HB2	2:J:98:TRP:CB	2.42	0.49
1:A:153:TRP:HA	1:A:157:ARG:O	2.13	0.49
1:A:576:ILE:CG1	2:J:53:TYR:HB2	2.41	0.49
1:A:658:LEU:O	1:A:659:ASP:C	2.54	0.49
1:A:767:GLN:CG	1:A:768:MET:N	2.75	0.49
1:B:143:PHE:CD1	1:B:143:PHE:N	2.81	0.49
1:C:77:ASP:C	1:C:78:LEU:HD23	2.37	0.49
1:C:595:THR:HG23	1:C:596:PRO:CA	2.43	0.49
1:D:77:ASP:C	1:D:78:LEU:HD23	2.37	0.49
1:D:595:THR:HG23	1:D:596:PRO:CA	2.43	0.49
1:D:610:ASP:HB3	2:I:53:TYR:CD1	2.47	0.49
1:A:143:PHE:N	1:A:143:PHE:CD1	2.81	0.49
1:B:12:GLN:HG3	1:B:13:ARG:N	2.27	0.49
1:B:153:TRP:HA	1:B:157:ARG:O	2.13	0.49
1:C:105:TYR:CE2	1:C:199:ASP:HB2	2.48	0.49
2:K:33:TYR:HB2	2:K:98:TRP:CB	2.42	0.49
1:A:30:HIS:ND1	1:A:31:PRO:O	2.40	0.49
1:B:835:LEU:CD1	1:B:857:ARG:HB2	2.43	0.49
1:D:584:PRO:HB3	2:I:30:THR:HA	1.94	0.49
1:A:830:LEU:HD22	1:A:835:LEU:HB2	1.95	0.48
1:A:835:LEU:CD1	1:A:857:ARG:HB2	2.43	0.48
1:B:652:LEU:HD12	1:B:699:ARG:O	2.12	0.48
1:C:433:LEU:O	1:C:437:SER:HB3	2.12	0.48
1:A:12:GLN:HG3	1:A:13:ARG:N	2.27	0.48
1:A:646:HIS:O	1:A:648:ASP:N	2.46	0.48
1:A:652:LEU:HD12	1:A:699:ARG:O	2.12	0.48
1:B:595:THR:HG23	1:B:596:PRO:CA	2.43	0.48
1:C:30:HIS:ND1	1:C:31:PRO:O	2.40	0.48
1:C:610:ASP:N	2:H:53:TYR:OH	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:835:LEU:CD1	1:D:857:ARG:HB2	2.43	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: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: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:A:423:MET:HB2	1:D:282:ARG:CG	2.43	0.48
1:A:668:VAL:CG1	1:A:669:PRO:HD2	2.44	0.48
1:B:100:TYR:CE1	1:B:602:CYS:HB3	2.49	0.48
1:C:12:GLN:HG3	1:C:13:ARG:N	2.27	0.48
1:C:26:ARG:HD3	1:C:169:SER:HB3	1.96	0.48
1:C:100:TYR:CE1	1:C:602:CYS:HB3	2.49	0.48
1:D:26:ARG:HD3	1:D:169:SER:HB3	1.96	0.48
1:D:30:HIS:ND1	1:D:31:PRO:O	2.40	0.48
1:D:95:TYR:CD1	1:D:95:TYR:N	2.79	0.48
1:A:100:TYR:CE1	1:A:602:CYS:HB3	2.49	0.48
1:A:105:TYR:CE2	1:A:199:ASP:HB2	2.48	0.48
1:B:30:HIS:ND1	1:B:31:PRO:O	2.40	0.48
1:C:748:CYS:C	1:C:749:ILE:HD12	2.39	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:D:100:TYR:CE1	1:D:602:CYS:HB3	2.49	0.48
1:A:257:THR:OG1	1:A:316:HIS:HE1	1.97	0.48
1:A:610:ASP:HB3	2:J:53:TYR:CE1	2.49	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:B:610:ASP:N	2:K:53:TYR:OH	2.46	0.48
1:D:153:TRP:HA	1:D:157:ARG:O	2.13	0.48
1:D:748:CYS:C	1:D:749:ILE:HD12	2.39	0.48
1:A:26:ARG:HD3	1:A:169:SER:HB3	1.96	0.48
1:C:95:TYR:CD1	1:C:95:TYR:N	2.79	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:A:651:LEU:HD23	1:A:653[A]:HIS:HE1	1.79	0.48
1:B:362:LEU:HD21	2:K:31:SER:CA	2.41	0.48
1:B:513:PRO:O	1:B:514:ALA:HB3	2.14	0.48
1:B:578:TYR:CE2	2:K:28:SER:HB3	2.49	0.48
1:B:583:ASN:CG	2:K:72:ASP:HA	2.38	0.48
1:C:153:TRP:HA	1:C:157:ARG:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:513:PRO:O	1:C:514:ALA:HB3	2.14	0.48
1:C:646:HIS:O	1:C:648:ASP:N	2.46	0.48
1:A:610:ASP:CB	2:J:53:TYR:CE1	2.97	0.48
1:A:970:THR:CG2	1:A:975:LEU:HB2	2.44	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:513:PRO:O	1:A:514:ALA:HB3	2.14	0.48
1:A:660:GLY:O	1:A:662:PRO:HD3	2.13	0.48
1:B:651:LEU:HD23	1:B:653[A]:HIS:HE1	1.79	0.48
1:B:970:THR:CG2	1:B:975:LEU:HB2	2.44	0.48
1:C:599:ARG:HD2	1:C:600:GLN:OE1	2.14	0.48
1:D:513:PRO:O	1:D:514:ALA:HB3	2.14	0.48
1:D:646:HIS:O	1:D:648:ASP:N	2.47	0.48
1:D:651:LEU:HD23	1:D:653[A]:HIS:HE1	1.79	0.48
1:D:830:LEU:HD22	1:D:835:LEU:HB2	1.95	0.48
1:A:305:ILE:HD11	1:A:645:ARG:HB3	1.96	0.47
1:A:573:GLN:HB2	1:A:602:CYS:O	2.14	0.47
1:C:210:ARG:NH1	1:C:358:GLU:OE1	2.47	0.47
1:D:210:ARG:NH1	1:D:358:GLU:OE1	2.47	0.47
1:D:599:ARG:HD2	1:D:600:GLN:OE1	2.14	0.47
1:D:660:GLY:O	1:D:662:PRO:HD3	2.13	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
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:D:610:ASP:HB3	2:I:53:TYR:CE1	2.49	0.47
1:A:210:ARG:NH1	1:A:358:GLU:OE1	2.47	0.47
1:A:748:CYS:C	1:A:749:ILE:HD12	2.39	0.47
1:A:882:ILE:O	1:A:882:ILE:HG22	2.12	0.47
1:B:210:ARG:NH1	1:B:358:GLU:OE1	2.47	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:C:305:ILE:HD11	1:C:645:ARG:HB3	1.96	0.47
2:K:28:SER:HA	2:K:76:ASN:HD21	1.79	0.47
1:A:568:TRP:HE1	1:A:604:ASN:HD22	1.62	0.47
1:B:882:ILE:HG22	1:B:882:ILE:O	2.12	0.47
1:D:3:ILE:C	1:D:5:ASP:H	2.22	0.47
1:D:856:TYR:HD2	1:D:864:MET:CE	2.27	0.47
1:B:748:CYS:C	1:B:749:ILE:HD12	2.39	0.47
1:C:143:PHE:N	1:C:143:PHE:CD1	2.81	0.47
1:C:660:GLY:O	1:C:662:PRO:HD3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:J:28:SER:HA	2:J:76:ASN:HD21	1.79	0.47
1:A:910:LEU:C	1:A:910:LEU:HD12	2.39	0.47
1:B:701:VAL:CG1	1:B:702:GLN:N	2.78	0.47
1:B:910:LEU:C	1:B:910:LEU:HD12	2.39	0.47
1:C:147:ASN:HA	1:C:148:SER:HA	1.66	0.47
1:C:668:VAL:CG1	1:C:669:PRO:HD2	2.44	0.47
1:C:856:TYR:HD2	1:C:864:MET:CE	2.27	0.47
1:D:143:PHE:N	1:D:143:PHE:CD1	2.81	0.47
1:D:573:GLN:HB2	1:D:602:CYS:O	2.14	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: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
1:A:635:THR:OG1	1:A:681:GLU:HG3	2.15	0.47
1:A:701:VAL:CG1	1:A:702:GLN:N	2.77	0.47
1:C:3:ILE:C	1:C:5:ASP:H	2.22	0.47
1:C:257:THR:OG1	1:C:316:HIS:HE1	1.97	0.47
1:C:573:GLN:HB2	1:C:602:CYS:O	2.14	0.47
1:C:609:ALA:C	2:H:53:TYR:CZ	2.93	0.47
1:C:701:VAL:CG1	1:C:702:GLN:N	2.77	0.47
1:D:251:ARG:HG2	1:D:251:ARG:HH11	1.79	0.47
1:D:701:VAL:CG1	1:D:702:GLN:N	2.77	0.47
1:D:970:THR:CG2	1:D:975:LEU:HB2	2.44	0.47
2:I:28:SER:HA	2:I:76:ASN:HD21	1.79	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
1:A:423:MET:HB2	1:D:282:ARG:HG2	1.97	0.47
1:B:742:THR:CG2	1:B:743:SER:N	2.77	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:C:583:ASN:CG	2:H:72:ASP:HA	2.39	0.47
1:D:127:PHE:HE1	1:D:184:LEU:HG	1.80	0.47
1:D:257:THR:OG1	1:D:316:HIS:HE1	1.97	0.47
1:D:610:ASP:CB	2:I:53:TYR:CE1	2.97	0.47
1:D:635:THR:OG1	1:D:681:GLU:HG3	2.15	0.47
1:D:910:LEU:C	1:D:910:LEU:HD12	2.39	0.47
2:H:28:SER:HA	2:H:76:ASN:HD21	1.79	0.47
1:B:80:GLU:OE1	1:B:80:GLU:N	2.29	0.47
1:B:635:THR:OG1	1:B:681:GLU:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:PHE:HE1	1:C:184:LEU:HG	1.80	0.47
1:C:630:ARG:HE	1:C:630:ARG:HB3	1.31	0.47
1:C:635:THR:OG1	1:C:681:GLU:HG3	2.15	0.47
1:D:568:TRP:HE1	1:D:604:ASN:HD22	1.62	0.47
1:A:80:GLU:OE1	1:A:80:GLU:N	2.29	0.47
1:A:441:THR:HG22	1:A:474:TRP:CH2	2.50	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:C:910:LEU:C	1:C:910:LEU:HD12	2.39	0.47
1:D:580:GLU:O	2:I:74:SER:HB2	2.13	0.47
1:A:599:ARG:HD2	1:A:600:GLN:OE1	2.14	0.46
1:B:3:ILE:C	1:B:5:ASP:H	2.22	0.46
1:A:3:ILE:C	1:A:5:ASP:H	2.22	0.46
1:A:780:LEU:HA	1:A:886:CYS:HB3	1.97	0.46
1:B:251:ARG:HG2	1:B:251:ARG:HH11	1.79	0.46
1:B:780:LEU:HA	1:B:886:CYS:HB3	1.97	0.46
1:D:134:LEU:N	1:D:134:LEU:CD1	2.73	0.46
1:A:13:ARG:NH1	1:D:13:ARG:NH1	2.63	0.46
1:B:599:ARG:HD2	1:B:600:GLN:OE1	2.14	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:A:945:ASN:OD1	1:A:950:GLN:HB2	2.16	0.46
1:B:63:PHE:HB3	1:B:64:PRO:CD	2.45	0.46
1:B:234:ASP:O	1:B:235:PHE:HB2	2.15	0.46
1:B:945:ASN:OD1	1:B:950:GLN:HB2	2.16	0.46
1:C:134:LEU:N	1:C:134:LEU:CD1	2.73	0.46
1:C:369:GLU:O	1:C:373:VAL:HG23	2.16	0.46
1:C:945:ASN:OD1	1:C: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
1:A:620:ALA:O	1:A:624:GLN:HG3	2.16	0.46
1:B:230:ARG:CG	1:B:230:ARG:NH1	2.79	0.46
1:C:620:ALA:O	1:C:624:GLN:HG3	2.16	0.46
1:C:849:LEU:N	1:C:849:LEU:HD23	2.30	0.46
1:D:111:PRO:HA	1:D:112:PRO:HA	1.56	0.46
1:D:369:GLU:O	1:D:373:VAL:HG23	2.16	0.46
1:D:584:PRO:N	2:I:30:THR:HG22	2.28	0.46
1:D:620:ALA:O	1:D:624:GLN:HG3	2.16	0.46
1:D:630:ARG:HE	1:D:630:ARG:HB3	1.31	0.46
1:D:849:LEU:N	1:D:849:LEU:HD23	2.30	0.46
1:D:945:ASN:OD1	1:D:950:GLN:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:ARG:CG	1:A:230:ARG:NH1	2.79	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:B:894:ARG:NH2	1:B:921:PRO:HD3	2.31	0.46
1:D:11:LEU:HD11	1:D:187:MET:HE1	1.98	0.46
1:A:73:TRP:CE2	1:A:122:CYS:HB3	2.50	0.46
1:A:166:ARG:HG3	1:A:392:TYR:CG	2.51	0.46
1:A:894:ARG:NH2	1:A:921:PRO:HD3	2.31	0.46
1:B:734:SER:HB2	1:B:860:GLY:HA3	1.95	0.46
1:C:581:ASN:CB	2:H:72:ASP:OD1	2.55	0.46
1:C:588:TYR:O	1:C:589:GLY:C	2.59	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:A:3:ILE:HD12	1:A:3:ILE:O	2.16	0.46
1:A:127:PHE:HE1	1:A:184:LEU:HG	1.80	0.46
1:A:141:ILE:CG1	1:A:142:ILE:N	2.79	0.46
1:A:147:ASN:HA	1:A:148:SER:HA	1.65	0.46
1:A:282:ARG:HG2	1:D:423:MET:HB2	1.97	0.46
1:A:362:LEU:HD21	2:J:31:SER:C	2.34	0.46
1:B:73:TRP:CE2	1:B:122:CYS:HB3	2.51	0.46
1:B:141:ILE:CG1	1:B:142:ILE:N	2.79	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:B:651:LEU:HD12	1:B:651:LEU:HA	1.46	0.46
1:C:11:LEU:HD11	1:C:187:MET:HE1	1.98	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:588:TYR:O	1:D:589:GLY:C	2.59	0.46
1:D:834:VAL:CG1	1:D:835:LEU:N	2.79	0.46
1:A:272:ALA:HB1	1:A:273:PRO:CD	2.43	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:B:127:PHE:HE1	1:B:184:LEU:HG	1.80	0.46
1:B:316:HIS:HB2	1:B:321:THR:O	2.16	0.46
1:C:111:PRO:HA	1:C:112:PRO:HA	1.57	0.46
1:C:834:VAL:CG1	1:C:835:LEU:N	2.79	0.46
1:D:147:ASN:HA	1:D:148:SER:HA	1.65	0.46
2:I:29:ILE:H	2:I:76:ASN:HD21	1.63	0.46
1:A:230:ARG:HH11	1:A:230:ARG:HG2	1.81	0.46
1:B:429:ASP:OD1	1:B:431[A]:ARG:HG3	2.16	0.46
1:B:834:VAL:CG1	1:B:835:LEU:N	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:TRP:CE2	1:C:122:CYS:HB3	2.51	0.46
1:D:531:ARG:CB	1:D:532:PRO:HD2	2.46	0.46
2:H:29:ILE:H	2:H:76:ASN:HD21	1.63	0.46
1:A:227:VAL:HG12	1:A:228:ALA:N	2.31	0.45
1:A:261:TRP:CD1	1:A:261:TRP:N	2.83	0.45
1:A:429:ASP:OD1	1:A:431[A]:ARG:HG3	2.16	0.45
1:B:3:ILE:HD12	1:B:3:ILE:O	2.16	0.45
1:B:287:ASP:CG	1:C:425:ARG:HH22	2.23	0.45
1:D:73:TRP:CE2	1:D:122:CYS:HB3	2.51	0.45
1:D:870:VAL:CG1	1:D:871:GLU:N	2.79	0.45
1:A:67:GLU:HG2	1:A:67:GLU:H	1.15	0.45
1:A:369:GLU:OE1	3:N:53:GLN:NE2	2.49	0.45
1:A:610:ASP:N	2:J:53:TYR:OH	2.49	0.45
1:A:734:SER:HB2	1:A:860:GLY:HA3	1.95	0.45
1:A:873:ALA:O	1:A:876:THR:HG22	2.16	0.45
1:B:230:ARG:HH11	1:B:230:ARG:HG2	1.81	0.45
1:B:261:TRP:CD1	1:B:261:TRP:N	2.83	0.45
1:B:873:ALA:O	1:B:876:THR:HG22	2.16	0.45
1:C:38:ASN:ND2	1:C:41:GLU:HG3	2.31	0.45
1:C:226:HIS:CD2	1:C:226:HIS:N	2.83	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:C:870:VAL:CG1	1:C:871:GLU:N	2.79	0.45
1:D:230:ARG:HH11	1:D:230:ARG:HG2	1.81	0.45
1:A:834:VAL:CG1	1:A:835:LEU:N	2.79	0.45
1:A:856:TYR:HD2	1:A:864:MET:CE	2.27	0.45
1:B:369:GLU:O	1:B:373:VAL:HG23	2.16	0.45
1:B:908:ASP:HB3	1:B:1007:PHE:CD2	2.51	0.45
1:C:230:ARG:HH11	1:C:230:ARG:HG2	1.81	0.45
1:C:531:ARG:CB	1:C:532:PRO:HD2	2.46	0.45
1:C:908:ASP:HB3	1:C:1007:PHE:CD2	2.52	0.45
1:D:38:ASN:ND2	1:D:41:GLU:HG3	2.32	0.45
1:D:234:ASP:O	1:D:235:PHE:HB2	2.15	0.45
1:A:369:GLU:O	1:A:373:VAL:HG23	2.16	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:242:ALA:O	1:D:290:THR:HA	2.17	0.45
1:D:316:HIS:HB2	1:D:321:THR:O	2.16	0.45
1:D:908:ASP:HB3	1:D:1007:PHE:CD2	2.52	0.45
1:A:352:ARG:O	1:A:385:ASN:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:ARG:CB	1:A:532:PRO:HD2	2.46	0.45
1:A:762:SER:C	1:A:822:LEU:HD23	2.42	0.45
1:A:1018:LEU:HD23	1:A:1018:LEU:HA	1.53	0.45
1:B:287:ASP:OD2	1:C:425:ARG:NH2	2.50	0.45
1:B:352:ARG:O	1:B:385:ASN:HB2	2.17	0.45
1:B:531:ARG:CB	1:B:532:PRO:HD2	2.46	0.45
1:B:762:SER:C	1:B:822:LEU:HD23	2.42	0.45
1:C:441:THR:HG22	1:C:474:TRP:CH2	2.50	0.45
1:D:226:HIS:CD2	1:D:226:HIS:N	2.83	0.45
1:D:441:THR:HG22	1:D:474:TRP:CH2	2.51	0.45
1:D:694:LEU:HD12	1:D:694:LEU:HA	1.82	0.45
1:A:908:ASP:HB3	1:A:1007:PHE:CD2	2.52	0.45
1:B:856:TYR:HD2	1:B:864:MET:CE	2.27	0.45
1:B:915:PHE:O	1:B:916:ASP:HB2	2.17	0.45
1:C:166:ARG:HG3	1:C:392:TYR:CG	2.51	0.45
1:D:369:GLU:OE1	3:M:53:GLN:NE2	2.50	0.45
1:D:734:SER:HB2	1:D:860:GLY:HA3	1.95	0.45
1:A:84:VAL:HG13	1:A:85:VAL:N	2.31	0.45
1:B:701:VAL:O	1:B:703:PRO:HD3	2.16	0.45
1:C:362:LEU:HD21	2:H:31:SER:C	2.37	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:C:694:LEU:HD12	1:C:694:LEU:HA	1.82	0.45
1:D:3:ILE:HD12	1:D:3:ILE:O	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:D:609:ALA:C	2:I:53:TYR:CZ	2.80	0.45
1:A:214:LEU:HD23	1:A:214:LEU:HA	1.61	0.45
1:A:651:LEU:HD12	1:A:651:LEU:HA	1.46	0.45
1:A:685:LEU:CB	1:A:686:PRO:HD2	2.38	0.45
1:A:915:PHE:O	1:A:916:ASP:HB2	2.17	0.45
1:B:67:GLU:HG2	1:B:67:GLU:H	1.15	0.45
1:B:168:PRO:O	1:B:442:ARG:NH2	2.48	0.45
1:B:597:ASN:ND2	1:B:599:ARG:N	2.48	0.45
1:C:429:ASP:OD1	1:C:431[A]:ARG:HG3	2.16	0.45
1:C:734:SER:HB2	1:C:860:GLY:HA3	1.95	0.45
1:C:742:THR:CG2	1:C:743:SER:N	2.77	0.45
1:D:352:ARG:O	1:D:385:ASN:HB2	2.17	0.45
1:A:43:ARG:HD2	1:A:261:TRP:CD2	2.52	0.45
1:A:757:GLN:HG2	1:A:758:PHE:N	2.31	0.45
1:B:84:VAL:HG13	1:B:85:VAL:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:580:GLU:C	2:K:74:SER:HA	2.00	0.45
1:C:3:ILE:HD12	1:C:3:ILE:O	2.16	0.45
1:C:352:ARG:O	1:C:385:ASN:HB2	2.17	0.45
1:C:362:LEU:HD21	2:H:30:THR:O	2.17	0.45
1:C:576:ILE:HG21	2:H:30:THR:CB	2.43	0.45
1:C:580:GLU:C	2:H:74:SER:HA	1.95	0.45
1:D:742:THR:CG2	1:D:743:SER:N	2.77	0.45
3:L:24:ARG:HA	3:L:69:THR:O	2.17	0.45
3:M:24:ARG:HA	3:M:69:THR:O	2.17	0.45
1:A:128:ASN:HD22	1:A:180:GLY:C	2.25	0.45
1:A:168:PRO:O	1:A:442:ARG:NH2	2.48	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:B:395:HIS:HA	1:B:396:PRO:HD3	1.83	0.45
1:C:143:PHE:O	1:C:168:PRO:HA	2.17	0.45
1:C:578:TYR:CA	2:H:30:THR:HG21	2.47	0.45
1:C:658:LEU:HD23	1:C:661:LYS:HZ2	1.81	0.45
1:C:894:ARG:NH2	1:C:921:PRO:HD3	2.31	0.45
1:D:143:PHE:O	1:D:168:PRO:HA	2.17	0.45
1:D:894:ARG:NH2	1:D:921:PRO:HD3	2.31	0.45
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:C:576:ILE:HG22	2:H:30:THR:HB	1.85	0.44
1:D:86:VAL:HG13	1:D:87:PRO:HA	1.99	0.44
1:D:599:ARG:HB2	1:D:600:GLN:H	1.54	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
1:B:128:ASN:HD22	1:B:180:GLY:C	2.25	0.44
2:H:36:TRP:CE2	2:H:80:LEU:HB2	2.53	0.44
2:I:36:TRP:CE2	2:I:80:LEU:HB2	2.53	0.44
2:J:36:TRP:CE2	2:J:80:LEU:HB2	2.52	0.44
3:O:24:ARG:HA	3:O:69:THR:O	2.17	0.44
1:A:737:ILE:HA	1:A:738:PRO:HD3	1.78	0.44
1:B:30:HIS:CE1	1:B:33:PHE:CD2	3.06	0.44
1:B:38:ASN:ND2	1:B:41:GLU:HG3	2.32	0.44
1:B:242:ALA:O	1:B:290:THR:HA	2.16	0.44
1:B:881:ARG:HD3	1:B:987:ASP:OD2	2.17	0.44
1:C:395:HIS:HA	1:C:396:PRO:HD3	1.83	0.44
1:C:441:THR:HG22	1:C:474:TRP:CZ3	2.52	0.44
1:D:90:TRP:CD1	1:D:90:TRP:C	2.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:36:TRP:CE2	2:K:80:LEU:HB2	2.52	0.44
1:A:226:HIS:CD2	1:A:226:HIS:N	2.83	0.44
1:A:870:VAL:CG1	1:A:871:GLU:N	2.79	0.44
1:B:226:HIS:CD2	1:B:226:HIS:N	2.83	0.44
1:B:362:LEU:HD21	2:K:31:SER:HA	1.90	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:C:685:LEU:HA	1:C:686:PRO:HD3	1.84	0.44
1:C:708:TRP:CD1	1:C:708:TRP:N	2.85	0.44
1:D:378:LEU:HD23	1:D:378:LEU:HA	1.75	0.44
1:D:441:THR:HG22	1:D:474:TRP:CZ3	2.53	0.44
1:D:708:TRP:CD1	1:D:708:TRP:N	2.85	0.44
1:A:38:ASN:ND2	1:A:41:GLU:HG3	2.32	0.44
1:A:360:HIS:HA	1:A:361:PRO:HD3	1.88	0.44
1:A:395:HIS:HA	1:A:396:PRO:HD3	1.83	0.44
1:A:588:TYR:O	1:A:589:GLY:C	2.59	0.44
1:A:786:ARG:HH11	1:A:990:HIS:CE1	2.36	0.44
1:B:147:ASN:HA	1:B:148:SER:HA	1.65	0.44
1:B:579:ASP:CG	2:K:73:THR:OG1	2.50	0.44
1:B:650:GLU:HA	1:B:701:VAL:O	2.17	0.44
1:C:90:TRP:CD1	1:C:90:TRP:C	2.95	0.44
1:C:141:ILE:CG1	1:C:142:ILE:N	2.79	0.44
1:D:78:LEU:HB3	1:D:80:GLU:OE1	2.18	0.44
1:D:141:ILE:CG1	1:D:142:ILE:N	2.79	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
3:N:24:ARG:HA	3:N:69:THR:O	2.17	0.44
1:A:242:ALA:O	1:A:290:THR:HA	2.16	0.44
1:A:579:ASP:CG	1:A:583:ASN:HB2	2.42	0.44
1:A:645:ARG:NH2	1:A:650:GLU:OE2	2.51	0.44
1:B:584:PRO:HG2	2:K:71:ARG:HH12	1.66	0.44
1:B:588:TYR:O	1:B:589:GLY:C	2.59	0.44
1:B:645:ARG:NH2	1:B:650:GLU:OE2	2.51	0.44
1:C:645:ARG:NH2	1:C:650:GLU:OE1	2.46	0.44
1:C:645:ARG:NH2	1:C:650:GLU:OE2	2.51	0.44
1:C:915:PHE:O	1:C:916:ASP:HB2	2.17	0.44
1:D:43:ARG:HD2	1:D:261:TRP:CD2	2.52	0.44
1:D:63:PHE:N	1:D:63:PHE:CD1	2.86	0.44
1:D:650:GLU:HA	1:D:701:VAL:O	2.17	0.44
1:D:685:LEU:HA	1:D:686:PRO:HD3	1.84	0.44
1:A:11:LEU:HD11	1:A:187:MET:HE1	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:VAL:HA	1:A:115:PRO:HD3	1.77	0.44
1:A:989:PHE:CD1	1:A:989:PHE:N	2.86	0.44
1:B:11:LEU:HD11	1:B:187:MET:HE1	1.98	0.44
1:B:433:LEU:HB3	1:B:434:PRO:HD3	1.99	0.44
1:B:989:PHE:CD1	1:B:989:PHE:N	2.86	0.44
1:C:43:ARG:HD2	1:C:261:TRP:CD2	2.52	0.44
1:C:63:PHE:CD1	1:C:63:PHE:N	2.86	0.44
1:C:78:LEU:HB3	1:C:80:GLU:OE1	2.18	0.44
1:C:395:HIS:CG	1:C:396:PRO:HD2	2.53	0.44
1:C:679:LEU:HA	1:C:679:LEU:HD23	1.13	0.44
1:C:701:VAL:O	1:C:703:PRO:HD3	2.16	0.44
1:C:762:SER:C	1:C:822:LEU:HD23	2.42	0.44
1:D:30:HIS:CE1	1:D:33:PHE:CD2	3.06	0.44
1:D:395:HIS:CG	1:D:396:PRO:HD2	2.53	0.44
1:D:679:LEU:HA	1:D:679:LEU:HD23	1.13	0.44
1:A:395:HIS:CG	1:A:396:PRO:HD2	2.53	0.44
1:A:650:GLU:HA	1:A:701:VAL:O	2.17	0.44
1:A:995:GLY:O	1:A:996:ASP:C	2.61	0.44
1:B:134:LEU:N	1:B:134:LEU:CD1	2.73	0.44
1:B:742:THR:CG2	1:B:743:SER:H	2.31	0.44
1:B:995:GLY:O	1:B:996:ASP:C	2.61	0.44
1:B:1018:LEU:HD23	1:B:1018:LEU:HA	1.53	0.44
1:C:30:HIS:CE1	1:C:33:PHE:CD2	3.06	0.44
1:C:168:PRO:O	1:C:442:ARG:NH2	2.48	0.44
1:C:429:ASP:HA	1:C:430:PRO:HD3	1.82	0.44
1:C:650:GLU:HA	1:C:701:VAL:O	2.17	0.44
1:C:995:GLY:O	1:C:996:ASP:C	2.61	0.44
1:D:424:ASN:HD22	1:D:424:ASN:HA	1.40	0.44
1:D:429:ASP:HA	1:D:430:PRO:HD3	1.82	0.44
1:D:658:LEU:HD23	1:D:661:LYS:HZ2	1.82	0.44
1:D:915:PHE:O	1:D:916:ASP:HB2	2.17	0.44
1:A:78:LEU:HB3	1:A:80:GLU:OE1	2.18	0.44
1:A:90:TRP:CD1	1:A:90:TRP:C	2.95	0.44
1:A:597:ASN:ND2	1:A:599:ARG:N	2.49	0.44
1:A:742:THR:CG2	1:A:743:SER:H	2.31	0.44
1:B:214:LEU:HD23	1:B:214:LEU:HA	1.61	0.44
1:B:395:HIS:CG	1:B:396:PRO:HD2	2.53	0.44
1:B:579:ASP:CG	1:B:583:ASN:HB2	2.42	0.44
1:B:581:ASN:CB	2:K:72:ASP:OD1	2.56	0.44
1:B:786:ARG:HH11	1:B:990:HIS:CE1	2.36	0.44
1:C:79:PRO:HB2	1:C:80:GLU:HG3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:VAL:HG12	1:C:228:ALA:N	2.31	0.44
1:D:168:PRO:O	1:D:442:ARG:NH2	2.48	0.44
1:D:227:VAL:HG12	1:D:228:ALA:N	2.30	0.44
1:D:612:THR:HG21	2:I:56:SER:HB3	2.00	0.44
1:D:647:SER:HG	1:D:672:VAL:H	1.65	0.44
1:D:762:SER:C	1:D:822:LEU:HD23	2.42	0.44
1:D:995:GLY:O	1:D:996:ASP:C	2.61	0.44
1:D:1018:LEU:HD23	1:D:1018:LEU:HA	1.53	0.44
1:A:433:LEU:HB3	1:A:434:PRO:HD3	2.00	0.43
1:B:288:ARG:HH11	1:B:288:ARG:HD3	1.48	0.43
1:B:751:LEU:HD23	1:B:751:LEU:C	2.43	0.43
1:C:378:LEU:HD23	1:C:378:LEU:HA	1.75	0.43
1:C:757:GLN:HG2	1:C:758:PHE:N	2.31	0.43
1:D:79:PRO:HB2	1:D:80:GLU:HG3	2.00	0.43
1:D:433:LEU:HB3	1:D:434:PRO:HD3	2.00	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
2:I:97:ASN:ND2	2:I:102:TYR:H	2.16	0.43
1:A:86:VAL:HG13	1:A:87:PRO:HA	1.99	0.43
1:A:143:PHE:O	1:A:168:PRO:HA	2.17	0.43
1:A:441:THR:HG22	1:A:474:TRP:CZ3	2.52	0.43
1:A:507:ASP:C	1:A:519:SER:HB2	2.44	0.43
1:A:657:ALA:O	1:A:694:LEU:HD12	2.18	0.43
1:B:86:VAL:HG13	1:B:87:PRO:HA	1.99	0.43
1:B:90:TRP:C	1:B:90:TRP:CD1	2.95	0.43
1:B:145:GLY:HA3	1:B:210:ARG:HG3	2.00	0.43
1:B:657:ALA:O	1:B:694:LEU:HD12	2.18	0.43
1:B:925:MET:HE3	1:B:925:MET:HB3	1.83	0.43
1:C:63:PHE:HB3	1:C:64:PRO:CD	2.45	0.43
1:C:128:ASN:HD22	1:C:180:GLY:C	2.25	0.43
1:C:433:LEU:HB3	1:C:434:PRO:HD3	2.00	0.43
1:C:647:SER:HG	1:C:672:VAL:H	1.65	0.43
1:D:128:ASN:HD22	1:D:180:GLY:C	2.25	0.43
1:D:230:ARG:CG	1:D:230:ARG:NH1	2.79	0.43
1:D:822:LEU:HD13	1:D:822:LEU:HA	1.79	0.43
1:A:751:LEU:C	1:A:751:LEU:HD23	2.43	0.43
1:A:840:HIS:ND1	1:A:840:HIS:N	2.67	0.43
1:B:78:LEU:HB3	1:B:80:GLU:OE1	2.18	0.43
1:B:441:THR:HG22	1:B:474:TRP:CZ3	2.52	0.43
1:B:507:ASP:C	1:B:519:SER:HB2	2.44	0.43
1:B:737:ILE:HA	1:B:738:PRO:HD3	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:787:ALA:HA	1:B:788:PRO:HD3	1.66	0.43
1:C:424:ASN:HD22	1:C:424:ASN:HA	1.40	0.43
1:C:584:PRO:HB3	2:H:30:THR:HB	1.92	0.43
1:C:730:LEU:H	1:C:730:LEU:HG	1.41	0.43
1:C:822:LEU:HD13	1:C:822:LEU:HA	1.79	0.43
1:C:881:ARG:HD3	1:C:987:ASP:OD2	2.17	0.43
1:D:362:LEU:HD21	2:I:31:SER:C	2.35	0.43
1:D:787:ALA:HA	1:D:788:PRO:HD3	1.66	0.43
1:A:145:GLY:HA3	1:A:210:ARG:HG3	2.01	0.43
1:A:288:ARG:HH11	1:A:288:ARG:HD3	1.48	0.43
1:C:136:GLU:O	1:C:216:HIS:HE1	2.01	0.43
1:C:217:LYS:HB3	1:C:218:PRO:HD2	2.00	0.43
1:C:230:ARG:CG	1:C:230:ARG:NH1	2.79	0.43
1:C:1018:LEU:HD23	1:C:1018:LEU:HA	1.53	0.43
1:D:63:PHE:HB3	1:D:64:PRO:CD	2.45	0.43
1:D:751:LEU:C	1:D:751:LEU:HD23	2.43	0.43
1:A:285:TYR:OH	1:D:424:ASN:HB3	2.19	0.43
1:B:143:PHE:O	1:B:168:PRO:HA	2.17	0.43
1:B:840:HIS:ND1	1:B:840:HIS:N	2.67	0.43
1:C:354:VAL:HG22	1:C:355:ASN:N	2.34	0.43
1:C:645:ARG:NH2	1:C:650:GLU:CD	2.76	0.43
1:C:657:ALA:O	1:C:694:LEU:HD12	2.18	0.43
1:C:786:ARG:HH11	1:C:990:HIS:CE1	2.36	0.43
1:D:136:GLU:O	1:D:216:HIS:HE1	2.01	0.43
1:D:436:MET:HE1	1:D:467:ASN:HD22	1.81	0.43
1:D:576:ILE:HG22	2:I:30:THR:CB	2.34	0.43
1:D:657:ALA:O	1:D:694:LEU:HD12	2.18	0.43
1:D:786:ARG:HH11	1:D:990:HIS:CE1	2.36	0.43
1:A:134:LEU:N	1:A:134:LEU:CD1	2.73	0.43
1:A:925:MET:HE3	1:A:925:MET:HB3	1.82	0.43
1:B:225:PHE:HA	1:B:243:GLU:O	2.19	0.43
1:C:436:MET:HE1	1:C:467:ASN:HD22	1.81	0.43
1:C:634:GLN:NE2	1:C:682:LEU:O	2.51	0.43
1:C:751:LEU:HD23	1:C:751:LEU:C	2.43	0.43
1:D:217:LYS:HB3	1:D:218:PRO:HD2	2.00	0.43
1:D:354:VAL:HG22	1:D:355:ASN:N	2.34	0.43
1:D:634:GLN:NE2	1:D:682:LEU:O	2.52	0.43
1:D:881:ARG:HD3	1:D:987:ASP:OD2	2.18	0.43
1:A:225:PHE:HA	1:A:243:GLU:O	2.19	0.43
1:A:227:VAL:CG1	1:A:240:LEU:HD11	2.48	0.43
1:A:362:LEU:HD13	2:J:32:ASP:CA	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:957:PHE:CD2	1:A:957:PHE:C	2.95	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
1:C:989:PHE:N	1:C:989:PHE:CD1	2.86	0.43
1:D:362:LEU:HD13	2:I:32:ASP:CA	2.38	0.43
1:D:610:ASP:N	2:I:53:TYR:OH	2.49	0.43
1:D:612:THR:HG21	2:I:56:SER:CB	2.48	0.43
2:K:97:ASN:ND2	2:K:102:TYR:H	2.16	0.43
1:A:136:GLU:O	1:A:216:HIS:HE1	2.01	0.43
1:A:251:ARG:HH11	1:A:251:ARG:CG	2.32	0.43
1:A:257:THR:HA	1:A:270:GLY:O	2.19	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: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:C:18:ASN:HA	1:C:19:PRO:HD3	1.56	0.43
1:D:989:PHE:CD1	1:D:989:PHE:N	2.86	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:B:105:TYR:HA	1:B:106:PRO:HD3	1.91	0.43
1:B:708:TRP:CD1	1:B:708:TRP:N	2.85	0.43
1:B:957:PHE:CD2	1:B:957:PHE:C	2.95	0.43
1:D:308:LEU:HA	1:D:308:LEU:HD23	1.80	0.43
1:D:730:LEU:H	1:D:730:LEU:HG	1.41	0.43
3:L:76:ASN:C	3:L:76:ASN:ND2	2.77	0.43
1:A:79:PRO:HB2	1:A:80:GLU:HG3	2.00	0.42
1:A:187:MET:O	1:A:187:MET:HG3	2.19	0.42
1:A:354:VAL:HG22	1:A:355:ASN:N	2.34	0.42
1:A:612:THR:HG21	2:J:56:SER:CB	2.49	0.42
1:A:622:HIS:HD2	1:A:625:GLN:OE1	2.02	0.42
1:B:187:MET:O	1:B:187:MET:HG3	2.19	0.42
1:B:576:ILE:HD11	2:K:53:TYR:O	2.19	0.42
1:B:635:THR:HA	1:B:680:ILE:O	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
3:M:76:ASN:C	3:M:76:ASN:ND2	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:PHE:N	1:A:176:PHE:CD1	2.87	0.42
1:A:822:LEU:HD12	1:A:823:LEU:N	2.34	0.42
1:B:63:PHE:N	1:B:63:PHE:CD1	2.86	0.42
1:B:622:HIS:HD2	1:B:625:GLN:OE1	2.02	0.42
1:C:200:GLN:OE1	1:C:200:GLN:N	2.44	0.42
1:C:257:THR:HA	1:C:270:GLY:O	2.19	0.42
1:C:682:LEU:HA	1:C:683:PRO:HD3	1.91	0.42
1:D:257:THR:HA	1:D:270:GLY:O	2.19	0.42
1:A:282:ARG:NH1	1:D:418:HIS:O	2.52	0.42
1:A:570:TRP:CD1	1:A:571:VAL:HG22	2.54	0.42
1:A:584:PRO:N	2:J:30:THR:HG22	2.27	0.42
1:A:599:ARG:HB2	1:A:600:GLN:H	1.54	0.42
1:A:635:THR:HA	1:A:680:ILE:O	2.19	0.42
1:A:708:TRP:CD1	1:A:708:TRP:N	2.85	0.42
1:A:787:ALA:HA	1:A:788:PRO:HD3	1.66	0.42
1:B:18:ASN:HA	1:B:19:PRO:HD3	1.56	0.42
1:B:176:PHE:CD1	1:B:176:PHE:N	2.87	0.42
1:B:183:ARG:HH11	1:B:183:ARG:HD3	1.55	0.42
1:B:360:HIS:HE1	1:B:362:LEU:HB2	1.84	0.42
1:C:578:TYR:CD2	2:H:28:SER:HB3	2.54	0.42
1:C:988:GLY:C	1:C:989:PHE:CD1	2.97	0.42
1:D:102:ASN:C	1:D:102:ASN:HD22	2.27	0.42
1:A:63:PHE:N	1:A:63:PHE:CD1	2.86	0.42
1:A:105:TYR:HA	1:A:106:PRO:HD3	1.91	0.42
1:A:124:SER:HA	1:A:184:LEU:O	2.20	0.42
1:B:111:PRO:HA	1:B:112:PRO:HA	1.56	0.42
1:B:217:LYS:HB3	1:B:218:PRO:HD2	2.01	0.42
1:C:67:GLU:HG2	1:C:67:GLU:H	1.15	0.42
1:C:102:ASN:HD22	1:C:102:ASN:C	2.27	0.42
1:C:251:ARG:HH11	1:C:251:ARG:CG	2.32	0.42
1:C:472:TYR:O	1:C:476:LYS:HG2	2.20	0.42
1:D:38:ASN:ND2	1:D:38:ASN:C	2.77	0.42
1:D:145:GLY:HA3	1:D:210:ARG:HG3	2.00	0.42
1:D:622:HIS:HD2	1:D:625:GLN:OE1	2.02	0.42
1:D:988:GLY:C	1:D:989:PHE:CD1	2.97	0.42
1:A:685:LEU:HA	1:A:686:PRO:HD3	1.84	0.42
1:A:858:ILE:HG12	1:A:864:MET:HB3	2.02	0.42
1:B:262:GLN:O	1:B:262:GLN:HG2	2.19	0.42
1:B:429:ASP:HA	1:B:430:PRO:HD3	1.82	0.42
1:B:570:TRP:CD1	1:B:571:VAL:HG22	2.54	0.42
1:C:11:LEU:N	1:C:11:LEU:HD23	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:ASN:ND2	1:C:38:ASN:C	2.77	0.42
1:C:622:HIS:HD2	1:C:625:GLN:OE1	2.02	0.42
1:D:105:TYR:HB3	1:D:106:PRO:HD2	2.01	0.42
1:D:251:ARG:HH11	1:D:251:ARG:CG	2.32	0.42
1:D:472:TYR:O	1:D:476:LYS:HG2	2.20	0.42
1:A:111:PRO:HA	1:A:112:PRO:HA	1.56	0.42
1:A:262:GLN:O	1:A:262:GLN:HG2	2.19	0.42
1:B:7:LEU:HD23	1:B:7:LEU:HA	1.85	0.42
1:B:124:SER:HA	1:B:184:LEU:O	2.20	0.42
1:B:702:GLN:HA	1:B:703:PRO:HD3	1.82	0.42
1:B:858:ILE:HG12	1:B:864:MET:HB3	2.02	0.42
1:B:988:GLY:C	1:B:989:PHE:CD1	2.97	0.42
1:C:145:GLY:HA3	1:C:210:ARG:HG3	2.01	0.42
1:C:183:ARG:HH11	1:C:183:ARG:HD3	1.55	0.42
1:C:227:VAL:CG1	1:C:240:LEU:HD11	2.48	0.42
1:C:507:ASP:C	1:C:519:SER:HB2	2.43	0.42
1:C:635:THR:HA	1:C:680:ILE:O	2.19	0.42
1:C:858:ILE:HG12	1:C:864:MET:HB3	2.02	0.42
1:D:11:LEU:N	1:D:11:LEU:HD23	2.35	0.42
1:D:67:GLU:HG2	1:D:67:GLU:H	1.15	0.42
1:D:176:PHE:CD1	1:D:176:PHE:N	2.87	0.42
1:D:200:GLN:OE1	1:D:200:GLN:N	2.44	0.42
1:D:227:VAL:CG1	1:D:240:LEU:HD11	2.48	0.42
1:D:507:ASP:C	1:D:519:SER:HB2	2.44	0.42
1:D:570:TRP:CD1	1:D:571:VAL:HG22	2.54	0.42
1:D:576:ILE:HD13	1:D:584:PRO:HB2	2.02	0.42
1:D:635:THR:HA	1:D:680:ILE:O	2.19	0.42
1:D:878:HIS:HA	1:D:879:PRO:HD3	1.69	0.42
1:A:102:ASN:C	1:A:102:ASN:HD22	2.27	0.42
1:A:988:GLY:C	1:A:989:PHE:CD1	2.97	0.42
1:B:274:PHE:HB3	1:B:286:ALA:O	2.20	0.42
1:B:407:LEU:HA	1:B:407:LEU:HD23	1.86	0.42
1:C:176:PHE:N	1:C:176:PHE:CD1	2.87	0.42
1:C:187:MET:O	1:C:187:MET:HG3	2.19	0.42
1:C:570:TRP:CD1	1:C:571:VAL:HG22	2.54	0.42
1:C:576:ILE:HD13	1:C:584:PRO:HB2	2.02	0.42
1:D:80:GLU:OE1	1:D:80:GLU:N	2.29	0.42
1:D:187:MET:O	1:D:187:MET:HG3	2.19	0.42
1:D:682:LEU:HA	1:D:683:PRO:HD3	1.91	0.42
1:D:708:TRP:CD1	1:D:708:TRP:H	2.38	0.42
1:D:856:TYR:N	1:D:856:TYR:CD1	2.88	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:A:360:HIS:HE1	1:A:362:LEU:HB2	1.84	0.42
1:A:429:ASP:HA	1:A:430:PRO:HD3	1.82	0.42
1:B:645:ARG:NH2	1:B:650:GLU:CD	2.76	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:C:708:TRP:CD1	1:C:708:TRP:H	2.38	0.42
1:C:856:TYR:N	1:C:856:TYR:CD1	2.88	0.42
1:C:878:HIS:HA	1:C:879:PRO:HD3	1.69	0.42
1:D:118:ASN:HA	1:D:119:PRO:HD2	1.61	0.42
1:D:183:ARG:HH11	1:D:183:ARG:HD3	1.56	0.42
1:B:102:ASN:C	1:B:102:ASN:HD22	2.27	0.42
1:B:227:VAL:CG1	1:B:228:ALA:N	2.83	0.42
1:B:378:LEU:HD23	1:B:378:LEU:HA	1.75	0.42
1:B:420:MET:HE3	1:B:420:MET:HB3	1.62	0.42
1:B:645:ARG:NH2	1:B:650:GLU:OE1	2.46	0.42
1:B:685:LEU:HA	1:B:686:PRO:HD3	1.84	0.42
1:B:822:LEU:HA	1:B:822:LEU:HD13	1.78	0.42
1:C:26:ARG:HD2	1:C:169:SER:HB3	2.02	0.42
1:C:214:LEU:HD23	1:C:214:LEU:HA	1.61	0.42
1:C:441:THR:O	1:C:445:GLN:HG3	2.20	0.42
1:C:822:LEU:HD12	1:C:823:LEU:N	2.34	0.42
1:D:26:ARG:HD2	1:D:169:SER:HB3	2.02	0.42
1:D:225:PHE:HA	1:D:243:GLU:O	2.19	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:D:858:ILE:HG12	1:D:864:MET:HB3	2.02	0.42
1:A:38:ASN:ND2	1:A:38:ASN:C	2.77	0.42
1:A:227:VAL:CG1	1:A:228:ALA:N	2.83	0.42
1:A:436:MET:HE1	1:A:467:ASN:HD22	1.81	0.42
1:A:576:ILE:HD13	1:A:584:PRO:HB2	2.02	0.42
1:A:645:ARG:NH2	1:A:650:GLU:CD	2.76	0.42
1:A:652:LEU:O	1:A:667:GLU:HA	2.20	0.42
1:B:576:ILE:HD13	1:B:584:PRO:HB2	2.02	0.42
1:C:118:ASN:HA	1:C:119:PRO:HD2	1.61	0.42
1:C:128:ASN:ND2	1:C:180:GLY:C	2.78	0.42
1:C:225:PHE:HA	1:C:243:GLU:O	2.19	0.42
1:C:568:TRP:CD1	1:C:568:TRP:C	2.98	0.42
1:D:128:ASN:ND2	1:D:180:GLY:C	2.78	0.42
1:D:581:ASN:O	2:I:73:THR:N	2.50	0.42
1:D:645:ARG:NH2	1:D:650:GLU:CD	2.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:822:LEU:HD12	1:D:823:LEU:N	2.34	0.42
1:A:200:GLN:OE1	1:A:200:GLN:N	2.44	0.41
1:A:420:MET:HE3	1:A:420:MET:HB3	1.62	0.41
1:A:617:LEU:HA	1:A:617:LEU:HD12	1.82	0.41
1:B:11:LEU:N	1:B:11:LEU:HD23	2.35	0.41
1:B:38:ASN:ND2	1:B:38:ASN:C	2.77	0.41
1:B:78:LEU:HA	1:B:79:PRO:HD2	1.58	0.41
1:B:436:MET:HE1	1:B:467:ASN:HD22	1.81	0.41
1:B:652:LEU:O	1:B:667:GLU:HA	2.21	0.41
1:C:80:GLU:OE1	1:C:80:GLU:N	2.29	0.41
1:C:579:ASP:CG	1:C:583:ASN:HB2	2.42	0.41
1:D:124:SER:HA	1:D:184:LEU:O	2.20	0.41
1:D:214:LEU:HD23	1:D:214:LEU:HA	1.61	0.41
1:D:652:LEU:O	1:D:667:GLU:HA	2.20	0.41
1:D:840:HIS:ND1	1:D:840:HIS:N	2.67	0.41
1:A:26:ARG:HD2	1:A:169:SER:HB3	2.02	0.41
1:A:436:MET:HE3	1:A:467:ASN:ND2	2.29	0.41
1:B:141:ILE:HG12	1:B:142:ILE:N	2.35	0.41
1:B:892:ALA:HB3	1:B:946:TYR:CE1	2.55	0.41
1:C:141:ILE:HG12	1:C:142:ILE:N	2.35	0.41
1:C:652:LEU:O	1:C:667:GLU:HA	2.20	0.41
1:D:141:ILE:HG12	1:D:142:ILE:N	2.35	0.41
3:L:83:PHE:CE2	3:L:106:ILE:HB	2.55	0.41
1:A:11:LEU:N	1:A:11:LEU:HD23	2.35	0.41
1:A:141:ILE:HG12	1:A:142:ILE:N	2.35	0.41
1:A:237:ARG:HH11	1:A:237:ARG:HB2	1.85	0.41
1:A:362:LEU:HD22	2:J:32:ASP:N	2.19	0.41
1:A:441:THR:O	1:A:445:GLN:HG3	2.20	0.41
1:A:849:LEU:N	1:A:849:LEU:HD23	2.30	0.41
1:A:892:ALA:HB3	1:A:946:TYR:CE1	2.55	0.41
1:B:26:ARG:HD2	1:B:169:SER:HB3	2.02	0.41
1:B:105:TYR:HB3	1:B:106:PRO:HD2	2.01	0.41
1:B:441:THR:O	1:B:445:GLN:HG3	2.20	0.41
1:C:124:SER:HA	1:C:184:LEU:O	2.20	0.41
1:C:840:HIS:N	1:C:840:HIS:ND1	2.67	0.41
1:D:649:ASN:O	1:D:702:GLN:HG3	2.20	0.41
2:J:49:GLY:HA2	3:N:94:TRP:CH2	2.56	0.41
3:L:35:TRP:CD2	3:L:73:LEU:HB2	2.55	0.41
3:M:35:TRP:CD2	3:M:73:LEU:HB2	2.55	0.41
3:M:83:PHE:CE2	3:M:106:ILE:HB	2.55	0.41
3:N:31:ASN:O	3:N:50:TYR:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:128:ASN:ND2	1:A:180:GLY:C	2.78	0.41
1:A:856:TYR:CD1	1:A:856:TYR:N	2.88	0.41
1:B:436:MET:HE3	1:B:467:ASN:ND2	2.29	0.41
1:C:149:ALA:O	1:C:150:PHE:HB3	2.21	0.41
1:D:579:ASP:CG	1:D:583:ASN:HB2	2.42	0.41
1:D:906:TYR:CB	1:D:907:PRO:CD	2.99	0.41
3:N:35:TRP:CD2	3:N:73:LEU:HB2	2.55	0.41
1:A:7:LEU:HD23	1:A:7:LEU:HA	1.85	0.41
1:A:105:TYR:HB3	1:A:106:PRO:HD2	2.01	0.41
1:B:128:ASN:ND2	1:B:180:GLY:C	2.78	0.41
1:B:649:ASN:O	1:B:702:GLN:HG3	2.20	0.41
1:C:274:PHE:HB3	1:C:286:ALA:O	2.20	0.41
1:C:533:LEU:C	1:C:533:LEU:CD1	2.93	0.41
2:K:49:GLY:HA2	3:O:94:TRP:CH2	2.56	0.41
1:A:63:PHE:HB3	1:A:64:PRO:CD	2.45	0.41
1:A:308:LEU:HA	1:A:308:LEU:HD23	1.80	0.41
1:A:454:ILE:C	1:A:455:ILE:HG13	2.46	0.41
1:A:474:TRP:CZ2	1:A:478:VAL:HG21	2.55	0.41
1:A:479:ASP:HA	1:A:480:PRO:HD2	1.73	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:A:835:LEU:HD12	1:A:857:ARG:HB2	2.03	0.41
1:A:949:HIS:CD2	1:A:1020:TRP:NE1	2.79	0.41
1:B:200:GLN:OE1	1:B:200:GLN:N	2.45	0.41
1:B:454:ILE:C	1:B:455:ILE:HG13	2.46	0.41
1:B:578:TYR:CA	2:K:30:THR:HG21	2.48	0.41
1:B:949:HIS:CD2	1:B:1020:TRP:NE1	2.79	0.41
1:C:649:ASN:O	1:C:702:GLN:HG3	2.21	0.41
1:C:742:THR:CG2	1:C:743:SER:H	2.31	0.41
1:D:274:PHE:HB3	1:D:286:ALA:O	2.20	0.41
1:D:370:GLN:CB	2:I:98:TRP:HH2	2.33	0.41
1:D:407:LEU:HD23	1:D:407:LEU:HA	1.86	0.41
1:D:533:LEU:C	1:D:533:LEU:CD1	2.93	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
2:K:78:TYR:OH	2:K:95:CYS:HB2	2.21	0.41
3:L:31:ASN:O	3:L:50:TYR:HA	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:TRP:CD1	1:A:568:TRP:C	2.98	0.41
1:A:619:GLU:HA	1:A:912:ALA:HB2	2.03	0.41
1:A:868:VAL:HG12	1:A:869:ASP:N	2.36	0.41
1:B:599:ARG:HB2	1:B:600:GLN:H	1.54	0.41
1:B:619:GLU:HA	1:B:912:ALA:HB2	2.03	0.41
1:B:778:THR:HG22	1:B:779:PRO:N	2.35	0.41
1:B:835:LEU:HD12	1:B:857:ARG:HB2	2.03	0.41
1:B:856:TYR:CD1	1:B:856:TYR:N	2.88	0.41
1:B:868:VAL:HG12	1:B:869:ASP:N	2.36	0.41
1:C:454:ILE:C	1:C:455:ILE:HG13	2.46	0.41
1:C:906:TYR:CB	1:C:907:PRO:CD	2.99	0.41
1:C:970:THR:HG22	1:C:972:HIS:O	2.21	0.41
1:D:149:ALA:O	1:D:150:PHE:HB3	2.21	0.41
1:D:454:ILE:C	1:D:455:ILE:HG13	2.46	0.41
1:D:612:THR:HA	1:D:613:PRO:HD3	1.90	0.41
1:A:78:LEU:HA	1:A:79:PRO:HD2	1.58	0.41
1:A:380:LYS:HE3	1:A:406:GLY:O	2.21	0.41
1:B:352:ARG:NH2	1:B:641:GLU:OE1	2.54	0.41
1:B:380:LYS:HE3	1:B:406:GLY:O	2.21	0.41
1:B:479:ASP:HA	1:B:480:PRO:HD2	1.73	0.41
1:B:568:TRP:CD1	1:B:568:TRP:C	2.98	0.41
1:B:736:ALA:C	1:B:737:ILE:HG22	2.46	0.41
1:B:956:GLN:CD	1:B:956:GLN:N	2.79	0.41
1:C:578:TYR:HA	1:C:583:ASN:O	2.20	0.41
1:C:655:MET:O	1:C:696:LEU:HD12	2.21	0.41
1:C:900:LEU:HA	1:C:900:LEU:HD23	1.83	0.41
1:D:568:TRP:CD1	1:D:568:TRP:C	2.98	0.41
1:D:619:GLU:HA	1:D:912:ALA:HB2	2.03	0.41
1:D:655:MET:O	1:D:696:LEU:HD12	2.21	0.41
1:D:892:ALA:HB3	1:D:946:TYR:CE1	2.56	0.41
1:D:900:LEU:HA	1:D:900:LEU:HD23	1.83	0.41
1:D:970:THR:HG22	1:D:972:HIS:O	2.21	0.41
2:I:78:TYR:OH	2:I:95:CYS:HB2	2.21	0.41
3:M:31:ASN:O	3:M:50:TYR:HA	2.20	0.41
3:N:11:LEU:HD23	3:N:12:SER:N	2.36	0.41
1:A:41:GLU:HG2	1:A:46:ARG:NH1	2.35	0.41
1:A:62:TRP:C	1:A:63:PHE:CD1	2.99	0.41
1:A:352:ARG:NH2	1:A:641:GLU:OE1	2.54	0.41
1:A:378:LEU:HD23	1:A:378:LEU:HA	1.75	0.41
1:A:578:TYR:HA	1:A:583:ASN:O	2.20	0.41
1:A:612:THR:HG21	2:J:56:SER:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:708:TRP:CD1	1:A:708:TRP:H	2.38	0.41
1:A:736:ALA:C	1:A:737:ILE:HG22	2.46	0.41
1:A:778:THR:HG22	1:A:779:PRO:N	2.35	0.41
1:A:832:ASP:OD1	1:A:832:ASP:N	2.50	0.41
1:A:917:ARG:NH2	1:A:943:GLU:OE2	2.54	0.41
1:A:956:GLN:CD	1:A:956:GLN:N	2.79	0.41
1:B:62:TRP:C	1:B:63:PHE:CD1	2.99	0.41
1:B:149:ALA:O	1:B:150:PHE:HB3	2.21	0.41
1:B:474:TRP:CZ2	1:B:478:VAL:HG21	2.55	0.41
1:B:655:MET:O	1:B:696:LEU:HD12	2.21	0.41
1:B:917:ARG:NH2	1:B:943:GLU:OE2	2.54	0.41
1:C:41:GLU:HG2	1:C:46:ARG:NH1	2.35	0.41
1:C:127:PHE:CE1	1:C:184:LEU:HG	2.56	0.41
1:C:262:GLN:O	1:C:262:GLN:HG2	2.19	0.41
1:C:578:TYR:CE2	2:H:28:SER:OG	2.51	0.41
1:C:612:THR:HA	1:C:613:PRO:HD3	1.90	0.41
1:C:619:GLU:HA	1:C:912:ALA:HB2	2.03	0.41
1:C:652:LEU:HD12	1:C:652:LEU:C	2.46	0.41
1:C:892:ALA:HB3	1:C:946:TYR:CE1	2.56	0.41
1:D:41:GLU:HG2	1:D:46:ARG:NH1	2.35	0.41
1:D:127:PHE:CE1	1:D:184:LEU:HG	2.56	0.41
1:D:578:TYR:HA	1:D:583:ASN:O	2.20	0.41
1:D:617:LEU:HD12	1:D:617:LEU:HA	1.83	0.41
1:D:652:LEU:HD12	1:D:652:LEU:C	2.46	0.41
1:D:742:THR:CG2	1:D:743:SER:H	2.32	0.41
2:H:78:TYR:OH	2:H:95:CYS:HB2	2.21	0.41
2:J:78:TYR:OH	2:J:95:CYS:HB2	2.21	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
3:O:83:PHE:CE2	3:O:106:ILE:HB	2.55	0.41
1:A:149:ALA:O	1:A:150:PHE:HB3	2.21	0.41
1:A:336:ARG:NH2	1:A:338:GLU:CD	2.79	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:41:GLU:HG2	1:B:46:ARG:NH1	2.35	0.41
1:B:63:PHE:HA	1:B:64:PRO:HD3	1.81	0.41
1:B:202:MET:HE2	1:B:202:MET:HB2	1.90	0.41
1:B:279:ILE:HD12	1:B:279:ILE:HG21	1.91	0.41
1:B:336:ARG:NH2	1:B:338:GLU:CD	2.79	0.41
1:B:472:TYR:O	1:B:476:LYS:HG2	2.20	0.41
1:B:576:ILE:CG1	2:K:53:TYR:HB2	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:708:TRP:CD1	1:B:708:TRP:H	2.38	0.41
1:B:849:LEU:N	1:B:849:LEU:HD23	2.30	0.41
1:C:27:LEU:HA	1:C:27:LEU:HD23	1.92	0.41
1:C:360:HIS:HE1	1:C:362:LEU:HB2	1.84	0.41
1:C:380:LYS:HE3	1:C:406:GLY:O	2.21	0.41
1:C:581:ASN:HD22	1:C:583:ASN:ND2	2.19	0.41
1:C:617:LEU:HD12	1:C:617:LEU:HA	1.83	0.41
1:D:27:LEU:HA	1:D:27:LEU:HD23	1.92	0.41
1:D:262:GLN:O	1:D:262:GLN:HG2	2.19	0.41
1:D:581:ASN:HD22	1:D:583:ASN:ND2	2.19	0.41
3:N:83:PHE:CE2	3:N:106:ILE:HB	2.55	0.41
1:A:202:MET:HE2	1:A:202:MET:HB2	1.90	0.40
1:A:225:PHE:C	1:A:226:HIS:CD2	2.99	0.40
1:B:69:VAL:HG13	1:B:70:PRO:HD2	2.03	0.40
1:B:486:TYR:CE2	1:B:488:GLY:HA3	2.56	0.40
1:B:832:ASP:OD1	1:B:832:ASP:N	2.49	0.40
1:B:844:HIS:ND1	1:B:845:GLN:HG2	2.36	0.40
1:C:89:ASN:O	1:C:92:MET:HB2	2.22	0.40
1:C:225:PHE:C	1:C:226:HIS:CD2	2.99	0.40
1:C:278:ILE:N	1:C:278:ILE:HD13	2.37	0.40
1:C:736:ALA:C	1:C:737:ILE:HG22	2.46	0.40
1:C:917:ARG:NH2	1:C:943:GLU:OE2	2.54	0.40
1:D:225:PHE:C	1:D:226:HIS:CD2	2.99	0.40
1:D:278:ILE:N	1:D:278:ILE:HD13	2.37	0.40
1:D:380:LYS:HE3	1:D:406:GLY:O	2.21	0.40
1:D:486:TYR:CE2	1:D:488:GLY:HA3	2.56	0.40
2:J:14:PRO:O	2:J:15:SER:HB3	2.21	0.40
1:A:69:VAL:HG13	1:A:70:PRO:HD2	2.03	0.40
1:A:229:THR:HG22	1:A:240:LEU:HD12	2.04	0.40
1:A:472:TYR:O	1:A:476:LYS:HG2	2.20	0.40
1:A:486:TYR:CE2	1:A:488:GLY:HA3	2.56	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:B:473:ARG:HD3	1:B:473:ARG:C	2.45	0.40
1:B:617:LEU:HD12	1:B:617:LEU:HA	1.82	0.40
1:C:229:THR:HG22	1:C:240:LEU:HD12	2.03	0.40
1:C:502:MET:HA	1:C:537:GLU:O	2.22	0.40
1:C:868:VAL:HG12	1:C:869:ASP:N	2.36	0.40
1:D:62:TRP:C	1:D:63:PHE:CD1	2.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:ALA:CB	1:D:66:PRO:CD	3.00	0.40
1:D:89:ASN:O	1:D:92:MET:HB2	2.22	0.40
1:D:844:HIS:ND1	1:D:845:GLN:HG2	2.36	0.40
1:D:868:VAL:HG12	1:D:869:ASP:N	2.36	0.40
1:D:917:ARG:NH2	1:D:943:GLU:OE2	2.54	0.40
1:D:949:HIS:CD2	1:D:1020:TRP:NE1	2.79	0.40
2:J:3:GLN:HB2	2:J:25:THR:OG1	2.22	0.40
2:K:3:GLN:HB2	2:K:25:THR:OG1	2.22	0.40
1:A:282:ARG:HG3	1:D:423:MET:HB2	2.03	0.40
1:A:581:ASN:HD22	1:A:583:ASN:ND2	2.19	0.40
1:A:694:LEU:HD12	1:A:694:LEU:HA	1.81	0.40
1:B:225:PHE:C	1:B:226:HIS:CD2	2.99	0.40
1:C:65:ALA:CB	1:C:66:PRO:CD	3.00	0.40
1:C:336:ARG:NH2	1:C:338:GLU:CD	2.79	0.40
1:C:407:LEU:HD23	1:C:407:LEU:HA	1.87	0.40
1:C:486:TYR:CE2	1:C:488:GLY:HA3	2.56	0.40
1:C:651:LEU:HD12	1:C:651:LEU:HA	1.46	0.40
1:C:844:HIS:ND1	1:C:845:GLN:HG2	2.36	0.40
1:C:949:HIS:CD2	1:C:1020:TRP:NE1	2.78	0.40
1:D:336:ARG:NH2	1:D:338:GLU:CD	2.79	0.40
1:D:502:MET:HA	1:D:537:GLU:O	2.22	0.40
1:D:524:LEU:O	1:D:561:ARG:NH2	2.50	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
3:N:76:ASN:C	3:N:76:ASN:ND2	2.77	0.40
1:A:100:TYR:O	1:A:597:ASN:HB2	2.22	0.40
1:A:173:LEU:HD23	1:A:173:LEU:HA	1.80	0.40
1:A:237:ARG:CB	1:A:237:ARG:NH1	2.79	0.40
1:A:272:ALA:HA	1:A:273:PRO:HD3	1.88	0.40
1:A:502:MET:HA	1:A:537:GLU:O	2.22	0.40
1:A:751:LEU:HD23	1:A:751:LEU:O	2.22	0.40
1:A:844:HIS:ND1	1:A:845:GLN:HG2	2.36	0.40
1:B:229:THR:HG22	1:B:240:LEU:HD12	2.04	0.40
1:B:581:ASN:HD22	1:B:583:ASN:ND2	2.19	0.40
1:B:658:LEU:HD23	1:B:661:LYS:HZ3	1.86	0.40
1:C:60:PHE:HA	1:C:122:CYS:O	2.22	0.40
1:C:244:VAL:O	1:C:288:ARG:HA	2.22	0.40
1:C:956:GLN:CD	1:C:956:GLN:N	2.79	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:D:360:HIS:HE1	1:D:362:LEU:HB2	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:736:ALA:C	1:D:737:ILE:HG22	2.46	0.40
1:D:956:GLN:CD	1:D:956:GLN:N	2.79	0.40
2:H:3:GLN:HB2	2:H:25:THR:OG1	2.22	0.40
2:I:3:GLN:HB2	2:I:25:THR:OG1	2.22	0.40
1:A:63:PHE:CB	1:A:64:PRO:CD	2.98	0.40
1:A:89:ASN:O	1:A:92:MET:HB2	2.21	0.40
1:A:473:ARG:HD3	1:A:473:ARG:C	2.45	0.40
1:A:652:LEU:HD12	1:A:652:LEU:C	2.46	0.40
1:A:682:LEU:HA	1:A:683:PRO:HD3	1.91	0.40
1:B:472:TYR:CD1	1:B:472:TYR:C	2.98	0.40
1:B:502:MET:HA	1:B:537:GLU:O	2.22	0.40
1:B:694:LEU:HD12	1:B:694:LEU:HA	1.82	0.40
1:C:62:TRP:C	1:C:63:PHE:CD1	2.99	0.40
1:C:778:THR:HG22	1:C:779:PRO:N	2.35	0.40
1:C:864:MET:HB2	1:C:864:MET:HE3	1.67	0.40
1:D:229:THR:HG22	1:D:240:LEU:HD12	2.04	0.40
1:D:778:THR:HG22	1:D:779:PRO:N	2.35	0.40
2:H:13:LYS:O	2:H:16:GLN:HG2	2.22	0.40
2:I:13:LYS:O	2:I:16:GLN:HG2	2.22	0.40
3:L:13:VAL:HG22	3:L:14:THR:N	2.35	0.40
3:O:14:THR:O	3:O:15:PRO:C	2.65	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%)	21	59
1	B	1026/1024 (100%)	953 (93%)	67 (6%)	6 (1%)	21	59
1	C	1026/1024 (100%)	953 (93%)	67 (6%)	6 (1%)	21	59
1	D	1026/1024 (100%)	953 (93%)	67 (6%)	6 (1%)	21	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	26	63

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 ⓘ

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%)	746 (85%)	134 (15%)	3	12
1	B	880/876 (100%)	746 (85%)	134 (15%)	3	12
1	C	880/876 (100%)	746 (85%)	134 (15%)	3	12
1	D	880/876 (100%)	746 (85%)	134 (15%)	3	12
2	H	102/102 (100%)	101 (99%)	1 (1%)	68	78
2	I	102/102 (100%)	101 (99%)	1 (1%)	68	78
2	J	102/102 (100%)	101 (99%)	1 (1%)	68	78
2	K	102/102 (100%)	101 (99%)	1 (1%)	68	78
3	L	94/94 (100%)	94 (100%)	0	100	100
3	M	94/94 (100%)	94 (100%)	0	100	100
3	N	94/94 (100%)	94 (100%)	0	100	100
3	O	94/94 (100%)	94 (100%)	0	100	100
All	All	4304/4288 (100%)	3764 (88%)	540 (12%)	6	16

All (540) 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	84	VAL
1	A	85	VAL
1	A	90	TRP

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Mol	Chain	Res	Type
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
1	A	219	THR
1	A	223	SER
1	A	230	ARG
1	A	237	ARG
1	A	245	GLN
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	291	LEU
1	A	310	ARG
1	A	322	LEU
1	A	333	ARG
1	A	347	LYS
1	A	357	HIS
1	A	385	ASN
1	A	424	ASN
1	A	437	SER
1	A	448	ARG
1	A	473	ARG
1	A	481	SER

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Mol	Chain	Res	Type
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	599	ARG
1	A	600	GLN
1	A	630	ARG
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	698	VAL
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	741	THR
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

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Mol	Chain	Res	Type
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	836	ILE
1	A	843	GLN
1	A	845	GLN
1	A	856	TYR
1	A	857	ARG
1	A	858	ILE
1	A	866	ILE
1	A	867	THR
1	A	874	SER
1	A	881	ARG
1	A	894	ARG
1	A	917	ARG
1	A	931	PHE
1	A	934	GLU
1	A	937	LEU
1	A	938	ARG
1	A	950	GLN
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	1018	LEU
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

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Mol	Chain	Res	Type
1	B	49	GLN
1	B	67	GLU
1	B	71	GLU
1	B	72	SER
1	B	80	GLU
1	B	84	VAL
1	B	85	VAL
1	B	90	TRP
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
1	B	219	THR
1	B	223	SER
1	B	230	ARG
1	B	237	ARG
1	B	245	GLN
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	291	LEU
1	B	310	ARG
1	B	322	LEU
1	B	333	ARG

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Mol	Chain	Res	Type
1	B	347	LYS
1	B	357	HIS
1	B	385	ASN
1	B	424	ASN
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	599	ARG
1	B	600	GLN
1	B	630	ARG
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	698	VAL
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	741	THR
1	B	743	SER

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Mol	Chain	Res	Type
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	836	ILE
1	B	843	GLN
1	B	845	GLN
1	B	856	TYR
1	B	857	ARG
1	B	858	ILE
1	B	866	ILE
1	B	867	THR
1	B	874	SER
1	B	881	ARG
1	B	894	ARG
1	B	917	ARG
1	B	931	PHE
1	B	934	GLU
1	B	937	LEU
1	B	938	ARG
1	B	950	GLN
1	B	969	GLU
1	B	986	ILE
1	B	991	MET
1	B	1004	SER
1	B	1006	GLU
1	B	1017	GLN

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Mol	Chain	Res	Type
1	B	1018	LEU
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	84	VAL
1	C	85	VAL
1	C	90	TRP
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
1	C	219	THR
1	C	223	SER
1	C	230	ARG
1	C	237	ARG
1	C	245	GLN
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

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Mol	Chain	Res	Type
1	C	278	ILE
1	C	279	ILE
1	C	282	ARG
1	C	288	ARG
1	C	291	LEU
1	C	310	ARG
1	C	322	LEU
1	C	333	ARG
1	C	347	LYS
1	C	357	HIS
1	C	385	ASN
1	C	424	ASN
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	599	ARG
1	C	600	GLN
1	C	630	ARG
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	698	VAL

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Mol	Chain	Res	Type
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	741	THR
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	836	ILE
1	C	843	GLN
1	C	845	GLN
1	C	856	TYR
1	C	857	ARG
1	C	858	ILE
1	C	866	ILE
1	C	867	THR
1	C	874	SER
1	C	881	ARG
1	C	894	ARG
1	C	917	ARG
1	C	931	PHE
1	C	934	GLU
1	C	937	LEU

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Mol	Chain	Res	Type
1	C	938	ARG
1	C	950	GLN
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	1018	LEU
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	84	VAL
1	D	85	VAL
1	D	90	TRP
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
1	D	219	THR
1	D	223	SER
1	D	230	ARG
1	D	237	ARG

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Mol	Chain	Res	Type
1	D	245	GLN
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	291	LEU
1	D	310	ARG
1	D	322	LEU
1	D	333	ARG
1	D	347	LYS
1	D	357	HIS
1	D	385	ASN
1	D	424	ASN
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	599	ARG
1	D	600	GLN
1	D	630	ARG
1	D	645	ARG
1	D	647	SER

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Mol	Chain	Res	Type
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	698	VAL
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	741	THR
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	836	ILE
1	D	843	GLN
1	D	845	GLN
1	D	856	TYR
1	D	857	ARG
1	D	858	ILE
1	D	866	ILE

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Mol	Chain	Res	Type
1	D	867	THR
1	D	874	SER
1	D	881	ARG
1	D	894	ARG
1	D	917	ARG
1	D	931	PHE
1	D	934	GLU
1	D	937	LEU
1	D	938	ARG
1	D	950	GLN
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	1018	LEU
1	D	1023	LYS
2	H	97	ASN
2	I	97	ASN
2	J	97	ASN
2	K	97	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (137) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	50	GLN
1	A	102	ASN
1	A	128	ASN
1	A	216	HIS
1	A	226	HIS
1	A	266	GLN
1	A	316	HIS
1	A	357	HIS
1	A	363	HIS
1	A	385	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	614	HIS
1	A	622	HIS
1	A	623	GLN
1	A	624	GLN
1	A	634	GLN
1	A	817	GLN
1	A	824	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	216	HIS
1	B	226	HIS
1	B	266	GLN
1	B	316	HIS
1	B	357	HIS
1	B	363	HIS
1	B	385	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	614	HIS
1	B	622	HIS
1	B	623	GLN
1	B	624	GLN
1	B	634	GLN
1	B	817	GLN
1	B	824	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

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Mol	Chain	Res	Type
1	C	102	ASN
1	C	128	ASN
1	C	216	HIS
1	C	226	HIS
1	C	266	GLN
1	C	316	HIS
1	C	357	HIS
1	C	363	HIS
1	C	385	ASN
1	C	424	ASN
1	C	445	GLN
1	C	467	ASN
1	C	554	GLN
1	C	581	ASN
1	C	597	ASN
1	C	604	ASN
1	C	614	HIS
1	C	622	HIS
1	C	624	GLN
1	C	634	GLN
1	C	817	GLN
1	C	824	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	266	GLN
1	D	316	HIS
1	D	357	HIS
1	D	363	HIS
1	D	385	ASN
1	D	424	ASN
1	D	467	ASN
1	D	554	GLN
1	D	581	ASN
1	D	597	ASN

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Mol	Chain	Res	Type
1	D	604	ASN
1	D	614	HIS
1	D	622	HIS
1	D	624	GLN
1	D	634	GLN
1	D	817	GLN
1	D	824	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	83	ASN
2	H	97	ASN
2	I	5	GLN
2	I	76	ASN
2	I	77	GLN
2	I	83	ASN
2	I	97	ASN
2	J	5	GLN
2	J	76	ASN
2	J	77	GLN
2	J	83	ASN
2	J	97	ASN
2	K	5	GLN
2	K	76	ASN
2	K	77	GLN
2	K	83	ASN
2	K	97	ASN
3	L	76	ASN
3	M	37	GLN
3	M	76	ASN
3	N	76	ASN
3	O	37	GLN
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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

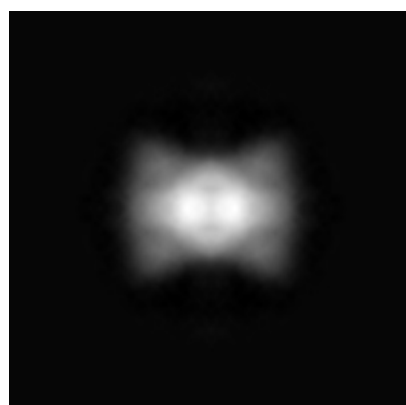
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2548. These allow visual inspection of the internal detail of the map and identification of artifacts.

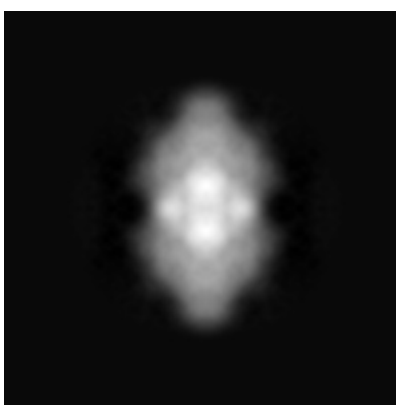
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

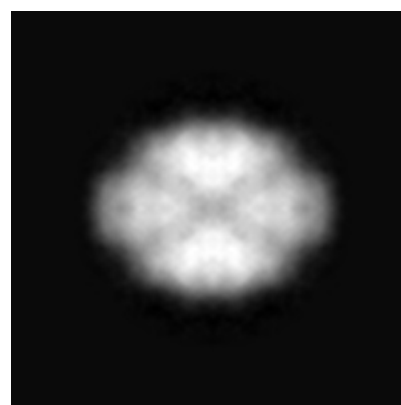
6.1.1 Primary map



X



Y

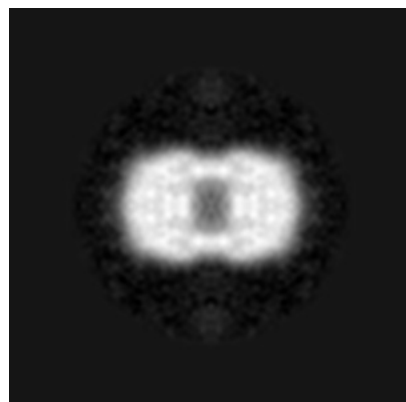


Z

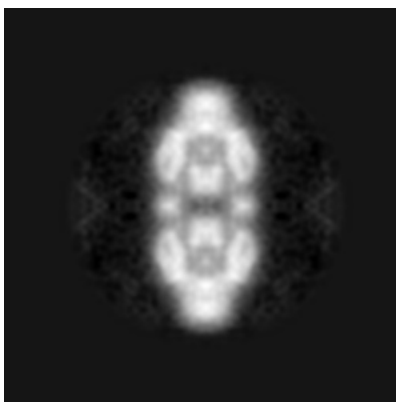
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 50



Y Index: 50

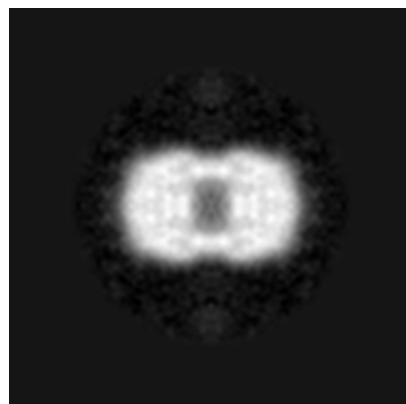


Z Index: 50

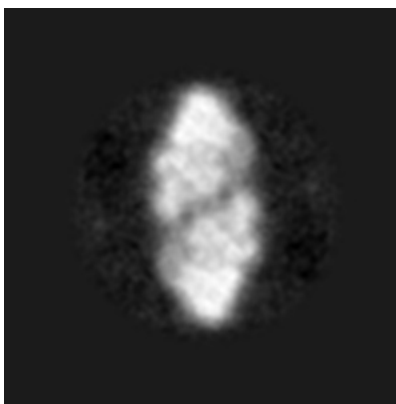
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 50



Y Index: 54



Z Index: 50

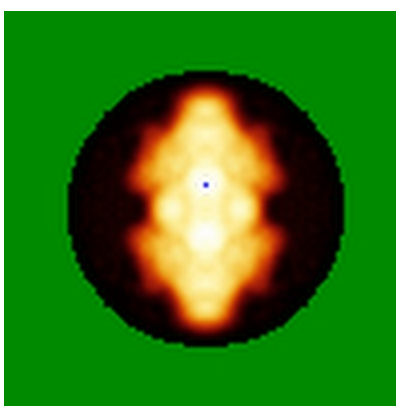
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

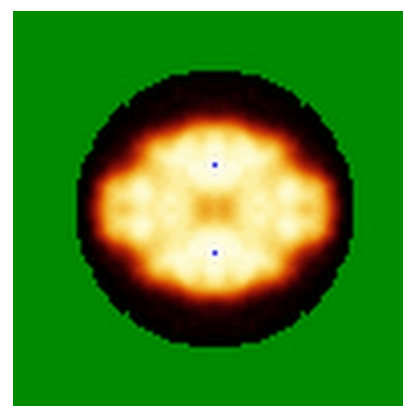
6.4.1 Primary map



X



Y

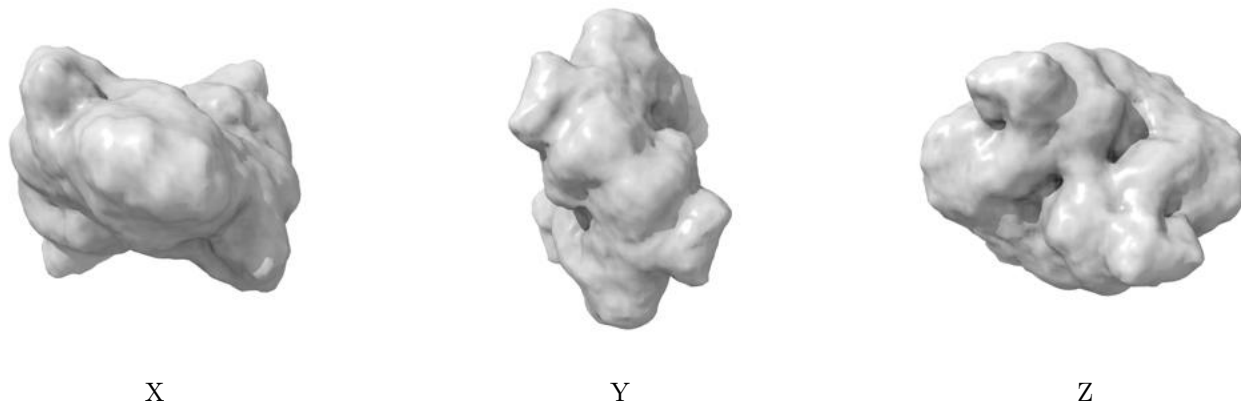


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.13. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

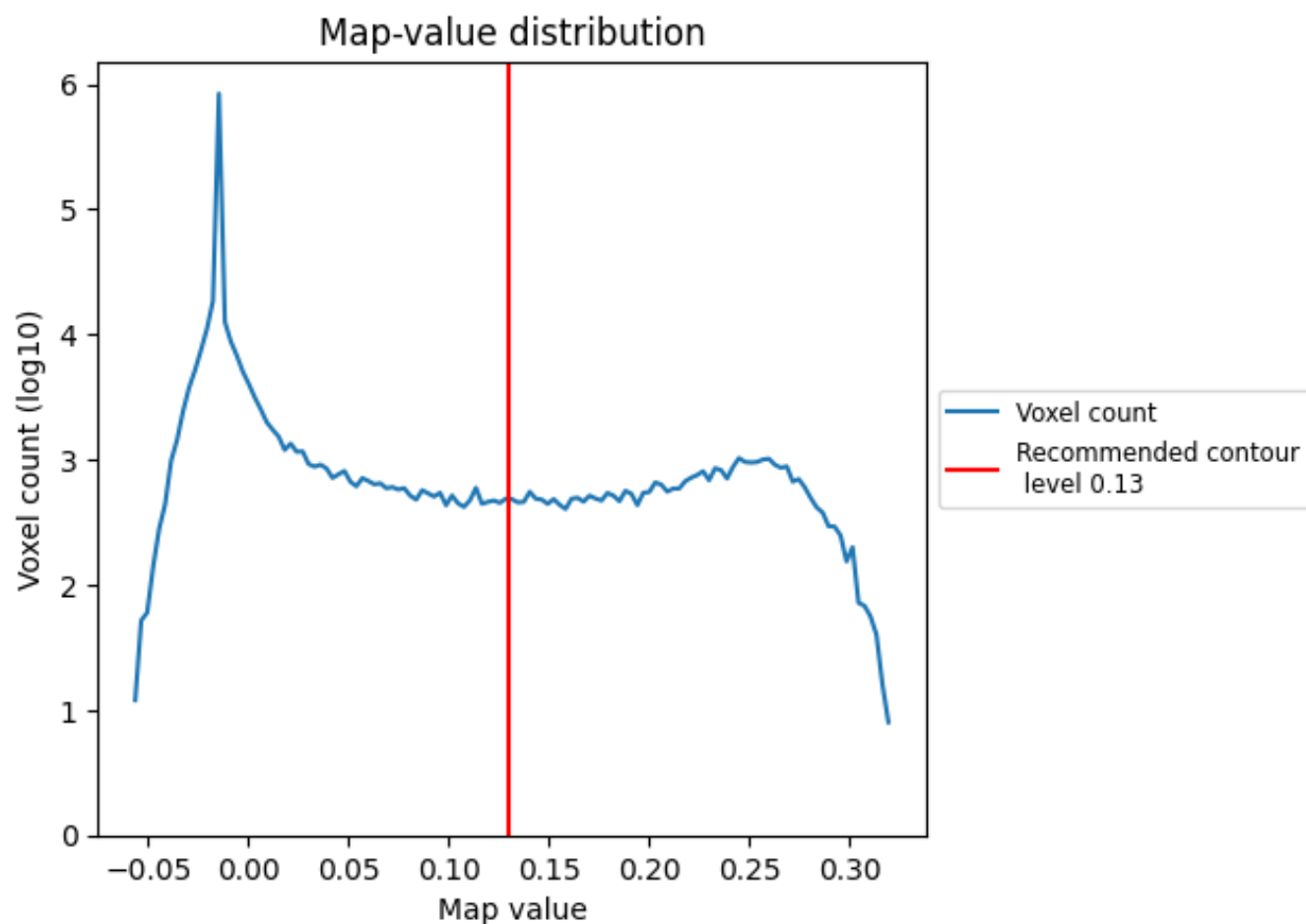
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

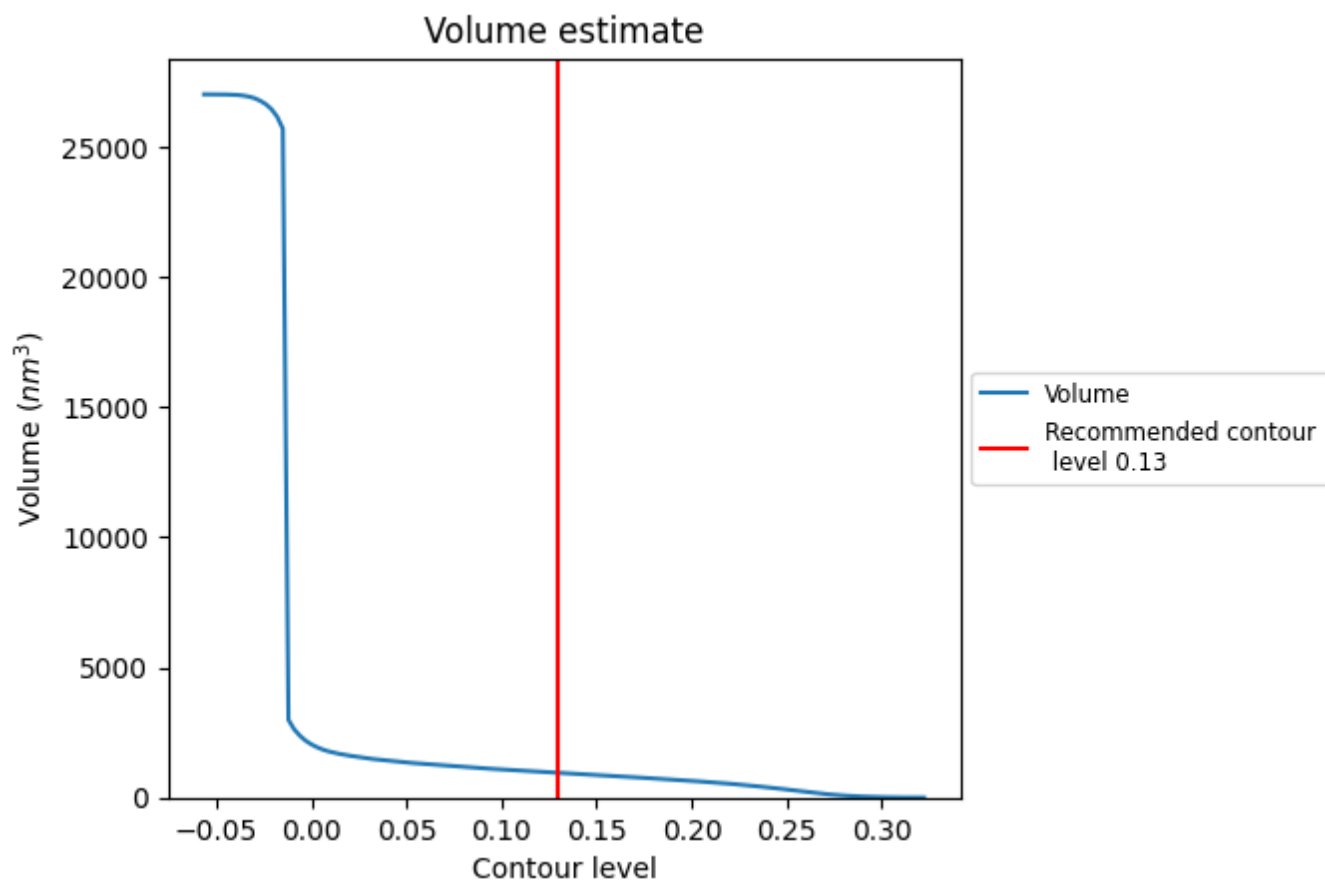
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

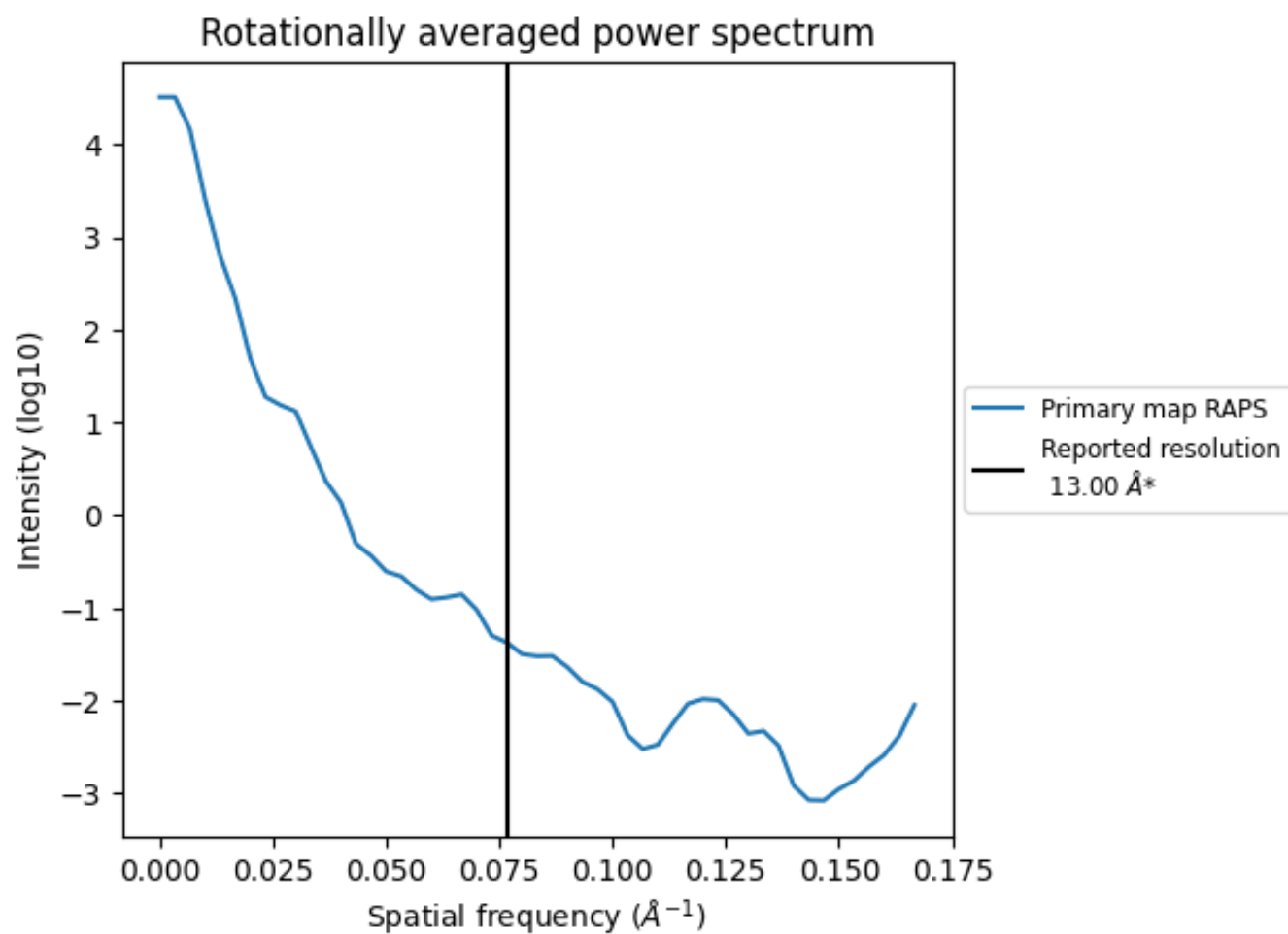
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 950 nm³; this corresponds to an approximate mass of 859 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.077 Å⁻¹

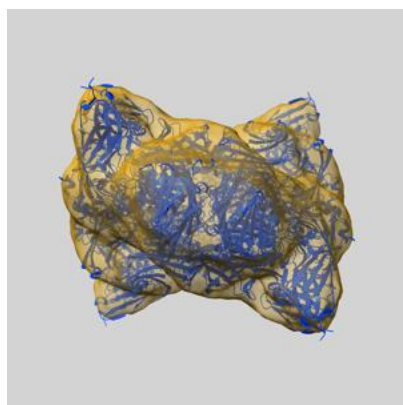
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

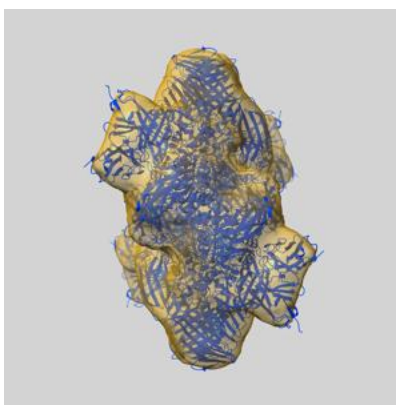
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-2548 and PDB model 4CKD. Per-residue inclusion information can be found in section [3](#) on page [5](#).

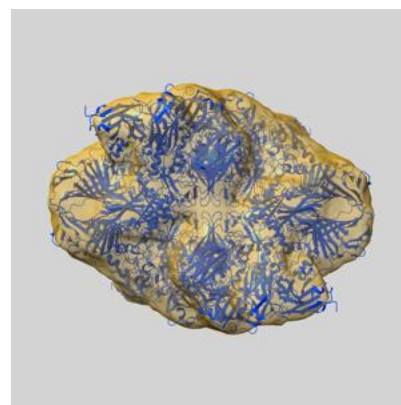
9.1 Map-model overlay [i](#)



X



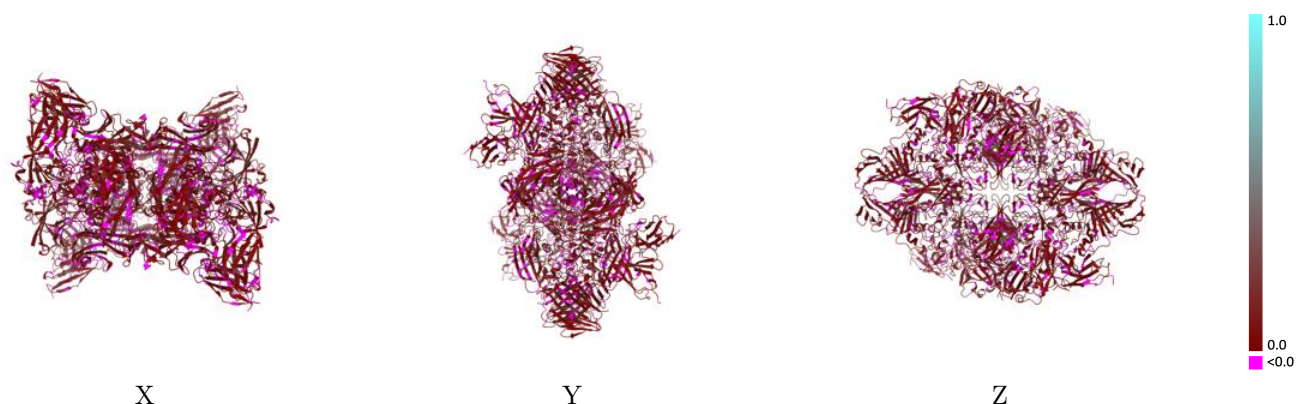
Y



Z

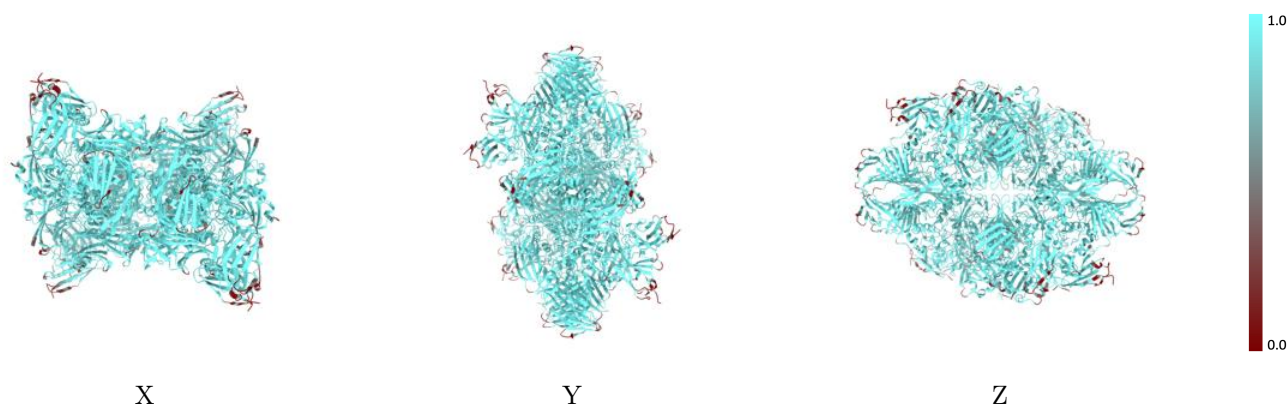
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



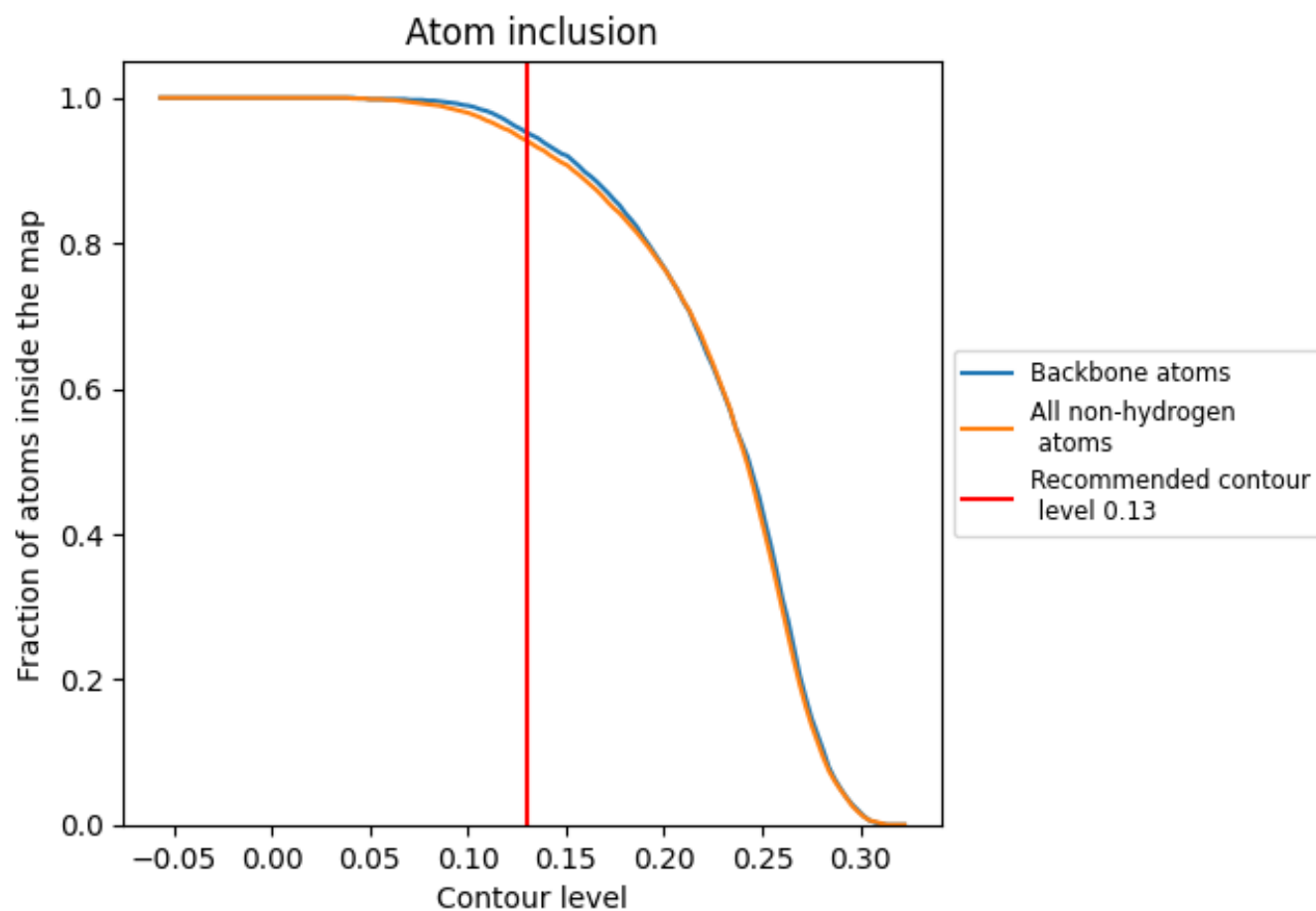
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.13).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9410	0.0750
A	0.9660	0.0760
B	0.9660	0.0790
C	0.9660	0.0750
D	0.9660	0.0790
H	0.7920	0.0510
I	0.7970	0.0590
J	0.7960	0.0580
K	0.7950	0.0660
L	0.8520	0.0580
M	0.8520	0.0740
N	0.8510	0.0590
O	0.8510	0.0700

