



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:04 PM UTC

PDB ID : 1U6G / pdb_00001u6g
Title : Crystal Structure of The Cand1-Cul1-Roc1 Complex
Authors : Goldenberg, S.J.; Shumway, S.D.; Cascio, T.C.; Garbutt, K.C.; Liu, J.; Xiong, Y.; Zheng, N.
Deposited on : 2004-07-29
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

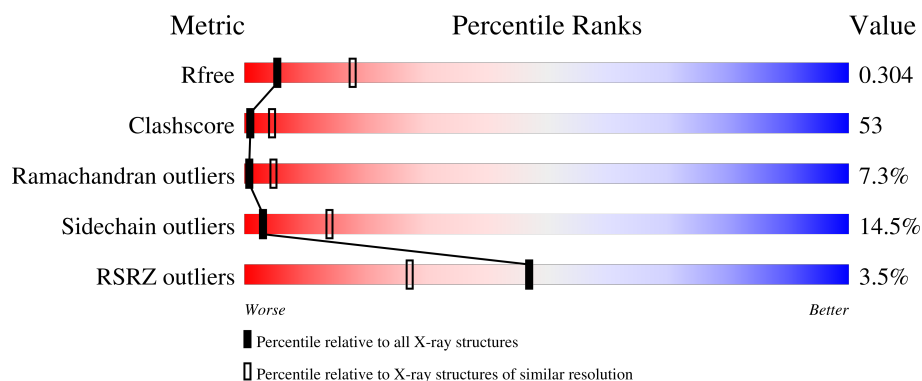
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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

Mol	Chain	Length	Quality of chain
1	A	776	4% 35% 41% 14% 8%
2	B	108	25% 40% 15% 19%
3	C	1230	3% 26% 49% 16% 7%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 15511 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cullin homolog 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	715	Total	C	N	O	S	0	0	0
			5855	3719	998	1109	29			

- Molecule 2 is a protein called RING-box protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	88	Total	C	N	O	S	0	0	0
			731	464	133	125	9			

- Molecule 3 is a protein called TIP120 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	1146	Total	C	N	O	S	0	0	0
			8904	5667	1509	1672	56			

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	3	Total	Zn	0	0
			3	3		

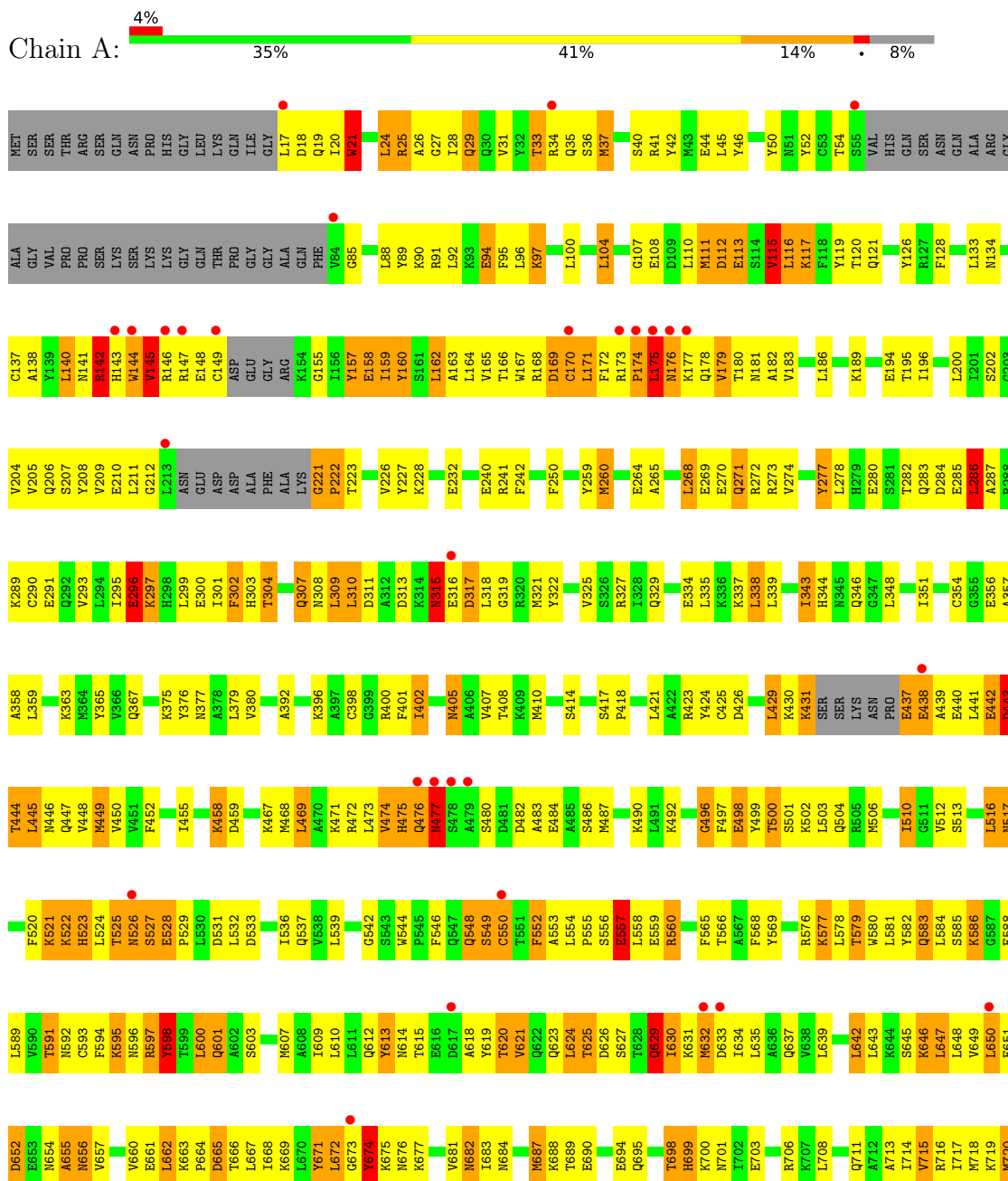
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	10	Total	O	0	0
			10	10		
5	B	3	Total	O	0	0
			3	3		
5	C	5	Total	O	0	0
			5	5		

3 Residue-property plots [i](#)

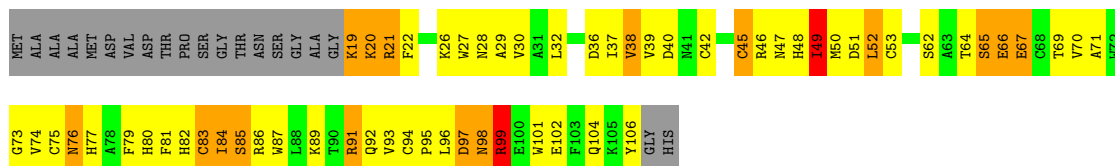
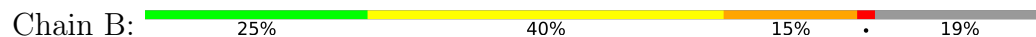
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Cullin homolog 1

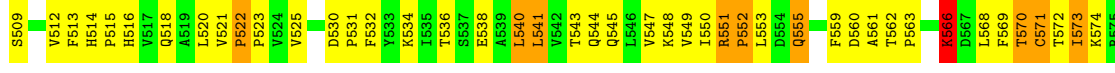
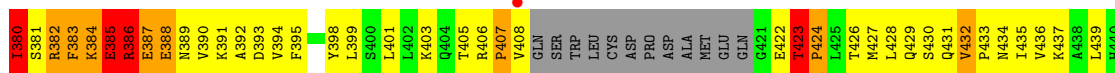
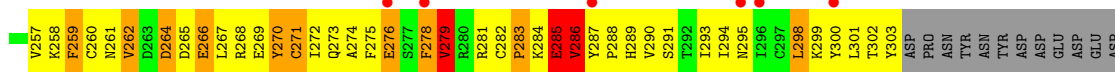


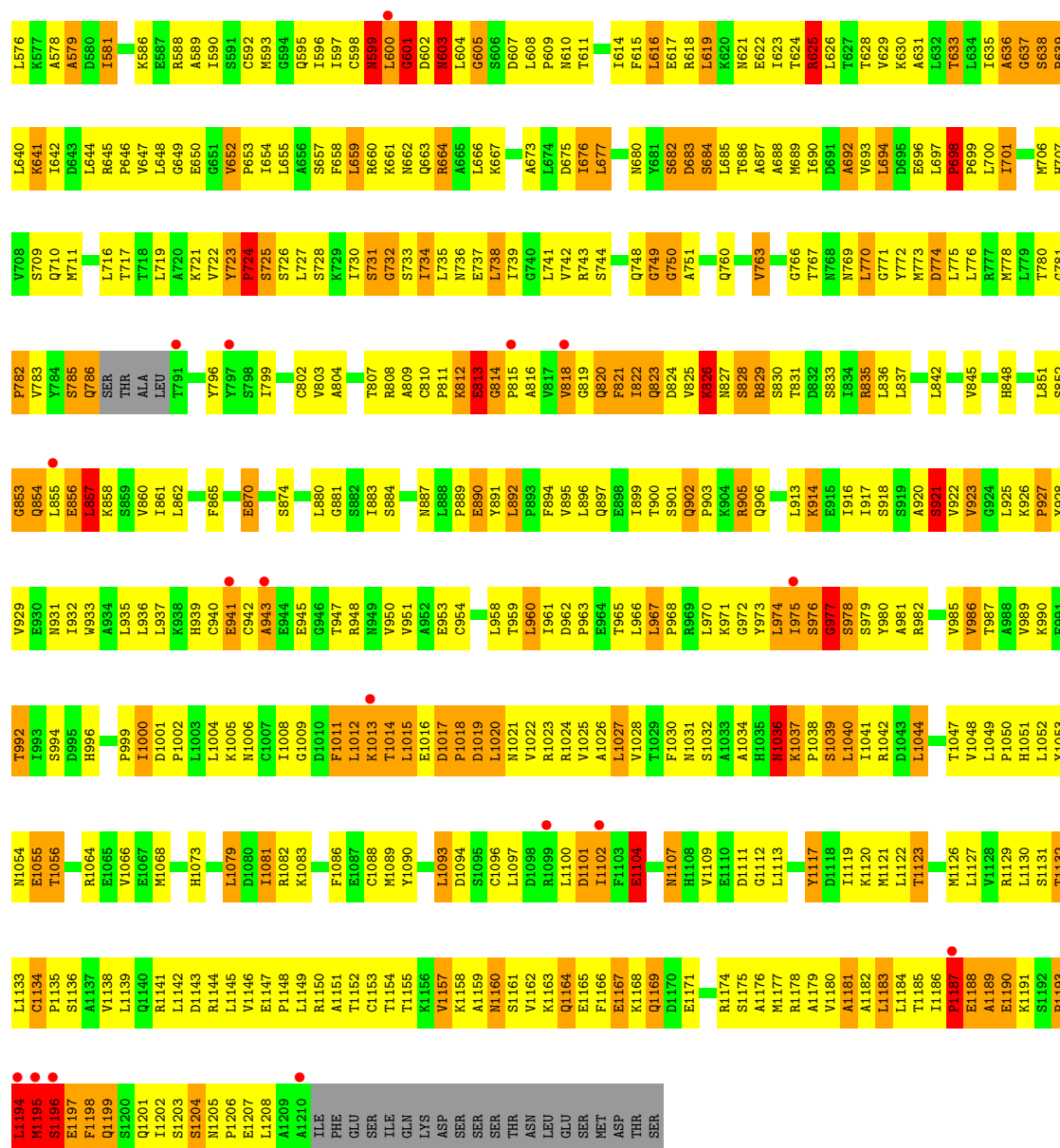


- Molecule 2: RING-box protein 1



- Molecule 3: TIP120 protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	108.47Å 151.33Å 215.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 50.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.10) 94.5 (50.00-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.84 (at 2.48Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.243 , 0.317 0.236 , 0.304	Depositor DCC
R_{free} test set	3108 reflections (2.95%)	wwPDB-VP
Wilson B-factor (Å ²)	56.5	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 68.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	15511	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.65	4/5949 (0.1%)	1.49	71/8007 (0.9%)
2	B	0.68	1/752 (0.1%)	1.27	9/1020 (0.9%)
3	C	0.59	5/9041 (0.1%)	1.25	113/12243 (0.9%)
All	All	0.62	10/15742 (0.1%)	1.35	193/21270 (0.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
3	C	0	2
All	All	0	3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	443	ASP	C-N	14.71	1.52	1.33
1	A	437	GLU	C-N	-14.37	1.13	1.33
3	C	601	GLY	C-N	-10.52	1.19	1.34
1	A	630	ILE	CG1-CD1	8.57	1.85	1.51
3	C	490	SER	N-CA	-8.11	1.36	1.46
3	C	375	VAL	N-CA	5.62	1.53	1.46
3	C	652	VAL	CA-CB	5.61	1.56	1.54
3	C	921	SER	C-N	-5.61	1.26	1.33
1	A	442	GLU	CA-CB	5.36	1.61	1.53
2	B	83	CYS	CA-CB	5.35	1.61	1.53

All (193) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	437	GLU	O-C-N	-72.55	6.91	123.00
1	A	476	GLN	N-CA-C	18.73	137.54	109.07
1	A	142	ARG	N-CA-C	14.29	128.83	111.40
1	A	721	ARG	N-CA-C	-14.03	88.06	109.24
3	C	487	LYS	CB-CA-C	12.51	135.31	110.42
3	C	1198	PHE	CA-CB-CG	-12.44	101.36	113.80
3	C	973	TYR	N-CA-C	-12.31	97.63	112.89
1	A	630	ILE	CB-CG1-CD1	-12.25	88.08	113.80
1	A	630	ILE	CB-CA-C	-12.23	96.77	111.08
1	A	111	MET	N-CA-C	12.04	129.92	114.75
3	C	117	LEU	C-N-CD	-11.81	76.58	125.00
3	C	380	ILE	N-CA-C	-11.75	101.46	111.56
3	C	117	LEU	CA-C-N	11.42	179.69	122.60
3	C	117	LEU	C-N-CA	11.42	179.69	122.60
1	A	113	GLU	N-CA-C	-11.16	98.48	112.88
2	B	45	CYS	N-CA-C	-10.99	91.32	109.24
3	C	377	PRO	CA-N-CD	-10.97	96.64	112.00
1	A	295	ILE	N-CA-C	10.67	120.54	111.90
3	C	423	THR	CA-C-N	10.61	130.01	118.97
3	C	423	THR	C-N-CA	10.61	130.01	118.97
1	A	637	GLN	OE1-CD-NE2	-10.60	112.00	122.60
1	A	33	THR	N-CA-C	-10.32	88.82	110.80
1	A	687	MET	N-CA-C	-10.21	95.17	110.28
3	C	488	SER	N-CA-C	10.21	125.96	110.14
3	C	1195	MET	N-CA-C	10.16	132.45	110.80
3	C	117	LEU	N-CA-C	10.14	121.80	110.13
3	C	940	CYS	N-CA-C	-9.83	101.92	112.93
1	A	315	ASN	N-CA-C	9.67	123.76	112.93
1	A	629	GLN	OE1-CD-NE2	-9.57	113.03	122.60
1	A	656	ASN	N-CA-C	-9.57	101.81	112.72
3	C	42	ASP	N-CA-C	-9.55	95.14	110.32
1	A	170	CYS	N-CA-C	-9.51	102.77	114.75
3	C	1198	PHE	CB-CA-C	-9.46	96.56	109.71
3	C	738	LEU	N-CA-C	-9.43	99.89	111.40
3	C	1199	GLN	OE1-CD-NE2	-9.38	113.22	122.60
3	C	599	ASN	N-CA-C	9.37	125.41	113.88
3	C	1189	ALA	N-CA-C	-9.26	99.27	113.89
1	A	286	LEU	N-CA-C	-9.20	101.34	111.36
1	A	115	VAL	N-CA-C	-9.03	101.41	110.62
3	C	813	GLU	N-CA-C	8.88	124.07	109.24
3	C	1196	SER	N-CA-C	8.82	123.42	109.39
3	C	147	ASP	N-CA-C	-8.79	93.67	108.26
3	C	375	VAL	CB-CA-C	-8.77	96.91	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	GLY	CA-C-N	8.76	130.79	119.84
1	A	221	GLY	C-N-CA	8.76	130.79	119.84
3	C	487	LYS	N-CA-C	-8.54	92.60	110.80
3	C	99	LYS	N-CA-C	-8.41	92.90	110.80
3	C	131	CYS	N-CA-C	-8.38	102.99	113.55
1	A	111	MET	CA-C-N	-8.27	111.48	121.90
1	A	111	MET	C-N-CA	-8.27	111.48	121.90
3	C	921	SER	N-CA-C	-8.22	93.29	110.80
3	C	941	GLU	N-CA-C	-8.22	93.29	110.80
3	C	601	GLY	O-C-N	-8.21	112.03	122.70
3	C	488	SER	CA-C-N	8.17	137.15	121.54
3	C	488	SER	C-N-CA	8.17	137.15	121.54
3	C	188	ARG	N-CA-C	-8.13	95.96	109.46
1	A	296	GLU	N-CA-C	8.10	123.21	113.16
1	A	552	PHE	N-CA-C	7.96	121.06	107.93
3	C	469	LEU	N-CA-C	7.91	122.52	113.02
3	C	923	VAL	N-CA-C	-7.80	105.10	111.81
1	A	647	LEU	N-CA-C	-7.76	102.84	114.64
3	C	43	ASP	N-CA-C	-7.59	104.43	112.93
1	A	18	ASP	N-CA-C	-7.51	104.36	113.97
1	A	301	ILE	N-CA-C	-7.43	103.70	111.58
3	C	271	CYS	N-CA-C	-7.42	103.12	111.14
2	B	80	HIS	N-CA-C	-7.39	99.34	110.28
1	A	169	ASP	N-CA-C	-7.33	104.29	112.57
3	C	279	VAL	N-CA-C	-7.30	106.78	113.71
3	C	1136	SER	N-CA-C	7.29	120.15	111.33
3	C	1160	ASN	N-CA-C	-7.26	104.42	113.20
3	C	285	GLU	N-CA-C	7.21	126.15	110.80
1	A	637	GLN	CG-CD-NE2	7.17	127.16	116.40
3	C	485	ASN	CA-C-N	-7.17	107.86	121.54
3	C	485	ASN	C-N-CA	-7.17	107.86	121.54
3	C	823	GLN	N-CA-C	-7.08	105.57	114.56
3	C	266	GLU	N-CA-C	-7.03	104.70	112.72
3	C	692	ALA	N-CA-C	-7.02	104.71	113.28
3	C	229	THR	N-CA-C	-6.92	103.86	112.72
3	C	622	GLU	N-CA-C	-6.91	103.20	112.94
3	C	603	ASN	N-CA-C	-6.84	103.51	112.41
1	A	297	LYS	N-CA-C	-6.84	104.55	113.17
1	A	157	TYR	N-CA-C	-6.84	100.09	110.14
3	C	744	SER	CA-C-N	6.83	126.46	119.56
3	C	744	SER	C-N-CA	6.83	126.46	119.56
3	C	1194	LEU	N-CA-C	-6.82	96.27	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1199	GLN	CG-CD-NE2	6.82	126.62	116.40
3	C	491	SER	N-CA-C	-6.81	104.86	113.72
2	B	45	CYS	CA-C-N	-6.80	109.70	122.27
2	B	45	CYS	C-N-CA	-6.80	109.70	122.27
3	C	814	GLY	N-CA-C	-6.80	98.48	112.34
3	C	818	VAL	N-CA-C	-6.79	103.86	110.72
3	C	16	THR	N-CA-C	-6.78	102.20	110.88
1	A	629	GLN	CG-CD-NE2	6.72	126.47	116.40
1	A	311	ASP	N-CA-C	-6.66	104.05	111.71
1	A	46	TYR	N-CA-C	-6.58	104.03	111.07
1	A	175	LEU	N-CA-C	6.53	124.71	110.80
1	A	316	GLU	N-CA-C	-6.52	105.46	113.41
3	C	375	VAL	N-CA-C	6.50	122.85	109.34
1	A	544	TRP	CA-C-N	6.41	126.04	119.56
1	A	544	TRP	C-N-CA	6.41	126.04	119.56
1	A	310	LEU	N-CA-C	-6.40	104.66	113.18
3	C	1014	THR	N-CA-C	-6.35	107.38	114.62
1	A	630	ILE	N-CA-CB	6.32	118.03	110.95
2	B	46	ARG	N-CA-C	6.32	120.91	111.81
3	C	118	PRO	CA-N-CD	-6.32	103.15	112.00
3	C	17	SER	N-CA-C	6.29	120.63	113.15
3	C	1104	GLU	N-CA-C	-6.27	104.44	111.28
1	A	722	LYS	N-CA-C	-6.18	106.06	113.97
3	C	601	GLY	CA-C-N	6.18	129.70	120.31
3	C	601	GLY	C-N-CA	6.18	129.70	120.31
3	C	636	ALA	N-CA-C	-6.15	101.86	110.35
3	C	1019	ASP	N-CA-C	6.13	118.50	109.24
1	A	497	PHE	N-CA-C	-6.10	105.07	113.18
3	C	81	GLU	N-CA-C	6.07	120.22	112.34
3	C	163	SER	N-CA-C	6.06	120.84	112.90
3	C	1044	LEU	N-CA-C	6.05	120.27	113.01
3	C	978	SER	N-CA-C	6.01	119.42	110.52
3	C	625	ARG	N-CA-C	6.01	123.60	110.80
3	C	633	THR	N-CA-C	-5.99	105.46	112.89
3	C	488	SER	O-C-N	5.99	130.82	123.10
3	C	381	SER	N-CA-C	-5.95	104.14	111.33
3	C	473	ILE	CA-C-N	5.92	125.54	119.56
3	C	473	ILE	C-N-CA	5.92	125.54	119.56
1	A	498	GLU	N-CA-C	-5.91	104.92	111.71
3	C	488	SER	CA-C-O	5.87	128.67	121.56
3	C	106	SER	N-CA-C	-5.87	104.96	111.36
3	C	1011	PHE	N-CA-C	-5.86	105.14	112.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	477	ASN	CA-CB-CG	-5.85	106.75	112.60
3	C	349	VAL	N-CA-C	-5.85	104.92	110.42
1	A	548	GLN	N-CA-C	-5.83	102.84	110.53
3	C	698	PRO	N-CA-C	5.82	117.80	110.70
3	C	468	ALA	N-CA-C	5.81	123.17	110.80
1	A	630	ILE	CA-C-N	5.72	132.47	121.54
1	A	630	ILE	C-N-CA	5.72	132.47	121.54
2	B	47	ASN	CA-C-N	-5.71	113.13	121.76
2	B	47	ASN	C-N-CA	-5.71	113.13	121.76
3	C	32	THR	N-CA-C	-5.71	105.05	111.28
3	C	977	GLY	N-CA-C	5.71	126.70	113.18
3	C	812	LYS	N-CA-C	-5.70	97.92	108.24
1	A	26	ALA	N-CA-C	-5.67	104.79	110.97
3	C	485	ASN	O-C-N	-5.67	115.32	121.95
1	A	112	ASP	N-CA-C	5.66	119.77	111.34
3	C	464	VAL	N-CA-C	-5.63	105.61	110.74
1	A	277	TYR	N-CA-C	5.62	121.40	113.02
3	C	478	PRO	N-CA-C	-5.62	105.72	113.53
3	C	347	TRP	N-CA-C	5.61	122.75	110.80
1	A	160	TYR	N-CA-C	-5.61	104.56	111.40
3	C	278	PHE	N-CA-C	5.58	118.89	112.97
1	A	401	PHE	N-CA-C	5.56	118.27	111.82
1	A	133	LEU	N-CA-C	-5.55	105.13	111.07
3	C	682	SER	N-CA-C	5.54	117.00	110.97
1	A	444	THR	N-CA-C	-5.53	104.47	111.11
3	C	1107	ASN	N-CA-C	-5.53	104.94	110.97
1	A	476	GLN	N-CA-CB	-5.47	102.52	111.66
1	A	443	ASP	N-CA-C	-5.47	104.96	111.03
1	A	655	ALA	N-CA-C	5.46	118.12	108.24
1	A	620	THR	N-CA-C	-5.46	102.81	110.50
3	C	1183	LEU	N-CA-C	-5.44	106.64	113.28
1	A	760	TYR	N-CA-C	-5.44	106.81	113.50
3	C	492	ASN	N-CA-C	-5.44	105.27	111.14
3	C	472	HIS	N-CA-C	5.41	121.73	113.19
3	C	857	LEU	N-CA-C	5.37	118.29	111.69
3	C	489	SER	CA-C-O	5.33	128.13	120.51
1	A	591	THR	N-CA-C	5.30	118.12	107.41
3	C	490	SER	N-CA-C	-5.30	97.21	107.44
3	C	1134	CYS	N-CA-C	5.30	121.52	109.81
1	A	627	SER	N-CA-C	5.29	116.73	110.97
3	C	210	LEU	N-CA-C	5.29	119.83	112.90
3	C	489	SER	O-C-N	5.28	129.61	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	576	ARG	N-CA-C	5.28	118.24	110.59
1	A	525	THR	N-CA-C	-5.26	105.55	111.28
3	C	1020	LEU	N-CA-C	5.25	117.85	109.02
2	B	99	ARG	N-CA-C	-5.25	100.05	108.55
3	C	821	PHE	N-CA-C	-5.19	106.02	112.93
3	C	981	ALA	N-CA-C	-5.18	105.54	111.14
3	C	365	HIS	N-CA-C	-5.18	105.25	112.45
1	A	721	ARG	CA-C-N	-5.18	113.62	122.11
1	A	721	ARG	C-N-CA	-5.18	113.62	122.11
3	C	474	PRO	N-CA-C	5.16	120.31	113.86
3	C	1036	ASN	N-CA-C	5.16	117.48	110.88
1	A	458	LYS	N-CA-C	5.16	117.64	111.71
3	C	230	TYR	N-CA-C	-5.14	105.66	112.34
3	C	222	ASP	N-CA-C	-5.13	99.63	108.56
3	C	1187	PRO	N-CA-C	5.11	123.00	112.47
1	A	175	LEU	CA-CB-CG	5.11	134.18	116.30
3	C	1175	SER	N-CA-C	-5.07	106.94	113.23
3	C	224	MET	N-CA-C	5.06	121.57	110.80
1	A	598	TYR	N-CA-C	5.03	117.06	109.41
2	B	51	ASP	N-CA-C	-5.02	102.36	110.14
1	A	264	GLU	N-CA-C	-5.01	105.71	111.07
1	A	699	HIS	N-CA-C	-5.01	105.47	111.03
1	A	302	PHE	N-CA-C	-5.00	105.91	111.36
3	C	921	SER	CB-CA-C	5.00	120.37	110.42

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	437	GLU	Mainchain
3	C	599	ASN	Mainchain
3	C	601	GLY	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5855	0	5900	541	0
2	B	731	0	689	81	0
3	C	8904	0	9249	1098	0
4	B	3	0	0	0	0
5	A	10	0	0	0	0
5	B	3	0	0	0	0
5	C	5	0	0	0	0
All	All	15511	0	15838	1668	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 53.

All (1668) 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)
3:C:373:LYS:CE	3:C:427:MET:HE3	1.25	1.60
3:C:373:LYS:HE3	3:C:427:MET:CE	1.36	1.54
3:C:373:LYS:CG	3:C:427:MET:HE1	1.36	1.52
1:A:630:ILE:CG1	1:A:630:ILE:CD1	1.85	1.51
3:C:373:LYS:CE	3:C:427:MET:CE	1.84	1.48
2:B:97:ASP:OD1	2:B:97:ASP:O	1.55	1.25
3:C:373:LYS:CG	3:C:427:MET:CE	2.19	1.18
3:C:373:LYS:CD	3:C:427:MET:HE1	1.73	1.17
3:C:600:LEU:O	3:C:602:ASP:N	1.81	1.13
3:C:375:VAL:HG13	3:C:379:LEU:HB2	1.19	1.12
3:C:38:SER:HB3	3:C:78:LYS:HD2	1.25	1.12
2:B:52:LEU:HD12	2:B:52:LEU:H	1.09	1.11
1:A:630:ILE:HG21	1:A:630:ILE:HD13	1.34	1.10
3:C:829:ARG:HH11	3:C:829:ARG:HB2	1.18	1.07
3:C:373:LYS:HG3	3:C:427:MET:HE1	1.08	1.06
1:A:597:ARG:HH11	1:A:597:ARG:HB2	1.14	1.06
3:C:377:PRO:HB3	3:C:431:GLN:OE1	1.54	1.05
3:C:1013:LYS:HE2	3:C:1047:THR:HG21	1.38	1.05
1:A:630:ILE:CD1	1:A:630:ILE:CB	2.35	1.04
1:A:625:THR:OG1	1:A:632:MET:HG2	1.58	1.02
3:C:211:ILE:O	3:C:215:LEU:HG	1.60	1.01
1:A:440:GLU:O	1:A:444:THR:N	1.94	0.99
3:C:1015:LEU:HD13	3:C:1018:PRO:HG3	1.41	0.99
3:C:1194:LEU:HD12	3:C:1194:LEU:O	1.63	0.99
3:C:1190:GLU:OE2	3:C:1191:LYS:HG2	1.63	0.98
1:A:441:LEU:O	1:A:445:LEU:HB2	1.63	0.97
3:C:373:LYS:HE2	3:C:427:MET:HE3	1.00	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:982:ARG:NH2	3:C:1018:PRO:HB2	1.79	0.97
3:C:287:TYR:HB2	3:C:288:PRO:HD3	1.43	0.96
3:C:85:GLU:HG3	3:C:133:LYS:HE2	1.46	0.96
3:C:294:ILE:HG21	3:C:357:LEU:HG	1.44	0.96
3:C:375:VAL:CG1	3:C:379:LEU:HB2	1.95	0.95
1:A:625:THR:HG21	1:A:632:MET:HG3	1.44	0.95
3:C:1081:ILE:HG13	3:C:1082:ARG:N	1.78	0.95
3:C:192:ARG:HH21	3:C:227:THR:HG21	1.33	0.94
1:A:600:LEU:H	1:A:600:LEU:HD23	1.32	0.93
3:C:373:LYS:HE3	3:C:427:MET:SD	2.09	0.93
3:C:1011:PHE:O	3:C:1015:LEU:HB2	1.66	0.93
3:C:385:GLU:HA	3:C:391:LYS:HE2	1.51	0.92
1:A:175:LEU:HD11	1:A:208:TYR:CE1	2.04	0.92
3:C:481:ILE:HD11	3:C:520:LEU:HD23	1.51	0.92
3:C:375:VAL:HG13	3:C:379:LEU:CB	1.99	0.91
1:A:592:ASN:HD21	2:B:21:ARG:HE	1.14	0.91
3:C:231:ILE:HG23	3:C:273:GLN:NE2	1.84	0.91
1:A:600:LEU:HD23	1:A:600:LEU:N	1.84	0.91
1:A:116:LEU:O	1:A:120:THR:HG23	1.71	0.91
3:C:551:ARG:NH1	3:C:553:LEU:HB2	1.85	0.91
3:C:432:VAL:HG13	3:C:435:ILE:HB	1.53	0.90
1:A:542:GLY:H	2:B:76:ASN:HD21	1.20	0.90
1:A:625:THR:OG1	1:A:632:MET:CG	2.19	0.90
3:C:270:TYR:HD1	3:C:270:TYR:H	1.19	0.90
3:C:187:PRO:HB2	3:C:188:ARG:HH11	1.36	0.90
1:A:175:LEU:HG	1:A:208:TYR:OH	1.73	0.89
3:C:1147:GLU:HB3	3:C:1148:PRO:HD3	1.54	0.89
1:A:672:LEU:N	1:A:672:LEU:HD12	1.87	0.88
3:C:975:ILE:HG23	3:C:976:SER:H	1.37	0.88
1:A:173:ARG:HB2	1:A:174:PRO:HD3	1.53	0.88
3:C:285:GLU:HA	3:C:287:TYR:CE2	2.09	0.88
3:C:349:VAL:HG23	3:C:350:ARG:H	1.37	0.88
3:C:485:ASN:O	3:C:486:ASP:HB3	1.72	0.88
3:C:249:LEU:HA	3:C:252:ILE:HG13	1.55	0.88
3:C:298:LEU:O	3:C:298:LEU:HD22	1.72	0.88
1:A:592:ASN:HA	1:A:597:ARG:HH12	1.38	0.87
3:C:211:ILE:HG12	3:C:244:ARG:HE	1.39	0.87
1:A:642:LEU:HB3	1:A:648:LEU:HD12	1.54	0.87
1:A:592:ASN:CA	1:A:597:ARG:HH12	1.87	0.87
1:A:630:ILE:CD1	1:A:630:ILE:HG21	2.04	0.87
1:A:631:LYS:O	1:A:635:LEU:N	2.06	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:432:VAL:HG12	3:C:436:VAL:HG23	1.57	0.87
3:C:548:LYS:HA	3:C:551:ARG:HG3	1.54	0.87
1:A:144:TRP:O	1:A:145:VAL:HG13	1.74	0.87
3:C:211:ILE:HG12	3:C:244:ARG:NE	1.89	0.87
3:C:270:TYR:HA	3:C:273:GLN:OE1	1.75	0.87
3:C:92:CYS:HB3	3:C:137:ARG:HG2	1.56	0.86
1:A:167:TRP:O	1:A:170:CYS:HB3	1.75	0.86
1:A:440:GLU:O	1:A:444:THR:OG1	1.91	0.86
2:B:49:ILE:HD13	2:B:50:MET:HG2	1.54	0.86
3:C:821:PHE:C	3:C:823:GLN:H	1.80	0.86
3:C:999:PRO:O	3:C:1002:PRO:HD2	1.76	0.86
3:C:1199:GLN:HB3	3:C:1202:ILE:HB	1.59	0.85
3:C:1037:LYS:HD2	3:C:1040:LEU:HD11	1.56	0.85
3:C:373:LYS:HG3	3:C:427:MET:CE	1.93	0.85
2:B:97:ASP:O	2:B:97:ASP:CG	2.18	0.85
3:C:373:LYS:HG2	3:C:427:MET:CE	2.06	0.85
3:C:379:LEU:HA	3:C:382:ARG:HB2	1.56	0.84
3:C:812:LYS:HG3	3:C:812:LYS:O	1.76	0.84
1:A:287:ALA:O	1:A:291:GLU:HG3	1.76	0.84
3:C:269:GLU:O	3:C:273:GLN:HG3	1.77	0.84
3:C:373:LYS:CD	3:C:427:MET:CE	2.42	0.84
1:A:300:GLU:O	1:A:304:THR:HG22	1.77	0.83
1:A:474:VAL:HG12	1:A:475:HIS:N	1.93	0.83
3:C:206:CYS:O	3:C:210:LEU:HB2	1.78	0.83
3:C:551:ARG:N	3:C:552:PRO:HD2	1.94	0.83
3:C:377:PRO:CB	3:C:431:GLN:OE1	2.27	0.83
3:C:473:ILE:O	3:C:477:VAL:HG23	1.79	0.83
3:C:590:ILE:HG21	3:C:628:THR:HG22	1.60	0.82
3:C:650:GLU:O	3:C:654:ILE:HG13	1.80	0.82
1:A:630:ILE:CD1	1:A:630:ILE:CG2	2.57	0.82
3:C:982:ARG:O	3:C:986:VAL:HG12	1.77	0.82
3:C:548:LYS:HA	3:C:551:ARG:CG	2.09	0.82
3:C:625:ARG:O	3:C:629:VAL:HG23	1.79	0.82
1:A:597:ARG:HB2	1:A:597:ARG:NH1	1.93	0.82
3:C:301:LEU:HD12	3:C:302:THR:H	1.44	0.82
3:C:386:ARG:HB2	3:C:386:ARG:CZ	2.09	0.82
3:C:673:ALA:HA	3:C:676:ILE:HD11	1.61	0.82
1:A:95:PHE:HD2	1:A:96:LEU:HD12	1.44	0.82
3:C:249:LEU:HA	3:C:252:ILE:CG1	2.09	0.82
3:C:1194:LEU:O	3:C:1195:MET:HB2	1.78	0.81
1:A:171:LEU:HG	1:A:175:LEU:HD22	1.60	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1012:LEU:O	3:C:1014:THR:N	2.14	0.81
3:C:375:VAL:O	3:C:379:LEU:N	2.13	0.81
3:C:566:LYS:HB2	3:C:566:LYS:HZ3	1.46	0.81
1:A:592:ASN:HD21	2:B:21:ARG:NE	1.78	0.81
2:B:52:LEU:HD12	2:B:52:LEU:N	1.93	0.81
3:C:1012:LEU:C	3:C:1014:THR:H	1.89	0.81
3:C:1139:LEU:HA	3:C:1142:LEU:HB2	1.63	0.80
3:C:181:LEU:HD13	3:C:217:GLU:HG3	1.60	0.80
1:A:27:GLY:O	1:A:31:VAL:HG23	1.81	0.80
3:C:967:LEU:N	3:C:968:PRO:HD2	1.97	0.80
3:C:566:LYS:H	3:C:566:LYS:HD3	1.45	0.80
3:C:187:PRO:HB2	3:C:188:ARG:NH1	1.96	0.80
3:C:601:GLY:O	3:C:604:LEU:N	2.15	0.79
1:A:145:VAL:O	1:A:146:ARG:HG3	1.82	0.79
3:C:1142:LEU:O	3:C:1146:VAL:HG23	1.82	0.79
1:A:672:LEU:HD12	1:A:672:LEU:H	1.45	0.79
3:C:1176:ALA:O	3:C:1180:VAL:HG23	1.82	0.79
3:C:1190:GLU:O	3:C:1193:PRO:HD2	1.79	0.79
3:C:1169:GLN:OE1	3:C:1169:GLN:HA	1.82	0.79
3:C:1199:GLN:O	3:C:1203:SER:HB3	1.82	0.79
3:C:970:LEU:HD22	3:C:985:VAL:HG23	1.64	0.79
1:A:614:ASN:ND2	2:B:21:ARG:HA	1.98	0.78
1:A:405:ASN:ND2	1:A:407:VAL:H	1.81	0.78
3:C:831:THR:HG22	3:C:833:SER:H	1.46	0.78
1:A:651:GLU:HA	1:A:669:LYS:HZ2	1.45	0.78
1:A:142:ARG:CZ	1:A:147:ARG:HG2	2.13	0.78
3:C:267:LEU:HA	3:C:270:TYR:CE1	2.17	0.78
2:B:52:LEU:H	2:B:52:LEU:CD1	1.90	0.78
3:C:551:ARG:HH11	3:C:553:LEU:HB2	1.44	0.78
3:C:1052:LEU:HD11	3:C:1088:CYS:HB3	1.65	0.78
1:A:297:LYS:O	1:A:297:LYS:HD3	1.84	0.78
3:C:231:ILE:HG23	3:C:273:GLN:CD	2.09	0.78
3:C:375:VAL:O	3:C:379:LEU:HB2	1.84	0.78
3:C:110:LEU:HD23	3:C:157:ILE:HD13	1.67	0.77
3:C:349:VAL:HG23	3:C:350:ARG:N	1.99	0.77
3:C:372:TYR:HA	3:C:377:PRO:HG2	1.64	0.77
3:C:423:THR:O	3:C:427:MET:HG3	1.83	0.77
3:C:1187:PRO:O	3:C:1189:ALA:N	2.17	0.77
3:C:432:VAL:CG1	3:C:436:VAL:HG23	2.13	0.77
1:A:577:LYS:HB2	2:B:36:ASP:HB3	1.65	0.77
3:C:170:VAL:HA	3:C:173:HIS:CD2	2.18	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:736:ASN:HD21	3:C:778:MET:HE1	1.50	0.77
1:A:528:GLU:O	1:A:528:GLU:HG2	1.84	0.77
3:C:1081:ILE:HG13	3:C:1082:ARG:H	1.48	0.77
1:A:577:LYS:NZ	1:A:578:LEU:H	1.82	0.77
1:A:618:ALA:HB2	1:A:669:LYS:HG2	1.66	0.77
3:C:982:ARG:HH21	3:C:1018:PRO:HB2	1.48	0.77
3:C:77:SER:O	3:C:78:LYS:HD3	1.82	0.77
1:A:621:VAL:HG23	1:A:668:ILE:HD11	1.65	0.76
3:C:600:LEU:O	3:C:601:GLY:C	2.28	0.76
3:C:723:TYR:H	3:C:724:PRO:HD3	1.51	0.76
3:C:1055:GLU:HG3	3:C:1081:ILE:HD12	1.66	0.76
3:C:686:THR:OG1	3:C:689:MET:HG3	1.86	0.76
3:C:1204:SER:O	3:C:1208:LEU:HD23	1.85	0.76
1:A:142:ARG:HH11	1:A:142:ARG:HB3	1.48	0.76
3:C:660:ARG:HD2	3:C:696:GLU:OE2	1.85	0.76
3:C:942:CYS:HA	3:C:948:ARG:HD2	1.67	0.76
1:A:614:ASN:HD21	2:B:22:PHE:H	1.34	0.76
3:C:481:ILE:HD12	3:C:523:PRO:HG3	1.67	0.76
1:A:630:ILE:HD13	1:A:630:ILE:CG2	2.12	0.75
3:C:1015:LEU:HD12	3:C:1022:VAL:HG12	1.68	0.75
3:C:1199:GLN:HG2	3:C:1202:ILE:HG12	1.68	0.75
2:B:81:PHE:O	2:B:85:SER:HB2	1.86	0.75
3:C:299:LYS:NZ	3:C:379:LEU:HD22	2.02	0.75
3:C:820:GLN:HB3	3:C:842:LEU:HD21	1.69	0.75
1:A:134:ASN:HA	1:A:159:ILE:HG21	1.69	0.75
1:A:134:ASN:HA	1:A:159:ILE:CG2	2.17	0.75
1:A:645:SER:O	1:A:646:LYS:HB3	1.87	0.75
3:C:611:THR:HA	3:C:614:ILE:HG12	1.69	0.75
1:A:438:GLU:HA	1:A:438:GLU:OE1	1.86	0.75
1:A:614:ASN:HD21	2:B:22:PHE:N	1.85	0.74
3:C:135:THR:CG2	3:C:176:ILE:HD11	2.18	0.74
3:C:618:ARG:HB3	3:C:624:THR:HG21	1.68	0.74
3:C:738:LEU:O	3:C:742:VAL:HG23	1.87	0.74
2:B:62:SER:O	2:B:66:GLU:HG3	1.88	0.74
1:A:676:ASN:HD22	1:A:677:LYS:N	1.86	0.74
3:C:827:ASN:O	3:C:829:ARG:N	2.20	0.74
1:A:117:LYS:NZ	1:A:121:GLN:HE21	1.85	0.74
1:A:173:ARG:CB	1:A:174:PRO:HD3	2.18	0.74
1:A:315:ASN:HB3	1:A:379:LEU:HD21	1.69	0.74
3:C:143:ALA:O	3:C:145:GLN:N	2.20	0.73
3:C:268:ARG:HE	3:C:348:LYS:HB3	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:640:LEU:O	3:C:642:ILE:N	2.20	0.73
1:A:625:THR:CG2	1:A:632:MET:HG3	2.18	0.73
3:C:211:ILE:CG1	3:C:244:ARG:HE	2.00	0.73
1:A:592:ASN:ND2	2:B:21:ARG:HE	1.86	0.73
3:C:618:ARG:CB	3:C:624:THR:HG21	2.19	0.73
3:C:36:LYS:HG3	3:C:37:ASP:OD2	1.89	0.73
3:C:94:ASN:HB3	3:C:102:LEU:HG	1.70	0.73
3:C:616:LEU:HD23	3:C:647:VAL:HG12	1.69	0.73
3:C:42:ASP:HB2	3:C:45:SER:HB2	1.71	0.73
1:A:720:MET:HE3	1:A:720:MET:O	1.88	0.73
3:C:249:LEU:HD22	3:C:250:GLU:OE1	1.89	0.73
3:C:551:ARG:HD2	3:C:551:ARG:C	2.14	0.73
3:C:226:THR:CG2	3:C:227:THR:N	2.52	0.72
3:C:226:THR:HG22	3:C:227:THR:N	2.05	0.72
3:C:974:LEU:HD21	3:C:1011:PHE:CD2	2.24	0.72
3:C:1151:ALA:O	3:C:1155:THR:HG23	1.88	0.72
1:A:405:ASN:C	1:A:405:ASN:HD22	1.97	0.72
1:A:107:GLY:HA2	1:A:110:LEU:HD12	1.71	0.72
3:C:1188:GLU:HA	3:C:1190:GLU:OE1	1.89	0.72
3:C:633:THR:HA	3:C:676:ILE:HD13	1.71	0.72
3:C:899:ILE:HG21	3:C:935:LEU:HD11	1.72	0.72
3:C:829:ARG:HH11	3:C:829:ARG:CB	2.00	0.72
3:C:813:GLU:CD	3:C:814:GLY:H	1.97	0.72
1:A:603:SER:HB3	1:A:684:ASN:OD1	1.89	0.72
3:C:814:GLY:N	3:C:815:PRO:HD2	2.05	0.72
3:C:825:VAL:C	3:C:827:ASN:H	1.98	0.72
1:A:339:LEU:O	1:A:343:ILE:HG22	1.90	0.72
3:C:262:VAL:O	3:C:267:LEU:HD11	1.89	0.72
3:C:825:VAL:CG2	3:C:860:VAL:HG22	2.20	0.72
1:A:33:THR:O	1:A:34:ARG:HD3	1.91	0.71
3:C:283:PRO:C	3:C:284:LYS:HD3	2.15	0.71
3:C:375:VAL:O	3:C:375:VAL:HG12	1.90	0.71
1:A:134:ASN:HD22	1:A:159:ILE:HG22	1.54	0.71
3:C:735:LEU:HD11	3:C:778:MET:SD	2.30	0.71
3:C:495:ILE:HD11	3:C:534:LYS:HB3	1.73	0.71
3:C:366:GLU:OE2	3:C:367:MET:HG3	1.91	0.71
1:A:175:LEU:HD23	1:A:176:ASN:N	2.06	0.71
1:A:186:LEU:HD11	1:A:196:ILE:HB	1.72	0.71
1:A:438:GLU:OE1	1:A:438:GLU:CA	2.37	0.71
3:C:857:LEU:HD23	3:C:858:LYS:N	2.05	0.71
1:A:228:LYS:HA	1:A:232:GLU:HB3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:GLU:OE1	1:A:282:THR:HG22	1.89	0.71
1:A:682:ASN:C	1:A:682:ASN:HD22	1.98	0.71
3:C:822:ILE:C	3:C:826:LYS:HB2	2.16	0.71
1:A:475:HIS:CE1	1:A:586:LYS:HD3	2.26	0.70
3:C:1188:GLU:HA	3:C:1190:GLU:CD	2.15	0.70
1:A:405:ASN:HD22	1:A:407:VAL:H	1.37	0.70
3:C:601:GLY:O	3:C:604:LEU:CB	2.39	0.70
1:A:533:ASP:OD2	2:B:26:LYS:HE3	1.92	0.70
3:C:375:VAL:HG22	3:C:379:LEU:HD12	1.74	0.70
1:A:557:GLU:CD	1:A:557:GLU:H	1.98	0.70
3:C:287:TYR:HB2	3:C:288:PRO:CD	2.21	0.70
3:C:270:TYR:N	3:C:270:TYR:CD1	2.58	0.70
1:A:475:HIS:NE2	1:A:584:LEU:C	2.50	0.70
3:C:375:VAL:CG1	3:C:375:VAL:O	2.37	0.70
1:A:446:ASN:OD1	1:A:490:LYS:HE2	1.92	0.69
1:A:717:ILE:HA	3:C:25:MET:CE	2.22	0.69
1:A:592:ASN:HB3	1:A:597:ARG:HH22	1.54	0.69
3:C:1049:LEU:HD11	3:C:1100:LEU:HD23	1.74	0.69
3:C:218:LEU:HD13	3:C:234:ILE:HD13	1.75	0.69
1:A:676:ASN:HD22	1:A:677:LYS:H	1.38	0.69
3:C:233:CYS:O	3:C:237:ILE:HG13	1.92	0.69
3:C:820:GLN:HA	3:C:823:GLN:HG3	1.73	0.69
3:C:532:PHE:CZ	3:C:534:LYS:HB2	2.28	0.69
1:A:467:LYS:HZ2	1:A:698:THR:HB	1.56	0.69
3:C:550:ILE:C	3:C:552:PRO:HD2	2.16	0.69
3:C:373:LYS:HE3	3:C:427:MET:HE1	1.51	0.69
3:C:239:ARG:CZ	3:C:276:GLU:HG2	2.23	0.69
3:C:600:LEU:C	3:C:602:ASP:H	2.01	0.69
3:C:818:VAL:HG22	3:C:854:GLN:OE1	1.92	0.69
3:C:1141:ARG:O	3:C:1145:LEU:HG	1.93	0.69
1:A:344:HIS:NE2	1:A:348:LEU:HD11	2.08	0.69
3:C:244:ARG:HH11	3:C:244:ARG:HG2	1.56	0.69
3:C:855:LEU:HD11	3:C:858:LYS:HD2	1.75	0.69
3:C:211:ILE:HD13	3:C:244:ARG:HH21	1.57	0.69
3:C:914:LYS:HD3	3:C:953:GLU:HG2	1.73	0.69
1:A:29:GLN:O	1:A:33:THR:HG23	1.93	0.68
3:C:690:ILE:HG13	3:C:719:LEU:HD11	1.74	0.68
1:A:174:PRO:O	1:A:178:GLN:HB3	1.93	0.68
1:A:517:ASN:HD21	1:A:536:ILE:H	1.41	0.68
1:A:660:VAL:HG12	1:A:661:GLU:N	2.08	0.68
3:C:38:SER:CB	3:C:78:LYS:HD2	2.15	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:601:GLY:O	3:C:604:LEU:HB2	1.92	0.68
1:A:718:MET:CE	1:A:771:TYR:HB2	2.23	0.68
3:C:736:ASN:ND2	3:C:778:MET:HE1	2.07	0.68
1:A:549:SER:O	1:A:550:CYS:C	2.34	0.68
3:C:905:ARG:HH11	3:C:905:ARG:CG	2.05	0.68
1:A:639:LEU:O	1:A:643:LEU:HG	1.94	0.68
3:C:209:ASP:O	3:C:213:HIS:NE2	2.27	0.68
3:C:551:ARG:HD2	3:C:551:ARG:O	1.94	0.68
1:A:536:ILE:HG12	1:A:537:GLN:H	1.58	0.68
3:C:4:ALA:O	3:C:40:LYS:HG3	1.94	0.68
3:C:633:THR:HG23	3:C:676:ILE:HG12	1.74	0.68
3:C:8:ILE:HD12	3:C:8:ILE:H	1.57	0.68
3:C:212:GLU:HB3	3:C:248:TYR:OH	1.93	0.68
3:C:905:ARG:HH11	3:C:905:ARG:HG3	1.58	0.68
1:A:24:LEU:O	1:A:28:ILE:HG12	1.93	0.68
3:C:551:ARG:N	3:C:552:PRO:CD	2.57	0.67
3:C:701:ILE:HG21	3:C:738:LEU:HD23	1.75	0.67
3:C:1008:ILE:HG23	3:C:1009:GLY:N	2.10	0.67
3:C:1097:LEU:HA	3:C:1100:LEU:HD12	1.76	0.67
3:C:206:CYS:CB	3:C:207:PHE:HA	2.24	0.67
3:C:350:ARG:HH21	3:C:386:ARG:HH12	1.41	0.67
3:C:826:LYS:HA	3:C:826:LYS:HE2	1.77	0.67
1:A:134:ASN:HD21	1:A:157:TYR:CB	2.08	0.67
1:A:357:ALA:H	3:C:489:SER:HB2	1.59	0.67
3:C:38:SER:HB3	3:C:78:LYS:CD	2.13	0.67
3:C:76:VAL:HG21	3:C:113:VAL:HG13	1.77	0.67
3:C:282:CYS:HB2	3:C:283:PRO:HD3	1.77	0.67
3:C:550:ILE:HD12	3:C:561:ALA:HB1	1.77	0.67
1:A:717:ILE:HA	3:C:25:MET:HE3	1.77	0.67
2:B:49:ILE:HD12	2:B:50:MET:H	1.60	0.67
3:C:33:GLU:C	3:C:35:GLN:H	2.01	0.67
3:C:253:ILE:O	3:C:257:VAL:HG23	1.94	0.67
3:C:385:GLU:CA	3:C:391:LYS:HE2	2.24	0.67
3:C:913:LEU:HD23	3:C:913:LEU:O	1.95	0.67
3:C:295:ASN:OD1	3:C:357:LEU:HD21	1.94	0.67
3:C:821:PHE:C	3:C:823:GLN:N	2.51	0.66
3:C:1015:LEU:CD1	3:C:1018:PRO:HG3	2.19	0.66
3:C:481:ILE:CD1	3:C:520:LEU:HD23	2.25	0.66
1:A:186:LEU:HG	1:A:196:ILE:HD12	1.77	0.66
1:A:583:GLN:H	1:A:583:GLN:HE21	1.43	0.66
3:C:373:LYS:HE2	3:C:427:MET:CE	1.84	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:829:ARG:HB2	3:C:829:ARG:NH1	2.03	0.66
1:A:718:MET:HE2	1:A:771:TYR:HB2	1.78	0.66
3:C:723:TYR:O	3:C:724:PRO:C	2.39	0.66
2:B:19:LYS:NZ	2:B:19:LYS:HB3	2.10	0.66
3:C:92:CYS:CB	3:C:137:ARG:HG2	2.26	0.66
3:C:724:PRO:O	3:C:726:SER:N	2.28	0.66
3:C:52:MET:HA	3:C:52:MET:HE3	1.78	0.66
3:C:825:VAL:O	3:C:827:ASN:N	2.26	0.66
3:C:148:VAL:O	3:C:151:GLN:N	2.28	0.66
1:A:719:LYS:HA	1:A:773:TYR:CD1	2.31	0.66
3:C:168:LEU:HD23	3:C:168:LEU:N	2.10	0.66
3:C:183:GLN:C	3:C:185:THR:H	2.02	0.66
3:C:881:GLY:O	3:C:884:SER:HB2	1.95	0.66
1:A:286:LEU:HD22	1:A:290:CYS:HG	1.61	0.65
3:C:723:TYR:H	3:C:724:PRO:CD	2.08	0.65
3:C:1036:ASN:O	3:C:1037:LYS:HB2	1.95	0.65
1:A:662:LEU:HD12	1:A:662:LEU:H	1.61	0.65
3:C:618:ARG:HB3	3:C:624:THR:CG2	2.26	0.65
1:A:630:ILE:HG22	1:A:635:LEU:HB2	1.78	0.65
3:C:407:PRO:HG2	3:C:408:VAL:H	1.60	0.65
3:C:1055:GLU:OE1	3:C:1055:GLU:HA	1.95	0.65
1:A:467:LYS:NZ	1:A:698:THR:HB	2.10	0.65
1:A:492:LYS:HD3	3:C:108:ILE:HD11	1.78	0.65
3:C:207:PHE:C	3:C:209:ASP:H	2.05	0.65
3:C:1107:ASN:CG	3:C:1141:ARG:HH12	2.04	0.65
3:C:1079:LEU:O	3:C:1079:LEU:HD22	1.97	0.65
3:C:390:VAL:O	3:C:394:VAL:HG23	1.96	0.65
1:A:104:LEU:HD23	1:A:173:ARG:HH11	1.61	0.65
3:C:148:VAL:HA	3:C:151:GLN:HE21	1.62	0.65
3:C:566:LYS:HB2	3:C:566:LYS:NZ	2.11	0.65
3:C:655:LEU:HA	3:C:658:PHE:CD2	2.32	0.65
3:C:822:ILE:HG22	3:C:826:LYS:HD2	1.78	0.65
3:C:989:VAL:O	3:C:992:THR:HB	1.96	0.65
1:A:591:THR:HG22	2:B:22:PHE:HE2	1.61	0.65
1:A:591:THR:HG22	2:B:22:PHE:CE2	2.31	0.64
3:C:905:ARG:HG3	3:C:905:ARG:NH1	2.11	0.64
3:C:1194:LEU:HD12	3:C:1194:LEU:C	2.21	0.64
1:A:37:MET:HE2	1:A:42:TYR:HA	1.79	0.64
1:A:134:ASN:HD21	1:A:157:TYR:HB2	1.63	0.64
3:C:631:ALA:O	3:C:635:ILE:HG13	1.97	0.64
3:C:818:VAL:C	3:C:820:GLN:H	2.05	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:SER:O	1:A:529:PRO:HD3	1.97	0.64
3:C:701:ILE:HD13	3:C:738:LEU:CD2	2.27	0.64
3:C:365:HIS:C	3:C:367:MET:H	2.04	0.64
3:C:722:VAL:O	3:C:723:TYR:HB2	1.97	0.64
1:A:498:GLU:O	1:A:502:LYS:HG3	1.97	0.64
3:C:206:CYS:HB3	3:C:207:PHE:HA	1.80	0.64
3:C:207:PHE:C	3:C:209:ASP:N	2.51	0.64
1:A:682:ASN:HD22	1:A:684:ASN:H	1.45	0.64
3:C:129:ASN:HA	3:C:132:LYS:CB	2.27	0.64
3:C:1008:ILE:HG23	3:C:1009:GLY:H	1.63	0.64
3:C:573:ILE:HD12	3:C:574:LYS:N	2.13	0.64
3:C:862:LEU:O	3:C:865:PHE:HB2	1.98	0.64
3:C:760:GLN:HG2	3:C:809:ALA:HB2	1.78	0.63
3:C:42:ASP:C	3:C:44:ASP:H	2.05	0.63
3:C:551:ARG:HD3	3:C:599:ASN:OD1	1.98	0.63
1:A:147:ARG:O	1:A:148:GLU:HB2	1.97	0.63
3:C:364:ARG:HA	3:C:364:ARG:NE	2.11	0.63
3:C:655:LEU:HA	3:C:658:PHE:HD2	1.62	0.63
3:C:210:LEU:HD23	3:C:213:HIS:ND1	2.14	0.63
3:C:1164:GLN:HA	3:C:1167:GLU:HG3	1.78	0.63
1:A:273:ARG:HG2	1:A:277:TYR:OH	1.99	0.63
2:B:97:ASP:OD1	2:B:99:ARG:HB2	1.98	0.63
3:C:551:ARG:HG2	3:C:599:ASN:ND2	2.14	0.63
1:A:417:SER:N	1:A:418:PRO:HD2	2.14	0.63
2:B:53:CYS:HB2	2:B:83:CYS:SG	2.38	0.63
3:C:129:ASN:HA	3:C:132:LYS:HB2	1.81	0.63
3:C:936:LEU:HD22	3:C:951:VAL:HG13	1.80	0.63
1:A:175:LEU:CD1	1:A:208:TYR:CE1	2.81	0.63
3:C:823:GLN:HA	3:C:823:GLN:HE21	1.63	0.62
1:A:592:ASN:HA	1:A:597:ARG:NH1	2.10	0.62
3:C:301:LEU:HD12	3:C:302:THR:N	2.11	0.62
3:C:385:GLU:O	3:C:386:ARG:HB3	1.99	0.62
3:C:1135:PRO:O	3:C:1138:VAL:HB	1.99	0.62
1:A:92:LEU:O	1:A:96:LEU:HD13	1.98	0.62
3:C:96:LEU:HD12	3:C:96:LEU:N	2.14	0.62
3:C:349:VAL:CG2	3:C:350:ARG:H	2.09	0.62
1:A:325:VAL:C	1:A:327:ARG:H	2.05	0.62
3:C:548:LYS:HG2	3:C:599:ASN:HD21	1.64	0.62
3:C:974:LEU:HD21	3:C:1011:PHE:CE2	2.34	0.62
3:C:1117:TYR:C	3:C:1117:TYR:CD2	2.77	0.62
2:B:48:HIS:ND1	2:B:49:ILE:HD12	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:48:HIS:CE1	2:B:50:MET:HB2	2.34	0.62
3:C:158:MET:O	3:C:162:LEU:HB2	1.98	0.62
3:C:294:ILE:CG2	3:C:357:LEU:HG	2.25	0.62
3:C:212:GLU:OE1	3:C:212:GLU:N	2.19	0.62
3:C:253:ILE:HD11	3:C:281:ARG:HH22	1.65	0.62
3:C:825:VAL:HG23	3:C:860:VAL:HG13	1.82	0.62
1:A:632:MET:HA	1:A:635:LEU:HB3	1.80	0.62
1:A:734:LEU:CD2	1:A:743:PRO:HD2	2.30	0.62
3:C:810:CYS:O	3:C:812:LYS:N	2.31	0.62
3:C:831:THR:HG22	3:C:833:SER:HB3	1.80	0.62
3:C:1177:MET:HG3	3:C:1205:ASN:HB3	1.82	0.62
1:A:344:HIS:CE1	1:A:348:LEU:HD11	2.34	0.62
1:A:711:GLN:HE22	1:A:758:LYS:NZ	1.97	0.62
3:C:153:GLU:O	3:C:157:ILE:HG13	2.00	0.62
1:A:577:LYS:HE2	1:A:577:LYS:HA	1.81	0.62
1:A:585:SER:HB2	2:B:29:ALA:HA	1.82	0.62
3:C:294:ILE:HG23	3:C:353:ALA:HA	1.82	0.62
3:C:942:CYS:CA	3:C:948:ARG:HD2	2.28	0.61
3:C:578:ALA:O	3:C:579:ALA:HB3	2.00	0.61
3:C:902:GLN:HE22	3:C:905:ARG:HH12	1.48	0.61
1:A:221:GLY:HA3	3:C:1167:GLU:CD	2.26	0.61
1:A:600:LEU:N	1:A:600:LEU:CD2	2.58	0.61
1:A:104:LEU:HD12	1:A:104:LEU:O	2.00	0.61
1:A:682:ASN:ND2	1:A:684:ASN:H	1.98	0.61
3:C:652:VAL:N	3:C:653:PRO:HD2	2.15	0.61
1:A:620:THR:OG1	1:A:623:GLN:HG3	1.99	0.61
3:C:570:THR:O	3:C:572:THR:N	2.34	0.61
3:C:821:PHE:HE2	3:C:842:LEU:HD22	1.65	0.61
1:A:210:GLU:HB2	3:C:1164:GLN:HG3	1.83	0.61
1:A:363:LYS:O	1:A:367:GLN:HB2	2.00	0.61
3:C:804:ALA:HA	3:C:845:VAL:HG22	1.82	0.61
3:C:218:LEU:HD23	3:C:230:TYR:HD1	1.66	0.61
3:C:735:LEU:C	3:C:735:LEU:HD13	2.25	0.61
1:A:260:MET:HE1	1:A:321:MET:HE2	1.83	0.61
1:A:577:LYS:HZ3	1:A:578:LEU:H	1.47	0.61
3:C:192:ARG:HH21	3:C:227:THR:CG2	2.11	0.61
3:C:573:ILE:HD12	3:C:574:LYS:H	1.66	0.61
3:C:689:MET:O	3:C:692:ALA:HB3	2.01	0.61
3:C:54:LEU:HD13	3:C:90:THR:HG21	1.82	0.61
3:C:423:THR:HG22	3:C:426:THR:H	1.64	0.61
3:C:1012:LEU:C	3:C:1014:THR:N	2.58	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1086:PHE:CD2	3:C:1089:MET:HE2	2.36	0.61
1:A:405:ASN:ND2	1:A:408:THR:H	1.99	0.60
1:A:603:SER:O	1:A:607:MET:HG3	2.01	0.60
3:C:42:ASP:HB2	3:C:45:SER:H	1.65	0.60
3:C:294:ILE:HD11	3:C:356:CYS:SG	2.41	0.60
3:C:710:GLN:HB3	3:C:751:ALA:HA	1.82	0.60
3:C:249:LEU:HD13	3:C:249:LEU:N	2.15	0.60
3:C:821:PHE:HE2	3:C:842:LEU:CD2	2.14	0.60
1:A:676:ASN:ND2	1:A:677:LYS:N	2.49	0.60
1:A:744:ARG:HG2	1:A:746:PRO:HD2	1.83	0.60
2:B:49:ILE:HD12	2:B:50:MET:N	2.15	0.60
3:C:281:ARG:HH21	3:C:284:LYS:HB3	1.66	0.60
3:C:625:ARG:HG3	3:C:658:PHE:CE1	2.36	0.60
3:C:902:GLN:NE2	3:C:905:ARG:NH1	2.50	0.60
3:C:959:THR:HA	3:C:966:LEU:HD13	1.83	0.60
1:A:452:PHE:HA	1:A:455:ILE:HD13	1.83	0.60
1:A:459:ASP:OD2	1:A:706:ARG:NE	2.23	0.60
3:C:33:GLU:O	3:C:35:GLN:N	2.33	0.60
3:C:265:ASP:HB3	3:C:345:MET:SD	2.42	0.60
3:C:270:TYR:O	3:C:273:GLN:HB2	2.02	0.60
3:C:451:ARG:HD2	3:C:483:SER:OG	2.02	0.60
3:C:460:GLU:O	3:C:464:VAL:HG23	2.01	0.60
1:A:717:ILE:HG12	3:C:25:MET:CE	2.32	0.60
3:C:284:LYS:HD3	3:C:284:LYS:N	2.16	0.60
3:C:469:LEU:H	3:C:508:HIS:CE1	2.20	0.60
3:C:469:LEU:H	3:C:508:HIS:HE1	1.47	0.60
3:C:521:VAL:HB	3:C:522:PRO:HD3	1.84	0.60
1:A:52:TYR:HD2	1:A:52:TYR:O	1.84	0.60
1:A:475:HIS:NE2	1:A:584:LEU:O	2.35	0.60
1:A:592:ASN:CB	1:A:597:ARG:HH12	2.15	0.60
1:A:717:ILE:HD13	1:A:732:GLU:HB3	1.84	0.60
3:C:551:ARG:O	3:C:552:PRO:C	2.45	0.60
3:C:376:SER:OG	3:C:377:PRO:HD2	2.02	0.60
3:C:481:ILE:CD1	3:C:523:PRO:HG3	2.30	0.60
3:C:959:THR:HG21	3:C:967:LEU:HD23	1.82	0.60
1:A:440:GLU:C	1:A:444:THR:HG1	2.08	0.60
3:C:294:ILE:HG23	3:C:353:ALA:CA	2.31	0.60
3:C:701:ILE:O	3:C:701:ILE:HG22	2.02	0.60
3:C:917:ILE:HD13	3:C:958:LEU:HG	1.84	0.60
3:C:942:CYS:O	3:C:943:ALA:C	2.45	0.60
1:A:117:LYS:HZ2	1:A:121:GLN:HE21	1.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ARG:HG3	1:A:148:GLU:N	2.16	0.59
3:C:41:LEU:HD22	3:C:46:GLU:HG2	1.84	0.59
3:C:135:THR:HG22	3:C:176:ILE:HD11	1.83	0.59
3:C:971:LYS:HA	3:C:974:LEU:HD23	1.83	0.59
3:C:144:LYS:O	3:C:145:GLN:C	2.45	0.59
3:C:285:GLU:C	3:C:285:GLU:OE2	2.45	0.59
3:C:350:ARG:NE	3:C:386:ARG:NH2	2.51	0.59
3:C:1177:MET:HE2	3:C:1177:MET:HA	1.85	0.59
1:A:405:ASN:HD22	1:A:407:VAL:N	1.99	0.59
2:B:42:CYS:O	2:B:45:CYS:O	2.20	0.59
3:C:246:GLY:O	3:C:249:LEU:HD11	2.03	0.59
3:C:376:SER:O	3:C:380:ILE:HB	2.03	0.59
3:C:965:THR:O	3:C:965:THR:HG22	2.01	0.59
3:C:431:GLN:O	3:C:434:ASN:HB2	2.02	0.59
3:C:551:ARG:NH1	3:C:553:LEU:H	2.00	0.59
1:A:88:LEU:HD23	1:A:140:LEU:HD23	1.84	0.59
3:C:131:CYS:HB3	3:C:161:MET:SD	2.42	0.59
3:C:370:GLU:O	3:C:374:THR:HG22	2.03	0.59
3:C:827:ASN:O	3:C:828:SER:C	2.45	0.59
3:C:1143:ASP:CG	3:C:1193:PRO:HB3	2.28	0.59
1:A:646:LYS:C	1:A:647:LEU:HD12	2.28	0.59
3:C:698:PRO:HB2	3:C:699:PRO:HD3	1.85	0.59
3:C:1093:LEU:HD11	3:C:1130:LEU:HD21	1.85	0.59
1:A:629:GLN:HA	1:A:629:GLN:OE1	2.03	0.59
3:C:652:VAL:O	3:C:655:LEU:HB2	2.02	0.59
1:A:85:GLY:HA3	1:A:144:TRP:CE3	2.38	0.59
3:C:346:SER:C	3:C:349:VAL:HG22	2.27	0.59
3:C:346:SER:O	3:C:349:VAL:HG22	2.02	0.59
1:A:499:TYR:CZ	1:A:503:LEU:HD21	2.38	0.59
3:C:211:ILE:CD1	3:C:244:ARG:HE	2.16	0.59
3:C:551:ARG:HG2	3:C:599:ASN:CG	2.28	0.59
3:C:1184:LEU:HD23	3:C:1190:GLU:HG3	1.84	0.59
3:C:894:PHE:O	3:C:897:GLN:HB3	2.02	0.58
3:C:928:TYR:O	3:C:932:ILE:HG12	2.03	0.58
2:B:62:SER:H	2:B:65:SER:HB3	1.68	0.58
3:C:168:LEU:HG	3:C:169:LEU:HD12	1.86	0.58
1:A:542:GLY:H	2:B:76:ASN:ND2	1.95	0.58
3:C:562:THR:OG1	3:C:563:PRO:HD3	2.02	0.58
3:C:600:LEU:C	3:C:602:ASP:N	2.57	0.58
1:A:430:LYS:HA	1:A:477:ASN:O	2.04	0.58
3:C:268:ARG:CD	3:C:348:LYS:HE3	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:459:THR:HG23	3:C:503:VAL:HG21	1.84	0.58
3:C:192:ARG:NH2	3:C:227:THR:HG21	2.14	0.58
3:C:611:THR:HA	3:C:614:ILE:CG1	2.33	0.58
3:C:1139:LEU:HD11	3:C:1189:ALA:HB3	1.86	0.58
3:C:188:ARG:HD2	3:C:188:ARG:N	2.18	0.58
3:C:226:THR:CG2	3:C:227:THR:H	2.15	0.58
3:C:608:LEU:HB3	3:C:609:PRO:HD3	1.85	0.58
3:C:285:GLU:C	3:C:287:TYR:H	2.12	0.58
3:C:192:ARG:O	3:C:196:ILE:HG13	2.03	0.58
3:C:1185:THR:HG22	3:C:1185:THR:O	2.04	0.58
1:A:577:LYS:HA	1:A:577:LYS:CE	2.34	0.58
1:A:37:MET:HB3	3:C:1068:MET:HA	1.84	0.58
1:A:317:ASP:OD2	1:A:317:ASP:N	2.35	0.58
1:A:634:ILE:HD11	1:A:687:MET:SD	2.44	0.58
3:C:7:HIS:HB3	3:C:8:ILE:HD12	1.84	0.58
1:A:177:LYS:HG3	1:A:177:LYS:O	2.04	0.57
3:C:597:ILE:HG21	3:C:635:ILE:HD13	1.86	0.57
3:C:722:VAL:O	3:C:722:VAL:HG23	2.02	0.57
1:A:40:SER:O	1:A:44:GLU:HG3	2.04	0.57
1:A:579:THR:HG23	2:B:32:LEU:HB2	1.85	0.57
3:C:15:MET:CG	3:C:56:LEU:HD11	2.34	0.57
3:C:82:TYR:O	3:C:85:GLU:HB3	2.04	0.57
1:A:717:ILE:HG12	3:C:25:MET:HE2	1.85	0.57
3:C:441:LYS:HB2	3:C:441:LYS:NZ	2.19	0.57
3:C:586:LYS:O	3:C:590:ILE:HG13	2.04	0.57
3:C:1052:LEU:HD21	3:C:1089:MET:HG2	1.87	0.57
3:C:1188:GLU:HA	3:C:1190:GLU:OE2	2.04	0.57
1:A:134:ASN:ND2	1:A:159:ILE:HG22	2.19	0.57
3:C:249:LEU:HD22	3:C:250:GLU:H	1.69	0.57
3:C:275:PHE:CE2	3:C:359:ALA:HB2	2.39	0.57
3:C:1037:LYS:CD	3:C:1040:LEU:HD11	2.32	0.57
1:A:635:LEU:HD13	1:A:635:LEU:O	2.04	0.57
1:A:756:ILE:HD13	1:A:761:LEU:HB2	1.86	0.57
3:C:365:HIS:C	3:C:367:MET:N	2.62	0.57
3:C:870:GLU:CD	3:C:870:GLU:H	2.12	0.57
1:A:155:GLY:HA3	3:C:1163:LYS:N	2.20	0.57
1:A:650:LEU:O	1:A:669:LYS:HD2	2.04	0.57
3:C:183:GLN:C	3:C:185:THR:N	2.61	0.57
3:C:551:ARG:HH11	3:C:553:LEU:CB	2.16	0.57
3:C:673:ALA:HA	3:C:676:ILE:CD1	2.34	0.57
3:C:1113:LEU:O	3:C:1120:LYS:HD3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:822:ILE:O	3:C:826:LYS:HB2	2.05	0.57
1:A:357:ALA:H	3:C:489:SER:CB	2.17	0.57
1:A:441:LEU:HD21	1:A:483:ALA:CB	2.35	0.57
1:A:539:LEU:O	2:B:32:LEU:HA	2.04	0.57
3:C:158:MET:O	3:C:158:MET:HE3	2.04	0.57
3:C:168:LEU:C	3:C:169:LEU:HD12	2.30	0.57
3:C:206:CYS:HA	3:C:211:ILE:HD11	1.87	0.57
3:C:210:LEU:HD23	3:C:213:HIS:CE1	2.39	0.57
3:C:982:ARG:O	3:C:985:VAL:HG12	2.05	0.57
1:A:37:MET:HE1	1:A:45:LEU:HD12	1.87	0.57
2:B:39:VAL:O	2:B:40:ASP:C	2.47	0.57
3:C:465:LEU:O	3:C:467:GLY:N	2.38	0.57
3:C:553:LEU:HD13	3:C:639:PRO:HD2	1.87	0.57
3:C:831:THR:CG2	3:C:833:SER:HB3	2.34	0.57
1:A:144:TRP:C	1:A:145:VAL:HG22	2.30	0.56
3:C:42:ASP:O	3:C:46:GLU:HG3	2.04	0.56
3:C:138:LEU:O	3:C:141:ALA:HB3	2.05	0.56
3:C:205:SER:O	3:C:206:CYS:HB2	2.04	0.56
3:C:207:PHE:O	3:C:210:LEU:N	2.36	0.56
3:C:967:LEU:N	3:C:968:PRO:CD	2.67	0.56
3:C:8:ILE:H	3:C:8:ILE:CD1	2.17	0.56
3:C:87:ILE:O	3:C:88:VAL:C	2.47	0.56
3:C:780:THR:HG22	3:C:837:LEU:HD21	1.87	0.56
1:A:354:CYS:HB3	1:A:358:ALA:HB2	1.87	0.56
1:A:473:LEU:HB3	1:A:510:ILE:HG13	1.87	0.56
1:A:577:LYS:HZ2	1:A:578:LEU:H	1.52	0.56
3:C:17:SER:O	3:C:19:ASP:N	2.36	0.56
3:C:36:LYS:NZ	3:C:36:LYS:HB3	2.20	0.56
3:C:289:HIS:O	3:C:293:ILE:HG13	2.05	0.56
3:C:299:LYS:HZ2	3:C:379:LEU:HD22	1.69	0.56
3:C:379:LEU:HD23	3:C:382:ARG:HG3	1.87	0.56
3:C:442:GLN:O	3:C:444:LYS:N	2.39	0.56
3:C:645:ARG:HD2	3:C:684:SER:HB2	1.88	0.56
3:C:1143:ASP:OD1	3:C:1193:PRO:HB3	2.04	0.56
3:C:1207:GLU:HG3	3:C:1208:LEU:HD22	1.88	0.56
1:A:762:GLU:HB3	1:A:774:LEU:HD12	1.88	0.56
3:C:1038:PRO:C	3:C:1040:LEU:H	2.13	0.56
1:A:513:SER:OG	1:A:537:GLN:HA	2.06	0.56
3:C:216:SER:O	3:C:220:LYS:HG3	2.05	0.56
3:C:717:THR:O	3:C:721:LYS:HB2	2.06	0.56
1:A:286:LEU:HD22	1:A:290:CYS:SG	2.46	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1199:GLN:HB3	3:C:1202:ILE:CB	2.35	0.56
1:A:143:HIS:O	1:A:145:VAL:N	2.37	0.56
1:A:296:GLU:HA	1:A:299:LEU:HG	1.85	0.56
3:C:933:TRP:CH2	3:C:966:LEU:HD22	2.41	0.56
2:B:87:TRP:CE2	2:B:91:ARG:HG3	2.41	0.56
1:A:625:THR:CG2	1:A:632:MET:CG	2.84	0.56
3:C:46:GLU:OE2	3:C:79:VAL:HA	2.06	0.56
3:C:375:VAL:O	3:C:379:LEU:CB	2.53	0.56
1:A:660:VAL:HG12	1:A:661:GLU:H	1.70	0.56
1:A:671:TYR:CD1	1:A:671:TYR:C	2.83	0.56
3:C:495:ILE:HG23	3:C:538:GLU:HG3	1.86	0.56
3:C:887:ASN:CG	3:C:890:GLU:HB2	2.31	0.56
3:C:1015:LEU:HD12	3:C:1022:VAL:CG1	2.36	0.56
1:A:612:GLN:C	1:A:614:ASN:H	2.14	0.55
3:C:220:LYS:C	3:C:222:ASP:H	2.14	0.55
3:C:143:ALA:C	3:C:145:GLN:H	2.13	0.55
3:C:979:SER:HB3	3:C:1020:LEU:HD11	1.89	0.55
3:C:1015:LEU:O	3:C:1018:PRO:HD2	2.07	0.55
1:A:142:ARG:NH2	1:A:147:ARG:HG2	2.20	0.55
1:A:643:LEU:HD23	1:A:648:LEU:HB2	1.86	0.55
3:C:206:CYS:HB3	3:C:207:PHE:C	2.31	0.55
3:C:248:TYR:C	3:C:249:LEU:HD13	2.31	0.55
3:C:350:ARG:CZ	3:C:386:ARG:HH22	2.20	0.55
3:C:79:VAL:HG22	3:C:83:GLN:HB2	1.87	0.55
3:C:799:ILE:HG22	3:C:837:LEU:HD11	1.88	0.55
3:C:1047:THR:O	3:C:1050:PRO:HD2	2.06	0.55
1:A:748:ILE:O	1:A:752:ILE:HG13	2.06	0.55
1:A:595:LYS:NZ	1:A:595:LYS:HB3	2.21	0.55
1:A:688:LYS:HD3	1:A:689:THR:N	2.21	0.55
3:C:8:ILE:HD12	3:C:8:ILE:N	2.22	0.55
3:C:35:GLN:O	3:C:36:LYS:HB3	2.06	0.55
3:C:1037:LYS:H	3:C:1038:PRO:HD3	1.71	0.55
3:C:86:THR:O	3:C:87:ILE:C	2.49	0.55
3:C:570:THR:O	3:C:571:CYS:C	2.50	0.55
1:A:171:LEU:HD12	1:A:175:LEU:HD13	1.88	0.55
1:A:601:GLN:O	1:A:683:ILE:HG12	2.07	0.55
3:C:268:ARG:HD2	3:C:348:LYS:HE3	1.87	0.55
3:C:383:PHE:HE2	3:C:386:ARG:HH21	1.54	0.55
3:C:601:GLY:HA2	3:C:604:LEU:HB2	1.89	0.55
3:C:804:ALA:HA	3:C:845:VAL:CG2	2.37	0.55
3:C:486:ASP:O	3:C:487:LYS:CB	2.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:858:LYS:HE2	3:C:891:TYR:CD2	2.41	0.55
3:C:1012:LEU:O	3:C:1015:LEU:N	2.37	0.55
1:A:426:ASP:CG	1:A:468:MET:HE2	2.32	0.55
3:C:259:PHE:HB3	3:C:270:TYR:HE2	1.71	0.55
3:C:282:CYS:O	3:C:284:LYS:N	2.40	0.55
3:C:551:ARG:CB	3:C:599:ASN:HB3	2.37	0.55
1:A:307:GLN:O	1:A:310:LEU:N	2.40	0.54
3:C:253:ILE:HG12	3:C:286:VAL:HG21	1.87	0.54
3:C:428:LEU:O	3:C:429:GLN:C	2.49	0.54
2:B:73:GLY:HA2	2:B:102:GLU:O	2.07	0.54
3:C:15:MET:HG2	3:C:56:LEU:HD11	1.89	0.54
3:C:75:LEU:O	3:C:78:LYS:N	2.39	0.54
3:C:254:PRO:O	3:C:258:LYS:HG3	2.07	0.54
3:C:290:VAL:O	3:C:291:SER:C	2.50	0.54
3:C:658:PHE:C	3:C:660:ARG:H	2.15	0.54
1:A:117:LYS:HZ2	1:A:121:GLN:NE2	2.04	0.54
3:C:361:VAL:HA	3:C:371:PHE:CE1	2.42	0.54
3:C:368:LEU:O	3:C:369:PRO:C	2.50	0.54
1:A:175:LEU:O	1:A:176:ASN:C	2.48	0.54
1:A:631:LYS:O	1:A:635:LEU:CB	2.55	0.54
3:C:271:CYS:HB2	3:C:352:ALA:HB1	1.89	0.54
3:C:405:THR:O	3:C:407:PRO:HD3	2.07	0.54
1:A:21:TRP:CZ2	1:A:91:ARG:HB3	2.42	0.54
1:A:446:ASN:CG	1:A:490:LYS:HE2	2.33	0.54
3:C:658:PHE:O	3:C:660:ARG:N	2.39	0.54
3:C:970:LEU:HB3	3:C:985:VAL:CG2	2.38	0.54
1:A:597:ARG:HH11	1:A:597:ARG:CB	2.04	0.54
3:C:372:TYR:HA	3:C:377:PRO:CG	2.37	0.54
3:C:465:LEU:HB2	3:C:468:ALA:HB2	1.90	0.54
3:C:1184:LEU:HD23	3:C:1190:GLU:CG	2.38	0.54
1:A:439:ALA:O	1:A:443:ASP:HB2	2.07	0.54
1:A:614:ASN:ND2	2:B:22:PHE:H	2.02	0.54
3:C:75:LEU:O	3:C:76:VAL:C	2.51	0.54
3:C:126:LEU:O	3:C:128:ALA:N	2.41	0.54
3:C:134:ILE:HG22	3:C:138:LEU:HD11	1.89	0.54
3:C:386:ARG:HG3	3:C:387:GLU:H	1.73	0.54
3:C:398:TYR:O	3:C:401:LEU:HB3	2.07	0.54
3:C:469:LEU:N	3:C:508:HIS:HE1	2.05	0.54
3:C:566:LYS:H	3:C:566:LYS:CD	2.16	0.54
3:C:660:ARG:HD2	3:C:696:GLU:CD	2.32	0.54
3:C:663:GLN:O	3:C:664:ARG:C	2.50	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:851:LEU:C	3:C:853:GLY:H	2.16	0.54
3:C:936:LEU:HD11	3:C:954:CYS:HB3	1.90	0.54
1:A:426:ASP:OD2	1:A:430:LYS:HE3	2.08	0.54
1:A:725:LYS:O	1:A:726:HIS:C	2.51	0.54
3:C:723:TYR:N	3:C:724:PRO:CD	2.70	0.54
3:C:975:ILE:HG23	3:C:976:SER:N	2.17	0.54
3:C:1205:ASN:C	3:C:1207:GLU:H	2.15	0.54
1:A:137:CYS:CB	1:A:159:ILE:HG12	2.38	0.54
1:A:713:ALA:O	1:A:717:ILE:HG13	2.08	0.54
3:C:88:VAL:CG1	3:C:134:ILE:HG12	2.38	0.54
1:A:443:ASP:O	1:A:446:ASN:N	2.40	0.53
1:A:651:GLU:O	1:A:652:ASP:O	2.26	0.53
2:B:64:THR:O	2:B:67:GLU:HB3	2.08	0.53
3:C:17:SER:C	3:C:19:ASP:H	2.15	0.53
3:C:188:ARG:N	3:C:188:ARG:CD	2.71	0.53
3:C:230:TYR:O	3:C:234:ILE:HG12	2.08	0.53
3:C:301:LEU:HD13	3:C:350:ARG:HH12	1.71	0.53
3:C:616:LEU:HD23	3:C:647:VAL:CG1	2.38	0.53
1:A:363:LYS:HA	1:A:424:TYR:CD2	2.44	0.53
1:A:631:LYS:O	1:A:635:LEU:HB2	2.08	0.53
3:C:41:LEU:HD22	3:C:46:GLU:CG	2.38	0.53
3:C:386:ARG:HD3	3:C:390:VAL:HG12	1.89	0.53
3:C:690:ILE:HG12	3:C:723:TYR:CE2	2.43	0.53
3:C:933:TRP:NE1	3:C:937:LEU:HD11	2.23	0.53
3:C:1142:LEU:HD22	3:C:1193:PRO:HG2	1.90	0.53
1:A:423:ARG:O	1:A:426:ASP:HB3	2.07	0.53
1:A:536:ILE:HG12	1:A:537:GLN:N	2.21	0.53
2:B:77:HIS:CE1	2:B:97:ASP:HB3	2.44	0.53
3:C:300:TYR:O	3:C:300:TYR:CD2	2.61	0.53
3:C:365:HIS:O	3:C:367:MET:N	2.42	0.53
1:A:270:GLU:O	1:A:274:VAL:HG23	2.07	0.53
1:A:405:ASN:ND2	1:A:405:ASN:C	2.64	0.53
3:C:208:VAL:HA	3:C:244:ARG:NH2	2.22	0.53
1:A:52:TYR:O	1:A:52:TYR:CD2	2.61	0.53
1:A:624:LEU:C	1:A:626:ASP:N	2.66	0.53
1:A:630:ILE:HG22	1:A:630:ILE:O	2.04	0.53
3:C:83:GLN:HA	3:C:86:THR:OG1	2.08	0.53
3:C:294:ILE:HD13	3:C:356:CYS:HB3	1.90	0.53
3:C:1159:ALA:HA	3:C:1166:PHE:HZ	1.72	0.53
3:C:229:THR:C	3:C:231:ILE:N	2.65	0.53
3:C:543:THR:O	3:C:547:VAL:HG23	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1149:LEU:HD13	3:C:1180:VAL:HG22	1.88	0.53
1:A:100:LEU:HD21	1:A:126:TYR:CE1	2.44	0.53
1:A:619:TYR:HD2	1:A:623:GLN:HE21	1.57	0.53
1:A:713:ALA:O	1:A:714:ILE:C	2.52	0.53
3:C:206:CYS:HB3	3:C:207:PHE:CA	2.37	0.53
3:C:269:GLU:O	3:C:272:ILE:HB	2.09	0.53
3:C:933:TRP:CZ3	3:C:966:LEU:HD22	2.44	0.53
3:C:982:ARG:HH22	3:C:1019:ASP:H	1.55	0.53
3:C:1023:ARG:O	3:C:1026:ALA:HB3	2.09	0.53
1:A:112:ASP:O	1:A:182:ALA:HB1	2.08	0.53
1:A:221:GLY:HA3	3:C:1167:GLU:OE1	2.09	0.53
1:A:662:LEU:HD12	1:A:662:LEU:N	2.22	0.53
2:B:64:THR:O	2:B:65:SER:C	2.52	0.53
3:C:85:GLU:CG	3:C:133:LYS:HE2	2.30	0.53
3:C:133:LYS:HB2	3:C:133:LYS:NZ	2.24	0.53
3:C:1205:ASN:C	3:C:1207:GLU:N	2.66	0.53
3:C:33:GLU:HA	3:C:36:LYS:HE2	1.90	0.53
3:C:299:LYS:HZ1	3:C:379:LEU:HD22	1.73	0.53
3:C:502:TYR:CE1	3:C:541:LEU:HD22	2.44	0.53
3:C:896:LEU:HD11	3:C:932:ILE:HD13	1.90	0.53
3:C:1015:LEU:CD1	3:C:1022:VAL:CG1	2.87	0.53
1:A:325:VAL:C	1:A:327:ARG:N	2.67	0.53
1:A:592:ASN:HB3	1:A:597:ARG:HH12	1.73	0.53
1:A:719:LYS:HG3	1:A:773:TYR:HE1	1.72	0.53
1:A:727:GLN:O	1:A:728:GLN:C	2.51	0.53
3:C:282:CYS:C	3:C:284:LYS:H	2.17	0.53
3:C:945:GLU:HA	3:C:948:ARG:HD3	1.90	0.53
1:A:134:ASN:ND2	1:A:160:TYR:HB2	2.25	0.52
1:A:734:LEU:HD23	1:A:743:PRO:HD2	1.91	0.52
1:A:767:GLU:HA	1:A:767:GLU:OE1	2.09	0.52
3:C:208:VAL:O	3:C:212:GLU:OE2	2.27	0.52
3:C:813:GLU:OE1	3:C:814:GLY:N	2.39	0.52
1:A:21:TRP:CD1	1:A:91:ARG:HD3	2.44	0.52
1:A:624:LEU:C	1:A:626:ASP:H	2.17	0.52
3:C:46:GLU:O	3:C:47:ARG:C	2.52	0.52
3:C:227:THR:HG22	3:C:229:THR:OG1	2.09	0.52
3:C:856:GLU:O	3:C:860:VAL:HG23	2.10	0.52
1:A:31:VAL:HA	3:C:1068:MET:HE1	1.92	0.52
1:A:719:LYS:HG3	1:A:773:TYR:CE1	2.44	0.52
3:C:126:LEU:C	3:C:128:ALA:H	2.18	0.52
3:C:551:ARG:HD3	3:C:599:ASN:CG	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:926:LYS:HB3	3:C:927:PRO:HD3	1.91	0.52
1:A:117:LYS:O	1:A:117:LYS:HD3	2.09	0.52
1:A:117:LYS:HZ1	1:A:121:GLN:HE21	1.57	0.52
1:A:186:LEU:O	1:A:189:LYS:HB2	2.10	0.52
1:A:472:ARG:NH1	1:A:484:GLU:OE1	2.43	0.52
1:A:592:ASN:HB3	1:A:597:ARG:NH2	2.23	0.52
1:A:630:ILE:O	1:A:635:LEU:HB2	2.09	0.52
3:C:19:ASP:OD1	3:C:21:ASP:HB2	2.10	0.52
3:C:253:ILE:CD1	3:C:281:ARG:HH22	2.21	0.52
3:C:701:ILE:HD13	3:C:738:LEU:HD21	1.89	0.52
3:C:1117:TYR:OH	3:C:1121:MET:HE2	2.10	0.52
1:A:660:VAL:HB	1:A:662:LEU:CD1	2.39	0.52
1:A:719:LYS:HE2	1:A:773:TYR:OH	2.10	0.52
2:B:37:ILE:HG23	2:B:38:VAL:HG13	1.91	0.52
3:C:38:SER:H	3:C:78:LYS:HZ3	1.57	0.52
3:C:727:LEU:HD13	3:C:767:THR:OG1	2.10	0.52
1:A:25:ARG:HD3	1:A:95:PHE:CD1	2.44	0.52
3:C:458:LEU:O	3:C:462:VAL:HG23	2.09	0.52
3:C:1094:ASP:CG	3:C:1129:ARG:HH22	2.17	0.52
3:C:1194:LEU:O	3:C:1195:MET:CB	2.44	0.52
1:A:107:GLY:HA2	1:A:110:LEU:CD1	2.37	0.52
1:A:175:LEU:CG	1:A:208:TYR:OH	2.52	0.52
1:A:492:LYS:HB3	3:C:108:ILE:CD1	2.39	0.52
3:C:239:ARG:NE	3:C:276:GLU:HG2	2.24	0.52
3:C:373:LYS:HE3	3:C:427:MET:HE3	1.09	0.52
3:C:548:LYS:CA	3:C:551:ARG:HG3	2.33	0.52
3:C:971:LYS:O	3:C:971:LYS:HG2	2.08	0.52
3:C:1152:THR:C	3:C:1154:THR:H	2.18	0.52
1:A:143:HIS:C	1:A:145:VAL:H	2.18	0.52
3:C:148:VAL:O	3:C:149:SER:C	2.53	0.52
3:C:213:HIS:O	3:C:217:GLU:HB2	2.10	0.52
3:C:626:LEU:HD23	3:C:666:LEU:HD12	1.91	0.52
3:C:824:ASP:O	3:C:825:VAL:C	2.53	0.52
1:A:21:TRP:NE1	1:A:91:ARG:HD3	2.25	0.52
1:A:50:TYR:CE1	1:A:54:THR:HG21	2.45	0.52
1:A:651:GLU:CA	1:A:669:LYS:HZ2	2.18	0.52
1:A:667:LEU:HB3	1:A:669:LYS:HE3	1.91	0.52
3:C:37:ASP:OD2	3:C:39:ILE:HG12	2.10	0.52
3:C:771:GLY:H	3:C:774:ASP:HB2	1.75	0.52
3:C:826:LYS:NZ	3:C:828:SER:HB2	2.23	0.52
3:C:903:PRO:HA	3:C:906:GLN:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:GLN:O	1:A:181:ASN:N	2.43	0.52
1:A:597:ARG:O	1:A:597:ARG:HG3	2.09	0.52
1:A:645:SER:O	1:A:646:LYS:CB	2.57	0.52
2:B:86:ARG:O	2:B:89:LYS:HB2	2.09	0.52
3:C:168:LEU:HG	3:C:169:LEU:CD1	2.39	0.52
3:C:373:LYS:HG2	3:C:427:MET:HE2	1.90	0.52
3:C:942:CYS:HB3	3:C:980:TYR:CD2	2.45	0.52
1:A:614:ASN:HA	2:B:20:LYS:O	2.10	0.51
3:C:225:SER:O	3:C:226:THR:O	2.28	0.51
3:C:385:GLU:HB3	3:C:442:GLN:OE1	2.10	0.51
3:C:925:LEU:O	3:C:926:LYS:C	2.53	0.51
1:A:286:LEU:O	1:A:290:CYS:SG	2.64	0.51
1:A:714:ILE:HD13	1:A:733:VAL:HG21	1.93	0.51
1:A:733:VAL:HG11	1:A:748:ILE:HD13	1.91	0.51
2:B:49:ILE:CD1	2:B:50:MET:HG2	2.34	0.51
3:C:1179:ALA:O	3:C:1180:VAL:C	2.52	0.51
1:A:158:GLU:O	1:A:162:LEU:N	2.44	0.51
1:A:649:VAL:HG23	1:A:671:TYR:HB2	1.92	0.51
1:A:654:ASN:HD22	1:A:656:ASN:ND2	2.09	0.51
1:A:717:ILE:HA	3:C:25:MET:HE2	1.92	0.51
3:C:701:ILE:HD13	3:C:738:LEU:HD23	1.92	0.51
3:C:913:LEU:CD2	3:C:917:ILE:HG13	2.40	0.51
3:C:947:THR:O	3:C:951:VAL:HG23	2.10	0.51
3:C:1104:GLU:OE1	3:C:1104:GLU:HA	2.11	0.51
1:A:17:LEU:N	1:A:19:GLN:HG2	2.25	0.51
1:A:227:TYR:HE1	1:A:282:THR:HG23	1.75	0.51
1:A:542:GLY:N	2:B:76:ASN:HD21	1.99	0.51
1:A:635:LEU:HD13	1:A:635:LEU:C	2.35	0.51
3:C:1158:LYS:C	3:C:1160:ASN:H	2.17	0.51
1:A:376:TYR:O	1:A:380:VAL:HG23	2.09	0.51
1:A:595:LYS:HG3	1:A:596:ASN:N	2.25	0.51
3:C:41:LEU:HD22	3:C:46:GLU:OE2	2.09	0.51
3:C:543:THR:HG23	3:C:568:LEU:HD22	1.93	0.51
3:C:610:ASN:O	3:C:614:ILE:HG12	2.11	0.51
3:C:961:ILE:O	3:C:962:ASP:HB3	2.10	0.51
3:C:994:SER:O	3:C:1037:LYS:HE2	2.11	0.51
3:C:245:ILE:HG12	3:C:245:ILE:O	2.11	0.51
3:C:374:THR:O	3:C:374:THR:HG23	2.10	0.51
3:C:473:ILE:N	3:C:474:PRO:CD	2.73	0.51
1:A:35:GLN:O	1:A:36:SER:C	2.53	0.51
1:A:660:VAL:CG1	1:A:661:GLU:N	2.72	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:301:LEU:HB2	3:C:350:ARG:NH1	2.25	0.51
3:C:351:ARG:HD3	3:C:393:ASP:OD2	2.10	0.51
3:C:933:TRP:CD1	3:C:937:LEU:HD11	2.46	0.51
3:C:1117:TYR:C	3:C:1117:TYR:HD2	2.18	0.51
1:A:145:VAL:C	1:A:146:ARG:HG3	2.34	0.51
1:A:319:GLY:O	1:A:322:TYR:HB3	2.10	0.51
3:C:236:ALA:HA	3:C:239:ARG:NH1	2.26	0.51
3:C:495:ILE:CD1	3:C:534:LYS:HB3	2.41	0.51
3:C:1024:ARG:O	3:C:1028:VAL:HG23	2.11	0.51
1:A:365:TYR:CE2	1:A:407:VAL:HG21	2.46	0.51
1:A:486:SER:O	1:A:490:LYS:HG3	2.11	0.51
3:C:129:ASN:HA	3:C:132:LYS:HB3	1.92	0.51
3:C:261:ASN:O	3:C:262:VAL:C	2.53	0.51
3:C:825:VAL:HG23	3:C:860:VAL:HG22	1.92	0.51
2:B:73:GLY:O	2:B:104:GLN:NE2	2.44	0.51
3:C:126:LEU:CD2	3:C:130:VAL:HG21	2.41	0.51
3:C:383:PHE:O	3:C:394:VAL:HG11	2.11	0.51
1:A:21:TRP:HE3	1:A:21:TRP:HA	1.75	0.50
1:A:672:LEU:H	1:A:672:LEU:CD1	2.16	0.50
1:A:726:HIS:HA	1:A:771:TYR:HE1	1.77	0.50
3:C:267:LEU:HA	3:C:270:TYR:CD1	2.46	0.50
3:C:1037:LYS:O	3:C:1040:LEU:HG	2.11	0.50
3:C:1112:GLY:O	3:C:1123:THR:CB	2.59	0.50
3:C:1190:GLU:O	3:C:1193:PRO:CD	2.55	0.50
1:A:503:LEU:HA	1:A:506:MET:HE3	1.94	0.50
3:C:970:LEU:C	3:C:972:GLY:H	2.18	0.50
1:A:308:ASN:C	1:A:310:LEU:H	2.18	0.50
1:A:741:PHE:O	1:A:743:PRO:HD3	2.11	0.50
3:C:52:MET:HE3	3:C:55:LYS:HB3	1.92	0.50
3:C:645:ARG:HD2	3:C:684:SER:CB	2.41	0.50
3:C:769:ASN:O	3:C:770:LEU:HD12	2.11	0.50
3:C:796:TYR:HD2	3:C:837:LEU:HB2	1.76	0.50
3:C:1031:ASN:OD1	3:C:1088:CYS:HA	2.10	0.50
1:A:21:TRP:HA	1:A:21:TRP:CE3	2.46	0.50
1:A:598:TYR:CD1	1:A:598:TYR:N	2.79	0.50
1:A:662:LEU:H	1:A:662:LEU:CD1	2.23	0.50
2:B:40:ASP:O	2:B:49:ILE:HD11	2.11	0.50
3:C:206:CYS:HB2	3:C:207:PHE:HA	1.92	0.50
3:C:244:ARG:HG2	3:C:244:ARG:NH1	2.24	0.50
3:C:384:LYS:C	3:C:385:GLU:HG3	2.36	0.50
1:A:299:LEU:O	1:A:303:HIS:CG	2.64	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:655:ALA:C	1:A:657:VAL:H	2.20	0.50
2:B:82:HIS:O	2:B:86:ARG:HB2	2.12	0.50
3:C:254:PRO:HB2	3:C:258:LYS:HE3	1.92	0.50
3:C:500:CYS:O	3:C:504:ILE:HG13	2.11	0.50
3:C:673:ALA:CA	3:C:676:ILE:HD11	2.37	0.50
3:C:857:LEU:HD11	3:C:883:ILE:HD13	1.93	0.50
1:A:21:TRP:CE3	1:A:21:TRP:O	2.65	0.50
1:A:227:TYR:CE1	1:A:282:THR:HG23	2.46	0.50
1:A:440:GLU:O	1:A:444:THR:CB	2.59	0.50
1:A:646:LYS:O	1:A:646:LYS:HG2	2.11	0.50
3:C:1202:ILE:HA	3:C:1205:ASN:HD22	1.76	0.50
1:A:309:LEU:HD13	1:A:317:ASP:HB2	1.92	0.50
1:A:309:LEU:CD1	1:A:317:ASP:HB2	2.42	0.50
1:A:441:LEU:HD21	1:A:483:ALA:HB2	1.93	0.50
1:A:703:GLU:OE1	1:A:703:GLU:HA	2.12	0.50
3:C:209:ASP:O	3:C:213:HIS:CD2	2.65	0.50
1:A:141:ASN:HD21	1:A:159:ILE:H	1.58	0.49
1:A:274:VAL:HA	1:A:278:LEU:HB2	1.93	0.49
1:A:521:LYS:HB3	1:A:521:LYS:NZ	2.27	0.49
1:A:522:LYS:O	1:A:525:THR:N	2.45	0.49
3:C:219:SER:O	3:C:222:ASP:HB2	2.12	0.49
3:C:814:GLY:O	3:C:818:VAL:HG23	2.12	0.49
2:B:97:ASP:O	2:B:99:ARG:N	2.45	0.49
3:C:151:GLN:O	3:C:154:ALA:N	2.44	0.49
3:C:223:SER:O	3:C:225:SER:N	2.45	0.49
3:C:350:ARG:NH2	3:C:386:ARG:HH22	2.10	0.49
3:C:1159:ALA:C	3:C:1161:SER:H	2.20	0.49
1:A:144:TRP:O	1:A:145:VAL:CG1	2.53	0.49
1:A:660:VAL:HB	1:A:662:LEU:HD11	1.94	0.49
3:C:851:LEU:C	3:C:853:GLY:N	2.68	0.49
3:C:887:ASN:OD1	3:C:889:PRO:HD2	2.11	0.49
3:C:1109:VAL:HG13	3:C:1123:THR:HG22	1.94	0.49
3:C:509:SER:O	3:C:512:VAL:HG23	2.11	0.49
3:C:697:LEU:CD1	3:C:716:LEU:HD21	2.42	0.49
3:C:697:LEU:O	3:C:700:LEU:N	2.38	0.49
3:C:821:PHE:CE1	3:C:857:LEU:HB2	2.46	0.49
3:C:902:GLN:HE22	3:C:905:ARG:NH1	2.11	0.49
3:C:1117:TYR:CZ	3:C:1121:MET:HE2	2.47	0.49
1:A:175:LEU:HG	1:A:208:TYR:CZ	2.48	0.49
1:A:430:LYS:HG2	1:A:477:ASN:O	2.12	0.49
1:A:431:LYS:HD2	1:A:431:LYS:C	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:621:VAL:HG11	1:A:632:MET:HE1	1.94	0.49
3:C:249:LEU:CB	3:C:281:ARG:NH2	2.75	0.49
3:C:1001:ASP:HB2	3:C:1002:PRO:HD3	1.93	0.49
1:A:598:TYR:CZ	1:A:675:LYS:HB3	2.48	0.49
1:A:720:MET:HE1	3:C:29:ASP:OD2	2.13	0.49
3:C:267:LEU:HD23	3:C:270:TYR:CZ	2.47	0.49
3:C:301:LEU:HB2	3:C:350:ARG:CZ	2.42	0.49
3:C:405:THR:O	3:C:406:ARG:C	2.55	0.49
3:C:763:VAL:HG13	3:C:775:LEU:HD12	1.93	0.49
3:C:818:VAL:C	3:C:820:GLN:N	2.70	0.49
2:B:48:HIS:O	2:B:50:MET:N	2.45	0.49
3:C:42:ASP:HB2	3:C:45:SER:CB	2.42	0.49
3:C:405:THR:O	3:C:407:PRO:N	2.46	0.49
3:C:1049:LEU:O	3:C:1050:PRO:C	2.55	0.49
3:C:1197:GLU:O	3:C:1198:PHE:C	2.54	0.49
1:A:452:PHE:O	1:A:458:LYS:NZ	2.46	0.49
1:A:492:LYS:HB3	3:C:108:ILE:HD11	1.95	0.49
1:A:593:CYS:HB2	2:B:20:LYS:H	1.78	0.49
1:A:609:ILE:HD11	1:A:635:LEU:CD2	2.42	0.49
1:A:615:THR:OG1	1:A:619:TYR:OH	2.31	0.49
1:A:618:ALA:CB	1:A:669:LYS:HG2	2.39	0.49
3:C:4:ALA:HB3	3:C:7:HIS:HB2	1.95	0.49
3:C:225:SER:O	3:C:226:THR:C	2.56	0.49
3:C:633:THR:HG23	3:C:676:ILE:CG1	2.41	0.49
1:A:134:ASN:ND2	1:A:157:TYR:HB2	2.27	0.49
3:C:386:ARG:HG3	3:C:386:ARG:HH11	1.77	0.49
3:C:615:PHE:O	3:C:616:LEU:C	2.55	0.49
3:C:808:ARG:HE	3:C:848:HIS:CG	2.31	0.49
1:A:178:GLN:O	1:A:179:VAL:C	2.56	0.48
3:C:374:THR:O	3:C:374:THR:CG2	2.61	0.48
3:C:1079:LEU:O	3:C:1079:LEU:CD2	2.60	0.48
1:A:170:CYS:O	1:A:174:PRO:HD2	2.12	0.48
1:A:643:LEU:HD23	1:A:648:LEU:CB	2.42	0.48
2:B:87:TRP:CZ2	2:B:95:PRO:HB3	2.48	0.48
3:C:547:VAL:HG12	3:C:599:ASN:HD22	1.77	0.48
3:C:830:SER:O	3:C:831:THR:C	2.54	0.48
3:C:1015:LEU:C	3:C:1018:PRO:HD2	2.39	0.48
3:C:1016:GLU:OE2	3:C:1016:GLU:HA	2.13	0.48
1:A:100:LEU:HD13	1:A:167:TRP:HA	1.96	0.48
1:A:556:SER:O	1:A:558:LEU:N	2.46	0.48
3:C:636:ALA:O	3:C:637:GLY:C	2.55	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1198:PHE:C	3:C:1198:PHE:CD1	2.62	0.48
1:A:117:LYS:HD3	1:A:117:LYS:C	2.37	0.48
1:A:178:GLN:O	1:A:180:THR:N	2.46	0.48
1:A:443:ASP:O	1:A:444:THR:C	2.56	0.48
1:A:475:HIS:CE1	1:A:585:SER:HA	2.47	0.48
1:A:619:TYR:HD2	1:A:623:GLN:NE2	2.11	0.48
1:A:647:LEU:HD12	1:A:647:LEU:N	2.28	0.48
1:A:660:VAL:CG1	1:A:661:GLU:H	2.26	0.48
3:C:249:LEU:HB3	3:C:281:ARG:CZ	2.43	0.48
3:C:299:LYS:HZ3	3:C:382:ARG:HD3	1.79	0.48
3:C:386:ARG:CZ	3:C:386:ARG:CB	2.80	0.48
3:C:578:ALA:O	3:C:579:ALA:CB	2.62	0.48
1:A:170:CYS:O	1:A:174:PRO:CD	2.61	0.48
1:A:186:LEU:HA	1:A:189:LYS:HG3	1.94	0.48
1:A:480:SER:C	1:A:482:ASP:H	2.22	0.48
3:C:600:LEU:N	3:C:600:LEU:HD23	2.27	0.48
3:C:601:GLY:CA	3:C:604:LEU:HB2	2.44	0.48
3:C:1013:LYS:HB2	3:C:1047:THR:HG21	1.95	0.48
1:A:178:GLN:C	1:A:180:THR:N	2.72	0.48
1:A:520:PHE:HD1	1:A:568:PHE:CG	2.30	0.48
3:C:249:LEU:HD22	3:C:250:GLU:N	2.27	0.48
3:C:599:ASN:C	3:C:600:LEU:HD23	2.39	0.48
1:A:356:GLU:O	1:A:357:ALA:C	2.57	0.48
3:C:1199:GLN:CG	3:C:1202:ILE:HG12	2.42	0.48
1:A:475:HIS:O	1:A:476:GLN:HG3	2.14	0.48
3:C:61:ASN:OD1	3:C:63:GLU:HB2	2.13	0.48
3:C:507:ASN:O	3:C:508:HIS:CG	2.66	0.48
3:C:633:THR:HG23	3:C:676:ILE:CD1	2.44	0.48
3:C:975:ILE:CG2	3:C:976:SER:H	2.19	0.48
1:A:202:SER:O	1:A:206:GLN:HG3	2.13	0.48
1:A:284:ASP:OD1	1:A:284:ASP:O	2.31	0.48
3:C:117:LEU:HD11	3:C:130:VAL:HG11	1.94	0.48
3:C:448:VAL:HG13	3:C:493:LEU:HD22	1.96	0.48
3:C:590:ILE:CD1	3:C:624:THR:HG23	2.44	0.48
3:C:821:PHE:CD2	3:C:821:PHE:N	2.79	0.48
1:A:147:ARG:C	1:A:149:CYS:H	2.21	0.48
1:A:250:PHE:CE2	1:A:259:TYR:HA	2.48	0.48
2:B:19:LYS:HB3	2:B:19:LYS:HZ3	1.76	0.48
3:C:134:ILE:O	3:C:137:ARG:N	2.46	0.48
3:C:181:LEU:HB3	3:C:217:GLU:OE1	2.14	0.48
3:C:226:THR:HG23	3:C:227:THR:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:294:ILE:HG23	3:C:353:ALA:HB1	1.96	0.48
3:C:521:VAL:HG13	3:C:525:VAL:HG23	1.94	0.48
3:C:633:THR:HA	3:C:676:ILE:CD1	2.42	0.48
3:C:1100:LEU:O	3:C:1102:ILE:HD13	2.14	0.48
1:A:104:LEU:O	1:A:108:GLU:HG3	2.14	0.47
1:A:212:GLY:C	1:A:223:THR:HG21	2.38	0.47
1:A:711:GLN:HE22	1:A:758:LYS:HZ2	1.62	0.47
1:A:734:LEU:HD23	1:A:734:LEU:HA	1.70	0.47
2:B:19:LYS:O	2:B:20:LYS:HB2	2.14	0.47
3:C:79:VAL:CG2	3:C:83:GLN:HB2	2.44	0.47
3:C:166:GLY:O	3:C:168:LEU:N	2.47	0.47
3:C:462:VAL:O	3:C:462:VAL:HG12	2.14	0.47
3:C:598:CYS:SG	3:C:638:SER:HB2	2.53	0.47
3:C:771:GLY:O	3:C:775:LEU:HG	2.13	0.47
1:A:289:LYS:O	1:A:293:VAL:HG12	2.14	0.47
1:A:472:ARG:O	1:A:473:LEU:C	2.57	0.47
1:A:630:ILE:CD1	1:A:630:ILE:HB	2.38	0.47
3:C:146:GLU:CD	3:C:146:GLU:N	2.72	0.47
3:C:380:ILE:HG23	3:C:394:VAL:HG12	1.96	0.47
3:C:592:CYS:O	3:C:596:ILE:HG13	2.14	0.47
3:C:648:LEU:HB3	3:C:689:MET:HE1	1.95	0.47
3:C:690:ILE:HG23	3:C:719:LEU:HD21	1.95	0.47
3:C:897:GLN:HE21	3:C:897:GLN:HA	1.79	0.47
3:C:1194:LEU:C	3:C:1194:LEU:CD1	2.87	0.47
1:A:405:ASN:ND2	1:A:408:THR:HG23	2.29	0.47
1:A:440:GLU:C	1:A:444:THR:OG1	2.55	0.47
2:B:87:TRP:CE2	2:B:95:PRO:HB3	2.48	0.47
3:C:514:HIS:CD2	3:C:559:PHE:HB2	2.49	0.47
3:C:698:PRO:CG	3:C:733:SER:HB2	2.43	0.47
3:C:823:GLN:HA	3:C:823:GLN:NE2	2.29	0.47
1:A:115:VAL:O	1:A:119:TYR:N	2.42	0.47
1:A:315:ASN:HB3	1:A:318:LEU:HD12	1.96	0.47
1:A:504:GLN:HA	1:A:504:GLN:NE2	2.29	0.47
2:B:36:ASP:C	2:B:36:ASP:OD2	2.57	0.47
3:C:195:THR:O	3:C:198:ALA:HB3	2.15	0.47
3:C:209:ASP:C	3:C:212:GLU:OE1	2.57	0.47
3:C:359:ALA:O	3:C:360:VAL:C	2.57	0.47
3:C:540:LEU:HD22	3:C:589:ALA:HA	1.96	0.47
3:C:1017:ASP:N	3:C:1018:PRO:CD	2.78	0.47
1:A:205:VAL:O	1:A:209:VAL:HG23	2.15	0.47
1:A:392:ALA:O	1:A:396:LYS:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:ASN:ND2	1:A:407:VAL:N	2.53	0.47
3:C:371:PHE:O	3:C:376:SER:OG	2.32	0.47
3:C:383:PHE:HD2	3:C:386:ARG:HE	1.55	0.47
3:C:386:ARG:HB2	3:C:386:ARG:NH1	2.29	0.47
3:C:428:LEU:O	3:C:431:GLN:HB2	2.15	0.47
3:C:508:HIS:O	3:C:509:SER:C	2.58	0.47
3:C:734:ILE:HG22	3:C:735:LEU:N	2.28	0.47
3:C:891:TYR:O	3:C:894:PHE:HB3	2.14	0.47
3:C:1019:ASP:O	3:C:1020:LEU:HG	2.15	0.47
3:C:257:VAL:O	3:C:260:CYS:N	2.47	0.47
3:C:621:ASN:HB2	3:C:624:THR:HB	1.96	0.47
3:C:724:PRO:O	3:C:727:LEU:HG	2.15	0.47
3:C:861:ILE:HG21	3:C:880:LEU:HB2	1.96	0.47
1:A:365:TYR:CD2	1:A:407:VAL:HG21	2.49	0.47
1:A:548:GLN:HA	1:A:581:LEU:HD22	1.96	0.47
1:A:632:MET:C	1:A:634:ILE:N	2.69	0.47
3:C:38:SER:H	3:C:78:LYS:NZ	2.12	0.47
3:C:211:ILE:HD12	3:C:211:ILE:N	2.29	0.47
3:C:275:PHE:C	3:C:275:PHE:CD2	2.93	0.47
3:C:281:ARG:HE	3:C:284:LYS:HG2	1.79	0.47
3:C:285:GLU:O	3:C:287:TYR:N	2.47	0.47
3:C:375:VAL:O	3:C:379:LEU:CA	2.61	0.47
3:C:385:GLU:HA	3:C:391:LYS:CE	2.34	0.47
3:C:465:LEU:CB	3:C:468:ALA:HB2	2.44	0.47
3:C:686:THR:C	3:C:688:ALA:N	2.70	0.47
3:C:857:LEU:O	3:C:858:LYS:C	2.57	0.47
3:C:1038:PRO:C	3:C:1040:LEU:N	2.72	0.47
3:C:1127:LEU:HD21	3:C:1145:LEU:HD13	1.96	0.47
3:C:1177:MET:O	3:C:1178:ARG:C	2.57	0.47
1:A:221:GLY:N	3:C:1171:GLU:OE2	2.48	0.47
1:A:445:LEU:HG	1:A:487:MET:SD	2.55	0.47
1:A:449:MET:SD	1:A:487:MET:HE1	2.54	0.47
1:A:556:SER:C	1:A:558:LEU:H	2.23	0.47
1:A:560:ARG:HG2	1:A:560:ARG:HH11	1.80	0.47
1:A:672:LEU:N	1:A:672:LEU:CD1	2.60	0.47
1:A:708:LEU:HD12	2:B:106:TYR:CD1	2.49	0.47
3:C:199:LEU:O	3:C:202:LEU:HB3	2.15	0.47
3:C:218:LEU:HD13	3:C:234:ILE:CD1	2.44	0.47
3:C:235:ALA:O	3:C:238:SER:HB2	2.14	0.47
3:C:375:VAL:HG13	3:C:379:LEU:HD12	1.96	0.47
3:C:590:ILE:HD11	3:C:624:THR:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:813:GLU:CD	3:C:814:GLY:N	2.70	0.47
1:A:734:LEU:O	1:A:735:THR:C	2.57	0.47
3:C:532:PHE:CE2	3:C:534:LYS:HB2	2.50	0.47
3:C:667:LYS:HE3	3:C:700:LEU:HD21	1.96	0.47
3:C:769:ASN:O	3:C:770:LEU:CD1	2.62	0.47
3:C:819:GLY:O	3:C:823:GLN:HG3	2.15	0.47
1:A:694:GLU:O	1:A:698:THR:HG23	2.15	0.47
3:C:287:TYR:CB	3:C:288:PRO:HD3	2.28	0.47
3:C:825:VAL:HG23	3:C:860:VAL:CG1	2.44	0.47
3:C:1157:VAL:HB	3:C:1166:PHE:HE2	1.79	0.47
3:C:1196:SER:O	3:C:1198:PHE:N	2.48	0.47
3:C:1199:GLN:HG3	3:C:1201:GLN:N	2.31	0.47
3:C:95:MET:HB2	3:C:96:LEU:HD12	1.97	0.46
3:C:200:GLY:O	3:C:203:VAL:HG22	2.15	0.46
3:C:405:THR:O	3:C:407:PRO:CD	2.63	0.46
3:C:590:ILE:HD13	3:C:628:THR:CG2	2.45	0.46
3:C:618:ARG:CG	3:C:624:THR:HG21	2.45	0.46
3:C:824:ASP:C	3:C:826:LYS:N	2.70	0.46
3:C:982:ARG:HH21	3:C:1018:PRO:CB	2.23	0.46
3:C:1157:VAL:HB	3:C:1166:PHE:CE2	2.50	0.46
3:C:1160:ASN:O	3:C:1160:ASN:CG	2.58	0.46
1:A:159:ILE:HD12	1:A:159:ILE:HA	1.78	0.46
1:A:167:TRP:O	1:A:170:CYS:N	2.48	0.46
1:A:171:LEU:CD1	1:A:175:LEU:HD13	2.46	0.46
1:A:408:THR:HB	1:A:414:SER:HA	1.96	0.46
3:C:38:SER:N	3:C:78:LYS:HZ3	2.13	0.46
3:C:253:ILE:HG21	3:C:286:VAL:HG11	1.96	0.46
3:C:432:VAL:HG11	3:C:436:VAL:HG23	1.97	0.46
3:C:560:ASP:OD1	3:C:562:THR:HG23	2.15	0.46
3:C:562:THR:N	3:C:563:PRO:HD2	2.30	0.46
3:C:576:LEU:HD22	3:C:593:MET:HG2	1.98	0.46
1:A:142:ARG:HH22	1:A:148:GLU:HG2	1.80	0.46
1:A:612:GLN:HB3	1:A:619:TYR:CE1	2.51	0.46
1:A:613:TYR:CE2	1:A:648:LEU:HD21	2.51	0.46
3:C:64:VAL:O	3:C:65:GLN:C	2.58	0.46
3:C:1015:LEU:C	3:C:1018:PRO:CD	2.88	0.46
3:C:1138:VAL:O	3:C:1142:LEU:N	2.48	0.46
1:A:37:MET:HE1	1:A:45:LEU:CD1	2.45	0.46
3:C:6:TYR:N	3:C:6:TYR:CD2	2.81	0.46
3:C:654:ILE:O	3:C:657:SER:HB3	2.16	0.46
3:C:1186:ILE:O	3:C:1187:PRO:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:821:PHE:O	3:C:823:GLN:N	2.44	0.46
3:C:1008:ILE:CG2	3:C:1009:GLY:N	2.78	0.46
3:C:1036:ASN:H	3:C:1036:ASN:ND2	2.14	0.46
3:C:1205:ASN:HB2	3:C:1206:PRO:CD	2.46	0.46
1:A:104:LEU:HD21	1:A:173:ARG:HB3	1.96	0.46
3:C:172:PHE:O	3:C:176:ILE:HG12	2.15	0.46
3:C:469:LEU:HD13	3:C:476:LEU:HD13	1.96	0.46
3:C:895:VAL:O	3:C:896:LEU:C	2.58	0.46
3:C:1202:ILE:O	3:C:1206:PRO:HD2	2.16	0.46
1:A:268:LEU:O	1:A:271:GLN:HB2	2.16	0.46
3:C:131:CYS:O	3:C:134:ILE:HB	2.16	0.46
3:C:206:CYS:CB	3:C:207:PHE:CA	2.94	0.46
3:C:441:LYS:HB2	3:C:441:LYS:HZ2	1.80	0.46
3:C:693:VAL:O	3:C:694:LEU:C	2.59	0.46
3:C:1086:PHE:HD2	3:C:1089:MET:HE2	1.80	0.46
3:C:1123:THR:HA	3:C:1126:MET:HB2	1.97	0.46
3:C:1183:LEU:O	3:C:1186:ILE:CG2	2.63	0.46
1:A:309:LEU:HB3	1:A:318:LEU:HD21	1.98	0.46
1:A:398:CYS:O	1:A:402:ILE:HG13	2.15	0.46
1:A:438:GLU:OE1	1:A:438:GLU:O	2.33	0.46
1:A:632:MET:O	1:A:633:ASP:C	2.59	0.46
3:C:171:ASN:OD1	3:C:171:ASN:N	2.49	0.46
3:C:186:SER:O	3:C:192:ARG:HD2	2.16	0.46
3:C:218:LEU:HD23	3:C:230:TYR:CD1	2.47	0.46
3:C:551:ARG:C	3:C:551:ARG:CD	2.84	0.46
3:C:1051:HIS:O	3:C:1054:ASN:N	2.49	0.46
1:A:553:ALA:HB2	1:A:629:GLN:HB2	1.97	0.46
2:B:74:VAL:HA	2:B:104:GLN:NE2	2.30	0.46
3:C:661:LYS:O	3:C:662:ASN:C	2.58	0.46
3:C:676:ILE:H	3:C:676:ILE:HG13	1.36	0.46
3:C:852:SER:HB2	3:C:887:ASN:HD22	1.81	0.46
3:C:1015:LEU:CD1	3:C:1022:VAL:HG12	2.41	0.46
3:C:1036:ASN:H	3:C:1036:ASN:HD22	1.62	0.46
1:A:171:LEU:CG	1:A:175:LEU:HD13	2.46	0.46
1:A:260:MET:HE1	1:A:321:MET:HB2	1.97	0.46
1:A:533:ASP:HB3	2:B:26:LYS:HG2	1.97	0.46
3:C:442:GLN:O	3:C:445:GLU:HB2	2.15	0.46
3:C:505:LEU:HD23	3:C:513:PHE:CE2	2.51	0.46
3:C:1079:LEU:CD2	3:C:1079:LEU:C	2.89	0.46
3:C:1181:ALA:O	3:C:1183:LEU:N	2.49	0.46
3:C:1184:LEU:CD2	3:C:1195:MET:HE2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:40:ASP:HB3	2:B:49:ILE:HD11	1.98	0.45
3:C:35:GLN:O	3:C:36:LYS:CB	2.65	0.45
3:C:247:GLU:HG3	3:C:248:TYR:CD1	2.51	0.45
3:C:825:VAL:C	3:C:827:ASN:N	2.64	0.45
3:C:1023:ARG:HD3	3:C:1055:GLU:OE2	2.15	0.45
1:A:624:LEU:O	1:A:626:ASP:N	2.50	0.45
3:C:33:GLU:C	3:C:35:GLN:N	2.67	0.45
3:C:126:LEU:C	3:C:128:ALA:N	2.74	0.45
3:C:173:HIS:HB3	3:C:210:LEU:HD13	1.98	0.45
3:C:208:VAL:HA	3:C:244:ARG:HH22	1.81	0.45
3:C:601:GLY:HA2	3:C:604:LEU:HD22	1.97	0.45
3:C:686:THR:O	3:C:689:MET:N	2.35	0.45
3:C:1147:GLU:HB3	3:C:1148:PRO:CD	2.38	0.45
1:A:21:TRP:O	1:A:21:TRP:CD2	2.69	0.45
1:A:400:ARG:HG2	1:A:400:ARG:HH11	1.81	0.45
3:C:168:LEU:O	3:C:169:LEU:HB2	2.16	0.45
3:C:189:LEU:HD13	3:C:192:ARG:CZ	2.47	0.45
3:C:205:SER:O	3:C:206:CYS:CB	2.63	0.45
3:C:249:LEU:HB2	3:C:281:ARG:NH2	2.31	0.45
3:C:579:ALA:HA	3:C:586:LYS:HE2	1.99	0.45
3:C:966:LEU:C	3:C:968:PRO:HD2	2.41	0.45
3:C:1026:ALA:O	3:C:1027:LEU:C	2.57	0.45
3:C:933:TRP:HE1	3:C:937:LEU:HD11	1.81	0.45
3:C:985:VAL:HG13	3:C:986:VAL:N	2.31	0.45
3:C:1036:ASN:ND2	3:C:1036:ASN:N	2.60	0.45
3:C:1037:LYS:N	3:C:1038:PRO:HD3	2.31	0.45
3:C:1146:VAL:O	3:C:1147:GLU:C	2.59	0.45
1:A:145:VAL:O	1:A:146:ARG:CG	2.59	0.45
1:A:688:LYS:HD3	1:A:688:LYS:C	2.41	0.45
3:C:735:LEU:C	3:C:737:GLU:H	2.24	0.45
3:C:990:LYS:C	3:C:992:THR:H	2.24	0.45
1:A:609:ILE:O	1:A:610:LEU:C	2.59	0.45
3:C:209:ASP:O	3:C:212:GLU:CD	2.60	0.45
3:C:218:LEU:O	3:C:222:ASP:OD2	2.35	0.45
3:C:813:GLU:OE2	3:C:815:PRO:HG2	2.16	0.45
3:C:1199:GLN:HG3	3:C:1201:GLN:H	1.81	0.45
3:C:1208:LEU:HD22	3:C:1208:LEU:N	2.31	0.45
1:A:37:MET:HE3	1:A:41:ARG:HG3	1.99	0.45
1:A:240:GLU:CD	1:A:289:LYS:NZ	2.74	0.45
3:C:176:ILE:O	3:C:179:CYS:SG	2.75	0.45
3:C:373:LYS:CE	3:C:427:MET:HE1	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:545:GLN:O	3:C:549:VAL:HG23	2.17	0.45
3:C:562:THR:OG1	3:C:563:PRO:CD	2.65	0.45
3:C:1034:ALA:O	3:C:1038:PRO:HG3	2.17	0.45
1:A:682:ASN:HD21	1:A:684:ASN:HB3	1.82	0.45
2:B:70:VAL:HG12	2:B:71:ALA:N	2.32	0.45
3:C:100:GLU:C	3:C:102:LEU:N	2.72	0.45
3:C:229:THR:C	3:C:231:ILE:H	2.24	0.45
3:C:433:PRO:HB2	3:C:437:LYS:HE3	1.99	0.45
3:C:576:LEU:CD2	3:C:593:MET:HG2	2.47	0.45
3:C:1051:HIS:O	3:C:1052:LEU:C	2.60	0.45
3:C:1132:THR:HG22	3:C:1133:LEU:N	2.32	0.45
3:C:1199:GLN:CG	3:C:1202:ILE:H	2.29	0.45
1:A:168:ARG:O	1:A:172:PHE:HD1	2.00	0.45
1:A:171:LEU:HD12	1:A:175:LEU:CD1	2.47	0.45
1:A:200:LEU:O	1:A:204:VAL:HG23	2.17	0.45
1:A:226:VAL:HG23	1:A:227:TYR:H	1.81	0.45
2:B:79:PHE:HE1	2:B:101:TRP:CZ3	2.35	0.45
3:C:169:LEU:HD12	3:C:169:LEU:N	2.32	0.45
3:C:186:SER:O	3:C:192:ARG:NH1	2.27	0.45
3:C:485:ASN:O	3:C:486:ASP:CB	2.34	0.45
3:C:514:HIS:HE1	3:C:549:VAL:O	2.00	0.45
3:C:569:PHE:CD1	3:C:593:MET:HE1	2.52	0.45
3:C:958:LEU:HD23	3:C:958:LEU:HA	1.72	0.45
3:C:975:ILE:O	3:C:976:SER:C	2.60	0.45
3:C:1079:LEU:HD22	3:C:1079:LEU:C	2.41	0.45
1:A:89:TYR:CZ	1:A:162:LEU:HG	2.52	0.45
1:A:546:PHE:CD2	1:A:584:LEU:HD11	2.52	0.45
1:A:585:SER:CB	2:B:29:ALA:HA	2.47	0.45
1:A:706:ARG:HG2	1:A:741:PHE:CE1	2.52	0.45
3:C:72:LEU:O	3:C:73:GLY:C	2.60	0.45
3:C:347:TRP:C	3:C:349:VAL:N	2.73	0.45
3:C:588:ARG:HG3	3:C:588:ARG:HH11	1.81	0.45
3:C:604:LEU:O	3:C:605:GLY:O	2.35	0.45
3:C:605:GLY:C	3:C:607:ASP:H	2.25	0.45
3:C:616:LEU:HD23	3:C:647:VAL:CB	2.46	0.45
1:A:595:LYS:HG3	1:A:596:ASN:H	1.82	0.44
1:A:600:LEU:HA	1:A:681:VAL:O	2.17	0.44
3:C:932:ILE:HB	3:C:958:LEU:HD11	1.99	0.44
3:C:982:ARG:HH22	3:C:1018:PRO:HB2	1.75	0.44
3:C:1199:GLN:HG3	3:C:1202:ILE:H	1.83	0.44
1:A:582:TYR:HA	1:A:585:SER:OG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:158:MET:HE2	3:C:162:LEU:HG	1.99	0.44
3:C:248:TYR:N	3:C:249:LEU:HD13	2.32	0.44
3:C:253:ILE:HD12	3:C:253:ILE:H	1.83	0.44
3:C:271:CYS:O	3:C:272:ILE:C	2.60	0.44
3:C:439:LEU:O	3:C:442:GLN:N	2.50	0.44
3:C:802:CYS:O	3:C:803:VAL:C	2.60	0.44
3:C:858:LYS:HD3	3:C:894:PHE:CE2	2.52	0.44
3:C:925:LEU:C	3:C:927:PRO:HD2	2.43	0.44
1:A:89:TYR:O	1:A:92:LEU:N	2.49	0.44
1:A:143:HIS:C	1:A:145:VAL:N	2.75	0.44
1:A:147:ARG:HG3	1:A:148:GLU:H	1.79	0.44
1:A:171:LEU:HG	1:A:175:LEU:HD13	1.99	0.44
1:A:351:ILE:CG2	1:A:407:VAL:HG23	2.48	0.44
1:A:472:ARG:NH1	1:A:484:GLU:OE2	2.49	0.44
1:A:500:THR:HG22	1:A:501:SER:N	2.32	0.44
1:A:632:MET:HE2	1:A:632:MET:HB3	1.71	0.44
1:A:657:VAL:HA	1:A:660:VAL:CG2	2.47	0.44
3:C:177:LEU:HD11	3:C:181:LEU:HD21	1.98	0.44
3:C:555:GLN:HE21	3:C:555:GLN:HB2	1.61	0.44
3:C:727:LEU:O	3:C:728:SER:C	2.60	0.44
3:C:799:ILE:CG2	3:C:837:LEU:HD11	2.47	0.44
3:C:1184:LEU:HD21	3:C:1195:MET:HE2	1.99	0.44
1:A:649:VAL:CG2	1:A:671:TYR:HB2	2.48	0.44
1:A:676:ASN:HB3	1:A:681:VAL:CG2	2.47	0.44
2:B:21:ARG:HG3	2:B:21:ARG:HH11	1.82	0.44
3:C:31:MET:HB2	3:C:71:CYS:SG	2.57	0.44
3:C:52:MET:O	3:C:55:LYS:HB3	2.18	0.44
3:C:134:ILE:O	3:C:135:THR:C	2.60	0.44
3:C:251:LYS:O	3:C:254:PRO:HG2	2.18	0.44
3:C:616:LEU:O	3:C:619:LEU:HB3	2.16	0.44
3:C:1008:ILE:HG23	3:C:1044:LEU:HD11	1.99	0.44
3:C:1083:LYS:O	3:C:1083:LYS:HD3	2.17	0.44
1:A:138:ALA:O	1:A:141:ASN:HB2	2.17	0.44
1:A:173:ARG:CB	1:A:174:PRO:CD	2.90	0.44
1:A:175:LEU:CG	1:A:208:TYR:CZ	3.01	0.44
1:A:588:GLU:OE2	2:B:26:LYS:HD3	2.17	0.44
1:A:724:LEU:HD22	1:A:728:GLN:HB3	1.99	0.44
3:C:264:ASP:CG	3:C:265:ASP:N	2.75	0.44
1:A:21:TRP:O	1:A:25:ARG:HB2	2.18	0.44
3:C:264:ASP:CG	3:C:266:GLU:H	2.25	0.44
3:C:270:TYR:HA	3:C:273:GLN:CD	2.40	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:786:GLN:HE21	3:C:786:GLN:HB2	1.63	0.44
3:C:813:GLU:C	3:C:815:PRO:HD2	2.42	0.44
3:C:1013:LYS:HB2	3:C:1047:THR:CG2	2.48	0.44
1:A:89:TYR:O	1:A:90:LYS:C	2.61	0.44
1:A:338:LEU:HD12	1:A:338:LEU:HA	1.83	0.44
1:A:687:MET:HB2	1:A:690:GLU:HB2	1.98	0.44
3:C:253:ILE:HD11	3:C:281:ARG:NH2	2.32	0.44
3:C:283:PRO:HD2	3:C:284:LYS:NZ	2.33	0.44
3:C:899:ILE:CG2	3:C:935:LEU:HD11	2.44	0.44
3:C:1181:ALA:C	3:C:1183:LEU:H	2.25	0.44
1:A:166:THR:O	1:A:169:ASP:HB2	2.17	0.44
3:C:294:ILE:HG23	3:C:353:ALA:CB	2.48	0.44
3:C:350:ARG:HE	3:C:386:ARG:NH2	2.15	0.44
3:C:385:GLU:HA	3:C:391:LYS:HG3	2.00	0.44
3:C:406:ARG:NH1	3:C:460:GLU:OE2	2.50	0.44
3:C:429:GLN:O	3:C:431:GLN:N	2.51	0.44
3:C:601:GLY:HA2	3:C:604:LEU:CD2	2.48	0.44
1:A:442:GLU:O	1:A:446:ASN:ND2	2.51	0.44
1:A:517:ASN:ND2	1:A:536:ILE:O	2.51	0.44
1:A:526:ASN:O	1:A:527:SER:HB3	2.17	0.44
2:B:83:CYS:HA	2:B:86:ARG:NH1	2.33	0.44
3:C:85:GLU:HG3	3:C:133:LYS:CE	2.33	0.44
3:C:181:LEU:N	3:C:182:PRO:HD2	2.32	0.44
3:C:686:THR:O	3:C:688:ALA:N	2.51	0.44
3:C:697:LEU:HB2	3:C:698:PRO:HD3	2.00	0.44
1:A:438:GLU:OE1	1:A:438:GLU:C	2.61	0.43
1:A:589:LEU:HD13	1:A:607:MET:HE2	2.00	0.43
1:A:625:THR:O	1:A:625:THR:HG22	2.17	0.43
3:C:148:VAL:O	3:C:150:VAL:N	2.51	0.43
3:C:228:ARG:O	3:C:228:ARG:CG	2.65	0.43
3:C:477:VAL:HB	3:C:478:PRO:HD3	2.00	0.43
3:C:572:THR:CG2	3:C:593:MET:HE2	2.48	0.43
3:C:638:SER:O	3:C:639:PRO:C	2.61	0.43
1:A:565:PHE:O	1:A:566:THR:C	2.61	0.43
3:C:164:ARG:HH11	3:C:164:ARG:HG3	1.83	0.43
3:C:227:THR:CG2	3:C:229:THR:OG1	2.66	0.43
3:C:386:ARG:HD3	3:C:390:VAL:CG1	2.48	0.43
3:C:683:ASP:C	3:C:685:LEU:H	2.27	0.43
3:C:771:GLY:N	3:C:774:ASP:HB2	2.33	0.43
3:C:785:SER:O	3:C:786:GLN:HG3	2.17	0.43
3:C:855:LEU:CD1	3:C:858:LYS:HD2	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1158:LYS:C	3:C:1160:ASN:N	2.76	0.43
3:C:97:SER:CB	3:C:102:LEU:HD23	2.47	0.43
3:C:170:VAL:HA	3:C:173:HIS:NE2	2.33	0.43
3:C:733:SER:O	3:C:737:GLU:HB2	2.18	0.43
3:C:835:ARG:HE	3:C:835:ARG:HB2	1.54	0.43
3:C:1032:SER:O	3:C:1036:ASN:ND2	2.52	0.43
1:A:95:PHE:CD2	1:A:96:LEU:HD12	2.36	0.43
1:A:425:CYS:O	1:A:429:LEU:HD22	2.18	0.43
2:B:82:HIS:HB3	2:B:86:ARG:HH21	1.83	0.43
3:C:88:VAL:HG13	3:C:134:ILE:HG12	2.01	0.43
3:C:218:LEU:CD2	3:C:230:TYR:HD1	2.29	0.43
3:C:386:ARG:HH11	3:C:386:ARG:CG	2.31	0.43
3:C:976:SER:O	3:C:977:GLY:O	2.36	0.43
3:C:1037:LYS:C	3:C:1039:SER:N	2.76	0.43
1:A:167:TRP:C	1:A:169:ASP:N	2.75	0.43
1:A:309:LEU:HB3	1:A:318:LEU:CD2	2.49	0.43
1:A:447:GLN:O	1:A:450:VAL:HB	2.18	0.43
1:A:510:ILE:HD13	1:A:510:ILE:HA	1.80	0.43
3:C:103:ARG:O	3:C:107:SER:HB2	2.19	0.43
3:C:388:GLU:O	3:C:389:ASN:C	2.62	0.43
3:C:423:THR:HA	3:C:424:PRO:HD3	1.81	0.43
3:C:423:THR:CG2	3:C:424:PRO:N	2.82	0.43
3:C:551:ARG:NH1	3:C:553:LEU:CB	2.71	0.43
3:C:601:GLY:C	3:C:604:LEU:HB2	2.43	0.43
3:C:676:ILE:O	3:C:677:LEU:C	2.61	0.43
3:C:710:GLN:HB3	3:C:751:ALA:CA	2.46	0.43
3:C:1166:PHE:O	3:C:1167:GLU:C	2.61	0.43
1:A:438:GLU:C	1:A:438:GLU:CD	2.86	0.43
1:A:597:ARG:NH1	1:A:597:ARG:CB	2.74	0.43
1:A:701:ASN:C	1:A:701:ASN:ND2	2.73	0.43
3:C:56:LEU:C	3:C:58:GLU:H	2.27	0.43
3:C:132:LYS:O	3:C:133:LYS:C	2.61	0.43
3:C:979:SER:OG	3:C:1020:LEU:HD21	2.18	0.43
1:A:107:GLY:CA	1:A:110:LEU:HD12	2.44	0.43
1:A:140:LEU:HA	1:A:140:LEU:HD22	1.80	0.43
1:A:376:TYR:HA	1:A:379:LEU:HB3	2.01	0.43
1:A:631:LYS:HB3	1:A:634:ILE:HG22	2.01	0.43
1:A:716:ARG:O	3:C:25:MET:HG3	2.18	0.43
1:A:720:MET:HG2	3:C:22:PHE:CE2	2.54	0.43
1:A:768:LYS:O	1:A:769:ASP:HB2	2.18	0.43
3:C:346:SER:O	3:C:348:LYS:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:355:LYS:O	3:C:358:ASP:HB3	2.18	0.43
3:C:623:ILE:O	3:C:624:THR:C	2.61	0.43
3:C:706:MET:O	3:C:707:HIS:C	2.61	0.43
3:C:769:ASN:HA	3:C:774:ASP:OD2	2.19	0.43
3:C:826:LYS:O	3:C:830:SER:HB2	2.18	0.43
1:A:167:TRP:C	1:A:167:TRP:CD1	2.96	0.43
3:C:37:ASP:OD1	3:C:39:ILE:HD13	2.17	0.43
3:C:46:GLU:CD	3:C:79:VAL:HG23	2.44	0.43
3:C:246:GLY:O	3:C:249:LEU:CD1	2.67	0.43
3:C:659:LEU:HD13	3:C:700:LEU:HD11	2.01	0.43
3:C:727:LEU:O	3:C:730:ILE:N	2.48	0.43
3:C:1141:ARG:NH1	3:C:1144:ARG:NH2	2.67	0.43
3:C:1181:ALA:C	3:C:1183:LEU:N	2.76	0.43
1:A:179:VAL:O	1:A:183:VAL:HG23	2.19	0.43
1:A:532:LEU:C	1:A:532:LEU:HD12	2.44	0.43
1:A:593:CYS:C	1:A:594:PHE:HD2	2.27	0.43
2:B:73:GLY:C	2:B:75:CYS:N	2.74	0.43
2:B:84:ILE:HG23	2:B:85:SER:N	2.34	0.43
3:C:389:ASN:O	3:C:392:ALA:HB3	2.18	0.43
3:C:459:THR:O	3:C:460:GLU:C	2.62	0.43
3:C:544:GLN:HG3	3:C:595:GLN:CB	2.49	0.43
3:C:551:ARG:HH12	3:C:553:LEU:HB2	1.79	0.43
3:C:913:LEU:HD23	3:C:917:ILE:HG13	1.99	0.43
1:A:625:THR:CB	1:A:632:MET:CG	2.97	0.43
1:A:708:LEU:HD22	2:B:81:PHE:CZ	2.54	0.43
3:C:143:ALA:C	3:C:145:GLN:N	2.76	0.43
3:C:481:ILE:HD11	3:C:520:LEU:CD2	2.36	0.43
3:C:1030:PHE:HE1	3:C:1041:ILE:HG23	1.83	0.43
1:A:95:PHE:CD2	1:A:95:PHE:C	2.97	0.42
1:A:157:TYR:N	1:A:157:TYR:CD1	2.86	0.42
1:A:162:LEU:HD22	1:A:162:LEU:O	2.20	0.42
1:A:280:GLU:HA	1:A:283:GLN:HE21	1.84	0.42
1:A:346:GLN:HG2	1:A:376:TYR:OH	2.19	0.42
1:A:377:ASN:C	1:A:379:LEU:H	2.26	0.42
1:A:496:GLY:H	1:A:740:ARG:NH2	2.17	0.42
1:A:516:LEU:HD11	1:A:569:TYR:HE1	1.84	0.42
1:A:593:CYS:CB	2:B:20:LYS:H	2.32	0.42
1:A:716:ARG:NE	1:A:736:GLN:HE22	2.17	0.42
1:A:749:LYS:C	1:A:751:CYS:N	2.75	0.42
2:B:94:CYS:C	2:B:96:LEU:H	2.27	0.42
3:C:260:CYS:HA	3:C:267:LEU:HD22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:268:ARG:O	3:C:272:ILE:HG12	2.18	0.42
3:C:274:ALA:O	3:C:278:PHE:HD1	2.02	0.42
3:C:547:VAL:HG13	3:C:600:LEU:HD21	2.01	0.42
3:C:548:LYS:HA	3:C:551:ARG:HG2	1.98	0.42
3:C:675:ASP:O	3:C:676:ILE:C	2.59	0.42
3:C:1183:LEU:HD23	3:C:1183:LEU:HA	1.84	0.42
1:A:171:LEU:CG	1:A:175:LEU:HD22	2.41	0.42
1:A:377:ASN:C	1:A:379:LEU:N	2.77	0.42
1:A:445:LEU:HD12	1:A:445:LEU:HA	1.88	0.42
3:C:257:VAL:O	3:C:258:LYS:C	2.62	0.42
3:C:367:MET:O	3:C:368:LEU:C	2.62	0.42
3:C:461:LEU:O	3:C:461:LEU:HD22	2.19	0.42
3:C:520:LEU:O	3:C:523:PRO:HG2	2.19	0.42
3:C:920:ALA:C	3:C:921:SER:OG	2.62	0.42
3:C:959:THR:O	3:C:960:LEU:C	2.62	0.42
2:B:37:ILE:HG12	2:B:37:ILE:O	2.20	0.42
3:C:89:ASP:OD1	3:C:137:ARG:NH1	2.51	0.42
3:C:127:ALA:HA	3:C:130:VAL:HB	2.00	0.42
3:C:461:LEU:HD22	3:C:461:LEU:C	2.45	0.42
3:C:640:LEU:O	3:C:641:LYS:C	2.63	0.42
3:C:813:GLU:CD	3:C:816:ALA:HB3	2.44	0.42
3:C:825:VAL:HG21	3:C:860:VAL:HG22	1.97	0.42
3:C:826:LYS:HA	3:C:826:LYS:CE	2.47	0.42
3:C:1008:ILE:CG2	3:C:1009:GLY:H	2.30	0.42
3:C:1048:VAL:O	3:C:1049:LEU:C	2.62	0.42
1:A:554:LEU:O	1:A:555:PRO:C	2.61	0.42
3:C:110:LEU:HD12	3:C:110:LEU:HA	1.80	0.42
3:C:148:VAL:HG12	3:C:152:LEU:HG	2.01	0.42
3:C:275:PHE:HE2	3:C:279:VAL:HG21	1.85	0.42
3:C:288:PRO:O	3:C:289:HIS:C	2.62	0.42
3:C:387:GLU:O	3:C:388:GLU:HG2	2.19	0.42
3:C:625:ARG:HH11	3:C:625:ARG:CG	2.32	0.42
3:C:730:ILE:O	3:C:730:ILE:HG22	2.19	0.42
3:C:731:SER:O	3:C:732:GLY:O	2.36	0.42
3:C:1037:LYS:C	3:C:1039:SER:H	2.27	0.42
3:C:1109:VAL:HG13	3:C:1123:THR:CG2	2.50	0.42
1:A:111:MET:HE3	1:A:111:MET:HB2	1.84	0.42
1:A:117:LYS:NZ	1:A:121:GLN:HG3	2.35	0.42
1:A:195:THR:HG21	3:C:1028:VAL:HG13	2.02	0.42
1:A:270:GLU:HA	1:A:273:ARG:HB2	2.01	0.42
1:A:588:GLU:CD	2:B:26:LYS:HD3	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:663:LYS:HB3	1:A:664:PRO:HD2	2.01	0.42
1:A:725:LYS:O	1:A:728:GLN:HB2	2.19	0.42
2:B:97:ASP:OD1	2:B:97:ASP:C	2.45	0.42
3:C:177:LEU:HG	3:C:181:LEU:HD11	2.01	0.42
3:C:602:ASP:HB3	3:C:640:LEU:HD13	2.01	0.42
3:C:1041:ILE:O	3:C:1042:ARG:C	2.61	0.42
1:A:469:LEU:HA	1:A:472:ARG:CZ	2.50	0.42
1:A:665:ASP:O	1:A:666:THR:C	2.62	0.42
3:C:168:LEU:CG	3:C:169:LEU:HD12	2.49	0.42
3:C:521:VAL:O	3:C:522:PRO:C	2.62	0.42
3:C:570:THR:C	3:C:572:THR:N	2.77	0.42
3:C:733:SER:O	3:C:734:ILE:C	2.63	0.42
3:C:939:HIS:C	3:C:941:GLU:H	2.26	0.42
3:C:1177:MET:C	3:C:1179:ALA:N	2.75	0.42
1:A:25:ARG:HD3	1:A:95:PHE:HD1	1.84	0.42
1:A:467:LYS:HZ2	1:A:698:THR:CB	2.29	0.42
1:A:475:HIS:HE1	1:A:585:SER:HA	1.83	0.42
1:A:522:LYS:O	1:A:524:LEU:N	2.53	0.42
1:A:667:LEU:CB	1:A:669:LYS:HE3	2.48	0.42
1:A:699:HIS:O	1:A:700:LYS:C	2.62	0.42
2:B:48:HIS:O	2:B:49:ILE:C	2.60	0.42
3:C:45:SER:O	3:C:49:VAL:HG23	2.20	0.42
3:C:168:LEU:C	3:C:169:LEU:CD1	2.93	0.42
3:C:174:PRO:HB3	3:C:210:LEU:HD21	2.00	0.42
3:C:252:ILE:H	3:C:252:ILE:HG12	1.73	0.42
3:C:617:GLU:O	3:C:618:ARG:C	2.62	0.42
3:C:637:GLY:H	3:C:680:ASN:HD22	1.67	0.42
3:C:814:GLY:N	3:C:815:PRO:CD	2.72	0.42
3:C:1150:ARG:O	3:C:1151:ALA:C	2.62	0.42
1:A:475:HIS:ND1	1:A:586:LYS:HD3	2.34	0.42
1:A:480:SER:C	1:A:482:ASP:N	2.77	0.42
3:C:104:ASP:O	3:C:108:ILE:HG12	2.20	0.42
3:C:781:GLY:O	3:C:783:VAL:N	2.52	0.42
1:A:128:PHE:CE1	3:C:1073:HIS:HB2	2.55	0.42
1:A:195:THR:CG2	3:C:1028:VAL:HG13	2.49	0.42
1:A:207:SER:O	1:A:208:TYR:C	2.61	0.42
1:A:583:GLN:H	1:A:583:GLN:NE2	2.12	0.42
1:A:646:LYS:O	1:A:646:LYS:CG	2.67	0.42
1:A:718:MET:HE1	1:A:771:TYR:HB2	1.99	0.42
3:C:56:LEU:C	3:C:58:GLU:N	2.73	0.42
3:C:536:THR:O	3:C:540:LEU:HD12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:572:THR:HG22	3:C:593:MET:HE2	2.01	0.42
3:C:914:LYS:HE2	3:C:914:LYS:HB3	1.90	0.42
3:C:987:THR:O	3:C:990:LYS:HB3	2.19	0.42
1:A:37:MET:CE	1:A:42:TYR:HA	2.49	0.42
1:A:472:ARG:NH1	1:A:484:GLU:CD	2.78	0.42
1:A:671:TYR:OH	1:A:674:TYR:HB2	2.19	0.42
3:C:92:CYS:HA	3:C:95:MET:HG3	2.02	0.42
3:C:388:GLU:OE2	3:C:388:GLU:HA	2.18	0.42
3:C:391:LYS:HG2	3:C:395:PHE:HE1	1.84	0.42
3:C:432:VAL:CG1	3:C:435:ILE:HB	2.36	0.42
3:C:472:HIS:C	3:C:474:PRO:CD	2.92	0.42
3:C:945:GLU:O	3:C:945:GLU:CD	2.62	0.42
3:C:1079:LEU:O	3:C:1083:LYS:HB2	2.20	0.42
3:C:1127:LEU:HD23	3:C:1127:LEU:HA	1.89	0.42
3:C:1203:SER:OG	3:C:1204:SER:N	2.51	0.42
1:A:280:GLU:OE1	3:C:1174:ARG:HD2	2.19	0.41
1:A:522:LYS:O	1:A:523:HIS:C	2.63	0.41
3:C:115:GLY:HA2	3:C:164:ARG:HD3	2.00	0.41
3:C:173:HIS:N	3:C:174:PRO:HD2	2.35	0.41
3:C:515:PRO:HG2	3:C:516:HIS:CD2	2.55	0.41
3:C:530:ASP:CG	3:C:531:PRO:HD2	2.45	0.41
3:C:611:THR:CA	3:C:614:ILE:HG12	2.45	0.41
3:C:926:LYS:O	3:C:927:PRO:C	2.63	0.41
1:A:556:SER:C	1:A:558:LEU:N	2.79	0.41
3:C:42:ASP:C	3:C:44:ASP:N	2.75	0.41
3:C:115:GLY:HA2	3:C:164:ARG:CD	2.50	0.41
3:C:368:LEU:O	3:C:371:PHE:HB2	2.20	0.41
3:C:399:LEU:O	3:C:403:LYS:HG3	2.20	0.41
3:C:540:LEU:CD2	3:C:589:ALA:HA	2.51	0.41
3:C:581:ILE:CD1	3:C:586:LYS:HE3	2.49	0.41
3:C:673:ALA:C	3:C:675:ASP:N	2.72	0.41
3:C:1101:ASP:OD1	3:C:1101:ASP:C	2.63	0.41
1:A:160:TYR:O	1:A:163:ALA:N	2.53	0.41
1:A:260:MET:CE	1:A:321:MET:HE2	2.48	0.41
1:A:375:LYS:HD3	1:A:376:TYR:CE1	2.55	0.41
1:A:476:GLN:O	1:A:477:ASN:HB2	2.20	0.41
3:C:237:ILE:HG13	3:C:237:ILE:H	1.72	0.41
3:C:914:LYS:HG2	3:C:954:CYS:SG	2.59	0.41
3:C:1000:ILE:HD13	3:C:1000:ILE:N	2.36	0.41
3:C:1009:GLY:C	3:C:1011:PHE:N	2.78	0.41
3:C:1053:TYR:O	3:C:1056:THR:HB	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1161:SER:HB3	3:C:1165:GLU:HB3	2.02	0.41
3:C:1205:ASN:O	3:C:1207:GLU:N	2.53	0.41
1:A:673:GLY:O	1:A:674:TYR:O	2.39	0.41
3:C:461:LEU:C	3:C:461:LEU:HD13	2.45	0.41
3:C:630:LYS:HG3	3:C:631:ALA:N	2.33	0.41
3:C:942:CYS:CB	3:C:948:ARG:HD2	2.50	0.41
3:C:1039:SER:C	3:C:1040:LEU:HD23	2.44	0.41
3:C:1186:ILE:O	3:C:1190:GLU:OE1	2.39	0.41
1:A:168:ARG:C	1:A:170:CYS:H	2.28	0.41
1:A:265:ALA:O	1:A:269:GLU:HG3	2.20	0.41
1:A:417:SER:N	1:A:418:PRO:CD	2.83	0.41
1:A:522:LYS:C	1:A:524:LEU:N	2.77	0.41
1:A:621:VAL:CG2	1:A:668:ILE:HD11	2.45	0.41
3:C:212:GLU:CD	3:C:212:GLU:H	2.18	0.41
3:C:302:THR:O	3:C:303:TYR:CB	2.69	0.41
3:C:775:LEU:O	3:C:776:LEU:C	2.64	0.41
3:C:814:GLY:O	3:C:815:PRO:C	2.60	0.41
3:C:926:LYS:N	3:C:927:PRO:CD	2.83	0.41
3:C:967:LEU:HD22	3:C:967:LEU:HA	1.79	0.41
3:C:978:SER:O	3:C:979:SER:C	2.64	0.41
3:C:1184:LEU:HA	3:C:1190:GLU:HG3	2.03	0.41
1:A:97:LYS:HB2	1:A:97:LYS:NZ	2.36	0.41
1:A:164:LEU:HD23	1:A:164:LEU:HA	1.85	0.41
1:A:344:HIS:CD2	1:A:348:LEU:HD11	2.55	0.41
1:A:354:CYS:CB	1:A:358:ALA:HB2	2.51	0.41
1:A:715:VAL:HG12	1:A:716:ARG:N	2.32	0.41
2:B:92:GLN:HG2	3:C:19:ASP:HA	2.03	0.41
3:C:281:ARG:HH21	3:C:284:LYS:CB	2.33	0.41
3:C:433:PRO:O	3:C:437:LYS:HG3	2.20	0.41
3:C:469:LEU:HD13	3:C:476:LEU:CD1	2.50	0.41
3:C:480:ILE:HG22	3:C:481:ILE:N	2.34	0.41
3:C:706:MET:O	3:C:709:SER:HB2	2.20	0.41
3:C:781:GLY:O	3:C:782:PRO:C	2.64	0.41
3:C:936:LEU:CD1	3:C:954:CYS:HB3	2.50	0.41
3:C:1017:ASP:N	3:C:1018:PRO:HD2	2.34	0.41
3:C:1152:THR:C	3:C:1154:THR:N	2.77	0.41
1:A:337:LYS:HE2	1:A:337:LYS:HB3	1.89	0.41
1:A:474:VAL:HG12	1:A:475:HIS:H	1.77	0.41
2:B:28:ASN:N	2:B:28:ASN:HD22	2.17	0.41
2:B:49:ILE:CD1	2:B:50:MET:N	2.82	0.41
3:C:743:ARG:CZ	3:C:782:PRO:HG2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:828:SER:C	3:C:829:ARG:HD3	2.45	0.41
3:C:889:PRO:HB3	3:C:928:TYR:OH	2.21	0.41
1:A:29:GLN:HE21	1:A:29:GLN:HB2	1.61	0.41
1:A:657:VAL:HA	1:A:660:VAL:HG23	2.03	0.41
1:A:694:GLU:O	1:A:698:THR:CG2	2.68	0.41
2:B:77:HIS:CD2	2:B:96:LEU:HD23	2.56	0.41
3:C:65:GLN:O	3:C:69:VAL:HG23	2.20	0.41
3:C:293:ILE:O	3:C:294:ILE:C	2.64	0.41
3:C:650:GLU:O	3:C:653:PRO:HG2	2.20	0.41
3:C:1090:TYR:O	3:C:1093:LEU:HB2	2.21	0.41
1:A:445:LEU:O	1:A:448:VAL:HB	2.21	0.41
1:A:580:TRP:CD1	1:A:580:TRP:N	2.88	0.41
1:A:589:LEU:HD23	1:A:610:LEU:HD12	2.03	0.41
1:A:714:ILE:HD13	1:A:733:VAL:CG2	2.51	0.41
1:A:749:LYS:C	1:A:751:CYS:H	2.29	0.41
2:B:73:GLY:C	2:B:75:CYS:H	2.28	0.41
3:C:166:GLY:C	3:C:168:LEU:N	2.78	0.41
3:C:267:LEU:HD23	3:C:270:TYR:CE1	2.56	0.41
3:C:268:ARG:HG3	3:C:269:GLU:N	2.35	0.41
3:C:386:ARG:NH1	3:C:386:ARG:CG	2.82	0.41
3:C:686:THR:C	3:C:688:ALA:H	2.29	0.41
3:C:710:GLN:CB	3:C:751:ALA:HA	2.47	0.41
3:C:1020:LEU:HB2	3:C:1021:ASN:H	1.66	0.41
3:C:1141:ARG:HH11	3:C:1144:ARG:NH2	2.18	0.41
3:C:1143:ASP:OD2	3:C:1193:PRO:HB3	2.21	0.41
3:C:1183:LEU:O	3:C:1186:ILE:HG22	2.19	0.41
1:A:94:GLU:O	1:A:95:PHE:C	2.64	0.41
1:A:137:CYS:HB3	1:A:159:ILE:HG12	2.02	0.41
1:A:226:VAL:HG23	1:A:227:TYR:N	2.35	0.41
1:A:321:MET:HE2	1:A:321:MET:HB2	1.97	0.41
1:A:618:ALA:HA	1:A:669:LYS:HA	2.02	0.41
3:C:180:LEU:C	3:C:182:PRO:HD2	2.46	0.41
3:C:602:ASP:OD1	3:C:603:ASN:N	2.53	0.41
3:C:644:LEU:O	3:C:647:VAL:HG23	2.21	0.41
3:C:658:PHE:C	3:C:660:ARG:N	2.78	0.41
3:C:667:LYS:HE3	3:C:700:LEU:CD2	2.51	0.41
3:C:682:SER:O	3:C:683:ASP:C	2.64	0.41
3:C:723:TYR:N	3:C:724:PRO:HD3	2.26	0.41
3:C:749:GLY:O	3:C:750:GLY:C	2.63	0.41
3:C:807:THR:C	3:C:809:ALA:N	2.78	0.41
3:C:1066:VAL:HB	3:C:1073:HIS:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1179:ALA:C	3:C:1181:ALA:N	2.79	0.41
1:A:648:LEU:HD23	1:A:648:LEU:HA	1.91	0.40
1:A:701:ASN:C	1:A:701:ASN:HD22	2.29	0.40
1:A:711:GLN:HE22	1:A:758:LYS:HZ3	1.65	0.40
3:C:347:TRP:C	3:C:349:VAL:H	2.29	0.40
3:C:481:ILE:O	3:C:482:PHE:C	2.61	0.40
3:C:858:LYS:HE2	3:C:891:TYR:HD2	1.82	0.40
3:C:892:LEU:HD23	3:C:892:LEU:O	2.21	0.40
1:A:27:GLY:O	1:A:28:ILE:C	2.64	0.40
3:C:212:GLU:O	3:C:213:HIS:C	2.64	0.40
3:C:220:LYS:O	3:C:222:ASP:N	2.55	0.40
3:C:294:ILE:O	3:C:298:LEU:N	2.54	0.40
3:C:639:PRO:O	3:C:641:LYS:N	2.54	0.40
3:C:724:PRO:O	3:C:725:SER:C	2.65	0.40
3:C:813:GLU:OE2	3:C:813:GLU:HA	2.16	0.40
3:C:1152:THR:O	3:C:1154:THR:N	2.55	0.40
1:A:241:ARG:O	1:A:242:PHE:C	2.63	0.40
1:A:299:LEU:HA	1:A:302:PHE:HB2	2.03	0.40
1:A:308:ASN:C	1:A:310:LEU:N	2.79	0.40
1:A:359:LEU:HD22	1:A:410:MET:SD	2.60	0.40
1:A:475:HIS:CE1	1:A:584:LEU:O	2.73	0.40
3:C:88:VAL:HG11	3:C:134:ILE:HG12	2.04	0.40
3:C:202:LEU:HD12	3:C:202:LEU:O	2.21	0.40
3:C:452:GLN:NE2	3:C:492:ASN:HB3	2.36	0.40
3:C:483:SER:C	3:C:485:ASN:H	2.28	0.40
3:C:652:VAL:N	3:C:653:PRO:CD	2.83	0.40
3:C:960:LEU:O	3:C:963:PRO:HD3	2.21	0.40
1:A:552:PHE:CD1	1:A:630:ILE:HG13	2.57	0.40
1:A:558:LEU:HD13	2:B:27:TRP:CE2	2.57	0.40
1:A:560:ARG:HG2	1:A:560:ARG:NH1	2.37	0.40
1:A:620:THR:HG22	1:A:667:LEU:CD2	2.52	0.40
3:C:74:PRO:O	3:C:78:LYS:HG2	2.21	0.40
3:C:252:ILE:O	3:C:253:ILE:C	2.64	0.40
3:C:456:ASN:HD22	3:C:456:ASN:HA	1.63	0.40
3:C:1177:MET:O	3:C:1179:ALA:N	2.54	0.40
1:A:753:ASP:O	1:A:756:ILE:N	2.48	0.40
3:C:66:ASN:HD22	3:C:66:ASN:HA	1.67	0.40
3:C:287:TYR:O	3:C:290:VAL:HB	2.22	0.40
3:C:492:ASN:O	3:C:493:LEU:C	2.64	0.40
3:C:682:SER:O	3:C:685:LEU:HG	2.22	0.40
3:C:696:GLU:OE1	3:C:696:GLU:HA	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:862:LEU:HD23	3:C:862:LEU:HA	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	705/776 (91%)	584 (83%)	91 (13%)	30 (4%)	2	12
2	B	86/108 (80%)	68 (79%)	13 (15%)	5 (6%)	1	8
3	C	1134/1230 (92%)	793 (70%)	236 (21%)	105 (9%)	0	3
All	All	1925/2114 (91%)	1445 (75%)	340 (18%)	140 (7%)	1	5

All (140) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	TRP
1	A	145	VAL
1	A	646	LYS
1	A	652	ASP
1	A	674	TYR
2	B	98	ASN
3	C	34	LEU
3	C	36	LYS
3	C	87	ILE
3	C	128	ALA
3	C	144	LYS
3	C	224	MET
3	C	226	THR
3	C	252	ILE
3	C	347	TRP
3	C	375	VAL

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Mol	Chain	Res	Type
3	C	443	MET
3	C	487	LYS
3	C	552	PRO
3	C	601	GLY
3	C	619	LEU
3	C	641	LYS
3	C	659	LEU
3	C	723	TYR
3	C	724	PRO
3	C	725	SER
3	C	828	SER
3	C	901	SER
3	C	943	ALA
3	C	976	SER
3	C	977	GLY
3	C	1013	LYS
3	C	1037	LYS
3	C	1187	PRO
3	C	1188	GLU
3	C	1195	MET
1	A	285	GLU
1	A	313	ASP
1	A	475	HIS
1	A	477	ASN
1	A	527	SER
1	A	550	CYS
1	A	557	GLU
2	B	20	LYS
2	B	67	GLU
3	C	76	VAL
3	C	88	VAL
3	C	127	ALA
3	C	146	GLU
3	C	149	SER
3	C	221	ASN
3	C	228	ARG
3	C	262	VAL
3	C	285	GLU
3	C	286	VAL
3	C	345	MET
3	C	346	SER
3	C	360	VAL

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Mol	Chain	Res	Type
3	C	386	ARG
3	C	388	GLU
3	C	430	SER
3	C	489	SER
3	C	570	THR
3	C	571	CYS
3	C	605	GLY
3	C	664	ARG
3	C	732	GLY
3	C	734	ILE
3	C	750	GLY
3	C	766	GLY
3	C	772	TYR
3	C	822	ILE
3	C	826	LYS
3	C	918	SER
3	C	975	ILE
3	C	1012	LEU
3	C	1018	PRO
3	C	1096	CYS
3	C	1197	GLU
1	A	174	PRO
1	A	175	LEU
1	A	559	GLU
1	A	767	GLU
3	C	7	HIS
3	C	167	GLY
3	C	283	PRO
3	C	366	GLU
3	C	407	PRO
3	C	466	PRO
3	C	566	LYS
3	C	649	GLY
3	C	684	SER
3	C	785	SER
3	C	811	PRO
3	C	853	GLY
3	C	1153	CYS
3	C	1181	ALA
3	C	1182	ALA
3	C	1204	SER
1	A	21	TRP

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Mol	Chain	Res	Type
1	A	176	ASN
1	A	474	VAL
1	A	549	SER
1	A	625	THR
1	A	650	LEU
1	A	662	LEU
2	B	49	ILE
3	C	18	SER
3	C	151	GLN
3	C	152	LEU
3	C	579	ALA
3	C	687	ALA
3	C	731	SER
3	C	960	LEU
3	C	1132	THR
1	A	523	HIS
1	A	695	GLN
3	C	385	GLU
3	C	637	GLY
3	C	677	LEU
3	C	1134	CYS
3	C	1194	LEU
1	A	222	PRO
1	A	613	TYR
3	C	646	PRO
3	C	694	LEU
3	C	782	PRO
3	C	1039	SER
3	C	1193	PRO
2	B	38	VAL
1	A	496	GLY
3	C	73	GLY
3	C	701	ILE
3	C	1017	ASP
1	A	179	VAL
1	A	715	VAL
3	C	551	ARG
3	C	749	GLY
3	C	916	ILE
3	C	927	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	650/698 (93%)	561 (86%)	89 (14%)	3	15
2	B	78/90 (87%)	62 (80%)	16 (20%)	1	5
3	C	1022/1098 (93%)	874 (86%)	148 (14%)	3	14
All	All	1750/1886 (93%)	1497 (86%)	253 (14%)	3	14

All (253) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ILE
1	A	21	TRP
1	A	24	LEU
1	A	25	ARG
1	A	29	GLN
1	A	37	MET
1	A	94	GLU
1	A	97	LYS
1	A	104	LEU
1	A	113	GLU
1	A	115	VAL
1	A	116	LEU
1	A	117	LYS
1	A	140	LEU
1	A	142	ARG
1	A	145	VAL
1	A	158	GLU
1	A	159	ILE
1	A	162	LEU
1	A	165	VAL
1	A	171	LEU
1	A	194	GLU
1	A	211	LEU
1	A	222	PRO
1	A	260	MET
1	A	268	LEU

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Mol	Chain	Res	Type
1	A	271	GLN
1	A	272	ARG
1	A	286	LEU
1	A	296	GLU
1	A	304	THR
1	A	307	GLN
1	A	309	LEU
1	A	315	ASN
1	A	317	ASP
1	A	329	GLN
1	A	334	GLU
1	A	335	LEU
1	A	338	LEU
1	A	343	ILE
1	A	402	ILE
1	A	405	ASN
1	A	421	LEU
1	A	429	LEU
1	A	431	LYS
1	A	438	GLU
1	A	443	ASP
1	A	445	LEU
1	A	449	MET
1	A	469	LEU
1	A	471	LYS
1	A	477	ASN
1	A	500	THR
1	A	510	ILE
1	A	512	VAL
1	A	516	LEU
1	A	517	ASN
1	A	521	LYS
1	A	522	LYS
1	A	526	ASN
1	A	528	GLU
1	A	531	ASP
1	A	557	GLU
1	A	560	ARG
1	A	577	LYS
1	A	579	THR
1	A	583	GLN
1	A	586	LYS

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Mol	Chain	Res	Type
1	A	595	LYS
1	A	597	ARG
1	A	598	TYR
1	A	600	LEU
1	A	601	GLN
1	A	621	VAL
1	A	624	LEU
1	A	629	GLN
1	A	632	MET
1	A	642	LEU
1	A	665	ASP
1	A	671	TYR
1	A	672	LEU
1	A	674	TYR
1	A	682	ASN
1	A	698	THR
1	A	720	MET
1	A	737	LEU
1	A	745	VAL
1	A	751	CYS
1	A	774	LEU
2	B	19	LYS
2	B	21	ARG
2	B	30	VAL
2	B	49	ILE
2	B	52	LEU
2	B	65	SER
2	B	66	GLU
2	B	69	THR
2	B	76	ASN
2	B	84	ILE
2	B	85	SER
2	B	91	ARG
2	B	93	VAL
2	B	97	ASP
2	B	98	ASN
2	B	99	ARG
3	C	7	HIS
3	C	36	LYS
3	C	57	LEU
3	C	66	ASN
3	C	69	VAL

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Mol	Chain	Res	Type
3	C	71	CYS
3	C	75	LEU
3	C	79	VAL
3	C	86	THR
3	C	96	LEU
3	C	116	GLU
3	C	118	PRO
3	C	133	LYS
3	C	144	LYS
3	C	146	GLU
3	C	162	LEU
3	C	168	LEU
3	C	171	ASN
3	C	189	LEU
3	C	192	ARG
3	C	194	ARG
3	C	204	MET
3	C	214	LEU
3	C	217	GLU
3	C	229	THR
3	C	243	HIS
3	C	249	LEU
3	C	259	PHE
3	C	264	ASP
3	C	270	TYR
3	C	276	GLU
3	C	279	VAL
3	C	286	VAL
3	C	298	LEU
3	C	344	ASP
3	C	345	MET
3	C	351	ARG
3	C	363	THR
3	C	364	ARG
3	C	366	GLU
3	C	377	PRO
3	C	380	ILE
3	C	382	ARG
3	C	383	PHE
3	C	384	LYS
3	C	385	GLU
3	C	386	ARG

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Mol	Chain	Res	Type
3	C	387	GLU
3	C	422	GLU
3	C	423	THR
3	C	424	PRO
3	C	432	VAL
3	C	441	LYS
3	C	456	ASN
3	C	461	LEU
3	C	472	HIS
3	C	491	SER
3	C	501	LEU
3	C	518	GLN
3	C	522	PRO
3	C	540	LEU
3	C	541	LEU
3	C	555	GLN
3	C	566	LYS
3	C	573	ILE
3	C	581	ILE
3	C	600	LEU
3	C	603	ASN
3	C	616	LEU
3	C	625	ARG
3	C	638	SER
3	C	639	PRO
3	C	676	ILE
3	C	683	ASP
3	C	698	PRO
3	C	711	MET
3	C	724	PRO
3	C	739	ILE
3	C	741	LEU
3	C	748	GLN
3	C	763	VAL
3	C	770	LEU
3	C	773	MET
3	C	774	ASP
3	C	786	GLN
3	C	813	GLU
3	C	820	GLN
3	C	826	LYS
3	C	829	ARG

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Mol	Chain	Res	Type
3	C	835	ARG
3	C	836	LEU
3	C	854	GLN
3	C	856	GLU
3	C	857	LEU
3	C	870	GLU
3	C	874	SER
3	C	890	GLU
3	C	892	LEU
3	C	900	THR
3	C	902	GLN
3	C	905	ARG
3	C	914	LYS
3	C	921	SER
3	C	922	VAL
3	C	923	VAL
3	C	929	VAL
3	C	931	ASN
3	C	950	VAL
3	C	967	LEU
3	C	974	LEU
3	C	986	VAL
3	C	992	THR
3	C	996	HIS
3	C	1000	ILE
3	C	1004	LEU
3	C	1005	LYS
3	C	1006	ASN
3	C	1015	LEU
3	C	1025	VAL
3	C	1027	LEU
3	C	1036	ASN
3	C	1040	LEU
3	C	1055	GLU
3	C	1056	THR
3	C	1064	ARG
3	C	1079	LEU
3	C	1081	ILE
3	C	1093	LEU
3	C	1101	ASP
3	C	1102	ILE
3	C	1104	GLU

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Mol	Chain	Res	Type
3	C	1111	ASP
3	C	1117	TYR
3	C	1119	ILE
3	C	1122	LEU
3	C	1123	THR
3	C	1131	SER
3	C	1157	VAL
3	C	1162	VAL
3	C	1164	GLN
3	C	1167	GLU
3	C	1168	LYS
3	C	1169	GLN
3	C	1187	PRO
3	C	1190	GLU
3	C	1194	LEU
3	C	1195	MET
3	C	1196	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	35	GLN
1	A	51	ASN
1	A	121	GLN
1	A	122	GLN
1	A	134	ASN
1	A	141	ASN
1	A	143	HIS
1	A	252	GLN
1	A	253	GLN
1	A	271	GLN
1	A	283	GLN
1	A	292	GLN
1	A	303	HIS
1	A	323	ASN
1	A	344	HIS
1	A	367	GLN
1	A	377	ASN
1	A	385	ASN
1	A	405	ASN
1	A	462	GLN

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Mol	Chain	Res	Type
1	A	476	GLN
1	A	477	ASN
1	A	504	GLN
1	A	517	ASN
1	A	526	ASN
1	A	548	GLN
1	A	573	HIS
1	A	583	GLN
1	A	592	ASN
1	A	596	ASN
1	A	614	ASN
1	A	622	GLN
1	A	623	GLN
1	A	656	ASN
1	A	676	ASN
1	A	682	ASN
1	A	701	ASN
1	A	711	GLN
1	A	727	GLN
1	A	728	GLN
1	A	736	GLN
2	B	28	ASN
2	B	76	ASN
2	B	104	GLN
3	C	28	ASN
3	C	66	ASN
3	C	83	GLN
3	C	101	GLN
3	C	151	GLN
3	C	173	HIS
3	C	221	ASN
3	C	365	HIS
3	C	442	GLN
3	C	452	GLN
3	C	456	ASN
3	C	463	ASN
3	C	472	HIS
3	C	508	HIS
3	C	511	GLN
3	C	514	HIS
3	C	544	GLN
3	C	555	GLN

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Mol	Chain	Res	Type
3	C	583	GLN
3	C	595	GLN
3	C	599	ASN
3	C	603	ASN
3	C	610	ASN
3	C	663	GLN
3	C	680	ASN
3	C	710	GLN
3	C	736	ASN
3	C	786	GLN
3	C	847	HIS
3	C	897	GLN
3	C	902	GLN
3	C	906	GLN
3	C	949	ASN
3	C	1036	ASN
3	C	1108	HIS
3	C	1164	GLN
3	C	1205	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	C	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	601:GLY	C	602:ASP	N	1.19
1	A	437:GLU	C	438:GLU	N	1.13

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	715/776 (92%)	-0.04	30 (4%) 40 22	13, 46, 129, 197	0
2	B	88/108 (81%)	-0.25	0 100 100	3, 38, 76, 151	0
3	C	1146/1230 (93%)	0.07	39 (3%) 48 28	14, 61, 122, 190	0
All	All	1949/2114 (92%)	0.01	69 (3%) 47 27	3, 55, 124, 197	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	478	SER	5.7
1	A	176	ASN	5.2
3	C	278	PHE	5.1
1	A	477	ASN	5.0
3	C	490	SER	4.9
3	C	374	THR	4.7
1	A	476	GLN	4.6
3	C	379	LEU	4.3
3	C	408	VAL	4.2
1	A	550	CYS	4.0
1	A	177	LYS	3.9
3	C	1194	LEU	3.9
3	C	1195	MET	3.7
3	C	600	LEU	3.6
1	A	479	ALA	3.5
3	C	818	VAL	3.4
1	A	170	CYS	3.2
1	A	143	HIS	3.2
3	C	377	PRO	3.2
1	A	55	SER	3.2
1	A	213	LEU	3.2
1	A	149	CYS	3.1
1	A	17	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
3	C	855	LEU	3.0
3	C	941	GLU	3.0
3	C	791	THR	3.0
3	C	1210	ALA	2.9
1	A	438	GLU	2.9
3	C	489	SER	2.9
3	C	975	ILE	2.9
3	C	375	VAL	2.9
1	A	173	ARG	2.8
1	A	84	VAL	2.8
3	C	167	GLY	2.8
1	A	144	TRP	2.8
3	C	1013	LYS	2.8
3	C	296	ILE	2.8
1	A	633	ASP	2.7
3	C	126	LEU	2.7
3	C	1102	ILE	2.7
1	A	147	ARG	2.6
3	C	943	ALA	2.6
3	C	226	THR	2.5
3	C	276	GLU	2.5
1	A	775	ALA	2.5
3	C	797	TYR	2.4
1	A	175	LEU	2.4
3	C	4	ALA	2.4
3	C	1187	PRO	2.4
3	C	222	ASP	2.4
3	C	815	PRO	2.3
1	A	617	ASP	2.3
3	C	20	LYS	2.3
1	A	673	GLY	2.3
3	C	1196	SER	2.3
1	A	632	MET	2.3
3	C	104	ASP	2.3
3	C	1099	ARG	2.3
1	A	174	PRO	2.3
3	C	300	TYR	2.3
3	C	295	ASN	2.3
1	A	316	GLU	2.2
3	C	466	PRO	2.2
3	C	287	TYR	2.1
1	A	526	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	128	ALA	2.1
1	A	34	ARG	2.1
1	A	650	LEU	2.0
1	A	146	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ZN	B	1230	1/1	0.97	0.05	56,56,56,56	0
4	ZN	B	1229	1/1	0.99	0.03	42,42,42,42	0
4	ZN	B	1231	1/1	1.00	0.02	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.