



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 5Y7O / pdb_00005y7o
Title : Crystal structure of folding sensor region of UGGT from *Thermomyces dupon-*
tii
Authors : Satoh, T.; Song, C.; Zhu, T.; Toshimori, T.; Murata, K.; Hayashi, Y.;
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Deposited on : 2017-08-17
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
Mogul	:	2022.3.0, CSD as543be (2022)
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

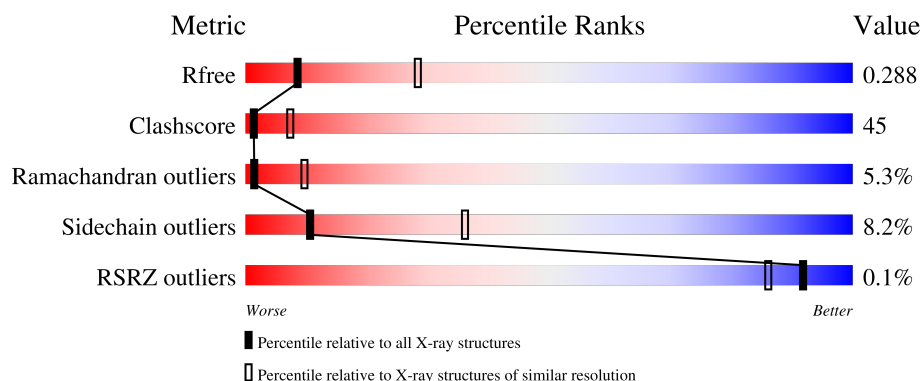
1 Overall quality at a glance

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)

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 14318 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 UGGT.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	913	Total	C	N	O	S	Se	0	0	0
			7159	4556	1224	1362	2	15			
1	B	913	Total	C	N	O	S	Se	0	0	0
			7159	4556	1224	1362	2	15			

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics

Property	Value	Source
Space group	P 32 1 2	Depositor
Cell constants a, b, c, α , β , γ	195.09Å 195.09Å 142.26Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.97 – 3.10 19.97 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.0 (19.97-3.10) 98.0 (19.97-3.10)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 3.09Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.232 , 0.278 0.232 , 0.288	Depositor DCC
R_{free} test set	2744 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	110.4	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 162.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.40$	Xtriage
Estimated twinning fraction	0.478 for -h,-k,l	Xtriage
Reported twinning fraction	0.500 for -h,-k,l	Depositor
Outliers	0 of 54601 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14318	wwPDB-VP
Average B, all atoms (Å ²)	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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.

4 Model quality

4.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.86	3/7286 (0.0%)	1.51	117/9871 (1.2%)
1	B	0.82	4/7286 (0.1%)	1.44	103/9871 (1.0%)
All	All	0.84	7/14572 (0.0%)	1.47	220/19742 (1.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	14
1	B	0	9
All	All	0	23

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	209	ALA	CA-CB	-9.38	1.37	1.53
1	A	100	ALA	CA-CB	-6.32	1.45	1.54
1	A	292	VAL	CA-CB	-6.11	1.48	1.55
1	B	292	VAL	CA-CB	-5.94	1.48	1.55
1	B	855	VAL	CA-CB	5.52	1.59	1.53
1	A	401	LEU	CG-CD2	-5.48	1.34	1.52
1	B	211	GLU	CB-CG	-5.17	1.36	1.52

All (220) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	664	ASP	CA-C-N	-15.82	100.06	119.84
1	B	664	ASP	C-N-CA	-15.82	100.06	119.84
1	A	804	ARG	N-CA-C	12.97	128.78	109.07
1	A	854	LYS	N-CA-C	-11.74	98.46	113.72
1	A	664	ASP	CA-C-N	-11.31	105.70	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	664	ASP	C-N-CA	-11.31	105.70	119.84
1	B	743	HIS	N-CA-C	11.14	127.86	111.81
1	A	581	VAL	N-CA-C	-11.13	100.40	113.42
1	A	337	LEU	N-CA-C	10.37	126.23	113.17
1	A	401	LEU	CB-CG-CD2	-10.29	79.83	110.70
1	A	786	TYR	N-CA-C	-10.03	100.31	111.14
1	A	113	SER	N-CA-C	9.96	125.52	113.16
1	A	394	ILE	N-CA-C	-9.94	98.68	112.50
1	B	859	VAL	N-CA-C	-9.91	100.71	110.72
1	A	974	GLU	N-CA-C	9.55	122.32	108.86
1	B	573	LEU	N-CA-C	-9.19	102.19	112.57
1	A	564	GLY	N-CA-C	9.09	134.73	113.18
1	B	336	PHE	N-CA-C	-8.95	101.21	110.97
1	A	893	LYS	N-CA-C	8.82	122.84	108.55
1	B	201	TYR	N-CA-C	-8.81	100.27	111.02
1	B	211	GLU	CA-CB-CG	-8.76	96.59	114.10
1	B	893	LYS	N-CA-C	8.75	122.94	107.80
1	B	674	VAL	N-CA-C	-8.66	91.33	109.34
1	A	579	GLU	CA-C-N	-8.65	109.50	122.83
1	A	579	GLU	C-N-CA	-8.65	109.50	122.83
1	B	440	ARG	N-CA-C	-8.49	101.99	111.07
1	A	816	VAL	CA-C-N	-8.47	109.25	119.84
1	A	816	VAL	C-N-CA	-8.47	109.25	119.84
1	A	205	LEU	N-CA-C	-8.43	102.99	113.28
1	B	675	GLN	N-CA-C	-8.43	102.78	113.23
1	B	743	HIS	CB-CA-C	-8.38	100.69	111.50
1	B	399	LEU	N-CA-C	-8.28	101.30	111.40
1	A	378	HIS	N-CA-C	-8.16	100.37	111.55
1	B	569	PHE	CB-CA-C	-8.05	106.22	115.79
1	A	895	TRP	N-CA-C	8.02	127.89	110.80
1	A	598	SER	CA-C-N	8.00	128.62	120.38
1	A	598	SER	C-N-CA	8.00	128.62	120.38
1	B	731	VAL	CA-C-N	7.99	129.82	119.84
1	B	731	VAL	C-N-CA	7.99	129.82	119.84
1	B	658	GLU	N-CA-C	-7.95	102.89	112.59
1	A	384	GLY	N-CA-C	-7.89	104.62	114.16
1	A	580	GLU	N-CA-C	7.83	121.42	112.57
1	B	911	SER	N-CA-C	-7.78	104.72	112.97
1	A	655	THR	N-CA-C	7.76	121.16	110.06
1	B	341	TYR	N-CA-C	-7.53	104.10	113.28
1	B	613	ASN	N-CA-C	-7.50	98.53	109.18
1	B	129	VAL	CB-CA-C	-7.49	105.34	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	592	LEU	N-CA-C	7.46	121.00	112.57
1	B	211	GLU	CB-CG-CD	7.41	125.20	112.60
1	B	207	ALA	N-CA-C	-7.39	104.36	113.15
1	B	365	ARG	CA-C-N	-7.34	111.63	122.86
1	B	365	ARG	C-N-CA	-7.34	111.63	122.86
1	B	129	VAL	N-CA-C	7.31	118.35	111.48
1	A	763	LEU	CB-CG-CD1	-7.30	88.80	110.70
1	B	837	LYS	N-CA-C	-7.29	104.41	112.72
1	A	343	ASN	N-CA-C	-7.28	104.54	113.50
1	A	348	LEU	CA-C-N	-7.24	110.79	119.84
1	A	348	LEU	C-N-CA	-7.24	110.79	119.84
1	B	657	ASN	N-CA-C	7.20	121.17	110.52
1	A	829	ILE	N-CA-C	-7.12	101.91	111.44
1	B	209	ALA	N-CA-C	-7.09	106.53	114.62
1	A	110	ALA	N-CA-C	-7.03	103.97	112.54
1	A	528	LEU	N-CA-C	6.98	121.38	113.01
1	B	974	GLU	N-CA-C	-6.94	96.02	110.80
1	B	821	THR	N-CA-C	6.92	120.95	112.23
1	A	94	GLY	N-CA-C	-6.91	106.27	115.32
1	A	542	ASP	N-CA-C	-6.88	101.65	110.53
1	A	703	VAL	N-CA-C	-6.85	98.50	108.71
1	B	453	GLN	N-CA-C	6.83	123.42	108.66
1	A	678	GLU	N-CA-C	-6.73	105.05	112.72
1	B	707	ASP	N-CA-C	-6.72	104.83	113.16
1	B	194	ALA	N-CA-C	-6.70	104.06	111.36
1	B	798	GLY	N-CA-C	-6.67	100.00	111.47
1	A	218	VAL	N-CA-C	6.67	117.72	107.99
1	B	388	LYS	N-CA-C	-6.65	104.10	111.82
1	B	398	ASP	N-CA-C	-6.64	105.58	113.21
1	B	637	ALA	N-CA-C	-6.62	99.77	109.18
1	A	725	HIS	CA-C-N	6.62	127.79	120.45
1	A	725	HIS	C-N-CA	6.62	127.79	120.45
1	A	905	SER	N-CA-C	6.61	118.91	108.79
1	B	184	ALA	CA-C-N	-6.60	112.86	119.99
1	B	184	ALA	C-N-CA	-6.60	112.86	119.99
1	A	1001	PRO	CA-C-N	6.57	126.51	119.28
1	A	1001	PRO	C-N-CA	6.57	126.51	119.28
1	A	292	VAL	N-CA-C	6.57	117.91	111.67
1	A	455	THR	N-CA-C	-6.56	100.81	110.52
1	A	284	LEU	N-CA-C	-6.48	103.84	111.03
1	A	827	LEU	CA-C-N	-6.48	112.37	122.67
1	A	827	LEU	C-N-CA	-6.48	112.37	122.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	545	ALA	N-CA-C	-6.46	104.31	111.36
1	B	816	VAL	CA-C-N	6.45	127.90	119.84
1	B	816	VAL	C-N-CA	6.45	127.90	119.84
1	A	912	ILE	CA-C-N	-6.44	113.92	123.00
1	A	912	ILE	C-N-CA	-6.44	113.92	123.00
1	B	180	GLY	N-CA-C	-6.44	104.57	112.68
1	A	382	PHE	N-CA-C	-6.43	104.27	111.28
1	A	656	ARG	N-CA-C	6.42	124.48	110.80
1	B	599	PRO	CA-C-N	6.41	127.86	119.84
1	B	599	PRO	C-N-CA	6.41	127.86	119.84
1	B	103	SER	N-CA-C	6.41	118.35	111.36
1	B	338	ASP	CA-C-N	-6.41	112.08	122.26
1	B	338	ASP	C-N-CA	-6.41	112.08	122.26
1	A	609	GLY	N-CA-C	-6.40	102.07	111.03
1	B	453	GLN	CB-CA-C	-6.38	104.02	110.65
1	A	734	HIS	N-CA-C	6.36	118.61	109.14
1	A	837	LYS	N-CA-C	-6.34	105.50	112.72
1	A	527	GLY	N-CA-C	6.33	128.18	113.18
1	B	892	ILE	CA-C-N	-6.30	113.30	122.44
1	B	892	ILE	C-N-CA	-6.30	113.30	122.44
1	A	836	SER	CB-CA-C	-6.30	107.58	115.89
1	A	570	GLU	CB-CA-C	-6.29	108.31	115.79
1	B	1001	PRO	CA-C-N	6.27	126.17	119.28
1	B	1001	PRO	C-N-CA	6.27	126.17	119.28
1	B	770	LYS	N-CA-C	-6.22	105.51	113.23
1	A	731	VAL	CA-C-N	6.20	126.16	120.03
1	A	731	VAL	C-N-CA	6.20	126.16	120.03
1	A	580	GLU	CA-C-N	-6.19	114.48	121.85
1	A	580	GLU	C-N-CA	-6.19	114.48	121.85
1	A	728	ILE	N-CA-C	6.15	117.34	108.48
1	A	105	PHE	N-CA-C	-6.13	104.52	111.14
1	A	798	GLY	N-CA-C	-6.13	100.93	111.47
1	A	205	LEU	CA-CB-CG	-6.12	94.90	116.30
1	B	562	LEU	N-CA-C	6.12	123.83	110.80
1	A	814	GLY	CA-C-N	6.11	127.48	119.84
1	A	814	GLY	C-N-CA	6.11	127.48	119.84
1	B	563	ARG	CB-CG-CD	6.11	125.36	111.30
1	B	836	SER	CB-CA-C	-6.10	107.84	115.89
1	B	560	ARG	CB-CG-CD	6.07	125.27	111.30
1	B	568	SER	N-CA-C	6.07	123.72	110.80
1	B	593	ASP	N-CA-C	6.06	119.92	111.74
1	A	861	PHE	N-CA-C	-6.05	104.25	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	101	ASP	N-CA-C	-6.05	104.01	111.33
1	B	698	LEU	N-CA-C	6.04	118.70	110.55
1	A	785	ALA	N-CA-C	6.02	123.63	110.80
1	A	584	LYS	N-CA-C	-5.91	104.92	111.36
1	B	451	LEU	N-CA-C	-5.88	96.84	107.60
1	A	706	PHE	N-CA-C	-5.87	101.72	110.23
1	B	513	LYS	N-CA-C	-5.85	104.54	111.03
1	A	333	THR	N-CA-C	5.81	118.50	109.60
1	A	396	ALA	CA-C-N	-5.81	111.43	121.66
1	A	396	ALA	C-N-CA	-5.81	111.43	121.66
1	A	285	LYS	CA-C-N	5.80	127.09	119.84
1	A	285	LYS	C-N-CA	5.80	127.09	119.84
1	B	292	VAL	N-CA-C	5.80	116.55	111.56
1	B	563	ARG	CG-CD-NE	5.77	124.69	112.00
1	B	851	LEU	N-CA-C	-5.74	101.90	110.23
1	A	703	VAL	CB-CA-C	5.73	119.06	110.98
1	A	210	LYS	CB-CG-CD	5.72	124.45	111.30
1	A	847	LYS	N-CA-C	-5.70	98.66	110.80
1	B	745	SER	N-CA-C	-5.70	104.53	112.45
1	B	238	VAL	N-CA-C	5.69	116.20	107.77
1	B	361	GLN	N-CA-C	5.68	118.24	110.24
1	B	67	ARG	N-CA-C	5.67	117.27	111.14
1	A	911	SER	N-CA-C	-5.66	106.97	112.97
1	B	340	TYR	CA-CB-CG	-5.65	103.72	113.90
1	A	618	LEU	N-CA-C	-5.65	104.81	110.97
1	B	561	VAL	N-CA-C	-5.62	103.90	111.44
1	A	141	CYS	CA-C-N	5.62	126.86	119.84
1	A	141	CYS	C-N-CA	5.62	126.86	119.84
1	A	895	TRP	CB-CA-C	-5.61	99.26	110.42
1	B	543	LYS	N-CA-C	5.59	118.58	109.24
1	A	204	LYS	CA-CB-CG	5.59	125.28	114.10
1	A	229	ARG	CA-C-N	-5.59	114.99	120.52
1	A	229	ARG	C-N-CA	-5.59	114.99	120.52
1	A	610	ARG	N-CA-C	-5.59	106.47	113.28
1	B	753	ARG	N-CA-C	-5.58	98.92	110.80
1	A	708	SER	N-CA-C	5.57	115.46	108.45
1	A	892	ILE	N-CA-C	5.53	116.31	110.72
1	B	195	SER	CA-C-N	5.52	125.61	119.87
1	B	195	SER	C-N-CA	5.52	125.61	119.87
1	A	797	LEU	N-CA-C	-5.50	104.77	112.25
1	A	828	GLU	CB-CG-CD	-5.48	103.29	112.60
1	A	115	VAL	CB-CA-C	-5.46	108.56	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	810	GLY	N-CA-C	-5.44	100.29	113.18
1	B	478	ASN	N-CA-C	5.43	118.40	109.76
1	B	960	ARG	N-CA-C	5.43	116.40	108.14
1	A	36	LEU	N-CA-C	5.42	117.25	108.26
1	B	909	ASP	N-CA-C	-5.41	104.13	111.55
1	A	181	ASP	CA-C-N	5.39	126.58	119.84
1	A	181	ASP	C-N-CA	5.39	126.58	119.84
1	A	851	LEU	N-CA-C	5.39	122.27	110.80
1	B	456	TYR	CA-C-N	-5.36	106.47	120.25
1	B	456	TYR	C-N-CA	-5.36	106.47	120.25
1	A	503	LEU	CA-C-N	-5.35	117.55	123.43
1	A	503	LEU	C-N-CA	-5.35	117.55	123.43
1	B	210	LYS	CD-CE-NZ	-5.34	94.80	111.90
1	A	504	VAL	CA-C-O	5.34	123.01	119.38
1	B	233	LEU	N-CA-C	5.34	117.38	109.69
1	A	747	GLN	N-CA-C	-5.33	106.73	113.18
1	A	995	THR	N-CA-C	5.33	117.21	108.52
1	A	720	LYS	N-CA-C	-5.30	105.61	111.71
1	B	976	GLY	N-CA-C	5.30	125.73	113.18
1	A	636	ASP	CA-C-N	-5.29	113.59	123.01
1	A	636	ASP	C-N-CA	-5.29	113.59	123.01
1	A	341	TYR	N-CA-C	-5.27	106.98	113.41
1	A	532	MSE	N-CA-C	-5.27	105.43	111.07
1	B	338	ASP	N-CA-C	5.25	117.80	111.40
1	A	767	GLN	N-CA-C	-5.24	106.73	113.23
1	B	728	ILE	N-CA-C	5.22	116.41	109.37
1	A	398	ASP	N-CA-C	-5.20	106.91	113.20
1	A	48	GLU	N-CA-C	-5.18	105.75	111.71
1	B	972	PHE	N-CA-C	5.17	117.03	108.49
1	B	567	GLN	N-CA-C	5.17	117.59	110.35
1	A	834	GLU	N-CA-C	-5.17	106.10	112.72
1	B	477	THR	N-CA-C	-5.16	107.11	113.41
1	B	638	VAL	N-CA-C	-5.16	102.24	108.53
1	B	339	GLU	N-CA-C	5.15	120.42	113.72
1	B	248	ILE	N-CA-C	-5.14	101.23	109.20
1	A	85	ARG	N-CA-C	-5.13	106.85	113.01
1	B	401	LEU	CB-CA-C	-5.11	101.26	109.89
1	B	903	THR	N-CA-C	-5.11	102.82	110.23
1	A	151	GLN	CA-C-N	5.11	130.61	122.59
1	A	151	GLN	C-N-CA	5.11	130.61	122.59
1	A	698	LEU	N-CA-C	-5.10	103.96	110.53
1	B	895	TRP	N-CA-C	-5.08	99.98	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	979	ASN	N-CA-C	5.08	118.49	109.96
1	A	388	LYS	CA-CB-CG	-5.07	103.95	114.10
1	B	455	THR	N-CA-C	-5.04	100.06	110.80
1	B	836	SER	N-CA-C	5.03	117.47	109.02
1	B	456	TYR	CB-CA-C	-5.01	100.30	110.17

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	150	MSE	Peptide
1	A	151	GLN	Peptide
1	A	204	LYS	Peptide
1	A	391	LEU	Peptide
1	A	456	TYR	Peptide
1	A	562	LEU	Peptide
1	A	580	GLU	Peptide
1	A	816	VAL	Peptide
1	A	845	VAL	Peptide
1	A	846	MSE	Peptide
1	A	849	LEU	Peptide
1	A	852	GLY	Peptide
1	A	891	ALA	Peptide
1	A	974	GLU	Peptide
1	B	198	PHE	Peptide
1	B	207	ALA	Peptide
1	B	208	MSE	Peptide
1	B	209	ALA	Peptide
1	B	210	LYS	Peptide
1	B	211	GLU	Peptide
1	B	638	VAL	Peptide
1	B	743	HIS	Peptide
1	B	820	SER	Peptide

4.2 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	7159	0	7156	704	0
1	B	7159	0	7156	600	1
All	All	14318	0	14312	1297	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 45.

All (1297) 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:703:VAL:HG22	1:A:804:ARG:HH11	1.15	1.10
1:A:380:ARG:HH11	1:A:912:ILE:HD12	1.02	1.07
1:B:210:LYS:HB2	1:B:211:GLU:HG2	1.11	1.06
1:A:433:ASN:HD22	1:A:500:ARG:HA	1.21	1.04
1:B:420:ARG:HE	1:B:649:LEU:HD21	1.22	1.00
1:A:380:ARG:NH1	1:A:912:ILE:HD12	1.78	0.97
1:A:703:VAL:HG13	1:A:804:ARG:HE	1.27	0.95
1:B:453:GLN:HE21	1:B:453:GLN:HA	1.31	0.94
1:B:613:ASN:OD1	1:B:616:GLN:NE2	2.01	0.94
1:A:386:PHE:HA	1:A:388:LYS:HE2	1.50	0.94
1:B:385:GLN:HA	1:B:388:LYS:HD2	1.48	0.94
1:A:913:ASN:HA	1:A:942:ASN:OD1	1.68	0.94
1:B:845:VAL:HA	1:B:848:ASP:HB2	1.46	0.94
1:A:748:LEU:HD12	1:A:751:LEU:HD21	1.52	0.92
1:B:202:HIS:O	1:B:206:SER:N	2.03	0.92
1:A:378:HIS:HA	1:A:381:GLN:HE22	1.34	0.91
1:A:809:ASN:HB3	1:A:839:LEU:HD11	1.52	0.91
1:B:170:ALA:HB1	1:B:186:LEU:HD23	1.50	0.91
1:A:200:GLU:OE1	1:A:203:ARG:NH1	2.02	0.91
1:A:813:VAL:HG23	1:A:814:GLY:H	1.35	0.90
1:B:918:ILE:HD13	1:B:945:ILE:HG23	1.54	0.90
1:B:452:LEU:O	1:B:453:GLN:NE2	2.02	0.90
1:A:208:MSE:H	1:A:210:LYS:HZ2	1.17	0.90
1:A:151:GLN:HG2	1:A:152:TYR:H	1.36	0.89
1:B:211:GLU:HG3	1:B:212:GLY:N	1.86	0.89
1:A:559:ALA:HB1	1:A:563:ARG:HA	1.52	0.89
1:B:522:LEU:HD23	1:B:531:MSE:HA	1.54	0.88
1:B:249:MSE:SE	1:B:292:VAL:HG21	2.24	0.88
1:B:519:ALA:HB1	1:B:531:MSE:HE3	1.56	0.88
1:A:339:GLU:HA	1:A:342:ALA:HB3	1.54	0.87
1:A:716:ILE:HG22	1:A:767:GLN:HE21	1.39	0.87
1:B:108:SER:HA	1:B:373:LEU:HD21	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:LYS:HD2	1:A:389:LEU:HD13	1.57	0.86
1:A:710:ALA:HA	1:A:713:ASN:HB2	1.58	0.86
1:B:752:LEU:C	1:B:754:THR:H	1.82	0.86
1:A:111:ILE:O	1:A:113:SER:N	2.08	0.86
1:A:755:GLU:CD	1:A:755:GLU:H	1.83	0.85
1:A:956:LEU:HD12	1:A:957:PRO:HD2	1.57	0.85
1:A:847:LYS:NZ	1:A:854:LYS:H	1.73	0.85
1:B:335:GLU:HA	1:B:338:ASP:HB3	1.58	0.85
1:A:100:ALA:HB1	1:A:380:ARG:HH21	1.38	0.84
1:A:672:ASN:C	1:A:675:GLN:HE22	1.84	0.84
1:B:451:LEU:HG	1:B:460:LEU:HD13	1.58	0.84
1:A:131:PRO:O	1:B:508:HIS:NE2	2.10	0.84
1:A:580:GLU:HA	1:A:580:GLU:OE1	1.76	0.84
1:B:297:MSE:HE2	1:B:951:ARG:HA	1.61	0.82
1:A:98:ASP:CG	1:A:101:ASP:H	1.86	0.82
1:A:202:HIS:O	1:A:206:SER:N	2.13	0.82
1:A:246:ASP:H	1:A:285:LYS:HD2	1.44	0.82
1:A:847:LYS:HB3	1:A:850:ASN:O	1.78	0.82
1:B:98:ASP:HB2	1:B:101:ASP:HB2	1.62	0.82
1:B:444:PHE:O	1:B:464:ARG:NE	2.13	0.82
1:A:151:GLN:HG2	1:A:152:TYR:N	1.95	0.82
1:A:587:ARG:O	1:A:591:ARG:N	2.13	0.81
1:A:80:LYS:NZ	1:A:84:ASP:OD2	2.14	0.81
1:B:767:GLN:HA	1:B:770:LYS:HG2	1.59	0.81
1:B:208:MSE:HA	1:B:210:LYS:HE3	1.62	0.81
1:B:340:TYR:OH	1:B:948:THR:HA	1.79	0.81
1:B:520:ARG:NH1	1:B:523:GLN:O	2.14	0.81
1:A:332:VAL:HG22	1:A:336:PHE:HB2	1.61	0.81
1:B:1008:PRO:HA	1:B:1033:TYR:HA	1.61	0.81
1:A:808:LEU:HD21	1:A:831:LEU:HD23	1.63	0.80
1:A:521:TYR:CE1	1:A:568:SER:HB3	2.16	0.80
1:A:385:GLN:O	1:A:388:LYS:HG2	1.80	0.80
1:A:446:SER:HA	1:A:463:VAL:HG13	1.62	0.80
1:A:747:GLN:NE2	1:A:750:GLN:O	2.14	0.80
1:B:536:GLN:OE1	1:B:537:ARG:NH1	2.14	0.80
1:A:860:GLU:HA	1:A:863:LYS:HD2	1.64	0.80
1:B:209:ALA:N	1:B:210:LYS:HD2	1.96	0.80
1:A:98:ASP:OD1	1:A:101:ASP:N	2.16	0.79
1:A:396:ALA:O	1:A:399:LEU:HB3	1.82	0.79
1:B:65:LEU:HD12	1:B:68:ILE:HD11	1.63	0.79
1:A:721:PHE:CZ	1:A:828:GLU:HB3	2.18	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:561:VAL:HG13	1:B:562:LEU:HD13	1.65	0.79
1:B:453:GLN:HA	1:B:453:GLN:NE2	1.92	0.78
1:A:242:LEU:HD23	1:A:245:THR:HG21	1.64	0.78
1:A:549:GLN:HE22	1:A:571:GLU:HA	1.49	0.78
1:B:672:ASN:OD1	1:B:673:LEU:N	2.16	0.78
1:B:511:PRO:O	1:B:515:GLN:N	2.17	0.78
1:A:546:ARG:NH1	1:B:119:GLU:OE2	2.18	0.77
1:A:748:LEU:HA	1:A:751:LEU:HD21	1.66	0.77
1:A:471:VAL:HB	1:A:602:LEU:HB2	1.66	0.77
1:B:292:VAL:HA	1:B:295:LEU:HB2	1.67	0.77
1:B:295:LEU:HD11	1:B:324:SER:HB2	1.67	0.77
1:A:388:LYS:HG3	1:A:389:LEU:H	1.49	0.77
1:A:48:GLU:HG3	1:A:114:ALA:HB3	1.66	0.77
1:B:208:MSE:HA	1:B:210:LYS:CE	2.14	0.77
1:A:560:ARG:HH21	1:A:561:VAL:HG13	1.48	0.77
1:B:787:TRP:O	1:B:789:GLN:N	2.17	0.77
1:B:846:MSE:O	1:B:849:LEU:HG	1.85	0.76
1:A:335:GLU:HA	1:A:338:ASP:OD1	1.85	0.76
1:B:655:THR:OG1	1:B:656:ARG:NH1	2.19	0.76
1:A:151:GLN:CG	1:A:152:TYR:H	1.96	0.76
1:A:336:PHE:CD2	1:A:337:LEU:HD13	2.19	0.76
1:B:453:GLN:HE21	1:B:453:GLN:CA	1.99	0.76
1:B:858:SER:HA	1:B:861:PHE:HB3	1.67	0.76
1:B:917:THR:HB	1:B:948:THR:HG21	1.68	0.76
1:A:847:LYS:HE3	1:A:853:HIS:CD2	2.22	0.75
1:B:249:MSE:HB2	1:B:956:LEU:HD22	1.66	0.75
1:B:310:PHE:HB2	1:B:902:ILE:HG21	1.69	0.75
1:B:190:TYR:OH	1:B:219:ARG:NH1	2.18	0.74
1:B:710:ALA:O	1:B:712:LEU:N	2.19	0.74
1:A:104:SER:HB3	1:A:377:ARG:NH2	2.02	0.74
1:A:104:SER:HB3	1:A:377:ARG:HH21	1.51	0.74
1:A:803:THR:HB	1:A:815:PRO:HG3	1.69	0.74
1:B:210:LYS:HB2	1:B:211:GLU:CG	2.06	0.74
1:B:672:ASN:OD1	1:B:863:LYS:NZ	2.14	0.74
1:A:580:GLU:OE1	1:A:584:LYS:N	2.21	0.74
1:B:244:ARG:HB3	1:B:993:LEU:HB2	1.69	0.74
1:B:428:VAL:HG13	1:B:585:THR:HG22	1.70	0.74
1:B:387:ARG:HA	1:B:391:LEU:H	1.52	0.74
1:B:722:ARG:NH1	1:B:728:ILE:O	2.21	0.74
1:B:836:SER:OG	1:B:837:LYS:N	2.15	0.73
1:B:893:LYS:HE3	1:B:895:TRP:CD1	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:788:ALA:O	1:A:792:GLN:NE2	2.21	0.73
1:A:94:GLY:HA2	1:A:97:ASN:OD1	1.89	0.73
1:A:401:LEU:HD21	1:A:893:LYS:HD3	1.69	0.73
1:B:144:TRP:CE3	1:B:151:GLN:HG3	2.22	0.73
1:A:336:PHE:CE2	1:A:337:LEU:HD13	2.24	0.73
1:A:342:ALA:O	1:A:896:ASN:ND2	2.22	0.73
1:B:510:GLU:O	1:B:514:SER:OG	2.05	0.73
1:A:465:ARG:HE	1:A:644:LEU:HD11	1.54	0.73
1:A:654:LEU:HB2	1:A:656:ARG:HH22	1.53	0.73
1:B:589:ILE:HG23	1:B:594:LEU:HB2	1.71	0.73
1:A:698:LEU:HD13	1:A:839:LEU:HD21	1.71	0.72
1:B:209:ALA:HB2	1:B:216:TYR:HB3	1.70	0.72
1:B:452:LEU:C	1:B:453:GLN:HE21	1.97	0.72
1:B:474:ILE:HD11	1:B:485:VAL:HG21	1.71	0.72
1:B:817:PRO:HD2	1:B:821:THR:HG21	1.69	0.72
1:B:33:ASN:N	1:B:1029:VAL:O	2.23	0.72
1:B:146:HIS:HB3	1:B:188:ILE:HB	1.71	0.72
1:B:767:GLN:OE1	1:B:767:GLN:N	2.21	0.72
1:B:204:LYS:O	1:B:208:MSE:N	2.23	0.72
1:B:376:LEU:HG	1:B:912:ILE:HD13	1.72	0.72
1:B:210:LYS:HD3	1:B:211:GLU:HG2	1.70	0.72
1:B:349:PRO:HB2	1:B:352:ARG:HE	1.54	0.72
1:A:170:ALA:HB1	1:A:186:LEU:HD23	1.71	0.72
1:A:791:LYS:HE3	1:A:801:SER:HA	1.71	0.71
1:A:209:ALA:HB3	1:A:210:LYS:HE3	1.70	0.71
1:B:76:ALA:HB2	1:B:85:ARG:HD2	1.72	0.71
1:B:473:PRO:HA	1:B:504:VAL:HG22	1.72	0.71
1:B:612:ASP:CG	1:B:616:GLN:HE22	1.97	0.71
1:B:1003:SER:HA	1:B:1039:LEU:HG	1.72	0.71
1:A:433:ASN:HB3	1:A:500:ARG:HG3	1.73	0.71
1:B:420:ARG:NE	1:B:649:LEU:HD21	2.03	0.71
1:A:667:LYS:HE3	1:A:669:ARG:HD3	1.72	0.71
1:B:853:HIS:NE2	1:B:855:VAL:O	2.24	0.71
1:A:80:LYS:HA	1:A:83:TYR:HB3	1.71	0.71
1:A:111:ILE:HG23	1:A:112:ARG:NH1	2.05	0.70
1:A:523:GLN:NE2	1:A:527:GLY:O	2.23	0.70
1:B:289:SER:OG	1:B:290:SER:N	2.21	0.70
1:B:483:TYR:O	1:B:487:GLN:N	2.22	0.70
1:B:179:LEU:HG	1:B:209:ALA:CB	2.21	0.70
1:A:315:LYS:H	1:A:315:LYS:HD2	1.56	0.70
1:B:393:ASN:ND2	1:B:909:ASP:OD1	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:582:MSE:O	1:A:586:GLY:N	2.18	0.70
1:B:632:SER:OG	1:B:633:ILE:N	2.23	0.70
1:A:473:PRO:O	1:A:610:ARG:NH2	2.25	0.70
1:B:751:LEU:CD1	1:B:752:LEU:H	2.05	0.70
1:A:245:THR:HA	1:A:285:LYS:HD3	1.74	0.70
1:B:558:SER:O	1:B:561:VAL:HG12	1.92	0.70
1:B:734:HIS:CD2	1:B:735:THR:H	2.10	0.70
1:B:629:ILE:HD13	1:B:644:LEU:HD22	1.73	0.70
1:B:660:ILE:HG21	1:B:829:ILE:HG23	1.74	0.70
1:A:287:LEU:HD12	1:A:288:SER:H	1.57	0.69
1:A:156:THR:O	1:A:157:LEU:HG	1.91	0.69
1:B:293:ALA:HA	1:B:953:LEU:H	1.57	0.69
1:A:428:VAL:HG13	1:A:585:THR:HG22	1.72	0.69
1:A:208:MSE:HG3	1:A:213:GLN:HB2	1.73	0.69
1:A:591:ARG:HH21	1:A:655:THR:HB	1.57	0.69
1:A:185:PRO:HB2	1:A:214:VAL:HA	1.75	0.69
1:A:292:VAL:HA	1:A:295:LEU:HB2	1.74	0.69
1:A:638:VAL:HG21	1:A:642:THR:HG21	1.75	0.69
1:B:737:ASP:CG	1:B:791:LYS:HZ3	2.00	0.69
1:A:346:ALA:CB	1:A:895:TRP:HB2	2.23	0.69
1:A:367:VAL:O	1:A:927:ARG:NH2	2.26	0.69
1:A:750:GLN:HG3	1:A:753:ARG:HD3	1.74	0.69
1:A:529:ALA:O	1:A:533:LYS:HG2	1.92	0.68
1:A:399:LEU:O	1:A:401:LEU:N	2.24	0.68
1:A:526:HIS:O	1:A:562:LEU:HD21	1.93	0.68
1:A:539:LEU:HA	1:A:544:LEU:HD11	1.74	0.68
1:B:208:MSE:HG2	1:B:210:LYS:HE3	1.75	0.68
1:A:546:ARG:HD3	1:B:228:PHE:HE2	1.58	0.68
1:A:974:GLU:HB3	1:A:976:GLY:H	1.59	0.68
1:A:385:GLN:NE2	1:A:673:LEU:HB3	2.08	0.68
1:A:562:LEU:O	1:A:563:ARG:HD3	1.92	0.68
1:A:632:SER:O	1:A:637:ALA:HB2	1.94	0.68
1:B:36:LEU:HD23	1:B:233:LEU:HB2	1.76	0.68
1:A:30:SER:OG	1:A:31:SER:N	2.22	0.68
1:A:735:THR:N	1:A:804:ARG:HH22	1.92	0.68
1:A:752:LEU:CD2	1:A:760:SER:HB3	2.24	0.68
1:A:388:LYS:HG3	1:A:389:LEU:N	2.05	0.68
1:A:703:VAL:HG22	1:A:804:ARG:NH1	2.00	0.68
1:B:250:ILE:HD12	1:B:289:SER:HB2	1.75	0.67
1:B:520:ARG:HA	1:B:520:ARG:HH11	1.60	0.67
1:B:644:LEU:O	1:B:647:TYR:N	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:GLN:HG2	1:A:102:LEU:HD21	1.76	0.67
1:A:205:LEU:O	1:A:210:LYS:NZ	2.26	0.67
1:A:523:GLN:HG3	1:A:528:LEU:HA	1.76	0.67
1:A:703:VAL:HG13	1:A:804:ARG:NE	2.07	0.67
1:A:836:SER:OG	1:A:837:LYS:N	2.27	0.67
1:A:695:THR:OG1	1:A:696:ASN:N	2.24	0.67
1:A:433:ASN:ND2	1:A:500:ARG:HA	2.03	0.67
1:A:800:PRO:O	1:A:803:THR:OG1	2.08	0.67
1:B:517:LYS:NZ	1:B:578:LEU:HD12	2.10	0.67
1:A:82:LEU:O	1:A:86:PHE:HB2	1.95	0.67
1:B:83:TYR:CZ	1:B:87:LEU:HD11	2.30	0.67
1:B:210:LYS:CB	1:B:211:GLU:HG2	2.07	0.67
1:B:293:ALA:HA	1:B:953:LEU:N	2.09	0.67
1:B:1019:ARG:HG2	1:B:1021:SER:HB3	1.76	0.66
1:A:752:LEU:HD23	1:A:760:SER:HB3	1.77	0.66
1:B:78:THR:CG2	1:B:81:GLU:HG3	2.25	0.66
1:A:721:PHE:CE1	1:A:828:GLU:HB3	2.30	0.66
1:A:846:MSE:HG2	1:A:847:LYS:H	1.61	0.66
1:A:681:ASP:OD2	1:A:683:THR:HG23	1.95	0.66
1:A:974:GLU:HG2	1:A:976:GLY:N	2.09	0.66
1:B:559:ALA:HA	1:B:562:LEU:HB2	1.77	0.66
1:B:709:GLU:CD	1:B:709:GLU:H	1.99	0.66
1:B:398:ASP:O	1:B:401:LEU:HG	1.96	0.66
1:B:589:ILE:HA	1:B:594:LEU:HD12	1.78	0.66
1:A:675:GLN:C	1:A:677:ALA:H	2.03	0.66
1:B:672:ASN:HD22	1:B:866:SER:CB	2.09	0.66
1:B:179:LEU:HG	1:B:209:ALA:HB3	1.78	0.65
1:A:455:THR:OG1	1:A:457:PRO:HD2	1.96	0.65
1:A:435:LEU:HA	1:A:441:TYR:HD2	1.59	0.65
1:A:381:GLN:O	1:A:385:GLN:N	2.28	0.65
1:A:237:GLY:N	1:A:999:ASP:O	2.27	0.65
1:B:148:ASP:OD1	1:B:149:GLY:N	2.29	0.65
1:B:580:GLU:O	1:B:584:LYS:HD3	1.96	0.65
1:B:853:HIS:CE1	1:B:855:VAL:HG22	2.32	0.65
1:A:428:VAL:CG2	1:A:584:LYS:HG2	2.26	0.65
1:B:817:PRO:O	1:B:818:SER:OG	2.12	0.65
1:A:698:LEU:HB2	1:A:728:ILE:HD11	1.78	0.65
1:B:91:GLN:HG2	1:B:97:ASN:OD1	1.97	0.65
1:B:439:LYS:O	1:B:442:SER:OG	2.10	0.65
1:A:734:HIS:CE1	1:A:749:TYR:OH	2.50	0.65
1:B:672:ASN:CG	1:B:673:LEU:H	2.01	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:SER:OG	1:A:290:SER:N	2.30	0.64
1:A:665:PRO:O	1:A:667:LYS:N	2.25	0.64
1:B:243:LYS:HB3	1:B:993:LEU:HB3	1.80	0.64
1:B:536:GLN:HB2	1:B:537:ARG:HD2	1.79	0.64
1:A:635:GLN:HG2	1:A:636:ASP:H	1.61	0.64
1:A:816:VAL:HB	1:A:817:PRO:HD3	1.77	0.64
1:A:797:LEU:HD22	1:A:807:LEU:HD11	1.79	0.64
1:B:241:THR:OG1	1:B:995:THR:HB	1.97	0.64
1:A:113:SER:O	1:A:116:PRO:HD2	1.98	0.64
1:A:247:TYR:HB2	1:A:286:PRO:HG2	1.78	0.64
1:B:492:PHE:HB3	1:B:497:ILE:HD12	1.79	0.64
1:B:534:TYR:HA	1:B:555:THR:HG21	1.79	0.64
1:B:956:LEU:HD12	1:B:957:PRO:HD2	1.79	0.64
1:A:523:GLN:HE22	1:A:531:MSE:H	1.43	0.64
1:B:208:MSE:HA	1:B:210:LYS:CD	2.28	0.64
1:A:294:ARG:NH1	1:A:328:ALA:O	2.31	0.64
1:A:767:GLN:N	1:A:767:GLN:OE1	2.28	0.64
1:B:68:ILE:HG22	1:B:73:LEU:HD13	1.79	0.64
1:B:523:GLN:O	1:B:524:MSE:HG3	1.96	0.64
1:A:418:ASP:HA	1:A:649:LEU:HD11	1.80	0.64
1:A:702:VAL:O	1:A:732:PRO:HA	1.98	0.64
1:A:831:LEU:O	1:A:835:PHE:N	2.26	0.64
1:A:84:ASP:HA	1:A:87:LEU:HD12	1.79	0.64
1:A:431:TRP:CE3	1:A:500:ARG:HG2	2.33	0.64
1:B:44:PRO:HG2	1:B:47:LEU:HD12	1.80	0.64
1:B:100:ALA:O	1:B:104:SER:N	2.25	0.63
1:B:751:LEU:HD12	1:B:752:LEU:H	1.62	0.63
1:A:358:ASN:N	1:A:913:ASN:O	2.16	0.63
1:A:606:VAL:HG11	1:A:621:ARG:HG2	1.80	0.63
1:A:672:ASN:OD1	1:A:673:LEU:N	2.31	0.63
1:B:48:GLU:OE2	1:B:112:ARG:HD3	1.99	0.63
1:B:787:TRP:HD1	1:B:790:THR:HG1	1.47	0.63
1:A:208:MSE:N	1:A:210:LYS:HZ2	1.92	0.63
1:A:239:GLU:HG2	1:A:960:ARG:NH2	2.12	0.63
1:A:432:LEU:HD11	1:A:503:LEU:HD11	1.81	0.63
1:A:721:PHE:HZ	1:A:828:GLU:HB3	1.63	0.63
1:A:301:SER:HB3	1:A:333:THR:HG23	1.81	0.63
1:A:335:GLU:HB2	1:A:900:SER:HB3	1.81	0.63
1:A:702:VAL:HG11	1:A:718:ALA:HB1	1.80	0.63
1:B:30:SER:OG	1:B:31:SER:N	2.31	0.63
1:A:76:ALA:HB3	1:A:81:GLU:OE1	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:827:LEU:O	1:A:830:LEU:HB3	1.99	0.63
1:B:606:VAL:HG11	1:B:621:ARG:HD3	1.81	0.63
1:B:973:ASP:O	1:B:974:GLU:HB2	1.98	0.63
1:A:580:GLU:OE2	1:A:583:ASP:HB2	1.99	0.62
1:B:698:LEU:HB2	1:B:728:ILE:HG12	1.81	0.62
1:B:787:TRP:CD1	1:B:790:THR:HG1	2.17	0.62
1:A:546:ARG:HD3	1:B:228:PHE:CE2	2.33	0.62
1:B:418:ASP:OD1	1:B:655:THR:HG22	1.98	0.62
1:B:849:LEU:O	1:B:851:LEU:N	2.31	0.62
1:B:905:SER:HB2	1:B:942:ASN:HA	1.81	0.62
1:A:428:VAL:HG22	1:A:584:LYS:HG2	1.80	0.62
1:B:927:ARG:HH12	1:B:999:ASP:CG	2.08	0.62
1:A:108:SER:HA	1:A:111:ILE:HB	1.82	0.62
1:A:532:MSE:O	1:A:536:GLN:N	2.29	0.62
1:A:847:LYS:HZ2	1:A:854:LYS:H	1.47	0.62
1:A:246:ASP:N	1:A:285:LYS:HD2	2.13	0.62
1:B:221:ARG:NH1	1:B:222:PRO:O	2.33	0.62
1:B:639:GLU:CD	1:B:639:GLU:H	2.07	0.62
1:B:293:ALA:HB1	1:B:952:ILE:HG13	1.81	0.62
1:A:147:MSE:O	1:A:149:GLY:N	2.33	0.62
1:A:639:GLU:CD	1:A:639:GLU:H	2.07	0.62
1:A:207:ALA:CA	1:A:210:LYS:HG3	2.29	0.62
1:B:586:GLY:O	1:B:590:LYS:HD3	2.00	0.62
1:A:249:MSE:CE	1:A:292:VAL:HG21	2.29	0.62
1:A:804:ARG:H	1:A:815:PRO:HB3	1.65	0.62
1:A:817:PRO:CD	1:A:818:SER:H	2.12	0.62
1:B:78:THR:OG1	1:B:976:GLY:O	2.16	0.62
1:B:533:LYS:HA	1:B:536:GLN:HG3	1.82	0.62
1:B:1004:TRP:CD1	1:B:1038:ILE:HD11	2.35	0.62
1:A:173:LEU:N	1:A:176:ASP:OD2	2.33	0.62
1:B:249:MSE:SE	1:B:292:VAL:HG11	2.50	0.62
1:B:449:ASP:O	1:B:452:LEU:HD21	2.00	0.62
1:B:33:ASN:O	1:B:1031:ALA:N	2.26	0.61
1:A:85:ARG:O	1:A:89:ILE:HD13	2.00	0.61
1:A:466:ASP:O	1:A:645:PRO:HD3	2.01	0.61
1:A:111:ILE:C	1:A:112:ARG:HG3	2.25	0.61
1:A:676:VAL:HA	1:A:680:HIS:CE1	2.35	0.61
1:B:210:LYS:HD3	1:B:211:GLU:CG	2.30	0.61
1:B:923:GLU:HG3	1:B:958:ILE:HA	1.80	0.61
1:A:672:ASN:CG	1:A:673:LEU:H	2.07	0.61
1:B:239:GLU:O	1:B:240:LEU:HD23	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:LYS:HD2	1:A:315:LYS:N	2.16	0.61
1:B:339:GLU:HA	1:B:342:ALA:HB3	1.81	0.61
1:B:463:VAL:C	1:B:465:ARG:H	2.08	0.61
1:B:770:LYS:O	1:B:773:SER:OG	2.19	0.61
1:A:106:LYS:HD3	1:A:106:LYS:H	1.65	0.61
1:A:381:GLN:OE1	1:A:382:PHE:N	2.34	0.61
1:A:817:PRO:HD2	1:A:818:SER:H	1.66	0.61
1:B:558:SER:C	1:B:560:ARG:HG2	2.26	0.61
1:A:635:GLN:O	1:A:637:ALA:N	2.33	0.61
1:A:794:ALA:O	1:A:797:LEU:HD12	2.01	0.61
1:A:910:ALA:C	1:A:912:ILE:H	2.09	0.61
1:B:736:SER:O	1:B:791:LYS:HD3	2.00	0.61
1:A:153:CYS:O	1:A:201:TYR:OH	2.17	0.60
1:B:748:LEU:O	1:B:751:LEU:N	2.34	0.60
1:A:209:ALA:H	1:A:210:LYS:NZ	1.98	0.60
1:A:387:ARG:CZ	1:A:393:ASN:HD21	2.13	0.60
1:B:205:LEU:HA	1:B:208:MSE:HB2	1.82	0.60
1:A:74:ASP:OD2	1:A:196:PRO:HB3	2.01	0.60
1:A:444:PHE:HD2	1:A:462:ALA:HB3	1.66	0.60
1:B:737:ASP:OD2	1:B:801:SER:HB3	2.01	0.60
1:A:521:TYR:CE1	1:A:525:THR:HG21	2.36	0.60
1:A:847:LYS:HZ1	1:A:854:LYS:H	1.47	0.60
1:A:249:MSE:HE2	1:A:292:VAL:HG21	1.83	0.60
1:A:709:GLU:O	1:A:711:GLY:N	2.33	0.60
1:B:34:VAL:HG22	1:B:1031:ALA:HB3	1.83	0.60
1:B:555:THR:HA	1:B:558:SER:HB3	1.82	0.60
1:A:517:LYS:HG2	1:A:582:MSE:HE2	1.83	0.60
1:B:143:VAL:HG23	1:B:191:ALA:HB2	1.84	0.60
1:B:764:GLU:O	1:B:767:GLN:NE2	2.31	0.60
1:A:293:ALA:HA	1:A:953:LEU:H	1.66	0.60
1:A:393:ASN:HA	1:A:396:ALA:H	1.67	0.60
1:A:83:TYR:O	1:A:87:LEU:HD12	2.01	0.60
1:A:560:ARG:NH2	1:A:561:VAL:HG13	2.15	0.60
1:A:704:GLY:C	1:A:804:ARG:HD3	2.26	0.60
1:A:665:PRO:C	1:A:667:LYS:H	2.10	0.59
1:B:250:ILE:H	1:B:289:SER:HA	1.65	0.59
1:B:250:ILE:HG13	1:B:288:SER:O	2.01	0.59
1:B:420:ARG:HE	1:B:649:LEU:CD2	2.04	0.59
1:B:917:THR:HB	1:B:948:THR:CG2	2.31	0.59
1:A:846:MSE:HG2	1:A:847:LYS:N	2.17	0.59
1:B:80:LYS:HB2	1:B:972:PHE:CB	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:698:LEU:HB2	1:A:728:ILE:CD1	2.32	0.59
1:A:130:GLU:HA	1:A:133:LEU:HD12	1.83	0.59
1:A:589:ILE:O	1:A:593:ASP:N	2.36	0.59
1:B:29:ASP:OD1	1:B:30:SER:N	2.30	0.59
1:A:515:GLN:NE2	1:A:547:PRO:HB3	2.17	0.59
1:B:294:ARG:HD2	1:B:298:ASN:HD21	1.68	0.59
1:A:57:ASN:CG	1:A:95:HIS:HB3	2.27	0.59
1:A:542:ASP:O	1:A:543:LYS:HD3	2.03	0.59
1:A:351:GLY:H	1:A:951:ARG:HH12	1.50	0.59
1:A:567:GLN:OE1	1:A:568:SER:N	2.35	0.59
1:B:789:GLN:C	1:B:793:LEU:HG	2.28	0.59
1:B:906:HIS:NE2	1:B:910:ALA:HB2	2.17	0.59
1:B:1019:ARG:O	1:B:1022:SER:N	2.27	0.59
1:A:83:TYR:CE1	1:A:87:LEU:HD11	2.37	0.59
1:A:799:TYR:N	1:A:800:PRO:HD3	2.18	0.59
1:B:705:ASP:O	1:B:707:ASP:N	2.36	0.59
1:B:848:ASP:O	1:B:850:ASN:N	2.36	0.59
1:A:706:PHE:CD2	1:A:734:HIS:HB3	2.37	0.59
1:A:816:VAL:HB	1:A:817:PRO:CD	2.31	0.59
1:B:156:THR:O	1:B:157:LEU:HG	2.03	0.59
1:B:431:TRP:CZ3	1:B:500:ARG:HG2	2.38	0.59
1:A:179:LEU:N	1:A:216:TYR:O	2.34	0.58
1:A:523:GLN:CG	1:A:528:LEU:HA	2.32	0.58
1:A:244:ARG:O	1:A:992:ALA:HB1	2.04	0.58
1:B:100:ALA:HB2	1:B:939:ASN:OD1	2.03	0.58
1:B:234:ALA:O	1:B:370:TYR:OH	2.20	0.58
1:B:762:ILE:O	1:B:766:ILE:HG23	2.04	0.58
1:A:208:MSE:H	1:A:210:LYS:NZ	1.95	0.58
1:A:621:ARG:HA	1:A:624:ILE:HD12	1.84	0.58
1:B:185:PRO:HG2	1:B:214:VAL:HG22	1.85	0.58
1:B:752:LEU:C	1:B:754:THR:N	2.55	0.58
1:A:813:VAL:HG23	1:A:814:GLY:N	2.14	0.58
1:B:56:GLU:N	1:B:56:GLU:OE1	2.37	0.58
1:B:346:ALA:HB3	1:B:893:LYS:HE2	1.84	0.58
1:B:597:ARG:HG3	1:B:598:SER:N	2.19	0.58
1:A:385:GLN:HE22	1:A:673:LEU:HB3	1.67	0.58
1:A:845:VAL:HA	1:A:848:ASP:HB2	1.85	0.58
1:A:905:SER:CB	1:A:942:ASN:HA	2.34	0.58
1:A:972:PHE:O	1:A:979:ASN:ND2	2.30	0.58
1:A:1003:SER:O	1:A:1038:ILE:HB	2.03	0.58
1:B:393:ASN:ND2	1:B:911:SER:HB2	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:GLN:O	1:A:453:GLN:HG2	2.04	0.58
1:A:716:ILE:O	1:A:720:LYS:HG2	2.04	0.58
1:A:851:LEU:HG	1:A:852:GLY:N	2.19	0.58
1:B:342:ALA:HB1	1:B:895:TRP:CH2	2.39	0.58
1:A:142:PRO:O	1:A:221:ARG:NH1	2.37	0.57
1:A:825:ASP:N	1:A:825:ASP:OD1	2.35	0.57
1:B:723:LEU:HD11	1:B:761:GLU:HB3	1.86	0.57
1:A:527:GLY:C	1:A:562:LEU:HD11	2.29	0.57
1:B:309:PRO:HB2	1:B:902:ILE:HD12	1.86	0.57
1:B:483:TYR:CZ	1:B:487:GLN:HG2	2.38	0.57
1:B:797:LEU:HD22	1:B:807:LEU:HD11	1.87	0.57
1:A:209:ALA:H	1:A:210:LYS:HZ1	1.52	0.57
1:B:986:SER:O	1:B:987:ARG:HB3	2.04	0.57
1:B:661:MSE:O	1:B:661:MSE:HG3	2.05	0.57
1:A:644:LEU:HD12	1:A:644:LEU:H	1.68	0.57
1:B:548:ASP:OD1	1:B:551:LEU:HB2	2.05	0.57
1:A:65:LEU:HA	1:A:68:ILE:HG12	1.85	0.57
1:A:377:ARG:NH2	1:A:380:ARG:NH2	2.52	0.57
1:A:392:SER:O	1:A:395:GLU:HG2	2.03	0.57
1:A:492:PHE:HB3	1:A:497:ILE:HD12	1.85	0.57
1:A:707:ASP:OD2	1:A:745:SER:HB3	2.03	0.57
1:B:211:GLU:OE2	1:B:213:GLN:HB2	2.05	0.57
1:B:824:GLU:CD	1:B:824:GLU:H	2.13	0.57
1:A:704:GLY:O	1:A:804:ARG:NH2	2.38	0.57
1:A:482:VAL:HG12	1:A:539:LEU:HD22	1.87	0.57
1:A:703:VAL:HG12	1:A:805:GLY:O	2.05	0.57
1:A:790:THR:O	1:A:794:ALA:N	2.38	0.57
1:A:839:LEU:HD12	1:A:865:THR:HB	1.87	0.57
1:B:107:PHE:HD2	1:B:373:LEU:HD13	1.69	0.57
1:A:358:ASN:OD1	1:A:913:ASN:N	2.31	0.56
1:A:431:TRP:CZ3	1:A:500:ARG:HG2	2.39	0.56
1:A:245:THR:HG22	1:A:247:TYR:H	1.70	0.56
1:A:990:GLU:HG2	1:A:1020:LEU:HB2	1.87	0.56
1:A:388:LYS:HZ2	1:A:389:LEU:HD22	1.70	0.56
1:A:629:ILE:HG12	1:A:647:TYR:CD2	2.40	0.56
1:B:185:PRO:O	1:B:215:SER:OG	2.23	0.56
1:B:340:TYR:HH	1:B:948:THR:HA	1.70	0.56
1:A:918:ILE:HD13	1:A:945:ILE:HG23	1.86	0.56
1:A:1037:HIS:CG	1:A:1038:ILE:H	2.24	0.56
1:B:799:TYR:HA	1:B:803:THR:HG21	1.87	0.56
1:B:929:VAL:HB	1:B:930:PRO:HD3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:GLU:OE1	1:B:510:GLU:N	2.37	0.56
1:A:207:ALA:HA	1:A:210:LYS:HG3	1.86	0.56
1:B:298:ASN:HD22	1:B:330:TYR:H	1.52	0.56
1:B:733:LEU:HD23	1:B:794:ALA:HB2	1.87	0.56
1:A:64:LEU:O	1:A:68:ILE:HG23	2.05	0.56
1:A:431:TRP:HH2	1:A:469:ASN:HB3	1.70	0.56
1:A:751:LEU:HD22	1:A:763:LEU:HD11	1.87	0.56
1:A:627:GLN:O	1:A:631:GLN:N	2.30	0.56
1:A:676:VAL:HA	1:A:680:HIS:NE2	2.21	0.56
1:A:803:THR:HB	1:A:815:PRO:CG	2.35	0.56
1:B:712:LEU:O	1:B:716:ILE:N	2.24	0.56
1:B:917:THR:C	1:B:918:ILE:HD12	2.31	0.56
1:A:927:ARG:HD2	1:A:999:ASP:OD1	2.06	0.56
1:B:847:LYS:NZ	1:B:853:HIS:HB3	2.21	0.56
1:A:562:LEU:C	1:A:563:ARG:HD3	2.30	0.56
1:A:735:THR:HG23	1:A:791:LYS:HD2	1.86	0.56
1:A:804:ARG:O	1:A:815:PRO:HA	2.06	0.56
1:B:517:LYS:HZ3	1:B:578:LEU:HD12	1.70	0.56
1:A:614:PHE:O	1:A:618:LEU:N	2.29	0.56
1:A:927:ARG:O	1:A:930:PRO:HD2	2.05	0.56
1:B:787:TRP:HB2	1:B:790:THR:CG2	2.36	0.56
1:A:528:LEU:N	1:A:562:LEU:HD11	2.22	0.55
1:A:709:GLU:C	1:A:711:GLY:H	2.14	0.55
1:B:927:ARG:O	1:B:930:PRO:HD2	2.06	0.55
1:B:46:LEU:O	1:B:50:LEU:N	2.32	0.55
1:B:117:ARG:CZ	1:B:177:ARG:NH2	2.69	0.55
1:B:533:LYS:O	1:B:533:LYS:HG3	2.05	0.55
1:A:559:ALA:HB1	1:A:563:ARG:HG3	1.88	0.55
1:B:476:LEU:HD11	1:B:505:PRO:HB3	1.88	0.55
1:A:102:LEU:O	1:A:106:LYS:NZ	2.39	0.55
1:A:387:ARG:NH1	1:A:393:ASN:ND2	2.54	0.55
1:A:847:LYS:HD2	1:A:851:LEU:HB3	1.87	0.55
1:B:645:PRO:O	1:B:649:LEU:N	2.35	0.55
1:B:825:ASP:OD1	1:B:825:ASP:N	2.40	0.55
1:A:393:ASN:HB3	1:A:396:ALA:HB3	1.89	0.55
1:A:674:VAL:HG23	1:A:674:VAL:O	2.07	0.55
1:A:734:HIS:CE1	1:A:749:TYR:HH	2.22	0.55
1:B:418:ASP:CG	1:B:655:THR:HG22	2.32	0.55
1:B:721:PHE:O	1:B:725:HIS:N	2.37	0.55
1:B:125:TYR:CZ	1:B:221:ARG:HG3	2.40	0.55
1:B:705:ASP:HA	1:B:734:HIS:HD2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:635:GLN:HB3	1:A:636:ASP:OD1	2.06	0.55
1:A:765:LYS:HD2	1:A:765:LYS:N	2.22	0.55
1:A:247:TYR:CE2	1:A:321:PRO:HB3	2.42	0.55
1:A:481:ASP:CG	1:A:610:ARG:HH12	2.15	0.55
1:A:660:ILE:O	1:A:811:ARG:NH2	2.40	0.55
1:A:751:LEU:HD22	1:A:763:LEU:CD1	2.37	0.55
1:B:558:SER:HA	1:B:560:ARG:HD2	1.87	0.55
1:A:579:GLU:O	1:A:583:ASP:N	2.39	0.55
1:A:643:TRP:CZ2	1:A:645:PRO:HB2	2.42	0.55
1:B:623:ALA:O	1:B:626:LEU:HB3	2.07	0.55
1:A:1038:ILE:HG13	1:A:1039:LEU:H	1.71	0.55
1:A:301:SER:OG	1:A:333:THR:N	2.30	0.54
1:A:387:ARG:NH1	1:A:393:ASN:HD21	2.05	0.54
1:A:560:ARG:HG2	1:A:561:VAL:N	2.21	0.54
1:A:718:ALA:O	1:A:721:PHE:HB3	2.06	0.54
1:B:291:GLU:HA	1:B:294:ARG:HH11	1.72	0.54
1:A:247:TYR:CD2	1:A:321:PRO:HB3	2.42	0.54
1:A:401:LEU:HD21	1:A:893:LYS:CD	2.35	0.54
1:B:41:ASP:HA	1:B:231:LEU:HB2	1.89	0.54
1:B:71:GLY:C	1:B:73:LEU:H	2.15	0.54
1:B:188:ILE:HG23	1:B:217:VAL:HG22	1.88	0.54
1:A:1001:PRO:HB2	1:A:1004:TRP:CD1	2.42	0.54
1:B:84:ASP:HA	1:B:87:LEU:HD12	1.88	0.54
1:B:85:ARG:O	1:B:89:ILE:HD13	2.07	0.54
1:A:655:THR:H	1:A:656:ARG:NH1	2.06	0.54
1:A:750:GLN:N	1:A:750:GLN:OE1	2.40	0.54
1:B:853:HIS:CE1	1:B:855:VAL:H	2.24	0.54
1:A:513:LYS:O	1:A:517:LYS:N	2.36	0.54
1:B:186:LEU:HD11	1:B:217:VAL:CG1	2.37	0.54
1:A:111:ILE:O	1:A:111:ILE:HG22	2.07	0.54
1:A:132:ARG:HD2	1:A:168:LEU:HD22	1.88	0.54
1:A:761:GLU:O	1:A:765:LYS:NZ	2.38	0.54
1:A:990:GLU:O	1:A:992:ALA:N	2.40	0.54
1:B:209:ALA:CA	1:B:210:LYS:HD2	2.38	0.54
1:B:243:LYS:N	1:B:993:LEU:O	2.35	0.54
1:B:420:ARG:NH2	1:B:650:SER:HB3	2.22	0.54
1:A:110:ALA:HB2	1:A:969:GLU:C	2.33	0.54
1:A:444:PHE:CD2	1:A:462:ALA:HB3	2.42	0.54
1:B:520:ARG:NH1	1:B:523:GLN:HG3	2.23	0.54
1:A:444:PHE:O	1:A:464:ARG:HG3	2.08	0.54
1:B:536:GLN:O	1:B:539:LEU:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:922:SER:O	1:B:925:SER:OG	2.26	0.54
1:A:734:HIS:HA	1:A:804:ARG:NH1	2.23	0.54
1:A:734:HIS:HE1	1:A:749:TYR:CE1	2.25	0.54
1:B:179:LEU:HG	1:B:209:ALA:HB1	1.90	0.54
1:B:334:GLN:HA	1:B:337:LEU:HD13	1.90	0.54
1:A:106:LYS:HD3	1:A:106:LYS:N	2.19	0.54
1:A:510:GLU:HB3	1:A:511:PRO:HD3	1.89	0.54
1:A:672:ASN:ND2	1:A:863:LYS:HA	2.23	0.54
1:A:293:ALA:HB1	1:A:952:ILE:HA	1.90	0.53
1:A:939:ASN:OD1	1:A:939:ASN:C	2.51	0.53
1:B:476:LEU:HB3	1:B:535:PHE:CE1	2.43	0.53
1:A:48:GLU:CG	1:A:114:ALA:HB3	2.37	0.53
1:A:283:ASP:O	1:A:989:PRO:HA	2.07	0.53
1:A:523:GLN:OE1	1:A:531:MSE:HB2	2.07	0.53
1:A:733:LEU:HG	1:A:790:THR:HB	1.90	0.53
1:A:846:MSE:SE	1:A:848:ASP:HA	2.59	0.53
1:A:918:ILE:O	1:A:947:LEU:HA	2.07	0.53
1:A:1037:HIS:CD2	1:A:1038:ILE:H	2.26	0.53
1:A:107:PHE:O	1:A:111:ILE:HB	2.08	0.53
1:A:735:THR:CB	1:A:804:ARG:HH22	2.22	0.53
1:B:558:SER:HA	1:B:560:ARG:HG2	1.90	0.53
1:B:244:ARG:O	1:B:992:ALA:HA	2.09	0.53
1:B:703:VAL:HG23	1:B:733:LEU:HB3	1.91	0.53
1:A:102:LEU:O	1:A:106:LYS:HD3	2.09	0.53
1:A:1038:ILE:HD12	1:A:1039:LEU:HB2	1.90	0.53
1:B:669:ARG:NH2	1:B:797:LEU:O	2.42	0.53
1:A:150:MSE:O	1:A:151:GLN:HB2	2.06	0.53
1:A:905:SER:HB3	1:A:942:ASN:HB2	1.91	0.53
1:B:705:ASP:C	1:B:707:ASP:H	2.16	0.53
1:A:119:GLU:O	1:A:123:GLN:HG3	2.09	0.53
1:A:474:ILE:O	1:A:506:LEU:N	2.34	0.53
1:A:533:LYS:HA	1:A:536:GLN:HG3	1.91	0.53
1:A:583:ASP:O	1:A:587:ARG:N	2.34	0.53
1:A:643:TRP:CD1	1:A:645:PRO:HD2	2.44	0.53
1:A:926:GLN:HE22	1:A:958:ILE:HD11	1.73	0.53
1:B:292:VAL:HG23	1:B:293:ALA:H	1.73	0.53
1:A:581:VAL:O	1:A:585:THR:HG23	2.09	0.53
1:A:944:LYS:HE2	1:A:946:PHE:CZ	2.44	0.53
1:B:107:PHE:CD2	1:B:373:LEU:HD13	2.43	0.53
1:B:210:LYS:HD3	1:B:211:GLU:CD	2.34	0.53
1:B:607:LEU:O	1:B:608:LEU:HD23	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:LEU:HD11	1:A:1006:VAL:HG21	1.91	0.53
1:B:380:ARG:HB2	1:B:912:ILE:HD11	1.91	0.53
1:B:558:SER:CA	1:B:560:ARG:HG2	2.39	0.53
1:B:1025:GLU:C	1:B:1027:SER:H	2.16	0.53
1:B:705:ASP:HA	1:B:734:HIS:CD2	2.45	0.52
1:B:763:LEU:O	1:B:766:ILE:HG12	2.09	0.52
1:A:247:TYR:CE2	1:A:956:LEU:HD21	2.44	0.52
1:B:100:ALA:HA	1:B:103:SER:HB3	1.90	0.52
1:B:125:TYR:CD2	1:B:222:PRO:HD3	2.44	0.52
1:B:249:MSE:HE2	1:B:956:LEU:N	2.24	0.52
1:B:703:VAL:HG21	1:B:794:ALA:CB	2.40	0.52
1:A:707:ASP:CG	1:A:745:SER:HB3	2.33	0.52
1:B:147:MSE:O	1:B:149:GLY:N	2.37	0.52
1:B:581:VAL:O	1:B:585:THR:HG23	2.09	0.52
1:B:711:GLY:O	1:B:714:LEU:HB3	2.09	0.52
1:A:990:GLU:HG2	1:A:1020:LEU:CB	2.40	0.52
1:B:130:GLU:HA	1:B:133:LEU:HD12	1.91	0.52
1:A:314:THR:O	1:A:318:GLN:HG3	2.09	0.52
1:A:974:GLU:CB	1:A:976:GLY:H	2.23	0.52
1:A:378:HIS:HA	1:A:381:GLN:NE2	2.15	0.52
1:A:32:VAL:HB	1:A:985:PHE:HB2	1.90	0.52
1:B:250:ILE:N	1:B:289:SER:HA	2.24	0.52
1:B:432:LEU:CD1	1:B:503:LEU:HD13	2.40	0.52
1:A:292:VAL:HG23	1:A:293:ALA:H	1.74	0.52
1:A:377:ARG:C	1:A:379:GLU:H	2.17	0.52
1:B:240:LEU:HD12	1:B:988:LEU:HD21	1.91	0.52
1:B:339:GLU:HG3	1:B:900:SER:OG	2.10	0.52
1:B:434:ASP:N	1:B:438:ASP:OD2	2.39	0.52
1:B:1008:PRO:HB3	1:B:1033:TYR:CE1	2.45	0.52
1:A:247:TYR:CZ	1:A:956:LEU:HD21	2.45	0.52
1:A:247:TYR:OH	1:A:956:LEU:HD11	2.10	0.52
1:B:290:SER:HA	1:B:292:VAL:HG22	1.91	0.52
1:B:672:ASN:ND2	1:B:866:SER:OG	2.39	0.52
1:A:52:ALA:HB2	1:A:114:ALA:HB2	1.91	0.51
1:A:93:GLU:HB2	1:A:96:ILE:HG22	1.92	0.51
1:A:239:GLU:HG2	1:A:960:ARG:HH21	1.74	0.51
1:A:763:LEU:HA	1:A:766:ILE:HD12	1.91	0.51
1:A:1000:VAL:HG22	1:A:1001:PRO:HD2	1.92	0.51
1:B:56:GLU:OE2	1:B:105:PHE:HA	2.10	0.51
1:B:200:GLU:HB3	1:B:203:ARG:HD3	1.92	0.51
1:B:597:ARG:NH1	1:B:658:GLU:OE1	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:LEU:HG	1:A:340:TYR:HB3	1.92	0.51
1:A:390:GLY:O	1:A:854:LYS:HD3	2.10	0.51
1:B:490:GLN:O	1:B:493:ILE:HB	2.10	0.51
1:A:208:MSE:CG	1:A:213:GLN:HB2	2.40	0.51
1:A:346:ALA:HB1	1:A:895:TRP:HB2	1.93	0.51
1:A:951:ARG:HD3	1:A:951:ARG:H	1.75	0.51
1:B:393:ASN:HD22	1:B:911:SER:HB2	1.74	0.51
1:B:764:GLU:OE1	1:B:767:GLN:NE2	2.44	0.51
1:B:789:GLN:HB2	1:B:793:LEU:HD21	1.91	0.51
1:A:38:ALA:HA	1:A:1035:LEU:HB3	1.93	0.51
1:A:111:ILE:O	1:A:111:ILE:CG2	2.58	0.51
1:A:465:ARG:HE	1:A:644:LEU:CD1	2.22	0.51
1:B:203:ARG:O	1:B:207:ALA:N	2.36	0.51
1:A:638:VAL:HG21	1:A:642:THR:CG2	2.39	0.51
1:A:734:HIS:NE2	1:A:749:TYR:OH	2.41	0.51
1:B:244:ARG:CB	1:B:993:LEU:HB2	2.40	0.51
1:B:465:ARG:NH1	1:B:642:THR:O	2.44	0.51
1:B:558:SER:C	1:B:560:ARG:N	2.66	0.51
1:A:305:ASP:OD2	1:A:330:TYR:OH	2.13	0.51
1:B:124:TYR:CZ	1:B:173:LEU:HD11	2.45	0.51
1:A:102:LEU:C	1:A:106:LYS:HZ3	2.18	0.51
1:B:32:VAL:HG22	1:B:1029:VAL:HB	1.91	0.51
1:B:78:THR:HG22	1:B:81:GLU:HG3	1.92	0.51
1:B:432:LEU:HD11	1:B:503:LEU:HD13	1.92	0.51
1:B:449:ASP:OD1	1:B:633:ILE:HD13	2.11	0.51
1:B:483:TYR:O	1:B:484:MSE:C	2.54	0.51
1:B:735:THR:HG21	1:B:802:GLY:N	2.24	0.51
1:A:370:TYR:HH	1:A:1004:TRP:HZ2	1.58	0.51
1:B:200:GLU:OE1	1:B:203:ARG:HD3	2.11	0.51
1:B:206:SER:O	1:B:210:LYS:N	2.43	0.51
1:B:493:ILE:O	1:B:496:LEU:N	2.42	0.51
1:B:647:TYR:HA	1:B:651:GLN:NE2	2.25	0.51
1:A:31:SER:O	1:A:1028:ASP:HB2	2.10	0.51
1:A:435:LEU:HA	1:A:441:TYR:CD2	2.44	0.51
1:A:459:GLN:O	1:A:460:LEU:HB2	2.10	0.51
1:B:63:PRO:O	1:B:66:ASP:HB2	2.10	0.51
1:B:353:ASN:OD1	1:B:918:ILE:HA	2.10	0.51
1:A:791:LYS:O	1:A:794:ALA:HB3	2.11	0.51
1:B:339:GLU:OE2	1:B:898:ALA:HB3	2.11	0.51
1:B:347:SER:OG	1:B:893:LYS:HG3	2.11	0.51
1:B:578:LEU:HA	1:B:582:MSE:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:911:SER:O	1:B:912:ILE:HG13	2.10	0.51
1:A:532:MSE:O	1:A:535:PHE:N	2.44	0.50
1:B:334:GLN:O	1:B:337:LEU:HB2	2.11	0.50
1:B:347:SER:O	1:B:348:LEU:HB2	2.09	0.50
1:B:463:VAL:C	1:B:465:ARG:N	2.69	0.50
1:A:284:LEU:O	1:A:285:LYS:HB2	2.09	0.50
1:A:569:PHE:CD1	1:A:570:GLU:HB3	2.45	0.50
1:A:804:ARG:N	1:A:815:PRO:HB3	2.24	0.50
1:B:106:LYS:O	1:B:970:PRO:HD3	2.10	0.50
1:A:427:ASP:OD1	1:A:584:LYS:NZ	2.35	0.50
1:A:673:LEU:N	1:A:675:GLN:HE22	2.07	0.50
1:B:521:TYR:HE2	1:B:556:ILE:HD11	1.76	0.50
1:B:612:ASP:OD1	1:B:616:GLN:NE2	2.42	0.50
1:B:672:ASN:CG	1:B:673:LEU:N	2.69	0.50
1:A:533:LYS:HE2	1:A:561:VAL:CG2	2.41	0.50
1:B:48:GLU:OE2	1:B:112:ARG:NH2	2.44	0.50
1:B:866:SER:O	1:B:870:LEU:HD13	2.11	0.50
1:B:497:ILE:HG22	1:B:499:VAL:HG23	1.93	0.50
1:A:427:ASP:O	1:A:520:ARG:NH2	2.45	0.50
1:A:427:ASP:H	1:A:584:LYS:NZ	2.09	0.50
1:A:565:LYS:HG2	1:A:566:ALA:H	1.76	0.50
1:A:587:ARG:NH2	1:A:590:LYS:HE3	2.26	0.50
1:B:488:HIS:N	1:B:488:HIS:CD2	2.79	0.50
1:B:834:GLU:O	1:B:838:ARG:HB3	2.12	0.50
1:A:83:TYR:CZ	1:A:87:LEU:HD11	2.47	0.50
1:A:705:ASP:OD1	1:A:736:SER:OG	2.29	0.50
1:A:1006:VAL:HA	1:A:1034:GLU:O	2.12	0.50
1:B:232:PHE:CD2	1:B:980:ARG:HB2	2.47	0.50
1:B:525:THR:O	1:B:564:GLY:HA2	2.12	0.50
1:B:1010:GLU:CD	1:B:1010:GLU:H	2.19	0.50
1:A:433:ASN:CB	1:A:501:PHE:H	2.25	0.49
1:B:195:SER:O	1:B:198:PHE:HD2	1.95	0.49
1:B:200:GLU:HA	1:B:203:ARG:H	1.77	0.49
1:A:209:ALA:N	1:A:210:LYS:HG2	2.27	0.49
1:A:319:ASP:OD2	1:A:963:ARG:NH2	2.46	0.49
1:A:591:ARG:O	1:A:656:ARG:HA	2.13	0.49
1:A:725:HIS:CE1	1:A:828:GLU:CD	2.91	0.49
1:B:47:LEU:O	1:B:51:GLU:N	2.34	0.49
1:B:208:MSE:C	1:B:210:LYS:HD2	2.36	0.49
1:A:292:VAL:C	1:A:294:ARG:N	2.70	0.49
1:A:679:SER:O	1:A:681:ASP:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:VAL:HG21	1:B:205:LEU:HD11	1.95	0.49
1:A:388:LYS:HE3	1:A:389:LEU:HD22	1.94	0.49
1:B:392:SER:HB3	1:B:395:GLU:HG3	1.94	0.49
1:B:1028:ASP:N	1:B:1028:ASP:OD1	2.44	0.49
1:A:100:ALA:HB1	1:A:380:ARG:NH2	2.17	0.49
1:A:202:HIS:CE1	1:A:206:SER:HB2	2.47	0.49
1:A:704:GLY:N	1:A:733:LEU:O	2.40	0.49
1:A:831:LEU:HA	1:A:834:GLU:HB3	1.93	0.49
1:B:713:ASN:HA	1:B:716:ILE:HG12	1.95	0.49
1:A:309:PRO:HG2	1:A:902:ILE:HG23	1.93	0.49
1:A:338:ASP:OD1	1:A:338:ASP:N	2.38	0.49
1:A:851:LEU:HD23	1:A:854:LYS:HG3	1.95	0.49
1:A:100:ALA:CB	1:A:380:ARG:HH21	2.17	0.49
1:A:632:SER:OG	1:A:633:ILE:N	2.44	0.49
1:A:753:ARG:HG2	1:A:753:ARG:O	2.12	0.49
1:A:951:ARG:HB2	1:A:952:ILE:HG22	1.94	0.49
1:B:443:ASP:OD1	1:B:443:ASP:N	2.42	0.49
1:A:207:ALA:C	1:A:210:LYS:HG3	2.38	0.49
1:A:393:ASN:OD1	1:A:393:ASN:N	2.45	0.49
1:A:402:HIS:C	1:A:402:HIS:CD2	2.90	0.49
1:B:205:LEU:O	1:B:208:MSE:C	2.55	0.49
1:B:705:ASP:OD1	1:B:734:HIS:NE2	2.45	0.49
1:A:96:ILE:O	1:A:102:LEU:HB2	2.12	0.49
1:A:530:ALA:H	1:A:562:LEU:HD22	1.78	0.49
1:A:696:ASN:O	1:A:858:SER:HB3	2.11	0.49
1:A:735:THR:HB	1:A:804:ARG:NH2	2.28	0.49
1:A:785:ALA:HA	1:A:787:TRP:CE2	2.48	0.49
1:A:917:THR:C	1:A:918:ILE:HD12	2.37	0.49
1:B:67:ARG:HG3	1:B:72:VAL:HG21	1.93	0.49
1:B:204:LYS:O	1:B:208:MSE:HB2	2.13	0.49
1:B:657:ASN:HB3	1:B:659:LEU:H	1.76	0.49
1:A:427:ASP:H	1:A:584:LYS:HZ1	1.60	0.48
1:B:292:VAL:HG23	1:B:293:ALA:N	2.28	0.48
1:B:349:PRO:HB3	1:B:352:ARG:HH11	1.77	0.48
1:B:360:LEU:HD12	1:B:890:SER:N	2.27	0.48
1:B:657:ASN:HB3	1:B:659:LEU:HB3	1.95	0.48
1:A:463:VAL:HG12	1:A:465:ARG:HG3	1.95	0.48
1:A:504:VAL:HG11	1:A:588:TYR:CE2	2.48	0.48
1:A:704:GLY:HA2	1:A:804:ARG:HG2	1.95	0.48
1:B:90:VAL:HB	1:B:95:HIS:HE1	1.78	0.48
1:A:849:LEU:N	1:A:849:LEU:HD23	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:849:LEU:O	1:A:850:ASN:HB2	2.12	0.48
1:B:555:THR:HA	1:B:558:SER:CB	2.43	0.48
1:A:487:GLN:O	1:A:491:THR:HG23	2.13	0.48
1:A:807:LEU:HD23	1:A:812:ALA:HA	1.95	0.48
1:B:476:LEU:O	1:B:515:GLN:HG2	2.14	0.48
1:B:857:GLY:O	1:B:861:PHE:N	2.46	0.48
1:B:974:GLU:HG2	1:B:977:ALA:HB3	1.96	0.48
1:B:35:ALA:N	1:B:1031:ALA:O	2.38	0.48
1:B:249:MSE:SE	1:B:292:VAL:CG2	3.07	0.48
1:B:353:ASN:HA	1:B:917:THR:O	2.13	0.48
1:B:485:VAL:HA	1:B:489:ILE:CG1	2.43	0.48
1:A:111:ILE:HG22	1:A:113:SER:OG	2.13	0.48
1:A:237:GLY:O	1:A:999:ASP:N	2.42	0.48
1:A:388:LYS:CE	1:A:389:LEU:HD22	2.44	0.48
1:A:449:ASP:HA	1:A:633:ILE:HD11	1.96	0.48
1:A:657:ASN:OD1	1:A:659:LEU:N	2.36	0.48
1:A:672:ASN:C	1:A:675:GLN:NE2	2.64	0.48
1:A:710:ALA:N	1:A:819:THR:OG1	2.47	0.48
1:B:75:ASP:CG	1:B:85:ARG:HH21	2.21	0.48
1:B:629:ILE:C	1:B:631:GLN:N	2.69	0.48
1:B:749:TYR:N	1:B:749:TYR:CD1	2.79	0.48
1:A:485:VAL:HA	1:A:489:ILE:CG1	2.44	0.48
1:A:587:ARG:O	1:A:587:ARG:HG3	2.13	0.48
1:B:29:ASP:HA	1:B:1026:GLY:H	1.77	0.48
1:B:147:MSE:HG2	1:B:148:ASP:N	2.28	0.48
1:B:659:LEU:HD22	1:B:821:THR:OG1	2.12	0.48
1:A:152:TYR:OH	1:B:707:ASP:O	2.32	0.48
1:A:185:PRO:HB2	1:A:214:VAL:HG13	1.95	0.48
1:A:540:GLU:O	1:A:543:LYS:HE3	2.13	0.48
1:A:633:ILE:HA	1:A:637:ALA:CB	2.44	0.48
1:A:667:LYS:HE3	1:A:669:ARG:CD	2.43	0.48
1:A:705:ASP:O	1:A:708:SER:OG	2.27	0.48
1:A:712:LEU:O	1:A:716:ILE:N	2.26	0.48
1:B:355:LEU:HD21	1:B:357:ILE:HG13	1.95	0.48
1:A:56:GLU:CD	1:A:104:SER:OG	2.56	0.48
1:A:107:PHE:CE2	1:A:111:ILE:HD11	2.49	0.48
1:B:92:ASP:OD1	1:B:92:ASP:N	2.47	0.48
1:B:712:LEU:HA	1:B:715:LEU:HB3	1.95	0.48
1:B:893:LYS:NZ	1:B:895:TRP:HB3	2.29	0.48
1:A:660:ILE:O	1:A:662:PRO:HD3	2.14	0.47
1:A:998:MSE:HE3	1:A:998:MSE:HB3	1.70	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:PHE:O	1:B:323:TYR:N	2.47	0.47
1:A:388:LYS:CD	1:A:389:LEU:HD13	2.37	0.47
1:A:527:GLY:HA3	1:A:562:LEU:HD11	1.96	0.47
1:A:108:SER:CA	1:A:111:ILE:HB	2.43	0.47
1:A:226:ALA:O	1:A:229:ARG:NH1	2.47	0.47
1:A:309:PRO:HB2	1:A:902:ILE:HD12	1.96	0.47
1:A:333:THR:O	1:A:336:PHE:HB3	2.14	0.47
1:A:748:LEU:CA	1:A:751:LEU:HD21	2.42	0.47
1:B:54:ALA:HA	1:B:57:ASN:O	2.14	0.47
1:B:110:ALA:HB2	1:B:970:PRO:HD3	1.95	0.47
1:B:635:GLN:O	1:B:637:ALA:N	2.47	0.47
1:A:357:ILE:O	1:A:360:LEU:HB3	2.15	0.47
1:B:628:LEU:O	1:B:631:GLN:HB3	2.13	0.47
1:A:600:PRO:HB2	1:A:607:LEU:HD22	1.95	0.47
1:A:897:GLY:O	1:A:898:ALA:C	2.57	0.47
1:B:41:ASP:CG	1:B:230:PRO:HA	2.40	0.47
1:B:146:HIS:ND1	1:B:188:ILE:HD12	2.30	0.47
1:B:154:SER:O	1:B:156:THR:N	2.43	0.47
1:B:439:LYS:HD3	1:B:439:LYS:N	2.29	0.47
1:B:993:LEU:O	1:B:994:LEU:HD23	2.15	0.47
1:A:78:THR:HG23	1:A:81:GLU:HG3	1.96	0.47
1:A:292:VAL:O	1:A:295:LEU:N	2.47	0.47
1:A:380:ARG:HH12	1:A:941:VAL:CG2	2.28	0.47
1:A:599:PRO:O	1:A:610:ARG:HD3	2.15	0.47
1:A:918:ILE:N	1:A:946:PHE:O	2.46	0.47
1:A:926:GLN:OE1	1:A:958:ILE:HD13	2.15	0.47
1:B:669:ARG:NH1	1:B:813:VAL:O	2.47	0.47
1:B:735:THR:HG22	1:B:791:LYS:NZ	2.29	0.47
1:B:799:TYR:OH	1:B:813:VAL:N	2.30	0.47
1:A:203:ARG:O	1:A:206:SER:HB3	2.15	0.47
1:A:289:SER:O	1:A:292:VAL:HG13	2.14	0.47
1:A:349:PRO:HA	1:A:352:ARG:NH2	2.29	0.47
1:A:351:GLY:HA2	1:A:948:THR:O	2.13	0.47
1:A:355:LEU:O	1:A:362:ILE:N	2.36	0.47
1:A:416:ARG:NH2	1:A:604:ASN:O	2.44	0.47
1:B:46:LEU:O	1:B:49:LEU:HB2	2.15	0.47
1:B:627:GLN:HA	1:B:630:GLN:HB2	1.97	0.47
1:B:745:SER:O	1:B:749:TYR:CZ	2.68	0.47
1:A:39:SER:HB3	1:A:1036:GLU:HA	1.96	0.47
1:A:77:VAL:HA	1:A:82:LEU:HD23	1.96	0.47
1:A:210:LYS:CD	1:A:210:LYS:H	2.09	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:791:LYS:O	1:A:795:ALA:N	2.32	0.47
1:B:424:GLU:HG2	1:B:588:TYR:N	2.30	0.47
1:B:572:ALA:C	1:B:574:SER:H	2.22	0.47
1:B:789:GLN:O	1:B:793:LEU:HG	2.14	0.47
1:A:98:ASP:OD1	1:A:98:ASP:C	2.57	0.47
1:A:303:ILE:HD13	1:A:313:LEU:CD1	2.45	0.47
1:A:804:ARG:HG3	1:A:805:GLY:H	1.80	0.47
1:B:55:ALA:HB1	1:B:377:ARG:HH22	1.79	0.47
1:B:109:LEU:HB2	1:B:970:PRO:HG3	1.97	0.47
1:B:401:LEU:O	1:B:402:HIS:CD2	2.68	0.47
1:B:460:LEU:HA	1:B:460:LEU:HD23	1.63	0.47
1:B:521:TYR:HE1	1:B:568:SER:HB3	1.79	0.47
1:A:90:VAL:HB	1:A:96:ILE:HG21	1.96	0.47
1:A:1028:ASP:OD1	1:A:1028:ASP:N	2.48	0.47
1:B:353:ASN:HB3	1:B:928:TRP:CZ3	2.50	0.47
1:A:293:ALA:HA	1:A:953:LEU:N	2.30	0.46
1:A:797:LEU:HD22	1:A:807:LEU:CD1	2.44	0.46
1:B:467:VAL:O	1:B:645:PRO:HG3	2.15	0.46
1:B:696:ASN:OD1	1:B:858:SER:OG	2.33	0.46
1:B:698:LEU:O	1:B:729:GLU:N	2.37	0.46
1:B:703:VAL:HG21	1:B:794:ALA:HB2	1.97	0.46
1:B:792:GLN:HG2	1:B:795:ALA:HB3	1.96	0.46
1:A:363:ASP:OD1	1:A:364:SER:N	2.48	0.46
1:A:679:SER:C	1:A:681:ASP:H	2.24	0.46
1:B:211:GLU:OE2	1:B:213:GLN:N	2.49	0.46
1:B:826:ASP:O	1:B:829:ILE:HG22	2.16	0.46
1:A:152:TYR:HE1	1:B:709:GLU:OE2	1.99	0.46
1:A:934:THR:HG21	1:A:966:LEU:HG	1.97	0.46
1:A:990:GLU:C	1:A:992:ALA:H	2.23	0.46
1:B:484:MSE:SE	1:B:610:ARG:HH12	2.48	0.46
1:B:549:GLN:HA	1:B:552:PHE:HB3	1.98	0.46
1:A:435:LEU:H	1:A:500:ARG:HD2	1.81	0.46
1:A:763:LEU:HD12	1:A:766:ILE:HD12	1.98	0.46
1:B:111:ILE:HD11	1:B:369:ALA:HB1	1.97	0.46
1:B:291:GLU:HB3	1:B:328:ALA:HB1	1.97	0.46
1:B:298:ASN:OD1	1:B:298:ASN:N	2.49	0.46
1:B:562:LEU:HB3	1:B:563:ARG:H	1.29	0.46
1:B:847:LYS:HE3	1:B:852:GLY:C	2.39	0.46
1:B:1008:PRO:HB3	1:B:1033:TYR:CZ	2.50	0.46
1:A:223:PRO:HB2	1:A:227:SER:OG	2.16	0.46
1:A:236:TYR:HB3	1:A:1000:VAL:HG23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:712:LEU:O	1:A:716:ILE:HG23	2.15	0.46
1:B:135:THR:HG21	1:B:139:ALA:N	2.30	0.46
1:B:237:GLY:HA3	1:B:962:TYR:OH	2.16	0.46
1:B:463:VAL:HG12	1:B:463:VAL:O	2.15	0.46
1:B:593:ASP:OD2	1:B:658:GLU:HG3	2.15	0.46
1:B:636:ASP:OD1	1:B:636:ASP:N	2.48	0.46
1:B:672:ASN:HB2	1:B:866:SER:HB3	1.96	0.46
1:B:718:ALA:O	1:B:721:PHE:HB3	2.15	0.46
1:B:1037:HIS:CG	1:B:1038:ILE:H	2.34	0.46
1:A:48:GLU:CD	1:A:115:VAL:HG23	2.41	0.46
1:A:377:ARG:HD3	1:A:380:ARG:HB2	1.97	0.46
1:A:481:ASP:OD1	1:A:610:ARG:NH1	2.48	0.46
1:A:530:ALA:HA	1:A:533:LYS:HG3	1.95	0.46
1:A:951:ARG:HD3	1:A:951:ARG:N	2.31	0.46
1:B:39:SER:OG	1:B:40:PHE:N	2.49	0.46
1:B:996:LEU:HD13	1:B:1015:LEU:HD22	1.98	0.46
1:A:240:LEU:HD23	1:A:240:LEU:HA	1.62	0.46
1:A:927:ARG:HD2	1:A:999:ASP:CG	2.41	0.46
1:B:712:LEU:H	1:B:712:LEU:HD12	1.79	0.46
1:A:291:GLU:O	1:A:294:ARG:HB3	2.15	0.46
1:A:487:GLN:OE1	1:A:488:HIS:HB3	2.16	0.46
1:B:84:ASP:HA	1:B:87:LEU:CD1	2.46	0.46
1:B:522:LEU:HB3	1:B:531:MSE:HB2	1.98	0.46
1:B:957:PRO:O	1:B:958:ILE:C	2.58	0.46
1:A:102:LEU:HG	1:A:106:LYS:HZ1	1.81	0.46
1:A:188:ILE:HD13	1:A:219:ARG:NH1	2.31	0.46
1:A:296:GLY:HA3	1:A:953:LEU:HD11	1.98	0.46
1:A:911:SER:O	1:A:912:ILE:HG13	2.16	0.46
1:B:80:LYS:HB2	1:B:972:PHE:CG	2.50	0.46
1:B:338:ASP:CG	1:B:339:GLU:HG2	2.39	0.46
1:A:336:PHE:CG	1:A:337:LEU:HD13	2.50	0.46
1:A:530:ALA:H	1:A:562:LEU:CD2	2.28	0.46
1:B:211:GLU:HG3	1:B:212:GLY:H	1.78	0.46
1:B:608:LEU:HD13	1:B:617:GLU:HB2	1.98	0.46
1:B:716:ILE:O	1:B:720:LYS:HG3	2.16	0.46
1:A:460:LEU:HD21	1:A:626:LEU:HD11	1.98	0.45
1:A:957:PRO:O	1:A:958:ILE:C	2.59	0.45
1:B:349:PRO:CB	1:B:352:ARG:HE	2.25	0.45
1:B:487:GLN:HB3	1:B:488:HIS:HD2	1.81	0.45
1:B:766:ILE:O	1:B:769:ILE:HG12	2.17	0.45
1:B:836:SER:HG	1:B:837:LYS:H	1.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:630:GLN:O	1:A:634:VAL:HG22	2.16	0.45
1:A:655:THR:H	1:A:656:ARG:CZ	2.29	0.45
1:B:987:ARG:CG	1:B:987:ARG:O	2.65	0.45
1:A:292:VAL:HG23	1:A:293:ALA:N	2.30	0.45
1:A:793:LEU:O	1:A:797:LEU:HD11	2.17	0.45
1:B:632:SER:O	1:B:637:ALA:HB2	2.15	0.45
1:B:733:LEU:HD11	1:B:790:THR:HA	1.97	0.45
1:B:903:THR:HG22	1:B:944:LYS:HD3	1.97	0.45
1:A:113:SER:C	1:A:116:PRO:HD2	2.41	0.45
1:A:447:ASP:HB2	1:A:450:ALA:HB3	1.97	0.45
1:A:699:LEU:O	1:A:809:ASN:N	2.49	0.45
1:A:735:THR:HG23	1:A:791:LYS:CD	2.46	0.45
1:B:342:ALA:HB1	1:B:895:TRP:HH2	1.80	0.45
1:A:290:SER:HA	1:A:292:VAL:HG22	1.98	0.45
1:A:380:ARG:O	1:A:384:GLY:N	2.48	0.45
1:A:766:ILE:O	1:A:769:ILE:HG12	2.17	0.45
1:B:29:ASP:HA	1:B:1025:GLU:HG2	1.98	0.45
1:B:78:THR:HG23	1:B:81:GLU:HG3	1.95	0.45
1:B:171:ARG:O	1:B:173:LEU:HG	2.17	0.45
1:B:204:LYS:HD2	1:B:208:MSE:HG3	1.97	0.45
1:B:463:VAL:HB	1:B:498:PRO:HB2	1.98	0.45
1:B:672:ASN:O	1:B:674:VAL:N	2.50	0.45
1:B:710:ALA:HA	1:B:713:ASN:OD1	2.16	0.45
1:B:799:TYR:HE1	1:B:813:VAL:HG23	1.81	0.45
1:B:1023:LEU:HD11	1:B:1029:VAL:HG23	1.99	0.45
1:A:206:SER:C	1:A:210:LYS:HD2	2.41	0.45
1:A:310:PHE:O	1:A:313:LEU:HB3	2.16	0.45
1:A:444:PHE:HB3	1:A:462:ALA:O	2.17	0.45
1:A:660:ILE:HD13	1:A:660:ILE:HA	1.85	0.45
1:A:772:THR:O	1:A:773:SER:OG	2.23	0.45
1:B:62:PHE:O	1:B:66:ASP:N	2.42	0.45
1:B:150:MSE:HB3	1:B:151:GLN:H	1.61	0.45
1:B:167:ASP:O	1:B:168:LEU:HD23	2.16	0.45
1:B:465:ARG:NH2	1:B:640:GLU:OE2	2.49	0.45
1:B:708:SER:OG	1:B:710:ALA:N	2.49	0.45
1:B:734:HIS:CD2	1:B:735:THR:N	2.82	0.45
1:B:786:TYR:HB2	1:B:787:TRP:HE3	1.82	0.45
1:A:187:ALA:N	1:A:215:SER:O	2.33	0.45
1:A:515:GLN:CD	1:A:547:PRO:HB3	2.42	0.45
1:A:523:GLN:HG3	1:A:527:GLY:C	2.41	0.45
1:A:643:TRP:CE3	1:A:646:SER:HB3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:GLU:C	1:A:711:GLY:N	2.69	0.45
1:B:91:GLN:HG2	1:B:97:ASN:CG	2.42	0.45
1:B:445:PRO:HG2	1:B:462:ALA:HB2	1.98	0.45
1:B:558:SER:O	1:B:560:ARG:HG2	2.17	0.45
1:A:516:ALA:O	1:A:520:ARG:HG2	2.16	0.45
1:A:530:ALA:HB2	1:A:562:LEU:CD2	2.47	0.45
1:A:569:PHE:HD1	1:A:570:GLU:HB3	1.82	0.45
1:A:855:VAL:HG13	1:A:860:GLU:HG3	1.99	0.45
1:B:787:TRP:HE3	1:B:787:TRP:H	1.64	0.45
1:A:62:PHE:CD1	1:A:179:LEU:HD22	2.51	0.45
1:A:515:GLN:HG3	1:A:535:PHE:CZ	2.52	0.45
1:A:702:VAL:HG11	1:A:718:ALA:CB	2.47	0.45
1:A:789:GLN:HB3	1:A:793:LEU:HD22	1.97	0.45
1:B:178:LYS:HE3	1:B:178:LYS:HB3	1.47	0.45
1:B:502:GLY:C	1:B:503:LEU:HD12	2.42	0.45
1:A:249:MSE:HE1	1:A:292:VAL:HG21	1.98	0.45
1:A:351:GLY:N	1:A:951:ARG:HH12	2.14	0.45
1:B:698:LEU:HD13	1:B:808:LEU:HD11	1.99	0.45
1:A:616:GLN:O	1:A:620:MSE:N	2.47	0.44
1:A:1014:ASP:HB3	1:A:1017:ASN:HB2	2.00	0.44
1:B:202:HIS:CE1	1:B:206:SER:HB2	2.52	0.44
1:A:209:ALA:H	1:A:210:LYS:CE	2.31	0.44
1:A:460:LEU:HD23	1:A:460:LEU:HA	1.76	0.44
1:B:599:PRO:HA	1:B:600:PRO:HD3	1.76	0.44
1:A:78:THR:HG22	1:A:81:GLU:OE1	2.16	0.44
1:A:401:LEU:O	1:A:402:HIS:HB3	2.17	0.44
1:A:733:LEU:HD21	1:A:790:THR:HA	1.99	0.44
1:A:792:GLN:C	1:A:794:ALA:N	2.76	0.44
1:B:111:ILE:O	1:B:112:ARG:HB2	2.17	0.44
1:B:111:ILE:HG22	1:B:113:SER:HB3	1.99	0.44
1:B:147:MSE:HA	1:B:186:LEU:O	2.17	0.44
1:B:616:GLN:H	1:B:616:GLN:HG3	1.42	0.44
1:A:747:GLN:CD	1:A:747:GLN:O	2.60	0.44
1:A:859:VAL:O	1:A:862:ALA:HB3	2.17	0.44
1:B:146:HIS:CD2	1:B:146:HIS:C	2.95	0.44
1:B:246:ASP:O	1:B:248:ILE:N	2.49	0.44
1:B:293:ALA:CB	1:B:952:ILE:HG13	2.45	0.44
1:B:450:ALA:HA	1:B:452:LEU:HG	2.00	0.44
1:B:459:GLN:O	1:B:460:LEU:HB2	2.18	0.44
1:B:858:SER:HA	1:B:861:PHE:CB	2.41	0.44
1:A:107:PHE:CD1	1:A:968:PRO:HA	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ALA:HB2	1:A:970:PRO:N	2.32	0.44
1:A:169:GLU:OE1	1:A:171:ARG:HB2	2.18	0.44
1:A:334:GLN:HG3	1:A:335:GLU:OE1	2.17	0.44
1:A:530:ALA:HB2	1:A:562:LEU:HD23	1.99	0.44
1:A:616:GLN:O	1:A:620:MSE:HG3	2.17	0.44
1:A:855:VAL:HA	1:A:860:GLU:CD	2.43	0.44
1:A:936:SER:HB3	1:A:943:VAL:HB	1.99	0.44
1:B:313:LEU:HD21	1:B:929:VAL:HG22	1.99	0.44
1:B:602:LEU:HA	1:B:602:LEU:HD23	1.59	0.44
1:A:485:VAL:HA	1:A:489:ILE:HB	1.99	0.44
1:A:672:ASN:CA	1:A:675:GLN:HE22	2.27	0.44
1:B:83:TYR:O	1:B:87:LEU:HD12	2.18	0.44
1:B:188:ILE:HD13	1:B:219:ARG:CZ	2.47	0.44
1:B:190:TYR:CZ	1:B:219:ARG:HD2	2.51	0.44
1:B:666:SER:OG	1:B:668:ILE:HD11	2.18	0.44
1:A:419:TRP:CZ3	1:A:649:LEU:HD13	2.53	0.44
1:A:448:ILE:HG22	1:A:465:ARG:CD	2.48	0.44
1:A:703:VAL:HG23	1:A:733:LEU:HB3	1.99	0.44
1:B:298:ASN:ND2	1:B:327:VAL:O	2.50	0.44
1:B:387:ARG:C	1:B:390:GLY:H	2.26	0.44
1:B:558:SER:C	1:B:560:ARG:H	2.24	0.44
1:B:746:SER:HA	1:B:749:TYR:CG	2.53	0.44
1:B:789:GLN:N	1:B:789:GLN:OE1	2.50	0.44
1:B:910:ALA:C	1:B:912:ILE:H	2.24	0.44
1:A:62:PHE:N	1:A:63:PRO:HD2	2.32	0.44
1:A:784:LEU:HB3	1:A:787:TRP:CH2	2.53	0.44
1:B:675:GLN:O	1:B:680:HIS:ND1	2.37	0.44
1:B:929:VAL:O	1:B:933:ARG:N	2.42	0.44
1:A:84:ASP:HA	1:A:87:LEU:CD1	2.48	0.44
1:A:109:LEU:C	1:A:111:ILE:N	2.75	0.44
1:A:298:ASN:OD1	1:A:298:ASN:N	2.50	0.44
1:A:515:GLN:HE22	1:A:547:PRO:HB3	1.82	0.44
1:B:105:PHE:O	1:B:109:LEU:HD12	2.18	0.44
1:B:113:SER:O	1:B:116:PRO:HD2	2.18	0.44
1:B:203:ARG:HG2	1:B:204:LYS:N	2.32	0.44
1:B:417:TYR:N	1:B:605:GLY:O	2.51	0.44
1:B:537:ARG:NH2	1:B:540:GLU:OE1	2.51	0.44
1:B:807:LEU:HD23	1:B:812:ALA:HA	1.99	0.44
1:A:310:PHE:CZ	1:A:933:ARG:HB2	2.53	0.43
1:A:351:GLY:N	1:A:951:ARG:HH22	2.16	0.43
1:A:836:SER:HB3	1:A:838:ARG:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:TYR:O	1:B:49:LEU:HG	2.18	0.43
1:B:125:TYR:CE2	1:B:221:ARG:HG3	2.53	0.43
1:B:151:GLN:O	1:B:152:TYR:HD1	2.00	0.43
1:B:232:PHE:C	1:B:233:LEU:HD23	2.43	0.43
1:B:467:VAL:O	1:B:648:PHE:HE2	2.01	0.43
1:B:513:LYS:O	1:B:516:ALA:N	2.50	0.43
1:A:188:ILE:HG21	1:A:219:ARG:NH1	2.32	0.43
1:A:532:MSE:O	1:A:536:GLN:HG3	2.18	0.43
1:A:974:GLU:OE1	1:A:977:ALA:O	2.36	0.43
1:B:106:LYS:HB3	1:B:969:GLU:HB3	1.99	0.43
1:B:371:SER:OG	1:B:372:LEU:N	2.49	0.43
1:B:842:VAL:O	1:B:846:MSE:HB2	2.18	0.43
1:A:418:ASP:HB3	1:A:655:THR:HG22	1.99	0.43
1:A:950:VAL:HB	1:A:953:LEU:HG	1.99	0.43
1:A:1000:VAL:HG21	1:A:1004:TRP:CE3	2.53	0.43
1:B:250:ILE:N	1:B:288:SER:O	2.47	0.43
1:B:353:ASN:HB3	1:B:928:TRP:CE3	2.52	0.43
1:B:477:THR:HA	1:B:544:LEU:O	2.18	0.43
1:B:720:LYS:HG3	1:B:720:LYS:H	1.63	0.43
1:B:847:LYS:C	1:B:849:LEU:N	2.76	0.43
1:B:1036:GLU:O	1:B:1037:HIS:HB2	2.19	0.43
1:A:433:ASN:HB3	1:A:501:PHE:H	1.84	0.43
1:A:527:GLY:CA	1:A:562:LEU:HD11	2.47	0.43
1:A:575:SER:C	1:A:577:THR:H	2.26	0.43
1:B:105:PHE:CE2	1:B:109:LEU:HD11	2.54	0.43
1:B:113:SER:C	1:B:116:PRO:HD2	2.43	0.43
1:B:204:LYS:O	1:B:208:MSE:CB	2.66	0.43
1:B:349:PRO:CB	1:B:352:ARG:HH11	2.32	0.43
1:B:370:TYR:O	1:B:373:LEU:HB3	2.17	0.43
1:B:903:THR:HG22	1:B:944:LYS:CD	2.49	0.43
1:A:532:MSE:C	1:A:536:GLN:HG3	2.43	0.43
1:A:567:GLN:OE1	1:A:569:PHE:N	2.52	0.43
1:A:672:ASN:HA	1:A:675:GLN:NE2	2.33	0.43
1:A:792:GLN:O	1:A:795:ALA:N	2.52	0.43
1:B:399:LEU:O	1:B:401:LEU:HB2	2.18	0.43
1:B:550:ALA:O	1:B:554:GLU:HB2	2.19	0.43
1:B:1023:LEU:HD13	1:B:1028:ASP:HA	2.01	0.43
1:A:98:ASP:CG	1:A:100:ALA:N	2.76	0.43
1:A:244:ARG:HB2	1:A:993:LEU:HB2	2.01	0.43
1:A:851:LEU:CD2	1:A:854:LYS:HG3	2.48	0.43
1:A:862:ALA:O	1:A:865:THR:OG1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:SER:O	1:B:1028:ASP:HB2	2.18	0.43
1:B:72:VAL:HG23	1:B:73:LEU:HD12	1.99	0.43
1:B:455:THR:HB	1:B:456:TYR:H	1.62	0.43
1:B:551:LEU:HD23	1:B:551:LEU:HA	1.87	0.43
1:B:965:VAL:HG22	1:B:982:GLY:C	2.43	0.43
1:B:354:VAL:HG23	1:B:356:TRP:CH2	2.53	0.43
1:B:923:GLU:OE2	1:B:959:LYS:HG2	2.19	0.43
1:A:63:PRO:O	1:A:66:ASP:HB2	2.19	0.43
1:A:175:PHE:HE1	1:A:219:ARG:HG2	1.83	0.43
1:A:376:LEU:HG	1:A:912:ILE:CD1	2.49	0.43
1:B:78:THR:HG22	1:B:81:GLU:OE2	2.19	0.43
1:B:205:LEU:O	1:B:216:TYR:CD2	2.71	0.43
1:B:377:ARG:HA	1:B:380:ARG:NH1	2.34	0.43
1:A:107:PHE:O	1:A:111:ILE:N	2.52	0.43
1:A:706:PHE:CE2	1:A:734:HIS:HB3	2.54	0.43
1:A:811:ARG:HB2	1:A:834:GLU:OE2	2.18	0.43
1:B:244:ARG:N	1:B:993:LEU:HB2	2.34	0.43
1:B:355:LEU:HG	1:B:915:VAL:O	2.19	0.43
1:A:98:ASP:CG	1:A:99:ALA:N	2.72	0.43
1:A:349:PRO:HA	1:A:352:ARG:HH22	1.83	0.43
1:A:380:ARG:HH12	1:A:941:VAL:HG22	1.83	0.43
1:B:34:VAL:HA	1:B:1031:ALA:HB3	1.99	0.43
1:B:644:LEU:C	1:B:646:SER:N	2.76	0.43
1:A:176:ASP:HB3	1:A:217:VAL:HG21	2.02	0.42
1:A:344:ARG:HA	1:A:348:LEU:HG	2.01	0.42
1:A:522:LEU:O	1:A:526:HIS:N	2.45	0.42
1:A:562:LEU:O	1:A:563:ARG:NH2	2.52	0.42
1:A:629:ILE:O	1:A:633:ILE:HG22	2.18	0.42
1:A:672:ASN:HD21	1:A:863:LYS:HA	1.84	0.42
1:A:1000:VAL:CG2	1:A:1004:TRP:CE3	3.02	0.42
1:B:83:TYR:CE2	1:B:87:LEU:HD11	2.53	0.42
1:B:209:ALA:HB2	1:B:216:TYR:CB	2.45	0.42
1:B:242:LEU:HD11	1:B:961:PHE:CE1	2.54	0.42
1:B:377:ARG:HG3	1:B:380:ARG:HH22	1.83	0.42
1:B:537:ARG:HD2	1:B:537:ARG:N	2.33	0.42
1:B:705:ASP:C	1:B:707:ASP:N	2.77	0.42
1:B:851:LEU:O	1:B:852:GLY:C	2.60	0.42
1:A:169:GLU:HG2	1:A:170:ALA:H	1.84	0.42
1:A:635:GLN:HG2	1:A:636:ASP:N	2.31	0.42
1:A:1005:LEU:HD23	1:A:1005:LEU:HA	1.85	0.42
1:B:571:GLU:C	1:B:573:LEU:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:712:LEU:N	1:B:712:LEU:HD12	2.34	0.42
1:B:913:ASN:HD22	1:B:942:ASN:HB3	1.84	0.42
1:B:958:ILE:CD1	1:B:960:ARG:HG2	2.49	0.42
1:A:177:ARG:H	1:A:217:VAL:HG23	1.83	0.42
1:A:242:LEU:HB3	1:A:245:THR:OG1	2.19	0.42
1:A:393:ASN:HB3	1:A:396:ALA:CB	2.48	0.42
1:A:603:ALA:O	1:A:606:VAL:HG12	2.18	0.42
1:B:57:ASN:O	1:B:60:SER:OG	2.36	0.42
1:B:205:LEU:C	1:B:208:MSE:H	2.28	0.42
1:B:298:ASN:ND2	1:B:330:TYR:H	2.16	0.42
1:A:191:ALA:N	1:A:221:ARG:HG2	2.34	0.42
1:A:703:VAL:HA	1:A:733:LEU:O	2.20	0.42
1:A:806:VAL:H	1:A:813:VAL:HG21	1.84	0.42
1:B:32:VAL:HG13	1:B:1029:VAL:HB	2.00	0.42
1:B:181:ASP:OD1	1:B:212:GLY:HA2	2.20	0.42
1:B:343:ASN:OD1	1:B:344:ARG:HG2	2.18	0.42
1:B:418:ASP:OD2	1:B:591:ARG:NH2	2.51	0.42
1:B:430:ILE:HD13	1:B:531:MSE:HE1	2.01	0.42
1:B:459:GLN:O	1:B:459:GLN:HG2	2.19	0.42
1:A:34:VAL:CG2	1:A:996:LEU:HD11	2.50	0.42
1:A:241:THR:HA	1:A:960:ARG:HA	2.01	0.42
1:A:433:ASN:HD22	1:A:500:ARG:CA	2.09	0.42
1:A:794:ALA:O	1:A:796:ASP:N	2.53	0.42
1:A:974:GLU:HG3	1:A:975:HIS:N	2.34	0.42
1:B:181:ASP:O	1:B:183:THR:N	2.52	0.42
1:B:700:MSE:SE	1:B:806:VAL:HG21	2.70	0.42
1:A:320:PHE:CD2	1:A:958:ILE:HG23	2.54	0.42
1:A:320:PHE:HB3	1:A:958:ILE:HG13	2.01	0.42
1:A:828:GLU:HG3	1:A:828:GLU:O	2.20	0.42
1:A:903:THR:HG22	1:A:944:LYS:HD2	2.01	0.42
1:B:520:ARG:CZ	1:B:524:MSE:HE3	2.49	0.42
1:B:575:SER:C	1:B:577:THR:H	2.27	0.42
1:A:847:LYS:HB2	1:A:853:HIS:CD2	2.54	0.42
1:A:892:ILE:O	1:A:893:LYS:HD3	2.19	0.42
1:A:974:GLU:HG3	1:A:975:HIS:H	1.84	0.42
1:B:179:LEU:HD23	1:B:216:TYR:HD2	1.85	0.42
1:B:516:ALA:O	1:B:519:ALA:HB3	2.20	0.42
1:B:521:TYR:CE2	1:B:556:ILE:HD11	2.55	0.42
1:B:735:THR:HG22	1:B:791:LYS:HZ1	1.85	0.42
1:A:46:LEU:O	1:A:49:LEU:HB2	2.20	0.42
1:A:183:THR:OG1	1:A:185:PRO:HD2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:ASP:OD2	1:A:194:ALA:HB3	2.20	0.42
1:A:351:GLY:HA3	1:A:951:ARG:HH22	1.85	0.42
1:A:451:LEU:HG	1:A:460:LEU:HD22	2.01	0.42
1:A:696:ASN:OD1	1:A:697:SER:N	2.41	0.42
1:A:792:GLN:HB2	1:A:793:LEU:H	1.54	0.42
1:A:823:ALA:O	1:A:826:ASP:HB2	2.19	0.42
1:A:847:LYS:C	1:A:849:LEU:N	2.72	0.42
1:A:931:ILE:HA	1:A:966:LEU:HD23	2.01	0.42
1:A:497:ILE:HG22	1:A:499:VAL:HG23	2.02	0.42
1:A:602:LEU:HD23	1:A:602:LEU:HA	1.75	0.42
1:A:707:ASP:OD1	1:A:745:SER:HB3	2.20	0.42
1:A:951:ARG:H	1:A:951:ARG:CD	2.31	0.42
1:A:1038:ILE:CG1	1:A:1039:LEU:H	2.33	0.42
1:B:37:GLN:O	1:B:1034:GLU:HG3	2.20	0.42
1:B:62:PHE:N	1:B:63:PRO:HD2	2.34	0.42
1:B:292:VAL:O	1:B:295:LEU:N	2.53	0.42
1:B:669:ARG:HH12	1:B:814:GLY:HA2	1.85	0.42
1:A:89:ILE:HG22	1:A:90:VAL:N	2.35	0.42
1:A:905:SER:HB3	1:A:942:ASN:HA	2.02	0.42
1:B:292:VAL:C	1:B:294:ARG:N	2.72	0.42
1:B:300:ALA:O	1:B:303:ILE:N	2.53	0.42
1:B:430:ILE:HD11	1:B:520:ARG:HD3	2.02	0.42
1:B:672:ASN:HD21	1:B:863:LYS:HA	1.84	0.42
1:B:799:TYR:CE1	1:B:813:VAL:HG23	2.54	0.42
1:A:39:SER:OG	1:A:40:PHE:N	2.53	0.41
1:A:79:GLU:HA	1:A:82:LEU:HD11	2.02	0.41
1:A:147:MSE:C	1:A:149:GLY:H	2.28	0.41
1:A:419:TRP:CE3	1:A:649:LEU:HD13	2.55	0.41
1:A:516:ALA:HB3	1:A:582:MSE:HE1	2.01	0.41
1:A:523:GLN:O	1:A:524:MSE:HB2	2.20	0.41
1:A:533:LYS:HE2	1:A:561:VAL:HG23	2.02	0.41
1:A:806:VAL:O	1:A:813:VAL:HG22	2.20	0.41
1:A:851:LEU:O	1:A:853:HIS:HD2	2.03	0.41
1:A:974:GLU:CG	1:A:975:HIS:N	2.83	0.41
1:B:69:ALA:HB1	1:B:199:GLY:O	2.20	0.41
1:B:455:THR:HG22	1:B:456:TYR:CD2	2.55	0.41
1:A:240:LEU:HD23	1:A:995:THR:O	2.20	0.41
1:A:620:MSE:O	1:A:624:ILE:HG13	2.20	0.41
1:A:654:LEU:HB3	1:A:655:THR:HG23	2.02	0.41
1:A:655:THR:H	1:A:656:ARG:NH2	2.18	0.41
1:A:1037:HIS:CG	1:A:1038:ILE:N	2.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:PRO:HG2	1:B:47:LEU:CD1	2.46	0.41
1:B:510:GLU:HB3	1:B:511:PRO:HD3	2.02	0.41
1:B:551:LEU:O	1:B:555:THR:N	2.42	0.41
1:A:393:ASN:C	1:A:395:GLU:N	2.77	0.41
1:A:633:ILE:HA	1:A:637:ALA:HB3	2.02	0.41
1:A:847:LYS:HE3	1:A:847:LYS:HB2	1.62	0.41
1:A:953:LEU:H	1:A:953:LEU:HD12	1.85	0.41
1:B:29:ASP:CG	1:B:30:SER:N	2.77	0.41
1:B:75:ASP:OD1	1:B:76:ALA:N	2.51	0.41
1:B:786:TYR:HB2	1:B:787:TRP:CE3	2.55	0.41
1:B:991:ASP:N	1:B:991:ASP:OD1	2.52	0.41
1:A:102:LEU:HG	1:A:106:LYS:NZ	2.35	0.41
1:A:240:LEU:HD12	1:A:985:PHE:CD2	2.55	0.41
1:A:351:GLY:CA	1:A:951:ARG:HH22	2.33	0.41
1:A:377:ARG:HD3	1:A:377:ARG:HA	1.80	0.41
1:A:433:ASN:ND2	1:A:499:VAL:O	2.54	0.41
1:A:622:VAL:O	1:A:626:LEU:N	2.38	0.41
1:A:725:HIS:NE2	1:A:828:GLU:CD	2.79	0.41
1:A:824:GLU:CD	1:A:824:GLU:H	2.28	0.41
1:A:828:GLU:HA	1:A:831:LEU:H	1.85	0.41
1:B:40:PHE:CD1	1:B:40:PHE:C	2.99	0.41
1:B:66:ASP:OD1	1:B:202:HIS:NE2	2.43	0.41
1:B:71:GLY:C	1:B:73:LEU:N	2.76	0.41
1:B:199:GLY:C	1:B:200:GLU:HG2	2.45	0.41
1:B:347:SER:HB2	1:B:895:TRP:HE1	1.85	0.41
1:B:569:PHE:C	1:B:570:GLU:HG2	2.46	0.41
1:A:124:TYR:CE2	1:A:173:LEU:HD11	2.55	0.41
1:A:785:ALA:HA	1:A:787:TRP:CZ2	2.54	0.41
1:A:815:PRO:O	1:A:816:VAL:HG22	2.21	0.41
1:A:930:PRO:HG2	1:A:964:HIS:HB2	2.03	0.41
1:A:974:GLU:CD	1:A:977:ALA:O	2.63	0.41
1:B:211:GLU:OE1	1:B:213:GLN:NE2	2.54	0.41
1:B:934:THR:HG21	1:B:966:LEU:HG	2.03	0.41
1:A:34:VAL:HG22	1:A:996:LEU:HD11	2.02	0.41
1:A:240:LEU:HD23	1:A:995:THR:C	2.45	0.41
1:A:247:TYR:CZ	1:A:321:PRO:HA	2.55	0.41
1:A:359:GLY:O	1:A:891:ALA:HB3	2.21	0.41
1:A:376:LEU:O	1:A:379:GLU:HB3	2.21	0.41
1:A:452:LEU:HB2	1:A:453:GLN:CD	2.46	0.41
1:A:494:LYS:C	1:A:496:LEU:H	2.29	0.41
1:A:993:LEU:O	1:A:994:LEU:HD23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:GLU:CD	1:B:377:ARG:NH1	2.79	0.41
1:B:301:SER:O	1:B:305:ASP:N	2.51	0.41
1:B:451:LEU:N	1:B:452:LEU:HG	2.36	0.41
1:B:847:LYS:HZ2	1:B:853:HIS:HB3	1.85	0.41
1:A:147:MSE:C	1:A:149:GLY:N	2.79	0.41
1:A:383:ILE:C	1:A:385:GLN:N	2.78	0.41
1:A:418:ASP:HA	1:A:649:LEU:CD1	2.49	0.41
1:A:764:GLU:HA	1:A:764:GLU:OE1	2.21	0.41
1:A:1001:PRO:HA	1:A:1002:PRO:HD3	1.77	0.41
1:B:77:VAL:HG23	1:B:78:THR:H	1.85	0.41
1:B:207:ALA:C	1:B:210:LYS:HG3	2.46	0.41
1:B:346:ALA:C	1:B:893:LYS:HG2	2.45	0.41
1:B:419:TRP:CH2	1:B:649:LEU:HB2	2.56	0.41
1:B:485:VAL:HA	1:B:489:ILE:HG12	2.02	0.41
1:A:169:GLU:HG2	1:A:170:ALA:N	2.36	0.41
1:A:761:GLU:CD	1:A:761:GLU:H	2.29	0.41
1:A:935:LEU:O	1:A:938:LEU:HB2	2.20	0.41
1:B:588:TYR:CZ	1:B:592:LEU:HD12	2.56	0.41
1:B:629:ILE:HG22	1:B:647:TYR:HD2	1.85	0.41
1:B:733:LEU:HD21	1:B:793:LEU:HB2	2.02	0.41
1:B:817:PRO:C	1:B:818:SER:HG	2.22	0.41
1:A:141:CYS:HA	1:A:142:PRO:HD3	1.66	0.41
1:A:287:LEU:O	1:A:325:SER:HB2	2.21	0.41
1:A:463:VAL:CG1	1:A:465:ARG:HG3	2.51	0.41
1:A:521:TYR:HE1	1:A:568:SER:HB3	1.78	0.41
1:A:591:ARG:HG3	1:A:655:THR:O	2.21	0.41
1:A:630:GLN:O	1:A:634:VAL:HG13	2.20	0.41
1:A:632:SER:C	1:A:637:ALA:HB2	2.46	0.41
1:B:384:GLY:HA2	1:B:387:ARG:NH2	2.36	0.41
1:B:575:SER:C	1:B:577:THR:N	2.79	0.41
1:B:669:ARG:NH1	1:B:814:GLY:HA2	2.36	0.41
1:B:867:LEU:O	1:B:870:LEU:HB2	2.21	0.41
1:B:918:ILE:O	1:B:947:LEU:HA	2.20	0.41
1:A:491:THR:O	1:A:495:ARG:N	2.43	0.41
1:A:654:LEU:HB2	1:A:656:ARG:NH2	2.29	0.41
1:B:80:LYS:HD2	1:B:972:PHE:HB2	2.03	0.41
1:B:542:ASP:O	1:B:543:LYS:HD3	2.21	0.41
1:B:938:LEU:HB2	1:B:941:VAL:HB	2.02	0.41
1:B:1009:LYS:HG3	1:B:1032:ILE:O	2.21	0.41
1:A:246:ASP:OD2	1:A:285:LYS:HE3	2.22	0.40
1:A:419:TRP:CD1	1:A:419:TRP:C	2.98	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:ASP:OD1	1:A:477:THR:HB	2.21	0.40
1:A:644:LEU:HB2	1:A:645:PRO:HD3	2.03	0.40
1:A:784:LEU:O	1:A:786:TYR:N	2.54	0.40
1:B:382:PHE:CE1	1:B:386:PHE:HE2	2.39	0.40
1:B:787:TRP:CE3	1:B:787:TRP:N	2.86	0.40
1:B:929:VAL:O	1:B:932:LEU:HB2	2.22	0.40
1:B:998:MSE:HE3	1:B:998:MSE:HB2	1.51	0.40
1:B:1039:LEU:O	1:B:1040:ILE:HD13	2.20	0.40
1:A:132:ARG:HH11	1:A:168:LEU:HB3	1.86	0.40
1:A:433:ASN:HB2	1:A:501:PHE:H	1.86	0.40
1:A:720:LYS:HG3	1:A:824:GLU:HG2	2.03	0.40
1:A:969:GLU:HG2	1:A:970:PRO:HD2	2.03	0.40
1:B:400:LEU:H	1:B:400:LEU:HG	1.26	0.40
1:B:474:ILE:HD12	1:B:503:LEU:HG	2.03	0.40
1:B:624:ILE:O	1:B:627:GLN:N	2.55	0.40
1:B:817:PRO:CD	1:B:821:THR:HG21	2.46	0.40
1:A:45:TYR:HB2	1:A:79:GLU:OE2	2.21	0.40
1:A:353:ASN:HB3	1:A:928:TRP:CH2	2.55	0.40
1:A:492:PHE:HZ	1:A:615:LEU:HD11	1.86	0.40
1:A:567:GLN:CD	1:A:569:PHE:HD2	2.30	0.40
1:A:846:MSE:HE2	1:A:847:LYS:O	2.21	0.40
1:A:1003:SER:HA	1:A:1039:LEU:HD12	2.04	0.40
1:B:714:LEU:HA	1:B:714:LEU:HD12	1.81	0.40
1:A:421:ASP:HB3	1:A:429:ILE:HG13	2.03	0.40
1:A:456:TYR:C	1:A:458:GLY:N	2.79	0.40
1:A:679:SER:C	1:A:681:ASP:N	2.79	0.40
1:A:712:LEU:HA	1:A:715:LEU:HB3	2.04	0.40
1:B:56:GLU:OE1	1:B:377:ARG:NH1	2.54	0.40
1:B:459:GLN:HE22	1:B:498:PRO:HG2	1.87	0.40
1:A:179:LEU:HD23	1:A:216:TYR:CD2	2.56	0.40
1:A:188:ILE:HD13	1:A:219:ARG:CZ	2.51	0.40
1:A:241:THR:HG22	1:A:960:ARG:HB2	2.03	0.40
1:A:657:ASN:OD1	1:A:657:ASN:C	2.64	0.40
1:A:974:GLU:CG	1:A:976:GLY:H	2.35	0.40
1:B:1000:VAL:HG22	1:B:1001:PRO:HD2	2.04	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)
1:B:456:TYR:OH	1:B:456:TYR:OH[5_554]	2.09	0.11

4.3 Torsion angles

4.3.1 Protein backbone

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	893/1130 (79%)	685 (77%)	155 (17%)	53 (6%)	1	8
1	B	893/1130 (79%)	696 (78%)	155 (17%)	42 (5%)	2	11
All	All	1786/2260 (79%)	1381 (77%)	310 (17%)	95 (5%)	1	10

All (95) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	GLU
1	A	61	TYR
1	A	148	ASP
1	A	348	LEU
1	A	524	MSE
1	A	527	GLY
1	A	544	LEU
1	A	560	ARG
1	A	563	ARG
1	A	636	ASP
1	A	652	ALA
1	A	674	VAL
1	A	680	HIS
1	A	710	ALA
1	A	785	ALA
1	A	816	VAL
1	A	850	ASN
1	A	851	LEU
1	A	898	ALA
1	A	908	ASP
1	A	958	ILE
1	B	210	LYS
1	B	213	GLN
1	B	612	ASP
1	B	664	ASP

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Mol	Chain	Res	Type
1	B	673	LEU
1	B	706	PHE
1	B	786	TYR
1	B	788	ALA
1	B	803	THR
1	B	811	ARG
1	B	850	ASN
1	B	906	HIS
1	B	958	ILE
1	B	974	GLU
1	B	990	GLU
1	A	75	ASP
1	A	400	LEU
1	A	707	ASP
1	A	991	ASP
1	B	56	GLU
1	B	524	MSE
1	B	636	ASP
1	B	711	GLY
1	B	751	LEU
1	B	815	PRO
1	B	818	SER
1	B	849	LEU
1	B	898	ALA
1	A	112	ARG
1	A	151	GLN
1	A	347	SER
1	A	442	SER
1	A	566	ALA
1	A	654	LEU
1	A	846	MSE
1	A	993	LEU
1	A	1021	SER
1	B	61	TYR
1	B	456	TYR
1	B	459	GLN
1	B	597	ARG
1	B	652	ALA
1	B	677	ALA
1	A	210	LYS
1	A	297	MSE
1	A	460	LEU

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Mol	Chain	Res	Type
1	A	673	LEU
1	A	697	SER
1	A	792	GLN
1	B	148	ASP
1	B	285	LYS
1	B	348	LEU
1	B	616	GLN
1	A	401	LEU
1	A	422	GLU
1	A	453	GLN
1	A	666	SER
1	A	966	LEU
1	B	632	SER
1	A	309	PRO
1	A	676	VAL
1	A	857	GLY
1	B	460	LEU
1	B	484	MSE
1	B	544	LEU
1	B	600	PRO
1	A	564	GLY
1	B	309	PRO
1	A	813	VAL
1	B	892	ILE
1	A	367	VAL
1	A	600	PRO
1	A	817	PRO
1	B	142	PRO

4.3.2 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	782/948 (82%)	713 (91%)	69 (9%)	9	33
1	B	782/948 (82%)	722 (92%)	60 (8%)	12	38
All	All	1564/1896 (82%)	1435 (92%)	129 (8%)	10	36

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	SER
1	A	64	LEU
1	A	70	GLU
1	A	81	GLU
1	A	82	LEU
1	A	89	ILE
1	A	106	LYS
1	A	112	ARG
1	A	169	GLU
1	A	193	VAL
1	A	204	LYS
1	A	208	MSE
1	A	210	LYS
1	A	248	ILE
1	A	249	MSE
1	A	250	ILE
1	A	332	VAL
1	A	335	GLU
1	A	380	ARG
1	A	389	LEU
1	A	393	ASN
1	A	394	ILE
1	A	401	LEU
1	A	420	ARG
1	A	437	LYS
1	A	447	ASP
1	A	474	ILE
1	A	477	THR
1	A	484	MSE
1	A	544	LEU
1	A	556	ILE
1	A	561	VAL
1	A	562	LEU
1	A	573	LEU
1	A	580	GLU
1	A	581	VAL
1	A	610	ARG
1	A	629	ILE
1	A	639	GLU
1	A	657	ASN
1	A	667	LYS
1	A	673	LEU

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Mol	Chain	Res	Type
1	A	674	VAL
1	A	703	VAL
1	A	712	LEU
1	A	742	THR
1	A	754	THR
1	A	762	ILE
1	A	763	LEU
1	A	786	TYR
1	A	793	LEU
1	A	804	ARG
1	A	816	VAL
1	A	821	THR
1	A	828	GLU
1	A	837	LYS
1	A	839	LEU
1	A	847	LYS
1	A	892	ILE
1	A	906	HIS
1	A	912	ILE
1	A	914	ILE
1	A	924	ARG
1	A	927	ARG
1	A	939	ASN
1	A	951	ARG
1	A	974	GLU
1	A	1006	VAL
1	A	1038	ILE
1	B	82	LEU
1	B	89	ILE
1	B	111	ILE
1	B	150	MSE
1	B	169	GLU
1	B	178	LYS
1	B	193	VAL
1	B	203	ARG
1	B	210	LYS
1	B	213	GLN
1	B	217	VAL
1	B	249	MSE
1	B	250	ILE
1	B	332	VAL
1	B	376	LEU

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Mol	Chain	Res	Type
1	B	432	LEU
1	B	453	GLN
1	B	488	HIS
1	B	504	VAL
1	B	533	LYS
1	B	544	LEU
1	B	562	LEU
1	B	563	ARG
1	B	576	THR
1	B	579	GLU
1	B	617	GLU
1	B	629	ILE
1	B	634	VAL
1	B	638	VAL
1	B	639	GLU
1	B	658	GLU
1	B	667	LYS
1	B	668	ILE
1	B	676	VAL
1	B	678	GLU
1	B	679	SER
1	B	709	GLU
1	B	727	GLU
1	B	745	SER
1	B	746	SER
1	B	751	LEU
1	B	761	GLU
1	B	803	THR
1	B	804	ARG
1	B	816	VAL
1	B	820	SER
1	B	824	GLU
1	B	831	LEU
1	B	846	MSE
1	B	855	VAL
1	B	866	SER
1	B	870	LEU
1	B	914	ILE
1	B	958	ILE
1	B	963	ARG
1	B	986	SER
1	B	998	MSE

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Mol	Chain	Res	Type
1	B	1006	VAL
1	B	1010	GLU
1	B	1041	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	213	GLN
1	A	378	HIS
1	A	433	ASN
1	A	488	HIS
1	A	675	GLN
1	A	734	HIS
1	A	853	HIS
1	A	975	HIS
1	A	1013	HIS
1	B	353	ASN
1	B	375	HIS
1	B	453	GLN
1	B	459	GLN
1	B	488	HIS
1	B	616	GLN
1	B	631	GLN
1	B	635	GLN
1	B	896	ASN
1	B	913	ASN
1	B	1013	HIS
1	B	1037	HIS

4.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

4.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

4.6 Ligand geometry

There are no ligands in this entry.

4.7 Other polymers

There are no such residues in this entry.

4.8 Polymer linkage issues

There are no chain breaks in this entry.

5 Fit of model and data [i](#)

5.1 Protein, DNA and RNA chains [i](#)

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	898/1130 (79%)	-1.13	0	100	100	70, 117, 187, 345	0
1	B	898/1130 (79%)	-1.11	1 (0%)	92	86	76, 115, 181, 279	0
All	All	1796/2260 (79%)	-1.12	1 (0%)	92	86	70, 116, 185, 345	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	94	GLY	3.2

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

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

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 Ligands [i](#)

There are no ligands in this entry.

5.5 Other polymers [i](#)

There are no such residues in this entry.