



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:09 AM UTC

PDB ID : 2HYE / pdb_00002hye
Title : Crystal Structure of the DDB1-Cul4A-Rbx1-SV5V Complex
Authors : Angers, S.; Li, T.; Yi, X.; MacCoss, M.J.; Moon, R.T.; Zheng, N.
Deposited on : 2006-08-05
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

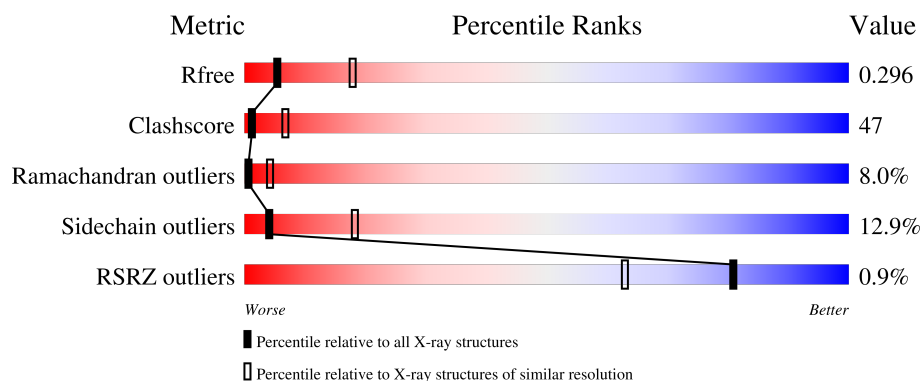
1 Overall quality at a glance

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	1140	32% 51% 15% .
2	B	222	3% 18% 45% 14% . 19%
3	C	759	29% 47% 17% . 5%
4	D	108	3% 30% 26% 20% 7% 17%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16943 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 DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1140	Total	C	N	O	S	0	0	0
			8920	5645	1503	1723	49			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	422	TYR	ASP	conflict	UNP Q16531
A	898	ASP	GLU	conflict	UNP Q16531
A	899	VAL	LEU	conflict	UNP Q16531

- Molecule 2 is a protein called Nonstructural protein V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	180	Total	C	N	O	S	0	0	0
			1373	856	237	272	8			

- Molecule 3 is a protein called Cullin-4A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	719	Total	C	N	O	S	0	0	0
			5899	3753	1023	1089	34			

- Molecule 4 is a protein called RING-box protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	90	Total	C	N	O	S	0	0	0
			746	472	137	128	9			

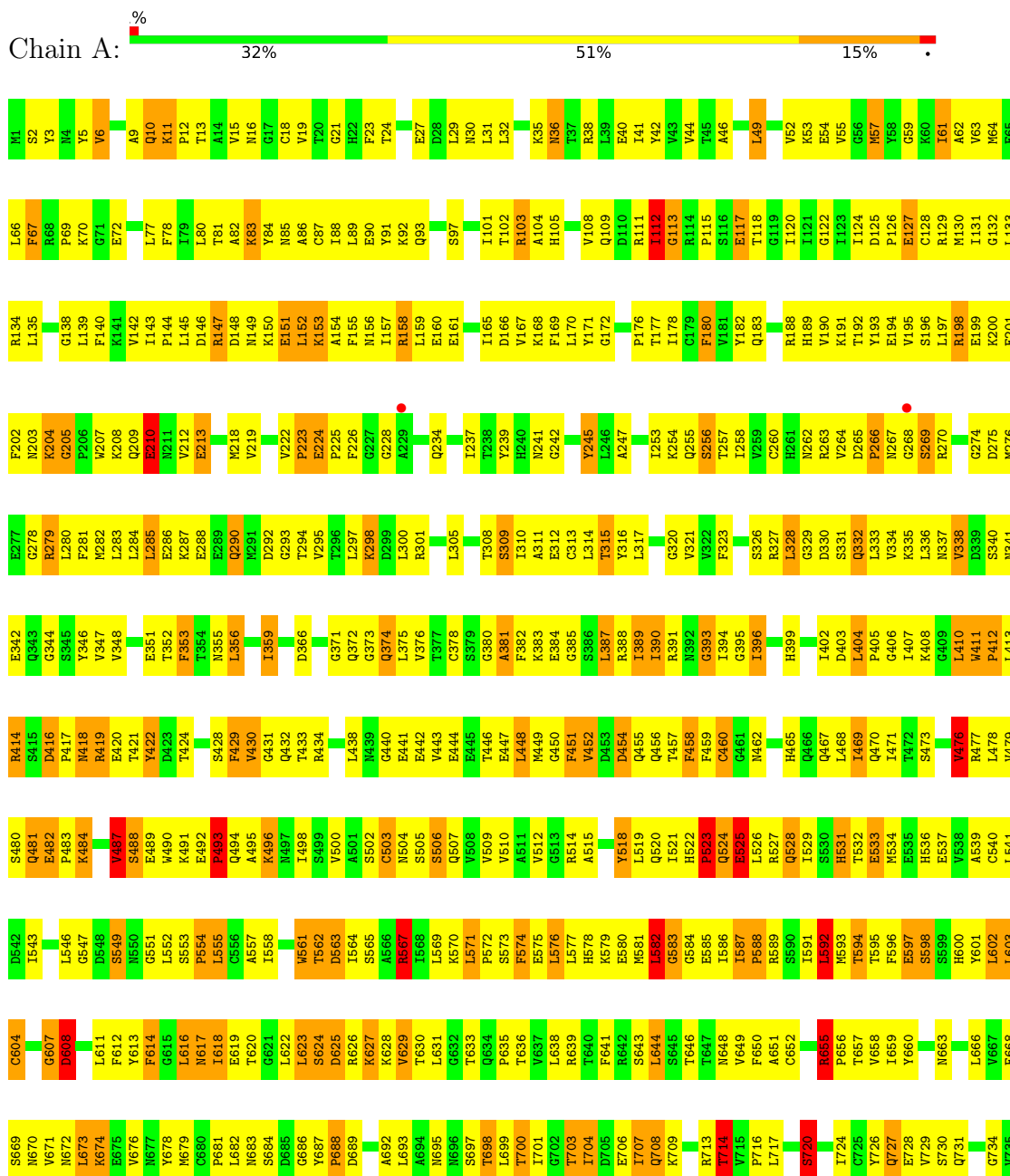
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

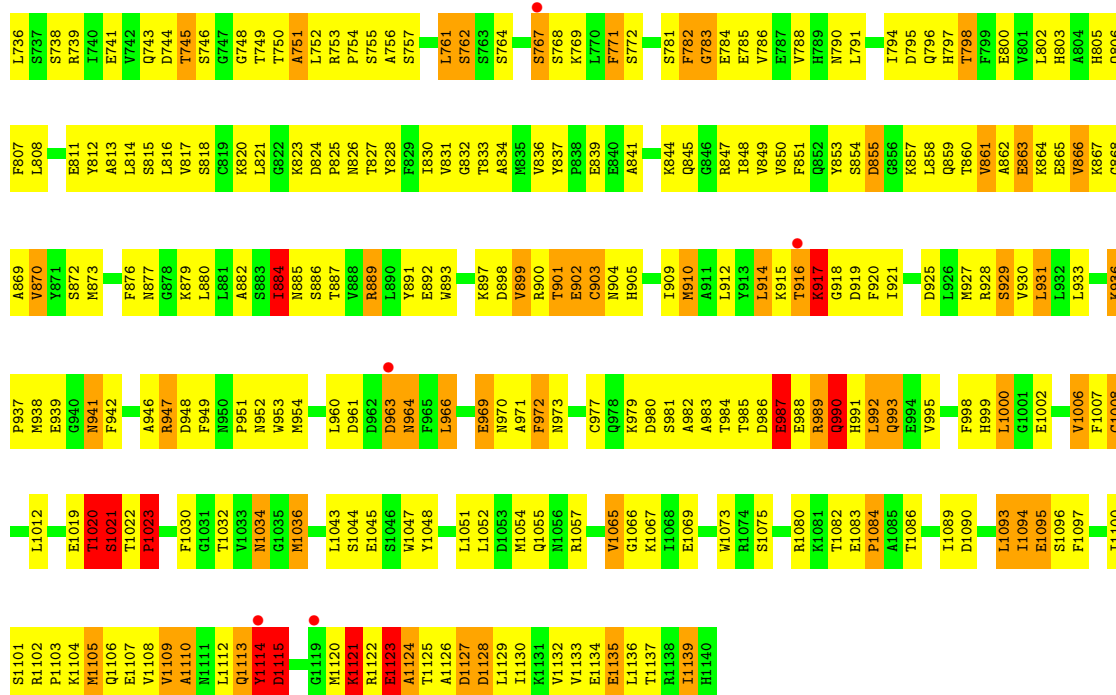
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total 2	Zn 2	0	0
5	D	3	Total 3	Zn 3	0	0

3 Residue-property plots

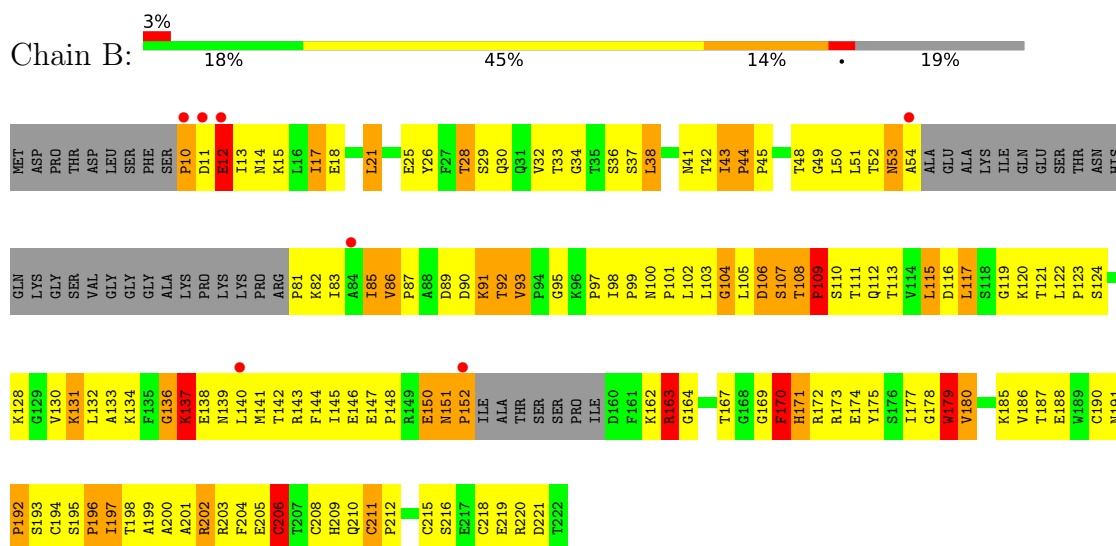
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: DNA damage-binding protein 1

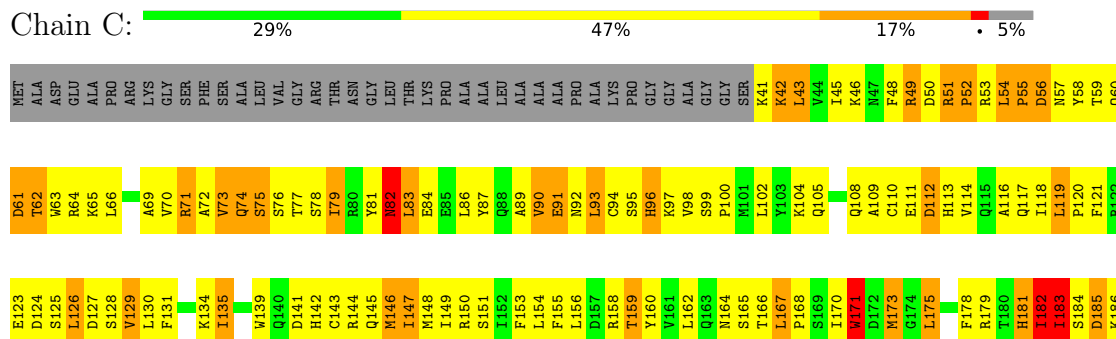


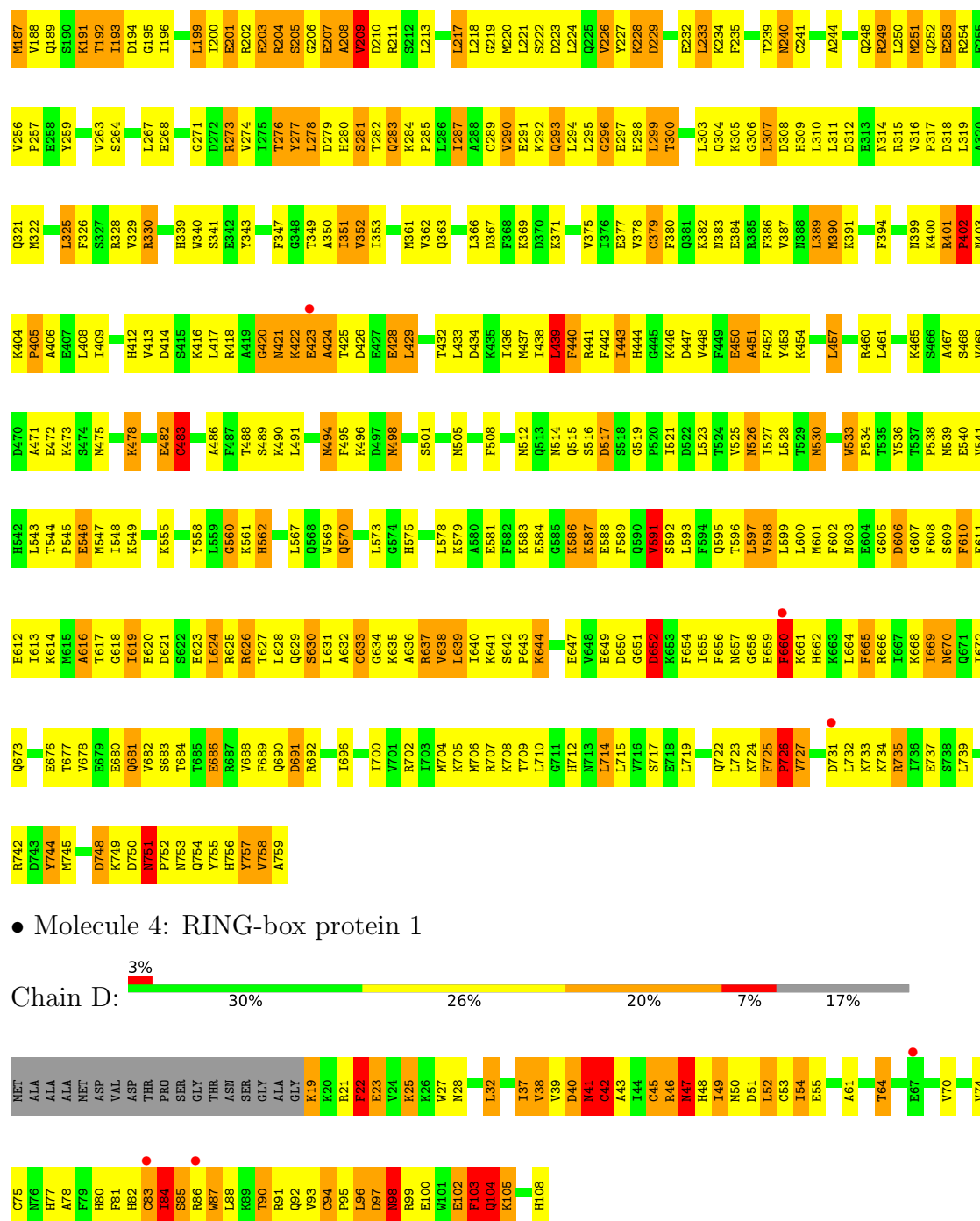


• Molecule 2: Nonstructural protein V



• Molecule 3: Cullin-4A





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	83.45Å 203.16Å 424.88Å 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) 90.5 (50.00-3.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 3.07Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.250 , 0.316 0.244 , 0.296	Depositor DCC
R_{free} test set	3109 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	80.8	Xtriage
Anisotropy	0.441	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 52.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16943	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.64	9/9086 (0.1%)	1.34	128/12311 (1.0%)
2	B	0.74	3/1401 (0.2%)	1.48	24/1899 (1.3%)
3	C	0.62	10/6007 (0.2%)	1.29	84/8068 (1.0%)
4	D	0.87	2/768 (0.3%)	1.55	18/1040 (1.7%)
All	All	0.65	24/17262 (0.1%)	1.35	254/23318 (1.1%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	179	TRP	C-N	-11.28	1.22	1.33
4	D	47	ASN	N-CA	-9.27	1.40	1.46
1	A	582	LEU	C-N	8.05	1.45	1.33
3	C	83	LEU	C-N	-6.69	1.25	1.33
1	A	767	SER	C-O	-6.24	1.17	1.24
3	C	298	HIS	CA-C	-6.09	1.44	1.52
1	A	381	ALA	N-CA	6.04	1.52	1.46
1	A	916	THR	C-N	-6.00	1.25	1.33
3	C	420	GLY	C-N	5.70	1.41	1.34
1	A	1114	TYR	N-CA	5.69	1.53	1.46
2	B	109	PRO	CA-C	-5.68	1.47	1.52
3	C	126	LEU	N-CA	5.59	1.53	1.46
2	B	107	SER	N-CA	-5.55	1.39	1.45
3	C	183	ILE	N-CA	-5.54	1.40	1.46
4	D	46	ARG	C-N	-5.51	1.27	1.34
1	A	709	LYS	N-CA	-5.45	1.38	1.45
1	A	916	THR	N-CA	5.45	1.52	1.46
3	C	181	HIS	CB-CG	5.28	1.57	1.50
3	C	616	ALA	C-N	-5.25	1.26	1.33
1	A	708	GLN	C-N	-5.18	1.26	1.33
1	A	1114	TYR	CA-C	5.18	1.59	1.52
3	C	421	ASN	N-CA	5.12	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	420	GLY	CA-C	5.10	1.59	1.51
3	C	126	LEU	C-N	-5.04	1.26	1.33

All (254) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	561	TRP	N-CA-C	33.35	153.04	113.02
1	A	151	GLU	N-CA-C	-30.65	66.15	110.59
3	C	182	ILE	N-CA-C	25.13	136.10	110.72
1	A	916	THR	N-CA-C	19.12	137.54	112.88
3	C	73	VAL	N-CA-C	-18.50	96.91	111.90
1	A	767	SER	N-CA-C	-18.24	78.68	108.41
2	B	10	PRO	CA-N-CD	-17.89	86.95	112.00
2	B	107	SER	N-CA-C	-17.41	83.43	110.42
1	A	561	TRP	CB-CA-C	-17.38	79.43	110.37
2	B	179	TRP	CB-CA-C	-16.44	85.59	111.74
2	B	109	PRO	CA-N-CD	-15.82	89.85	112.00
4	D	42	CYS	N-CA-C	-14.56	91.31	110.24
3	C	420	GLY	CA-C-N	14.07	140.54	120.28
3	C	420	GLY	C-N-CA	14.07	140.54	120.28
1	A	1115	ASP	N-CA-C	13.47	139.48	110.80
1	A	916	THR	CB-CA-C	-13.28	88.27	110.72
4	D	22	PHE	CB-CA-C	-12.96	84.63	110.42
1	A	767	SER	CB-CA-C	-12.81	88.89	110.16
3	C	616	ALA	N-CA-C	12.56	128.38	113.18
1	A	1114	TYR	CA-C-N	12.16	144.76	121.54
1	A	1114	TYR	C-N-CA	12.16	144.76	121.54
3	C	126	LEU	CB-CA-C	-11.48	87.58	110.42
4	D	98	ASN	N-CA-C	-11.32	100.18	114.56
3	C	296	GLY	N-CA-C	-11.07	99.19	111.93
1	A	781	SER	N-CA-C	11.00	126.53	112.89
1	A	1023	PRO	CA-N-CD	-10.92	96.71	112.00
3	C	298	HIS	CB-CA-C	-10.77	88.98	110.42
3	C	206	GLY	N-CA-C	10.47	130.38	115.30
3	C	252	GLN	OE1-CD-NE2	-10.33	112.27	122.60
2	B	152	PRO	CA-N-CD	-10.22	97.69	112.00
1	A	1114	TYR	N-CA-C	10.16	132.44	110.80
3	C	126	LEU	N-CA-C	9.84	131.75	110.80
3	C	130	LEU	N-CA-C	-9.78	99.47	111.40
4	D	103	PHE	N-CA-C	9.78	131.62	110.80
1	A	708	GLN	OE1-CD-NE2	-9.75	112.85	122.60
4	D	104	GLN	OE1-CD-NE2	-9.72	112.88	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	GLN	OE1-CD-NE2	-9.72	112.88	122.60
4	D	47	ASN	N-CA-C	-9.67	94.12	108.34
1	A	266	PRO	CA-N-CD	-9.62	98.53	112.00
1	A	524	GLN	OE1-CD-NE2	-9.58	113.02	122.60
3	C	187	MET	N-CA-C	-9.48	100.83	111.82
1	A	624	SER	N-CA-C	8.94	129.84	110.80
3	C	182	ILE	N-CA-CB	-8.93	97.19	110.58
1	A	117	GLU	N-CA-C	-8.92	97.66	110.59
3	C	167	LEU	CA-C-N	8.91	129.61	119.99
3	C	167	LEU	C-N-CA	8.91	129.61	119.99
3	C	637	ARG	N-CA-C	8.84	125.78	114.56
1	A	411	TRP	CA-C-N	8.70	130.71	119.84
1	A	411	TRP	C-N-CA	8.70	130.71	119.84
3	C	146	MET	N-CA-C	-8.65	102.47	113.72
1	A	1115	ASP	CA-CB-CG	-8.57	104.03	112.60
1	A	1113	GLN	OE1-CD-NE2	-8.54	114.06	122.60
3	C	74	GLN	N-CA-C	-8.47	96.64	109.60
1	A	381	ALA	N-CA-C	8.44	123.92	111.34
4	D	104	GLN	N-CA-C	8.38	128.64	110.80
3	C	690	GLN	N-CA-C	-8.36	97.92	109.71
2	B	109	PRO	N-CA-CB	8.25	108.20	102.35
3	C	665	PHE	N-CA-C	-8.20	96.52	109.23
1	A	688	PRO	N-CA-C	8.13	129.22	112.47
1	A	689	ASP	N-CA-C	-8.08	93.58	110.80
3	C	83	LEU	N-CA-C	8.03	127.91	110.80
1	A	720	SER	N-CA-C	7.99	119.78	109.64
3	C	253	GLU	N-CA-C	7.98	123.32	113.50
3	C	362	VAL	N-CA-C	7.96	117.90	110.42
1	A	1020	THR	N-CA-C	7.82	127.46	110.80
4	D	103	PHE	CB-CA-C	-7.78	94.94	110.42
3	C	560	GLY	N-CA-C	-7.71	101.58	112.37
1	A	1022	THR	CA-C-N	7.62	127.66	119.28
1	A	1022	THR	C-N-CA	7.62	127.66	119.28
3	C	689	PHE	N-CA-C	-7.59	102.35	111.69
2	B	179	TRP	N-CA-C	7.59	124.24	108.53
1	A	1020	THR	CB-CA-C	-7.54	95.42	110.42
1	A	338	VAL	N-CA-C	-7.35	102.58	113.39
1	A	451	PHE	N-CA-C	7.30	119.95	110.53
2	B	12	GLU	N-CA-C	7.26	126.26	110.80
3	C	203	GLU	N-CA-C	-7.26	104.68	113.97
1	A	222	VAL	CA-C-N	7.24	127.16	120.21
1	A	222	VAL	C-N-CA	7.24	127.16	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	638	VAL	N-CA-CB	-7.21	105.73	111.64
4	D	85	SER	N-CA-C	-7.20	103.76	112.54
1	A	709	LYS	N-CA-C	-7.18	98.49	109.41
3	C	443	ILE	N-CA-C	7.16	119.32	109.80
1	A	655	ARG	CA-C-N	7.15	128.78	119.84
1	A	655	ARG	C-N-CA	7.15	128.78	119.84
1	A	562	THR	N-CA-CB	-7.13	98.44	110.49
3	C	84	GLU	N-CA-CB	-7.12	99.65	110.12
3	C	181	HIS	CB-CA-C	7.11	124.56	110.42
3	C	403	ASN	N-CA-C	7.09	123.05	113.97
3	C	379	CYS	N-CA-C	7.08	120.81	111.75
1	A	990	GLN	N-CA-C	-7.02	104.18	112.89
2	B	180	VAL	N-CA-CB	-6.95	103.33	111.39
2	B	150	GLU	CB-CA-C	6.94	124.24	110.42
3	C	465	LYS	N-CA-C	6.88	119.20	110.33
3	C	165	SER	N-CA-C	-6.86	103.83	111.71
3	C	252	GLN	CG-CD-NE2	6.85	126.68	116.40
1	A	524	GLN	CG-CD-NE2	6.85	126.67	116.40
1	A	332	GLN	N-CA-C	6.82	118.51	108.14
3	C	277	TYR	N-CA-C	6.75	121.22	113.19
3	C	725	PHE	CA-C-N	6.74	128.27	119.84
3	C	725	PHE	C-N-CA	6.74	128.27	119.84
1	A	209	GLN	CG-CD-NE2	6.68	126.42	116.40
1	A	698	THR	N-CA-C	6.68	119.48	108.99
4	D	41	ASN	CA-C-N	-6.68	111.01	120.82
4	D	41	ASN	C-N-CA	-6.68	111.01	120.82
1	A	376	VAL	N-CA-C	-6.67	98.83	108.17
1	A	1113	GLN	CG-CD-NE2	6.66	126.39	116.40
1	A	917	LYS	N-CA-C	6.61	124.87	110.80
1	A	791	LEU	N-CA-C	-6.61	98.13	108.90
3	C	192	THR	N-CA-C	-6.59	105.25	113.55
3	C	125	SER	CA-C-N	6.54	134.03	121.54
3	C	125	SER	C-N-CA	6.54	134.03	121.54
3	C	400	LYS	N-CA-C	-6.51	105.30	113.18
1	A	378	CYS	N-CA-C	-6.50	98.59	108.67
1	A	917	LYS	N-CA-CB	-6.46	99.57	110.49
1	A	708	GLN	CG-CD-NE2	6.43	126.04	116.40
1	A	309	SER	N-CA-C	-6.42	100.48	110.17
1	A	15	VAL	N-CA-C	6.38	116.60	106.32
4	D	97	ASP	N-CA-C	-6.36	99.96	109.94
1	A	458	PHE	N-CA-C	-6.36	106.11	114.31
3	C	533	TRP	CA-C-N	6.31	127.73	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	533	TRP	C-N-CA	6.31	127.73	119.84
1	A	768	SER	N-CA-C	-6.30	97.38	110.80
1	A	393	GLY	N-CA-C	6.30	120.33	111.14
1	A	688	PRO	CA-N-CD	-6.26	103.23	112.00
1	A	1096	SER	N-CA-C	-6.24	105.65	113.20
3	C	352	VAL	N-CA-C	6.21	118.14	112.43
1	A	429	PHE	N-CA-C	-6.19	100.39	109.18
1	A	714	THR	N-CA-C	6.16	118.93	108.90
4	D	104	GLN	CG-CD-NE2	6.13	125.60	116.40
1	A	1019	GLU	CA-C-N	6.13	133.24	121.54
1	A	1019	GLU	C-N-CA	6.13	133.24	121.54
1	A	1095	GLU	N-CA-C	-6.11	107.06	114.75
1	A	886	SER	N-CA-C	-6.07	105.70	113.23
1	A	571	LEU	N-CA-C	6.07	123.21	109.81
1	A	709	LYS	CB-CA-C	6.05	122.28	110.30
2	B	179	TRP	N-CA-CB	6.04	120.87	111.64
3	C	351	ILE	N-CA-C	-6.03	106.93	112.96
3	C	84	GLU	N-CA-C	6.03	117.85	111.28
2	B	12	GLU	CB-CA-C	-6.01	98.45	110.42
1	A	749	THR	N-CA-C	6.00	119.31	109.76
3	C	439	LEU	N-CA-C	-5.99	103.52	111.24
1	A	824	ASP	CA-C-N	5.96	125.58	119.56
1	A	824	ASP	C-N-CA	5.96	125.58	119.56
3	C	630	SER	N-CA-C	-5.92	100.68	109.86
1	A	963	ASP	N-CA-C	5.90	120.64	113.38
1	A	223	PRO	N-CA-C	5.90	119.48	111.22
1	A	574	PHE	N-CA-C	-5.89	106.05	113.23
1	A	525	GLU	N-CA-C	5.89	118.23	108.99
4	D	61	ALA	N-CA-C	-5.88	104.98	114.09
3	C	183	ILE	CA-C-O	5.88	124.54	118.96
1	A	205	GLY	CA-C-N	5.87	125.55	119.56
1	A	205	GLY	C-N-CA	5.87	125.55	119.56
1	A	989	ARG	N-CA-C	-5.86	105.90	114.39
1	A	1114	TYR	CB-CA-C	-5.83	98.81	110.42
3	C	170	ILE	N-CA-C	-5.82	104.69	110.62
4	D	47	ASN	N-CA-CB	5.82	117.00	111.59
3	C	401	ARG	CA-C-N	5.81	127.10	119.84
3	C	401	ARG	C-N-CA	5.81	127.10	119.84
1	A	83	LYS	N-CA-C	-5.80	106.01	112.57
1	A	380	GLY	CA-C-N	-5.79	114.60	121.90
1	A	380	GLY	C-N-CA	-5.79	114.60	121.90
1	A	757	SER	N-CA-C	5.79	118.53	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	VAL	N-CA-C	5.78	116.94	107.24
1	A	651	ALA	N-CA-C	5.77	118.55	108.52
1	A	210	GLU	N-CA-C	5.75	123.06	110.80
1	A	624	SER	CB-CA-C	-5.75	98.97	110.42
1	A	9	ALA	N-CA-C	-5.73	106.27	113.72
2	B	44	PRO	CA-C-N	5.71	126.98	119.84
2	B	44	PRO	C-N-CA	5.71	126.98	119.84
3	C	314	ASN	N-CA-C	5.71	119.57	111.92
1	A	555	LEU	N-CA-C	5.70	118.97	110.14
3	C	591	VAL	N-CA-C	5.69	117.54	108.89
3	C	669	ILE	N-CA-C	-5.67	104.72	113.16
2	B	91	LYS	N-CA-C	-5.66	106.72	113.97
1	A	523	PRO	CA-N-CD	-5.66	104.08	112.00
1	A	269	SER	N-CA-C	-5.63	98.80	110.80
3	C	62	THR	N-CA-C	-5.60	106.58	113.41
3	C	109	ALA	N-CA-C	-5.60	105.09	111.14
1	A	295	VAL	N-CA-C	5.58	116.34	108.36
1	A	528	GLN	N-CA-C	5.56	117.97	109.62
1	A	487	VAL	N-CA-C	5.56	117.54	112.43
3	C	751	ASN	CA-C-N	5.56	126.79	119.84
3	C	751	ASN	C-N-CA	5.56	126.79	119.84
1	A	127	GLU	N-CA-C	-5.55	106.58	113.19
1	A	752	LEU	N-CA-C	-5.55	107.14	114.31
1	A	941	ASN	N-CA-C	5.55	115.88	108.38
3	C	617	THR	N-CA-C	-5.55	98.97	110.80
1	A	607	GLY	N-CA-C	-5.51	107.07	115.66
1	A	1128	ASP	N-CA-C	-5.49	105.38	112.68
1	A	506	SER	N-CA-C	5.48	119.97	113.12
1	A	889	ARG	N-CA-C	5.48	119.04	110.32
1	A	582	LEU	O-C-N	5.47	129.87	122.59
1	A	929	SER	CB-CA-C	-5.46	108.68	115.89
1	A	523	PRO	N-CA-C	5.46	123.71	112.47
3	C	299	LEU	N-CA-C	-5.46	99.18	110.80
3	C	208	ALA	N-CA-C	-5.45	102.10	109.95
1	A	625	ASP	N-CA-C	-5.44	99.21	110.80
3	C	636	ALA	CA-C-N	-5.44	113.76	122.08
3	C	636	ALA	C-N-CA	-5.44	113.76	122.08
3	C	273	ARG	N-CA-C	-5.43	105.45	112.68
3	C	686	GLU	N-CA-C	-5.43	105.44	111.36
2	B	150	GLU	CA-CB-CG	-5.41	103.28	114.10
3	C	402	PRO	N-CA-C	5.41	123.61	112.47
1	A	524	GLN	N-CA-C	-5.40	104.11	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	416	ASP	CA-C-N	5.40	125.07	119.56
1	A	416	ASP	C-N-CA	5.40	125.07	119.56
1	A	359	ILE	N-CA-C	-5.39	100.57	108.54
3	C	183	ILE	N-CA-C	-5.39	107.56	113.43
2	B	150	GLU	CB-CG-CD	5.37	121.73	112.60
1	A	256	SER	N-CA-C	5.37	115.37	108.34
1	A	866	VAL	N-CA-C	5.37	114.25	107.70
3	C	61	ASP	N-CA-C	-5.33	106.78	113.28
3	C	744	TYR	N-CA-C	-5.31	107.17	113.97
3	C	181	HIS	CA-C-N	5.31	127.96	120.42
3	C	181	HIS	C-N-CA	5.31	127.96	120.42
1	A	794	ILE	N-CA-C	5.29	116.11	108.48
1	A	588	PRO	N-CA-C	-5.28	103.15	111.34
1	A	782	PHE	CA-CB-CG	5.28	119.08	113.80
1	A	836	VAL	N-CA-C	5.26	115.88	108.36
1	A	608	ASP	N-CA-C	-5.26	105.44	111.07
3	C	207	GLU	N-CA-C	-5.25	102.13	109.69
1	A	687	TYR	CA-C-N	5.25	126.40	119.84
1	A	687	TYR	C-N-CA	5.25	126.40	119.84
3	C	147	ILE	N-CA-C	-5.25	104.95	112.35
1	A	484	LYS	N-CA-C	5.23	117.56	111.02
2	B	170	PHE	N-CA-C	5.23	117.03	108.55
2	B	34	GLY	N-CA-C	-5.21	106.34	112.64
3	C	183	ILE	N-CA-CB	-5.21	106.48	112.21
1	A	942	PHE	N-CA-C	5.19	118.16	110.48
4	D	97	ASP	CB-CA-C	5.18	123.82	112.63
1	A	554	PRO	N-CA-C	-5.18	106.98	114.18
2	B	106	ASP	N-CA-C	5.18	117.10	107.99
1	A	476	VAL	N-CA-C	-5.17	100.96	109.12
1	A	604	CYS	N-CA-C	-5.16	103.12	110.59
3	C	204	ARG	N-CA-C	-5.15	107.16	112.93
3	C	424	ALA	N-CA-C	5.15	119.43	113.20
2	B	37	SER	N-CA-C	5.13	117.10	108.73
1	A	987	GLU	N-CA-C	-5.13	107.68	114.04
1	A	387	LEU	N-CA-C	-5.12	101.53	109.72
3	C	82	ASN	CA-C-N	5.10	131.29	121.54
3	C	82	ASN	C-N-CA	5.10	131.29	121.54
1	A	523	PRO	N-CA-CB	-5.10	97.90	103.25
1	A	1115	ASP	CB-CA-C	-5.09	100.29	110.42
1	A	567	ARG	N-CA-C	5.08	117.61	110.14
4	D	22	PHE	N-CA-C	5.06	121.59	110.80
3	C	278	LEU	N-CA-C	5.06	118.26	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	179	TRP	CA-CB-CG	5.06	123.21	113.60
2	B	211	CYS	CA-C-N	5.04	126.13	119.84
2	B	211	CYS	C-N-CA	5.04	126.13	119.84
3	C	183	ILE	O-C-N	5.03	127.33	122.25
1	A	496	LYS	N-CA-C	-5.03	103.89	110.53
1	A	1023	PRO	CA-CB-CG	-5.01	94.98	104.50
4	D	45	CYS	CA-CB-SG	5.01	125.92	114.40
3	C	708	LYS	N-CA-C	5.01	118.85	112.34

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8920	0	8880	845	0
2	B	1373	0	1356	184	0
3	C	5899	0	5977	539	1
4	D	746	0	699	83	0
5	B	2	0	0	0	0
5	D	3	0	0	0	0
All	All	16943	0	16912	1606	1

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 47.

All (1606) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1114:TYR:O	1:A:1114:TYR:CD1	1.68	1.47
1:A:381:ALA:O	1:A:720:SER:HB3	1.35	1.23
3:C:422:LYS:NZ	3:C:422:LYS:HB3	1.30	1.22
1:A:381:ALA:O	1:A:720:SER:CB	1.90	1.18
1:A:1120:MET:HE2	1:A:1122:ARG:CZ	1.77	1.15
1:A:889:ARG:HD3	1:A:904:ASN:HD21	1.16	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:69:ALA:HA	3:C:79:ILE:HG21	1.33	1.10
4:D:25:LYS:HE3	4:D:25:LYS:HA	1.30	1.10
1:A:189:HIS:ND1	1:A:210:GLU:O	1.85	1.09
1:A:1120:MET:HE2	1:A:1122:ARG:NE	1.67	1.08
3:C:54:LEU:HB2	3:C:55:PRO:HD3	1.40	1.04
1:A:889:ARG:HD2	1:A:901:THR:HG23	1.36	1.03
2:B:151:ASN:OD1	2:B:170:PHE:HZ	1.42	1.03
1:A:112:ILE:HD13	1:A:112:ILE:H	1.24	1.01
3:C:118:ILE:HD11	3:C:181:HIS:HB3	1.38	1.01
3:C:422:LYS:NZ	3:C:422:LYS:CB	2.20	1.01
3:C:626:ARG:HA	3:C:629:GLN:HB2	1.41	1.00
1:A:771:PHE:HE2	1:A:845:GLN:HB3	1.24	0.99
2:B:85:ILE:HD12	2:B:85:ILE:H	1.28	0.99
3:C:657:ASN:HD21	3:C:659:GLU:HB2	1.28	0.99
1:A:889:ARG:HD3	1:A:904:ASN:ND2	1.79	0.98
1:A:328:LEU:HD12	1:A:328:LEU:H	1.27	0.97
1:A:226:PHE:CE1	1:A:268:GLY:O	2.17	0.97
4:D:41:ASN:ND2	4:D:47:ASN:O	1.98	0.96
3:C:491:LEU:HA	3:C:494:MET:HG3	1.47	0.96
1:A:1120:MET:CE	1:A:1122:ARG:CZ	2.44	0.96
3:C:638:VAL:HG12	3:C:639:LEU:HD23	1.47	0.95
3:C:642:SER:HB2	3:C:643:PRO:HD3	1.46	0.95
1:A:1114:TYR:O	1:A:1114:TYR:CG	2.20	0.95
2:B:30:GLN:HE21	2:B:36:SER:HB3	1.30	0.94
2:B:170:PHE:O	2:B:193:SER:HB2	1.67	0.94
1:A:465:HIS:ND1	1:A:523:PRO:HD3	1.82	0.93
3:C:251:MET:HE2	3:C:251:MET:HA	1.50	0.93
2:B:38:LEU:HD22	2:B:131:LYS:HZ2	1.34	0.92
1:A:985:THR:HG22	1:A:987:GLU:H	1.35	0.92
1:A:866:VAL:HG21	1:A:884:ILE:HG12	1.50	0.91
3:C:422:LYS:HB3	3:C:422:LYS:HZ3	1.09	0.91
1:A:507:GLN:NE2	1:A:552:LEU:HA	1.85	0.91
1:A:149:ASN:C	1:A:151:GLU:O	2.14	0.91
3:C:704:MET:HG3	3:C:745:MET:HE2	1.52	0.90
1:A:444:GLU:HB3	3:C:46:LYS:HB2	1.54	0.90
1:A:335:LYS:HB3	1:A:348:VAL:HG23	1.54	0.90
3:C:99:SER:HB2	3:C:100:PRO:HD3	1.53	0.89
4:D:94:CYS:SG	4:D:97:ASP:HB2	2.12	0.89
4:D:102:GLU:O	4:D:103:PHE:HB2	1.69	0.89
1:A:465:HIS:CE1	1:A:523:PRO:HD3	2.07	0.89
3:C:635:LYS:HD3	3:C:637:ARG:HD2	1.53	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:745:MET:HA	3:C:757:TYR:O	1.71	0.88
4:D:49:ILE:HD12	4:D:70:VAL:HG22	1.54	0.88
1:A:24:THR:H	1:A:30:ASN:ND2	1.71	0.88
1:A:649:VAL:HG12	1:A:650:PHE:H	1.39	0.88
1:A:176:PRO:HB2	1:A:195:VAL:HG22	1.56	0.88
1:A:578:HIS:CD2	1:A:623:LEU:HD12	2.09	0.87
1:A:1100:ILE:O	1:A:1105:MET:HE1	1.74	0.87
3:C:422:LYS:HB3	3:C:422:LYS:HZ2	1.10	0.87
1:A:482:GLU:CD	1:A:483:PRO:HD3	2.00	0.87
1:A:1120:MET:HG3	1:A:1122:ARG:HG2	1.55	0.87
4:D:41:ASN:HB3	4:D:42:CYS:O	1.75	0.87
3:C:538:PRO:HA	3:C:570:GLN:HE22	1.40	0.86
1:A:928:ARG:HH12	1:A:947:ARG:NH2	1.74	0.86
3:C:274:VAL:HA	3:C:278:LEU:HB2	1.57	0.86
3:C:213:LEU:O	3:C:217:LEU:HD12	1.76	0.85
1:A:771:PHE:CE2	1:A:845:GLN:HB3	2.10	0.85
3:C:605:GLY:O	3:C:606:ASP:HB2	1.75	0.85
1:A:507:GLN:HE22	1:A:553:SER:H	1.25	0.85
2:B:51:LEU:HD22	2:B:141:MET:HA	1.59	0.85
1:A:736:LEU:HD11	1:A:815:SER:O	1.78	0.84
4:D:42:CYS:O	4:D:46:ARG:HA	1.77	0.84
3:C:144:ARG:HA	3:C:147:ILE:HD12	1.57	0.84
2:B:51:LEU:HD11	2:B:143:ARG:H	1.42	0.84
1:A:224:GLU:HB2	1:A:225:PRO:HD3	1.59	0.84
2:B:15:LYS:O	2:B:15:LYS:HG3	1.78	0.84
1:A:520:GLN:HG3	1:A:529:ILE:HG13	1.60	0.84
2:B:177:ILE:HG12	2:B:186:VAL:HG22	1.59	0.83
1:A:1080:ARG:NH1	2:B:120:LYS:H	1.74	0.83
1:A:963:ASP:C	1:A:964:ASN:HD22	1.86	0.83
1:A:1032:THR:HG22	1:A:1034:ASN:H	1.42	0.83
1:A:19:VAL:HG12	1:A:64:MET:HE3	1.61	0.82
1:A:1127:ASP:HA	1:A:1130:ILE:HD12	1.58	0.82
1:A:270:ARG:HG2	1:A:284:LEU:HG	1.60	0.82
3:C:199:LEU:O	3:C:209:VAL:HG11	1.79	0.82
3:C:119:LEU:HB2	3:C:120:PRO:HD3	1.59	0.82
3:C:284:LYS:HB3	3:C:285:PRO:HD3	1.62	0.82
1:A:534:MET:HE1	1:A:569:LEU:HD21	1.62	0.82
1:A:602:LEU:C	1:A:603:LEU:HD23	2.04	0.82
2:B:196:PRO:HD2	2:B:204:PHE:HE2	1.45	0.82
1:A:736:LEU:HG	1:A:816:LEU:HD22	1.62	0.81
3:C:183:ILE:HD11	3:C:220:MET:SD	2.20	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:THR:HG22	1:A:447:GLU:H	1.43	0.81
1:A:889:ARG:HG2	1:A:891:TYR:CE1	2.15	0.81
2:B:170:PHE:HA	2:B:212:PRO:CD	2.09	0.81
1:A:413:LEU:HB2	1:A:424:THR:HB	1.63	0.81
1:A:262:ASN:ND2	1:A:316:TYR:H	1.78	0.81
3:C:757:TYR:HE1	3:C:759:ALA:HA	1.46	0.80
3:C:366:LEU:HD23	3:C:439:LEU:HD12	1.62	0.80
1:A:381:ALA:O	1:A:720:SER:OG	1.99	0.80
1:A:969:GLU:HG2	1:A:971:ALA:H	1.46	0.80
1:A:189:HIS:HD1	1:A:210:GLU:C	1.89	0.80
3:C:678:VAL:O	3:C:682:VAL:HG23	1.81	0.80
1:A:985:THR:HB	1:A:988:GLU:HG3	1.62	0.80
1:A:328:LEU:HD12	1:A:328:LEU:N	1.97	0.80
1:A:509:VAL:HG23	1:A:543:ILE:HD13	1.62	0.80
1:A:808:LEU:HG	1:A:847:ARG:HH21	1.47	0.80
1:A:340:SER:OG	1:A:344:GLY:HA2	1.82	0.79
1:A:909:ILE:HG12	1:A:928:ARG:HD2	1.63	0.79
1:A:1114:TYR:O	1:A:1114:TYR:HD1	1.63	0.79
3:C:680:GLU:O	3:C:684:THR:HG22	1.81	0.79
3:C:239:THR:C	3:C:241:CYS:H	1.91	0.79
1:A:176:PRO:HB2	1:A:195:VAL:CG2	2.13	0.78
3:C:593:LEU:HD21	4:D:27:TRP:HE1	1.48	0.78
4:D:41:ASN:O	4:D:42:CYS:C	2.19	0.78
1:A:166:ASP:HB3	1:A:219:VAL:HG23	1.65	0.78
3:C:599:LEU:HD21	3:C:631:LEU:HD12	1.64	0.78
1:A:167:VAL:O	1:A:168:LYS:HG2	1.83	0.78
3:C:274:VAL:HG11	3:C:283:GLN:HE21	1.49	0.78
1:A:859:GLN:HE22	3:C:281:SER:HB2	1.47	0.78
1:A:24:THR:H	1:A:30:ASN:HD21	1.30	0.78
3:C:211:ARG:HD2	3:C:276:THR:HG21	1.64	0.78
1:A:889:ARG:HH11	1:A:904:ASN:HD21	1.29	0.78
3:C:329:VAL:HG12	3:C:330:ARG:H	1.49	0.78
1:A:578:HIS:NE2	1:A:623:LEU:HD12	1.99	0.77
1:A:1094:ILE:HG22	1:A:1094:ILE:O	1.82	0.77
3:C:296:GLY:O	3:C:297:GLU:HB2	1.82	0.77
2:B:32:VAL:HG23	2:B:33:THR:HG23	1.66	0.77
1:A:59:GLY:HA2	1:A:1073:TRP:CZ3	2.19	0.77
2:B:52:THR:HG21	2:B:85:ILE:HG13	1.67	0.77
1:A:910:MET:HE3	1:A:912:LEU:HD21	1.67	0.77
3:C:422:LYS:CB	3:C:422:LYS:HZ2	1.93	0.77
3:C:527:ILE:HD11	3:C:567:LEU:HD22	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:649:VAL:HG12	1:A:650:PHE:N	2.00	0.76
2:B:87:PRO:HB2	2:B:198:THR:HG22	1.65	0.76
3:C:578:LEU:HD11	3:C:596:THR:HG23	1.67	0.76
1:A:507:GLN:HE22	1:A:552:LEU:HA	1.49	0.76
2:B:151:ASN:OD1	2:B:170:PHE:CZ	2.34	0.76
2:B:89:ASP:CG	2:B:90:ASP:H	1.93	0.76
1:A:300:LEU:HD23	1:A:300:LEU:H	1.50	0.76
3:C:294:LEU:O	3:C:295:LEU:HD23	1.86	0.75
1:A:1080:ARG:HD2	2:B:119:GLY:HA3	1.68	0.75
3:C:186:LYS:HB3	3:C:188:VAL:HG23	1.68	0.75
1:A:469:ILE:HD11	1:A:476:VAL:HG23	1.69	0.75
3:C:279:ASP:OD1	3:C:281:SER:HB3	1.87	0.75
1:A:90:GLU:OE2	1:A:92:LYS:HE3	1.87	0.75
3:C:423:GLU:OE1	3:C:467:ALA:HB2	1.87	0.75
4:D:25:LYS:HA	4:D:25:LYS:CE	2.15	0.75
1:A:450:GLY:HA3	1:A:479:VAL:CG2	2.17	0.74
3:C:601:MET:HE1	3:C:613:ILE:HA	1.69	0.74
1:A:452:VAL:HG12	1:A:454:ASP:OD2	1.86	0.74
1:A:149:ASN:O	1:A:151:GLU:O	2.04	0.74
1:A:1120:MET:HE3	1:A:1122:ARG:NH2	2.02	0.74
1:A:1120:MET:CG	1:A:1122:ARG:HG2	2.17	0.74
1:A:36:ASN:O	1:A:61:ILE:HG12	1.88	0.74
1:A:862:ALA:HB2	1:A:893:TRP:HH2	1.51	0.74
2:B:202:ARG:HB2	2:B:204:PHE:HE1	1.51	0.74
4:D:49:ILE:HD12	4:D:70:VAL:CG2	2.16	0.74
1:A:633:THR:HB	3:C:162:LEU:CD2	2.18	0.74
1:A:1120:MET:HG3	1:A:1122:ARG:NH1	2.03	0.74
1:A:451:PHE:CD1	1:A:470:GLN:HB2	2.23	0.73
1:A:743:GLN:HB3	1:A:783:GLY:HA2	1.68	0.73
3:C:630:SER:HB3	3:C:672:ILE:HD11	1.71	0.73
1:A:57:MET:HE3	1:A:1065:VAL:HB	1.68	0.73
1:A:657:THR:HG22	1:A:658:VAL:H	1.54	0.73
3:C:595:GLN:HE22	3:C:669:ILE:HG22	1.52	0.73
3:C:635:LYS:HG2	3:C:637:ARG:HG3	1.68	0.73
4:D:91:ARG:HG2	4:D:92:GLN:H	1.53	0.73
1:A:964:ASN:HD22	1:A:964:ASN:N	1.87	0.73
1:A:1109:VAL:HG21	1:A:1125:THR:HA	1.71	0.73
1:A:1120:MET:CE	1:A:1122:ARG:NH2	2.51	0.73
4:D:41:ASN:C	4:D:42:CYS:O	2.21	0.73
2:B:26:TYR:CE1	2:B:38:LEU:HD21	2.23	0.73
3:C:422:LYS:CB	3:C:422:LYS:HZ3	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:38:LEU:HD22	2:B:131:LYS:NZ	2.03	0.72
1:A:1082:THR:HG22	1:A:1082:THR:O	1.89	0.72
3:C:609:SER:O	3:C:612:GLU:HG2	1.87	0.72
1:A:465:HIS:HB2	1:A:467:GLN:HE21	1.54	0.72
2:B:117:LEU:HD13	2:B:137:LYS:NZ	2.03	0.72
1:A:578:HIS:CD2	1:A:623:LEU:H	2.06	0.72
3:C:77:THR:HG22	3:C:78:SER:H	1.53	0.72
1:A:130:MET:HE2	1:A:142:VAL:HG13	1.72	0.72
1:A:356:LEU:HB3	1:A:359:ILE:HD11	1.71	0.72
1:A:876:PHE:HD1	1:A:916:THR:HG23	1.51	0.72
3:C:276:THR:HG22	3:C:277:TYR:N	2.02	0.72
1:A:448:LEU:HB3	1:A:451:PHE:HD2	1.52	0.72
1:A:465:HIS:O	1:A:467:GLN:HG3	1.89	0.72
3:C:127:ASP:O	3:C:129:VAL:N	2.22	0.72
3:C:696:ILE:O	3:C:700:ILE:HG12	1.88	0.72
1:A:192:THR:OG1	1:A:205:GLY:HA3	1.90	0.72
3:C:240:ASN:OD1	3:C:289:CYS:HB3	1.90	0.72
1:A:726:TYR:OH	1:A:796:GLN:NE2	2.22	0.72
3:C:447:ASP:OD2	3:C:725:PHE:HB3	1.90	0.72
2:B:195:SER:HB3	2:B:204:PHE:CD2	2.25	0.72
3:C:49:ARG:HD2	3:C:51:ARG:NH2	2.05	0.72
3:C:340:TRP:CH2	3:C:390:MET:HB2	2.25	0.72
3:C:602:PHE:HD2	3:C:656:PHE:HB2	1.54	0.72
4:D:83:CYS:O	4:D:84:ILE:HB	1.89	0.72
2:B:43:ILE:HD12	2:B:44:PRO:HD2	1.72	0.71
4:D:55:GLU:HG3	4:D:86:ARG:NH2	2.06	0.71
1:A:579:LYS:HG2	1:A:581:MET:HE3	1.73	0.71
1:A:971:ALA:O	1:A:972:PHE:HB2	1.89	0.71
1:A:1002:GLU:HB3	1:A:1032:THR:HG21	1.71	0.71
2:B:206:CYS:SG	2:B:211:CYS:HB2	2.30	0.71
3:C:316:VAL:HB	3:C:317:PRO:HD3	1.71	0.71
3:C:660:PHE:O	3:C:662:HIS:N	2.23	0.71
1:A:275:ASP:CB	1:A:279:ARG:HB2	2.21	0.71
1:A:451:PHE:CE1	1:A:470:GLN:HB2	2.26	0.71
2:B:198:THR:C	2:B:200:ALA:H	1.98	0.71
4:D:70:VAL:CG1	4:D:78:ALA:HB1	2.20	0.71
1:A:399:HIS:NE2	1:A:703:THR:HG22	2.06	0.71
1:A:633:THR:HB	3:C:162:LEU:HD23	1.72	0.71
1:A:652:CYS:HB3	1:A:676:VAL:O	1.91	0.71
1:A:532:THR:HG22	1:A:533:GLU:N	2.06	0.70
1:A:828:TYR:HB3	1:A:851:PHE:O	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:SER:O	1:A:484:LYS:HA	1.92	0.70
1:A:864:LYS:HB2	1:A:899:VAL:HG23	1.72	0.70
2:B:92:THR:O	2:B:93:VAL:HG13	1.91	0.70
1:A:81:THR:HG22	1:A:82:ALA:N	2.06	0.70
3:C:587:LYS:H	3:C:587:LYS:HD2	1.57	0.70
1:A:469:ILE:HD13	1:A:470:GLN:N	2.06	0.70
3:C:578:LEU:HD13	3:C:591:VAL:CG2	2.21	0.70
1:A:125:ASP:OD2	1:A:127:GLU:HB2	1.90	0.70
1:A:450:GLY:HA3	1:A:479:VAL:HG21	1.73	0.70
2:B:208:CYS:O	2:B:210:GLN:N	2.24	0.70
1:A:32:LEU:HD22	1:A:41:ILE:HG12	1.74	0.70
1:A:834:ALA:HB2	1:A:869:ALA:HA	1.73	0.69
1:A:862:ALA:HB2	1:A:893:TRP:CH2	2.27	0.69
1:A:592:LEU:HD23	1:A:593:MET:O	1.92	0.69
3:C:602:PHE:O	4:D:21:ARG:HD2	1.91	0.69
1:A:596:PHE:HE2	1:A:648:ASN:HA	1.57	0.69
1:A:704:ILE:HD12	1:A:704:ILE:H	1.57	0.69
1:A:724:ILE:HA	1:A:734:GLY:O	1.92	0.69
3:C:643:PRO:CD	3:C:652:ASP:HA	2.21	0.69
1:A:1115:ASP:CA	1:A:1120:MET:O	2.41	0.69
3:C:734:LYS:HA	3:C:737:GLU:CD	2.18	0.69
1:A:158:ARG:HB3	1:A:158:ARG:NH1	2.06	0.69
1:A:815:SER:HB2	1:A:832:GLY:HA3	1.75	0.69
1:A:889:ARG:HD2	1:A:901:THR:CG2	2.21	0.69
3:C:432:THR:O	3:C:436:ILE:HG13	1.91	0.69
1:A:1007:PHE:O	1:A:1008:CYS:HB3	1.93	0.69
2:B:143:ARG:NH2	2:B:145:ILE:HD11	2.08	0.69
2:B:115:LEU:HD22	2:B:115:LEU:C	2.18	0.69
3:C:630:SER:C	3:C:632:ALA:H	2.01	0.69
1:A:767:SER:O	1:A:767:SER:OG	1.91	0.68
3:C:329:VAL:HG12	3:C:330:ARG:N	2.08	0.68
3:C:619:ILE:HG22	3:C:620:GLU:H	1.57	0.68
1:A:739:ARG:NH1	1:A:790:ASN:HD21	1.92	0.68
4:D:19:LYS:HE3	4:D:19:LYS:HA	1.76	0.68
1:A:24:THR:HG23	1:A:91:TYR:CE2	2.29	0.68
1:A:762:SER:HB2	1:A:803:HIS:ND1	2.09	0.68
1:A:864:LYS:HB2	1:A:899:VAL:CG2	2.24	0.68
1:A:618:ILE:HG13	1:A:619:GLU:N	2.08	0.68
1:A:876:PHE:CD1	1:A:916:THR:HG23	2.29	0.68
2:B:92:THR:O	2:B:92:THR:HG22	1.94	0.68
3:C:555:LYS:HD2	3:C:569:TRP:HZ3	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:560:GLY:O	3:C:561:LYS:HB2	1.93	0.68
3:C:630:SER:CB	3:C:672:ILE:HD11	2.24	0.68
3:C:751:ASN:O	3:C:753:ASN:N	2.27	0.68
1:A:452:VAL:HG23	1:A:470:GLN:OE1	1.93	0.67
1:A:903:CYS:SG	1:A:941:ASN:HA	2.33	0.67
3:C:601:MET:HE3	3:C:616:ALA:HB3	1.76	0.67
1:A:157:ILE:HG22	1:A:158:ARG:N	2.08	0.67
1:A:743:GLN:HE22	1:A:748:GLY:HA2	1.59	0.67
2:B:111:THR:HB	2:B:188:GLU:HG2	1.77	0.67
1:A:440:GLY:O	1:A:686:GLY:HA3	1.94	0.67
3:C:249:ARG:O	3:C:253:GLU:HB2	1.95	0.67
2:B:144:PHE:O	2:B:145:ILE:HD12	1.94	0.67
3:C:366:LEU:CD2	3:C:439:LEU:HD12	2.25	0.67
1:A:130:MET:HE2	1:A:142:VAL:CG1	2.25	0.67
1:A:310:ILE:HG13	1:A:384:GLU:OE2	1.95	0.67
3:C:274:VAL:HG11	3:C:283:GLN:HB2	1.76	0.67
1:A:49:LEU:HD22	1:A:49:LEU:N	2.08	0.67
1:A:105:HIS:CA	1:A:152:LEU:HD12	2.25	0.67
3:C:609:SER:H	3:C:612:GLU:CD	2.03	0.67
1:A:112:ILE:H	1:A:112:ILE:CD1	2.01	0.67
2:B:98:ILE:HB	2:B:201:ALA:HB1	1.76	0.67
3:C:512:MET:HE2	3:C:512:MET:HA	1.77	0.66
3:C:714:LEU:HD12	3:C:714:LEU:N	2.10	0.66
1:A:422:TYR:CE2	1:A:683:ASN:HB3	2.31	0.66
1:A:889:ARG:HH11	1:A:904:ASN:ND2	1.94	0.66
4:D:52:LEU:N	4:D:52:LEU:HD22	2.10	0.66
4:D:94:CYS:SG	4:D:97:ASP:CB	2.81	0.66
4:D:104:GLN:O	4:D:105:LYS:HB2	1.93	0.66
2:B:196:PRO:HD2	2:B:204:PHE:CE2	2.28	0.66
1:A:394:ILE:HD12	1:A:706:GLU:HA	1.77	0.66
1:A:1007:PHE:HD2	1:A:1030:PHE:HB3	1.61	0.66
1:A:312:GLU:HG3	1:A:327:ARG:HB2	1.76	0.66
1:A:1130:ILE:O	1:A:1134:GLU:HB3	1.96	0.66
1:A:412:PRO:HB2	1:A:422:TYR:CD1	2.30	0.66
3:C:538:PRO:CA	3:C:570:GLN:HE22	2.08	0.66
1:A:460:CYS:HA	1:A:469:ILE:O	1.95	0.66
1:A:864:LYS:HG3	1:A:865:GLU:H	1.60	0.66
1:A:884:ILE:N	1:A:884:ILE:HD12	2.11	0.66
3:C:409:ILE:HG13	3:C:443:ILE:CD1	2.26	0.66
3:C:630:SER:O	3:C:631:LEU:HB2	1.95	0.66
4:D:95:PRO:O	4:D:96:LEU:HG	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:841:ALA:HA	2:B:45:PRO:HG2	1.76	0.66
1:A:914:LEU:O	1:A:915:LYS:HG2	1.96	0.65
2:B:208:CYS:C	2:B:210:GLN:H	2.02	0.65
3:C:79:ILE:H	3:C:79:ILE:HD12	1.60	0.65
3:C:635:LYS:CD	3:C:637:ARG:HD2	2.26	0.65
1:A:927:MET:HE2	2:B:123:PRO:HG2	1.78	0.65
4:D:93:VAL:O	4:D:94:CYS:C	2.38	0.65
1:A:1120:MET:HG2	1:A:1121:LYS:H	1.61	0.65
2:B:51:LEU:HB2	2:B:141:MET:HE3	1.79	0.65
2:B:170:PHE:N	2:B:170:PHE:CD2	2.63	0.65
3:C:461:LEU:HB3	3:C:498:MET:HE2	1.79	0.65
3:C:233:LEU:O	3:C:234:LYS:C	2.39	0.65
1:A:507:GLN:HE22	1:A:553:SER:N	1.94	0.65
1:A:828:TYR:CE2	1:A:861:VAL:HG21	2.32	0.65
1:A:1057:ARG:NH2	1:A:1112:LEU:HA	2.11	0.65
1:A:1023:PRO:HG2	1:A:1135:GLU:OE2	1.96	0.65
1:A:520:GLN:HG3	1:A:529:ILE:CG1	2.27	0.65
1:A:1100:ILE:HG13	1:A:1105:MET:CE	2.27	0.65
1:A:23:PHE:H	1:A:30:ASN:HD22	1.45	0.64
1:A:582:LEU:O	1:A:583:GLY:O	2.14	0.64
3:C:312:ASP:HB3	3:C:343:TYR:OH	1.96	0.64
1:A:601:TYR:CE2	1:A:666:LEU:HD21	2.32	0.64
3:C:69:ALA:O	3:C:73:VAL:HG23	1.97	0.64
3:C:49:ARG:HD2	3:C:51:ARG:HH21	1.60	0.64
1:A:280:LEU:HB2	1:A:308:THR:HG23	1.80	0.64
1:A:564:ILE:HG22	1:A:564:ILE:O	1.96	0.64
3:C:249:ARG:HH11	3:C:249:ARG:HB3	1.62	0.64
4:D:49:ILE:CD1	4:D:70:VAL:HG22	2.25	0.64
1:A:5:TYR:CZ	1:A:1136:LEU:HD21	2.31	0.64
1:A:727:GLN:OE1	1:A:827:THR:HG22	1.98	0.64
3:C:74:GLN:HB3	3:C:113:HIS:CD2	2.32	0.64
1:A:518:TYR:HD2	1:A:519:LEU:N	1.95	0.64
3:C:437:MET:HE1	3:C:475:MET:CE	2.28	0.64
1:A:692:ALA:C	1:A:693:LEU:HD23	2.23	0.64
2:B:89:ASP:OD2	2:B:90:ASP:N	2.30	0.64
3:C:642:SER:CB	3:C:643:PRO:HD3	2.24	0.64
1:A:118:THR:HG21	1:A:165:ILE:O	1.99	0.63
1:A:985:THR:HG22	1:A:987:GLU:N	2.10	0.63
1:A:1100:ILE:HG13	1:A:1105:MET:HE2	1.80	0.63
3:C:757:TYR:O	3:C:758:VAL:HB	1.99	0.63
1:A:808:LEU:HD12	1:A:847:ARG:HE	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:998:PHE:CZ	1:A:1090:ASP:HB3	2.33	0.63
2:B:163:ARG:HA	2:B:167:THR:HB	1.81	0.63
3:C:310:LEU:HD22	3:C:315:ARG:HB2	1.80	0.63
3:C:538:PRO:HA	3:C:570:GLN:NE2	2.12	0.63
4:D:37:ILE:CD1	4:D:43:ALA:HB2	2.29	0.63
1:A:81:THR:HG22	1:A:82:ALA:H	1.64	0.63
1:A:177:THR:C	1:A:178:ILE:HD12	2.23	0.63
1:A:993:GLN:O	1:A:995:VAL:HG13	1.98	0.63
3:C:539:MET:HE1	3:C:619:ILE:HG23	1.79	0.63
2:B:117:LEU:HD13	2:B:137:LYS:HZ2	1.62	0.63
3:C:404:LYS:N	3:C:405:PRO:HD2	2.14	0.63
1:A:285:LEU:HD22	1:A:297:LEU:HD11	1.81	0.63
1:A:476:VAL:HG13	1:A:490:TRP:HB3	1.81	0.63
3:C:66:LEU:HD23	3:C:86:LEU:HD22	1.81	0.63
4:D:87:TRP:CZ2	4:D:95:PRO:HB3	2.34	0.63
1:A:617:ASN:HD21	1:A:619:GLU:HB2	1.64	0.62
1:A:67:PHE:HZ	1:A:88:ILE:HD13	1.62	0.62
1:A:169:PHE:CE2	1:A:178:ILE:HD11	2.34	0.62
3:C:164:ASN:OD1	3:C:166:THR:HB	1.99	0.62
1:A:374:GLN:HG2	1:A:391:ARG:NH1	2.13	0.62
1:A:507:GLN:NE2	1:A:553:SER:H	1.94	0.62
1:A:591:ILE:O	1:A:592:LEU:HB2	2.00	0.62
1:A:741:GLU:OE1	1:A:788:VAL:HG21	1.99	0.62
1:A:833:THR:O	1:A:870:VAL:HG23	1.99	0.62
3:C:523:LEU:HD11	3:C:525:VAL:HG22	1.81	0.62
1:A:482:GLU:OE2	1:A:483:PRO:HD3	1.99	0.62
1:A:414:ARG:CB	1:A:462:ASN:HD21	2.12	0.62
1:A:1093:LEU:C	1:A:1095:GLU:H	2.08	0.62
3:C:77:THR:HG22	3:C:78:SER:N	2.13	0.62
3:C:251:MET:HA	3:C:251:MET:CE	2.27	0.62
3:C:292:LYS:HD2	3:C:292:LYS:O	1.99	0.62
3:C:540:GLU:CD	3:C:540:GLU:H	2.08	0.62
4:D:37:ILE:HD11	4:D:43:ALA:HB2	1.80	0.62
1:A:536:HIS:CD2	1:A:563:ASP:HB3	2.34	0.62
1:A:582:LEU:HD13	1:A:583:GLY:H	1.65	0.62
3:C:148:MET:O	3:C:151:SER:OG	2.17	0.62
3:C:437:MET:HE1	3:C:475:MET:HE3	1.81	0.62
3:C:724:LYS:HE2	3:C:724:LYS:HA	1.82	0.62
1:A:731:GLN:O	1:A:796:GLN:HB2	2.00	0.62
1:A:1097:PHE:CE1	1:A:1105:MET:HG3	2.35	0.62
4:D:85:SER:HA	4:D:88:LEU:HD12	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:LEU:O	1:A:153:LYS:C	2.43	0.61
1:A:180:PHE:HE2	1:A:191:LYS:HG3	1.65	0.61
1:A:312:GLU:HG3	1:A:327:ARG:CB	2.29	0.61
1:A:1126:ALA:O	1:A:1128:ASP:N	2.33	0.61
3:C:409:ILE:O	3:C:413:VAL:HG23	2.00	0.61
1:A:391:ARG:HG3	1:A:391:ARG:HH11	1.65	0.61
3:C:726:PRO:O	3:C:727:VAL:HB	2.00	0.61
1:A:207:TRP:CD1	1:A:208:LYS:N	2.68	0.61
3:C:108:GLN:HA	3:C:111:GLU:HB3	1.81	0.61
3:C:228:LYS:HD3	3:C:232:GLU:HG2	1.81	0.61
1:A:10:GLN:NE2	1:A:11:LYS:O	2.33	0.61
1:A:120:ILE:HD12	1:A:135:LEU:HD22	1.83	0.61
1:A:408:LYS:HZ1	3:C:92:ASN:HA	1.64	0.61
2:B:205:GLU:O	2:B:206:CYS:HB2	2.00	0.61
3:C:183:ILE:CD1	3:C:220:MET:SD	2.89	0.61
3:C:282:THR:O	3:C:285:PRO:HD2	2.01	0.61
1:A:142:VAL:O	1:A:154:ALA:HB1	2.00	0.61
1:A:828:TYR:HE2	1:A:861:VAL:HG21	1.66	0.61
2:B:171:HIS:NE2	2:B:212:PRO:HB2	2.16	0.61
1:A:86:ALA:O	1:A:87:CYS:HB3	2.01	0.61
1:A:564:ILE:HG22	1:A:582:LEU:CD1	2.31	0.61
1:A:669:SER:O	1:A:670:ASN:C	2.43	0.61
2:B:115:LEU:C	2:B:115:LEU:CD2	2.72	0.61
3:C:527:ILE:HD11	3:C:567:LEU:CD2	2.31	0.61
3:C:624:LEU:CD2	3:C:628:LEU:HG	2.30	0.61
1:A:446:THR:HG22	1:A:447:GLU:N	2.16	0.60
1:A:341:ASN:ND2	1:A:342:GLU:HG2	2.15	0.60
1:A:396:ILE:HD13	1:A:396:ILE:H	1.66	0.60
1:A:518:TYR:C	1:A:518:TYR:CD2	2.79	0.60
1:A:589:ARG:HD3	3:C:87:TYR:OH	2.01	0.60
1:A:81:THR:HB	1:A:85:ASN:HB2	1.82	0.60
1:A:373:GLY:O	1:A:1012:LEU:HD23	2.01	0.60
1:A:573:SER:OG	1:A:575:GLU:HB2	2.01	0.60
1:A:657:THR:HG21	1:A:668:PHE:HB3	1.82	0.60
2:B:15:LYS:HD2	2:B:82:LYS:HB2	1.81	0.60
3:C:461:LEU:HD22	3:C:498:MET:HE2	1.83	0.60
3:C:692:ARG:O	3:C:696:ILE:HG12	2.02	0.60
1:A:18:CYS:N	1:A:313:CYS:SG	2.75	0.60
1:A:24:THR:HA	1:A:91:TYR:CD2	2.36	0.60
1:A:492:GLU:HG3	1:A:496:LYS:HB2	1.83	0.60
2:B:215:CYS:HB3	2:B:218:CYS:SG	2.42	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:204:ARG:CG	3:C:273:ARG:HH12	2.15	0.60
3:C:751:ASN:C	3:C:753:ASN:H	2.10	0.60
1:A:105:HIS:C	1:A:152:LEU:HD12	2.27	0.60
2:B:169:GLY:O	2:B:212:PRO:HD3	2.01	0.60
3:C:296:GLY:O	3:C:297:GLU:CB	2.50	0.60
2:B:170:PHE:HA	2:B:212:PRO:HD3	1.81	0.60
3:C:276:THR:HG22	3:C:277:TYR:H	1.67	0.60
3:C:417:LEU:HD23	3:C:460:ARG:HH12	1.66	0.60
3:C:751:ASN:N	3:C:751:ASN:HD22	2.00	0.60
1:A:716:PRO:O	1:A:717:LEU:HD23	2.01	0.60
1:A:741:GLU:HG2	1:A:751:ALA:HA	1.83	0.60
3:C:228:LYS:HA	3:C:232:GLU:HB2	1.84	0.60
3:C:305:LYS:O	3:C:305:LYS:HG3	2.02	0.60
3:C:204:ARG:HG3	3:C:273:ARG:HH12	1.65	0.60
3:C:490:LYS:HE3	4:D:104:GLN:O	2.01	0.60
1:A:441:GLU:O	1:A:441:GLU:HG2	2.02	0.59
1:A:864:LYS:HG3	1:A:865:GLU:N	2.17	0.59
1:A:1115:ASP:CB	1:A:1120:MET:O	2.50	0.59
3:C:587:LYS:H	3:C:587:LYS:CD	2.15	0.59
3:C:602:PHE:CD2	3:C:656:PHE:HB2	2.35	0.59
1:A:53:LYS:HE3	1:A:55:VAL:HG13	1.83	0.59
1:A:90:GLU:CD	1:A:92:LYS:HE3	2.27	0.59
3:C:340:TRP:HH2	3:C:390:MET:HB2	1.65	0.59
1:A:280:LEU:HD22	1:A:308:THR:HG21	1.84	0.59
1:A:356:LEU:O	1:A:359:ILE:HD13	2.03	0.59
2:B:17:ILE:HD13	2:B:17:ILE:N	2.16	0.59
2:B:108:THR:HB	2:B:109:PRO:HD2	1.84	0.59
3:C:51:ARG:H	3:C:52:PRO:HD2	1.67	0.59
3:C:192:THR:O	3:C:196:ILE:HG13	2.03	0.59
3:C:486:ALA:HA	3:C:489:SER:HB2	1.84	0.59
3:C:640:ILE:O	3:C:654:PHE:HA	2.01	0.59
1:A:443:VAL:CG1	3:C:45:ILE:HG12	2.32	0.59
1:A:498:ILE:HD12	1:A:498:ILE:N	2.18	0.59
1:A:930:VAL:CG1	1:A:954:MET:HE2	2.32	0.59
2:B:100:ASN:OD1	2:B:102:LEU:HB2	2.02	0.59
3:C:725:PHE:HB2	3:C:726:PRO:HD2	1.85	0.59
3:C:732:LEU:O	3:C:733:LYS:C	2.45	0.59
1:A:305:LEU:HD13	1:A:336:LEU:HD21	1.84	0.59
3:C:597:LEU:O	3:C:598:VAL:C	2.45	0.59
1:A:1055:GLN:HE21	1:A:1089:ILE:HG23	1.67	0.59
1:A:889:ARG:CD	1:A:904:ASN:HD21	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:454:LYS:HD2	3:C:534:PRO:HG3	1.83	0.59
4:D:42:CYS:SG	4:D:45:CYS:N	2.76	0.59
4:D:45:CYS:HB2	4:D:47:ASN:HD21	1.66	0.59
1:A:847:ARG:NH1	1:A:849:VAL:HG22	2.18	0.59
1:A:1121:LYS:HB2	1:A:1121:LYS:NZ	2.18	0.59
4:D:41:ASN:CG	4:D:47:ASN:O	2.46	0.59
1:A:930:VAL:HG13	1:A:954:MET:HE2	1.83	0.59
1:A:316:TYR:HE1	1:A:320:GLY:HA2	1.67	0.59
1:A:726:TYR:HE1	1:A:796:GLN:HE21	1.50	0.59
3:C:589:PHE:CD2	3:C:669:ILE:HD11	2.37	0.59
1:A:953:TRP:HB2	1:A:970:ASN:OD1	2.02	0.58
3:C:228:LYS:HE2	3:C:232:GLU:OE2	2.03	0.58
3:C:642:SER:C	3:C:644:LYS:H	2.11	0.58
1:A:414:ARG:HB3	1:A:462:ASN:HD21	1.68	0.58
1:A:588:PRO:HB3	1:A:604:CYS:SG	2.43	0.58
3:C:228:LYS:CE	3:C:232:GLU:HG2	2.34	0.58
3:C:244:ALA:HA	3:C:293:GLN:OE1	2.03	0.58
1:A:81:THR:HG22	1:A:83:LYS:H	1.68	0.58
1:A:407:ILE:HG21	1:A:410:LEU:HD23	1.84	0.58
1:A:553:SER:O	1:A:571:LEU:HD12	2.03	0.58
1:A:1002:GLU:OE1	1:A:1032:THR:HG21	2.04	0.58
1:A:1075:SER:HA	1:A:1084:PRO:O	2.03	0.58
2:B:52:THR:O	2:B:54:ALA:N	2.37	0.58
2:B:119:GLY:C	2:B:121:THR:H	2.11	0.58
3:C:249:ARG:HH11	3:C:249:ARG:CB	2.16	0.58
3:C:429:LEU:O	3:C:433:LEU:HB2	2.03	0.58
1:A:1000:LEU:HD11	1:A:1030:PHE:CZ	2.38	0.58
3:C:239:THR:O	3:C:241:CYS:N	2.36	0.58
3:C:421:ASN:O	3:C:424:ALA:HB2	2.03	0.58
3:C:521:ILE:HD12	3:C:521:ILE:N	2.18	0.58
1:A:414:ARG:HG2	1:A:414:ARG:HH11	1.69	0.58
1:A:753:ARG:HG3	1:A:754:PRO:O	2.03	0.58
3:C:135:ILE:HD11	3:C:188:VAL:CG1	2.34	0.58
3:C:468:SER:HB3	3:C:471:ALA:HB2	1.85	0.58
1:A:5:TYR:OH	1:A:1136:LEU:HD21	2.03	0.58
1:A:806:GLN:HG2	1:A:807:PHE:N	2.18	0.58
2:B:177:ILE:HG22	2:B:179:TRP:CZ3	2.38	0.58
3:C:369:LYS:HE2	3:C:390:MET:CE	2.33	0.58
1:A:125:ASP:HB2	1:A:169:PHE:CD2	2.39	0.58
1:A:963:ASP:HA	1:A:979:LYS:HE2	1.86	0.58
1:A:1126:ALA:C	1:A:1128:ASP:H	2.10	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ILE:HG12	1:A:154:ALA:HB2	1.85	0.58
1:A:155:PHE:HE1	1:A:157:ILE:HG12	1.69	0.58
3:C:405:PRO:O	3:C:409:ILE:HG12	2.02	0.58
1:A:81:THR:CB	1:A:85:ASN:HB2	2.33	0.58
1:A:138:GLY:O	1:A:139:LEU:HD23	2.04	0.58
1:A:429:PHE:O	1:A:430:VAL:O	2.22	0.58
1:A:477:ARG:HG2	1:A:489:GLU:HG3	1.86	0.58
1:A:673:LEU:HD23	1:A:674:LYS:H	1.67	0.58
1:A:859:GLN:NE2	3:C:281:SER:HB2	2.18	0.58
1:A:1007:PHE:CD2	1:A:1030:PHE:HB3	2.37	0.58
3:C:240:ASN:ND2	3:C:289:CYS:SG	2.77	0.58
1:A:265:ASP:C	1:A:267:ASN:H	2.10	0.57
1:A:330:ASP:OD1	1:A:388:ARG:NH2	2.37	0.57
1:A:987:GLU:C	1:A:989:ARG:H	2.11	0.57
3:C:700:ILE:HD13	3:C:719:LEU:HD21	1.85	0.57
1:A:706:GLU:O	1:A:706:GLU:HG2	2.04	0.57
1:A:854:SER:O	1:A:855:ASP:OD1	2.22	0.57
2:B:107:SER:HB2	2:B:203:ARG:HH22	1.69	0.57
3:C:155:PHE:O	3:C:159:THR:HB	2.04	0.57
1:A:929:SER:OG	1:A:930:VAL:N	2.36	0.57
3:C:528:LEU:HD22	3:C:533:TRP:CZ2	2.40	0.57
2:B:177:ILE:HG22	2:B:179:TRP:HZ3	1.68	0.57
3:C:621:ASP:O	3:C:625:ARG:HG2	2.03	0.57
1:A:502:SER:O	1:A:503:CYS:HB2	2.04	0.57
1:A:1002:GLU:OE1	1:A:1034:ASN:HB2	2.03	0.57
3:C:665:PHE:O	3:C:666:ARG:HB2	2.04	0.57
1:A:158:ARG:HB3	1:A:158:ARG:HH11	1.68	0.57
1:A:200:LYS:O	1:A:201:GLU:HG3	2.04	0.57
1:A:432:GLN:HA	1:A:455:GLN:O	2.04	0.57
1:A:578:HIS:CE1	1:A:623:LEU:HD12	2.39	0.57
1:A:798:THR:OG1	1:A:800:GLU:HG2	2.04	0.57
3:C:601:MET:HB3	3:C:608:PHE:HE1	1.69	0.57
1:A:157:ILE:HG21	1:A:202:PHE:CD1	2.40	0.57
2:B:108:THR:HG22	2:B:109:PRO:HD3	1.86	0.57
3:C:159:THR:HG22	3:C:160:TYR:N	2.18	0.57
1:A:218:MET:HE1	1:A:260:CYS:HA	1.86	0.57
1:A:430:VAL:HG12	1:A:431:GLY:N	2.19	0.57
1:A:443:VAL:HG12	3:C:45:ILE:HG12	1.86	0.57
1:A:600:HIS:HB2	1:A:616:LEU:O	2.04	0.57
1:A:671:VAL:O	1:A:673:LEU:N	2.38	0.57
1:A:695:ASN:OD1	1:A:697:SER:N	2.30	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:198:THR:C	2:B:200:ALA:N	2.59	0.57
3:C:57:ASN:O	3:C:59:THR:N	2.28	0.57
1:A:12:PRO:HG3	1:A:1036:MET:HB2	1.87	0.57
1:A:850:VAL:HB	1:A:862:ALA:HB3	1.85	0.57
1:A:228:GLY:HA3	1:A:239:TYR:HE1	1.69	0.56
1:A:622:LEU:C	1:A:622:LEU:HD12	2.29	0.56
1:A:761:LEU:HB2	1:A:802:LEU:O	2.05	0.56
2:B:102:LEU:C	2:B:104:GLY:H	2.13	0.56
1:A:388:ARG:HH11	1:A:714:THR:HB	1.70	0.56
1:A:432:GLN:NE2	3:C:52:PRO:HG2	2.19	0.56
1:A:982:ALA:C	1:A:984:THR:H	2.13	0.56
2:B:86:VAL:CG1	2:B:198:THR:HA	2.35	0.56
3:C:49:ARG:CD	3:C:51:ARG:HH21	2.18	0.56
1:A:127:GLU:HB3	1:A:129:ARG:HH11	1.70	0.56
1:A:167:VAL:C	1:A:168:LYS:HG2	2.30	0.56
1:A:255:GLN:HE21	1:A:279:ARG:HH22	1.53	0.56
1:A:280:LEU:HG	1:A:305:LEU:HD12	1.85	0.56
2:B:87:PRO:HB2	2:B:198:THR:CG2	2.33	0.56
2:B:197:ILE:HG12	2:B:197:ILE:O	2.06	0.56
3:C:51:ARG:O	3:C:53:ARG:N	2.36	0.56
1:A:433:THR:HG22	1:A:434:ARG:H	1.68	0.56
1:A:454:ASP:OD2	1:A:454:ASP:N	2.28	0.56
1:A:503:CYS:SG	1:A:504:ASN:N	2.78	0.56
1:A:936:LYS:HB3	1:A:939:GLU:HB2	1.88	0.56
2:B:137:LYS:O	2:B:137:LYS:HD3	2.05	0.56
2:B:172:ARG:NH1	2:B:197:ILE:HG22	2.20	0.56
2:B:197:ILE:HD13	2:B:197:ILE:N	2.19	0.56
3:C:541:VAL:HG12	3:C:618:GLY:O	2.05	0.56
3:C:643:PRO:HD2	3:C:652:ASP:HA	1.86	0.56
1:A:255:GLN:HG3	1:A:279:ARG:NH2	2.20	0.56
1:A:293:GLY:O	1:A:294:THR:HG23	2.05	0.56
1:A:335:LYS:HB3	1:A:348:VAL:CG2	2.30	0.56
1:A:806:GLN:HG2	1:A:807:PHE:H	1.69	0.56
2:B:117:LEU:HD23	2:B:134:LYS:NZ	2.21	0.56
3:C:748:ASP:O	3:C:749:LYS:HB2	2.06	0.56
4:D:84:ILE:O	4:D:88:LEU:HG	2.05	0.56
1:A:112:ILE:HD13	1:A:112:ILE:N	2.08	0.56
2:B:100:ASN:OD1	2:B:102:LEU:N	2.39	0.56
3:C:65:LYS:HD2	3:C:81:TYR:CD2	2.41	0.56
3:C:221:LEU:HD22	3:C:226:VAL:HG23	1.87	0.56
3:C:239:THR:C	3:C:241:CYS:N	2.60	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:420:GLY:O	3:C:423:GLU:HG3	2.06	0.56
3:C:657:ASN:ND2	3:C:659:GLU:HB2	2.11	0.56
1:A:1020:THR:O	1:A:1021:SER:C	2.46	0.56
3:C:227:TYR:C	3:C:227:TYR:CD2	2.83	0.56
3:C:390:MET:O	3:C:394:PHE:HB2	2.06	0.56
3:C:439:LEU:O	3:C:440:PHE:C	2.49	0.56
1:A:300:LEU:H	1:A:300:LEU:CD2	2.19	0.56
1:A:534:MET:HE2	1:A:558:ILE:HD13	1.87	0.56
2:B:11:ASP:HB3	2:B:85:ILE:HD11	1.86	0.56
1:A:884:ILE:HG22	1:A:885:ASN:OD1	2.05	0.56
1:A:493:PRO:HB2	1:A:494:GLN:HE22	1.70	0.56
1:A:813:ALA:HA	1:A:833:THR:HG22	1.88	0.56
3:C:48:PHE:O	3:C:50:ASP:N	2.39	0.56
3:C:660:PHE:C	3:C:662:HIS:H	2.14	0.56
3:C:757:TYR:CE1	3:C:759:ALA:HA	2.36	0.56
4:D:86:ARG:C	4:D:88:LEU:H	2.14	0.56
1:A:192:THR:O	1:A:193:TYR:CD2	2.59	0.55
1:A:928:ARG:NH1	1:A:947:ARG:NH2	2.50	0.55
3:C:586:LYS:O	3:C:586:LYS:HG2	2.06	0.55
1:A:525:GLU:OE1	1:A:527:ARG:NH2	2.39	0.55
1:A:948:ASP:N	1:A:992:LEU:HD11	2.20	0.55
1:A:276:MET:HG2	1:A:276:MET:O	2.06	0.55
1:A:490:TRP:CG	1:A:491:LYS:H	2.23	0.55
1:A:493:PRO:HB2	1:A:494:GLN:NE2	2.21	0.55
1:A:633:THR:HB	3:C:162:LEU:HD21	1.88	0.55
1:A:1002:GLU:HB3	1:A:1032:THR:CG2	2.36	0.55
3:C:72:ALA:HB3	3:C:79:ILE:HG23	1.87	0.55
3:C:227:TYR:HD2	3:C:228:LYS:N	2.04	0.55
3:C:287:ILE:O	3:C:291:GLU:HG3	2.07	0.55
2:B:216:SER:HA	2:B:219:GLU:OE1	2.06	0.55
3:C:267:LEU:HD23	3:C:290:VAL:HG11	1.87	0.55
1:A:78:PHE:HD1	1:A:87:CYS:O	1.90	0.55
1:A:408:LYS:HZ1	3:C:92:ASN:ND2	2.04	0.55
1:A:502:SER:OG	1:A:543:ILE:HG12	2.07	0.55
2:B:21:LEU:N	2:B:21:LEU:HD23	2.22	0.55
1:A:16:ASN:ND2	1:A:36:ASN:HA	2.21	0.55
1:A:84:TYR:CD2	1:A:135:LEU:HD13	2.42	0.55
1:A:334:VAL:HG11	1:A:347:VAL:HG13	1.88	0.55
1:A:848:ILE:O	1:A:848:ILE:HG22	2.05	0.55
2:B:48:THR:OG1	2:B:81:PRO:HB2	2.06	0.55
2:B:51:LEU:HD13	2:B:141:MET:HE2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:94:CYS:SG	3:C:156:LEU:HD13	2.47	0.55
1:A:59:GLY:HA2	1:A:1073:TRP:CE3	2.41	0.55
1:A:442:GLU:HG2	3:C:46:LYS:HE2	1.89	0.55
1:A:969:GLU:CD	1:A:971:ALA:HB3	2.32	0.55
2:B:52:THR:HB	2:B:85:ILE:HG23	1.88	0.55
3:C:89:ALA:O	3:C:93:LEU:HB2	2.07	0.55
3:C:193:ILE:HG22	3:C:194:ASP:N	2.21	0.55
4:D:93:VAL:HG12	4:D:100:GLU:HA	1.89	0.55
1:A:782:PHE:O	1:A:783:GLY:C	2.50	0.55
1:A:226:PHE:CZ	1:A:268:GLY:O	2.59	0.55
1:A:402:ILE:HD13	3:C:43:LEU:HB3	1.87	0.55
1:A:522:HIS:HB3	1:A:523:PRO:HD2	1.89	0.55
1:A:928:ARG:HH12	1:A:947:ARG:CZ	2.19	0.55
1:A:946:ALA:O	1:A:947:ARG:HB3	2.06	0.55
1:A:987:GLU:HA	1:A:990:GLN:NE2	2.22	0.55
2:B:136:GLY:O	2:B:139:ASN:O	2.25	0.55
2:B:164:GLY:HA2	2:B:194:CYS:O	2.06	0.55
3:C:733:LYS:O	3:C:737:GLU:HG3	2.07	0.55
1:A:170:LEU:HB2	1:A:177:THR:OG1	2.06	0.55
2:B:198:THR:O	2:B:200:ALA:N	2.40	0.55
3:C:292:LYS:HG3	3:C:330:ARG:NH2	2.22	0.55
3:C:643:PRO:HG2	3:C:652:ASP:HA	1.88	0.55
3:C:676:GLU:HA	3:C:680:GLU:OE1	2.06	0.55
1:A:267:ASN:O	1:A:268:GLY:C	2.50	0.54
1:A:434:ARG:NH2	3:C:50:ASP:HA	2.22	0.54
1:A:448:LEU:HD23	1:A:451:PHE:CE2	2.42	0.54
1:A:532:THR:CG2	1:A:533:GLU:N	2.69	0.54
1:A:614:PHE:CD1	1:A:614:PHE:N	2.75	0.54
1:A:659:ILE:HG22	1:A:660:TYR:N	2.21	0.54
1:A:1109:VAL:HB	1:A:1124:ALA:O	2.07	0.54
3:C:448:VAL:O	3:C:452:PHE:HD1	1.90	0.54
1:A:29:LEU:HD23	1:A:44:VAL:HG21	1.89	0.54
1:A:142:VAL:HB	1:A:155:PHE:CE1	2.42	0.54
1:A:977:CYS:HB3	1:A:992:LEU:HD13	1.89	0.54
2:B:171:HIS:CD2	2:B:171:HIS:H	2.23	0.54
3:C:437:MET:HE3	3:C:478:LYS:HB3	1.89	0.54
2:B:85:ILE:H	2:B:85:ILE:CD1	2.02	0.54
3:C:267:LEU:HD13	3:C:328:ARG:NH1	2.22	0.54
1:A:138:GLY:HA2	1:A:159:LEU:HB2	1.88	0.54
1:A:433:THR:HG22	1:A:434:ARG:N	2.22	0.54
1:A:1066:GLY:O	1:A:1067:LYS:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:472:GLU:HG2	3:C:495:PHE:HZ	1.72	0.54
3:C:657:ASN:HD21	3:C:659:GLU:CB	2.10	0.54
1:A:182:TYR:CE1	1:A:189:HIS:HB2	2.43	0.54
1:A:402:ILE:CD1	3:C:43:LEU:HB3	2.38	0.54
1:A:518:TYR:CD2	1:A:519:LEU:N	2.75	0.54
3:C:42:LYS:O	3:C:43:LEU:HD23	2.07	0.54
3:C:183:ILE:HD11	3:C:220:MET:CE	2.37	0.54
3:C:630:SER:OG	3:C:672:ILE:HD11	2.08	0.54
1:A:182:TYR:CZ	1:A:189:HIS:HB2	2.43	0.54
1:A:557:ALA:HB2	1:A:593:MET:HE2	1.89	0.54
1:A:1108:VAL:C	1:A:1110:ALA:H	2.13	0.54
1:A:1114:TYR:O	1:A:1114:TYR:CE1	2.48	0.54
3:C:57:ASN:C	3:C:59:THR:H	2.14	0.54
1:A:864:LYS:HD3	1:A:899:VAL:O	2.08	0.54
1:A:909:ILE:HD11	2:B:124:SER:HA	1.89	0.54
2:B:21:LEU:HD12	2:B:25:GLU:HB3	1.90	0.54
3:C:404:LYS:O	3:C:405:PRO:C	2.49	0.54
1:A:198:ARG:CA	1:A:198:ARG:HH11	2.21	0.54
1:A:1120:MET:HG2	1:A:1121:LYS:N	2.22	0.54
3:C:655:ILE:HD12	3:C:655:ILE:N	2.23	0.54
4:D:70:VAL:HG13	4:D:78:ALA:HB1	1.90	0.54
1:A:42:TYR:HB3	1:A:49:LEU:HB3	1.89	0.54
1:A:532:THR:OG1	1:A:574:PHE:HD1	1.90	0.54
2:B:111:THR:HB	2:B:188:GLU:CG	2.38	0.54
3:C:581:GLU:HB2	4:D:21:ARG:HA	1.89	0.54
1:A:128:CYS:O	1:A:145:LEU:HD23	2.08	0.54
1:A:403:ASP:HA	1:A:698:THR:HG22	1.88	0.54
1:A:596:PHE:CZ	1:A:649:VAL:HG23	2.43	0.54
1:A:808:LEU:HG	1:A:847:ARG:NH2	2.21	0.54
1:A:837:TYR:HB3	1:A:839:GLU:OE1	2.08	0.54
2:B:139:ASN:O	2:B:141:MET:N	2.41	0.54
3:C:73:VAL:C	3:C:74:GLN:O	2.45	0.53
3:C:347:PHE:CE2	3:C:351:ILE:HD11	2.43	0.53
1:A:388:ARG:HD3	1:A:714:THR:HB	1.90	0.53
1:A:431:GLY:O	1:A:432:GLN:HB3	2.07	0.53
1:A:525:GLU:OE1	1:A:527:ARG:NE	2.41	0.53
1:A:582:LEU:CD1	1:A:583:GLY:H	2.19	0.53
1:A:1120:MET:HG2	1:A:1122:ARG:H	1.73	0.53
3:C:316:VAL:CB	3:C:317:PRO:HD3	2.38	0.53
3:C:628:LEU:O	3:C:630:SER:O	2.26	0.53
1:A:77:LEU:HD23	1:A:89:LEU:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:VAL:HA	1:A:334:VAL:O	2.09	0.53
4:D:53:CYS:HB3	4:D:80:HIS:ND1	2.22	0.53
1:A:203:ASN:O	1:A:204:LYS:HB2	2.08	0.53
1:A:479:VAL:HG12	1:A:480:SER:N	2.22	0.53
1:A:602:LEU:O	1:A:603:LEU:HD23	2.07	0.53
3:C:74:GLN:O	3:C:75:SER:C	2.50	0.53
3:C:100:PRO:HG3	3:C:160:TYR:CZ	2.43	0.53
4:D:51:ASP:O	4:D:52:LEU:C	2.50	0.53
1:A:539:ALA:HB2	1:A:561:TRP:CD1	2.44	0.53
1:A:112:ILE:HG12	1:A:113:GLY:N	2.23	0.53
2:B:10:PRO:N	2:B:85:ILE:HD13	2.23	0.53
3:C:54:LEU:HB2	3:C:55:PRO:CD	2.25	0.53
1:A:375:LEU:O	1:A:389:ILE:HA	2.09	0.53
1:A:1106:GLN:C	1:A:1108:VAL:H	2.14	0.53
3:C:363:GLN:NE2	3:C:367:ASP:OD1	2.42	0.53
4:D:102:GLU:O	4:D:103:PHE:CB	2.47	0.53
1:A:487:VAL:O	1:A:488:SER:HB2	2.09	0.53
1:A:658:VAL:HG12	1:A:658:VAL:O	2.09	0.53
2:B:21:LEU:HG	2:B:26:TYR:CE2	2.43	0.53
2:B:91:LYS:C	2:B:93:VAL:H	2.15	0.53
3:C:139:TRP:HD1	3:C:178:PHE:CE2	2.27	0.53
3:C:406:ALA:HB2	3:C:443:ILE:HG21	1.91	0.53
3:C:468:SER:HB3	3:C:471:ALA:CB	2.39	0.53
3:C:731:ASP:O	3:C:734:LYS:HB3	2.08	0.53
4:D:104:GLN:O	4:D:105:LYS:CB	2.55	0.53
1:A:408:LYS:NZ	3:C:92:ASN:ND2	2.57	0.53
1:A:985:THR:HB	1:A:988:GLU:CG	2.36	0.53
4:D:37:ILE:O	4:D:37:ILE:HG12	2.08	0.53
1:A:821:LEU:HD11	1:A:830:ILE:HD11	1.91	0.53
1:A:866:VAL:CG2	1:A:884:ILE:HG12	2.32	0.53
1:A:1123:GLU:HG2	1:A:1124:ALA:N	2.24	0.53
3:C:248:GLN:O	3:C:249:ARG:C	2.52	0.53
3:C:544:THR:O	3:C:547:MET:HB2	2.09	0.53
1:A:188:ARG:O	1:A:212:VAL:HG22	2.09	0.52
1:A:196:SER:OG	1:A:199:GLU:HB2	2.09	0.52
1:A:900:ARG:O	1:A:901:THR:C	2.51	0.52
1:A:910:MET:CE	1:A:912:LEU:HD21	2.38	0.52
1:A:1126:ALA:O	1:A:1130:ILE:HG13	2.10	0.52
2:B:136:GLY:O	2:B:139:ASN:N	2.38	0.52
3:C:382:LYS:O	3:C:383:ASN:C	2.50	0.52
3:C:643:PRO:CG	3:C:652:ASP:HA	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:39:VAL:O	4:D:40:ASP:C	2.51	0.52
4:D:54:ILE:HG22	4:D:55:GLU:N	2.24	0.52
4:D:90:THR:OG1	4:D:91:ARG:N	2.42	0.52
1:A:602:LEU:C	1:A:602:LEU:HD13	2.33	0.52
2:B:18:GLU:HB2	2:B:42:THR:HG22	1.90	0.52
3:C:100:PRO:O	3:C:104:LYS:HG3	2.08	0.52
3:C:579:LYS:O	4:D:22:PHE:HA	2.09	0.52
3:C:660:PHE:C	3:C:662:HIS:N	2.67	0.52
3:C:735:ARG:HA	3:C:735:ARG:NE	2.24	0.52
1:A:127:GLU:HB3	1:A:129:ARG:NH1	2.24	0.52
1:A:288:GLU:CD	1:A:298:LYS:HG2	2.34	0.52
2:B:144:PHE:C	2:B:145:ILE:HD12	2.35	0.52
3:C:119:LEU:HB2	3:C:120:PRO:CD	2.37	0.52
3:C:705:LYS:C	3:C:705:LYS:HD3	2.35	0.52
1:A:24:THR:HG23	1:A:91:TYR:HE2	1.73	0.52
1:A:728:GLU:O	1:A:728:GLU:HG3	2.08	0.52
2:B:97:PRO:HA	2:B:202:ARG:HA	1.91	0.52
2:B:128:LYS:HE2	2:B:146:GLU:OE1	2.09	0.52
3:C:182:ILE:HG22	3:C:183:ILE:HG13	1.89	0.52
3:C:299:LEU:HD23	3:C:326:PHE:CE2	2.45	0.52
3:C:390:MET:C	3:C:390:MET:HE2	2.35	0.52
3:C:587:LYS:HE3	3:C:664:LEU:O	2.09	0.52
3:C:630:SER:C	3:C:632:ALA:N	2.67	0.52
4:D:47:ASN:HD22	4:D:47:ASN:H	1.57	0.52
2:B:43:ILE:HD12	2:B:44:PRO:CD	2.39	0.52
2:B:50:LEU:CD1	2:B:145:ILE:HD13	2.40	0.52
2:B:202:ARG:CB	2:B:204:PHE:HE1	2.22	0.52
3:C:41:LYS:O	3:C:42:LYS:O	2.26	0.52
1:A:594:THR:CG2	1:A:595:THR:N	2.73	0.52
1:A:631:LEU:O	1:A:655:ARG:HB2	2.10	0.52
1:A:679:MET:SD	1:A:679:MET:C	2.92	0.52
2:B:89:ASP:CG	2:B:90:ASP:N	2.63	0.52
2:B:117:LEU:HD13	2:B:137:LYS:HZ3	1.75	0.52
1:A:23:PHE:N	1:A:30:ASN:HD22	2.08	0.52
1:A:150:LYS:N	1:A:151:GLU:O	2.42	0.52
1:A:450:GLY:HA3	1:A:479:VAL:HG22	1.91	0.52
1:A:953:TRP:O	1:A:969:GLU:HB2	2.09	0.52
3:C:227:TYR:O	3:C:229:ASP:N	2.37	0.52
1:A:262:ASN:HD22	1:A:316:TYR:H	1.57	0.52
1:A:949:PHE:C	2:B:122:LEU:HD21	2.35	0.52
2:B:219:GLU:O	2:B:220:ARG:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:63:TRP:HZ3	3:C:105:GLN:HG3	1.75	0.52
4:D:84:ILE:O	4:D:84:ILE:HD13	2.10	0.52
1:A:62:ALA:HB3	1:A:80:LEU:O	2.10	0.52
1:A:256:SER:HB3	1:A:275:ASP:OD1	2.10	0.52
1:A:422:TYR:CD2	1:A:422:TYR:N	2.77	0.52
1:A:444:GLU:CB	3:C:46:LYS:HB2	2.33	0.52
1:A:571:LEU:O	1:A:572:PRO:C	2.50	0.52
1:A:585:GLU:OE2	3:C:147:ILE:HG23	2.09	0.52
2:B:49:GLY:HA3	2:B:141:MET:HE1	1.92	0.52
2:B:208:CYS:C	2:B:210:GLN:N	2.66	0.52
3:C:228:LYS:NZ	3:C:232:GLU:HG2	2.24	0.52
1:A:180:PHE:N	1:A:180:PHE:CD2	2.77	0.52
1:A:902:GLU:O	1:A:903:CYS:HB2	2.08	0.52
3:C:121:PHE:HE2	3:C:134:LYS:HB3	1.74	0.52
1:A:225:PRO:HG2	1:A:267:ASN:CB	2.40	0.51
1:A:402:ILE:O	1:A:698:THR:HB	2.10	0.51
1:A:578:HIS:CE1	1:A:623:LEU:CD1	2.93	0.51
1:A:1093:LEU:O	1:A:1095:GLU:N	2.42	0.51
2:B:102:LEU:HD13	2:B:180:VAL:HG23	1.92	0.51
2:B:179:TRP:N	2:B:179:TRP:CE3	2.78	0.51
3:C:583:LYS:O	3:C:584:GLU:HB2	2.10	0.51
3:C:676:GLU:O	3:C:676:GLU:HG3	2.09	0.51
3:C:702:ARG:HD2	3:C:722:GLN:HE22	1.75	0.51
1:A:1112:LEU:O	1:A:1123:GLU:HA	2.10	0.51
1:A:1135:GLU:OE1	1:A:1135:GLU:O	2.27	0.51
2:B:174:GLU:O	2:B:188:GLU:HA	2.10	0.51
3:C:99:SER:HB2	3:C:100:PRO:CD	2.35	0.51
3:C:251:MET:HE3	3:C:259:TYR:CZ	2.46	0.51
3:C:625:ARG:O	3:C:629:GLN:N	2.43	0.51
1:A:1051:LEU:CD2	1:A:1094:ILE:HG21	2.40	0.51
3:C:390:MET:O	3:C:390:MET:HE2	2.09	0.51
3:C:609:SER:H	3:C:612:GLU:CG	2.23	0.51
1:A:471:ILE:HA	1:A:476:VAL:HA	1.92	0.51
2:B:48:THR:O	2:B:144:PHE:HA	2.10	0.51
3:C:501:SER:O	3:C:505:MET:HB2	2.11	0.51
1:A:81:THR:CG2	1:A:82:ALA:N	2.73	0.51
1:A:285:LEU:HD12	1:A:285:LEU:O	2.10	0.51
1:A:490:TRP:CG	1:A:491:LYS:N	2.79	0.51
1:A:659:ILE:HD12	1:A:659:ILE:H	1.75	0.51
1:A:866:VAL:HG22	1:A:867:LYS:N	2.25	0.51
1:A:1120:MET:HE3	1:A:1122:ARG:CZ	2.33	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:145:ILE:HG23	2:B:172:ARG:HD3	1.92	0.51
2:B:178:GLY:C	2:B:179:TRP:HE3	2.18	0.51
3:C:228:LYS:CD	3:C:232:GLU:HG2	2.41	0.51
3:C:352:VAL:HG12	3:C:361:MET:SD	2.50	0.51
4:D:82:HIS:O	4:D:84:ILE:N	2.43	0.51
1:A:451:PHE:HD1	1:A:470:GLN:HB2	1.73	0.51
1:A:1136:LEU:HD23	1:A:1136:LEU:C	2.35	0.51
2:B:50:LEU:O	2:B:51:LEU:HG	2.11	0.51
3:C:55:PRO:O	3:C:56:ASP:HB2	2.11	0.51
3:C:141:ASP:C	3:C:143:CYS:N	2.64	0.51
1:A:155:PHE:CE1	1:A:157:ILE:HG12	2.46	0.51
1:A:282:MET:HG3	1:A:284:LEU:CD1	2.41	0.51
1:A:769:LYS:HB3	1:A:772:SER:OG	2.10	0.51
1:A:897:LYS:O	1:A:898:ASP:OD2	2.29	0.51
2:B:170:PHE:HA	2:B:212:PRO:CG	2.41	0.51
3:C:742:ARG:HD3	4:D:64:THR:HG21	1.92	0.51
1:A:157:ILE:CG2	1:A:158:ARG:N	2.73	0.51
1:A:180:PHE:N	1:A:180:PHE:HD2	2.08	0.51
1:A:224:GLU:HB2	1:A:225:PRO:CD	2.37	0.51
1:A:270:ARG:HG2	1:A:284:LEU:CG	2.34	0.51
1:A:283:LEU:C	1:A:283:LEU:HD23	2.36	0.51
1:A:831:VAL:HG12	1:A:832:GLY:N	2.26	0.51
2:B:30:GLN:HE21	2:B:36:SER:CB	2.13	0.51
3:C:257:PRO:HB3	3:C:318:ASP:OD1	2.10	0.51
1:A:459:PHE:CD2	1:A:460:CYS:N	2.79	0.51
1:A:805:HIS:HB2	1:A:858:LEU:HD12	1.93	0.51
1:A:815:SER:O	1:A:816:LEU:HB2	2.11	0.51
2:B:92:THR:C	2:B:93:VAL:HG22	2.36	0.51
2:B:172:ARG:O	2:B:190:CYS:HA	2.11	0.51
3:C:390:MET:HE2	3:C:391:LYS:HA	1.92	0.51
3:C:757:TYR:HD1	3:C:758:VAL:N	2.09	0.51
1:A:404:LEU:HD21	3:C:45:ILE:HD11	1.93	0.50
1:A:408:LYS:HA	1:A:678:TYR:CE1	2.45	0.50
1:A:448:LEU:HD23	1:A:451:PHE:HE2	1.75	0.50
1:A:570:LYS:O	1:A:574:PHE:N	2.41	0.50
3:C:202:ARG:O	3:C:207:GLU:HB2	2.11	0.50
3:C:602:PHE:N	3:C:602:PHE:CD1	2.79	0.50
3:C:696:ILE:HD11	3:C:727:VAL:HG22	1.92	0.50
1:A:795:ASP:OD1	1:A:798:THR:HG23	2.11	0.50
3:C:688:VAL:O	3:C:692:ARG:HG3	2.11	0.50
1:A:408:LYS:NZ	3:C:92:ASN:HA	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:HIS:HD2	1:A:623:LEU:H	1.56	0.50
1:A:771:PHE:N	1:A:771:PHE:CD1	2.79	0.50
1:A:844:LYS:O	1:A:867:LYS:HA	2.11	0.50
1:A:893:TRP:CE3	1:A:899:VAL:HG13	2.46	0.50
1:A:1108:VAL:C	1:A:1110:ALA:N	2.69	0.50
3:C:748:ASP:C	3:C:750:ASP:H	2.16	0.50
1:A:275:ASP:HB2	1:A:279:ARG:HB2	1.92	0.50
1:A:279:ARG:HB3	1:A:281:PHE:CE1	2.46	0.50
1:A:280:LEU:HD22	1:A:308:THR:CG2	2.41	0.50
1:A:388:ARG:NH1	1:A:714:THR:HB	2.26	0.50
1:A:573:SER:O	1:A:574:PHE:HB2	2.10	0.50
3:C:638:VAL:HG12	3:C:639:LEU:CD2	2.31	0.50
3:C:696:ILE:CD1	3:C:727:VAL:HG22	2.42	0.50
2:B:52:THR:HG21	2:B:85:ILE:CG1	2.38	0.50
3:C:271:GLY:C	3:C:273:ARG:H	2.20	0.50
1:A:52:VAL:HG23	1:A:53:LYS:N	2.27	0.50
1:A:109:GLN:HE22	1:A:111:ARG:HH11	1.59	0.50
1:A:422:TYR:CE1	1:A:682:LEU:HA	2.46	0.50
3:C:516:SER:O	3:C:517:ASP:O	2.29	0.50
3:C:632:ALA:O	3:C:633:CYS:C	2.54	0.50
1:A:416:ASP:OD1	1:A:418:ASN:HB2	2.11	0.50
3:C:417:LEU:HD23	3:C:460:ARG:NH1	2.26	0.50
3:C:457:LEU:HD22	3:C:461:LEU:HD12	1.94	0.50
1:A:198:ARG:HH11	1:A:198:ARG:N	2.10	0.50
1:A:257:THR:HG22	1:A:258:ILE:O	2.12	0.50
1:A:279:ARG:HB3	1:A:281:PHE:HE1	1.76	0.50
1:A:328:LEU:N	1:A:328:LEU:CD1	2.67	0.50
2:B:162:LYS:O	2:B:162:LYS:HG3	2.12	0.50
3:C:347:PHE:O	3:C:351:ILE:HG13	2.12	0.50
3:C:726:PRO:O	3:C:727:VAL:CB	2.60	0.50
1:A:81:THR:OG1	1:A:85:ASN:HB2	2.12	0.49
1:A:155:PHE:CD1	1:A:155:PHE:C	2.89	0.49
1:A:869:ALA:O	1:A:884:ILE:HA	2.12	0.49
3:C:380:PHE:CD1	3:C:386:PHE:CD2	3.00	0.49
3:C:505:MET:HE3	3:C:525:VAL:O	2.13	0.49
4:D:37:ILE:O	4:D:38:VAL:C	2.55	0.49
4:D:51:ASP:OD1	4:D:52:LEU:HD23	2.12	0.49
1:A:66:LEU:HD23	1:A:77:LEU:HA	1.93	0.49
1:A:612:PHE:CE2	1:A:628:LYS:HD2	2.46	0.49
3:C:149:ILE:O	3:C:150:ARG:C	2.55	0.49
3:C:696:ILE:HD11	3:C:725:PHE:HE1	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:GLU:HB3	1:A:42:TYR:CE1	2.47	0.49
1:A:226:PHE:CE2	1:A:287:LYS:HB3	2.48	0.49
1:A:245:TYR:C	1:A:245:TYR:HD2	2.21	0.49
1:A:755:SER:O	1:A:756:ALA:C	2.55	0.49
1:A:1097:PHE:HD2	1:A:1133:VAL:HG21	1.77	0.49
2:B:50:LEU:C	2:B:51:LEU:HD12	2.37	0.49
3:C:173:MET:O	3:C:173:MET:HG2	2.11	0.49
1:A:1044:SER:O	1:A:1045:GLU:C	2.56	0.49
1:A:1101:SER:O	1:A:1105:MET:HE3	2.12	0.49
3:C:440:PHE:CE2	3:C:446:LYS:HD3	2.47	0.49
4:D:45:CYS:C	4:D:46:ARG:HG2	2.36	0.49
1:A:178:ILE:HD12	1:A:178:ILE:N	2.27	0.49
1:A:180:PHE:CE2	1:A:191:LYS:HG3	2.47	0.49
1:A:736:LEU:HD11	1:A:816:LEU:HB2	1.93	0.49
1:A:960:LEU:HD21	1:A:966:LEU:HB2	1.93	0.49
2:B:50:LEU:HD11	2:B:145:ILE:HD13	1.94	0.49
2:B:52:THR:OG1	2:B:85:ILE:HA	2.13	0.49
2:B:91:LYS:O	2:B:93:VAL:N	2.45	0.49
2:B:116:ASP:OD2	2:B:116:ASP:C	2.53	0.49
2:B:143:ARG:HH22	2:B:145:ILE:HD11	1.76	0.49
1:A:13:THR:OG1	1:A:355:ASN:HA	2.12	0.49
1:A:161:GLU:HG2	1:A:182:TYR:CE2	2.48	0.49
1:A:168:LYS:HG3	1:A:219:VAL:O	2.12	0.49
1:A:194:GLU:HG3	1:A:204:LYS:O	2.13	0.49
1:A:194:GLU:HB2	1:A:203:ASN:HB2	1.95	0.49
1:A:265:ASP:C	1:A:267:ASN:N	2.71	0.49
1:A:613:TYR:CE1	1:A:627:LYS:HB2	2.46	0.49
1:A:649:VAL:CG1	1:A:650:PHE:H	2.17	0.49
1:A:971:ALA:O	1:A:972:PHE:CB	2.60	0.49
2:B:38:LEU:CD2	2:B:131:LYS:HZ2	2.16	0.49
3:C:48:PHE:O	3:C:49:ARG:C	2.55	0.49
3:C:49:ARG:CD	3:C:51:ARG:NH2	2.75	0.49
3:C:469:VAL:HG12	3:C:473:LYS:HE3	1.94	0.49
3:C:732:LEU:O	3:C:735:ARG:N	2.45	0.49
1:A:146:ASP:C	1:A:148:ASP:H	2.20	0.49
1:A:514:ARG:HG3	1:A:514:ARG:HH11	1.78	0.49
1:A:668:PHE:N	1:A:668:PHE:CD1	2.80	0.49
2:B:174:GLU:HG3	2:B:191:ASN:HB2	1.93	0.49
3:C:369:LYS:HE2	3:C:390:MET:HE1	1.94	0.49
1:A:72:GLU:CD	1:A:103:ARG:HH22	2.21	0.49
1:A:490:TRP:CD2	1:A:491:LYS:N	2.81	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:VAL:HB	1:A:515:ALA:HB3	1.94	0.49
1:A:630:THR:HG21	1:A:797:HIS:HB3	1.94	0.49
2:B:38:LEU:CD2	2:B:131:LYS:NZ	2.75	0.49
3:C:193:ILE:C	3:C:195:GLY:N	2.68	0.49
3:C:307:LEU:O	3:C:308:ASP:C	2.56	0.49
1:A:399:HIS:CE1	1:A:703:THR:HG22	2.47	0.49
1:A:492:GLU:CG	1:A:496:LYS:HB2	2.42	0.49
1:A:641:PHE:CE2	1:A:650:PHE:HB2	2.48	0.49
1:A:657:THR:HG22	1:A:658:VAL:N	2.24	0.49
1:A:1129:LEU:N	1:A:1129:LEU:HD22	2.28	0.49
1:A:103:ARG:NH1	1:A:103:ARG:HG3	2.28	0.49
1:A:394:ILE:HG22	1:A:395:GLY:N	2.27	0.49
1:A:587:ILE:H	1:A:587:ILE:HD12	1.77	0.49
1:A:873:MET:HA	1:A:882:ALA:HA	1.95	0.49
3:C:300:THR:O	3:C:304:GLN:HB2	2.13	0.49
1:A:596:PHE:CE1	1:A:659:ILE:HG22	2.48	0.48
1:A:855:ASP:C	1:A:857:LYS:H	2.21	0.48
1:A:951:PRO:HD2	1:A:1080:ARG:NH1	2.27	0.48
1:A:992:LEU:HD12	1:A:992:LEU:O	2.13	0.48
3:C:251:MET:HE3	3:C:259:TYR:CE1	2.48	0.48
3:C:330:ARG:H	3:C:330:ARG:CD	2.26	0.48
3:C:545:PRO:O	3:C:546:GLU:C	2.56	0.48
4:D:47:ASN:ND2	4:D:47:ASN:N	2.61	0.48
1:A:117:GLU:O	1:A:118:THR:HB	2.13	0.48
1:A:459:PHE:O	1:A:460:CYS:HB3	2.13	0.48
1:A:594:THR:HG23	1:A:595:THR:N	2.28	0.48
1:A:743:GLN:NE2	1:A:748:GLY:HA2	2.26	0.48
1:A:808:LEU:CG	1:A:847:ARG:HH21	2.24	0.48
1:A:823:LYS:HD2	1:A:823:LYS:N	2.28	0.48
1:A:868:GLY:O	1:A:884:ILE:HG23	2.13	0.48
1:A:917:LYS:O	1:A:920:PHE:HB2	2.13	0.48
3:C:649:GLU:HB2	3:C:652:ASP:OD2	2.13	0.48
3:C:71:ARG:NH2	3:C:74:GLN:OE1	2.45	0.48
1:A:81:THR:CG2	1:A:82:ALA:H	2.25	0.48
1:A:104:ALA:O	1:A:105:HIS:HB3	2.13	0.48
1:A:157:ILE:HG21	1:A:202:PHE:CE1	2.48	0.48
1:A:1129:LEU:HD22	1:A:1129:LEU:H	1.77	0.48
1:A:1136:LEU:O	1:A:1139:ILE:HD12	2.13	0.48
1:A:3:TYR:CE2	1:A:1045:GLU:HG3	2.48	0.48
1:A:36:ASN:ND2	1:A:1002:GLU:OE2	2.46	0.48
1:A:587:ILE:HD12	1:A:587:ILE:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:876:PHE:HD1	1:A:916:THR:CG2	2.23	0.48
3:C:512:MET:HE2	3:C:512:MET:CA	2.44	0.48
3:C:541:VAL:HG23	3:C:543:LEU:CD2	2.44	0.48
3:C:634:GLY:O	3:C:635:LYS:HB3	2.14	0.48
3:C:751:ASN:O	3:C:751:ASN:ND2	2.46	0.48
1:A:161:GLU:N	1:A:161:GLU:OE1	2.47	0.48
1:A:596:PHE:HZ	1:A:649:VAL:HG23	1.78	0.48
1:A:985:THR:HG22	1:A:986:ASP:N	2.27	0.48
1:A:1126:ALA:C	1:A:1128:ASP:N	2.72	0.48
2:B:147:GLU:OE1	2:B:163:ARG:HD3	2.13	0.48
3:C:203:GLU:C	3:C:205:SER:H	2.20	0.48
3:C:349:THR:C	3:C:351:ILE:H	2.21	0.48
1:A:268:GLY:C	1:A:285:LEU:HD11	2.39	0.48
2:B:85:ILE:HD12	2:B:85:ILE:N	2.12	0.48
3:C:515:GLN:HG2	3:C:515:GLN:O	2.14	0.48
3:C:587:LYS:HD2	3:C:587:LYS:N	2.26	0.48
1:A:340:SER:HB2	1:A:346:TYR:CE1	2.48	0.48
1:A:659:ILE:O	1:A:660:TYR:HB3	2.13	0.48
1:A:808:LEU:CD1	1:A:847:ARG:HE	2.25	0.48
1:A:931:LEU:HG	1:A:947:ARG:NH2	2.29	0.48
2:B:86:VAL:HG13	2:B:87:PRO:HD2	1.96	0.48
2:B:143:ARG:NH2	2:B:174:GLU:OE1	2.41	0.48
3:C:315:ARG:O	3:C:319:LEU:HG	2.14	0.48
3:C:601:MET:HB3	3:C:608:PHE:CE1	2.49	0.48
3:C:609:SER:O	3:C:610:PHE:C	2.57	0.48
1:A:138:GLY:C	1:A:159:LEU:HB2	2.38	0.48
1:A:245:TYR:C	1:A:245:TYR:CD2	2.91	0.48
2:B:103:LEU:O	2:B:105:LEU:HG	2.13	0.48
3:C:751:ASN:N	3:C:751:ASN:ND2	2.61	0.48
1:A:433:THR:O	1:A:434:ARG:HG3	2.14	0.48
1:A:641:PHE:HB2	1:A:681:PRO:HG3	1.95	0.48
1:A:847:ARG:HH11	1:A:849:VAL:HG22	1.79	0.48
3:C:453:TYR:CD1	3:C:453:TYR:C	2.91	0.48
3:C:599:LEU:HB3	4:D:22:PHE:CE1	2.49	0.48
1:A:16:ASN:ND2	1:A:35:LYS:O	2.47	0.47
1:A:198:ARG:N	1:A:198:ARG:NH1	2.61	0.47
1:A:286:GLU:CG	1:A:301:ARG:HH12	2.26	0.47
3:C:450:GLU:OE2	3:C:454:LYS:HE3	2.14	0.47
3:C:719:LEU:HD22	3:C:723:LEU:HD21	1.96	0.47
1:A:443:VAL:HG12	1:A:443:VAL:O	2.13	0.47
2:B:89:ASP:O	2:B:198:THR:HG21	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:GLY:O	2:B:194:CYS:HB3	2.13	0.47
3:C:482:GLU:O	3:C:483:CYS:HB2	2.14	0.47
3:C:588:GLU:O	3:C:666:ARG:HA	2.14	0.47
3:C:651:GLY:O	3:C:652:ASP:C	2.57	0.47
4:D:47:ASN:HD22	4:D:47:ASN:N	2.11	0.47
4:D:91:ARG:HB2	4:D:91:ARG:NH1	2.30	0.47
1:A:316:TYR:HE1	1:A:320:GLY:CA	2.27	0.47
1:A:479:VAL:CG1	1:A:480:SER:N	2.77	0.47
3:C:412:HIS:HE1	3:C:416:LYS:HE3	1.77	0.47
3:C:642:SER:HB2	3:C:643:PRO:CD	2.32	0.47
1:A:459:PHE:CG	1:A:460:CYS:N	2.82	0.47
1:A:579:LYS:HE3	1:A:581:MET:CE	2.45	0.47
1:A:929:SER:HB2	1:A:952:ASN:HB2	1.97	0.47
3:C:193:ILE:C	3:C:195:GLY:H	2.22	0.47
3:C:592:SER:HB2	3:C:673:GLN:NE2	2.29	0.47
1:A:182:TYR:HE2	1:A:191:LYS:HG2	1.80	0.47
1:A:611:LEU:C	1:A:611:LEU:HD23	2.40	0.47
1:A:731:GLN:O	1:A:796:GLN:CB	2.61	0.47
1:A:1082:THR:O	1:A:1082:THR:CG2	2.61	0.47
3:C:641:LYS:HE2	3:C:647:GLU:O	2.14	0.47
1:A:207:TRP:CE3	1:A:242:GLY:HA2	2.48	0.47
1:A:282:MET:CB	1:A:305:LEU:HD21	2.45	0.47
1:A:396:ILE:HD13	1:A:396:ILE:O	2.15	0.47
1:A:403:ASP:O	1:A:405:PRO:HD3	2.15	0.47
1:A:729:VAL:HG23	1:A:730:SER:N	2.28	0.47
1:A:884:ILE:N	1:A:884:ILE:CD1	2.77	0.47
2:B:102:LEU:CD1	2:B:180:VAL:HG23	2.44	0.47
2:B:107:SER:HB2	2:B:203:ARG:NH2	2.30	0.47
3:C:417:LEU:CD2	3:C:460:ARG:HH12	2.27	0.47
3:C:629:GLN:O	3:C:633:CYS:HB2	2.15	0.47
1:A:264:VAL:HG13	1:A:316:TYR:CG	2.49	0.47
1:A:407:ILE:CD1	1:A:699:LEU:HB2	2.45	0.47
1:A:457:THR:HG22	1:A:458:PHE:N	2.29	0.47
1:A:812:TYR:O	1:A:833:THR:HB	2.14	0.47
1:A:847:ARG:NH1	1:A:849:VAL:CG2	2.78	0.47
1:A:925:ASP:CB	1:A:928:ARG:HB3	2.45	0.47
1:A:1107:GLU:O	1:A:1107:GLU:HG2	2.14	0.47
2:B:86:VAL:HG13	2:B:197:ILE:O	2.15	0.47
2:B:113:THR:O	2:B:185:LYS:HA	2.15	0.47
3:C:263:VAL:HG11	3:C:295:LEU:HD21	1.97	0.47
3:C:341:SER:HB3	3:C:389:LEU:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:624:LEU:HD22	3:C:628:LEU:CD1	2.44	0.47
1:A:589:ARG:NH1	3:C:87:TYR:HE2	2.13	0.47
2:B:52:THR:O	2:B:53:ASN:C	2.57	0.47
3:C:184:SER:O	3:C:185:ASP:C	2.58	0.47
3:C:329:VAL:CG1	3:C:330:ARG:H	2.23	0.47
3:C:401:ARG:NH2	3:C:404:LYS:HG3	2.30	0.47
3:C:457:LEU:O	3:C:460:ARG:N	2.47	0.47
1:A:183:GLN:HB2	1:A:188:ARG:HG2	1.96	0.47
1:A:311:ALA:HB1	1:A:314:LEU:HD13	1.97	0.47
1:A:366:ASP:OD1	1:A:371:GLY:N	2.48	0.47
1:A:374:GLN:HG2	1:A:391:ARG:HH11	1.79	0.47
1:A:589:ARG:HD3	3:C:87:TYR:CZ	2.50	0.47
1:A:707:ILE:O	1:A:708:GLN:C	2.58	0.47
3:C:544:THR:HG23	3:C:545:PRO:HD2	1.96	0.47
1:A:140:PHE:HE2	1:A:178:ILE:HG12	1.80	0.47
2:B:92:THR:O	2:B:92:THR:CG2	2.63	0.47
3:C:329:VAL:CG1	3:C:330:ARG:N	2.78	0.47
4:D:50:MET:SD	4:D:108:HIS:CE1	3.08	0.47
1:A:207:TRP:HD1	1:A:208:LYS:N	2.13	0.46
1:A:225:PRO:HG2	1:A:267:ASN:HB2	1.97	0.46
1:A:356:LEU:HD11	1:A:390:ILE:HD12	1.98	0.46
1:A:656:PRO:HG2	1:A:676:VAL:HG23	1.97	0.46
3:C:276:THR:CG2	3:C:277:TYR:N	2.71	0.46
3:C:627:THR:O	3:C:631:LEU:HD23	2.14	0.46
3:C:705:LYS:HB2	3:C:757:TYR:HE2	1.79	0.46
1:A:189:HIS:HD1	1:A:210:GLU:HA	1.81	0.46
1:A:450:GLY:O	1:A:477:ARG:NH2	2.46	0.46
3:C:308:ASP:OD1	3:C:343:TYR:HD1	1.97	0.46
1:A:2:SER:HB3	1:A:995:VAL:HG23	1.97	0.46
1:A:31:LEU:HD13	1:A:317:LEU:HD21	1.97	0.46
1:A:169:PHE:CD2	1:A:178:ILE:HD11	2.51	0.46
1:A:353:PHE:N	1:A:353:PHE:CD1	2.84	0.46
1:A:512:VAL:O	1:A:515:ALA:HB3	2.15	0.46
1:A:808:LEU:O	1:A:811:GLU:HB3	2.15	0.46
3:C:91:GLU:HA	3:C:155:PHE:CD2	2.50	0.46
3:C:200:ILE:O	3:C:201:GLU:C	2.59	0.46
3:C:203:GLU:OE1	3:C:277:TYR:OH	2.29	0.46
4:D:74:VAL:CG2	4:D:102:GLU:HB3	2.46	0.46
1:A:93:GLN:HG3	1:A:97:SER:O	2.16	0.46
1:A:189:HIS:HD1	1:A:210:GLU:CA	2.28	0.46
1:A:596:PHE:CZ	1:A:659:ILE:HG22	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:638:LEU:O	1:A:639:ARG:HG2	2.14	0.46
3:C:448:VAL:O	3:C:451:ALA:HB3	2.14	0.46
3:C:702:ARG:NH1	3:C:722:GLN:HE21	2.14	0.46
3:C:702:ARG:NH1	3:C:722:GLN:NE2	2.64	0.46
3:C:705:LYS:HA	3:C:757:TYR:CD2	2.50	0.46
3:C:714:LEU:N	3:C:714:LEU:CD1	2.77	0.46
1:A:402:ILE:HG22	1:A:403:ASP:H	1.80	0.46
1:A:438:LEU:CD1	1:A:684:SER:HB2	2.45	0.46
1:A:633:THR:O	3:C:158:ARG:NH1	2.47	0.46
1:A:931:LEU:HD23	1:A:946:ALA:O	2.16	0.46
1:A:985:THR:CB	1:A:988:GLU:HG3	2.41	0.46
1:A:998:PHE:HZ	1:A:1090:ASP:HB3	1.77	0.46
1:A:1129:LEU:O	1:A:1130:ILE:C	2.58	0.46
3:C:587:LYS:HB2	3:C:660:PHE:CE1	2.51	0.46
4:D:91:ARG:CG	4:D:92:GLN:H	2.25	0.46
1:A:315:THR:HG22	1:A:323:PHE:HB3	1.98	0.46
1:A:414:ARG:HB3	1:A:462:ASN:ND2	2.29	0.46
1:A:641:PHE:CD1	1:A:641:PHE:C	2.93	0.46
1:A:641:PHE:HB3	1:A:679:MET:HE1	1.98	0.46
1:A:764:SER:O	1:A:805:HIS:HA	2.15	0.46
1:A:802:LEU:HD13	1:A:853:TYR:OH	2.16	0.46
1:A:1057:ARG:CB	1:A:1108:VAL:HG13	2.45	0.46
3:C:141:ASP:O	3:C:142:HIS:C	2.58	0.46
3:C:341:SER:CB	3:C:389:LEU:HD12	2.46	0.46
3:C:757:TYR:CD1	3:C:758:VAL:N	2.83	0.46
1:A:32:LEU:CD2	1:A:41:ILE:HG23	2.46	0.46
1:A:531:HIS:ND1	1:A:532:THR:N	2.63	0.46
1:A:815:SER:HB2	1:A:832:GLY:CA	2.45	0.46
1:A:936:LYS:CB	1:A:939:GLU:HB2	2.46	0.46
1:A:1101:SER:OG	1:A:1104:LYS:HD2	2.15	0.46
3:C:433:LEU:HD23	3:C:478:LYS:HE3	1.97	0.46
3:C:440:PHE:CZ	3:C:446:LYS:HD3	2.51	0.46
3:C:587:LYS:HD3	3:C:660:PHE:CE1	2.51	0.46
4:D:52:LEU:N	4:D:52:LEU:CD2	2.78	0.46
3:C:141:ASP:OD2	3:C:144:ARG:NH2	2.46	0.46
3:C:256:VAL:O	3:C:257:PRO:C	2.56	0.46
3:C:321:GLN:O	3:C:325:LEU:HD12	2.16	0.46
1:A:197:LEU:HB2	1:A:198:ARG:HH12	1.81	0.46
1:A:332:GLN:HE21	1:A:352:THR:HG22	1.81	0.46
1:A:411:TRP:HB2	1:A:460:CYS:SG	2.56	0.46
1:A:443:VAL:O	3:C:45:ILE:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1102:ARG:N	1:A:1103:PRO:CD	2.79	0.46
2:B:132:LEU:O	2:B:133:ALA:C	2.59	0.46
1:A:52:VAL:HG23	1:A:53:LYS:H	1.81	0.46
1:A:143:ILE:HG12	1:A:154:ALA:CB	2.46	0.46
2:B:171:HIS:HD1	2:B:215:CYS:HB3	1.81	0.46
3:C:219:GLY:O	3:C:220:MET:C	2.57	0.46
3:C:375:VAL:HG13	3:C:379:CYS:HB2	1.98	0.46
1:A:334:VAL:HG12	1:A:335:LYS:N	2.31	0.45
1:A:442:GLU:HG3	1:A:443:VAL:H	1.81	0.45
1:A:1115:ASP:HA	1:A:1120:MET:O	2.14	0.45
1:A:1133:VAL:O	1:A:1137:THR:HG23	2.16	0.45
3:C:114:VAL:O	3:C:117:GLN:N	2.50	0.45
3:C:700:ILE:CG2	3:C:745:MET:HE1	2.46	0.45
1:A:5:TYR:CE2	1:A:1136:LEU:HD21	2.51	0.45
1:A:148:ASP:N	1:A:148:ASP:OD2	2.46	0.45
1:A:407:ILE:HD11	1:A:699:LEU:HB2	1.98	0.45
1:A:490:TRP:O	1:A:491:LYS:HB2	2.15	0.45
1:A:629:VAL:HG23	1:A:630:THR:N	2.31	0.45
2:B:41:ASN:HD21	2:B:139:ASN:HD21	1.63	0.45
2:B:171:HIS:CD2	2:B:171:HIS:N	2.84	0.45
3:C:55:PRO:O	3:C:56:ASP:CB	2.64	0.45
3:C:110:CYS:O	3:C:111:GLU:C	2.58	0.45
3:C:303:LEU:HD23	3:C:322:MET:CE	2.46	0.45
3:C:578:LEU:HD13	3:C:591:VAL:HG21	1.99	0.45
1:A:253:ILE:O	1:A:254:LYS:C	2.58	0.45
1:A:1093:LEU:C	1:A:1095:GLU:N	2.74	0.45
3:C:90:VAL:O	3:C:91:GLU:C	2.58	0.45
3:C:208:ALA:O	3:C:209:VAL:HG13	2.16	0.45
3:C:227:TYR:CD2	3:C:228:LYS:N	2.83	0.45
3:C:241:CYS:O	3:C:244:ALA:HB3	2.15	0.45
3:C:460:ARG:NH1	3:C:472:GLU:OE2	2.49	0.45
4:D:98:ASN:HD22	4:D:98:ASN:HA	1.52	0.45
1:A:880:LEU:HG	1:A:880:LEU:O	2.17	0.45
1:A:982:ALA:O	1:A:984:THR:N	2.44	0.45
2:B:110:SER:N	2:B:221:ASP:HB3	2.30	0.45
2:B:141:MET:O	2:B:179:TRP:HH2	1.99	0.45
3:C:79:ILE:H	3:C:79:ILE:CD1	2.23	0.45
3:C:274:VAL:CG1	3:C:283:GLN:HE21	2.23	0.45
3:C:696:ILE:HD11	3:C:725:PHE:CE1	2.50	0.45
1:A:108:VAL:HG21	1:A:133:LEU:HD23	1.99	0.45
1:A:1112:LEU:HD12	1:A:1113:GLN:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:52:THR:CG2	2:B:85:ILE:HG13	2.42	0.45
2:B:137:LYS:C	2:B:137:LYS:CD	2.90	0.45
3:C:595:GLN:HE22	3:C:669:ILE:CG2	2.27	0.45
3:C:757:TYR:O	3:C:758:VAL:CB	2.64	0.45
1:A:32:LEU:CD2	1:A:41:ILE:HG12	2.45	0.45
1:A:528:GLN:O	1:A:528:GLN:HG2	2.17	0.45
1:A:576:LEU:C	1:A:577:LEU:HD23	2.41	0.45
1:A:893:TRP:CZ3	1:A:899:VAL:HG13	2.52	0.45
2:B:28:THR:HG22	2:B:29:SER:N	2.30	0.45
2:B:169:GLY:C	2:B:212:PRO:HD3	2.41	0.45
3:C:534:PRO:HB2	3:C:536:TYR:CE1	2.51	0.45
4:D:45:CYS:O	4:D:46:ARG:C	2.60	0.45
4:D:75:CYS:CB	4:D:97:ASP:OD2	2.64	0.45
1:A:476:VAL:HG22	1:A:526:LEU:CD1	2.47	0.45
2:B:11:ASP:C	2:B:12:GLU:HG3	2.42	0.45
2:B:99:PRO:O	2:B:100:ASN:C	2.60	0.45
2:B:219:GLU:C	2:B:221:ASP:H	2.25	0.45
3:C:54:LEU:CB	3:C:55:PRO:HD3	2.27	0.45
3:C:200:ILE:O	3:C:202:ARG:N	2.50	0.45
3:C:610:PHE:CE2	3:C:614:LYS:HE3	2.52	0.45
1:A:396:ILE:N	1:A:396:ILE:CD1	2.79	0.45
1:A:534:MET:CE	1:A:569:LEU:HD11	2.47	0.45
1:A:597:GLU:O	1:A:598:SER:HB3	2.16	0.45
1:A:659:ILE:CG2	1:A:660:TYR:N	2.79	0.45
2:B:205:GLU:O	2:B:206:CYS:CB	2.65	0.45
3:C:98:VAL:O	3:C:99:SER:C	2.60	0.45
1:A:102:THR:HG23	1:A:104:ALA:O	2.17	0.45
1:A:103:ARG:HH11	1:A:103:ARG:CG	2.30	0.45
1:A:263:ARG:CG	1:A:265:ASP:O	2.65	0.45
1:A:383:LYS:C	1:A:385:GLY:H	2.24	0.45
1:A:478:LEU:HB3	1:A:488:SER:HB3	1.99	0.45
1:A:695:ASN:OD1	1:A:698:THR:N	2.42	0.45
1:A:1104:LYS:HA	1:A:1107:GLU:HB3	1.98	0.45
3:C:57:ASN:C	3:C:59:THR:N	2.74	0.45
3:C:267:LEU:CD2	3:C:290:VAL:HG11	2.47	0.45
3:C:303:LEU:HD13	3:C:339:HIS:CD2	2.51	0.45
3:C:725:PHE:HB2	3:C:726:PRO:CD	2.47	0.45
1:A:66:LEU:HD21	1:A:77:LEU:HD13	1.99	0.45
1:A:258:ILE:HA	1:A:274:GLY:O	2.17	0.45
1:A:546:LEU:O	1:A:549:SER:HB3	2.17	0.45
1:A:557:ALA:N	1:A:593:MET:HE2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:195:SER:CB	2:B:204:PHE:CD2	2.97	0.45
3:C:234:LYS:O	3:C:235:PHE:C	2.59	0.45
3:C:758:VAL:O	3:C:758:VAL:HG12	2.17	0.45
1:A:63:VAL:HB	1:A:80:LEU:HB3	1.98	0.44
1:A:138:GLY:HA2	1:A:159:LEU:CB	2.47	0.44
1:A:586:ILE:HG22	1:A:607:GLY:H	1.82	0.44
1:A:889:ARG:NH1	1:A:904:ASN:HD21	2.04	0.44
2:B:142:THR:HG22	2:B:179:TRP:CH2	2.52	0.44
3:C:264:SER:O	3:C:268:GLU:HG2	2.17	0.44
4:D:41:ASN:CB	4:D:42:CYS:O	2.57	0.44
4:D:52:LEU:HD22	4:D:52:LEU:H	1.83	0.44
1:A:263:ARG:HG2	1:A:265:ASP:O	2.18	0.44
1:A:396:ILE:HD13	1:A:396:ILE:N	2.29	0.44
1:A:830:ILE:HG12	1:A:850:VAL:HG22	1.98	0.44
2:B:136:GLY:O	2:B:137:LYS:C	2.59	0.44
3:C:200:ILE:C	3:C:202:ARG:N	2.74	0.44
3:C:496:LYS:HD3	3:C:496:LYS:HA	1.84	0.44
1:A:16:ASN:HD22	1:A:36:ASN:HA	1.81	0.44
1:A:587:ILE:H	1:A:587:ILE:CD1	2.29	0.44
1:A:987:GLU:HA	1:A:990:GLN:HE21	1.81	0.44
3:C:491:LEU:HA	3:C:494:MET:CG	2.33	0.44
3:C:700:ILE:HG22	3:C:745:MET:HE1	2.00	0.44
1:A:643:SER:O	1:A:644:LEU:C	2.59	0.44
1:A:673:LEU:HD23	1:A:674:LYS:N	2.33	0.44
2:B:148:PRO:C	2:B:150:GLU:H	2.23	0.44
3:C:51:ARG:N	3:C:52:PRO:HD2	2.32	0.44
3:C:146:MET:HE2	3:C:149:ILE:HD12	1.99	0.44
3:C:179:ARG:O	3:C:184:SER:HB3	2.16	0.44
3:C:218:LEU:HD12	3:C:277:TYR:HB2	2.00	0.44
3:C:579:LYS:HE3	4:D:23:GLU:OE2	2.18	0.44
1:A:2:SER:HB3	1:A:995:VAL:CG2	2.48	0.44
1:A:117:GLU:O	1:A:118:THR:CB	2.65	0.44
1:A:429:PHE:O	1:A:456:GLN:HG3	2.18	0.44
1:A:532:THR:CG2	1:A:533:GLU:H	2.31	0.44
1:A:580:GLU:OE2	1:A:626:ARG:HD2	2.17	0.44
1:A:821:LEU:HD11	1:A:830:ILE:CD1	2.48	0.44
1:A:877:ASN:C	1:A:879:LYS:H	2.25	0.44
1:A:905:HIS:CD2	1:A:933:LEU:HD21	2.52	0.44
3:C:70:VAL:O	3:C:72:ALA:N	2.50	0.44
3:C:143:CYS:O	3:C:147:ILE:HG13	2.18	0.44
3:C:610:PHE:C	3:C:610:PHE:CD2	2.94	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:757:TYR:CD1	3:C:757:TYR:C	2.95	0.44
4:D:53:CYS:HB2	4:D:83:CYS:SG	2.57	0.44
1:A:130:MET:HB2	1:A:143:ILE:O	2.17	0.44
1:A:419:ARG:HD3	1:A:421:THR:O	2.18	0.44
1:A:607:GLY:HA2	1:A:635:PRO:HB3	1.99	0.44
2:B:119:GLY:C	2:B:121:THR:N	2.76	0.44
3:C:61:ASP:O	3:C:65:LYS:HG3	2.17	0.44
3:C:65:LYS:HD2	3:C:81:TYR:HD2	1.79	0.44
3:C:95:SER:O	3:C:96:HIS:C	2.61	0.44
3:C:121:PHE:C	3:C:123:GLU:H	2.25	0.44
3:C:292:LYS:O	3:C:293:GLN:HG2	2.17	0.44
3:C:707:ARG:HD2	3:C:710:LEU:HD13	2.00	0.44
1:A:157:ILE:HG22	1:A:158:ARG:H	1.78	0.44
1:A:171:TYR:CZ	1:A:223:PRO:HG3	2.53	0.44
1:A:257:THR:HG22	1:A:258:ILE:N	2.33	0.44
3:C:113:HIS:O	3:C:117:GLN:HG2	2.16	0.44
3:C:428:GLU:O	3:C:432:THR:HG23	2.18	0.44
3:C:434:ASP:O	3:C:438:ILE:HG13	2.18	0.44
3:C:527:ILE:O	3:C:527:ILE:CG2	2.65	0.44
3:C:668:LYS:NZ	3:C:670:ASN:HB3	2.32	0.44
2:B:162:LYS:O	2:B:164:GLY:N	2.51	0.44
3:C:294:LEU:C	3:C:295:LEU:HD23	2.41	0.44
3:C:409:ILE:HG13	3:C:443:ILE:HD11	1.98	0.44
3:C:544:THR:O	3:C:545:PRO:C	2.60	0.44
3:C:555:LYS:HD2	3:C:569:TRP:CZ3	2.47	0.44
1:A:67:PHE:CE1	1:A:145:LEU:HD21	2.53	0.44
1:A:447:GLU:O	1:A:448:LEU:HD12	2.18	0.44
1:A:657:THR:CG2	1:A:668:PHE:HB3	2.48	0.44
1:A:876:PHE:HZ	1:A:919:ASP:HA	1.82	0.44
3:C:184:SER:O	3:C:186:LYS:N	2.50	0.44
3:C:227:TYR:C	3:C:229:ASP:H	2.24	0.44
3:C:578:LEU:HD13	3:C:591:VAL:HG23	2.00	0.44
3:C:712:HIS:CD2	3:C:712:HIS:C	2.95	0.44
1:A:146:ASP:O	1:A:148:ASP:N	2.45	0.43
1:A:239:TYR:CZ	1:A:241:ASN:HB2	2.53	0.43
1:A:643:SER:OG	1:A:644:LEU:N	2.46	0.43
2:B:119:GLY:O	2:B:121:THR:N	2.46	0.43
3:C:311:LEU:HD11	3:C:340:TRP:HD1	1.83	0.43
3:C:412:HIS:CE1	3:C:416:LYS:HE3	2.53	0.43
3:C:555:LYS:HB2	3:C:569:TRP:HH2	1.83	0.43
1:A:430:VAL:O	1:A:456:GLN:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:823:LYS:O	1:A:825:PRO:HD3	2.18	0.43
1:A:973:ASN:OD1	1:A:999:HIS:ND1	2.43	0.43
3:C:240:ASN:CG	3:C:289:CYS:HB3	2.43	0.43
3:C:523:LEU:HD11	3:C:525:VAL:CG2	2.48	0.43
4:D:81:PHE:O	4:D:84:ILE:HG22	2.18	0.43
1:A:744:ASP:O	1:A:745:THR:C	2.61	0.43
2:B:51:LEU:HD11	2:B:143:ARG:N	2.22	0.43
2:B:143:ARG:HA	2:B:175:TYR:O	2.17	0.43
3:C:171:TRP:CZ3	3:C:175:LEU:HD11	2.52	0.43
4:D:21:ARG:O	4:D:22:PHE:CD2	2.71	0.43
1:A:112:ILE:HG12	1:A:113:GLY:H	1.83	0.43
1:A:726:TYR:CE1	1:A:796:GLN:NE2	2.86	0.43
1:A:1057:ARG:HB3	1:A:1108:VAL:HG13	2.00	0.43
3:C:110:CYS:C	3:C:112:ASP:N	2.76	0.43
3:C:704:MET:CG	3:C:745:MET:HE2	2.37	0.43
1:A:134:ARG:HH11	1:A:134:ARG:HG3	1.82	0.43
1:A:500:VAL:HG12	1:A:541:LEU:HD12	2.01	0.43
1:A:582:LEU:CD1	1:A:583:GLY:N	2.81	0.43
3:C:530:MET:HG2	4:D:32:LEU:HB3	2.01	0.43
3:C:702:ARG:HD2	3:C:722:GLN:NE2	2.33	0.43
4:D:47:ASN:HB2	4:D:48:HIS:H	1.65	0.43
1:A:126:PRO:C	1:A:128:CYS:H	2.25	0.43
1:A:446:THR:CG2	1:A:447:GLU:H	2.05	0.43
1:A:567:ARG:HB3	1:A:579:LYS:HA	2.01	0.43
1:A:750:THR:HG22	1:A:751:ALA:N	2.33	0.43
3:C:204:ARG:NE	3:C:273:ARG:HH12	2.17	0.43
3:C:295:LEU:HD11	3:C:325:LEU:HD22	1.99	0.43
3:C:440:PHE:O	3:C:442:PHE:N	2.51	0.43
1:A:326:SER:HB3	1:A:329:GLY:O	2.19	0.43
1:A:579:LYS:CG	1:A:581:MET:HE3	2.47	0.43
1:A:655:ARG:HH11	1:A:655:ARG:CG	2.31	0.43
1:A:692:ALA:O	1:A:693:LEU:HD23	2.17	0.43
1:A:869:ALA:O	1:A:884:ILE:HG23	2.17	0.43
1:A:951:PRO:HG2	2:B:119:GLY:HA2	2.00	0.43
1:A:1034:ASN:HD22	1:A:1034:ASN:HA	1.55	0.43
1:A:1047:TRP:HZ3	1:A:1132:VAL:HG13	1.83	0.43
2:B:98:ILE:N	2:B:201:ALA:O	2.32	0.43
3:C:437:MET:O	3:C:440:PHE:HB3	2.19	0.43
1:A:393:GLY:O	1:A:708:GLN:HA	2.19	0.43
1:A:407:ILE:HD13	1:A:699:LEU:HD23	2.01	0.43
1:A:451:PHE:HE1	1:A:470:GLN:HB2	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:GLU:CD	1:A:496:LYS:HB2	2.44	0.43
1:A:564:ILE:O	1:A:582:LEU:HD12	2.18	0.43
1:A:602:LEU:HD22	1:A:603:LEU:N	2.34	0.43
1:A:697:SER:C	1:A:698:THR:HG23	2.44	0.43
1:A:1102:ARG:O	1:A:1105:MET:HB2	2.18	0.43
3:C:118:ILE:O	3:C:119:LEU:C	2.62	0.43
3:C:222:SER:O	3:C:224:LEU:N	2.51	0.43
3:C:309:HIS:CD2	3:C:309:HIS:C	2.97	0.43
3:C:681:GLN:C	3:C:681:GLN:HE21	2.27	0.43
3:C:686:GLU:C	3:C:688:VAL:H	2.27	0.43
4:D:77:HIS:CE1	4:D:97:ASP:OD1	2.72	0.43
1:A:109:GLN:HE22	1:A:111:ARG:NH1	2.16	0.43
1:A:1114:TYR:CD1	1:A:1114:TYR:C	2.52	0.43
2:B:112:GLN:NE2	2:B:187:THR:HG23	2.34	0.43
3:C:399:ASN:ND2	3:C:444:HIS:CE1	2.87	0.43
3:C:452:PHE:O	3:C:453:TYR:C	2.61	0.43
3:C:583:LYS:O	3:C:584:GLU:CB	2.66	0.43
3:C:657:ASN:CG	3:C:658:GLY:N	2.76	0.43
1:A:553:SER:HA	1:A:554:PRO:HD3	1.80	0.43
2:B:148:PRO:C	2:B:150:GLU:N	2.76	0.43
3:C:90:VAL:O	3:C:92:ASN:N	2.51	0.43
3:C:141:ASP:O	3:C:145:GLN:HG2	2.19	0.43
3:C:186:LYS:CB	3:C:188:VAL:HG23	2.44	0.43
3:C:203:GLU:HB2	3:C:209:VAL:HG21	2.00	0.43
3:C:709:THR:HA	3:C:755:TYR:O	2.19	0.43
3:C:709:THR:HG23	3:C:756:HIS:CD2	2.53	0.43
1:A:70:LYS:O	1:A:147:ARG:NH2	2.49	0.42
1:A:190:VAL:HG13	1:A:190:VAL:O	2.19	0.42
1:A:494:GLN:O	1:A:495:ALA:HB3	2.19	0.42
1:A:505:SER:OG	1:A:506:SER:N	2.52	0.42
1:A:1020:THR:O	1:A:1020:THR:OG1	2.24	0.42
3:C:123:GLU:HB3	3:C:124:ASP:H	1.61	0.42
3:C:592:SER:OG	3:C:595:GLN:HG3	2.19	0.42
1:A:6:VAL:HG13	1:A:6:VAL:O	2.19	0.42
1:A:239:TYR:CE2	1:A:297:LEU:HD13	2.54	0.42
1:A:275:ASP:CG	1:A:279:ARG:HB2	2.43	0.42
1:A:428:SER:OG	1:A:456:GLN:HG2	2.18	0.42
1:A:586:ILE:HG21	1:A:608:ASP:N	2.34	0.42
2:B:170:PHE:N	2:B:170:PHE:HD2	2.13	0.42
2:B:204:PHE:CD1	2:B:204:PHE:N	2.87	0.42
3:C:450:GLU:HG3	3:C:451:ALA:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:624:LEU:HD22	3:C:628:LEU:HG	2.01	0.42
3:C:692:ARG:HG2	3:C:725:PHE:CE2	2.54	0.42
1:A:80:LEU:HD11	1:A:84:TYR:HA	2.01	0.42
1:A:351:GLU:HG2	1:A:352:THR:N	2.34	0.42
1:A:507:GLN:HE22	1:A:552:LEU:CA	2.27	0.42
1:A:1006:VAL:CG2	1:A:1007:PHE:N	2.81	0.42
3:C:72:ALA:HB1	3:C:77:THR:HB	2.01	0.42
3:C:539:MET:HE3	3:C:619:ILE:HA	2.02	0.42
3:C:597:LEU:HA	3:C:600:LEU:HD12	2.02	0.42
3:C:603:ASN:OD1	4:D:22:PHE:HB2	2.19	0.42
1:A:105:HIS:HA	1:A:152:LEU:HD12	1.98	0.42
1:A:335:LYS:O	1:A:348:VAL:HG22	2.18	0.42
1:A:537:GLU:OE1	3:C:82:ASN:HB2	2.20	0.42
2:B:172:ARG:HG2	2:B:173:ARG:N	2.34	0.42
3:C:51:ARG:C	3:C:53:ARG:H	2.26	0.42
3:C:623:GLU:O	3:C:624:LEU:C	2.61	0.42
1:A:124:ILE:HG12	1:A:131:ILE:HG23	2.01	0.42
1:A:255:GLN:HE21	1:A:279:ARG:NH2	2.16	0.42
1:A:534:MET:HE2	1:A:569:LEU:HD11	2.00	0.42
1:A:1106:GLN:C	1:A:1108:VAL:N	2.78	0.42
3:C:42:LYS:O	3:C:43:LEU:CD2	2.67	0.42
3:C:74:GLN:HB3	3:C:113:HIS:NE2	2.34	0.42
1:A:699:LEU:HD13	1:A:700:THR:N	2.35	0.42
1:A:859:GLN:HA	1:A:859:GLN:OE1	2.19	0.42
1:A:961:ASP:OD2	1:A:964:ASN:N	2.51	0.42
1:A:1047:TRP:CZ3	1:A:1132:VAL:HG13	2.55	0.42
1:A:1121:LYS:HB2	1:A:1121:LYS:HZ2	1.83	0.42
3:C:59:THR:O	3:C:63:TRP:HD1	2.02	0.42
3:C:279:ASP:O	3:C:281:SER:N	2.52	0.42
3:C:541:VAL:HG23	3:C:543:LEU:HD21	2.02	0.42
3:C:640:ILE:O	3:C:655:ILE:HD12	2.20	0.42
3:C:735:ARG:HA	3:C:735:ARG:HE	1.84	0.42
1:A:197:LEU:O	1:A:200:LYS:HG3	2.19	0.42
1:A:422:TYR:CE1	1:A:683:ASN:N	2.84	0.42
1:A:1048:TYR:CZ	1:A:1052:LEU:HD22	2.54	0.42
1:A:1101:SER:CB	1:A:1103:PRO:HD2	2.49	0.42
2:B:83:ILE:CD1	2:B:141:MET:HE1	2.49	0.42
2:B:119:GLY:O	2:B:120:LYS:HB2	2.18	0.42
3:C:536:TYR:CD2	3:C:573:LEU:HD11	2.54	0.42
1:A:278:GLY:O	1:A:279:ARG:C	2.63	0.42
1:A:416:ASP:OD1	1:A:416:ASP:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1055:GLN:NE2	1:A:1089:ILE:HA	2.34	0.42
2:B:179:TRP:N	2:B:179:TRP:HE3	2.18	0.42
3:C:75:SER:O	3:C:77:THR:N	2.53	0.42
3:C:182:ILE:CG2	3:C:183:ILE:HG13	2.50	0.42
3:C:643:PRO:O	3:C:644:LYS:C	2.62	0.42
4:D:75:CYS:HB2	4:D:97:ASP:OD2	2.19	0.42
1:A:963:ASP:N	1:A:963:ASP:OD2	2.53	0.42
2:B:86:VAL:HG11	2:B:198:THR:HA	1.99	0.42
2:B:136:GLY:O	2:B:138:GLU:N	2.53	0.42
3:C:227:TYR:C	3:C:229:ASP:N	2.78	0.42
3:C:250:LEU:HD22	3:C:254:ARG:HD3	2.01	0.42
3:C:425:THR:HG22	3:C:426:ASP:N	2.35	0.42
3:C:575:HIS:CE1	4:D:28:ASN:HB2	2.55	0.42
1:A:59:GLY:HA3	1:A:81:THR:HG23	2.02	0.42
1:A:265:ASP:O	1:A:267:ASN:N	2.53	0.42
1:A:270:ARG:HG2	1:A:284:LEU:CD2	2.50	0.42
1:A:754:PRO:O	1:A:755:SER:HB3	2.20	0.42
2:B:103:LEU:O	2:B:104:GLY:C	2.63	0.42
3:C:488:THR:O	3:C:489:SER:C	2.63	0.42
4:D:37:ILE:HG23	4:D:40:ASP:HA	2.02	0.42
1:A:92:LYS:HD2	1:A:101:ILE:HD13	2.02	0.41
1:A:565:SER:CB	1:A:567:ARG:HH11	2.33	0.41
1:A:41:ILE:O	1:A:52:VAL:HG22	2.19	0.41
1:A:1065:VAL:HG12	1:A:1065:VAL:O	2.20	0.41
2:B:175:TYR:HE2	2:B:188:GLU:OE1	2.03	0.41
3:C:95:SER:O	3:C:96:HIS:O	2.38	0.41
3:C:284:LYS:HB2	3:C:284:LYS:HE3	1.88	0.41
3:C:543:LEU:HD22	3:C:543:LEU:N	2.36	0.41
3:C:650:ASP:OD2	3:C:650:ASP:N	2.53	0.41
3:C:707:ARG:HG3	3:C:707:ARG:O	2.19	0.41
4:D:87:TRP:CH2	4:D:93:VAL:O	2.74	0.41
1:A:38:ARG:HH21	1:A:54:GLU:CD	2.28	0.41
1:A:67:PHE:C	1:A:69:PRO:HD3	2.45	0.41
1:A:132:GLY:O	1:A:133:LEU:HD12	2.19	0.41
1:A:228:GLY:HA3	1:A:239:TYR:CE1	2.54	0.41
1:A:892:GLU:O	1:A:899:VAL:HA	2.20	0.41
1:A:980:ASP:OD1	1:A:981:SER:N	2.53	0.41
1:A:404:LEU:HD12	1:A:429:PHE:CZ	2.56	0.41
1:A:557:ALA:H	1:A:593:MET:HE2	1.85	0.41
1:A:565:SER:OG	1:A:567:ARG:NH1	2.54	0.41
2:B:137:LYS:HD3	2:B:137:LYS:C	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:600:LEU:O	3:C:601:MET:C	2.62	0.41
3:C:751:ASN:HD21	3:C:754:GLN:HB2	1.86	0.41
1:A:138:GLY:CA	1:A:159:LEU:HB2	2.50	0.41
1:A:728:GLU:O	1:A:728:GLU:CG	2.68	0.41
1:A:1136:LEU:HD23	1:A:1136:LEU:O	2.21	0.41
3:C:131:PHE:O	3:C:134:LYS:HB2	2.21	0.41
3:C:141:ASP:CG	3:C:144:ARG:HH12	2.28	0.41
1:A:134:ARG:HD2	1:A:134:ARG:C	2.45	0.41
1:A:234:GLN:O	1:A:253:ILE:HG22	2.20	0.41
1:A:331:SER:O	1:A:332:GLN:HB3	2.20	0.41
1:A:448:LEU:HD12	1:A:448:LEU:HA	1.81	0.41
1:A:523:PRO:HB3	1:A:524:GLN:NE2	2.35	0.41
1:A:844:LYS:O	1:A:867:LYS:CA	2.69	0.41
1:A:1095:GLU:C	1:A:1097:PHE:H	2.28	0.41
2:B:100:ASN:HA	2:B:101:PRO:HD3	1.91	0.41
2:B:102:LEU:C	2:B:104:GLY:N	2.78	0.41
2:B:115:LEU:HG	2:B:130:VAL:HG13	2.03	0.41
2:B:204:PHE:N	2:B:204:PHE:HD1	2.19	0.41
3:C:526:ASN:HD22	3:C:526:ASN:HA	1.61	0.41
3:C:739:LEU:HD23	3:C:739:LEU:HA	1.91	0.41
4:D:45:CYS:CB	4:D:47:ASN:HD21	2.31	0.41
1:A:32:LEU:CD1	1:A:77:LEU:HD13	2.50	0.41
1:A:487:VAL:O	1:A:487:VAL:HG23	2.20	0.41
1:A:580:GLU:C	1:A:581:MET:HE2	2.45	0.41
2:B:98:ILE:HA	2:B:99:PRO:HD3	1.85	0.41
3:C:232:GLU:O	3:C:235:PHE:HB3	2.20	0.41
3:C:587:LYS:HB2	3:C:660:PHE:CZ	2.55	0.41
3:C:734:LYS:HD3	3:C:737:GLU:OE2	2.20	0.41
1:A:63:VAL:HG11	1:A:122:GLY:HA3	2.02	0.41
1:A:237:ILE:O	1:A:247:ALA:HA	2.20	0.41
1:A:263:ARG:HD2	1:A:265:ASP:O	2.21	0.41
1:A:388:ARG:NH1	1:A:714:THR:CB	2.84	0.41
1:A:414:ARG:HH11	1:A:414:ARG:CG	2.32	0.41
1:A:921:ILE:N	1:A:921:ILE:HD12	2.36	0.41
2:B:44:PRO:HA	2:B:45:PRO:HD2	1.77	0.41
3:C:508:PHE:O	3:C:512:MET:HB2	2.21	0.41
1:A:21:GLY:O	1:A:30:ASN:HB2	2.20	0.41
1:A:102:THR:HG21	1:A:1067:LYS:HG3	2.03	0.41
1:A:144:PRO:HD2	1:A:149:ASN:ND2	2.36	0.41
1:A:212:VAL:O	1:A:213:GLU:C	2.64	0.41
1:A:265:ASP:OD2	1:A:270:ARG:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:SER:HG	1:A:344:GLY:HA2	1.82	0.41
1:A:404:LEU:HD13	1:A:404:LEU:HA	1.89	0.41
1:A:413:LEU:HD13	1:A:468:LEU:HD23	2.03	0.41
1:A:429:PHE:O	1:A:430:VAL:C	2.64	0.41
1:A:498:ILE:N	1:A:498:ILE:CD1	2.84	0.41
1:A:532:THR:HG22	1:A:533:GLU:H	1.80	0.41
1:A:876:PHE:CE1	1:A:918:GLY:O	2.74	0.41
1:A:949:PHE:CD1	1:A:991:HIS:CE1	3.08	0.41
2:B:86:VAL:CG1	2:B:197:ILE:O	2.69	0.41
2:B:111:THR:O	2:B:187:THR:HA	2.21	0.41
3:C:96:HIS:O	3:C:97:LYS:HB3	2.21	0.41
3:C:167:LEU:HA	3:C:168:PRO:HD3	1.49	0.41
3:C:282:THR:O	3:C:283:GLN:C	2.63	0.41
3:C:329:VAL:O	3:C:330:ARG:O	2.39	0.41
3:C:450:GLU:O	3:C:451:ALA:C	2.63	0.41
3:C:536:TYR:CD2	3:C:573:LEU:HD21	2.56	0.41
3:C:707:ARG:CD	3:C:710:LEU:HD13	2.50	0.41
3:C:744:TYR:O	3:C:757:TYR:O	2.38	0.41
1:A:987:GLU:C	1:A:989:ARG:N	2.79	0.41
3:C:63:TRP:CZ3	3:C:105:GLN:HG3	2.55	0.41
3:C:70:VAL:C	3:C:72:ALA:N	2.77	0.41
3:C:528:LEU:HB2	4:D:32:LEU:HD23	2.03	0.41
3:C:715:LEU:C	3:C:717:SER:N	2.77	0.41
1:A:382:PHE:N	1:A:382:PHE:CD1	2.88	0.40
1:A:452:VAL:HG22	1:A:477:ARG:NH1	2.36	0.40
1:A:469:ILE:HD13	1:A:469:ILE:C	2.46	0.40
3:C:232:GLU:O	3:C:233:LEU:C	2.64	0.40
3:C:279:ASP:C	3:C:281:SER:N	2.79	0.40
4:D:39:VAL:O	4:D:39:VAL:HG12	2.21	0.40
1:A:72:GLU:CD	1:A:103:ARG:NH2	2.79	0.40
1:A:257:THR:O	1:A:276:MET:N	2.54	0.40
1:A:300:LEU:CD2	1:A:300:LEU:N	2.84	0.40
1:A:301:ARG:HH11	1:A:301:ARG:HG2	1.86	0.40
1:A:451:PHE:HD1	1:A:470:GLN:CB	2.34	0.40
1:A:785:GLU:C	1:A:786:VAL:HG23	2.46	0.40
2:B:13:ILE:C	2:B:15:LYS:H	2.29	0.40
2:B:177:ILE:HG12	2:B:186:VAL:CG2	2.41	0.40
3:C:45:ILE:HG21	3:C:48:PHE:HD1	1.87	0.40
3:C:49:ARG:NE	3:C:49:ARG:HA	2.37	0.40
3:C:96:HIS:C	3:C:98:VAL:H	2.29	0.40
3:C:187:MET:O	3:C:191:LYS:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:303:LEU:HD23	3:C:322:MET:HE1	2.03	0.40
3:C:311:LEU:HA	3:C:311:LEU:HD23	1.79	0.40
3:C:408:LEU:O	3:C:409:ILE:C	2.63	0.40
4:D:80:HIS:O	4:D:81:PHE:C	2.64	0.40
1:A:40:GLU:HB3	1:A:42:TYR:HE1	1.85	0.40
1:A:67:PHE:N	1:A:67:PHE:CD2	2.90	0.40
1:A:167:VAL:HG13	1:A:180:PHE:HB3	2.04	0.40
1:A:290:GLN:HG3	1:A:294:THR:O	2.21	0.40
1:A:592:LEU:HD23	1:A:592:LEU:C	2.46	0.40
1:A:1044:SER:O	1:A:1047:TRP:N	2.54	0.40
3:C:114:VAL:C	3:C:116:ALA:N	2.79	0.40
3:C:209:VAL:O	3:C:210:ASP:HB3	2.21	0.40
3:C:267:LEU:HD21	3:C:290:VAL:HG12	2.03	0.40
3:C:390:MET:HE3	3:C:394:PHE:CD1	2.56	0.40
3:C:454:LYS:HE2	3:C:490:LYS:HD2	2.02	0.40
3:C:457:LEU:CD2	3:C:461:LEU:HG	2.52	0.40
3:C:515:GLN:C	3:C:517:ASP:H	2.30	0.40
3:C:548:ILE:O	3:C:549:LYS:C	2.65	0.40
3:C:558:TYR:O	3:C:562:HIS:HB2	2.21	0.40
1:A:125:ASP:HA	1:A:126:PRO:HD3	2.00	0.40
1:A:412:PRO:HG2	1:A:412:PRO:O	2.22	0.40
1:A:457:THR:CG2	1:A:459:PHE:O	2.69	0.40
1:A:1043:LEU:HD23	1:A:1043:LEU:HA	1.88	0.40
3:C:384:GLU:HA	3:C:387:VAL:HG23	2.04	0.40
3:C:414:ASP:O	3:C:418:ARG:HG3	2.21	0.40
1:A:57:MET:HG3	1:A:61:ILE:HD11	2.02	0.40
1:A:67:PHE:O	1:A:69:PRO:HD3	2.21	0.40
1:A:105:HIS:HA	1:A:152:LEU:CD1	2.52	0.40
1:A:111:ARG:HD2	1:A:111:ARG:HA	1.63	0.40
1:A:337:ASN:ND2	1:A:348:VAL:HG11	2.36	0.40
1:A:411:TRP:HA	1:A:412:PRO:HD3	1.90	0.40
1:A:413:LEU:HD23	1:A:413:LEU:HA	1.83	0.40
1:A:416:ASP:HA	1:A:417:PRO:HD3	1.88	0.40
1:A:603:LEU:HD23	1:A:603:LEU:N	2.34	0.40
1:A:699:LEU:HD13	1:A:699:LEU:C	2.46	0.40
1:A:990:GLN:HE21	1:A:990:GLN:HB2	1.65	0.40
3:C:153:PHE:O	3:C:154:LEU:C	2.64	0.40
3:C:188:VAL:O	3:C:192:THR:OG1	2.29	0.40
3:C:274:VAL:HG21	3:C:283:GLN:HB2	2.04	0.40
3:C:527:ILE:O	3:C:527:ILE:HG23	2.21	0.40
3:C:591:VAL:CG1	3:C:669:ILE:HD12	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:94:CYS:HA	4:D:95:PRO:HD2	1.91	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:60:GLN:NE2	3:C:60:GLN:NE2[3_554]	2.09	0.11

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	1138/1140 (100%)	869 (76%)	201 (18%)	68 (6%)	1	7
2	B	174/222 (78%)	119 (68%)	37 (21%)	18 (10%)	0	2
3	C	717/759 (94%)	516 (72%)	132 (18%)	69 (10%)	0	3
4	D	88/108 (82%)	47 (53%)	27 (31%)	14 (16%)	0	0
All	All	2117/2229 (95%)	1551 (73%)	397 (19%)	169 (8%)	1	4

All (169) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	ILE
1	A	290	GLN
1	A	292	ASP
1	A	430	VAL
1	A	583	GLY
1	A	598	SER
1	A	672	ASN
1	A	746	SER
1	A	761	LEU

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Mol	Chain	Res	Type
1	A	826	ASN
1	A	1020	THR
1	A	1094	ILE
1	A	1110	ALA
1	A	1115	ASP
1	A	1127	ASP
2	B	53	ASN
2	B	92	THR
2	B	163	ARG
2	B	206	CYS
2	B	209	HIS
3	C	42	LYS
3	C	49	ARG
3	C	56	ASP
3	C	58	TYR
3	C	76	SER
3	C	82	ASN
3	C	83	LEU
3	C	96	HIS
3	C	126	LEU
3	C	128	SER
3	C	185	ASP
3	C	191	LYS
3	C	276	THR
3	C	330	ARG
3	C	483	CYS
3	C	517	ASP
3	C	587	LYS
3	C	606	ASP
3	C	633	CYS
3	C	644	LYS
3	C	660	PHE
3	C	661	LYS
3	C	752	PRO
4	D	22	PHE
4	D	38	VAL
4	D	84	ILE
4	D	104	GLN
1	A	46	ALA
1	A	147	ARG
1	A	172	GLY
1	A	279	ARG

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Mol	Chain	Res	Type
1	A	549	SER
1	A	584	GLY
1	A	674	LYS
1	A	860	THR
1	A	863	GLU
1	A	983	ALA
1	A	1084	PRO
1	A	1121	LYS
1	A	1123	GLU
2	B	38	LEU
2	B	104	GLY
2	B	137	LYS
2	B	171	HIS
3	C	129	VAL
3	C	209	VAL
3	C	229	ASP
3	C	240	ASN
3	C	280	HIS
3	C	441	ARG
3	C	598	VAL
3	C	607	GLY
3	C	652	ASP
3	C	670	ASN
3	C	691	ASP
4	D	90	THR
4	D	96	LEU
4	D	105	LYS
1	A	36	ASN
1	A	113	GLY
1	A	115	PRO
1	A	213	GLU
1	A	418	ASN
1	A	449	MET
1	A	481	GLN
1	A	547	GLY
1	A	624	SER
1	A	644	LEU
1	A	738	SER
1	A	861	VAL
1	A	901	THR
1	A	910	MET
1	A	917	LYS

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Mol	Chain	Res	Type
1	A	947	ARG
1	A	1021	SER
1	A	1124	ALA
2	B	140	LEU
2	B	199	ALA
3	C	55	PRO
3	C	71	ARG
3	C	75	SER
3	C	119	LEU
3	C	223	ASP
3	C	293	GLN
3	C	350	ALA
3	C	402	PRO
3	C	451	ALA
3	C	586	LYS
3	C	727	VAL
3	C	757	TYR
3	C	758	VAL
4	D	52	LEU
4	D	83	CYS
4	D	87	TRP
1	A	153	LYS
1	A	204	LYS
1	A	488	SER
1	A	503	CYS
1	A	751	ALA
1	A	783	GLY
1	A	1008	CYS
1	A	1114	TYR
3	C	54	LEU
3	C	91	GLU
3	C	189	GLN
3	C	201	GLU
3	C	205	SER
3	C	228	LYS
3	C	325	LEU
3	C	377	GLU
3	C	514	ASN
3	C	610	PHE
3	C	726	PRO
4	D	102	GLU
1	A	224	GLU

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Mol	Chain	Res	Type
1	A	592	LEU
1	A	745	THR
1	A	884	ILE
1	A	972	PHE
2	B	12	GLU
2	B	108	THR
2	B	192	PRO
3	C	171	TRP
3	C	233	LEU
3	C	378	VAL
3	C	440	PHE
3	C	597	LEU
4	D	40	ASP
4	D	103	PHE
1	A	460	CYS
1	A	903	CYS
1	A	937	PRO
2	B	95	GLY
2	B	136	GLY
2	B	196	PRO
3	C	51	ARG
1	A	61	ILE
1	A	493	PRO
1	A	551	GLY
3	C	52	PRO
3	C	619	ILE
4	D	94	CYS
3	C	306	GLY
1	A	406	GLY
1	A	523	PRO
1	A	707	ILE
2	B	151	ASN
3	C	405	PRO
3	C	519	GLY

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	999/999 (100%)	859 (86%)	140 (14%)	3	15
2	B	157/191 (82%)	135 (86%)	22 (14%)	3	15
3	C	656/679 (97%)	589 (90%)	67 (10%)	7	28
4	D	79/90 (88%)	64 (81%)	15 (19%)	1	7
All	All	1891/1959 (96%)	1647 (87%)	244 (13%)	4	18

All (244) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	11	LYS
1	A	27	GLU
1	A	49	LEU
1	A	57	MET
1	A	67	PHE
1	A	103	ARG
1	A	112	ILE
1	A	152	LEU
1	A	156	ASN
1	A	158	ARG
1	A	160	GLU
1	A	180	PHE
1	A	198	ARG
1	A	210	GLU
1	A	245	TYR
1	A	266	PRO
1	A	269	SER
1	A	285	LEU
1	A	298	LYS
1	A	309	SER
1	A	315	THR
1	A	328	LEU
1	A	333	LEU
1	A	338	VAL
1	A	353	PHE
1	A	356	LEU
1	A	372	GLN
1	A	374	GLN
1	A	387	LEU
1	A	389	ILE
1	A	390	ILE
1	A	396	ILE

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Mol	Chain	Res	Type
1	A	404	LEU
1	A	410	LEU
1	A	412	PRO
1	A	414	ARG
1	A	419	ARG
1	A	420	GLU
1	A	422	TYR
1	A	448	LEU
1	A	452	VAL
1	A	454	ASP
1	A	469	ILE
1	A	473	SER
1	A	476	VAL
1	A	481	GLN
1	A	482	GLU
1	A	487	VAL
1	A	493	PRO
1	A	510	VAL
1	A	518	TYR
1	A	521	ILE
1	A	523	PRO
1	A	525	GLU
1	A	531	HIS
1	A	533	GLU
1	A	540	CYS
1	A	555	LEU
1	A	562	THR
1	A	563	ASP
1	A	567	ARG
1	A	576	LEU
1	A	582	LEU
1	A	587	ILE
1	A	592	LEU
1	A	594	THR
1	A	597	GLU
1	A	602	LEU
1	A	603	LEU
1	A	608	ASP
1	A	614	PHE
1	A	616	LEU
1	A	617	ASN
1	A	618	ILE

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Mol	Chain	Res	Type
1	A	620	THR
1	A	623	LEU
1	A	625	ASP
1	A	627	LYS
1	A	629	VAL
1	A	636	THR
1	A	646	THR
1	A	655	ARG
1	A	663	ASN
1	A	673	LEU
1	A	688	PRO
1	A	700	THR
1	A	701	ILE
1	A	703	THR
1	A	704	ILE
1	A	713	ARG
1	A	714	THR
1	A	720	SER
1	A	727	GLN
1	A	762	SER
1	A	771	PHE
1	A	784	GLU
1	A	798	THR
1	A	814	LEU
1	A	817	VAL
1	A	818	SER
1	A	820	LYS
1	A	855	ASP
1	A	863	GLU
1	A	870	VAL
1	A	872	SER
1	A	884	ILE
1	A	887	THR
1	A	899	VAL
1	A	902	GLU
1	A	914	LEU
1	A	931	LEU
1	A	936	LYS
1	A	938	MET
1	A	964	ASN
1	A	966	LEU
1	A	969	GLU

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Mol	Chain	Res	Type
1	A	987	GLU
1	A	990	GLN
1	A	992	LEU
1	A	993	GLN
1	A	1000	LEU
1	A	1006	VAL
1	A	1021	SER
1	A	1023	PRO
1	A	1034	ASN
1	A	1036	MET
1	A	1054	MET
1	A	1065	VAL
1	A	1069	GLU
1	A	1083	GLU
1	A	1086	THR
1	A	1093	LEU
1	A	1105	MET
1	A	1109	VAL
1	A	1115	ASP
1	A	1121	LYS
1	A	1123	GLU
1	A	1135	GLU
1	A	1139	ILE
2	B	14	ASN
2	B	17	ILE
2	B	21	LEU
2	B	28	THR
2	B	43	ILE
2	B	85	ILE
2	B	86	VAL
2	B	93	VAL
2	B	106	ASP
2	B	109	PRO
2	B	115	LEU
2	B	117	LEU
2	B	131	LYS
2	B	137	LYS
2	B	152	PRO
2	B	163	ARG
2	B	170	PHE
2	B	179	TRP
2	B	192	PRO

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Mol	Chain	Res	Type
2	B	197	ILE
2	B	202	ARG
2	B	206	CYS
3	C	43	LEU
3	C	62	THR
3	C	64	ARG
3	C	79	ILE
3	C	90	VAL
3	C	93	LEU
3	C	102	LEU
3	C	112	ASP
3	C	135	ILE
3	C	159	THR
3	C	171	TRP
3	C	173	MET
3	C	175	LEU
3	C	182	ILE
3	C	183	ILE
3	C	193	ILE
3	C	199	LEU
3	C	209	VAL
3	C	217	LEU
3	C	226	VAL
3	C	249	ARG
3	C	251	MET
3	C	281	SER
3	C	283	GLN
3	C	287	ILE
3	C	290	VAL
3	C	300	THR
3	C	307	LEU
3	C	353	ILE
3	C	371	LYS
3	C	389	LEU
3	C	390	MET
3	C	402	PRO
3	C	422	LYS
3	C	423	GLU
3	C	428	GLU
3	C	429	LEU
3	C	439	LEU
3	C	450	GLU

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Mol	Chain	Res	Type
3	C	457	LEU
3	C	478	LYS
3	C	482	GLU
3	C	483	CYS
3	C	494	MET
3	C	498	MET
3	C	526	ASN
3	C	530	MET
3	C	546	GLU
3	C	562	HIS
3	C	570	GLN
3	C	591	VAL
3	C	611	GLU
3	C	624	LEU
3	C	626	ARG
3	C	639	LEU
3	C	652	ASP
3	C	660	PHE
3	C	677	THR
3	C	681	GLN
3	C	683	SER
3	C	691	ASP
3	C	706	MET
3	C	714	LEU
3	C	726	PRO
3	C	735	ARG
3	C	748	ASP
3	C	751	ASN
4	D	19	LYS
4	D	23	GLU
4	D	25	LYS
4	D	32	LEU
4	D	37	ILE
4	D	41	ASN
4	D	42	CYS
4	D	47	ASN
4	D	49	ILE
4	D	54	ILE
4	D	64	THR
4	D	84	ILE
4	D	98	ASN
4	D	99	ARG

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Mol	Chain	Res	Type
4	D	103	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	16	ASN
1	A	30	ASN
1	A	85	ASN
1	A	93	GLN
1	A	105	HIS
1	A	109	GLN
1	A	203	ASN
1	A	234	GLN
1	A	255	GLN
1	A	262	ASN
1	A	332	GLN
1	A	343	GLN
1	A	372	GLN
1	A	374	GLN
1	A	432	GLN
1	A	455	GLN
1	A	462	ASN
1	A	467	GLN
1	A	481	GLN
1	A	494	GLN
1	A	507	GLN
1	A	524	GLN
1	A	578	HIS
1	A	634	GLN
1	A	663	ASN
1	A	677	ASN
1	A	708	GLN
1	A	727	GLN
1	A	790	ASN
1	A	796	GLN
1	A	809	GLN
1	A	810	ASN
1	A	859	GLN
1	A	904	ASN
1	A	907	ASN
1	A	964	ASN

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Mol	Chain	Res	Type
1	A	990	GLN
1	A	1016	ASN
1	A	1034	ASN
1	A	1055	GLN
1	A	1056	ASN
1	A	1077	HIS
2	B	30	GLN
2	B	31	GLN
2	B	41	ASN
2	B	112	GLN
2	B	191	ASN
2	B	210	GLN
3	C	92	ASN
3	C	115	GLN
3	C	283	GLN
3	C	309	HIS
3	C	333	GLN
3	C	338	GLN
3	C	339	HIS
3	C	363	GLN
3	C	399	ASN
3	C	412	HIS
3	C	511	HIS
3	C	514	ASN
3	C	526	ASN
3	C	551	GLN
3	C	570	GLN
3	C	575	HIS
3	C	595	GLN
3	C	629	GLN
3	C	657	ASN
3	C	670	ASN
3	C	681	GLN
3	C	712	HIS
3	C	722	GLN
3	C	751	ASN
3	C	754	GLN
3	C	756	HIS
4	D	28	ASN
4	D	41	ASN
4	D	47	ASN
4	D	48	HIS

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Mol	Chain	Res	Type
4	D	98	ASN
4	D	108	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	1140/1140 (100%)	-0.24	7 (0%) 85 70	22, 68, 125, 202	0
2	B	180/222 (81%)	0.20	7 (3%) 43 24	32, 86, 135, 167	0
3	C	719/759 (94%)	-0.27	3 (0%) 88 76	23, 71, 126, 173	0
4	D	90/108 (83%)	0.14	3 (3%) 49 29	44, 75, 117, 140	0
All	All	2129/2229 (95%)	-0.19	20 (0%) 81 63	22, 71, 126, 202	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	423	GLU	4.7
2	B	152	PRO	3.6
2	B	84	ALA	3.0
2	B	12	GLU	2.9
1	A	1119	GLY	2.8
2	B	10	PRO	2.5
2	B	54	ALA	2.5
1	A	1114	TYR	2.5
1	A	268	GLY	2.5
1	A	767	SER	2.4
1	A	229	ALA	2.3
1	A	963	ASP	2.3
3	C	731	ASP	2.3
4	D	83	CYS	2.2
3	C	660	PHE	2.2
2	B	11	ASP	2.2
2	B	140	LEU	2.1
4	D	86	ARG	2.1
1	A	916	THR	2.0
4	D	67	GLU	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
5	ZN	D	4001	1/1	0.95	0.06	77,77,77,77	0
5	ZN	B	3001	1/1	0.96	0.05	114,114,114,114	0
5	ZN	D	4002	1/1	0.98	0.06	99,99,99,99	0
5	ZN	D	4003	1/1	0.99	0.06	84,84,84,84	0
5	ZN	B	3002	1/1	0.99	0.03	91,91,91,91	0

6.5 Other polymers [i](#)

There are no such residues in this entry.