



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 06:18 AM UTC

PDB ID : 3M8L / pdb_00003m8l
Title : Crystal Structure Analysis of the Feline Calicivirus Capsid Protein
Authors : Zhou, Y.; Prasad, B.V.V.
Deposited on : 2010-03-18
Resolution : 3.40 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

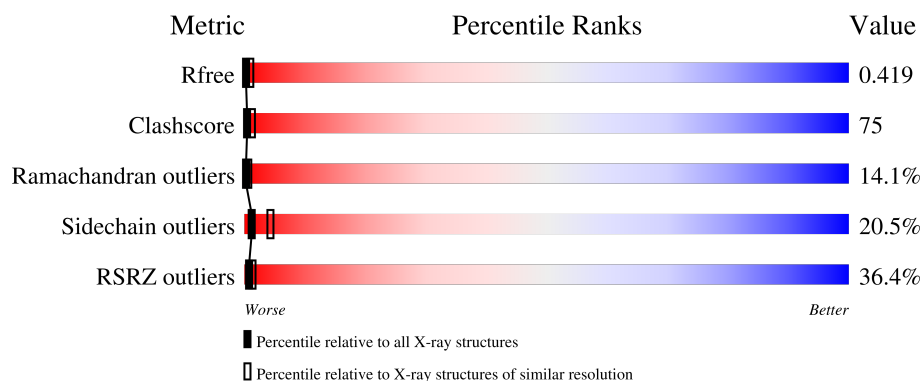
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	534	35% 22% 51% 22% 5%
1	B	534	37% 19% 52% 24% 5%
1	C	534	37% 20% 54% 21% 5%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12360 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.

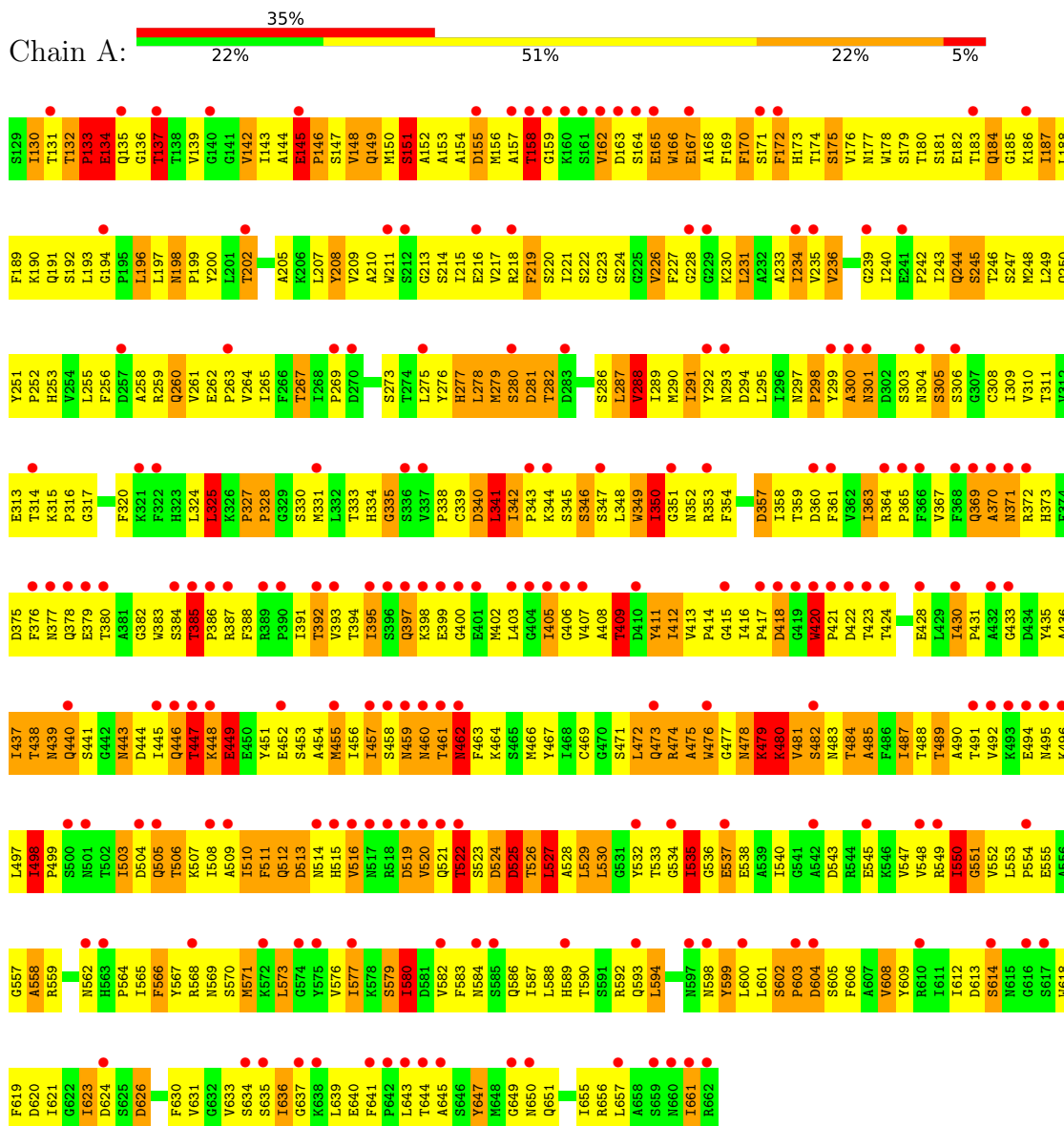
- Molecule 1 is a protein called Capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	534	Total	C	N	O	S	0	0	0
			4129	2632	687	796	14			
1	B	530	Total	C	N	O	S	0	0	0
			4101	2615	683	789	14			
1	C	534	Total	C	N	O	S	0	0	0
			4130	2632	687	797	14			

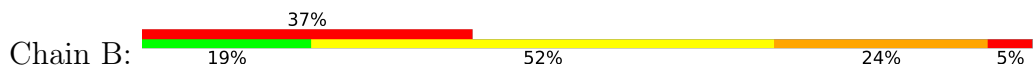
3 Residue-property plots

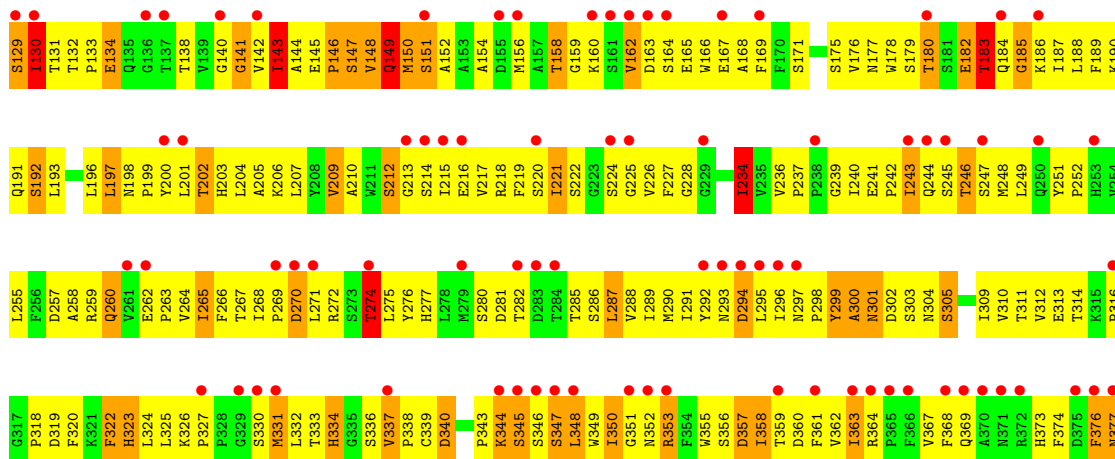
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

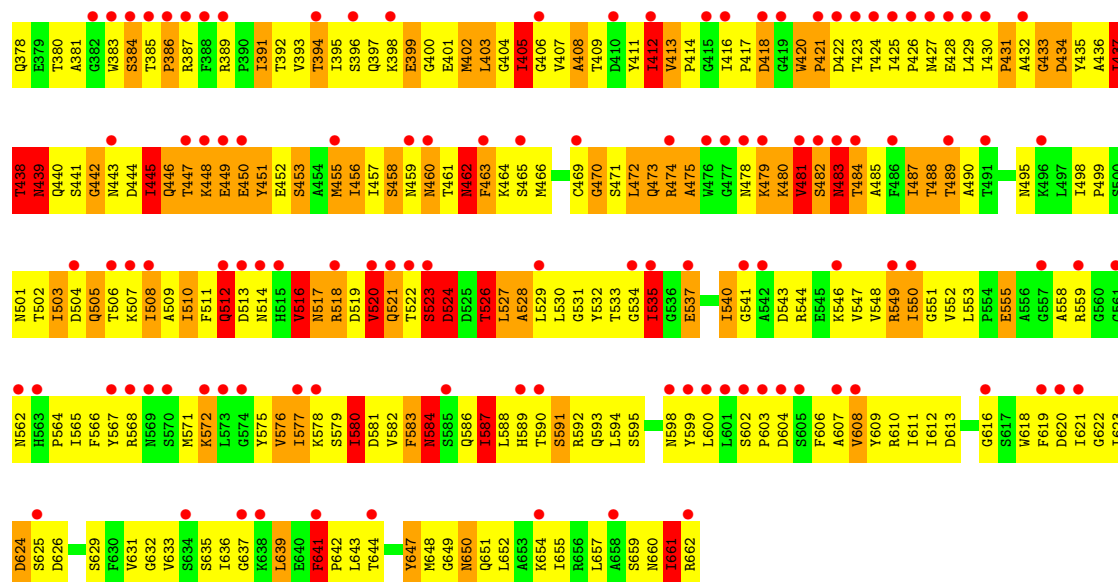
• Molecule 1: Capsid protein



• Molecule 1: Capsid protein







4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	427.08Å 450.73Å 467.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.40 30.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.40) 88.9 (30.00-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 3.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.390 , 0.370 0.420 , 0.419	Depositor DCC
R_{free} test set	27284 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	85.6	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.017 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.39	EDS
Total number of atoms	12360	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.87	7/4229 (0.2%)	1.21	42/5759 (0.7%)
1	B	1.16	15/4201 (0.4%)	1.21	40/5719 (0.7%)
1	C	0.91	11/4230 (0.3%)	1.28	51/5759 (0.9%)
All	All	0.99	33/12660 (0.3%)	1.23	133/17237 (0.8%)

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	B	0	1

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	624	ASP	CB-CG	28.32	2.22	1.52
1	B	606	PHE	CE1-CZ	15.16	1.84	1.38
1	B	606	PHE	CE2-CZ	13.81	1.80	1.38
1	B	606	PHE	CD2-CE2	13.68	1.79	1.38
1	B	606	PHE	CD1-CE1	13.66	1.79	1.38
1	B	437	ILE	CA-CB	9.99	1.68	1.54
1	B	606	PHE	CG-CD1	9.94	1.59	1.38
1	B	606	PHE	CG-CD2	9.62	1.59	1.38
1	A	132	THR	CA-CB	9.28	1.66	1.53
1	B	445	ILE	CA-CB	8.59	1.66	1.54
1	C	520	VAL	CA-CB	7.40	1.63	1.54
1	C	502	THR	CA-CB	7.32	1.63	1.53
1	C	535	ILE	CA-CB	6.98	1.64	1.54
1	B	234	ILE	CA-CB	-6.65	1.48	1.55
1	A	516	VAL	CA-CB	6.54	1.61	1.54
1	C	437	ILE	CA-CB	6.40	1.63	1.54
1	A	522	THR	CA-CB	6.39	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	288	VAL	CA-CB	-6.29	1.49	1.55
1	B	457	ILE	CA-CB	6.18	1.62	1.54
1	C	274	THR	CA-CB	6.12	1.61	1.53
1	C	162	VAL	CA-CB	6.12	1.61	1.54
1	A	535	ILE	CA-CB	6.05	1.62	1.54
1	C	145	GLU	CA-C	5.91	1.60	1.52
1	B	445	ILE	CA-C	5.80	1.60	1.52
1	A	623	ILE	CA-CB	-5.80	1.48	1.54
1	C	455	MET	SD-CE	5.69	1.93	1.79
1	B	447	THR	CA-C	5.61	1.58	1.53
1	C	156	MET	SD-CE	5.49	1.93	1.79
1	B	577	ILE	CA-CB	5.48	1.61	1.54
1	C	331	MET	SD-CE	5.33	1.92	1.79
1	A	430	ILE	CA-CB	5.16	1.60	1.54
1	B	459	ASN	CA-C	5.15	1.54	1.52
1	C	445	ILE	CA-CB	5.09	1.61	1.54

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	438	THR	CB-CA-C	18.35	146.94	110.42
1	A	439	ASN	N-CA-CB	-13.86	87.07	110.49
1	C	512	GLN	N-CA-C	11.70	123.19	108.45
1	B	360	ASP	N-CA-C	10.88	133.98	110.80
1	C	446	GLN	N-CA-C	-10.75	99.83	113.16
1	C	451	TYR	CB-CA-C	-9.22	92.67	110.65
1	C	145	GLU	N-CA-C	9.18	130.11	109.81
1	A	198	ASN	CA-C-N	8.92	128.52	119.24
1	A	198	ASN	C-N-CA	8.92	128.52	119.24
1	C	478	ASN	N-CA-C	8.65	119.35	108.19
1	A	165	GLU	N-CA-C	-8.52	102.79	113.01
1	C	389	ARG	CA-C-N	8.46	128.52	119.89
1	C	389	ARG	C-N-CA	8.46	128.52	119.89
1	C	487	ILE	N-CA-C	8.10	118.70	108.82
1	C	442	GLY	N-CA-C	-8.01	103.38	114.67
1	B	517	ASN	N-CA-C	7.96	127.76	110.80
1	B	624	ASP	CA-CB-CG	7.80	120.40	112.60
1	C	531	GLY	N-CA-C	7.78	122.02	111.20
1	C	517	ASN	N-CA-C	7.57	122.20	113.19
1	C	480	LYS	N-CA-C	7.36	126.48	110.80
1	C	143	ILE	N-CA-C	-7.35	105.55	112.83
1	C	439	ASN	N-CA-C	7.32	126.38	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	438	THR	N-CA-C	-7.11	95.65	110.80
1	C	483	ASN	N-CA-C	7.10	125.93	110.80
1	A	512	GLN	N-CA-C	7.09	118.02	108.23
1	A	288	VAL	N-CA-C	7.09	117.66	107.88
1	A	402	MET	N-CA-C	-7.06	99.44	109.96
1	A	438	THR	N-CA-C	-6.98	95.93	110.80
1	C	337	VAL	CA-C-N	6.95	126.63	119.82
1	C	337	VAL	C-N-CA	6.95	126.63	119.82
1	A	420	TRP	CA-C-N	6.92	126.84	119.85
1	A	420	TRP	C-N-CA	6.92	126.84	119.85
1	B	455	MET	N-CA-C	-6.92	103.31	112.72
1	C	145	GLU	C-N-CD	-6.88	105.47	120.60
1	C	518	ARG	N-CA-C	-6.83	104.68	112.87
1	C	520	VAL	N-CA-C	-6.77	100.43	109.30
1	A	151	SER	N-CA-C	-6.74	96.44	110.80
1	C	241	GLU	CA-C-N	6.73	126.69	119.76
1	C	241	GLU	C-N-CA	6.73	126.69	119.76
1	A	608	VAL	N-CA-C	6.73	117.14	108.12
1	B	361	PHE	CA-C-N	-6.66	112.69	122.68
1	B	361	PHE	C-N-CA	-6.66	112.69	122.68
1	B	361	PHE	N-CA-C	6.65	124.97	110.80
1	B	608	VAL	N-CA-C	6.64	118.16	108.53
1	A	550	ILE	N-CA-C	-6.62	106.54	111.90
1	A	260	GLN	CA-C-N	-6.62	116.14	123.16
1	A	260	GLN	C-N-CA	-6.62	116.14	123.16
1	C	147	SER	N-CA-C	-6.61	102.56	112.54
1	C	447	THR	N-CA-C	6.44	119.92	110.59
1	C	528	ALA	CA-C-O	6.43	121.67	117.94
1	A	411	TYR	N-CA-C	6.39	119.13	109.23
1	B	515	HIS	N-CA-C	6.39	124.41	110.80
1	B	624	ASP	OD1-CG-OD2	-6.38	107.59	122.90
1	C	524	ASP	N-CA-C	6.32	124.25	110.80
1	B	327	PRO	CA-C-N	6.29	127.70	119.84
1	B	327	PRO	C-N-CA	6.29	127.70	119.84
1	A	327	PRO	CA-C-N	6.26	127.67	119.84
1	A	327	PRO	C-N-CA	6.26	127.67	119.84
1	B	416	ILE	CA-C-N	6.26	127.66	119.84
1	B	416	ILE	C-N-CA	6.26	127.66	119.84
1	C	148	VAL	N-CA-C	6.23	116.42	108.82
1	C	526	THR	N-CA-C	6.20	119.26	110.14
1	B	446	GLN	N-CA-C	-6.19	103.80	113.02
1	B	480	LYS	N-CA-C	6.14	123.89	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	563	HIS	CA-C-N	6.09	126.00	119.85
1	B	563	HIS	C-N-CA	6.09	126.00	119.85
1	C	470	GLY	N-CA-C	-6.07	105.65	112.33
1	C	484	THR	N-CA-C	5.98	123.55	110.80
1	A	443	ASN	N-CA-C	-5.98	103.36	111.55
1	A	503	ILE	N-CA-C	5.98	116.22	107.37
1	C	503	ILE	N-CA-C	5.97	116.70	107.99
1	C	353	ARG	N-CA-C	-5.92	106.22	113.50
1	B	456	ILE	N-CA-CB	-5.91	105.83	112.45
1	A	147	SER	N-CA-C	5.82	117.98	110.65
1	C	587	ILE	N-CA-C	-5.81	101.09	108.93
1	B	268	ILE	CA-C-N	5.79	125.80	119.90
1	B	268	ILE	C-N-CA	5.79	125.80	119.90
1	A	208	TYR	N-CA-C	5.64	117.19	109.18
1	B	420	TRP	CA-C-N	5.62	126.87	119.84
1	B	420	TRP	C-N-CA	5.62	126.87	119.84
1	C	334	HIS	N-CA-C	5.62	117.76	108.48
1	C	234	ILE	N-CA-C	5.61	116.36	108.17
1	C	271	LEU	N-CA-C	-5.57	100.16	109.24
1	A	134	GLU	N-CA-C	5.53	117.78	107.99
1	C	481	VAL	N-CA-C	5.53	120.84	109.34
1	C	183	THR	N-CA-C	5.50	117.99	110.24
1	C	149	GLN	N-CA-C	5.49	122.50	110.80
1	A	547	VAL	N-CA-C	5.49	116.34	108.93
1	B	235	VAL	CA-C-N	-5.48	118.00	123.04
1	B	235	VAL	C-N-CA	-5.48	118.00	123.04
1	A	385	THR	CA-C-N	5.46	126.67	119.84
1	A	385	THR	C-N-CA	5.46	126.67	119.84
1	A	248	MET	N-CA-C	-5.45	105.74	112.38
1	A	163	ASP	N-CA-C	-5.44	105.08	112.26
1	A	516	VAL	N-CA-C	5.42	116.57	109.58
1	A	159	GLY	N-CA-C	-5.37	107.79	115.64
1	B	608	VAL	CB-CA-C	-5.36	102.66	110.81
1	A	236	VAL	CA-C-N	5.32	123.49	119.66
1	A	236	VAL	C-N-CA	5.32	123.49	119.66
1	A	492	VAL	N-CA-C	5.30	116.39	108.54
1	B	300	ALA	N-CA-C	-5.29	99.54	110.80
1	C	377	ASN	N-CA-C	-5.28	106.70	112.72
1	A	325	LEU	N-CA-C	5.27	118.26	110.46
1	C	277	HIS	N-CA-C	5.26	117.30	109.25
1	A	472	LEU	N-CA-C	-5.25	102.91	111.04
1	B	641	PHE	N-CA-C	5.24	121.39	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	478	ASN	N-CA-C	5.23	121.95	110.80
1	A	487	ILE	N-CA-C	5.23	116.43	108.80
1	B	445	ILE	N-CA-C	5.23	120.21	109.34
1	C	641	PHE	N-CA-C	5.21	121.31	109.81
1	B	344	LYS	N-CA-C	5.20	117.02	111.36
1	B	141	GLY	CA-C-N	5.18	131.29	121.97
1	B	141	GLY	C-N-CA	5.18	131.29	121.97
1	A	530	LEU	CA-C-N	-5.17	117.87	122.47
1	A	530	LEU	C-N-CA	-5.17	117.87	122.47
1	B	641	PHE	CA-C-N	-5.13	113.42	119.84
1	B	641	PHE	C-N-CA	-5.13	113.42	119.84
1	B	487	ILE	N-CA-C	5.12	119.99	109.34
1	C	420	TRP	CA-C-N	5.12	126.24	119.84
1	C	420	TRP	C-N-CA	5.12	126.24	119.84
1	B	650	ASN	N-CA-C	5.12	116.20	108.07
1	C	148	VAL	CA-C-N	5.10	131.28	121.54
1	C	148	VAL	C-N-CA	5.10	131.28	121.54
1	A	154	ALA	N-CA-C	-5.08	106.85	113.16
1	B	145	GLU	N-CA-C	5.08	116.05	109.65
1	C	641	PHE	CA-C-N	-5.06	113.52	119.84
1	C	641	PHE	C-N-CA	-5.06	113.52	119.84
1	A	327	PRO	N-CA-C	-5.06	104.53	110.70
1	C	528	ALA	N-CA-C	5.03	112.91	108.78
1	A	282	THR	N-CA-C	5.02	116.84	111.36
1	B	401	GLU	N-CA-C	5.02	121.50	110.80
1	C	381	ALA	N-CA-C	-5.01	106.43	112.54
1	B	288	VAL	N-CA-C	5.00	115.57	108.42

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	200	TYR	Sidechain

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	4129	0	4062	636	0
1	B	4101	0	4033	645	6
1	C	4130	0	4062	598	7
All	All	12360	0	12157	1829	7

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 75.

All (1829) 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:B:606:PHE:CE1	1:B:606:PHE:CZ	1.84	1.62
1:B:606:PHE:CE1	1:B:606:PHE:CD1	1.79	1.62
1:B:606:PHE:CE2	1:B:606:PHE:CD2	1.79	1.62
1:B:606:PHE:CZ	1:B:606:PHE:CE2	1.80	1.61
1:B:606:PHE:CZ	1:B:624:ASP:CG	1.87	1.52
1:B:606:PHE:CZ	1:B:624:ASP:CB	1.88	1.51
1:B:606:PHE:CE2	1:B:624:ASP:CB	1.92	1.50
1:B:606:PHE:CE1	1:B:624:ASP:CG	1.88	1.49
1:B:606:PHE:CE2	1:B:624:ASP:CG	1.97	1.42
1:B:606:PHE:CD1	1:B:624:ASP:CG	2.02	1.37
1:B:606:PHE:CE1	1:B:624:ASP:CB	2.10	1.34
1:B:606:PHE:CZ	1:B:624:ASP:HB3	1.53	1.30
1:B:606:PHE:CD2	1:B:624:ASP:CG	2.11	1.29
1:B:606:PHE:CD1	1:B:624:ASP:HA	1.66	1.28
1:B:606:PHE:CD2	1:B:624:ASP:CB	2.20	1.24
1:B:606:PHE:CE1	1:B:624:ASP:OD2	1.91	1.23
1:A:209:VAL:HG22	1:A:324:LEU:O	1.36	1.23
1:B:606:PHE:CG	1:B:624:ASP:CG	2.20	1.20
1:C:437:ILE:CD1	1:C:457:ILE:HD11	1.73	1.19
1:B:436:ALA:HB3	1:B:461:THR:HA	1.18	1.17
1:B:453:SER:CB	1:B:456:ILE:HD13	1.76	1.15
1:B:606:PHE:CD2	1:B:624:ASP:OD1	1.98	1.14
1:B:606:PHE:CD1	1:B:624:ASP:CA	2.32	1.13
1:B:624:ASP:CG	1:B:624:ASP:CB	2.22	1.12
1:C:358:ILE:HD12	1:C:358:ILE:H	1.07	1.11
1:A:405:ILE:HD12	1:A:510:ILE:HG12	1.28	1.11
1:A:474:ARG:HH21	1:A:523:SER:HB3	1.03	1.11
1:B:606:PHE:CD2	1:B:624:ASP:HB2	1.84	1.11
1:A:474:ARG:HD3	1:A:523:SER:HA	1.35	1.08
1:A:175:SER:HB3	1:A:311:THR:HG22	1.33	1.08
1:B:606:PHE:CD1	1:B:624:ASP:CB	2.37	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:ASN:HB2	1:A:456:ILE:HA	1.35	1.07
1:B:396:SER:HA	1:B:521:GLN:HE21	1.14	1.07
1:B:606:PHE:CE2	1:B:624:ASP:HB2	1.69	1.07
1:A:535:ILE:HG13	1:A:536:GLY:H	1.18	1.06
1:B:395:ILE:HG12	1:B:396:SER:H	1.04	1.06
1:B:623:ILE:H	1:B:623:ILE:HD12	1.15	1.06
1:B:606:PHE:CZ	1:B:624:ASP:OD2	2.09	1.05
1:A:456:ILE:O	1:A:458:SER:N	1.89	1.05
1:C:437:ILE:HD12	1:C:457:ILE:HD11	1.09	1.04
1:B:449:GLU:O	1:B:450:GLU:HB2	1.53	1.03
1:B:402:MET:HE2	1:B:511:PHE:HA	1.39	1.03
1:B:213:GLY:HA3	1:B:320:PHE:HA	1.40	1.03
1:B:349:TRP:HE3	1:B:358:ILE:HD13	1.23	1.02
1:C:448:LYS:HE3	1:C:537:GLU:OE2	1.60	1.02
1:A:399:GLU:HG3	1:A:516:VAL:HG21	1.40	1.01
1:B:185:GLY:H	1:B:291:ILE:HG13	1.24	1.01
1:A:438:THR:HG21	1:A:458:SER:HA	1.40	1.00
1:C:287:LEU:HD12	1:C:288:VAL:N	1.75	1.00
1:A:406:GLY:H	1:A:508:ILE:HD11	1.26	1.00
1:C:587:ILE:H	1:C:587:ILE:HD12	1.25	0.99
1:B:453:SER:HB3	1:B:456:ILE:HD13	1.40	0.99
1:B:606:PHE:CG	1:B:624:ASP:CB	2.45	0.99
1:C:550:ILE:O	1:C:550:ILE:HD13	1.61	0.98
1:B:393:VAL:HA	1:B:409:THR:HG21	1.43	0.98
1:A:130:ILE:HG13	1:A:131:THR:H	1.29	0.97
1:A:474:ARG:NH2	1:A:523:SER:HB3	1.78	0.97
1:A:438:THR:HG22	1:A:457:ILE:O	1.65	0.96
1:B:385:THR:HG22	1:B:386:PRO:HD2	1.45	0.96
1:C:149:GLN:O	1:C:152:ALA:HB2	1.65	0.96
1:B:190:LYS:HE3	1:B:242:PRO:HB2	1.43	0.96
1:B:452:GLU:O	1:B:453:SER:HB2	1.63	0.96
1:B:346:SER:HB3	1:B:643:LEU:HB2	1.48	0.95
1:A:189:PHE:CZ	1:A:191:GLN:HB2	2.01	0.95
1:A:405:ILE:HG13	1:A:509:ALA:HA	1.49	0.94
1:B:395:ILE:HG12	1:B:396:SER:N	1.82	0.94
1:C:416:ILE:HD12	1:C:503:ILE:HG12	1.50	0.94
1:B:358:ILE:HG13	1:B:359:THR:H	1.32	0.94
1:C:397:GLN:HB2	1:C:521:GLN:HA	1.47	0.94
1:C:577:ILE:HG13	1:C:578:LYS:H	1.33	0.94
1:A:148:VAL:HG22	1:A:149:GLN:H	1.33	0.94
1:B:636:ILE:H	1:B:636:ILE:HD13	1.28	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:638:LYS:H	1:B:638:LYS:HD2	1.33	0.93
1:B:446:GLN:NE2	1:B:447:THR:HG23	1.83	0.93
1:C:544:ARG:HD3	1:C:553:LEU:HD21	1.50	0.93
1:A:445:ILE:O	1:A:445:ILE:HG13	1.69	0.92
1:A:506:THR:O	1:A:507:LYS:HD2	1.67	0.92
1:B:606:PHE:CG	1:B:624:ASP:OD1	2.21	0.92
1:A:487:ILE:HG22	1:A:510:ILE:HA	1.50	0.92
1:B:661:ILE:HD13	1:B:661:ILE:H	1.33	0.91
1:C:221:ILE:HD13	1:C:221:ILE:H	1.34	0.91
1:B:353:ARG:H	1:B:584:ASN:ND2	1.68	0.91
1:C:352:ASN:ND2	1:C:586:GLN:H	1.67	0.91
1:C:219:PHE:HB3	1:C:312:VAL:HA	1.50	0.91
1:B:439:ASN:HD22	1:B:443:ASN:HD21	1.18	0.91
1:C:448:LYS:CE	1:C:537:GLU:OE2	2.19	0.91
1:A:350:ILE:HA	1:A:357:ASP:HA	1.52	0.91
1:B:470:GLY:H	1:B:528:ALA:H	1.13	0.91
1:B:146:PRO:HB2	1:B:149:GLN:CD	1.96	0.90
1:A:246:THR:O	1:A:249:LEU:HB2	1.69	0.90
1:C:144:ALA:HB1	1:C:147:SER:HB3	1.52	0.90
1:C:448:LYS:O	1:C:449:GLU:HB2	1.70	0.90
1:B:349:TRP:CE3	1:B:358:ILE:HD13	2.07	0.90
1:B:352:ASN:HD21	1:B:369:GLN:HE22	1.17	0.90
1:C:474:ARG:H	1:C:524:ASP:HA	1.33	0.90
1:A:273:SER:O	1:B:275:LEU:HD12	1.71	0.90
1:B:226:VAL:HG12	1:B:298:PRO:HG2	1.51	0.90
1:C:437:ILE:CD1	1:C:457:ILE:CD1	2.51	0.89
1:C:451:TYR:H	1:C:458:SER:HB2	1.36	0.89
1:C:358:ILE:HD12	1:C:358:ILE:N	1.86	0.89
1:A:213:GLY:HA3	1:A:320:PHE:HA	1.54	0.89
1:A:405:ILE:HB	1:A:508:ILE:HG13	1.53	0.89
1:B:255:LEU:HB2	1:C:131:THR:HG23	1.55	0.89
1:C:236:VAL:HG23	1:C:286:SER:HB2	1.54	0.89
1:C:464:LYS:HA	1:C:533:THR:HG21	1.52	0.89
1:A:148:VAL:HG13	1:A:149:GLN:HG3	1.56	0.88
1:A:476:TRP:CD1	1:A:520:VAL:HB	2.09	0.88
1:B:623:ILE:HD12	1:B:623:ILE:N	1.89	0.88
1:C:437:ILE:HD12	1:C:457:ILE:CD1	2.02	0.87
1:A:454:ALA:O	1:A:455:MET:HG3	1.75	0.87
1:B:192:SER:HA	1:B:286:SER:HB3	1.57	0.86
1:A:503:ILE:HG22	1:A:549:ARG:O	1.76	0.86
1:B:210:ALA:HB3	1:B:323:HIS:HB2	1.54	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:349:TRP:HB3	1:C:358:ILE:HD13	1.55	0.86
1:A:378:GLN:HG3	1:C:654:LYS:NZ	1.90	0.86
1:C:287:LEU:HD12	1:C:288:VAL:H	1.38	0.85
1:A:447:THR:O	1:A:447:THR:HG22	1.76	0.85
1:B:417:PRO:HB2	1:B:420:TRP:HB2	1.58	0.85
1:A:459:ASN:O	1:A:460:ASN:CG	2.19	0.85
1:C:631:VAL:HG12	1:C:633:VAL:H	1.41	0.85
1:B:243:ILE:HG22	1:B:245:SER:H	1.40	0.85
1:C:358:ILE:H	1:C:358:ILE:CD1	1.89	0.85
1:C:391:ILE:HD12	1:C:391:ILE:N	1.90	0.85
1:A:438:THR:CG2	1:A:458:SER:HA	2.06	0.84
1:B:383:TRP:CD1	1:B:384:SER:HG	1.94	0.84
1:A:416:ILE:HD12	1:A:503:ILE:HG12	1.57	0.84
1:B:394:THR:HG22	1:B:522:THR:HG23	1.58	0.84
1:B:353:ARG:H	1:B:584:ASN:HD22	1.25	0.84
1:C:221:ILE:HG22	1:C:310:VAL:HG22	1.57	0.84
1:B:451:TYR:HE1	1:B:457:ILE:HD11	1.43	0.84
1:B:521:GLN:HG2	1:B:522:THR:H	1.43	0.84
1:C:451:TYR:HD1	1:C:457:ILE:CA	1.91	0.84
1:A:346:SER:HB3	1:A:643:LEU:HB2	1.58	0.84
1:B:606:PHE:CE1	1:B:624:ASP:CA	2.61	0.83
1:B:490:ALA:HB1	1:B:498:ILE:O	1.78	0.83
1:C:451:TYR:N	1:C:458:SER:HB2	1.91	0.83
1:B:623:ILE:H	1:B:623:ILE:CD1	1.81	0.83
1:A:394:THR:OG1	1:A:407:VAL:HG11	1.78	0.82
1:A:473:GLN:HB3	1:A:482:SER:HA	1.60	0.82
1:C:572:LYS:H	1:C:572:LYS:HD2	1.44	0.82
1:C:141:GLY:HA3	1:C:144:ALA:HB3	1.61	0.82
1:B:553:LEU:HD12	1:B:554:PRO:HD2	1.62	0.82
1:B:327:PRO:O	1:B:330:SER:HB2	1.79	0.81
1:B:453:SER:CB	1:B:456:ILE:CD1	2.57	0.81
1:A:397:GLN:HE22	1:A:520:VAL:HG23	1.44	0.81
1:B:397:GLN:OE1	1:B:521:GLN:HB3	1.80	0.81
1:B:533:THR:O	1:B:535:ILE:HG23	1.79	0.81
1:A:405:ILE:CD1	1:A:510:ILE:HG12	2.10	0.81
1:B:463:PHE:HB3	1:B:466:MET:HG3	1.62	0.81
1:A:234:ILE:HD13	1:A:234:ILE:N	1.96	0.81
1:C:608:VAL:HB	1:C:648:MET:HB2	1.63	0.81
1:A:535:ILE:HG13	1:A:536:GLY:N	1.94	0.81
1:C:424:THR:OG1	1:C:489:THR:HG23	1.80	0.80
1:B:411:TYR:CZ	1:B:417:PRO:HA	2.16	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:PHE:HB2	1:C:311:THR:O	1.79	0.80
1:C:187:ILE:HG12	1:C:244:GLN:HG2	1.64	0.80
1:A:353:ARG:H	1:A:584:ASN:ND2	1.79	0.80
1:B:451:TYR:CE1	1:B:457:ILE:CD1	2.64	0.80
1:A:184:GLN:HE21	1:A:293:ASN:HA	1.47	0.80
1:B:439:ASN:ND2	1:B:456:ILE:HG13	1.97	0.80
1:C:221:ILE:H	1:C:221:ILE:CD1	1.95	0.79
1:C:210:ALA:HB3	1:C:324:LEU:H	1.46	0.79
1:A:476:TRP:CE3	1:A:522:THR:HB	2.17	0.79
1:B:171:SER:O	1:B:313:GLU:HB3	1.82	0.79
1:B:606:PHE:CE1	1:B:624:ASP:HB3	2.17	0.79
1:A:393:VAL:O	1:A:525:ASP:HB3	1.83	0.79
1:B:158:THR:C	1:B:160:LYS:H	1.90	0.79
1:B:407:VAL:O	1:B:409:THR:HG22	1.82	0.79
1:C:532:TYR:OH	1:C:535:ILE:HD13	1.81	0.79
1:C:451:TYR:HD1	1:C:457:ILE:CB	1.95	0.79
1:B:174:THR:HG22	1:B:175:SER:H	1.45	0.79
1:A:566:PHE:CE2	1:A:583:PHE:HB3	2.18	0.79
1:A:447:THR:O	1:A:447:THR:CG2	2.31	0.79
1:A:571:MET:HB3	1:A:580:ILE:HD11	1.65	0.78
1:B:146:PRO:O	1:B:149:GLN:HG2	1.84	0.78
1:A:278:LEU:HD23	1:A:278:LEU:H	1.47	0.78
1:C:451:TYR:HD1	1:C:457:ILE:HA	1.47	0.78
1:B:451:TYR:HE1	1:B:457:ILE:CD1	1.96	0.78
1:A:239:GLY:O	1:B:333:THR:HG22	1.83	0.78
1:C:471:SER:HB3	1:C:527:LEU:HB3	1.64	0.78
1:C:473:GLN:HA	1:C:524:ASP:OD1	1.84	0.78
1:B:287:LEU:HD12	1:B:288:VAL:H	1.48	0.78
1:A:327:PRO:HG2	1:A:330:SER:OG	1.84	0.78
1:C:349:TRP:HB3	1:C:358:ILE:CD1	2.14	0.78
1:B:476:TRP:CD1	1:B:520:VAL:HB	2.20	0.77
1:A:406:GLY:N	1:A:508:ILE:HD11	1.99	0.77
1:C:150:MET:C	1:C:152:ALA:H	1.90	0.77
1:C:487:ILE:HG22	1:C:510:ILE:HG22	1.66	0.77
1:A:130:ILE:CG1	1:A:131:THR:H	1.96	0.77
1:B:424:THR:HG22	1:B:489:THR:HG23	1.67	0.77
1:C:397:GLN:HG2	1:C:523:SER:HB2	1.64	0.77
1:A:631:VAL:HA	1:A:657:LEU:HD12	1.66	0.77
1:B:310:VAL:O	1:B:310:VAL:HG13	1.85	0.77
1:A:234:ILE:HD13	1:A:234:ILE:H	1.50	0.77
1:A:236:VAL:HG11	1:A:242:PRO:HG3	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:ARG:HD2	1:A:475:ALA:H	1.48	0.77
1:B:576:VAL:O	1:B:576:VAL:HG12	1.83	0.77
1:C:360:ASP:HB3	1:C:568:ARG:HB3	1.65	0.77
1:A:148:VAL:O	1:A:150:MET:N	2.18	0.76
1:B:397:GLN:HA	1:B:398:LYS:HZ2	1.48	0.76
1:B:487:ILE:CG2	1:B:510:ILE:HG22	2.15	0.76
1:A:459:ASN:O	1:A:460:ASN:CB	2.33	0.76
1:A:342:ILE:HD12	1:A:609:TYR:HD2	1.48	0.76
1:B:370:ALA:HB2	1:B:554:PRO:HD3	1.67	0.76
1:B:436:ALA:CB	1:B:461:THR:HA	2.10	0.76
1:B:397:GLN:CD	1:B:521:GLN:HB3	2.11	0.76
1:B:402:MET:HE2	1:B:511:PHE:CA	2.14	0.76
1:C:352:ASN:HD22	1:C:586:GLN:H	1.33	0.76
1:C:398:LYS:N	1:C:403:LEU:HD23	2.00	0.76
1:B:425:ILE:HG12	1:B:499:PRO:HB3	1.67	0.76
1:A:250:GLN:HB2	1:B:328:PRO:HG2	1.67	0.76
1:B:606:PHE:CG	1:B:624:ASP:CA	2.67	0.76
1:C:451:TYR:CD1	1:C:457:ILE:HB	2.21	0.76
1:A:221:ILE:HD12	1:A:221:ILE:O	1.86	0.75
1:B:341:LEU:HG	1:B:609:TYR:OH	1.86	0.75
1:B:453:SER:HB3	1:B:456:ILE:CD1	2.16	0.75
1:C:363:ILE:H	1:C:363:ILE:HD13	1.50	0.75
1:A:608:VAL:HG23	1:A:650:ASN:HA	1.68	0.75
1:B:606:PHE:CE2	1:B:624:ASP:HB3	2.16	0.75
1:B:451:TYR:CE1	1:B:457:ILE:HD11	2.20	0.75
1:C:395:ILE:HG22	1:C:406:GLY:HA3	1.66	0.75
1:C:401:GLU:OE1	1:C:402:MET:HB3	1.85	0.75
1:A:394:THR:O	1:A:407:VAL:HB	1.85	0.75
1:A:333:THR:HG22	1:C:239:GLY:HA2	1.65	0.75
1:C:587:ILE:HD12	1:C:587:ILE:N	2.01	0.75
1:B:439:ASN:OD1	1:B:456:ILE:HA	1.87	0.75
1:A:149:GLN:O	1:A:153:ALA:HB3	1.86	0.75
1:B:383:TRP:O	1:B:412:ILE:HD11	1.87	0.75
1:A:352:ASN:HB2	1:A:372:ARG:HB3	1.68	0.74
1:B:253:HIS:O	1:C:133:PRO:HB3	1.87	0.74
1:B:456:ILE:HG23	1:B:457:ILE:N	2.02	0.74
1:B:327:PRO:HG2	1:B:330:SER:HB2	1.70	0.74
1:C:350:ILE:HA	1:C:357:ASP:HA	1.69	0.74
1:A:624:ASP:OD2	1:A:626:ASP:HB2	1.87	0.74
1:B:354:PHE:C	1:B:356:SER:H	1.95	0.74
1:C:297:ASN:HD22	1:C:298:PRO:CD	1.99	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ILE:HD12	1:A:240:ILE:O	1.86	0.74
1:A:464:LYS:HA	1:A:533:THR:HG21	1.69	0.74
1:B:453:SER:HB3	1:B:456:ILE:HB	1.68	0.74
1:A:497:LEU:O	1:A:498:ILE:HG13	1.87	0.74
1:B:504:ASP:HB2	1:B:507:LYS:HD3	1.68	0.74
1:A:221:ILE:HD12	1:A:221:ILE:C	2.12	0.73
1:B:631:VAL:HG12	1:B:633:VAL:H	1.51	0.73
1:A:151:SER:O	1:A:152:ALA:HB3	1.88	0.73
1:A:197:LEU:HD12	1:A:215:ILE:HD12	1.69	0.73
1:B:185:GLY:N	1:B:291:ILE:HG13	2.01	0.73
1:C:535:ILE:HD12	1:C:546:LYS:NZ	2.03	0.73
1:A:378:GLN:HG3	1:C:654:LYS:HZ2	1.50	0.73
1:B:427:ASN:O	1:B:499:PRO:HD3	1.86	0.73
1:A:535:ILE:HD11	1:A:538:GLU:HB2	1.71	0.73
1:B:606:PHE:CG	1:B:624:ASP:HA	2.23	0.73
1:C:408:ALA:HB2	1:C:417:PRO:HG3	1.70	0.73
1:A:439:ASN:HB3	1:A:456:ILE:HG12	1.70	0.73
1:C:297:ASN:HD22	1:C:298:PRO:N	1.85	0.73
1:A:133:PRO:HB3	1:A:134:GLU:OE2	1.87	0.73
1:A:185:GLY:H	1:A:291:ILE:HG13	1.53	0.73
1:A:339:CYS:SG	1:A:647:TYR:HB2	2.28	0.73
1:A:287:LEU:HG	1:A:288:VAL:N	2.03	0.72
1:A:350:ILE:HG22	1:A:357:ASP:HB3	1.71	0.72
1:C:611:ILE:N	1:C:611:ILE:HD12	2.04	0.72
1:B:148:VAL:HG23	1:B:149:GLN:HE21	1.54	0.72
1:B:402:MET:CE	1:B:512:GLN:H	2.01	0.72
1:B:615:ASN:HB2	1:B:640:GLU:HG2	1.72	0.72
1:B:661:ILE:H	1:B:661:ILE:CD1	2.02	0.72
1:C:339:CYS:SG	1:C:649:GLY:HA2	2.29	0.72
1:C:447:THR:O	1:C:448:LYS:HB3	1.88	0.72
1:A:405:ILE:HD12	1:A:510:ILE:CG1	2.16	0.72
1:B:342:ILE:HD12	1:B:587:ILE:HD12	1.71	0.72
1:C:219:PHE:CB	1:C:312:VAL:HA	2.18	0.72
1:A:472:LEU:HD23	1:A:473:GLN:HG2	1.68	0.72
1:B:336:SER:H	1:B:599:TYR:HA	1.55	0.72
1:A:446:GLN:O	1:A:447:THR:C	2.33	0.72
1:B:579:SER:O	1:B:580:ILE:HG13	1.90	0.72
1:C:490:ALA:HB1	1:C:498:ILE:O	1.90	0.71
1:C:331:MET:HE3	1:C:332:LEU:H	1.54	0.71
1:A:335:GLY:HA3	1:A:600:LEU:H	1.54	0.71
1:A:438:THR:HG21	1:A:459:ASN:H	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:ASN:HB2	1:B:314:THR:OG1	1.90	0.71
1:B:656:ARG:O	1:B:657:LEU:HD23	1.89	0.71
1:C:201:LEU:HD11	1:C:316:PRO:HB3	1.72	0.71
1:B:412:ILE:HD13	1:B:413:VAL:HG23	1.71	0.71
1:B:452:GLU:O	1:B:453:SER:CB	2.37	0.71
1:A:562:ASN:OD1	1:A:657:LEU:HG	1.91	0.71
1:B:188:LEU:O	1:B:188:LEU:HD23	1.91	0.71
1:B:409:THR:O	1:B:410:ASP:HB2	1.89	0.71
1:B:656:ARG:C	1:B:657:LEU:HD23	2.15	0.71
1:C:130:ILE:HD13	1:C:130:ILE:H	1.56	0.71
1:C:175:SER:HB3	1:C:311:THR:HA	1.73	0.71
1:C:201:LEU:HD22	1:C:320:PHE:HE2	1.56	0.71
1:C:451:TYR:CD1	1:C:457:ILE:HA	2.25	0.71
1:A:398:LYS:N	1:A:403:LEU:HD22	2.06	0.71
1:A:472:LEU:O	1:A:473:GLN:HB3	1.87	0.71
1:A:565:ILE:HD12	1:A:566:PHE:N	2.05	0.71
1:C:334:HIS:HB3	1:C:600:LEU:HD11	1.73	0.71
1:B:374:PHE:H	1:B:586:GLN:HE22	1.39	0.71
1:B:439:ASN:HD21	1:B:456:ILE:HD11	1.56	0.71
1:C:529:LEU:C	1:C:530:LEU:HD12	2.16	0.71
1:A:393:VAL:C	1:A:525:ASP:HB3	2.14	0.70
1:B:289:ILE:HD12	1:B:289:ILE:N	2.06	0.70
1:B:451:TYR:CE1	1:B:457:ILE:HD12	2.25	0.70
1:A:474:ARG:HD3	1:A:523:SER:CA	2.16	0.70
1:B:350:ILE:HD12	1:B:588:LEU:HD23	1.72	0.70
1:A:131:THR:OG1	1:C:255:LEU:HB2	1.91	0.70
1:C:620:ASP:HB2	1:C:657:LEU:HB3	1.73	0.70
1:C:197:LEU:HD12	1:C:215:ILE:CD1	2.22	0.70
1:A:334:HIS:C	1:A:600:LEU:HD12	2.16	0.70
1:A:405:ILE:CG2	1:A:510:ILE:HG23	2.21	0.70
1:B:439:ASN:CG	1:B:456:ILE:HG13	2.16	0.70
1:B:580:ILE:HD12	1:B:580:ILE:O	1.91	0.70
1:C:471:SER:CB	1:C:527:LEU:HB3	2.21	0.70
1:A:132:THR:O	1:A:133:PRO:C	2.35	0.70
1:A:451:TYR:HA	1:A:452:GLU:HB2	1.72	0.70
1:C:189:PHE:HD1	1:C:289:ILE:HB	1.55	0.70
1:A:461:THR:HG22	1:A:464:LYS:HB3	1.73	0.70
1:B:178:TRP:CZ2	1:B:295:LEU:HB2	2.27	0.70
1:B:463:PHE:CB	1:B:466:MET:HG3	2.22	0.70
1:C:373:HIS:HA	1:C:586:GLN:OE1	1.92	0.70
1:A:164:SER:HA	1:A:166:TRP:CE3	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:655:ILE:HD12	1:A:655:ILE:O	1.90	0.70
1:B:221:ILE:H	1:B:221:ILE:HD12	1.57	0.70
1:C:567:TYR:OH	1:C:587:ILE:HD11	1.91	0.70
1:A:175:SER:HB3	1:A:311:THR:CG2	2.15	0.69
1:B:210:ALA:CB	1:B:323:HIS:HB2	2.22	0.69
1:C:425:ILE:HG13	1:C:499:PRO:HB3	1.74	0.69
1:B:425:ILE:HD13	1:B:425:ILE:N	2.07	0.69
1:C:508:ILE:HD13	1:C:508:ILE:N	2.07	0.69
1:A:420:TRP:CD1	1:A:421:PRO:HD2	2.26	0.69
1:C:397:GLN:HB2	1:C:520:VAL:O	1.92	0.69
1:A:251:TYR:CG	1:A:252:PRO:HD2	2.28	0.69
1:B:397:GLN:HE21	1:B:514:ASN:CG	1.99	0.69
1:B:453:SER:HB2	1:B:456:ILE:HD13	1.73	0.69
1:C:577:ILE:HG13	1:C:578:LYS:N	2.06	0.69
1:A:231:LEU:CD1	1:A:291:ILE:HA	2.23	0.69
1:A:406:GLY:H	1:A:508:ILE:CD1	2.04	0.69
1:A:460:ASN:O	1:A:462:ASN:N	2.26	0.69
1:B:503:ILE:HG22	1:B:549:ARG:O	1.93	0.69
1:B:606:PHE:CE2	1:B:624:ASP:OD1	2.45	0.69
1:C:150:MET:C	1:C:152:ALA:N	2.49	0.69
1:C:346:SER:HB2	1:C:643:LEU:HB2	1.75	0.69
1:C:578:LYS:O	1:C:579:SER:OG	2.09	0.69
1:A:145:GLU:O	1:A:146:PRO:C	2.35	0.69
1:A:601:LEU:HD11	1:A:606:PHE:O	1.92	0.69
1:B:513:ASP:HB2	1:B:515:HIS:NE2	2.08	0.69
1:C:353:ARG:H	1:C:584:ASN:ND2	1.90	0.69
1:C:587:ILE:H	1:C:587:ILE:CD1	2.00	0.69
1:C:345:SER:HA	1:C:644:THR:HG22	1.75	0.69
1:C:376:PHE:HB2	1:C:625:SER:O	1.92	0.69
1:C:567:TYR:CZ	1:C:587:ILE:HD11	2.28	0.69
1:A:352:ASN:ND2	1:A:586:GLN:H	1.90	0.68
1:B:611:ILE:HD12	1:B:611:ILE:N	2.09	0.68
1:C:450:GLU:O	1:C:451:TYR:HB2	1.92	0.68
1:B:637:GLY:O	1:B:639:LEU:HD22	1.94	0.68
1:C:474:ARG:HB2	1:C:524:ASP:C	2.19	0.68
1:A:350:ILE:CA	1:A:357:ASP:HA	2.22	0.68
1:B:396:SER:HB2	1:B:404:GLY:HA2	1.75	0.68
1:A:360:ASP:HB2	1:A:568:ARG:HD2	1.75	0.68
1:A:398:LYS:H	1:A:403:LEU:HD22	1.58	0.68
1:B:425:ILE:HG22	1:B:465:SER:HB2	1.76	0.68
1:B:566:PHE:CD2	1:B:583:PHE:HB3	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:288:VAL:C	1:C:289:ILE:HD12	2.19	0.68
1:A:411:TYR:CD1	1:A:418:ASP:N	2.61	0.68
1:B:365:PRO:O	1:B:366:PHE:HD1	1.77	0.68
1:B:468:ILE:HB	1:B:531:GLY:H	1.57	0.68
1:A:656:ARG:O	1:A:657:LEU:HD23	1.94	0.67
1:C:431:PRO:HB3	1:C:511:PHE:CZ	2.28	0.67
1:A:438:THR:HG21	1:A:458:SER:CA	2.20	0.67
1:B:428:GLU:HG3	1:B:498:ILE:HG22	1.75	0.67
1:B:472:LEU:HD22	1:B:473:GLN:N	2.08	0.67
1:C:401:GLU:CD	1:C:402:MET:H	2.03	0.67
1:A:189:PHE:CE2	1:A:191:GLN:HB2	2.29	0.67
1:B:145:GLU:OE1	1:B:146:PRO:HD2	1.94	0.67
1:B:437:ILE:O	1:B:438:THR:HB	1.94	0.67
1:B:368:PHE:O	1:B:369:GLN:HB3	1.95	0.67
1:C:412:ILE:HD12	1:C:413:VAL:HG22	1.77	0.67
1:A:408:ALA:HB2	1:A:417:PRO:HG3	1.77	0.67
1:A:448:LYS:O	1:A:449:GLU:CB	2.42	0.67
1:C:463:PHE:HB2	1:C:466:MET:HG3	1.76	0.67
1:A:535:ILE:CD1	1:A:538:GLU:HB2	2.25	0.67
1:A:352:ASN:H	1:A:584:ASN:HD22	1.41	0.67
1:A:580:ILE:HD12	1:A:580:ILE:C	2.20	0.67
1:B:473:GLN:HE21	1:B:475:ALA:N	1.92	0.67
1:B:624:ASP:O	1:B:627:GLY:N	2.20	0.67
1:C:470:GLY:H	1:C:530:LEU:HD13	1.58	0.67
1:C:287:LEU:CD1	1:C:288:VAL:N	2.56	0.67
1:C:296:ILE:HD12	1:C:296:ILE:O	1.95	0.67
1:A:472:LEU:HD22	1:A:524:ASP:HB3	1.77	0.66
1:C:344:LYS:O	1:C:345:SER:HB2	1.95	0.66
1:C:540:ILE:HB	1:C:582:VAL:CG1	2.26	0.66
1:A:457:ILE:O	1:A:457:ILE:HG13	1.94	0.66
1:B:516:VAL:O	1:B:516:VAL:HG13	1.96	0.66
1:C:472:LEU:HD13	1:C:472:LEU:C	2.20	0.66
1:A:341:LEU:HB2	1:A:609:TYR:OH	1.96	0.66
1:C:408:ALA:HB1	1:C:411:TYR:CD2	2.29	0.66
1:C:448:LYS:O	1:C:449:GLU:CB	2.41	0.66
1:B:446:GLN:HE22	1:B:447:THR:HG23	1.60	0.66
1:A:197:LEU:HD12	1:A:215:ILE:CD1	2.26	0.66
1:A:428:GLU:HG2	1:A:499:PRO:HD2	1.76	0.66
1:A:439:ASN:CG	1:A:440:GLN:H	2.03	0.66
1:B:158:THR:O	1:B:160:LYS:N	2.29	0.66
1:C:332:LEU:HD23	1:C:334:HIS:H	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:THR:CG2	1:A:464:LYS:HB3	2.26	0.66
1:A:490:ALA:HB1	1:A:498:ILE:O	1.95	0.66
1:A:209:VAL:HG22	1:A:324:LEU:C	2.20	0.66
1:A:469:CYS:O	1:A:485:ALA:CB	2.44	0.66
1:A:142:VAL:O	1:A:143:ILE:HG22	1.94	0.66
1:A:349:TRP:CE3	1:A:358:ILE:HD12	2.31	0.66
1:A:189:PHE:HB3	1:A:289:ILE:CD1	2.26	0.66
1:A:367:VAL:HG13	1:A:566:PHE:CE1	2.31	0.66
1:A:431:PRO:HB3	1:A:511:PHE:CE1	2.30	0.66
1:B:366:PHE:CE2	1:C:414:PRO:HD3	2.31	0.66
1:B:385:THR:HG22	1:B:386:PRO:CD	2.24	0.66
1:A:342:ILE:HD12	1:A:609:TYR:CD2	2.30	0.65
1:B:425:ILE:HD11	1:B:490:ALA:HB2	1.78	0.65
1:A:393:VAL:HA	1:A:409:THR:HG22	1.79	0.65
1:A:439:ASN:CB	1:A:456:ILE:HA	2.20	0.65
1:C:398:LYS:H	1:C:403:LEU:HD23	1.60	0.65
1:C:387:ARG:HH21	1:C:592:ARG:HD3	1.61	0.65
1:A:456:ILE:O	1:A:456:ILE:HG22	1.96	0.65
1:B:363:ILE:O	1:B:363:ILE:HD13	1.96	0.65
1:B:439:ASN:HD21	1:B:456:ILE:CD1	2.09	0.65
1:B:453:SER:HB2	1:B:456:ILE:CG1	2.27	0.65
1:C:353:ARG:H	1:C:584:ASN:HD21	1.42	0.65
1:B:602:SER:C	1:B:604:ASP:H	2.05	0.65
1:B:251:TYR:CG	1:B:252:PRO:HD2	2.32	0.65
1:C:149:GLN:O	1:C:152:ALA:CB	2.42	0.65
1:C:565:ILE:HD11	1:C:629:SER:HB3	1.78	0.65
1:A:209:VAL:CG2	1:A:324:LEU:O	2.30	0.65
1:A:474:ARG:C	1:A:524:ASP:HB2	2.22	0.65
1:A:170:PHE:N	1:A:170:PHE:CD1	2.65	0.65
1:A:172:PHE:CD1	1:A:172:PHE:N	2.65	0.65
1:B:633:VAL:HG12	1:B:634:SER:N	2.12	0.65
1:B:472:LEU:HD12	1:B:526:THR:HB	1.79	0.64
1:B:606:PHE:HB3	1:B:622:GLY:O	1.97	0.64
1:A:148:VAL:HG22	1:A:149:GLN:N	2.11	0.64
1:A:459:ASN:HD22	1:A:459:ASN:N	1.95	0.64
1:A:498:ILE:HD12	1:A:499:PRO:O	1.96	0.64
1:B:472:LEU:C	1:B:472:LEU:HD13	2.21	0.64
1:B:623:ILE:HA	1:B:628:PHE:O	1.97	0.64
1:A:407:VAL:HG12	1:A:408:ALA:N	2.13	0.64
1:A:469:CYS:HB3	1:A:527:LEU:HB2	1.79	0.64
1:C:166:TRP:C	1:C:168:ALA:H	2.04	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:LEU:HD23	1:A:278:LEU:N	2.11	0.64
1:B:453:SER:HB2	1:B:456:ILE:CD1	2.26	0.64
1:B:544:ARG:HH22	1:C:505:GLN:HE22	1.45	0.64
1:B:580:ILE:HD12	1:B:580:ILE:C	2.23	0.64
1:C:209:VAL:HG23	1:C:324:LEU:CB	2.27	0.64
1:A:459:ASN:N	1:A:459:ASN:ND2	2.45	0.64
1:C:439:ASN:HD21	1:C:440:GLN:HE22	1.46	0.64
1:B:550:ILE:O	1:B:550:ILE:HD13	1.97	0.64
1:A:334:HIS:HA	1:A:600:LEU:HD12	1.78	0.64
1:A:405:ILE:HD13	1:A:405:ILE:N	2.13	0.64
1:A:353:ARG:H	1:A:584:ASN:HD22	1.45	0.64
1:B:222:SER:O	1:B:308:CYS:HB2	1.97	0.64
1:C:395:ILE:HD13	1:C:403:LEU:CD1	2.28	0.64
1:C:437:ILE:O	1:C:461:THR:HB	1.98	0.64
1:A:461:THR:O	1:A:463:PHE:N	2.30	0.64
1:A:535:ILE:CG1	1:A:536:GLY:H	2.02	0.64
1:A:569:ASN:ND2	1:A:570:SER:H	1.96	0.64
1:B:158:THR:C	1:B:160:LYS:N	2.55	0.64
1:B:349:TRP:HB3	1:B:358:ILE:CG2	2.28	0.64
1:B:639:LEU:HD23	1:B:639:LEU:N	2.12	0.64
1:C:435:TYR:CD1	1:C:435:TYR:O	2.50	0.64
1:A:353:ARG:HE	1:A:422:ASP:HB2	1.63	0.63
1:C:540:ILE:HB	1:C:582:VAL:HG13	1.78	0.63
1:C:613:ASP:HA	1:C:643:LEU:HD23	1.80	0.63
1:A:130:ILE:HG13	1:A:131:THR:N	2.09	0.63
1:A:277:HIS:H	1:A:277:HIS:CD2	2.16	0.63
1:A:550:ILE:O	1:A:550:ILE:HD13	1.98	0.63
1:A:571:MET:O	1:A:579:SER:O	2.16	0.63
1:B:470:GLY:N	1:B:528:ALA:H	1.89	0.63
1:C:297:ASN:HD22	1:C:298:PRO:HD2	1.62	0.63
1:A:424:THR:HG23	1:A:548:VAL:HG22	1.80	0.63
1:C:393:VAL:HG22	1:C:408:ALA:HA	1.81	0.63
1:C:473:GLN:HB3	1:C:482:SER:HA	1.80	0.63
1:C:661:ILE:HG12	1:C:662:ARG:N	2.12	0.63
1:A:590:THR:O	1:A:594:LEU:HB2	1.99	0.63
1:B:251:TYR:CD1	1:C:327:PRO:HB3	2.33	0.63
1:B:395:ILE:O	1:B:521:GLN:HG3	1.98	0.63
1:B:411:TYR:HD1	1:B:418:ASP:HB2	1.64	0.63
1:B:437:ILE:HD11	1:B:440:GLN:HA	1.80	0.63
1:C:482:SER:O	1:C:483:ASN:HB3	1.99	0.63
1:C:526:THR:C	1:C:527:LEU:HD23	2.23	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:VAL:HG12	1:A:408:ALA:H	1.61	0.63
1:C:471:SER:O	1:C:482:SER:HB2	1.98	0.63
1:B:400:GLY:C	1:B:401:GLU:HG3	2.23	0.63
1:A:614:SER:HB2	1:A:640:GLU:OE1	1.97	0.63
1:B:565:ILE:HD11	1:B:629:SER:HB2	1.79	0.63
1:C:331:MET:HE3	1:C:332:LEU:N	2.13	0.63
1:C:504:ASP:O	1:C:506:THR:N	2.32	0.63
1:A:205:ALA:C	1:A:207:LEU:H	2.07	0.63
1:A:433:GLY:HA3	1:A:462:ASN:CG	2.23	0.63
1:A:512:GLN:OE1	1:A:514:ASN:HB2	1.98	0.63
1:B:256:PHE:CE1	1:B:264:VAL:HB	2.34	0.63
1:B:453:SER:O	1:B:456:ILE:CG2	2.46	0.63
1:C:391:ILE:N	1:C:391:ILE:CD1	2.60	0.63
1:C:451:TYR:CD1	1:C:457:ILE:CA	2.78	0.63
1:C:481:VAL:O	1:C:481:VAL:HG13	1.97	0.63
1:A:364:ARG:HB3	1:A:365:PRO:HD2	1.80	0.62
1:A:408:ALA:HB1	1:A:411:TYR:CD2	2.33	0.62
1:A:540:ILE:HB	1:A:582:VAL:HG13	1.80	0.62
1:B:151:SER:C	1:B:153:ALA:H	2.07	0.62
1:B:487:ILE:HG22	1:B:509:ALA:O	1.99	0.62
1:C:187:ILE:N	1:C:244:GLN:HE21	1.97	0.62
1:C:580:ILE:C	1:C:580:ILE:HD12	2.24	0.62
1:C:610:ARG:HH21	1:C:648:MET:HE2	1.63	0.62
1:B:384:SER:HA	1:B:418:ASP:OD1	1.99	0.62
1:C:607:ALA:HB3	1:C:623:ILE:HG12	1.81	0.62
1:B:437:ILE:CD1	1:B:440:GLN:HA	2.29	0.62
1:C:349:TRP:O	1:C:350:ILE:HG12	2.00	0.62
1:C:351:GLY:HA3	1:C:584:ASN:OD1	1.99	0.62
1:B:615:ASN:HB2	1:B:640:GLU:CG	2.30	0.62
1:B:453:SER:CB	1:B:456:ILE:HB	2.29	0.62
1:C:610:ARG:C	1:C:611:ILE:HD12	2.25	0.62
1:A:152:ALA:O	1:A:155:ASP:HB2	2.00	0.62
1:A:464:LYS:HA	1:A:533:THR:CG2	2.29	0.62
1:B:611:ILE:CD1	1:B:621:ILE:HD13	2.29	0.62
1:C:297:ASN:HD22	1:C:297:ASN:C	2.05	0.62
1:C:598:ASN:C	1:C:598:ASN:HD22	2.07	0.62
1:A:297:ASN:ND2	1:A:298:PRO:HD2	2.15	0.62
1:B:238:PRO:HB3	1:B:284:THR:HA	1.82	0.62
1:C:447:THR:O	1:C:448:LYS:CB	2.48	0.62
1:A:378:GLN:HG3	1:C:654:LYS:HZ1	1.64	0.62
1:B:636:ILE:H	1:B:636:ILE:CD1	2.06	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:TRP:CE2	1:B:508:ILE:HG22	2.34	0.62
1:B:569:ASN:HD22	1:B:570:SER:N	1.97	0.62
1:C:236:VAL:HG11	1:C:242:PRO:HG3	1.80	0.62
1:C:327:PRO:HG2	1:C:330:SER:HB2	1.81	0.62
1:A:144:ALA:C	1:A:145:GLU:HG3	2.25	0.61
1:A:460:ASN:O	1:A:461:THR:C	2.41	0.61
1:B:148:VAL:O	1:B:149:GLN:C	2.41	0.61
1:C:187:ILE:O	1:C:188:LEU:HD23	1.99	0.61
1:C:300:ALA:O	1:C:301:ASN:HB2	1.98	0.61
1:C:562:ASN:OD1	1:C:657:LEU:HG	2.01	0.61
1:A:310:VAL:HG12	1:A:311:THR:N	2.14	0.61
1:A:221:ILE:HD12	1:A:223:GLY:H	1.66	0.61
1:A:334:HIS:CA	1:A:600:LEU:HD12	2.30	0.61
1:A:438:THR:HG21	1:A:459:ASN:N	2.15	0.61
1:B:254:VAL:C	1:B:255:LEU:HD22	2.25	0.61
1:B:586:GLN:OE1	1:B:591:SER:HB3	1.99	0.61
1:B:358:ILE:HG13	1:B:359:THR:N	2.07	0.61
1:A:210:ALA:CB	1:A:278:LEU:HA	2.31	0.61
1:A:641:PHE:O	1:A:643:LEU:HG	2.01	0.61
1:B:517:ASN:CG	1:B:518:ARG:H	2.08	0.61
1:B:652:LEU:CD2	1:B:654:LYS:HD3	2.30	0.61
1:B:237:PRO:HD2	1:B:240:ILE:HD11	1.82	0.61
1:B:535:ILE:HG13	1:B:536:GLY:O	2.00	0.61
1:C:186:LYS:H	1:C:290:MET:HG3	1.66	0.61
1:C:401:GLU:CD	1:C:402:MET:N	2.58	0.61
1:A:405:ILE:HG23	1:A:510:ILE:HG12	1.82	0.61
1:A:411:TYR:CG	1:A:417:PRO:HA	2.36	0.61
1:A:484:THR:O	1:A:485:ALA:HB3	2.00	0.61
1:B:287:LEU:HD12	1:B:288:VAL:N	2.14	0.61
1:B:390:PRO:C	1:B:391:ILE:HD12	2.26	0.61
1:C:197:LEU:HD12	1:C:215:ILE:HD12	1.83	0.61
1:B:412:ILE:HD13	1:B:412:ILE:H	1.65	0.61
1:A:171:SER:O	1:A:313:GLU:HA	2.01	0.61
1:A:399:GLU:HG3	1:A:516:VAL:CG2	2.24	0.61
1:B:373:HIS:CG	1:B:586:GLN:HE21	2.19	0.60
1:B:391:ILE:HD12	1:B:391:ILE:N	2.16	0.60
1:B:251:TYR:HE1	1:C:325:LEU:O	1.84	0.60
1:B:411:TYR:CE2	1:B:417:PRO:HA	2.34	0.60
1:C:205:ALA:HA	1:C:322:PHE:HE2	1.67	0.60
1:C:452:GLU:HB2	1:C:456:ILE:HD13	1.84	0.60
1:B:179:SER:HB3	1:B:182:GLU:OE1	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:451:TYR:CD1	1:B:457:ILE:HD12	2.36	0.60
1:C:144:ALA:CB	1:C:147:SER:HB3	2.27	0.60
1:C:218:ARG:HB2	1:C:265:ILE:HG23	1.82	0.60
1:C:445:ILE:C	1:C:447:THR:H	2.06	0.60
1:A:363:ILE:HD11	1:A:635:SER:HA	1.84	0.60
1:B:424:THR:HB	1:B:425:ILE:HD13	1.83	0.60
1:C:251:TYR:CG	1:C:252:PRO:HD2	2.36	0.60
1:C:504:ASP:C	1:C:506:THR:H	2.08	0.60
1:A:183:THR:C	1:A:291:ILE:HD12	2.27	0.60
1:A:454:ALA:O	1:A:455:MET:CG	2.48	0.60
1:B:160:LYS:HE3	1:B:163:ASP:HA	1.82	0.60
1:B:220:SER:O	1:B:310:VAL:HG23	2.02	0.60
1:B:394:THR:HG22	1:B:522:THR:CG2	2.32	0.60
1:B:661:ILE:HD13	1:B:661:ILE:N	2.12	0.60
1:A:438:THR:CG2	1:A:458:SER:CA	2.79	0.60
1:B:412:ILE:CD1	1:B:413:VAL:HG23	2.32	0.60
1:C:451:TYR:CE1	1:C:457:ILE:HB	2.37	0.60
1:A:134:GLU:CD	1:A:134:GLU:N	2.60	0.60
1:C:180:THR:HA	1:C:295:LEU:HB3	1.83	0.60
1:C:362:VAL:HG12	1:C:364:ARG:HG2	1.83	0.60
1:B:141:GLY:O	1:B:143:ILE:HG12	2.01	0.60
1:A:250:GLN:O	1:B:328:PRO:HD2	2.01	0.60
1:B:443:ASN:ND2	1:B:447:THR:HG21	2.17	0.60
1:B:448:LYS:HA	1:B:448:LYS:NZ	2.17	0.60
1:C:162:VAL:HG12	1:C:164:SER:H	1.66	0.59
1:C:464:LYS:HA	1:C:533:THR:CG2	2.31	0.59
1:C:532:TYR:CD2	1:C:540:ILE:HD11	2.37	0.59
1:C:612:ILE:HG22	1:C:618:TRP:HB3	1.84	0.59
1:A:178:TRP:CZ2	1:A:295:LEU:HB2	2.37	0.59
1:A:234:ILE:N	1:A:234:ILE:CD1	2.65	0.59
1:A:498:ILE:HD12	1:A:498:ILE:C	2.27	0.59
1:C:162:VAL:HG12	1:C:164:SER:OG	2.03	0.59
1:C:166:TRP:HA	1:C:169:PHE:CE2	2.36	0.59
1:C:299:TYR:N	1:C:299:TYR:CD1	2.69	0.59
1:C:517:ASN:C	1:C:519:ASP:H	2.08	0.59
1:A:130:ILE:CG1	1:A:131:THR:N	2.65	0.59
1:A:190:LYS:HG3	1:A:651:GLN:HE22	1.68	0.59
1:A:423:THR:HB	1:A:467:TYR:HE1	1.68	0.59
1:B:261:VAL:HG12	1:B:262:GLU:N	2.17	0.59
1:B:574:GLY:O	1:B:575:TYR:HB2	2.02	0.59
1:A:220:SER:HB3	1:A:263:PRO:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:ARG:CZ	1:A:521:GLN:O	2.51	0.59
1:A:540:ILE:HG13	1:A:582:VAL:HG22	1.84	0.59
1:A:661:ILE:N	1:A:661:ILE:HD12	2.17	0.59
1:C:221:ILE:CD1	1:C:221:ILE:N	2.62	0.59
1:C:304:ASN:O	1:C:305:SER:C	2.44	0.59
1:C:535:ILE:HD12	1:C:546:LYS:HZ3	1.66	0.59
1:A:392:THR:O	1:A:409:THR:HG23	2.01	0.59
1:A:461:THR:O	1:A:461:THR:HG23	2.03	0.59
1:C:236:VAL:CG2	1:C:286:SER:HB2	2.29	0.59
1:A:256:PHE:HE1	1:A:264:VAL:HG23	1.67	0.59
1:A:411:TYR:HD1	1:A:418:ASP:HB3	1.67	0.59
1:A:573:LEU:HG	1:A:580:ILE:HG23	1.84	0.59
1:B:184:GLN:HG3	1:B:292:TYR:O	2.02	0.59
1:B:210:ALA:HB3	1:B:324:LEU:H	1.66	0.59
1:B:237:PRO:CD	1:B:240:ILE:HD11	2.32	0.59
1:B:395:ILE:C	1:B:521:GLN:HG3	2.28	0.59
1:B:449:GLU:HB3	1:B:452:GLU:HG2	1.84	0.59
1:A:222:SER:C	1:A:308:CYS:SG	2.86	0.59
1:A:457:ILE:CG1	1:A:460:ASN:HD22	2.16	0.59
1:C:474:ARG:HD3	1:C:523:SER:O	2.03	0.59
1:A:359:THR:CG2	1:A:568:ARG:HG2	2.32	0.59
1:B:398:LYS:NZ	1:B:398:LYS:H	2.00	0.59
1:A:167:GLU:HA	1:A:316:PRO:HG2	1.85	0.59
1:A:193:LEU:HG	1:A:194:GLY:N	2.16	0.59
1:B:260:GLN:NE2	1:C:129:SER:HA	2.18	0.59
1:C:288:VAL:HG12	1:C:289:ILE:N	2.17	0.59
1:C:361:PHE:CE1	1:C:619:PHE:HZ	2.20	0.59
1:A:179:SER:N	1:A:182:GLU:OE1	2.34	0.58
1:A:193:LEU:HD12	1:A:197:LEU:HD11	1.85	0.58
1:A:472:LEU:CD2	1:A:473:GLN:HG2	2.33	0.58
1:B:214:SER:O	1:B:215:ILE:HD13	2.02	0.58
1:B:453:SER:O	1:B:456:ILE:HG22	2.02	0.58
1:B:469:CYS:HB2	1:B:527:LEU:HB3	1.86	0.58
1:C:220:SER:HB3	1:C:263:PRO:HA	1.85	0.58
1:A:231:LEU:HD12	1:A:291:ILE:HA	1.84	0.58
1:A:255:LEU:H	1:A:255:LEU:HD12	1.67	0.58
1:A:333:THR:CG2	1:C:239:GLY:HA2	2.33	0.58
1:C:187:ILE:CG1	1:C:244:GLN:HG2	2.32	0.58
1:B:491:THR:O	1:B:497:LEU:HA	2.03	0.58
1:C:221:ILE:HG22	1:C:310:VAL:HG13	1.85	0.58
1:A:180:THR:HG23	1:A:306:SER:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:SER:HA	1:C:243:ILE:HD11	1.85	0.58
1:A:377:ASN:HB2	1:A:379:GLU:HG3	1.84	0.58
1:A:415:GLY:HA3	1:A:505:GLN:HG3	1.85	0.58
1:A:474:ARG:HH21	1:A:523:SER:CB	1.96	0.58
1:A:587:ILE:O	1:A:590:THR:HB	2.04	0.58
1:B:146:PRO:HB2	1:B:149:GLN:OE1	2.03	0.58
1:B:194:GLY:HA2	1:B:211:TRP:CH2	2.39	0.58
1:B:395:ILE:CG1	1:B:396:SER:H	1.94	0.58
1:B:412:ILE:H	1:B:412:ILE:CD1	2.16	0.58
1:B:218:ARG:HD3	1:B:265:ILE:HG12	1.86	0.58
1:C:187:ILE:H	1:C:244:GLN:HE21	1.51	0.58
1:C:221:ILE:CG2	1:C:310:VAL:HG22	2.32	0.58
1:B:146:PRO:O	1:B:149:GLN:CG	2.49	0.58
1:B:438:THR:HG23	1:B:457:ILE:CG2	2.32	0.58
1:C:661:ILE:H	1:C:661:ILE:HD13	1.68	0.58
1:B:440:GLN:OE1	1:B:455:MET:HE3	2.04	0.58
1:C:349:TRP:CB	1:C:358:ILE:HD13	2.29	0.58
1:B:178:TRP:CE2	1:B:295:LEU:HB2	2.39	0.58
1:B:439:ASN:ND2	1:B:443:ASN:HD21	1.96	0.58
1:C:404:GLY:HA2	1:C:510:ILE:HG12	1.84	0.58
1:C:474:ARG:N	1:C:524:ASP:HA	2.13	0.58
1:A:391:ILE:N	1:A:391:ILE:HD12	2.19	0.58
1:A:408:ALA:HB1	1:A:411:TYR:HD2	1.69	0.58
1:A:433:GLY:HA3	1:A:462:ASN:ND2	2.19	0.58
1:B:146:PRO:O	1:B:149:GLN:NE2	2.37	0.58
1:B:455:MET:HG2	1:B:455:MET:O	2.04	0.58
1:C:399:GLU:HB2	1:C:519:ASP:OD1	2.04	0.58
1:B:233:ALA:O	1:B:234:ILE:HG23	2.04	0.57
1:B:446:GLN:HE21	1:B:447:THR:HG23	1.64	0.57
1:B:503:ILE:O	1:B:503:ILE:HG13	2.02	0.57
1:C:482:SER:O	1:C:483:ASN:CB	2.52	0.57
1:A:353:ARG:N	1:A:584:ASN:ND2	2.49	0.57
1:A:377:ASN:HB3	1:C:559:ARG:HD3	1.85	0.57
1:A:457:ILE:HD11	1:A:460:ASN:ND2	2.19	0.57
1:B:237:PRO:HB2	1:C:324:LEU:HD13	1.86	0.57
1:B:611:ILE:HD12	1:B:611:ILE:H	1.67	0.57
1:C:214:SER:HB3	1:C:269:PRO:HA	1.86	0.57
1:C:257:ASP:OD1	1:C:258:ALA:N	2.37	0.57
1:C:484:THR:HG23	1:C:485:ALA:H	1.69	0.57
1:A:438:THR:CG2	1:A:459:ASN:H	2.17	0.57
1:B:396:SER:HA	1:B:521:GLN:NE2	1.99	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:ALA:HA	1:C:322:PHE:CE2	2.39	0.57
1:C:580:ILE:HD12	1:C:581:ASP:N	2.20	0.57
1:A:187:ILE:HD11	1:A:244:GLN:HA	1.85	0.57
1:B:214:SER:H	1:B:319:ASP:CG	2.12	0.57
1:B:480:LYS:O	1:B:481:VAL:HG12	2.03	0.57
1:C:249:LEU:C	1:C:251:TYR:H	2.13	0.57
1:C:368:PHE:HB3	1:C:544:ARG:NH1	2.19	0.57
1:C:439:ASN:CB	1:C:457:ILE:HG12	2.34	0.57
1:C:517:ASN:C	1:C:519:ASP:N	2.61	0.57
1:B:591:SER:HA	1:B:594:LEU:HD12	1.85	0.57
1:B:633:VAL:HG12	1:B:634:SER:H	1.69	0.57
1:C:297:ASN:C	1:C:297:ASN:ND2	2.59	0.57
1:A:194:GLY:HA2	1:A:211:TRP:CZ2	2.40	0.57
1:A:349:TRP:C	1:A:350:ILE:HG23	2.30	0.57
1:A:532:TYR:HB2	1:A:571:MET:HE3	1.86	0.57
1:B:472:LEU:HD22	1:B:473:GLN:H	1.66	0.57
1:C:408:ALA:HB1	1:C:411:TYR:HD2	1.70	0.57
1:C:416:ILE:CD1	1:C:503:ILE:HG12	2.29	0.57
1:C:481:VAL:O	1:C:482:SER:C	2.47	0.57
1:C:591:SER:HA	1:C:594:LEU:HD12	1.86	0.57
1:A:189:PHE:HB3	1:A:289:ILE:HD12	1.86	0.57
1:A:459:ASN:O	1:A:460:ASN:HB2	2.04	0.57
1:A:474:ARG:O	1:A:524:ASP:HB2	2.05	0.57
1:A:550:ILE:HD13	1:A:550:ILE:C	2.29	0.57
1:A:609:TYR:CE1	1:A:647:TYR:HB3	2.40	0.57
1:C:659:SER:OG	1:C:661:ILE:HD12	2.04	0.57
1:A:183:THR:HA	1:A:294:ASP:OD1	2.05	0.57
1:A:412:ILE:HD12	1:A:413:VAL:HG23	1.86	0.57
1:B:407:VAL:HG13	1:B:408:ALA:N	2.19	0.57
1:B:439:ASN:ND2	1:B:456:ILE:CG1	2.68	0.57
1:B:655:ILE:HD12	1:B:655:ILE:O	2.05	0.57
1:B:344:LYS:NZ	1:B:647:TYR:OH	2.37	0.57
1:B:449:GLU:HB2	1:B:452:GLU:CD	2.30	0.57
1:C:240:ILE:O	1:C:240:ILE:HG13	2.03	0.57
1:C:399:GLU:CG	1:C:519:ASP:HA	2.33	0.57
1:A:297:ASN:HD22	1:A:298:PRO:HD2	1.70	0.56
1:A:333:THR:HG22	1:C:239:GLY:CA	2.34	0.56
1:C:602:SER:C	1:C:604:ASP:H	2.13	0.56
1:A:325:LEU:HD12	1:A:325:LEU:H	1.70	0.56
1:A:360:ASP:HB2	1:A:568:ARG:CD	2.36	0.56
1:A:405:ILE:HG23	1:A:510:ILE:HG23	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:MET:HB2	1:A:582:VAL:HG23	1.88	0.56
1:B:153:ALA:O	1:B:156:MET:HB2	2.06	0.56
1:B:394:THR:CG2	1:B:522:THR:HG23	2.32	0.56
1:B:588:LEU:C	1:B:590:THR:H	2.11	0.56
1:C:352:ASN:HB3	1:C:586:GLN:O	2.04	0.56
1:C:391:ILE:HD12	1:C:391:ILE:H	1.66	0.56
1:A:436:ALA:HB2	1:A:462:ASN:HB2	1.87	0.56
1:A:567:TYR:CE1	1:A:586:GLN:HA	2.40	0.56
1:C:189:PHE:CD1	1:C:289:ILE:HB	2.38	0.56
1:C:453:SER:O	1:C:456:ILE:O	2.24	0.56
1:A:397:GLN:NE2	1:A:520:VAL:HG23	2.18	0.56
1:B:411:TYR:CD1	1:B:418:ASP:HB2	2.41	0.56
1:B:423:THR:HA	1:B:546:LYS:O	2.05	0.56
1:B:453:SER:CB	1:B:456:ILE:CG1	2.84	0.56
1:B:454:ALA:C	1:B:456:ILE:H	2.14	0.56
1:B:487:ILE:HG22	1:B:510:ILE:HG22	1.88	0.56
1:A:297:ASN:HD22	1:A:298:PRO:CD	2.18	0.56
1:A:405:ILE:HG13	1:A:508:ILE:O	2.06	0.56
1:B:554:PRO:HB2	1:B:628:PHE:HZ	1.71	0.56
1:B:652:LEU:HD23	1:B:654:LYS:HD3	1.87	0.56
1:C:176:VAL:HG12	1:C:177:ASN:N	2.20	0.56
1:C:199:PRO:O	1:C:202:THR:HG22	2.06	0.56
1:C:424:THR:HG22	1:C:425:ILE:N	2.20	0.56
1:C:533:THR:O	1:C:535:ILE:HG23	2.05	0.56
1:C:641:PHE:C	1:C:643:LEU:H	2.14	0.56
1:A:256:PHE:CE1	1:A:264:VAL:HG23	2.41	0.56
1:B:179:SER:OG	1:B:180:THR:N	2.37	0.56
1:B:370:ALA:HB2	1:B:554:PRO:CD	2.35	0.56
1:B:391:ILE:HG22	1:B:391:ILE:O	2.06	0.56
1:B:600:LEU:HD13	1:B:600:LEU:C	2.30	0.56
1:C:272:ARG:HD2	1:C:274:THR:O	2.04	0.56
1:C:403:LEU:CD2	1:C:514:ASN:HD21	2.18	0.56
1:A:397:GLN:HE22	1:A:520:VAL:CG2	2.18	0.56
1:B:620:ASP:C	1:B:621:ILE:HD12	2.31	0.56
1:C:474:ARG:O	1:C:475:ALA:HB2	2.06	0.56
1:A:589:HIS:CD2	1:A:593:GLN:HE21	2.24	0.56
1:A:612:ILE:HG22	1:A:618:TRP:CB	2.36	0.56
1:B:192:SER:HA	1:B:286:SER:CB	2.31	0.56
1:B:353:ARG:N	1:B:584:ASN:ND2	2.46	0.56
1:C:439:ASN:ND2	1:C:440:GLN:HE22	2.03	0.56
1:A:405:ILE:HG21	1:A:509:ALA:C	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:THR:HG22	1:B:489:THR:O	2.06	0.56
1:B:449:GLU:CB	1:B:452:GLU:CG	2.84	0.56
1:B:573:LEU:HD12	1:B:579:SER:OG	2.05	0.56
1:C:236:VAL:HB	1:C:240:ILE:HD11	1.87	0.56
1:C:339:CYS:HB3	1:C:647:TYR:HB2	1.87	0.56
1:A:474:ARG:NH1	1:A:520:VAL:O	2.38	0.55
1:C:221:ILE:HG22	1:C:310:VAL:CG2	2.33	0.55
1:C:427:ASN:HB3	1:C:429:LEU:CD2	2.35	0.55
1:A:399:GLU:O	1:A:516:VAL:HG11	2.05	0.55
1:A:422:ASP:O	1:A:548:VAL:HG23	2.06	0.55
1:B:327:PRO:HG2	1:B:330:SER:CB	2.36	0.55
1:B:453:SER:HB2	1:B:456:ILE:HG12	1.87	0.55
1:A:189:PHE:HB3	1:A:289:ILE:HD13	1.89	0.55
1:A:428:GLU:CG	1:A:499:PRO:HD2	2.36	0.55
1:B:255:LEU:HB2	1:C:131:THR:CG2	2.32	0.55
1:B:436:ALA:HB3	1:B:461:THR:CA	2.12	0.55
1:C:610:ARG:HH21	1:C:648:MET:CE	2.18	0.55
1:A:251:TYR:CD2	1:A:252:PRO:HD2	2.42	0.55
1:A:579:SER:O	1:A:580:ILE:HG13	2.06	0.55
1:B:354:PHE:O	1:B:356:SER:N	2.40	0.55
1:B:407:VAL:HG22	1:B:408:ALA:H	1.71	0.55
1:C:578:LYS:C	1:C:579:SER:OG	2.49	0.55
1:A:191:GLN:HE21	1:A:192:SER:H	1.54	0.55
1:B:148:VAL:HG23	1:B:149:GLN:NE2	2.21	0.55
1:A:216:GLU:HG2	1:A:267:THR:HG23	1.87	0.55
1:A:571:MET:HB2	1:A:582:VAL:CG2	2.37	0.55
1:B:168:ALA:HA	1:B:315:LYS:NZ	2.22	0.55
1:B:393:VAL:HG23	1:B:407:VAL:O	2.06	0.55
1:B:393:VAL:CA	1:B:409:THR:HG21	2.29	0.55
1:B:525:ASP:O	1:B:526:THR:C	2.49	0.55
1:A:391:ILE:O	1:A:527:LEU:HD12	2.06	0.55
1:A:469:CYS:O	1:A:485:ALA:HB1	2.05	0.55
1:A:636:ILE:HD13	1:A:636:ILE:H	1.72	0.55
1:C:184:GLN:HG3	1:C:292:TYR:O	2.07	0.55
1:C:337:VAL:CG1	1:C:338:PRO:HD2	2.37	0.55
1:C:398:LYS:H	1:C:403:LEU:CD2	2.20	0.55
1:C:401:GLU:OE1	1:C:402:MET:N	2.38	0.55
1:C:441:SER:C	1:C:443:ASN:H	2.15	0.55
1:C:612:ILE:HG13	1:C:612:ILE:O	2.06	0.55
1:A:430:ILE:HG22	1:A:495:ASN:O	2.07	0.55
1:B:397:GLN:HE21	1:B:514:ASN:ND2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:517:ASN:CG	1:B:518:ARG:N	2.64	0.55
1:C:403:LEU:HD21	1:C:514:ASN:HD21	1.71	0.55
1:C:470:GLY:H	1:C:530:LEU:CD1	2.20	0.55
1:B:431:PRO:HB3	1:B:511:PHE:CZ	2.42	0.55
1:C:234:ILE:HD12	1:C:234:ILE:O	2.07	0.55
1:A:193:LEU:CD1	1:A:215:ILE:HD12	2.37	0.55
1:A:343:PRO:C	1:A:345:SER:H	2.15	0.55
1:B:174:THR:HG22	1:B:175:SER:N	2.18	0.55
1:B:349:TRP:HB3	1:B:358:ILE:HG23	1.89	0.55
1:B:438:THR:OG1	1:B:460:ASN:O	2.24	0.55
1:C:411:TYR:CD1	1:C:418:ASP:HB3	2.42	0.55
1:C:451:TYR:CD1	1:C:458:SER:N	2.72	0.55
1:C:482:SER:OG	1:C:483:ASN:N	2.39	0.55
1:A:173:HIS:O	1:A:174:THR:HB	2.06	0.54
1:A:375:ASP:CG	1:A:376:PHE:N	2.65	0.54
1:A:528:ALA:O	1:A:530:LEU:CD1	2.55	0.54
1:C:132:THR:HB	1:C:133:PRO:HD2	1.88	0.54
1:C:443:ASN:ND2	1:C:446:GLN:HB3	2.22	0.54
1:C:451:TYR:CD1	1:C:457:ILE:CB	2.77	0.54
1:C:465:SER:HA	1:C:532:TYR:CZ	2.41	0.54
1:C:566:PHE:CD2	1:C:583:PHE:HB3	2.42	0.54
1:A:488:THR:H	1:A:509:ALA:HB3	1.72	0.54
1:A:601:LEU:HD21	1:A:605:SER:O	2.06	0.54
1:A:603:PRO:HG2	1:A:604:ASP:H	1.71	0.54
1:B:217:VAL:HG21	1:B:268:ILE:HD11	1.89	0.54
1:B:608:VAL:HG12	1:B:609:TYR:N	2.22	0.54
1:C:237:PRO:O	1:C:240:ILE:HG12	2.08	0.54
1:C:395:ILE:HD13	1:C:403:LEU:HD11	1.89	0.54
1:A:151:SER:O	1:A:152:ALA:CB	2.55	0.54
1:C:221:ILE:HD13	1:C:221:ILE:N	2.10	0.54
1:C:349:TRP:C	1:C:350:ILE:HG12	2.32	0.54
1:A:472:LEU:O	1:A:473:GLN:CB	2.55	0.54
1:B:339:CYS:SG	1:B:649:GLY:HA2	2.46	0.54
1:A:210:ALA:HB2	1:A:278:LEU:HA	1.88	0.54
1:A:236:VAL:HB	1:A:240:ILE:CD1	2.37	0.54
1:A:573:LEU:HD21	1:A:580:ILE:HG21	1.88	0.54
1:B:180:THR:HG22	1:B:295:LEU:O	2.08	0.54
1:C:285:THR:HG22	1:C:286:SER:N	2.21	0.54
1:C:397:GLN:HG2	1:C:523:SER:CB	2.36	0.54
1:B:354:PHE:C	1:B:356:SER:N	2.61	0.54
1:C:216:GLU:HA	1:C:267:THR:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:451:TYR:O	1:C:456:ILE:O	2.24	0.54
1:A:469:CYS:HB2	1:A:485:ALA:HB1	1.89	0.54
1:A:550:ILE:HG23	1:A:551:GLY:N	2.22	0.54
1:A:565:ILE:HD12	1:A:565:ILE:C	2.33	0.54
1:A:598:ASN:HB2	1:C:654:LYS:HG3	1.90	0.54
1:C:448:LYS:NZ	1:C:537:GLU:OE2	2.40	0.54
1:A:148:VAL:HG13	1:A:149:GLN:N	2.23	0.54
1:A:383:TRP:HB2	1:A:413:VAL:HG21	1.88	0.54
1:A:479:LYS:C	1:A:480:LYS:HG3	2.32	0.54
1:B:473:GLN:HE21	1:B:474:ARG:C	2.15	0.54
1:C:392:THR:O	1:C:409:THR:HG22	2.08	0.54
1:B:565:ILE:HG12	1:B:629:SER:O	2.08	0.54
1:C:501:ASN:O	1:C:548:VAL:HG13	2.08	0.54
1:A:335:GLY:HA3	1:A:600:LEU:N	2.23	0.53
1:B:239:GLY:HA2	1:C:333:THR:HG22	1.88	0.53
1:B:240:ILE:HB	1:C:330:SER:OG	2.08	0.53
1:B:398:LYS:HG2	1:B:399:GLU:H	1.72	0.53
1:A:392:THR:HA	1:A:526:THR:HA	1.90	0.53
1:B:339:CYS:SG	1:B:647:TYR:HB2	2.48	0.53
1:B:569:ASN:HD22	1:B:570:SER:H	1.56	0.53
1:C:228:GLY:O	1:C:296:ILE:HG13	2.08	0.53
1:B:438:THR:HG23	1:B:457:ILE:HG22	1.90	0.53
1:B:625:SER:O	1:B:626:ASP:C	2.52	0.53
1:A:234:ILE:O	1:A:288:VAL:HG23	2.08	0.53
1:C:426:PRO:O	1:C:427:ASN:HB2	2.08	0.53
1:C:439:ASN:HB3	1:C:457:ILE:HG12	1.91	0.53
1:A:661:ILE:HD12	1:A:661:ILE:H	1.73	0.53
1:B:333:THR:HG23	1:B:334:HIS:N	2.24	0.53
1:B:360:ASP:OD2	1:B:360:ASP:N	2.41	0.53
1:B:624:ASP:O	1:B:625:SER:C	2.51	0.53
1:C:398:LYS:HB2	1:C:403:LEU:HB3	1.91	0.53
1:C:469:CYS:O	1:C:485:ALA:HB3	2.08	0.53
1:A:481:VAL:HG13	1:A:481:VAL:O	2.07	0.53
1:B:553:LEU:CD1	1:B:554:PRO:HD2	2.38	0.53
1:B:621:ILE:HA	1:B:630:PHE:O	2.08	0.53
1:B:641:PHE:O	1:B:643:LEU:HG	2.09	0.53
1:B:200:TYR:O	1:B:201:LEU:C	2.52	0.53
1:B:234:ILE:O	1:B:287:LEU:HD12	2.09	0.53
1:C:358:ILE:HG22	1:C:359:THR:N	2.24	0.53
1:C:433:GLY:O	1:C:434:ASP:O	2.26	0.53
1:C:469:CYS:HA	1:C:530:LEU:HD13	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:550:ILE:O	1:C:550:ILE:CD1	2.48	0.53
1:C:641:PHE:N	1:C:642:PRO:HD3	2.23	0.53
1:A:339:CYS:O	1:A:340:ASP:HB3	2.08	0.53
1:A:484:THR:HG21	1:A:512:GLN:NE2	2.24	0.53
1:B:512:GLN:CD	1:B:513:ASP:H	2.16	0.53
1:C:187:ILE:HG21	1:C:190:LYS:HG3	1.91	0.53
1:C:367:VAL:HG22	1:C:566:PHE:CE1	2.44	0.53
1:A:612:ILE:HG22	1:A:618:TRP:HB3	1.91	0.53
1:B:368:PHE:HA	1:B:554:PRO:O	2.09	0.53
1:C:448:LYS:HE3	1:C:537:GLU:CD	2.33	0.53
1:A:209:VAL:O	1:A:279:MET:HG2	2.09	0.53
1:A:443:ASN:OD1	1:A:443:ASN:O	2.27	0.53
1:B:198:ASN:HB3	1:B:201:LEU:HD12	1.90	0.53
1:B:199:PRO:O	1:B:202:THR:HB	2.09	0.53
1:C:142:VAL:HG12	1:C:143:ILE:HD13	1.91	0.53
1:C:353:ARG:HH12	1:C:541:GLY:HA3	1.74	0.53
1:C:404:GLY:O	1:C:405:ILE:HD12	2.09	0.53
1:A:178:TRP:CZ3	1:A:231:LEU:HD22	2.44	0.52
1:A:477:GLY:HA3	1:A:520:VAL:HG21	1.91	0.52
1:B:426:PRO:HB3	1:B:546:LYS:HE2	1.92	0.52
1:B:457:ILE:HG23	1:B:459:ASN:H	1.73	0.52
1:A:130:ILE:HA	1:C:260:GLN:OE1	2.09	0.52
1:A:228:GLY:O	1:A:295:LEU:HD12	2.08	0.52
1:A:438:THR:CG2	1:A:459:ASN:N	2.72	0.52
1:A:506:THR:C	1:A:507:LYS:HD2	2.31	0.52
1:B:476:TRP:NE1	1:B:520:VAL:HB	2.23	0.52
1:B:571:MET:O	1:B:579:SER:O	2.26	0.52
1:C:590:THR:O	1:C:591:SER:C	2.51	0.52
1:A:397:GLN:HA	1:A:403:LEU:HD13	1.92	0.52
1:A:498:ILE:O	1:A:498:ILE:HD12	2.10	0.52
1:B:325:LEU:HD23	1:B:325:LEU:C	2.34	0.52
1:B:607:ALA:O	1:B:623:ILE:HD12	2.09	0.52
1:C:143:ILE:HD13	1:C:143:ILE:N	2.24	0.52
1:C:402:MET:SD	1:C:402:MET:C	2.92	0.52
1:B:327:PRO:O	1:B:327:PRO:HG2	2.10	0.52
1:B:332:LEU:HB3	1:B:335:GLY:O	2.09	0.52
1:C:337:VAL:HG13	1:C:338:PRO:HD2	1.91	0.52
1:C:509:ALA:C	1:C:510:ILE:HG23	2.34	0.52
1:C:540:ILE:O	1:C:582:VAL:HG13	2.09	0.52
1:A:325:LEU:HD12	1:A:325:LEU:N	2.24	0.52
1:A:342:ILE:HG23	1:A:609:TYR:CE2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:ALA:HB3	1:A:461:THR:HA	1.90	0.52
1:C:204:LEU:HD23	1:C:204:LEU:C	2.34	0.52
1:C:209:VAL:HG23	1:C:324:LEU:HB3	1.91	0.52
1:C:612:ILE:HG22	1:C:618:TRP:CB	2.39	0.52
1:A:155:ASP:O	1:A:156:MET:C	2.53	0.52
1:C:450:GLU:O	1:C:451:TYR:CB	2.57	0.52
1:A:476:TRP:HD1	1:A:520:VAL:HB	1.72	0.52
1:A:576:VAL:HG12	1:A:577:ILE:N	2.24	0.52
1:B:209:VAL:O	1:B:278:LEU:HA	2.09	0.52
1:B:394:THR:O	1:B:406:GLY:HA2	2.10	0.52
1:B:395:ILE:CG2	1:B:521:GLN:HB2	2.38	0.52
1:C:197:LEU:HD12	1:C:215:ILE:HD13	1.90	0.52
1:C:334:HIS:HB3	1:C:600:LEU:CD1	2.38	0.52
1:C:368:PHE:HB3	1:C:544:ARG:HH12	1.74	0.52
1:C:398:LYS:O	1:C:399:GLU:HB3	2.09	0.52
1:C:427:ASN:HB3	1:C:429:LEU:HD21	1.92	0.52
1:C:469:CYS:HB2	1:C:528:ALA:O	2.10	0.52
1:C:484:THR:HG21	1:C:512:GLN:HA	1.92	0.52
1:A:149:GLN:HA	1:A:153:ALA:CB	2.40	0.52
1:A:240:ILE:HG22	1:B:332:LEU:HA	1.91	0.52
1:A:297:ASN:ND2	1:A:298:PRO:CD	2.72	0.52
1:A:461:THR:HG21	1:A:533:THR:HG22	1.92	0.52
1:B:374:PHE:H	1:B:586:GLN:NE2	2.06	0.52
1:B:610:ARG:NH2	1:B:618:TRP:CH2	2.78	0.52
1:A:193:LEU:HD11	1:A:215:ILE:HD12	1.91	0.52
1:B:249:LEU:C	1:B:251:TYR:H	2.17	0.52
1:B:611:ILE:HD11	1:B:621:ILE:HD13	1.91	0.52
1:A:130:ILE:O	1:A:131:THR:HG23	2.10	0.52
1:B:426:PRO:HD3	1:B:465:SER:OG	2.10	0.52
1:B:432:ALA:HB3	1:B:462:ASN:CB	2.40	0.52
1:B:481:VAL:O	1:B:481:VAL:HG13	2.10	0.52
1:C:216:GLU:HG2	1:C:267:THR:HG22	1.91	0.52
1:A:230:LYS:HD2	1:A:293:ASN:HD22	1.75	0.51
1:A:491:THR:HG22	1:A:498:ILE:HG13	1.92	0.51
1:B:402:MET:HE2	1:B:512:GLN:H	1.74	0.51
1:C:221:ILE:HD13	1:C:221:ILE:O	2.09	0.51
1:C:460:ASN:CG	1:C:461:THR:H	2.19	0.51
1:A:214:SER:OG	1:A:269:PRO:HA	2.10	0.51
1:A:571:MET:HG3	1:A:582:VAL:HG21	1.92	0.51
1:B:187:ILE:HB	1:B:244:GLN:NE2	2.24	0.51
1:B:487:ILE:HG21	1:B:510:ILE:HG22	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:LEU:HD22	1:C:320:PHE:CE2	2.43	0.51
1:C:282:THR:HB	1:C:650:ASN:HD21	1.75	0.51
1:C:299:TYR:O	1:C:300:ALA:O	2.29	0.51
1:A:327:PRO:HG2	1:A:330:SER:HG	1.74	0.51
1:A:393:VAL:HG12	1:A:394:THR:O	2.09	0.51
1:A:439:ASN:HD22	1:A:456:ILE:CG1	2.23	0.51
1:B:292:TYR:HD2	1:B:293:ASN:ND2	2.09	0.51
1:C:144:ALA:HB1	1:C:147:SER:CB	2.34	0.51
1:C:217:VAL:HG12	1:C:219:PHE:CD2	2.45	0.51
1:C:540:ILE:HD12	1:C:582:VAL:HG21	1.91	0.51
1:C:593:GLN:O	1:C:594:LEU:C	2.54	0.51
1:C:608:VAL:O	1:C:609:TYR:HD1	1.94	0.51
1:A:145:GLU:H	1:A:146:PRO:CD	2.24	0.51
1:A:641:PHE:O	1:A:643:LEU:N	2.44	0.51
1:B:146:PRO:HB2	1:B:149:GLN:NE2	2.26	0.51
1:B:164:SER:C	1:B:166:TRP:H	2.18	0.51
1:B:349:TRP:HB3	1:B:358:ILE:HG21	1.92	0.51
1:B:393:VAL:HA	1:B:409:THR:CG2	2.29	0.51
1:C:148:VAL:O	1:C:150:MET:N	2.44	0.51
1:C:397:GLN:CB	1:C:520:VAL:O	2.59	0.51
1:C:437:ILE:HD11	1:C:457:ILE:CD1	2.40	0.51
1:A:504:ASP:O	1:A:507:LYS:HB2	2.10	0.51
1:B:155:ASP:O	1:B:158:THR:N	2.38	0.51
1:B:247:SER:O	1:B:250:GLN:HB2	2.11	0.51
1:B:377:ASN:C	1:B:379:GLU:H	2.19	0.51
1:B:411:TYR:CD1	1:B:418:ASP:N	2.73	0.51
1:B:449:GLU:HB3	1:B:452:GLU:CG	2.40	0.51
1:C:150:MET:O	1:C:152:ALA:N	2.44	0.51
1:C:198:ASN:O	1:C:202:THR:HB	2.11	0.51
1:C:488:THR:OG1	1:C:489:THR:N	2.44	0.51
1:A:209:VAL:HG23	1:A:210:ALA:N	2.25	0.51
1:A:287:LEU:HG	1:A:288:VAL:H	1.73	0.51
1:A:478:ASN:O	1:A:479:LYS:O	2.29	0.51
1:A:540:ILE:CG1	1:A:582:VAL:HG22	2.39	0.51
1:B:363:ILE:O	1:B:364:ARG:HD3	2.11	0.51
1:B:449:GLU:HB2	1:B:452:GLU:CG	2.41	0.51
1:B:521:GLN:C	1:B:523:SER:N	2.66	0.51
1:C:214:SER:HB2	1:C:268:ILE:O	2.11	0.51
1:A:335:GLY:HA3	1:A:600:LEU:HB2	1.92	0.51
1:A:448:LYS:O	1:A:449:GLU:HB3	2.11	0.51
1:A:471:SER:HB2	1:A:485:ALA:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:405:ILE:HA	1:B:508:ILE:O	2.11	0.51
1:B:647:TYR:N	1:B:647:TYR:CD1	2.78	0.51
1:C:463:PHE:O	1:C:466:MET:CG	2.59	0.51
1:C:466:MET:O	1:C:532:TYR:HA	2.11	0.51
1:B:288:VAL:HG12	1:B:289:ILE:N	2.26	0.51
1:B:539:ALA:HB3	1:B:583:PHE:HE1	1.75	0.51
1:C:452:GLU:HB2	1:C:456:ILE:CD1	2.40	0.51
1:C:622:GLY:O	1:C:623:ILE:HD13	2.11	0.51
1:A:219:PHE:C	1:A:219:PHE:CD2	2.82	0.51
1:A:287:LEU:HD23	1:A:287:LEU:C	2.36	0.51
1:A:422:ASP:C	1:A:548:VAL:HG23	2.36	0.51
1:C:228:GLY:HA3	1:C:296:ILE:HD11	1.93	0.51
1:C:402:MET:SD	1:C:403:LEU:N	2.84	0.51
1:A:227:PHE:HE1	1:A:308:CYS:HB2	1.76	0.51
1:B:150:MET:O	1:B:153:ALA:HB3	2.11	0.51
1:C:383:TRP:HA	1:C:413:VAL:HG11	1.92	0.51
1:A:149:GLN:C	1:A:153:ALA:HB3	2.36	0.50
1:A:526:THR:O	1:A:527:LEU:HG	2.11	0.50
1:B:288:VAL:C	1:B:289:ILE:HD12	2.36	0.50
1:A:359:THR:O	1:A:641:PHE:CZ	2.64	0.50
1:A:363:ILE:HG22	1:A:565:ILE:HG22	1.93	0.50
1:A:393:VAL:HG22	1:A:411:TYR:HE2	1.76	0.50
1:A:399:GLU:HA	1:A:516:VAL:CG2	2.41	0.50
1:B:355:TRP:H	1:B:355:TRP:CD1	2.27	0.50
1:B:393:VAL:O	1:B:525:ASP:HB3	2.11	0.50
1:C:420:TRP:CG	1:C:421:PRO:HD2	2.46	0.50
1:C:440:GLN:HB3	1:C:443:ASN:HB3	1.91	0.50
1:A:157:ALA:O	1:A:158:THR:OG1	2.28	0.50
1:A:277:HIS:CD2	1:A:277:HIS:N	2.80	0.50
1:A:643:LEU:O	1:A:644:THR:HG23	2.11	0.50
1:C:293:ASN:O	1:C:294:ASP:O	2.29	0.50
1:C:393:VAL:HG13	1:C:407:VAL:O	2.12	0.50
1:A:369:GLN:N	1:A:553:LEU:HD11	2.26	0.50
1:A:438:THR:HB	1:A:456:ILE:HG22	1.92	0.50
1:A:439:ASN:OD1	1:A:440:GLN:HG3	2.12	0.50
1:B:521:GLN:C	1:B:523:SER:H	2.18	0.50
1:C:555:GLU:C	1:C:555:GLU:CD	2.79	0.50
1:A:133:PRO:CB	1:A:134:GLU:OE2	2.58	0.50
1:C:183:THR:O	1:C:291:ILE:HD11	2.11	0.50
1:C:484:THR:OG1	1:C:485:ALA:N	2.39	0.50
1:A:253:HIS:ND1	1:A:253:HIS:N	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:THR:HB	1:A:526:THR:HG22	1.93	0.50
1:B:190:LYS:HA	1:B:288:VAL:HG22	1.92	0.50
1:B:325:LEU:HD23	1:B:326:LYS:N	2.27	0.50
1:B:371:ASN:ND2	1:B:383:TRP:CZ2	2.80	0.50
1:A:166:TRP:HE1	1:A:200:TYR:HB3	1.77	0.50
1:A:474:ARG:O	1:A:475:ALA:HB2	2.10	0.50
1:A:474:ARG:HA	1:A:524:ASP:H	1.76	0.50
1:A:528:ALA:O	1:A:530:LEU:HD12	2.12	0.50
1:B:162:VAL:O	1:B:163:ASP:C	2.55	0.50
1:B:341:LEU:HG	1:B:609:TYR:HH	1.75	0.50
1:A:200:TYR:N	1:A:200:TYR:CD1	2.80	0.50
1:A:308:CYS:SG	1:A:309:ILE:N	2.84	0.50
1:A:359:THR:HG22	1:A:568:ARG:C	2.36	0.50
1:A:416:ILE:HG23	1:A:503:ILE:HD11	1.94	0.50
1:B:489:THR:HG21	1:B:548:VAL:HG21	1.93	0.50
1:C:193:LEU:HD12	1:C:215:ILE:HD12	1.94	0.50
1:A:246:THR:O	1:A:249:LEU:N	2.34	0.50
1:A:300:ALA:O	1:A:301:ASN:HB2	2.10	0.50
1:C:166:TRP:HA	1:C:169:PHE:HE2	1.77	0.50
1:C:196:LEU:HA	1:C:202:THR:OG1	2.12	0.50
1:C:439:ASN:ND2	1:C:440:GLN:NE2	2.60	0.50
1:C:647:TYR:CD1	1:C:647:TYR:N	2.78	0.50
1:A:292:TYR:O	1:A:292:TYR:HD1	1.93	0.49
1:A:333:THR:HG22	1:C:239:GLY:C	2.36	0.49
1:B:342:ILE:HD12	1:B:587:ILE:CD1	2.40	0.49
1:A:370:ALA:HB2	1:A:554:PRO:HD2	1.93	0.49
1:B:334:HIS:O	1:B:600:LEU:HB2	2.13	0.49
1:B:362:VAL:HG23	1:B:568:ARG:HB2	1.94	0.49
1:C:393:VAL:CG1	1:C:394:THR:N	2.74	0.49
1:A:133:PRO:C	1:A:134:GLU:CD	2.81	0.49
1:A:221:ILE:C	1:A:221:ILE:CD1	2.80	0.49
1:A:350:ILE:HD12	1:A:351:GLY:O	2.13	0.49
1:B:430:ILE:HG22	1:B:496:LYS:HA	1.94	0.49
1:C:633:VAL:HG12	1:C:635:SER:H	1.76	0.49
1:A:399:GLU:CG	1:A:516:VAL:HG21	2.29	0.49
1:A:509:ALA:O	1:A:510:ILE:HG23	2.12	0.49
1:A:580:ILE:HD12	1:A:580:ILE:O	2.12	0.49
1:B:201:LEU:HD21	1:B:316:PRO:HB3	1.94	0.49
1:B:358:ILE:CG1	1:B:359:THR:H	2.16	0.49
1:C:549:ARG:HD3	1:C:553:LEU:HD13	1.93	0.49
1:A:550:ILE:CG2	1:A:551:GLY:N	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:SER:C	1:B:153:ALA:N	2.71	0.49
1:B:310:VAL:O	1:B:310:VAL:CG1	2.57	0.49
1:A:191:GLN:NE2	1:A:192:SER:H	2.10	0.49
1:A:391:ILE:O	1:A:526:THR:HA	2.13	0.49
1:A:398:LYS:C	1:A:400:GLY:H	2.19	0.49
1:B:320:PHE:O	1:B:321:LYS:HB2	2.12	0.49
1:B:605:SER:HA	1:B:652:LEU:HA	1.94	0.49
1:C:162:VAL:CG1	1:C:164:SER:OG	2.60	0.49
1:C:358:ILE:HG22	1:C:360:ASP:H	1.77	0.49
1:A:200:TYR:HD1	1:A:200:TYR:H	1.60	0.49
1:A:243:ILE:O	1:A:245:SER:N	2.41	0.49
1:A:287:LEU:O	1:A:288:VAL:HG13	2.13	0.49
1:A:412:ILE:C	1:A:413:VAL:HG23	2.38	0.49
1:B:295:LEU:HD12	1:B:296:ILE:H	1.78	0.49
1:C:352:ASN:HD22	1:C:586:GLN:N	2.05	0.49
1:C:442:GLY:C	1:C:444:ASP:H	2.21	0.49
1:A:255:LEU:HD12	1:A:255:LEU:N	2.28	0.49
1:A:304:ASN:O	1:A:305:SER:C	2.55	0.49
1:A:352:ASN:N	1:A:584:ASN:HD22	2.10	0.49
1:B:187:ILE:HG21	1:B:190:LYS:HB2	1.95	0.49
1:B:393:VAL:HG23	1:B:409:THR:CG2	2.43	0.49
1:C:166:TRP:C	1:C:168:ALA:N	2.71	0.49
1:C:216:GLU:HG2	1:C:267:THR:CG2	2.42	0.49
1:C:436:ALA:HB1	1:C:461:THR:HA	1.93	0.49
1:C:506:THR:OG1	1:C:507:LYS:HD2	2.12	0.49
1:A:190:LYS:HG3	1:A:651:GLN:NE2	2.28	0.48
1:A:566:PHE:CD2	1:A:583:PHE:HB3	2.48	0.48
1:B:344:LYS:HE3	1:B:647:TYR:OH	2.13	0.48
1:B:402:MET:HA	1:B:402:MET:HE3	1.94	0.48
1:B:432:ALA:O	1:B:433:GLY:C	2.55	0.48
1:B:657:LEU:O	1:B:658:ALA:O	2.31	0.48
1:C:431:PRO:HD2	1:C:495:ASN:O	2.12	0.48
1:A:130:ILE:HD11	1:C:255:LEU:O	2.12	0.48
1:B:198:ASN:HB2	1:B:314:THR:HG1	1.78	0.48
1:B:521:GLN:HG2	1:B:522:THR:N	2.22	0.48
1:C:187:ILE:HG22	1:C:188:LEU:N	2.26	0.48
1:C:203:HIS:O	1:C:206:LYS:HB2	2.13	0.48
1:C:374:PHE:CZ	1:C:386:PRO:HD3	2.48	0.48
1:C:487:ILE:CG2	1:C:510:ILE:HG22	2.40	0.48
1:A:164:SER:HA	1:A:166:TRP:HE3	1.73	0.48
1:B:437:ILE:C	1:B:439:ASN:H	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:463:PHE:HB3	1:B:466:MET:CE	2.43	0.48
1:A:187:ILE:CD1	1:A:290:MET:HE3	2.44	0.48
1:A:222:SER:O	1:A:308:CYS:SG	2.71	0.48
1:A:565:ILE:HG21	1:A:631:VAL:HG23	1.95	0.48
1:B:287:LEU:C	1:B:288:VAL:HG23	2.38	0.48
1:C:424:THR:CG2	1:C:425:ILE:N	2.76	0.48
1:C:451:TYR:HB3	1:C:457:ILE:HA	1.96	0.48
1:C:526:THR:HG22	1:C:527:LEU:H	1.78	0.48
1:C:618:TRP:CE2	1:C:660:ASN:HB2	2.49	0.48
1:A:273:SER:HA	1:B:276:TYR:CE1	2.49	0.48
1:A:624:ASP:C	1:A:626:ASP:H	2.20	0.48
1:B:611:ILE:HD13	1:B:621:ILE:HD13	1.94	0.48
1:C:661:ILE:H	1:C:661:ILE:CD1	2.25	0.48
1:A:143:ILE:HG23	1:A:143:ILE:O	2.13	0.48
1:B:142:VAL:O	1:B:142:VAL:CG1	2.62	0.48
1:B:587:ILE:HB	1:B:590:THR:OG1	2.13	0.48
1:C:440:GLN:OE1	1:C:456:ILE:HA	2.14	0.48
1:B:273:SER:O	1:C:275:LEU:HG	2.14	0.48
1:B:588:LEU:O	1:B:590:THR:N	2.47	0.48
1:B:658:ALA:O	1:B:659:SER:HB3	2.12	0.48
1:C:270:ASP:OD2	1:C:272:ARG:NH1	2.47	0.48
1:C:395:ILE:HD13	1:C:403:LEU:HD13	1.94	0.48
1:A:417:PRO:HG2	1:A:508:ILE:HG21	1.95	0.48
1:A:464:LYS:HD2	1:A:535:ILE:HG22	1.96	0.48
1:B:405:ILE:HD13	1:B:405:ILE:N	2.29	0.48
1:C:162:VAL:C	1:C:164:SER:H	2.22	0.48
1:C:393:VAL:HG12	1:C:394:THR:N	2.27	0.48
1:C:437:ILE:O	1:C:438:THR:HB	2.13	0.48
1:A:145:GLU:N	1:A:146:PRO:HD2	2.28	0.48
1:B:297:ASN:OD1	1:B:297:ASN:C	2.57	0.48
1:B:425:ILE:HD13	1:B:425:ILE:H	1.79	0.48
1:B:607:ALA:HA	1:B:650:ASN:CB	2.44	0.48
1:C:396:SER:O	1:C:403:LEU:CD2	2.62	0.48
1:C:403:LEU:CG	1:C:514:ASN:HD21	2.27	0.48
1:A:613:ASP:HB3	1:A:643:LEU:HD23	1.96	0.48
1:A:621:ILE:HA	1:A:630:PHE:O	2.13	0.48
1:B:272:ARG:O	1:C:276:TYR:HE1	1.97	0.48
1:B:402:MET:HB3	1:B:403:LEU:H	1.29	0.48
1:B:562:ASN:OD1	1:B:657:LEU:HG	2.13	0.48
1:C:191:GLN:HE21	1:C:197:LEU:CD2	2.25	0.48
1:C:209:VAL:HG23	1:C:324:LEU:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:397:GLN:HA	1:C:403:LEU:HD21	1.96	0.48
1:A:354:PHE:H	1:A:584:ASN:HD21	1.62	0.47
1:B:153:ALA:O	1:B:154:ALA:C	2.56	0.47
1:B:422:ASP:O	1:B:423:THR:C	2.56	0.47
1:B:610:ARG:HA	1:B:620:ASP:OD1	2.14	0.47
1:C:298:PRO:HB2	1:C:299:TYR:CE1	2.49	0.47
1:C:332:LEU:CD2	1:C:334:HIS:H	2.26	0.47
1:C:346:SER:HB2	1:C:643:LEU:CB	2.42	0.47
1:A:456:ILE:C	1:A:458:SER:N	2.69	0.47
1:A:476:TRP:CZ3	1:A:522:THR:HB	2.49	0.47
1:A:613:ASP:CG	1:A:614:SER:H	2.21	0.47
1:B:226:VAL:CG1	1:B:298:PRO:HG2	2.35	0.47
1:B:373:HIS:HD2	1:B:585:SER:HB2	1.79	0.47
1:B:395:ILE:HG23	1:B:521:GLN:HB2	1.97	0.47
1:B:606:PHE:CE1	1:B:624:ASP:C	2.92	0.47
1:C:451:TYR:C	1:C:453:SER:H	2.22	0.47
1:C:465:SER:HA	1:C:532:TYR:CE1	2.48	0.47
1:A:342:ILE:O	1:A:342:ILE:HD13	2.14	0.47
1:A:359:THR:HG23	1:A:360:ASP:N	2.28	0.47
1:A:451:TYR:HA	1:A:452:GLU:CB	2.37	0.47
1:B:168:ALA:HA	1:B:315:LYS:HZ3	1.78	0.47
1:B:353:ARG:N	1:B:584:ASN:HD22	2.03	0.47
1:B:353:ARG:HG2	1:B:353:ARG:NH1	2.29	0.47
1:B:420:TRP:CG	1:B:421:PRO:HD2	2.49	0.47
1:C:437:ILE:HD13	1:C:439:ASN:HB2	1.94	0.47
1:A:292:TYR:CD1	1:A:292:TYR:C	2.91	0.47
1:B:233:ALA:C	1:B:234:ILE:HG23	2.40	0.47
1:B:453:SER:C	1:B:456:ILE:HB	2.39	0.47
1:C:438:THR:C	1:C:457:ILE:HG13	2.38	0.47
1:C:602:SER:O	1:C:604:ASP:N	2.47	0.47
1:A:439:ASN:CB	1:A:456:ILE:HG12	2.41	0.47
1:C:362:VAL:HB	1:C:566:PHE:HB2	1.96	0.47
1:C:451:TYR:CA	1:C:458:SER:HB2	2.45	0.47
1:A:187:ILE:HD13	1:A:187:ILE:N	2.29	0.47
1:A:253:HIS:H	1:A:253:HIS:HD1	1.62	0.47
1:A:553:LEU:HD12	1:A:554:PRO:HD2	1.95	0.47
1:A:576:VAL:HG12	1:A:577:ILE:H	1.80	0.47
1:B:349:TRP:O	1:B:358:ILE:HG23	2.15	0.47
1:B:366:PHE:HE2	1:C:414:PRO:HD3	1.79	0.47
1:B:628:PHE:N	1:B:628:PHE:CD1	2.83	0.47
1:C:609:TYR:CE1	1:C:647:TYR:HB3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:VAL:HG12	1:A:177:ASN:N	2.29	0.47
1:A:179:SER:C	1:A:181:SER:H	2.23	0.47
1:A:236:VAL:HB	1:A:240:ILE:HD11	1.96	0.47
1:A:333:THR:HA	1:C:652:LEU:HD11	1.97	0.47
1:A:376:PHE:HE2	1:A:601:LEU:HD22	1.80	0.47
1:A:416:ILE:CD1	1:A:503:ILE:HG12	2.35	0.47
1:A:423:THR:HB	1:A:467:TYR:CE1	2.47	0.47
1:A:466:MET:HB2	1:A:533:THR:OG1	2.14	0.47
1:B:354:PHE:CE2	1:B:571:MET:HG2	2.49	0.47
1:B:360:ASP:OD2	1:B:568:ARG:HB3	2.14	0.47
1:B:368:PHE:O	1:B:369:GLN:CB	2.62	0.47
1:B:398:LYS:H	1:B:398:LYS:CD	2.27	0.47
1:C:130:ILE:H	1:C:130:ILE:CD1	2.25	0.47
1:C:385:THR:O	1:C:387:ARG:N	2.40	0.47
1:C:451:TYR:H	1:C:458:SER:CB	2.18	0.47
1:C:540:ILE:HB	1:C:582:VAL:CG2	2.45	0.47
1:A:338:PRO:HA	1:A:599:TYR:CD2	2.50	0.47
1:A:439:ASN:HD22	1:A:456:ILE:HG12	1.79	0.47
1:B:239:GLY:O	1:C:332:LEU:HA	2.15	0.47
1:B:287:LEU:C	1:B:288:VAL:CG2	2.88	0.47
1:B:451:TYR:O	1:B:453:SER:N	2.44	0.47
1:B:533:THR:O	1:B:535:ILE:CG2	2.56	0.47
1:C:246:THR:O	1:C:248:MET:N	2.47	0.47
1:C:618:TRP:NE1	1:C:660:ASN:HB2	2.30	0.47
1:A:193:LEU:HD12	1:A:197:LEU:CD1	2.44	0.47
1:B:430:ILE:HG13	1:B:431:PRO:O	2.14	0.47
1:B:587:ILE:O	1:B:590:THR:HB	2.15	0.47
1:C:199:PRO:HG2	1:C:200:TYR:H	1.80	0.47
1:C:385:THR:CG2	1:C:386:PRO:HD2	2.45	0.47
1:C:420:TRP:O	1:C:421:PRO:O	2.32	0.47
1:A:373:HIS:HA	1:A:586:GLN:OE1	2.15	0.47
1:A:405:ILE:CG1	1:A:509:ALA:HA	2.32	0.47
1:B:369:GLN:H	1:B:553:LEU:HD11	1.79	0.47
1:C:158:THR:O	1:C:160:LYS:N	2.48	0.47
1:C:340:ASP:O	1:C:340:ASP:CG	2.58	0.47
1:C:471:SER:HA	1:C:527:LEU:HA	1.97	0.47
1:A:411:TYR:HE1	1:A:418:ASP:O	1.98	0.46
1:A:469:CYS:HA	1:A:528:ALA:O	2.16	0.46
1:B:155:ASP:O	1:B:156:MET:C	2.58	0.46
1:B:272:ARG:C	1:C:276:TYR:HE1	2.24	0.46
1:B:506:THR:HG23	1:B:507:LYS:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:571:MET:HB3	1:B:580:ILE:HD11	1.97	0.46
1:C:133:PRO:O	1:C:134:GLU:HB2	2.15	0.46
1:C:473:GLN:HA	1:C:524:ASP:CG	2.40	0.46
1:C:530:LEU:HD12	1:C:530:LEU:N	2.30	0.46
1:A:353:ARG:NE	1:A:422:ASP:HB2	2.27	0.46
1:B:448:LYS:HD2	1:B:537:GLU:HG3	1.97	0.46
1:C:242:PRO:HG2	1:C:288:VAL:HG21	1.98	0.46
1:C:289:ILE:HD12	1:C:289:ILE:N	2.30	0.46
1:C:519:ASP:O	1:C:519:ASP:CG	2.58	0.46
1:C:552:VAL:HG12	1:C:553:LEU:H	1.80	0.46
1:A:142:VAL:O	1:A:142:VAL:HG22	2.13	0.46
1:A:278:LEU:H	1:A:278:LEU:CD2	2.16	0.46
1:A:375:ASP:CG	1:A:376:PHE:H	2.23	0.46
1:A:384:SER:HA	1:A:418:ASP:HB2	1.97	0.46
1:B:170:PHE:CE2	1:B:315:LYS:HB3	2.51	0.46
1:B:349:TRP:O	1:B:358:ILE:N	2.46	0.46
1:B:373:HIS:CD2	1:B:585:SER:HB2	2.50	0.46
1:B:398:LYS:HE3	1:B:403:LEU:HB2	1.97	0.46
1:B:636:ILE:HD13	1:B:636:ILE:N	2.09	0.46
1:C:178:TRP:CZ2	1:C:295:LEU:HB2	2.50	0.46
1:C:474:ARG:CB	1:C:523:SER:O	2.63	0.46
1:C:607:ALA:HA	1:C:649:GLY:O	2.14	0.46
1:C:610:ARG:HD3	1:C:620:ASP:OD1	2.15	0.46
1:C:631:VAL:HG12	1:C:632:GLY:N	2.30	0.46
1:C:474:ARG:HB2	1:C:524:ASP:CA	2.46	0.46
1:A:205:ALA:C	1:A:207:LEU:N	2.66	0.46
1:A:234:ILE:HG22	1:A:253:HIS:HB3	1.97	0.46
1:A:391:ILE:HG23	1:A:411:TYR:OH	2.15	0.46
1:B:264:VAL:HG21	1:C:130:ILE:HG21	1.98	0.46
1:A:199:PRO:HA	1:A:202:THR:HB	1.97	0.46
1:A:240:ILE:HD12	1:A:240:ILE:C	2.40	0.46
1:A:484:THR:OG1	1:A:511:PHE:O	2.32	0.46
1:B:220:SER:HB2	1:B:311:THR:OG1	2.15	0.46
1:B:239:GLY:HA2	1:C:333:THR:CG2	2.45	0.46
1:C:404:GLY:HA3	1:C:509:ALA:HA	1.98	0.46
1:C:416:ILE:HD12	1:C:503:ILE:CG1	2.34	0.46
1:C:471:SER:HB3	1:C:527:LEU:CB	2.42	0.46
1:C:621:ILE:CD1	1:C:631:VAL:HG22	2.46	0.46
1:A:196:LEU:H	1:A:196:LEU:HG	1.33	0.46
1:A:221:ILE:CD1	1:A:223:GLY:H	2.28	0.46
1:A:526:THR:C	1:A:527:LEU:HG	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:607:ALA:HA	1:B:650:ASN:HB3	1.97	0.46
1:A:376:PHE:CE2	1:A:601:LEU:HD22	2.51	0.46
1:B:209:VAL:HB	1:B:324:LEU:HB2	1.97	0.46
1:C:377:ASN:O	1:C:378:GLN:HB2	2.15	0.46
1:A:150:MET:O	1:A:151:SER:HB2	2.16	0.46
1:A:173:HIS:CE1	1:A:197:LEU:HA	2.51	0.46
1:A:415:GLY:O	1:A:416:ILE:C	2.59	0.46
1:B:210:ALA:HB3	1:B:323:HIS:CB	2.37	0.46
1:B:248:MET:O	1:B:250:GLN:N	2.48	0.46
1:B:272:ARG:C	1:C:276:TYR:CE1	2.94	0.46
1:B:544:ARG:HH22	1:C:505:GLN:NE2	2.11	0.46
1:C:326:LYS:HG2	1:C:327:PRO:N	2.31	0.46
1:C:343:PRO:HG3	1:C:589:HIS:CD2	2.51	0.46
1:C:348:LEU:O	1:C:348:LEU:CD1	2.64	0.46
1:C:453:SER:HB2	1:C:456:ILE:CG2	2.45	0.46
1:C:631:VAL:CG1	1:C:632:GLY:N	2.79	0.46
1:A:149:GLN:HA	1:A:153:ALA:HB3	1.97	0.46
1:A:327:PRO:HG2	1:A:327:PRO:O	2.16	0.46
1:A:636:ILE:HD13	1:A:636:ILE:N	2.30	0.46
1:B:402:MET:HE2	1:B:512:GLN:N	2.32	0.46
1:B:446:GLN:O	1:B:446:GLN:HG2	2.16	0.46
1:B:470:GLY:O	1:B:527:LEU:HA	2.15	0.46
1:C:424:THR:HG1	1:C:489:THR:HG23	1.80	0.46
1:A:176:VAL:HG11	1:A:188:LEU:HD22	1.98	0.45
1:A:278:LEU:O	1:A:280:SER:N	2.49	0.45
1:A:392:THR:O	1:A:409:THR:CG2	2.63	0.45
1:A:428:GLU:HB3	1:A:498:ILE:HG22	1.96	0.45
1:A:623:ILE:H	1:A:623:ILE:HG13	1.50	0.45
1:B:148:VAL:O	1:B:150:MET:N	2.49	0.45
1:C:192:SER:O	1:C:197:LEU:HD21	2.16	0.45
1:C:386:PRO:O	1:C:588:LEU:HD21	2.17	0.45
1:C:611:ILE:N	1:C:611:ILE:CD1	2.74	0.45
1:A:609:TYR:CD1	1:A:647:TYR:HB3	2.50	0.45
1:B:374:PHE:CE2	1:B:380:THR:HG21	2.51	0.45
1:B:588:LEU:C	1:B:590:THR:N	2.74	0.45
1:C:318:PRO:HG2	1:C:319:ASP:H	1.81	0.45
1:C:395:ILE:HD11	1:C:523:SER:HB3	1.98	0.45
1:C:469:CYS:CB	1:C:528:ALA:O	2.64	0.45
1:C:504:ASP:C	1:C:506:THR:N	2.71	0.45
1:A:371:ASN:C	1:A:373:HIS:H	2.24	0.45
1:A:377:ASN:CB	1:C:559:ARG:HD3	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:ILE:HG23	1:A:510:ILE:CG1	2.45	0.45
1:B:438:THR:HG23	1:B:457:ILE:HG23	1.97	0.45
1:C:179:SER:HB3	1:C:182:GLU:CD	2.41	0.45
1:C:297:ASN:ND2	1:C:298:PRO:HD2	2.31	0.45
1:C:346:SER:CB	1:C:643:LEU:HB2	2.44	0.45
1:C:353:ARG:NH2	1:C:540:ILE:O	2.49	0.45
1:C:404:GLY:CA	1:C:509:ALA:HA	2.46	0.45
1:C:503:ILE:HB	1:C:548:VAL:HG11	1.98	0.45
1:A:221:ILE:O	1:A:221:ILE:CD1	2.62	0.45
1:A:230:LYS:HD2	1:A:293:ASN:ND2	2.31	0.45
1:A:375:ASP:O	1:A:594:LEU:HD22	2.17	0.45
1:A:439:ASN:CG	1:A:440:GLN:N	2.71	0.45
1:A:478:ASN:HD22	1:A:478:ASN:N	2.15	0.45
1:A:535:ILE:HD11	1:A:538:GLU:CB	2.43	0.45
1:B:230:LYS:H	1:B:293:ASN:HB2	1.82	0.45
1:B:277:HIS:HB3	1:B:281:ASP:OD2	2.16	0.45
1:B:484:THR:OG1	1:B:485:ALA:N	2.49	0.45
1:B:590:THR:O	1:B:591:SER:C	2.60	0.45
1:B:618:TRP:NE1	1:B:660:ASN:HB2	2.32	0.45
1:B:633:VAL:CG1	1:B:634:SER:N	2.80	0.45
1:C:151:SER:O	1:C:152:ALA:C	2.60	0.45
1:C:243:ILE:HD13	1:C:243:ILE:N	2.32	0.45
1:C:296:ILE:HD12	1:C:296:ILE:C	2.40	0.45
1:C:374:PHE:CE2	1:C:595:SER:HB3	2.51	0.45
1:A:130:ILE:HD13	1:C:260:GLN:HE22	1.80	0.45
1:A:376:PHE:CD1	1:A:594:LEU:HD21	2.52	0.45
1:B:158:THR:O	1:B:158:THR:HG22	2.16	0.45
1:C:189:PHE:C	1:C:191:GLN:H	2.25	0.45
1:A:221:ILE:HD11	1:A:258:ALA:O	2.16	0.45
1:A:352:ASN:HD21	1:A:586:GLN:H	1.60	0.45
1:A:370:ALA:O	1:A:373:HIS:HB3	2.16	0.45
1:A:474:ARG:NH1	1:A:521:GLN:O	2.50	0.45
1:B:353:ARG:HB3	1:B:584:ASN:ND2	2.32	0.45
1:C:249:LEU:C	1:C:251:TYR:N	2.74	0.45
1:C:431:PRO:CD	1:C:495:ASN:O	2.65	0.45
1:A:631:VAL:HG12	1:A:633:VAL:HG23	1.98	0.45
1:B:606:PHE:CE1	1:B:625:SER:N	2.85	0.45
1:C:368:PHE:HD1	1:C:547:VAL:HG21	1.82	0.45
1:C:453:SER:HB2	1:C:456:ILE:HG23	1.98	0.45
1:C:588:LEU:HD23	1:C:588:LEU:C	2.41	0.45
1:A:385:THR:CB	1:A:386:PRO:HD2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:GLN:O	1:A:524:ASP:HB3	2.17	0.45
1:B:179:SER:O	1:B:182:GLU:HG2	2.17	0.45
1:B:248:MET:C	1:B:250:GLN:N	2.75	0.45
1:B:333:THR:HG23	1:B:334:HIS:H	1.82	0.45
1:B:439:ASN:ND2	1:B:456:ILE:CD1	2.79	0.45
1:B:591:SER:O	1:B:592:ARG:C	2.59	0.45
1:C:264:VAL:C	1:C:265:ILE:HG13	2.42	0.45
1:C:405:ILE:HA	1:C:508:ILE:HG12	1.99	0.45
1:C:479:LYS:HE3	1:C:516:VAL:HB	1.99	0.45
1:A:186:LYS:HA	1:A:244:GLN:HG2	1.98	0.45
1:A:223:GLY:CA	1:A:308:CYS:SG	3.05	0.45
1:A:460:ASN:C	1:A:462:ASN:N	2.73	0.45
1:A:483:ASN:HB3	1:A:484:THR:H	1.38	0.45
1:B:349:TRP:HB2	1:B:358:ILE:HG12	1.97	0.45
1:B:358:ILE:O	1:B:359:THR:CB	2.65	0.45
1:B:393:VAL:O	1:B:393:VAL:HG13	2.17	0.45
1:C:383:TRP:CD1	1:C:383:TRP:C	2.95	0.45
1:A:132:THR:O	1:A:133:PRO:O	2.34	0.45
1:A:341:LEU:HB3	1:A:342:ILE:H	1.63	0.45
1:A:405:ILE:HG23	1:A:510:ILE:CG2	2.46	0.45
1:A:472:LEU:HD23	1:A:472:LEU:C	2.41	0.45
1:B:201:LEU:HD22	1:B:320:PHE:HE2	1.82	0.45
1:B:449:GLU:CB	1:B:452:GLU:CD	2.89	0.45
1:B:519:ASP:HB3	1:B:520:VAL:H	1.44	0.45
1:C:171:SER:O	1:C:314:THR:N	2.43	0.45
1:C:324:LEU:HA	1:C:324:LEU:HD23	1.73	0.45
1:C:403:LEU:HG	1:C:514:ASN:HD21	1.82	0.45
1:C:427:ASN:HD22	1:C:429:LEU:HD21	1.82	0.45
1:C:451:TYR:HA	1:C:458:SER:N	2.32	0.45
1:C:474:ARG:O	1:C:475:ALA:CB	2.63	0.45
1:A:287:LEU:C	1:A:288:VAL:HG22	2.42	0.44
1:B:137:THR:HG22	1:B:138:THR:H	1.81	0.44
1:B:297:ASN:CG	1:B:300:ALA:HB2	2.43	0.44
1:B:342:ILE:HG23	1:B:587:ILE:HD12	1.99	0.44
1:B:344:LYS:CE	1:B:647:TYR:OH	2.65	0.44
1:C:451:TYR:HA	1:C:458:SER:HB2	1.98	0.44
1:A:157:ALA:C	1:A:158:THR:OG1	2.61	0.44
1:A:459:ASN:O	1:A:460:ASN:ND2	2.49	0.44
1:B:258:ALA:C	1:B:260:GLN:H	2.24	0.44
1:B:439:ASN:HD21	1:B:456:ILE:CG1	2.30	0.44
1:B:500:SER:HB2	1:B:502:THR:CG2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:VAL:CG1	1:C:177:ASN:N	2.80	0.44
1:A:184:GLN:NE2	1:A:292:TYR:O	2.50	0.44
1:A:193:LEU:CG	1:A:194:GLY:N	2.81	0.44
1:A:210:ALA:HB2	1:A:278:LEU:HB3	1.99	0.44
1:A:250:GLN:O	1:B:328:PRO:CD	2.65	0.44
1:A:259:ARG:O	1:A:260:GLN:C	2.61	0.44
1:A:369:GLN:O	1:A:554:PRO:HD2	2.17	0.44
1:A:393:VAL:N	1:A:525:ASP:HB2	2.32	0.44
1:A:408:ALA:CB	1:A:417:PRO:HG3	2.47	0.44
1:A:448:LYS:O	1:A:449:GLU:HB2	2.16	0.44
1:A:458:SER:C	1:A:459:ASN:ND2	2.75	0.44
1:A:601:LEU:HD23	1:A:602:SER:O	2.17	0.44
1:B:455:MET:HE2	1:B:455:MET:HB3	1.95	0.44
1:B:487:ILE:HG22	1:B:510:ILE:HA	1.98	0.44
1:B:573:LEU:HD23	1:B:573:LEU:HA	1.79	0.44
1:C:552:VAL:HG12	1:C:553:LEU:N	2.33	0.44
1:A:145:GLU:N	1:A:146:PRO:CD	2.80	0.44
1:A:223:GLY:HA2	1:A:308:CYS:SG	2.58	0.44
1:A:247:SER:C	1:A:249:LEU:N	2.70	0.44
1:A:346:SER:O	1:A:348:LEU:N	2.51	0.44
1:A:367:VAL:O	1:A:555:GLU:HA	2.17	0.44
1:A:412:ILE:O	1:A:413:VAL:CG2	2.65	0.44
1:C:300:ALA:O	1:C:301:ASN:CB	2.65	0.44
1:C:408:ALA:HB1	1:C:411:TYR:CE2	2.52	0.44
1:C:521:GLN:O	1:C:522:THR:C	2.61	0.44
1:C:565:ILE:HG13	1:C:629:SER:HB2	1.99	0.44
1:C:598:ASN:C	1:C:598:ASN:ND2	2.69	0.44
1:A:333:THR:N	1:C:239:GLY:O	2.48	0.44
1:B:391:ILE:N	1:B:391:ILE:CD1	2.80	0.44
1:B:472:LEU:HB3	1:B:526:THR:O	2.16	0.44
1:B:503:ILE:HB	1:B:548:VAL:CG1	2.47	0.44
1:B:525:ASP:O	1:B:527:LEU:HG	2.17	0.44
1:C:363:ILE:H	1:C:363:ILE:CD1	2.23	0.44
1:A:210:ALA:HB2	1:A:278:LEU:CA	2.47	0.44
1:B:352:ASN:HD21	1:B:369:GLN:NE2	1.99	0.44
1:B:602:SER:HB3	1:B:604:ASP:OD2	2.18	0.44
1:C:213:GLY:HA3	1:C:320:PHE:HA	2.00	0.44
1:A:231:LEU:HD12	1:A:231:LEU:HA	1.71	0.44
1:A:376:PHE:HD1	1:A:594:LEU:HD21	1.83	0.44
1:B:141:GLY:C	1:B:143:ILE:H	2.25	0.44
1:B:383:TRP:HD1	1:B:384:SER:HG	1.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:608:VAL:C	1:B:609:TYR:HD1	2.25	0.44
1:C:361:PHE:HE1	1:C:619:PHE:HZ	1.63	0.44
1:A:423:THR:HG22	1:A:424:THR:N	2.31	0.44
1:A:458:SER:O	1:A:459:ASN:CB	2.66	0.44
1:A:503:ILE:HB	1:A:548:VAL:CG1	2.48	0.44
1:B:139:VAL:HG12	1:B:140:GLY:N	2.32	0.44
1:C:344:LYS:O	1:C:345:SER:CB	2.64	0.44
1:A:170:PHE:CD2	1:A:315:LYS:HB2	2.53	0.44
1:A:371:ASN:HA	1:A:382:GLY:HA3	2.00	0.44
1:A:624:ASP:HB2	1:A:630:PHE:CE1	2.52	0.44
1:B:156:MET:C	1:B:158:THR:H	2.26	0.44
1:B:158:THR:HB	1:B:160:LYS:HB3	1.99	0.44
1:B:352:ASN:N	1:B:584:ASN:HD22	2.16	0.44
1:B:604:ASP:OD2	1:B:604:ASP:N	2.50	0.44
1:C:179:SER:N	1:C:182:GLU:OE2	2.43	0.44
1:C:193:LEU:HD12	1:C:193:LEU:HA	1.78	0.44
1:C:309:ILE:C	1:C:309:ILE:HD12	2.43	0.44
1:C:367:VAL:HG23	1:C:564:PRO:HB2	2.00	0.44
1:C:652:LEU:O	1:C:655:ILE:HG13	2.17	0.44
1:A:609:TYR:HA	1:A:647:TYR:HA	1.99	0.43
1:B:341:LEU:O	1:B:343:PRO:HD3	2.18	0.43
1:C:385:THR:C	1:C:387:ARG:H	2.25	0.43
1:A:214:SER:O	1:A:317:GLY:HA3	2.18	0.43
1:A:217:VAL:HG12	1:A:218:ARG:N	2.31	0.43
1:A:458:SER:C	1:A:459:ASN:CG	2.85	0.43
1:A:469:CYS:CB	1:A:527:LEU:HB2	2.48	0.43
1:B:602:SER:O	1:B:604:ASP:N	2.49	0.43
1:C:251:TYR:CD1	1:C:252:PRO:HD2	2.52	0.43
1:C:350:ILE:CA	1:C:357:ASP:HA	2.43	0.43
1:C:602:SER:C	1:C:604:ASP:N	2.76	0.43
1:C:610:ARG:NH2	1:C:648:MET:HE2	2.32	0.43
1:A:219:PHE:HB2	1:A:311:THR:O	2.17	0.43
1:A:221:ILE:HG13	1:A:256:PHE:HE2	1.83	0.43
1:A:393:VAL:H	1:A:525:ASP:HB2	1.83	0.43
1:A:436:ALA:O	1:A:437:ILE:C	2.60	0.43
1:A:504:ASP:O	1:A:505:GLN:C	2.61	0.43
1:A:525:ASP:O	1:A:526:THR:O	2.36	0.43
1:B:215:ILE:O	1:B:268:ILE:HG13	2.18	0.43
1:A:391:ILE:N	1:A:391:ILE:CD1	2.81	0.43
1:B:147:SER:O	1:B:148:VAL:O	2.37	0.43
1:B:474:ARG:HD3	1:B:525:ASP:OD1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:LEU:HD22	1:C:322:PHE:CZ	2.53	0.43
1:C:438:THR:O	1:C:438:THR:HG23	2.18	0.43
1:C:518:ARG:HD3	1:C:520:VAL:HG13	2.01	0.43
1:A:383:TRP:CZ3	1:A:550:ILE:HB	2.53	0.43
1:A:393:VAL:O	1:A:525:ASP:CB	2.59	0.43
1:B:147:SER:O	1:B:148:VAL:C	2.61	0.43
1:B:188:LEU:O	1:B:188:LEU:CD2	2.63	0.43
1:B:189:PHE:HD2	1:B:289:ILE:HD13	1.82	0.43
1:B:236:VAL:O	1:B:236:VAL:HG23	2.18	0.43
1:C:288:VAL:HG12	1:C:289:ILE:H	1.80	0.43
1:C:346:SER:O	1:C:347:SER:C	2.61	0.43
1:C:349:TRP:O	1:C:350:ILE:CG1	2.66	0.43
1:A:150:MET:O	1:A:151:SER:CB	2.66	0.43
1:A:166:TRP:NE1	1:A:200:TYR:HB3	2.34	0.43
1:A:183:THR:O	1:A:184:GLN:C	2.61	0.43
1:A:208:TYR:HA	1:A:325:LEU:HA	1.99	0.43
1:A:236:VAL:CG2	1:A:286:SER:HB2	2.48	0.43
1:A:433:GLY:HA3	1:A:462:ASN:OD1	2.18	0.43
1:A:624:ASP:C	1:A:626:ASP:N	2.76	0.43
1:B:154:ALA:O	1:B:155:ASP:C	2.62	0.43
1:B:414:PRO:O	1:B:416:ILE:HD12	2.19	0.43
1:B:470:GLY:N	1:B:528:ALA:O	2.51	0.43
1:C:576:VAL:HG12	1:C:577:ILE:HG12	2.01	0.43
1:C:619:PHE:CD1	1:C:619:PHE:C	2.97	0.43
1:A:484:THR:O	1:A:485:ALA:CB	2.65	0.43
1:A:513:ASP:OD2	1:A:513:ASP:N	2.50	0.43
1:A:528:ALA:O	1:A:530:LEU:HD13	2.19	0.43
1:B:358:ILE:O	1:B:359:THR:HB	2.18	0.43
1:B:383:TRP:HB2	1:B:413:VAL:HG21	2.01	0.43
1:C:392:THR:HG23	1:C:409:THR:CG2	2.48	0.43
1:C:460:ASN:C	1:C:461:THR:HG22	2.43	0.43
1:C:527:LEU:HD23	1:C:527:LEU:N	2.34	0.43
1:A:533:THR:O	1:A:535:ILE:N	2.51	0.43
1:A:639:LEU:HD23	1:A:639:LEU:H	1.83	0.43
1:B:146:PRO:O	1:B:149:GLN:CD	2.62	0.43
1:B:277:HIS:HB3	1:B:281:ASP:CG	2.44	0.43
1:B:393:VAL:CG2	1:B:406:GLY:C	2.92	0.43
1:B:474:ARG:O	1:B:475:ALA:HB2	2.19	0.43
1:B:505:GLN:HG3	1:B:506:THR:N	2.32	0.43
1:B:608:VAL:CG1	1:B:609:TYR:N	2.82	0.43
1:B:623:ILE:N	1:B:623:ILE:CD1	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:639:LEU:N	1:B:639:LEU:CD2	2.79	0.43
1:C:190:LYS:HD3	1:C:651:GLN:NE2	2.33	0.43
1:C:385:THR:HG23	1:C:386:PRO:HD2	2.01	0.43
1:C:591:SER:O	1:C:592:ARG:C	2.61	0.43
1:C:652:LEU:H	1:C:652:LEU:HD12	1.84	0.43
1:C:652:LEU:HD12	1:C:652:LEU:N	2.34	0.43
1:A:440:GLN:O	1:A:441:SER:HB2	2.19	0.43
1:A:571:MET:CB	1:A:580:ILE:HD11	2.43	0.43
1:A:608:VAL:C	1:A:609:TYR:HD1	2.25	0.43
1:B:146:PRO:O	1:B:147:SER:C	2.62	0.43
1:B:186:LYS:HB2	1:B:186:LYS:HE3	1.86	0.43
1:B:486:PHE:CD2	1:B:486:PHE:N	2.85	0.43
1:B:583:PHE:CD1	1:B:583:PHE:N	2.87	0.43
1:B:602:SER:C	1:B:604:ASP:N	2.73	0.43
1:C:398:LYS:O	1:C:399:GLU:CB	2.67	0.43
1:A:164:SER:C	1:A:166:TRP:N	2.75	0.43
1:A:383:TRP:HD1	1:A:418:ASP:HA	1.84	0.43
1:B:353:ARG:CB	1:B:584:ASN:ND2	2.82	0.43
1:C:297:ASN:ND2	1:C:298:PRO:N	2.60	0.43
1:C:398:LYS:N	1:C:403:LEU:CD2	2.76	0.43
1:C:435:TYR:O	1:C:436:ALA:C	2.62	0.43
1:C:582:VAL:HG12	1:C:583:PHE:N	2.33	0.43
1:B:257:ASP:OD1	1:B:258:ALA:N	2.51	0.42
1:B:443:ASN:CG	1:B:447:THR:HG21	2.44	0.42
1:B:444:ASP:O	1:B:446:GLN:N	2.52	0.42
1:B:611:ILE:HD13	1:B:619:PHE:HD1	1.84	0.42
1:C:353:ARG:HB2	1:C:369:GLN:HE22	1.83	0.42
1:C:449:GLU:O	1:C:450:GLU:OE2	2.36	0.42
1:C:512:GLN:HB3	1:C:514:ASN:OD1	2.19	0.42
1:A:151:SER:O	1:A:153:ALA:N	2.52	0.42
1:A:405:ILE:HG21	1:A:510:ILE:HG23	2.00	0.42
1:A:512:GLN:HB3	1:A:513:ASP:H	1.63	0.42
1:A:557:GLY:O	1:A:558:ALA:C	2.62	0.42
1:A:633:VAL:HG12	1:A:634:SER:N	2.34	0.42
1:B:389:ARG:HB3	1:B:390:PRO:HD2	2.00	0.42
1:C:280:SER:O	1:C:282:THR:HG23	2.19	0.42
1:C:383:TRP:CZ3	1:C:503:ILE:HG21	2.54	0.42
1:A:411:TYR:CE2	1:A:417:PRO:HB3	2.54	0.42
1:A:525:ASP:HB2	1:A:526:THR:H	1.34	0.42
1:A:564:PRO:HG3	1:A:630:PHE:CE2	2.54	0.42
1:B:198:ASN:OD1	1:B:200:TYR:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:ASN:HB3	1:B:586:GLN:O	2.20	0.42
1:B:491:THR:HG22	1:B:492:VAL:H	1.84	0.42
1:B:580:ILE:C	1:B:580:ILE:CD1	2.92	0.42
1:B:621:ILE:CG2	1:B:629:SER:HB3	2.48	0.42
1:C:175:SER:CB	1:C:311:THR:HA	2.47	0.42
1:C:262:GLU:OE1	1:C:262:GLU:HA	2.19	0.42
1:C:386:PRO:HG3	1:C:595:SER:OG	2.19	0.42
1:A:197:LEU:CD1	1:A:215:ILE:HD12	2.45	0.42
1:A:350:ILE:O	1:A:350:ILE:HG13	2.18	0.42
1:A:457:ILE:HD11	1:A:460:ASN:HD21	1.85	0.42
1:A:463:PHE:CD1	1:A:463:PHE:O	2.72	0.42
1:B:193:LEU:HD11	1:B:215:ILE:HG12	2.01	0.42
1:B:219:PHE:CD2	1:B:312:VAL:HG22	2.54	0.42
1:B:318:PRO:HG2	1:B:319:ASP:H	1.84	0.42
1:B:395:ILE:HD11	1:B:510:ILE:CD1	2.49	0.42
1:B:630:PHE:N	1:B:630:PHE:CD1	2.88	0.42
1:C:210:ALA:HB3	1:C:324:LEU:N	2.24	0.42
1:C:451:TYR:O	1:C:453:SER:N	2.44	0.42
1:C:460:ASN:ND2	1:C:461:THR:H	2.17	0.42
1:A:218:ARG:HB2	1:A:265:ILE:HG13	2.01	0.42
1:B:178:TRP:HD1	1:B:182:GLU:HG3	1.83	0.42
1:B:272:ARG:O	1:C:275:LEU:HD12	2.20	0.42
1:B:424:THR:O	1:B:465:SER:HB3	2.19	0.42
1:B:463:PHE:O	1:B:465:SER:N	2.52	0.42
1:C:374:PHE:CD2	1:C:380:THR:HB	2.54	0.42
1:C:403:LEU:H	1:C:403:LEU:HD12	1.83	0.42
1:C:430:ILE:O	1:C:462:ASN:ND2	2.53	0.42
1:C:463:PHE:O	1:C:466:MET:HG2	2.19	0.42
1:C:607:ALA:HB3	1:C:623:ILE:CG1	2.49	0.42
1:A:350:ILE:CD1	1:A:351:GLY:O	2.68	0.42
1:B:449:GLU:OE2	1:B:449:GLU:HA	2.20	0.42
1:C:397:GLN:HG3	1:C:521:GLN:C	2.44	0.42
1:C:470:GLY:N	1:C:530:LEU:HD13	2.31	0.42
1:A:341:LEU:CD1	1:A:590:THR:HG23	2.49	0.42
1:B:187:ILE:HB	1:B:244:GLN:HE21	1.85	0.42
1:B:237:PRO:HG2	1:B:240:ILE:HD11	2.01	0.42
1:B:295:LEU:HD12	1:B:296:ILE:N	2.35	0.42
1:B:392:THR:HA	1:B:526:THR:H	1.83	0.42
1:B:535:ILE:HD11	1:B:538:GLU:O	2.19	0.42
1:C:507:LYS:N	1:C:508:ILE:HD13	2.34	0.42
1:A:287:LEU:CG	1:A:288:VAL:N	2.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:CYS:O	1:A:485:ALA:HB3	2.18	0.42
1:A:488:THR:OG1	1:A:489:THR:N	2.51	0.42
1:A:509:ALA:C	1:A:510:ILE:HG23	2.45	0.42
1:A:523:SER:C	1:A:525:ASP:H	2.27	0.42
1:B:224:SER:O	1:B:225:GLY:C	2.62	0.42
1:B:370:ALA:HB1	1:B:381:ALA:HB3	2.02	0.42
1:B:395:ILE:HG21	1:B:523:SER:HB2	2.02	0.42
1:B:416:ILE:HA	1:B:417:PRO:HD3	1.89	0.42
1:B:484:THR:OG1	1:B:511:PHE:O	2.21	0.42
1:B:625:SER:O	1:B:627:GLY:N	2.53	0.42
1:C:234:ILE:HD11	1:C:288:VAL:HB	2.02	0.42
1:C:234:ILE:CD1	1:C:288:VAL:HB	2.50	0.42
1:C:450:GLU:C	1:C:451:TYR:CD2	2.98	0.42
1:C:599:TYR:CD1	1:C:599:TYR:N	2.87	0.42
1:A:399:GLU:HB2	1:A:519:ASP:CG	2.44	0.42
1:A:411:TYR:CE1	1:A:418:ASP:O	2.73	0.42
1:A:496:LYS:O	1:A:497:LEU:HD23	2.20	0.42
1:A:602:SER:HB2	1:A:605:SER:OG	2.19	0.42
1:B:167:GLU:HA	1:B:316:PRO:HG2	2.01	0.42
1:B:205:ALA:HA	1:B:322:PHE:HE2	1.84	0.42
1:B:421:PRO:HB2	1:B:422:ASP:H	1.74	0.42
1:B:612:ILE:HD11	1:B:644:THR:OG1	2.20	0.42
1:C:368:PHE:CD1	1:C:547:VAL:HG21	2.55	0.42
1:A:280:SER:O	1:A:281:ASP:O	2.37	0.42
1:A:484:THR:HG21	1:A:512:GLN:HE22	1.85	0.42
1:B:149:GLN:O	1:B:153:ALA:HB2	2.20	0.42
1:B:201:LEU:HD22	1:B:320:PHE:CE2	2.55	0.42
1:B:371:ASN:C	1:B:371:ASN:HD22	2.27	0.42
1:B:625:SER:C	1:B:627:GLY:N	2.76	0.42
1:C:255:LEU:HD12	1:C:255:LEU:N	2.34	0.42
1:C:425:ILE:HA	1:C:465:SER:OG	2.19	0.42
1:C:637:GLY:O	1:C:639:LEU:HD23	2.20	0.42
1:C:651:GLN:O	1:C:652:LEU:C	2.63	0.42
1:A:251:TYR:CE1	1:B:325:LEU:O	2.72	0.41
1:A:344:LYS:HA	1:A:645:ALA:O	2.19	0.41
1:A:412:ILE:C	1:A:413:VAL:CG2	2.92	0.41
1:A:436:ALA:CB	1:A:461:THR:HA	2.49	0.41
1:A:476:TRP:CD1	1:A:520:VAL:CB	2.92	0.41
1:B:192:SER:CA	1:B:286:SER:HB3	2.39	0.41
1:B:297:ASN:O	1:B:298:PRO:C	2.62	0.41
1:B:428:GLU:HA	1:B:498:ILE:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:613:ASP:HB2	1:B:640:GLU:O	2.20	0.41
1:C:359:THR:O	1:C:360:ASP:HB2	2.21	0.41
1:C:393:VAL:HG11	1:C:406:GLY:O	2.19	0.41
1:C:540:ILE:HB	1:C:582:VAL:HG22	2.02	0.41
1:A:233:ALA:HA	1:A:288:VAL:O	2.20	0.41
1:A:573:LEU:HA	1:A:573:LEU:HD23	1.61	0.41
1:B:187:ILE:HG23	1:B:288:VAL:CG1	2.50	0.41
1:B:191:GLN:HG2	1:B:197:LEU:CD2	2.50	0.41
1:B:373:HIS:ND1	1:B:586:GLN:NE2	2.68	0.41
1:B:448:LYS:HA	1:B:448:LYS:CE	2.47	0.41
1:B:466:MET:SD	1:B:486:PHE:HB3	2.59	0.41
1:B:539:ALA:CB	1:B:583:PHE:HE1	2.33	0.41
1:C:512:GLN:CD	1:C:513:ASP:H	2.28	0.41
1:C:641:PHE:N	1:C:642:PRO:CD	2.82	0.41
1:A:405:ILE:HG21	1:A:509:ALA:CA	2.50	0.41
1:A:488:THR:O	1:A:509:ALA:HB3	2.20	0.41
1:B:402:MET:CE	1:B:512:GLN:N	2.78	0.41
1:B:432:ALA:HB3	1:B:462:ASN:HB3	2.03	0.41
1:C:339:CYS:SG	1:C:649:GLY:CA	3.04	0.41
1:C:458:SER:O	1:C:459:ASN:HB3	2.20	0.41
1:C:624:ASP:C	1:C:626:ASP:N	2.77	0.41
1:A:136:GLY:O	1:A:137:THR:C	2.63	0.41
1:A:367:VAL:HG23	1:A:564:PRO:HB2	2.02	0.41
1:A:573:LEU:CG	1:A:580:ILE:HG23	2.47	0.41
1:A:613:ASP:HB2	1:A:640:GLU:O	2.20	0.41
1:B:233:ALA:O	1:B:234:ILE:CG2	2.68	0.41
1:B:248:MET:C	1:B:250:GLN:H	2.28	0.41
1:B:338:PRO:HD3	1:B:599:TYR:HB3	2.01	0.41
1:B:530:LEU:HD23	1:B:530:LEU:HA	1.92	0.41
1:B:638:LYS:C	1:B:639:LEU:HD23	2.45	0.41
1:C:130:ILE:HD13	1:C:130:ILE:N	2.29	0.41
1:C:185:GLY:HA2	1:C:290:MET:CG	2.50	0.41
1:A:198:ASN:HB2	1:A:314:THR:OG1	2.21	0.41
1:A:297:ASN:C	1:A:299:TYR:H	2.28	0.41
1:A:528:ALA:C	1:A:530:LEU:HD12	2.45	0.41
1:B:291:ILE:H	1:B:291:ILE:HG12	1.52	0.41
1:B:550:ILE:HD13	1:B:550:ILE:C	2.46	0.41
1:B:605:SER:HB3	1:B:651:GLN:O	2.21	0.41
1:B:618:TRP:CD1	1:B:660:ASN:HB2	2.54	0.41
1:C:212:SER:O	1:C:320:PHE:HA	2.20	0.41
1:C:490:ALA:HB1	1:C:499:PRO:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:519:ASP:O	1:C:520:VAL:C	2.64	0.41
1:A:190:LYS:CD	1:A:651:GLN:HE22	2.33	0.41
1:A:234:ILE:CG2	1:A:253:HIS:HB3	2.51	0.41
1:A:253:HIS:N	1:A:253:HIS:HD1	2.19	0.41
1:A:399:GLU:HA	1:A:516:VAL:HB	2.02	0.41
1:A:412:ILE:HD12	1:A:412:ILE:C	2.45	0.41
1:A:529:LEU:C	1:A:530:LEU:HD12	2.46	0.41
1:A:565:ILE:CD1	1:A:566:PHE:N	2.79	0.41
1:B:337:VAL:O	1:B:338:PRO:C	2.63	0.41
1:B:497:LEU:O	1:B:498:ILE:O	2.38	0.41
1:C:423:THR:HG22	1:C:546:LYS:O	2.21	0.41
1:C:484:THR:CG2	1:C:485:ALA:H	2.27	0.41
1:C:583:PHE:HB3	1:C:584:ASN:H	1.65	0.41
1:A:361:PHE:HE1	1:A:619:PHE:HZ	1.68	0.41
1:A:378:GLN:CG	1:C:654:LYS:HZ2	2.25	0.41
1:A:388:PHE:HE1	1:A:588:LEU:HD13	1.85	0.41
1:A:536:GLY:C	1:A:538:GLU:H	2.27	0.41
1:B:159:GLY:O	1:B:160:LYS:C	2.62	0.41
1:B:199:PRO:O	1:B:200:TYR:C	2.62	0.41
1:B:208:TYR:CD2	1:B:322:PHE:HB3	2.56	0.41
1:B:251:TYR:CD2	1:B:252:PRO:HD2	2.55	0.41
1:B:437:ILE:HG12	1:B:440:GLN:N	2.36	0.41
1:B:483:ASN:O	1:B:484:THR:O	2.39	0.41
1:B:534:GLY:HA2	1:B:573:LEU:HD22	2.03	0.41
1:A:287:LEU:HD21	1:A:289:ILE:HD11	2.03	0.41
1:A:437:ILE:HD12	1:A:439:ASN:O	2.21	0.41
1:A:440:GLN:H	1:A:440:GLN:HG3	1.70	0.41
1:A:565:ILE:HG21	1:A:631:VAL:CG2	2.50	0.41
1:B:166:TRP:CD1	1:B:200:TYR:CD2	3.09	0.41
1:B:620:ASP:O	1:B:621:ILE:HD12	2.21	0.41
1:C:140:GLY:O	1:C:141:GLY:O	2.38	0.41
1:C:151:SER:HA	1:C:154:ALA:HB3	2.03	0.41
1:C:383:TRP:O	1:C:413:VAL:HG21	2.21	0.41
1:C:451:TYR:O	1:C:456:ILE:HG12	2.21	0.41
1:A:275:LEU:HB2	1:A:276:TYR:CD2	2.56	0.41
1:A:293:ASN:O	1:A:294:ASP:C	2.64	0.41
1:A:324:LEU:HD23	1:A:324:LEU:HA	1.66	0.41
1:A:325:LEU:C	1:A:325:LEU:CD1	2.93	0.41
1:A:331:MET:H	1:C:243:ILE:HD11	1.86	0.41
1:A:394:THR:O	1:A:395:ILE:HG23	2.21	0.41
1:A:413:VAL:O	1:A:415:GLY:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:LEU:O	1:B:189:PHE:HB2	2.21	0.41
1:B:190:LYS:HZ3	1:B:651:GLN:CD	2.28	0.41
1:B:309:ILE:HG13	1:B:310:VAL:N	2.35	0.41
1:B:368:PHE:CD1	1:B:368:PHE:C	2.99	0.41
1:B:374:PHE:HA	1:B:380:THR:HB	2.02	0.41
1:B:448:LYS:HD3	1:B:537:GLU:CD	2.46	0.41
1:C:297:ASN:HA	1:C:298:PRO:HD3	1.95	0.41
1:C:367:VAL:HG13	1:C:566:PHE:CZ	2.55	0.41
1:C:404:GLY:O	1:C:405:ILE:C	2.63	0.41
1:C:408:ALA:CB	1:C:411:TYR:HD2	2.33	0.41
1:C:412:ILE:C	1:C:413:VAL:HG22	2.45	0.41
1:C:472:LEU:HD22	1:C:473:GLN:N	2.36	0.41
1:C:481:VAL:O	1:C:481:VAL:CG1	2.68	0.41
1:C:583:PHE:O	1:C:584:ASN:CG	2.64	0.41
1:C:584:ASN:HD22	1:C:584:ASN:HA	1.69	0.41
1:C:641:PHE:C	1:C:643:LEU:N	2.79	0.41
1:C:652:LEU:C	1:C:654:LYS:N	2.79	0.41
1:A:131:THR:OG1	1:C:255:LEU:CB	2.66	0.41
1:A:173:HIS:O	1:A:173:HIS:CD2	2.74	0.41
1:B:287:LEU:CD1	1:B:288:VAL:N	2.82	0.41
1:B:353:ARG:HH21	1:B:422:ASP:HB3	1.85	0.41
1:C:224:SER:C	1:C:226:VAL:N	2.79	0.41
1:C:224:SER:O	1:C:226:VAL:N	2.54	0.41
1:C:245:SER:OG	1:C:246:THR:N	2.54	0.41
1:C:422:ASP:OD1	1:C:422:ASP:C	2.64	0.41
1:C:516:VAL:CG1	1:C:520:VAL:HG21	2.51	0.41
1:C:587:ILE:O	1:C:588:LEU:C	2.64	0.41
1:A:339:CYS:SG	1:A:649:GLY:HA2	2.60	0.40
1:A:588:LEU:C	1:A:590:THR:N	2.77	0.40
1:B:190:LYS:HA	1:B:288:VAL:HG13	2.03	0.40
1:B:265:ILE:HG22	1:B:266:PHE:N	2.35	0.40
1:B:395:ILE:HD11	1:B:510:ILE:HD11	2.02	0.40
1:C:259:ARG:O	1:C:260:GLN:C	2.63	0.40
1:C:437:ILE:HD12	1:C:438:THR:N	2.36	0.40
1:C:535:ILE:CD1	1:C:546:LYS:NZ	2.81	0.40
1:C:621:ILE:HD13	1:C:621:ILE:HA	1.87	0.40
1:A:189:PHE:CE2	1:A:191:GLN:CB	3.02	0.40
1:A:224:SER:C	1:A:226:VAL:N	2.79	0.40
1:A:403:LEU:HD12	1:A:512:GLN:HG3	2.03	0.40
1:A:613:ASP:HA	1:A:643:LEU:HD23	2.03	0.40
1:B:151:SER:O	1:B:153:ALA:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:PHE:HB3	1:B:289:ILE:HD13	2.01	0.40
1:B:383:TRP:CD1	1:B:384:SER:OG	2.65	0.40
1:C:186:LYS:N	1:C:290:MET:HE2	2.35	0.40
1:C:287:LEU:C	1:C:288:VAL:CG2	2.95	0.40
1:A:198:ASN:HA	1:A:199:PRO:HD2	1.89	0.40
1:A:219:PHE:CD2	1:A:219:PHE:O	2.75	0.40
1:A:236:VAL:HG22	1:A:286:SER:O	2.22	0.40
1:A:251:TYR:HE1	1:B:325:LEU:O	2.05	0.40
1:A:473:GLN:CB	1:A:482:SER:HA	2.41	0.40
1:B:256:PHE:HD2	1:B:257:ASP:H	1.68	0.40
1:B:278:LEU:O	1:B:280:SER:N	2.55	0.40
1:B:604:ASP:O	1:B:652:LEU:HG	2.21	0.40
1:C:350:ILE:HA	1:C:356:SER:O	2.22	0.40
1:A:165:GLU:O	1:A:169:PHE:HE2	2.05	0.40
1:A:215:ILE:HG23	1:A:315:LYS:O	2.22	0.40
1:A:299:TYR:CD1	1:A:299:TYR:N	2.89	0.40
1:A:387:ARG:HB3	1:A:388:PHE:H	1.76	0.40
1:A:411:TYR:CD2	1:A:417:PRO:HA	2.56	0.40
1:A:438:THR:HG22	1:A:457:ILE:C	2.39	0.40
1:A:580:ILE:C	1:A:580:ILE:CD1	2.90	0.40
1:C:337:VAL:HG12	1:C:339:CYS:H	1.87	0.40
1:C:374:PHE:HZ	1:C:386:PRO:HD3	1.87	0.40
1:C:383:TRP:CD1	1:C:384:SER:HG	2.39	0.40
1:A:176:VAL:CG1	1:A:188:LEU:HD22	2.50	0.40
1:A:227:PHE:CE1	1:A:308:CYS:HB2	2.56	0.40
1:A:310:VAL:CG1	1:A:311:THR:N	2.82	0.40
1:B:214:SER:N	1:B:319:ASP:OD2	2.55	0.40
1:B:219:PHE:CE2	1:B:312:VAL:HG22	2.57	0.40
1:B:249:LEU:C	1:B:251:TYR:N	2.80	0.40
1:B:283:ASP:C	1:B:284:THR:HG23	2.47	0.40
1:B:463:PHE:HB3	1:B:466:MET:HE3	2.02	0.40
1:B:606:PHE:HB3	1:B:622:GLY:C	2.46	0.40
1:C:285:THR:CG2	1:C:286:SER:N	2.84	0.40
1:C:588:LEU:C	1:C:590:THR:N	2.80	0.40
1:C:608:VAL:C	1:C:609:TYR:HD1	2.30	0.40

All (7) 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:299:TYR:CE1	1:C:299:TYR:OH[2_555]	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:TYR:CD1	1:C:299:TYR:CZ[2_555]	1.97	0.23
1:B:229:GLY:N	1:C:222:SER:OG[2_555]	2.06	0.14
1:B:292:TYR:OH	1:C:313:GLU:OE1[2_555]	2.07	0.13
1:B:252:PRO:N	1:C:169:PHE:CE1[2_555]	2.10	0.10
1:C:480:LYS:CG	1:C:575:TYR:CD1[2_555]	2.17	0.03
1:B:299:TYR:CD1	1:C:299:TYR:OH[2_555]	2.18	0.02

5.3 Torsion angles

5.3.1 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	532/534 (100%)	310 (58%)	147 (28%)	75 (14%)	0	0
1	B	528/534 (99%)	321 (61%)	132 (25%)	75 (14%)	0	0
1	C	532/534 (100%)	332 (62%)	126 (24%)	74 (14%)	0	1
All	All	1592/1602 (99%)	963 (60%)	405 (25%)	224 (14%)	0	0

All (224) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	133	PRO
1	A	145	GLU
1	A	146	PRO
1	A	151	SER
1	A	279	MET
1	A	280	SER
1	A	281	ASP
1	A	300	ALA
1	A	303	SER
1	A	305	SER
1	A	340	ASP
1	A	341	LEU
1	A	347	SER

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Mol	Chain	Res	Type
1	A	350	ILE
1	A	457	ILE
1	A	461	THR
1	A	473	GLN
1	A	475	ALA
1	A	479	LYS
1	A	481	VAL
1	A	482	SER
1	A	484	THR
1	A	513	ASP
1	A	525	ASP
1	A	526	THR
1	A	534	GLY
1	A	580	ILE
1	B	142	VAL
1	B	147	SER
1	B	148	VAL
1	B	149	GLN
1	B	274	THR
1	B	298	PRO
1	B	302	ASP
1	B	340	ASP
1	B	399	GLU
1	B	401	GLU
1	B	402	MET
1	B	407	VAL
1	B	421	PRO
1	B	429	LEU
1	B	440	GLN
1	B	450	GLU
1	B	453	SER
1	B	475	ALA
1	B	481	VAL
1	B	484	THR
1	B	517	ASN
1	B	518	ARG
1	B	520	VAL
1	B	523	SER
1	B	580	ILE
1	B	625	SER
1	B	658	ALA
1	C	134	GLU

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Mol	Chain	Res	Type
1	C	146	PRO
1	C	149	GLN
1	C	294	ASP
1	C	300	ALA
1	C	301	ASN
1	C	303	SER
1	C	305	SER
1	C	340	ASP
1	C	345	SER
1	C	347	SER
1	C	350	ILE
1	C	421	PRO
1	C	434	ASP
1	C	438	THR
1	C	439	ASN
1	C	449	GLU
1	C	474	ARG
1	C	481	VAL
1	C	482	SER
1	C	505	GLN
1	C	523	SER
1	C	524	ASP
1	C	534	GLY
1	C	576	VAL
1	C	580	ILE
1	C	583	PHE
1	A	148	VAL
1	A	149	GLN
1	A	162	VAL
1	A	168	ALA
1	A	244	GLN
1	A	346	SER
1	A	371	ASN
1	A	437	ILE
1	A	447	THR
1	A	455	MET
1	A	460	ASN
1	A	462	ASN
1	A	485	ALA
1	A	515	HIS
1	A	522	THR
1	A	558	ALA

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Mol	Chain	Res	Type
1	A	592	ARG
1	A	637	GLY
1	B	150	MET
1	B	259	ARG
1	B	261	VAL
1	B	338	PRO
1	B	341	LEU
1	B	355	TRP
1	B	360	ASP
1	B	394	THR
1	B	408	ALA
1	B	433	GLY
1	B	445	ILE
1	B	457	ILE
1	B	460	ASN
1	B	464	LYS
1	B	485	ALA
1	B	498	ILE
1	B	524	ASP
1	B	526	THR
1	B	575	TYR
1	B	577	ILE
1	B	589	HIS
1	C	141	GLY
1	C	159	GLY
1	C	185	GLY
1	C	227	PHE
1	C	247	SER
1	C	322	PHE
1	C	323	HIS
1	C	355	TRP
1	C	400	GLY
1	C	405	ILE
1	C	433	GLY
1	C	460	ASN
1	C	463	PHE
1	C	475	ALA
1	C	479	LYS
1	C	483	ASN
1	C	516	VAL
1	C	577	ILE
1	A	137	THR

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Mol	Chain	Res	Type
1	A	158	THR
1	A	184	GLN
1	A	301	ASN
1	A	328	PRO
1	A	414	PRO
1	A	449	GLU
1	A	494	GLU
1	A	498	ILE
1	A	505	GLN
1	A	510	ILE
1	A	527	LEU
1	A	535	ILE
1	A	551	GLY
1	B	152	ALA
1	B	285	THR
1	B	328	PRO
1	B	359	THR
1	B	369	GLN
1	B	409	THR
1	B	414	PRO
1	B	449	GLU
1	B	452	GLU
1	B	461	THR
1	B	494	GLU
1	B	616	GLY
1	C	281	ASP
1	C	408	ALA
1	C	432	ALA
1	C	540	ILE
1	C	584	ASN
1	C	606	PHE
1	C	641	PHE
1	A	166	TRP
1	A	349	TRP
1	A	370	ALA
1	A	478	ASN
1	A	480	LYS
1	B	249	LEU
1	B	276	TYR
1	B	410	ASP
1	C	151	SER
1	C	167	GLU

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Mol	Chain	Res	Type
1	C	197	LEU
1	C	260	GLN
1	C	448	LYS
1	C	462	ASN
1	C	558	ALA
1	A	409	THR
1	A	435	TYR
1	A	448	LYS
1	A	476	TRP
1	A	537	GLU
1	B	165	GLU
1	B	305	SER
1	B	321	LYS
1	B	339	CYS
1	B	358	ILE
1	B	424	THR
1	B	487	ILE
1	B	519	ASP
1	C	386	PRO
1	C	412	ILE
1	C	428	GLU
1	C	437	ILE
1	C	488	THR
1	C	603	PRO
1	C	616	GLY
1	B	189	PHE
1	B	378	GLN
1	C	445	ILE
1	C	510	ILE
1	A	298	PRO
1	A	577	ILE
1	B	603	PRO
1	C	535	ILE
1	A	130	ILE
1	A	139	VAL
1	A	335	GLY
1	B	162	VAL
1	C	130	ILE
1	C	551	GLY
1	C	225	GLY
1	C	431	PRO
1	A	603	PRO

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Mol	Chain	Res	Type
1	C	661	ILE

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	461/461 (100%)	370 (80%)	91 (20%)	1	5
1	B	457/461 (99%)	350 (77%)	107 (23%)	1	2
1	C	461/461 (100%)	376 (82%)	85 (18%)	1	7
All	All	1379/1383 (100%)	1096 (80%)	283 (20%)	1	4

All (283) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	PRO
1	A	134	GLU
1	A	135	GLN
1	A	137	THR
1	A	142	VAL
1	A	145	GLU
1	A	155	ASP
1	A	158	THR
1	A	162	VAL
1	A	167	GLU
1	A	170	PHE
1	A	172	PHE
1	A	175	SER
1	A	187	ILE
1	A	196	LEU
1	A	202	THR
1	A	219	PHE
1	A	226	VAL
1	A	231	LEU
1	A	234	ILE
1	A	235	VAL

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Mol	Chain	Res	Type
1	A	245	SER
1	A	261	VAL
1	A	262	GLU
1	A	267	THR
1	A	277	HIS
1	A	278	LEU
1	A	282	THR
1	A	287	LEU
1	A	288	VAL
1	A	291	ILE
1	A	325	LEU
1	A	328	PRO
1	A	341	LEU
1	A	342	ILE
1	A	350	ILE
1	A	357	ASP
1	A	363	ILE
1	A	369	GLN
1	A	380	THR
1	A	385	THR
1	A	392	THR
1	A	395	ILE
1	A	397	GLN
1	A	405	ILE
1	A	409	THR
1	A	412	ILE
1	A	418	ASP
1	A	420	TRP
1	A	440	GLN
1	A	444	ASP
1	A	446	GLN
1	A	447	THR
1	A	449	GLU
1	A	453	SER
1	A	459	ASN
1	A	462	ASN
1	A	474	ARG
1	A	479	LYS
1	A	480	LYS
1	A	489	THR
1	A	498	ILE
1	A	506	THR

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Mol	Chain	Res	Type
1	A	511	PHE
1	A	519	ASP
1	A	520	VAL
1	A	524	ASP
1	A	525	ASP
1	A	527	LEU
1	A	529	LEU
1	A	537	GLU
1	A	543	ASP
1	A	545	GLU
1	A	550	ILE
1	A	552	VAL
1	A	559	ARG
1	A	566	PHE
1	A	571	MET
1	A	573	LEU
1	A	579	SER
1	A	580	ILE
1	A	594	LEU
1	A	599	TYR
1	A	602	SER
1	A	604	ASP
1	A	614	SER
1	A	620	ASP
1	A	626	ASP
1	A	636	ILE
1	A	647	TYR
1	A	661	ILE
1	B	137	THR
1	B	143	ILE
1	B	148	VAL
1	B	149	GLN
1	B	155	ASP
1	B	162	VAL
1	B	165	GLU
1	B	180	THR
1	B	181	SER
1	B	221	ILE
1	B	222	SER
1	B	226	VAL
1	B	246	THR
1	B	254	VAL

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Mol	Chain	Res	Type
1	B	265	ILE
1	B	266	PHE
1	B	277	HIS
1	B	279	MET
1	B	280	SER
1	B	286	SER
1	B	291	ILE
1	B	299	TYR
1	B	314	THR
1	B	331	MET
1	B	332	LEU
1	B	339	CYS
1	B	348	LEU
1	B	357	ASP
1	B	361	PHE
1	B	363	ILE
1	B	366	PHE
1	B	368	PHE
1	B	378	GLN
1	B	380	THR
1	B	384	SER
1	B	385	THR
1	B	388	PHE
1	B	392	THR
1	B	397	GLN
1	B	398	LYS
1	B	401	GLU
1	B	402	MET
1	B	405	ILE
1	B	407	VAL
1	B	412	ILE
1	B	425	ILE
1	B	435	TYR
1	B	438	THR
1	B	444	ASP
1	B	445	ILE
1	B	446	GLN
1	B	447	THR
1	B	448	LYS
1	B	449	GLU
1	B	450	GLU
1	B	452	GLU

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Mol	Chain	Res	Type
1	B	453	SER
1	B	456	ILE
1	B	457	ILE
1	B	458	SER
1	B	460	ASN
1	B	463	PHE
1	B	466	MET
1	B	471	SER
1	B	472	LEU
1	B	481	VAL
1	B	487	ILE
1	B	489	THR
1	B	491	THR
1	B	494	GLU
1	B	498	ILE
1	B	501	ASN
1	B	502	THR
1	B	508	ILE
1	B	511	PHE
1	B	512	GLN
1	B	513	ASP
1	B	519	ASP
1	B	523	SER
1	B	527	LEU
1	B	537	GLU
1	B	543	ASP
1	B	550	ILE
1	B	571	MET
1	B	579	SER
1	B	586	GLN
1	B	589	HIS
1	B	591	SER
1	B	600	LEU
1	B	602	SER
1	B	604	ASP
1	B	611	ILE
1	B	617	SER
1	B	619	PHE
1	B	623	ILE
1	B	624	ASP
1	B	626	ASP
1	B	636	ILE

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Mol	Chain	Res	Type
1	B	638	LYS
1	B	639	LEU
1	B	644	THR
1	B	647	TYR
1	B	652	LEU
1	B	654	LYS
1	B	657	LEU
1	B	660	ASN
1	B	661	ILE
1	C	129	SER
1	C	130	ILE
1	C	138	THR
1	C	143	ILE
1	C	146	PRO
1	C	150	MET
1	C	158	THR
1	C	163	ASP
1	C	165	GLU
1	C	180	THR
1	C	182	GLU
1	C	183	THR
1	C	192	SER
1	C	202	THR
1	C	207	LEU
1	C	209	VAL
1	C	212	SER
1	C	221	ILE
1	C	234	ILE
1	C	243	ILE
1	C	246	THR
1	C	265	ILE
1	C	266	PHE
1	C	270	ASP
1	C	274	THR
1	C	287	LEU
1	C	299	TYR
1	C	302	ASP
1	C	323	HIS
1	C	336	SER
1	C	344	LYS
1	C	348	LEU
1	C	357	ASP

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Mol	Chain	Res	Type
1	C	358	ILE
1	C	363	ILE
1	C	376	PHE
1	C	384	SER
1	C	391	ILE
1	C	394	THR
1	C	399	GLU
1	C	402	MET
1	C	403	LEU
1	C	405	ILE
1	C	412	ILE
1	C	413	VAL
1	C	418	ASP
1	C	438	THR
1	C	445	ILE
1	C	450	GLU
1	C	453	SER
1	C	455	MET
1	C	456	ILE
1	C	458	SER
1	C	462	ASN
1	C	472	LEU
1	C	473	GLN
1	C	489	THR
1	C	508	ILE
1	C	512	GLN
1	C	516	VAL
1	C	520	VAL
1	C	521	GLN
1	C	523	SER
1	C	524	ASP
1	C	526	THR
1	C	527	LEU
1	C	537	GLU
1	C	543	ASP
1	C	549	ARG
1	C	550	ILE
1	C	555	GLU
1	C	571	MET
1	C	572	LYS
1	C	580	ILE
1	C	584	ASN

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Mol	Chain	Res	Type
1	C	587	ILE
1	C	591	SER
1	C	608	VAL
1	C	624	ASP
1	C	636	ILE
1	C	639	LEU
1	C	641	PHE
1	C	647	TYR
1	C	650	ASN
1	C	661	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	173	HIS
1	A	184	GLN
1	A	191	GLN
1	A	203	HIS
1	A	260	GLN
1	A	277	HIS
1	A	293	ASN
1	A	297	ASN
1	A	304	ASN
1	A	323	HIS
1	A	371	ASN
1	A	377	ASN
1	A	397	GLN
1	A	439	ASN
1	A	440	GLN
1	A	443	ASN
1	A	459	ASN
1	A	460	ASN
1	A	478	ASN
1	A	501	ASN
1	A	514	ASN
1	A	521	GLN
1	A	569	ASN
1	A	584	ASN
1	A	593	GLN
1	A	598	ASN
1	B	135	GLN
1	B	149	GLN

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Mol	Chain	Res	Type
1	B	191	GLN
1	B	260	GLN
1	B	293	ASN
1	B	304	ASN
1	B	369	GLN
1	B	397	GLN
1	B	443	ASN
1	B	473	GLN
1	B	478	ASN
1	B	505	GLN
1	B	514	ASN
1	B	569	ASN
1	B	584	ASN
1	B	586	GLN
1	B	598	ASN
1	B	660	ASN
1	C	135	GLN
1	C	173	HIS
1	C	191	GLN
1	C	244	GLN
1	C	297	ASN
1	C	334	HIS
1	C	352	ASN
1	C	397	GLN
1	C	427	ASN
1	C	439	ASN
1	C	440	GLN
1	C	462	ASN
1	C	478	ASN
1	C	505	GLN
1	C	514	ASN
1	C	521	GLN
1	C	569	ASN
1	C	584	ASN
1	C	589	HIS
1	C	598	ASN
1	C	650	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 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	534/534 (100%)	1.79	189 (35%)  	48, 97, 120, 143	0
1	B	530/534 (99%)	1.72	197 (37%)  	48, 97, 112, 129	0
1	C	534/534 (100%)	1.77	195 (36%)  	49, 95, 113, 123	0
All	All	1598/1602 (99%)	1.76	581 (36%)  	48, 96, 115, 143	0

All (581) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	301	ASN	10.1
1	C	604	ASP	9.6
1	C	602	SER	9.3
1	A	637	GLY	8.5
1	C	513	ASP	7.0
1	A	404	GLY	6.9
1	A	644	THR	6.9
1	C	412	ILE	6.8
1	B	295	LEU	6.7
1	A	163	ASP	6.7
1	A	517	ASN	6.6
1	A	616	GLY	6.6
1	A	396	SER	6.4
1	A	167	GLU	6.3
1	A	300	ALA	6.2
1	B	654	LYS	6.1
1	A	164	SER	6.0
1	B	570	SER	5.8
1	C	534	GLY	5.5
1	B	477	GLY	5.4
1	A	406	GLY	5.3
1	C	283	ASP	5.2
1	B	164	SER	5.1

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Mol	Chain	Res	Type	RSRZ
1	C	419	GLY	5.1
1	C	514	ASN	5.1
1	C	270	ASP	5.0
1	A	171	SER	5.0
1	B	482	SER	5.0
1	A	165	GLU	5.0
1	B	378	GLN	5.0
1	B	555	GLU	5.0
1	B	478	ASN	4.9
1	C	425	ILE	4.9
1	A	460	ASN	4.8
1	C	567	TYR	4.8
1	C	541	GLY	4.8
1	C	600	LEU	4.8
1	A	514	ASN	4.8
1	C	214	SER	4.8
1	B	246	THR	4.7
1	C	365	PRO	4.7
1	B	567	TYR	4.6
1	C	427	ASN	4.6
1	C	426	PRO	4.6
1	A	235	VAL	4.6
1	A	482	SER	4.6
1	C	482	SER	4.6
1	A	515	HIS	4.5
1	B	434	ASP	4.5
1	A	299	TYR	4.5
1	A	366	PHE	4.5
1	C	459	ASN	4.4
1	A	424	THR	4.4
1	A	321	LYS	4.4
1	A	634	SER	4.4
1	B	435	TYR	4.4
1	A	379	GLU	4.4
1	B	188	LEU	4.4
1	B	660	ASN	4.4
1	C	331	MET	4.3
1	A	522	THR	4.3
1	B	569	ASN	4.3
1	C	382	GLY	4.3
1	B	315	LYS	4.3
1	A	505	GLN	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	642	PRO	4.3
1	C	601	LEU	4.3
1	A	386	PRO	4.2
1	C	369	GLN	4.2
1	A	361	PHE	4.2
1	A	433	GLY	4.2
1	C	506	THR	4.2
1	B	524	ASP	4.2
1	A	452	GLU	4.1
1	A	419	GLY	4.1
1	A	516	VAL	4.1
1	A	336	SER	4.1
1	B	560	GLY	4.1
1	B	525	ASP	4.1
1	A	534	GLY	4.1
1	A	659	SER	4.1
1	B	370	ALA	4.1
1	C	512	GLN	4.1
1	C	160	LYS	4.0
1	C	460	ASN	4.0
1	A	387	ARG	4.0
1	B	583	PHE	4.0
1	A	370	ALA	4.0
1	B	433	GLY	4.0
1	B	149	GLN	3.9
1	A	157	ALA	3.9
1	A	518	ARG	3.9
1	B	162	VAL	3.9
1	C	449	GLU	3.9
1	B	316	PRO	3.9
1	B	551	GLY	3.9
1	A	508	ILE	3.9
1	B	511	PHE	3.9
1	A	537	GLU	3.8
1	A	448	LYS	3.8
1	C	637	GLY	3.8
1	B	553	LEU	3.8
1	C	476	TRP	3.8
1	B	243	ILE	3.8
1	A	446	GLN	3.8
1	B	593	GLN	3.8
1	C	589	HIS	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	517	ASN	3.8
1	A	410	ASP	3.8
1	C	294	ASP	3.8
1	A	641	PHE	3.8
1	A	643	LEU	3.8
1	B	652	LEU	3.8
1	C	463	PHE	3.8
1	A	491	THR	3.8
1	B	267	THR	3.7
1	C	370	ALA	3.7
1	C	245	SER	3.7
1	B	307	GLY	3.7
1	C	316	PRO	3.7
1	B	305	SER	3.7
1	B	595	SER	3.7
1	C	238	PRO	3.7
1	B	216	GLU	3.7
1	C	225	GLY	3.7
1	A	473	GLN	3.6
1	A	159	GLY	3.6
1	B	459	ASN	3.6
1	C	562	ASN	3.6
1	A	642	PRO	3.6
1	C	129	SER	3.6
1	B	502	THR	3.6
1	C	415	GLY	3.6
1	A	509	ALA	3.6
1	C	616	GLY	3.6
1	B	206	LYS	3.6
1	B	634	SER	3.6
1	C	410	ASP	3.6
1	B	413	VAL	3.6
1	A	314	THR	3.6
1	A	161	SER	3.5
1	A	392	THR	3.5
1	A	378	GLN	3.5
1	B	574	GLY	3.5
1	C	450	GLU	3.5
1	C	329	GLY	3.5
1	B	408	ALA	3.5
1	C	253	HIS	3.5
1	B	169	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	530	LEU	3.4
1	C	282	THR	3.4
1	C	469	CYS	3.4
1	B	425	ILE	3.4
1	B	484	THR	3.4
1	A	155	ASP	3.4
1	A	400	GLY	3.4
1	A	501	ASN	3.4
1	B	283	ASP	3.4
1	A	542	ALA	3.4
1	B	557	GLY	3.4
1	A	347	SER	3.4
1	B	465	SER	3.4
1	B	163	ASP	3.4
1	C	162	VAL	3.4
1	A	158	THR	3.4
1	A	145	GLU	3.3
1	C	352	ASN	3.3
1	C	344	LYS	3.3
1	C	496	LYS	3.3
1	A	649	GLY	3.3
1	C	563	HIS	3.3
1	B	496	LYS	3.3
1	C	478	ASN	3.3
1	B	504	ASP	3.3
1	A	447	THR	3.3
1	B	566	PHE	3.3
1	A	337	VAL	3.3
1	B	584	ASN	3.3
1	B	406	GLY	3.3
1	A	662	ARG	3.2
1	B	568	ARG	3.2
1	B	458	SER	3.2
1	C	605	SER	3.2
1	C	137	THR	3.2
1	B	544	ARG	3.2
1	A	306	SER	3.2
1	B	146	PRO	3.2
1	C	422	ASP	3.2
1	A	415	GLY	3.2
1	B	640	GLU	3.2
1	A	597	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	398	LYS	3.2
1	A	369	GLN	3.2
1	A	504	ASP	3.2
1	B	364	ARG	3.2
1	B	428	GLU	3.2
1	C	216	GLU	3.2
1	A	280	SER	3.2
1	B	651	GLN	3.2
1	A	228	GLY	3.1
1	C	406	GLY	3.1
1	C	293	ASN	3.1
1	A	390	PRO	3.1
1	A	563	HIS	3.1
1	A	521	GLN	3.1
1	B	531	GLY	3.1
1	C	297	ASN	3.1
1	C	387	ARG	3.1
1	C	578	LYS	3.1
1	A	270	ASP	3.1
1	A	562	ASN	3.1
1	C	546	LYS	3.1
1	B	658	ALA	3.1
1	B	637	GLY	3.1
1	C	486	PHE	3.1
1	B	268	ILE	3.1
1	B	503	ILE	3.1
1	A	462	ASN	3.1
1	B	177	ASN	3.1
1	A	458	SER	3.1
1	A	283	ASP	3.1
1	B	352	ASN	3.0
1	C	371	ASN	3.0
1	C	261	VAL	3.0
1	A	322	PHE	3.0
1	B	241	GLU	3.0
1	A	445	ILE	3.0
1	B	460	ASN	3.0
1	B	589	HIS	3.0
1	C	363	ILE	3.0
1	B	426	PRO	3.0
1	C	327	PRO	3.0
1	C	599	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	304	ASN	3.0
1	A	368	PHE	3.0
1	C	296	ILE	3.0
1	B	147	SER	3.0
1	B	592	ARG	3.0
1	A	638	LYS	3.0
1	A	457	ILE	3.0
1	C	220	SER	3.0
1	A	418	ASP	3.0
1	C	620	ASP	3.0
1	B	506	THR	3.0
1	B	379	GLU	2.9
1	C	396	SER	2.9
1	B	373	HIS	2.9
1	B	520	VAL	2.9
1	C	535	ILE	2.9
1	C	550	ILE	2.9
1	C	429	LEU	2.9
1	C	474	ARG	2.9
1	A	384	SER	2.9
1	C	136	GLY	2.9
1	C	423	THR	2.9
1	C	537	GLU	2.9
1	A	577	ILE	2.9
1	C	598	ASN	2.9
1	B	339	CYS	2.9
1	C	559	ARG	2.9
1	C	625	SER	2.9
1	B	244	GLN	2.9
1	C	523	SER	2.8
1	A	257	ASP	2.8
1	C	163	ASP	2.8
1	A	660	ASN	2.8
1	B	245	SER	2.8
1	B	260	GLN	2.8
1	A	202	THR	2.8
1	A	422	ASP	2.8
1	C	353	ARG	2.8
1	C	383	TRP	2.8
1	B	186	LYS	2.8
1	C	244	GLN	2.8
1	B	585	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	554	PRO	2.8
1	B	507	LYS	2.8
1	B	519	ASP	2.8
1	A	459	ASN	2.8
1	C	508	ILE	2.8
1	A	617	SER	2.8
1	B	523	SER	2.8
1	C	573	LEU	2.8
1	A	376	PHE	2.8
1	B	228	GLY	2.8
1	C	574	GLY	2.8
1	C	448	LYS	2.8
1	A	492	VAL	2.8
1	A	614	SER	2.8
1	C	384	SER	2.8
1	A	399	GLU	2.8
1	B	598	ASN	2.7
1	A	589	HIS	2.7
1	B	505	GLN	2.7
1	C	345	SER	2.7
1	A	372	ARG	2.7
1	A	610	ARG	2.7
1	C	364	ARG	2.7
1	C	184	GLN	2.7
1	C	520	VAL	2.7
1	B	468	ILE	2.7
1	C	361	PHE	2.7
1	A	380	THR	2.7
1	B	344	LYS	2.7
1	A	432	ALA	2.7
1	C	130	ILE	2.7
1	C	140	GLY	2.7
1	C	229	GLY	2.7
1	C	428	GLU	2.7
1	C	477	GLY	2.7
1	B	464	LYS	2.7
1	C	585	SER	2.7
1	A	520	VAL	2.7
1	B	562	ASN	2.7
1	A	397	GLN	2.7
1	A	603	PRO	2.7
1	B	358	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	546	LYS	2.7
1	C	155	ASP	2.7
1	B	304	ASN	2.7
1	B	514	ASN	2.7
1	A	395	ILE	2.6
1	B	499	PRO	2.6
1	C	156	MET	2.6
1	C	262	GLU	2.6
1	A	331	MET	2.6
1	B	559	ARG	2.6
1	B	405	ILE	2.6
1	B	620	ASP	2.6
1	B	399	GLU	2.6
1	B	423	THR	2.6
1	C	489	THR	2.6
1	C	522	THR	2.6
1	C	161	SER	2.6
1	C	515	HIS	2.6
1	A	440	GLN	2.6
1	B	476	TRP	2.6
1	C	479	LYS	2.6
1	C	568	ARG	2.6
1	B	467	TYR	2.6
1	B	356	SER	2.6
1	C	386	PRO	2.6
1	A	604	ASP	2.6
1	A	624	ASP	2.6
1	B	649	GLY	2.6
1	B	495	ASN	2.6
1	C	201	LEU	2.6
1	B	518	ARG	2.6
1	A	183	THR	2.6
1	B	334	HIS	2.5
1	B	365	PRO	2.5
1	C	330	SER	2.5
1	A	519	ASP	2.5
1	C	518	ARG	2.5
1	C	654	LYS	2.5
1	A	476	TRP	2.5
1	B	412	ILE	2.5
1	C	491	THR	2.5
1	A	635	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	657	LEU	2.5
1	C	164	SER	2.5
1	A	584	ASN	2.5
1	C	432	ALA	2.5
1	B	178	TRP	2.5
1	C	359	THR	2.5
1	A	600	LEU	2.5
1	C	348	LEU	2.5
1	A	371	ASN	2.5
1	B	437	ILE	2.5
1	C	416	ILE	2.5
1	A	461	THR	2.5
1	A	269	PRO	2.5
1	A	575	TYR	2.5
1	B	603	PRO	2.5
1	B	372	ARG	2.5
1	B	223	GLY	2.5
1	B	561	GLY	2.5
1	C	151	SER	2.5
1	C	542	ALA	2.5
1	B	494	GLU	2.5
1	B	488	THR	2.5
1	C	590	THR	2.5
1	A	572	LYS	2.5
1	C	186	LYS	2.5
1	C	269	PRO	2.5
1	C	292	TYR	2.5
1	B	457	ILE	2.4
1	B	659	SER	2.4
1	C	243	ILE	2.4
1	A	364	ARG	2.4
1	B	360	ASP	2.4
1	A	393	VAL	2.4
1	B	382	GLY	2.4
1	C	455	MET	2.4
1	C	507	LYS	2.4
1	A	423	THR	2.4
1	B	422	ASP	2.4
1	C	621	ILE	2.4
1	A	216	GLU	2.4
1	B	160	LYS	2.4
1	C	638	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	374	PHE	2.4
1	B	214	SER	2.4
1	A	131	THR	2.4
1	A	344	LYS	2.4
1	A	496	LYS	2.4
1	A	549	ARG	2.4
1	B	369	GLN	2.4
1	C	250	GLN	2.4
1	C	167	GLU	2.4
1	B	175	SER	2.4
1	B	222	SER	2.4
1	C	224	SER	2.4
1	C	346	SER	2.4
1	C	465	SER	2.4
1	C	570	SER	2.4
1	B	337	VAL	2.4
1	C	421	PRO	2.4
1	B	272	ARG	2.3
1	A	403	LEU	2.3
1	B	184	GLN	2.3
1	B	512	GLN	2.3
1	A	420	TRP	2.3
1	B	282	THR	2.3
1	C	430	ILE	2.3
1	B	203	HIS	2.3
1	A	532	TYR	2.3
1	C	377	ASN	2.3
1	C	443	ASN	2.3
1	A	275	LEU	2.3
1	A	241	GLU	2.3
1	B	165	GLU	2.3
1	A	162	VAL	2.3
1	B	479	LYS	2.3
1	B	605	SER	2.3
1	C	215	ILE	2.3
1	C	180	THR	2.3
1	C	200	TYR	2.3
1	B	427	ASN	2.3
1	B	462	ASN	2.3
1	C	271	LEU	2.3
1	C	376	PHE	2.3
1	B	294	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	428	GLU	2.3
1	B	318	PRO	2.3
1	B	414	PRO	2.3
1	A	645	ALA	2.3
1	C	607	ALA	2.3
1	B	273	SER	2.3
1	B	614	SER	2.3
1	B	529	LEU	2.3
1	A	598	ASN	2.3
1	C	483	ASN	2.3
1	B	613	ASP	2.3
1	A	398	LYS	2.3
1	B	421	PRO	2.3
1	B	577	ILE	2.3
1	A	172	PHE	2.3
1	C	521	GLN	2.3
1	A	140	GLY	2.2
1	A	194	GLY	2.2
1	B	455	MET	2.2
1	C	658	ALA	2.2
1	C	295	LEU	2.2
1	C	274	THR	2.2
1	A	292	TYR	2.2
1	B	286	SER	2.2
1	A	389	ARG	2.2
1	B	259	ARG	2.2
1	C	372	ARG	2.2
1	C	481	VAL	2.2
1	B	513	ASP	2.2
1	A	661	ILE	2.2
1	A	263	PRO	2.2
1	B	141	GLY	2.2
1	B	351	GLY	2.2
1	C	424	THR	2.2
1	C	389	ARG	2.2
1	B	393	VAL	2.2
1	C	337	VAL	2.2
1	A	377	ASN	2.2
1	B	483	ASN	2.2
1	A	405	ILE	2.2
1	B	257	ASP	2.2
1	A	229	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	279	MET	2.2
1	B	516	VAL	2.2
1	B	135	GLN	2.2
1	A	365	PRO	2.2
1	A	421	PRO	2.2
1	B	645	ALA	2.2
1	C	418	ASP	2.2
1	C	169	PHE	2.2
1	C	549	ARG	2.2
1	A	407	VAL	2.2
1	C	608	VAL	2.2
1	B	508	ILE	2.2
1	C	247	SER	2.2
1	C	347	SER	2.2
1	A	494	GLU	2.2
1	A	186	LYS	2.2
1	A	574	GLY	2.2
1	B	269	PRO	2.2
1	A	218	ARG	2.2
1	A	360	ASP	2.2
1	C	368	PHE	2.2
1	A	548	VAL	2.1
1	B	639	LEU	2.1
1	A	160	LYS	2.1
1	B	306	SER	2.1
1	C	634	SER	2.1
1	A	343	PRO	2.1
1	B	630	PHE	2.1
1	C	619	PHE	2.1
1	C	641	PHE	2.1
1	B	410	ASP	2.1
1	A	211	TRP	2.1
1	B	180	THR	2.1
1	B	341	LEU	2.1
1	A	593	GLN	2.1
1	A	545	GLU	2.1
1	B	500	SER	2.1
1	C	603	PRO	2.1
1	A	650	ASN	2.1
1	C	366	PHE	2.1
1	B	515	HIS	2.1
1	A	234	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	271	LEU	2.1
1	C	394	THR	2.1
1	C	529	LEU	2.1
1	C	577	ILE	2.1
1	A	239	GLY	2.1
1	C	561	GLY	2.1
1	C	569	ASN	2.1
1	A	582	VAL	2.1
1	B	604	ASP	2.1
1	A	353	ARG	2.1
1	A	385	THR	2.1
1	B	392	THR	2.1
1	B	424	THR	2.1
1	C	447	THR	2.1
1	A	351	GLY	2.1
1	A	585	SER	2.1
1	A	293	ASN	2.1
1	A	493	LYS	2.1
1	A	495	ASN	2.1
1	B	215	ILE	2.1
1	C	504	ASP	2.1
1	B	292	TYR	2.1
1	C	484	THR	2.1
1	A	135	GLN	2.1
1	C	557	GLY	2.1
1	A	417	PRO	2.1
1	B	262	GLU	2.1
1	B	463	PHE	2.1
1	B	537	GLU	2.1
1	C	388	PHE	2.1
1	A	212	SER	2.0
1	A	500	SER	2.0
1	B	445	ILE	2.0
1	B	501	ASN	2.0
1	B	436	ALA	2.0
1	C	375	ASP	2.0
1	C	385	THR	2.0
1	C	644	THR	2.0
1	A	401	GLU	2.0
1	C	572	LYS	2.0
1	A	568	ARG	2.0
1	C	662	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	565	ILE	2.0
1	A	455	MET	2.0
1	A	137	THR	2.0
1	B	526	THR	2.0
1	B	644	THR	2.0
1	C	284	THR	2.0
1	C	213	GLY	2.0
1	C	351	GLY	2.0
1	B	576	VAL	2.0
1	C	142	VAL	2.0
1	A	430	ILE	2.0
1	B	187	ILE	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.