



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 12:14 AM UTC

PDB ID : 3P03 / pdb_00003p03
Title : Crystal structure of BetP-G153D with choline bound
Authors : Perez, C.; Ressler, S.; Ziegler, Z.
Deposited on : 2010-09-27
Resolution : 3.35 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

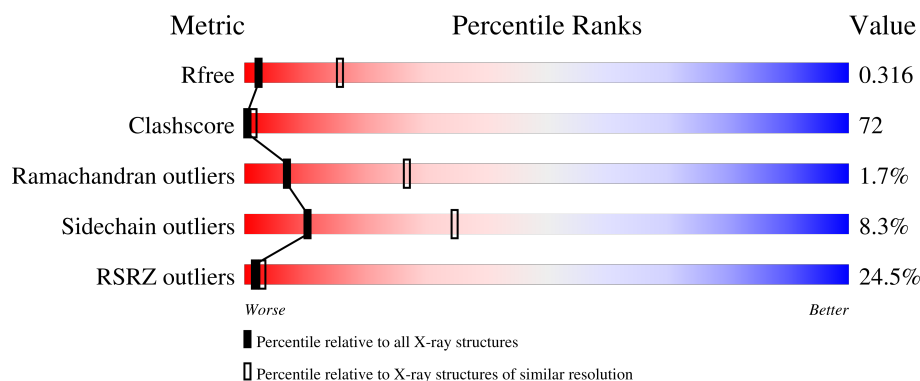
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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	566	25% 26% 56% 6% 11%
1	B	566	26% 26% 51% 7% 16%
1	C	566	13% 24% 54% 11% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CHT	C	2486	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11349 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.

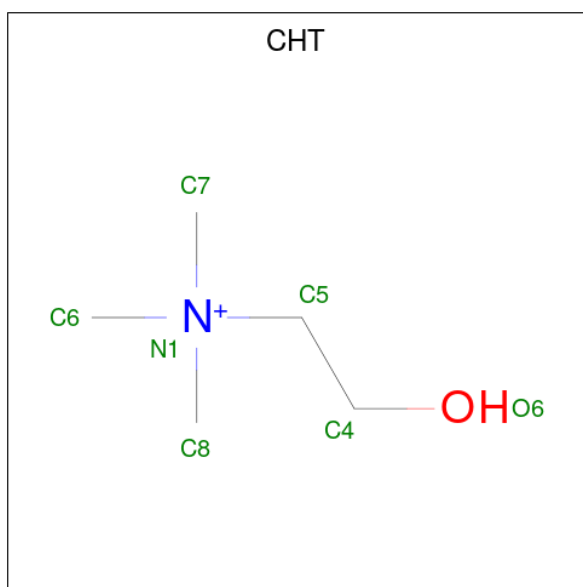
- Molecule 1 is a protein called Glycine betaine transporter BetP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	504	Total	C	N	O	S	0	0	0
			3868	2542	641	669	16			
1	B	476	Total	C	N	O	S	0	0	0
			3612	2391	577	628	16			
1	C	508	Total	C	N	O	S	0	0	0
			3862	2545	627	674	16			

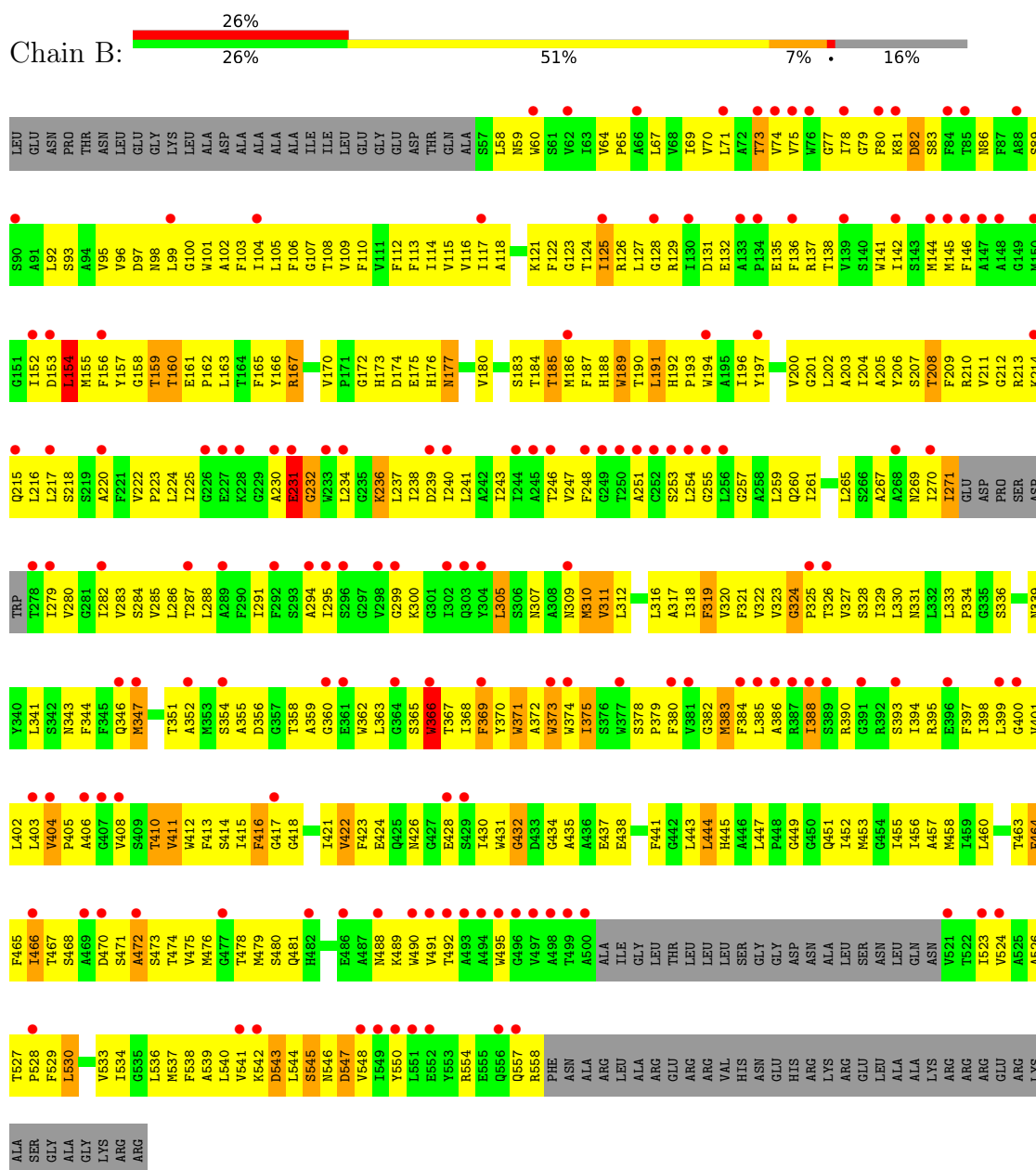
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	ALA	GLU	engineered mutation	UNP P54582
A	45	ALA	GLU	engineered mutation	UNP P54582
A	46	ALA	GLU	engineered mutation	UNP P54582
A	153	ASP	GLY	engineered mutation	UNP P54582
B	44	ALA	GLU	engineered mutation	UNP P54582
B	45	ALA	GLU	engineered mutation	UNP P54582
B	46	ALA	GLU	engineered mutation	UNP P54582
B	153	ASP	GLY	engineered mutation	UNP P54582
C	44	ALA	GLU	engineered mutation	UNP P54582
C	45	ALA	GLU	engineered mutation	UNP P54582
C	46	ALA	GLU	engineered mutation	UNP P54582
C	153	ASP	GLY	engineered mutation	UNP P54582

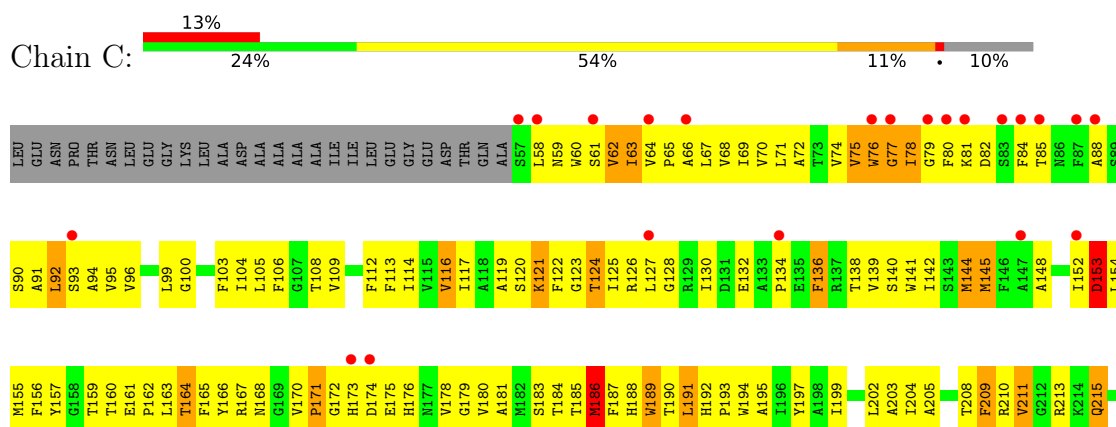
- Molecule 2 is CHOLINE ION (CCD ID: CHT) (formula: C₅H₁₄NO).

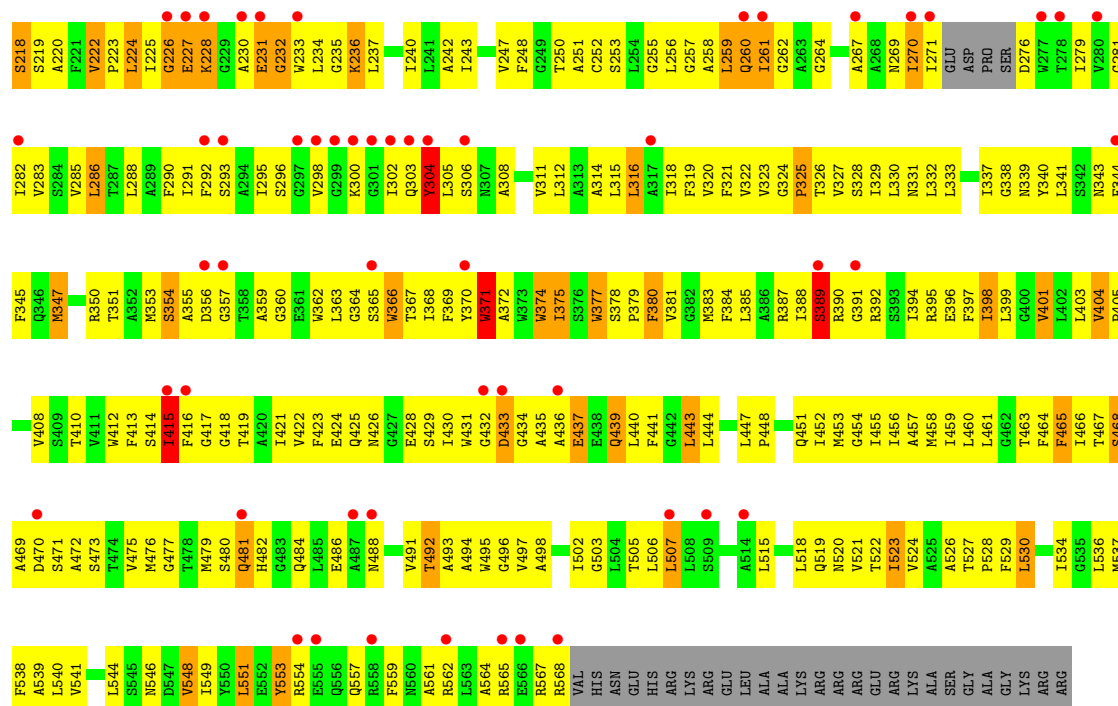


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	C	1	7	5	1	1	0	0



• Molecule 1: Glycine betaine transporter BetP





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.56Å 129.31Å 183.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.20 – 3.35 46.20 – 3.35	Depositor EDS
% Data completeness (in resolution range)	91.2 (46.20-3.35) 91.1 (46.20-3.35)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	15.91 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.6.2_432	Depositor
R, R_{free}	0.245 , 0.300 0.278 , 0.316	Depositor DCC
R_{free} test set	3712 reflections (9.95%)	wwPDB-VP
Wilson B-factor (Å ²)	70.2	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 115.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	11349	wwPDB-VP
Average B, all atoms (Å ²)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.43	1/3967 (0.0%)	0.96	15/5397 (0.3%)
1	B	0.47	0/3706	1.03	23/5051 (0.5%)
1	C	0.57	2/3960 (0.1%)	1.13	37/5396 (0.7%)
All	All	0.50	3/11633 (0.0%)	1.04	75/15844 (0.5%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	368	ILE	CA-CB	-7.01	1.44	1.54
1	C	366	TRP	CA-C	-6.50	1.48	1.52
1	C	371	TRP	C-O	-5.21	1.18	1.24

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	77	GLY	N-CA-C	10.54	125.37	112.73
1	C	415	ILE	N-CA-C	9.99	119.92	110.53
1	A	155	MET	N-CA-C	9.41	121.30	111.14
1	B	160	THR	N-CA-C	9.01	121.18	111.36
1	C	63	ILE	N-CA-C	8.88	118.94	110.42
1	A	352	ALA	N-CA-C	-8.75	101.71	112.38
1	C	260	GLN	N-CA-C	-8.72	101.86	111.36
1	B	366	TRP	N-CA-C	8.67	123.73	112.12
1	C	209	PHE	N-CA-C	8.61	120.75	111.36
1	C	366	TRP	CA-C-O	7.94	125.32	119.68
1	A	543	ASP	N-CA-C	7.81	119.87	111.36
1	C	228	LYS	N-CA-C	-7.76	101.26	111.74
1	C	236	LYS	N-CA-C	-7.76	101.80	111.11
1	C	403	LEU	N-CA-C	7.69	119.44	111.14
1	C	365	SER	N-CA-C	7.55	119.51	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	90	SER	N-CA-C	-7.54	104.22	113.41
1	C	401	VAL	N-CA-C	7.45	117.57	110.42
1	C	62	VAL	N-CA-C	7.12	118.76	111.00
1	C	93	SER	N-CA-C	-7.12	103.52	111.28
1	C	226	GLY	N-CA-C	-7.09	103.06	111.36
1	B	548	VAL	N-CA-C	7.04	117.80	110.62
1	C	99	LEU	N-CA-C	-6.96	102.89	113.89
1	B	81	LYS	N-CA-C	-6.90	104.60	113.16
1	C	261	ILE	N-CA-C	6.79	117.54	110.62
1	B	472	ALA	N-CA-C	-6.53	104.24	111.82
1	A	367	THR	CA-C-N	-6.53	109.06	120.29
1	A	367	THR	C-N-CA	-6.53	109.06	120.29
1	B	547	ASP	N-CA-C	-6.46	102.20	110.53
1	A	144	MET	N-CA-C	6.36	118.22	111.28
1	B	208	THR	N-CA-C	6.36	121.13	112.68
1	B	351	THR	N-CA-C	-6.32	101.58	110.50
1	C	356	ASP	N-CA-C	-6.30	105.54	113.23
1	B	236	LYS	N-CA-C	-6.22	104.50	111.28
1	C	404	VAL	N-CA-C	6.20	119.79	112.35
1	C	191	LEU	N-CA-C	6.12	117.95	111.28
1	A	95	VAL	N-CA-C	5.99	116.77	110.72
1	B	73	THR	N-CA-C	5.85	117.66	111.28
1	C	262	GLY	N-CA-C	-5.84	105.72	112.73
1	A	225	ILE	N-CA-C	-5.76	106.70	112.17
1	C	366	TRP	CB-CA-C	-5.68	104.24	114.52
1	B	324	GLY	N-CA-C	-5.67	100.76	112.34
1	A	296	SER	N-CA-C	5.61	117.47	111.36
1	C	389	SER	N-CA-C	5.60	117.39	111.28
1	C	127	LEU	N-CA-C	-5.54	102.19	110.23
1	A	566	GLU	N-CA-C	-5.49	104.94	111.03
1	C	78	ILE	N-CA-C	5.48	116.28	111.56
1	A	364	GLY	N-CA-C	-5.48	106.15	112.73
1	C	153	ASP	CA-C-N	-5.48	112.51	120.29
1	C	153	ASP	C-N-CA	-5.48	112.51	120.29
1	C	186	MET	N-CA-C	-5.47	105.31	111.28
1	B	449	GLY	N-CA-C	-5.47	107.70	115.30
1	C	300	LYS	CB-CA-C	-5.46	110.30	116.63
1	C	171	PRO	N-CA-C	-5.44	102.65	111.03
1	A	369	PHE	N-CA-C	5.44	117.91	111.33
1	C	338	GLY	N-CA-C	5.43	119.24	112.73
1	C	211	VAL	N-CA-C	-5.42	107.46	112.83
1	C	408	VAL	CB-CA-C	-5.41	104.77	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	HIS	N-CA-C	5.39	117.26	109.07
1	B	489	LYS	N-CA-C	5.39	117.15	111.28
1	B	189	TRP	N-CA-C	5.35	118.95	111.56
1	B	404	VAL	CB-CA-C	-5.35	108.68	114.35
1	C	145	MET	N-CA-C	5.33	117.09	111.28
1	B	174	ASP	N-CA-C	-5.32	102.58	110.46
1	A	485	LEU	N-CA-C	5.32	117.16	111.36
1	C	354	SER	N-CA-C	-5.23	101.18	109.96
1	B	159	THR	N-CA-C	5.16	116.99	111.36
1	B	231	GLU	N-CA-C	5.16	121.79	110.80
1	C	293	SER	N-CA-C	-5.15	106.10	112.38
1	B	344	PHE	N-CA-C	5.12	116.55	111.07
1	B	422	VAL	CB-CA-C	-5.10	105.34	112.02
1	B	416	PHE	N-CA-C	5.08	116.62	111.14
1	B	124	THR	N-CA-C	5.05	116.78	111.28
1	A	408	VAL	N-CA-C	-5.04	106.77	111.45
1	C	419	THR	N-CA-C	-5.03	107.28	113.41
1	B	167	ARG	N-CA-C	5.01	116.55	111.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3868	0	3897	529	0
1	B	3612	0	3647	560	0
1	C	3862	0	3899	600	0
2	C	7	0	14	6	0
All	All	11349	0	11457	1649	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 72.

All (1649) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:VAL:CG1	1:C:171:PRO:HD2	1.50	1.41
1:C:226:GLY:HA2	1:C:227:GLU:CB	1.47	1.40
1:C:247:VAL:HG12	1:C:502:ILE:CD1	1.54	1.35
1:B:69:ILE:O	1:B:73:THR:HG23	1.33	1.29
1:B:208:THR:HG22	1:B:213:ARG:O	1.32	1.27
1:C:173:HIS:HD2	1:C:180:VAL:CG1	1.47	1.25
1:C:363:LEU:CD2	1:C:367:THR:HG21	1.66	1.24
1:A:369:PHE:CE1	1:A:519:GLN:HB2	1.72	1.24
1:C:64:VAL:CG1	1:C:65:PRO:HD3	1.67	1.23
1:C:173:HIS:CD2	1:C:180:VAL:HG11	1.72	1.23
1:C:247:VAL:CG1	1:C:502:ILE:HD11	1.68	1.22
1:C:148:ALA:O	2:C:2486:CHT:H62	1.26	1.22
1:A:153:ASP:HA	1:A:156:PHE:CE2	1.79	1.17
1:C:64:VAL:HG13	1:C:65:PRO:HD3	1.22	1.17
1:B:309:ASN:ND2	1:B:464:PHE:HD2	1.41	1.16
1:A:418:GLY:O	1:A:422:VAL:HG23	1.41	1.15
1:C:173:HIS:CD2	1:C:180:VAL:CG1	2.27	1.15
1:C:170:VAL:HG12	1:C:171:PRO:CD	1.76	1.15
1:A:559:PHE:CE2	1:A:563:LEU:HD12	1.82	1.15
1:C:247:VAL:CG1	1:C:502:ILE:CD1	2.24	1.15
1:C:304:TYR:HD1	1:C:305:LEU:N	1.45	1.14
1:C:134:PRO:HA	1:C:391:GLY:HA3	1.31	1.12
1:A:343:ASN:O	1:A:347:MET:HG3	1.46	1.12
1:B:398:ILE:O	1:B:402:LEU:HD13	1.49	1.12
1:C:261:ILE:HD11	1:C:461:LEU:HB2	1.25	1.12
1:A:369:PHE:CZ	1:A:519:GLN:HB2	1.85	1.11
1:B:201:GLY:HA3	1:B:385:LEU:HD11	1.26	1.11
1:C:105:LEU:O	1:C:109:VAL:HG23	1.51	1.11
1:B:343:ASN:O	1:B:347:MET:HG2	1.51	1.10
1:C:226:GLY:CA	1:C:227:GLU:HB3	1.82	1.10
1:C:363:LEU:HD22	1:C:367:THR:HG21	1.09	1.09
1:C:144:MET:HG2	1:C:388:ILE:HD11	1.19	1.09
1:A:60:TRP:HA	1:A:63:ILE:HG22	1.27	1.09
1:B:92:LEU:HD11	1:B:523:ILE:HB	1.33	1.08
1:B:190:THR:O	1:B:194:TRP:HD1	1.34	1.08
1:B:196:ILE:HD11	1:B:374:TRP:HB3	1.34	1.07
1:C:237:LEU:O	1:C:240:ILE:HG22	1.55	1.07
1:B:312:LEU:HB3	1:B:460:LEU:HD21	1.12	1.07
1:A:570:HIS:O	1:A:574:ARG:HD3	1.55	1.06
1:C:173:HIS:HD2	1:C:180:VAL:HG11	0.99	1.06
1:A:351:THR:CG2	1:C:331:ASN:HB3	1.85	1.06
1:B:309:ASN:OD1	1:B:463:THR:HG21	1.56	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:GLY:CA	1:C:227:GLU:CB	2.31	1.06
1:A:89:SER:HA	1:A:520:ASN:HD21	1.20	1.05
1:B:141:TRP:HA	1:B:144:MET:HE2	1.39	1.04
1:B:208:THR:O	1:B:212:GLY:HA2	1.57	1.04
1:C:226:GLY:HA2	1:C:227:GLU:HB3	1.10	1.04
1:B:200:VAL:HG21	1:B:378:SER:HB3	1.04	1.04
1:C:224:LEU:HD11	1:C:539:ALA:N	1.71	1.03
1:C:304:TYR:CE1	1:C:305:LEU:HG	1.93	1.03
1:B:312:LEU:HB3	1:B:460:LEU:CD2	1.87	1.03
1:A:123:GLY:HA2	1:A:394:ILE:HB	1.37	1.03
1:B:114:ILE:O	1:B:117:ILE:HG22	1.58	1.03
1:C:144:MET:HG2	1:C:388:ILE:CD1	1.88	1.03
1:C:375:ILE:HD13	1:C:530:LEU:HA	1.39	1.02
1:A:478:THR:HA	1:A:481:GLN:NE2	1.72	1.02
1:A:329:ILE:HD11	1:A:419:THR:CG2	1.89	1.02
1:B:369:PHE:CD1	1:B:523:ILE:HD11	1.95	1.02
1:C:363:LEU:HA	1:C:367:THR:HG22	1.40	1.01
1:A:412:TRP:CE2	1:A:416:PHE:CE2	2.48	1.01
1:C:188:HIS:CG	1:C:370:TYR:CD2	2.49	1.01
1:C:224:LEU:HD11	1:C:539:ALA:CA	1.89	1.01
1:C:126:ARG:HD3	1:C:132:GLU:O	1.61	1.01
1:C:226:GLY:HA2	1:C:227:GLU:HB2	1.32	1.01
1:C:163:LEU:HG	1:C:431:TRP:HZ3	1.22	1.00
1:C:343:ASN:O	1:C:347:MET:HG2	1.60	1.00
1:A:64:VAL:HG23	1:A:65:PRO:HD3	1.44	1.00
1:C:295:ILE:HD11	1:C:493:ALA:HB2	1.38	1.00
1:C:76:TRP:HE1	1:C:85:THR:CB	1.73	1.00
1:A:412:TRP:CZ2	1:A:416:PHE:CE2	2.50	0.99
1:C:91:ALA:O	1:C:94:ALA:HB3	1.61	0.99
1:C:108:THR:HA	1:C:192:HIS:CE1	1.97	0.99
1:A:310:MET:O	1:A:314:ALA:HB3	1.63	0.99
1:A:481:GLN:O	1:A:482:HIS:HB2	1.62	0.98
1:B:200:VAL:HG11	1:B:378:SER:O	1.64	0.98
1:C:121:LYS:H	1:C:121:LYS:HD3	1.28	0.98
1:B:366:TRP:O	1:B:370:TYR:HB2	1.63	0.98
1:A:559:PHE:HE2	1:A:563:LEU:HD12	1.12	0.98
1:C:260:GLN:CD	1:C:461:LEU:HD21	1.89	0.98
1:A:344:PHE:C	1:A:344:PHE:HD2	1.70	0.97
1:A:309:ASN:CG	1:A:464:PHE:HE1	1.70	0.97
1:C:76:TRP:HE1	1:C:85:THR:CA	1.76	0.97
1:A:351:THR:HG21	1:C:331:ASN:HB3	1.43	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:LYS:HB2	1:A:84:PHE:HB2	1.46	0.97
1:B:473:SER:HB2	1:B:492:THR:O	1.63	0.97
1:C:188:HIS:CD2	1:C:370:TYR:CD2	2.53	0.97
1:C:61:SER:O	1:C:65:PRO:HG2	1.64	0.97
1:B:110:PHE:CD1	1:B:196:ILE:HG22	2.01	0.96
1:A:215:GLN:HB3	1:A:483:GLY:O	1.65	0.96
1:A:60:TRP:HA	1:A:63:ILE:CG2	1.95	0.96
1:C:81:LYS:HB3	1:C:84:PHE:HD2	1.29	0.96
1:A:344:PHE:C	1:A:344:PHE:CD2	2.40	0.95
1:C:92:LEU:HD13	1:C:520:ASN:HA	1.48	0.95
1:C:188:HIS:CD2	1:C:370:TYR:HD2	1.84	0.95
1:C:304:TYR:CD1	1:C:305:LEU:N	2.35	0.95
1:A:113:PHE:CE1	1:A:117:ILE:HD11	2.02	0.95
1:A:153:ASP:HA	1:A:156:PHE:HE2	1.16	0.94
1:B:320:VAL:HG23	1:B:415:ILE:CG2	1.98	0.94
1:B:114:ILE:HA	1:B:117:ILE:HG22	1.48	0.94
1:B:129:ARG:H	1:B:390:ARG:HH12	1.03	0.94
1:C:329:ILE:HD13	1:C:415:ILE:HG23	1.47	0.94
1:C:210:ARG:HH22	1:C:549:ILE:HD12	1.30	0.94
1:B:327:VAL:HG23	1:B:328:SER:H	1.30	0.94
1:B:488:ASN:OD1	1:B:490:TRP:HZ3	1.47	0.94
1:C:170:VAL:CG1	1:C:171:PRO:CD	2.41	0.93
1:A:445:HIS:HA	1:A:450:GLY:HA3	1.50	0.93
1:B:327:VAL:HG23	1:B:328:SER:N	1.82	0.93
1:B:411:VAL:O	1:B:415:ILE:HD12	1.68	0.93
1:A:305:LEU:HD22	1:A:467:THR:HG22	1.52	0.92
1:B:200:VAL:CG2	1:B:378:SER:HB3	1.99	0.92
1:B:186:MET:O	1:B:190:THR:HG23	1.69	0.92
1:B:411:VAL:HG13	1:B:415:ILE:CD1	2.00	0.92
1:C:144:MET:CG	1:C:388:ILE:CD1	2.46	0.92
1:B:92:LEU:CD1	1:B:523:ILE:HB	1.99	0.92
1:C:170:VAL:HG12	1:C:171:PRO:HD2	0.92	0.92
1:C:81:LYS:HB3	1:C:84:PHE:CD2	2.05	0.92
1:C:76:TRP:HE1	1:C:85:THR:HA	1.32	0.91
1:B:125:ILE:HG21	1:B:210:ARG:NH2	1.85	0.91
1:C:363:LEU:HD22	1:C:367:THR:CG2	1.97	0.91
1:B:186:MET:HG2	1:B:190:THR:HG21	1.52	0.91
1:C:64:VAL:HG13	1:C:65:PRO:CD	2.00	0.91
1:C:261:ILE:HD11	1:C:461:LEU:CB	2.01	0.91
1:C:144:MET:CG	1:C:388:ILE:HD11	2.00	0.90
1:C:381:VAL:HG12	1:C:385:LEU:HD12	1.54	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:THR:N	1:A:528:PRO:HD2	1.87	0.89
1:C:209:PHE:CZ	1:C:390:ARG:HB2	2.07	0.89
1:B:370:TYR:O	1:B:374:TRP:CD1	2.25	0.89
1:C:76:TRP:NE1	1:C:85:THR:HA	1.86	0.89
1:B:74:VAL:O	1:B:78:ILE:HG12	1.73	0.89
1:B:114:ILE:CA	1:B:117:ILE:HG22	2.03	0.89
1:B:316:LEU:HD22	1:B:460:LEU:CD1	2.01	0.89
1:C:103:PHE:CE2	1:C:530:LEU:CD2	2.56	0.89
1:B:161:GLU:HG2	1:B:185:THR:OG1	1.74	0.88
1:B:524:VAL:HA	1:B:527:THR:OG1	1.72	0.88
1:C:170:VAL:HG13	1:C:171:PRO:HD2	1.55	0.88
1:B:460:LEU:O	1:B:463:THR:HG22	1.72	0.88
1:C:188:HIS:CG	1:C:370:TYR:CE2	2.62	0.88
1:C:103:PHE:CE2	1:C:530:LEU:HD22	2.08	0.88
1:B:196:ILE:CD1	1:B:374:TRP:HB3	2.04	0.88
1:A:310:MET:O	1:A:314:ALA:CB	2.21	0.87
1:C:247:VAL:CG1	1:C:502:ILE:HD13	2.04	0.87
1:B:69:ILE:O	1:B:73:THR:CG2	2.21	0.87
1:C:114:ILE:HD12	1:C:117:ILE:HD11	1.55	0.87
1:C:250:THR:HG22	1:C:377:TRP:HE1	1.37	0.87
1:B:158:GLY:HA2	1:B:413:PHE:CE1	2.09	0.87
1:B:261:ILE:HG23	1:B:458:MET:HE1	1.57	0.86
1:C:363:LEU:CD2	1:C:367:THR:CG2	2.53	0.86
1:A:292:PHE:O	1:A:296:SER:HB3	1.76	0.86
1:A:156:PHE:CE1	1:A:157:TYR:CD2	2.64	0.86
1:C:247:VAL:HG12	1:C:502:ILE:HD11	0.88	0.86
1:A:209:PHE:CD2	1:A:390:ARG:HG2	2.10	0.86
1:B:78:ILE:HG22	1:B:79:GLY:N	1.90	0.85
1:A:574:ARG:N	1:A:574:ARG:CD	2.39	0.85
1:B:101:TRP:HA	1:B:104:ILE:HD11	1.57	0.85
1:B:92:LEU:CD1	1:B:524:VAL:HG13	2.06	0.85
1:C:228:LYS:O	1:C:228:LYS:HG2	1.77	0.85
1:B:114:ILE:C	1:B:117:ILE:HG22	2.01	0.85
1:B:317:ALA:O	1:B:320:VAL:HG22	1.77	0.85
1:B:320:VAL:CG2	1:B:415:ILE:CG2	2.53	0.85
1:C:64:VAL:HG12	1:C:65:PRO:HD3	1.55	0.85
1:B:78:ILE:HG22	1:B:79:GLY:H	1.41	0.85
1:C:148:ALA:O	2:C:2486:CHT:C6	2.21	0.85
1:A:527:THR:HG22	1:A:528:PRO:HD3	1.55	0.84
1:B:373:TRP:CD1	1:B:373:TRP:C	2.55	0.84
1:B:95:VAL:HG21	1:B:527:THR:CG2	2.08	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:GLN:HA	1:A:437:GLU:HG2	1.57	0.84
1:A:215:GLN:CB	1:A:483:GLY:O	2.24	0.84
1:A:222:VAL:HB	1:A:227:GLU:HA	1.59	0.84
1:C:311:VAL:HG23	1:C:312:LEU:HD12	1.60	0.84
1:B:146:PHE:HB3	1:B:310:MET:SD	2.18	0.84
1:B:372:ALA:CB	1:B:523:ILE:HG23	2.07	0.84
1:C:167:ARG:HG3	1:C:168:ASN:OD1	1.78	0.84
1:B:319:PHE:O	1:B:323:VAL:HG22	1.77	0.84
1:B:205:ALA:HB2	1:B:386:ALA:HB1	1.60	0.84
1:B:183:SER:OG	1:B:339:ASN:HB3	1.78	0.83
1:B:411:VAL:HG13	1:B:415:ILE:HD11	1.57	0.83
1:B:190:THR:O	1:B:194:TRP:CD1	2.26	0.83
1:C:173:HIS:HD2	1:C:180:VAL:HG13	1.43	0.83
1:C:397:PHE:O	1:C:401:VAL:HG23	1.77	0.83
1:A:369:PHE:HE1	1:A:519:GLN:HB2	1.33	0.83
1:C:224:LEU:HD12	1:C:539:ALA:HB2	1.59	0.83
1:A:123:GLY:HA2	1:A:394:ILE:CB	2.08	0.83
1:C:267:ALA:HB1	1:C:451:GLN:OE1	1.77	0.83
1:B:211:VAL:HG11	1:B:213:ARG:HE	1.44	0.83
1:C:337:ILE:HD11	1:C:410:THR:HG21	1.60	0.83
1:B:488:ASN:OD1	1:B:490:TRP:CZ3	2.30	0.83
1:C:329:ILE:HG21	1:C:415:ILE:HG12	1.61	0.83
1:C:103:PHE:CD2	1:C:530:LEU:HD22	2.13	0.83
1:C:126:ARG:CD	1:C:132:GLU:O	2.26	0.83
1:C:163:LEU:HG	1:C:431:TRP:CZ3	2.11	0.83
1:A:331:ASN:O	1:A:334:PRO:HD2	1.78	0.82
1:A:559:PHE:HE2	1:A:563:LEU:CD1	1.91	0.82
1:C:121:LYS:H	1:C:121:LYS:CD	1.88	0.82
1:C:134:PRO:HG3	1:C:391:GLY:O	1.79	0.82
1:C:173:HIS:CD2	1:C:180:VAL:CG2	2.62	0.82
1:A:89:SER:HA	1:A:520:ASN:ND2	1.93	0.82
1:C:192:HIS:N	1:C:193:PRO:HD2	1.95	0.82
1:B:153:ASP:OD1	1:B:154:LEU:N	2.12	0.81
1:A:352:ALA:O	1:A:357:GLY:HA2	1.79	0.81
1:B:309:ASN:OD1	1:B:463:THR:CG2	2.27	0.81
1:C:204:ILE:HD13	1:C:383:MET:HG2	1.59	0.81
1:C:252:CYS:SG	1:C:522:THR:HG21	2.20	0.81
1:C:298:VAL:HG23	1:C:302:ILE:HD13	1.60	0.81
1:C:74:VAL:HA	1:C:505:THR:HG21	1.62	0.81
1:C:319:PHE:CE2	1:C:453:MET:HG3	2.15	0.81
1:C:295:ILE:CD1	1:C:493:ALA:HB2	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:ILE:CG1	1:A:303:GLN:N	2.42	0.81
1:A:490:TRP:HD1	1:A:491:VAL:HG13	1.44	0.81
1:A:101:TRP:CE2	1:C:330:LEU:HD13	2.16	0.81
1:A:299:GLY:O	1:A:300:LYS:HB2	1.81	0.81
1:B:464:PHE:HA	1:B:467:THR:HG23	1.62	0.81
1:B:305:LEU:HD23	1:B:467:THR:HG22	1.61	0.81
1:C:116:VAL:O	1:C:120:SER:HB3	1.80	0.80
1:C:103:PHE:HZ	1:C:527:THR:HA	1.46	0.80
1:A:92:LEU:O	1:A:95:VAL:HG22	1.81	0.80
1:A:343:ASN:O	1:A:347:MET:CG	2.29	0.80
1:A:113:PHE:CE1	1:A:117:ILE:CD1	2.66	0.80
1:B:366:TRP:O	1:B:370:TYR:CB	2.30	0.80
1:C:228:LYS:O	1:C:228:LYS:CG	2.30	0.80
1:A:137:ARG:HD2	1:A:139:VAL:HG22	1.64	0.79
1:B:103:PHE:HD1	1:B:371:TRP:CB	1.95	0.79
1:C:190:THR:O	1:C:193:PRO:HG2	1.82	0.79
1:C:524:VAL:O	1:C:528:PRO:HD3	1.82	0.79
1:B:128:GLY:HA2	1:B:209:PHE:C	2.08	0.79
1:C:173:HIS:CD2	1:C:180:VAL:HG21	2.17	0.79
1:C:81:LYS:HD3	1:C:84:PHE:CD2	2.17	0.79
1:C:92:LEU:HD13	1:C:520:ASN:CA	2.13	0.79
1:C:163:LEU:HD11	1:C:424:GLU:HG3	1.63	0.79
1:B:103:PHE:HD1	1:B:371:TRP:HB3	1.46	0.79
1:B:106:PHE:CD1	1:B:534:ILE:HD12	2.17	0.79
1:C:144:MET:CG	1:C:388:ILE:HD13	2.13	0.79
1:C:205:ALA:O	1:C:209:PHE:HB2	1.83	0.79
1:B:123:GLY:HA2	1:B:394:ILE:HD11	1.65	0.79
1:B:206:TYR:CE2	1:B:543:ASP:OD2	2.36	0.79
1:B:366:TRP:O	1:B:370:TYR:CD2	2.36	0.79
1:C:173:HIS:CD2	1:C:180:VAL:HG13	2.17	0.79
1:A:350:ARG:HG2	1:A:363:LEU:HD11	1.66	0.79
1:B:475:VAL:O	1:B:479:MET:HG2	1.83	0.79
1:A:574:ARG:N	1:A:574:ARG:HD2	1.98	0.78
1:C:292:PHE:O	1:C:296:SER:HB3	1.83	0.78
1:A:261:ILE:HD11	1:A:461:LEU:HD21	1.65	0.78
1:B:200:VAL:HG21	1:B:378:SER:CB	2.01	0.78
1:A:64:VAL:CG2	1:A:65:PRO:HD3	2.14	0.78
1:B:128:GLY:HA2	1:B:209:PHE:O	1.84	0.78
1:A:327:VAL:HG11	1:B:97:ASP:O	1.82	0.78
1:C:215:GLN:HE22	1:C:387:ARG:HE	1.28	0.78
1:B:320:VAL:CG2	1:B:415:ILE:HG21	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:PHE:CE1	1:A:157:TYR:CG	2.72	0.78
1:A:285:VAL:HA	1:A:288:LEU:HG	1.66	0.78
1:A:422:VAL:HA	1:A:425:GLN:HG3	1.65	0.78
1:B:114:ILE:HA	1:B:117:ILE:CG2	2.13	0.78
1:A:59:ASN:OD1	1:A:482:HIS:CD2	2.36	0.78
1:A:295:ILE:HD13	1:A:492:THR:HG21	1.64	0.78
1:B:380:PHE:CE1	1:B:384:PHE:CE1	2.72	0.78
1:A:202:LEU:HD11	1:A:394:ILE:HG23	1.66	0.77
1:A:251:ALA:HA	1:A:254:LEU:HB2	1.66	0.77
1:B:201:GLY:CA	1:B:385:LEU:HD11	2.12	0.77
1:C:134:PRO:CD	1:C:391:GLY:O	2.32	0.77
1:C:264:GLY:HA3	1:C:441:PHE:CE1	2.19	0.77
1:C:269:ASN:O	1:C:270:ILE:HG13	1.84	0.77
1:B:309:ASN:ND2	1:B:464:PHE:CD2	2.30	0.77
1:B:453:MET:HE3	1:B:456:ILE:HD11	1.66	0.77
1:C:363:LEU:HD23	1:C:367:THR:HG21	1.62	0.77
1:A:155:MET:HE2	1:A:440:LEU:HD11	1.67	0.77
1:C:76:TRP:HD1	1:C:77:GLY:N	1.83	0.77
1:A:123:GLY:CA	1:A:394:ILE:HB	2.14	0.77
1:A:412:TRP:CZ2	1:A:416:PHE:CZ	2.72	0.77
1:B:457:ALA:HA	1:B:460:LEU:HD12	1.66	0.77
1:C:562:ARG:HA	1:C:565:ARG:HD2	1.67	0.77
1:B:129:ARG:N	1:B:390:ARG:HH12	1.82	0.76
1:A:92:LEU:HD23	1:A:520:ASN:OD1	1.86	0.76
1:A:156:PHE:HE1	1:A:157:TYR:CD2	2.03	0.76
1:B:127:LEU:HD11	1:B:205:ALA:HB1	1.67	0.76
1:B:379:PRO:HG3	1:B:529:PHE:CZ	2.20	0.76
1:C:59:ASN:O	1:C:63:ILE:HG13	1.84	0.76
1:B:145:MET:HE3	1:B:404:VAL:CG2	2.16	0.76
1:B:259:LEU:HD12	1:B:260:GLN:N	2.01	0.76
1:C:76:TRP:CD1	1:C:77:GLY:N	2.53	0.76
1:C:260:GLN:OE1	1:C:461:LEU:HD21	1.86	0.76
1:C:304:TYR:CD1	1:C:305:LEU:HG	2.20	0.76
1:C:471:SER:O	1:C:475:VAL:HG23	1.85	0.76
1:B:92:LEU:HD13	1:B:524:VAL:HG13	1.66	0.76
1:B:380:PHE:HE1	1:B:384:PHE:CE1	2.03	0.76
1:C:120:SER:OG	1:C:122:PHE:HD2	1.69	0.76
1:A:345:PHE:CE1	1:C:341:LEU:HD13	2.21	0.76
1:B:121:LYS:HZ1	1:B:550:TYR:HD1	1.32	0.76
1:B:152:ILE:HB	1:B:464:PHE:HE1	1.50	0.76
1:B:366:TRP:N	1:B:366:TRP:CD1	2.53	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:LEU:HD12	1:C:312:LEU:H	1.49	0.76
1:B:329:ILE:CD1	1:B:415:ILE:HG23	2.15	0.76
1:B:370:TYR:O	1:B:374:TRP:HD1	1.69	0.76
1:C:76:TRP:CD1	1:C:76:TRP:C	2.63	0.75
1:C:559:PHE:HA	1:C:562:ARG:HG2	1.67	0.75
1:C:363:LEU:HA	1:C:367:THR:CG2	2.17	0.75
1:B:114:ILE:O	1:B:117:ILE:CG2	2.33	0.75
1:A:92:LEU:HD13	1:A:96:VAL:HG21	1.67	0.75
1:B:211:VAL:HG11	1:B:213:ARG:NE	2.01	0.75
1:A:527:THR:N	1:A:528:PRO:CD	2.49	0.75
1:B:329:ILE:HD13	1:B:415:ILE:HG23	1.69	0.75
1:C:231:GLU:O	1:C:236:LYS:HG2	1.87	0.75
1:C:363:LEU:O	1:C:368:ILE:HG22	1.87	0.75
1:C:76:TRP:NE1	1:C:85:THR:CA	2.47	0.75
1:B:208:THR:CG2	1:B:213:ARG:O	2.25	0.75
1:B:451:GLN:CD	1:B:451:GLN:H	1.95	0.74
1:C:108:THR:CA	1:C:192:HIS:HE1	1.99	0.74
1:B:452:ILE:O	1:B:455:ILE:HG12	1.87	0.74
1:C:247:VAL:HG11	1:C:502:ILE:HD13	1.69	0.74
1:C:389:SER:O	1:C:390:ARG:C	2.30	0.74
1:A:309:ASN:CG	1:A:464:PHE:CE1	2.62	0.74
1:C:193:PRO:HB3	1:C:374:TRP:CD1	2.21	0.74
1:C:308:ALA:O	1:C:312:LEU:HD13	1.87	0.74
1:A:329:ILE:HG21	1:A:415:ILE:HG22	1.69	0.74
1:C:224:LEU:HD11	1:C:539:ALA:HA	1.70	0.74
1:A:81:LYS:CB	1:A:84:PHE:HB2	2.17	0.74
1:A:329:ILE:HD11	1:A:419:THR:HG22	1.70	0.74
1:B:404:VAL:O	1:B:408:VAL:HG22	1.88	0.74
1:B:476:MET:HE2	1:B:495:TRP:CE3	2.21	0.74
1:A:295:ILE:HD11	1:A:470:ASP:HA	1.69	0.74
1:B:161:GLU:HB3	1:B:162:PRO:HD3	1.70	0.74
1:B:300:LYS:O	1:B:300:LYS:HG2	1.87	0.74
1:C:64:VAL:CG1	1:C:65:PRO:CD	2.58	0.74
1:B:96:VAL:HG13	1:B:368:ILE:HG21	1.67	0.74
1:B:327:VAL:CG2	1:B:328:SER:H	1.99	0.74
1:C:231:GLU:HG3	1:C:236:LYS:HE2	1.70	0.74
1:B:64:VAL:HB	1:B:65:PRO:HD3	1.68	0.74
1:B:401:VAL:O	1:B:405:PRO:HG2	1.88	0.74
1:B:527:THR:HB	1:B:528:PRO:HD3	1.70	0.74
1:A:309:ASN:OD1	1:A:464:PHE:CE1	2.41	0.74
1:A:301:GLY:O	1:A:302:ILE:HG12	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:LEU:O	1:A:534:ILE:HG12	1.88	0.73
1:B:92:LEU:HD11	1:B:523:ILE:CB	2.13	0.73
1:C:108:THR:HA	1:C:192:HIS:HE1	1.49	0.73
1:C:134:PRO:HG3	1:C:392:ARG:HD3	1.70	0.73
1:C:264:GLY:HA3	1:C:441:PHE:CZ	2.23	0.73
1:A:68:VAL:O	1:A:72:ALA:HB2	1.88	0.73
1:C:288:LEU:O	1:C:291:ILE:HG22	1.88	0.73
1:B:92:LEU:O	1:B:95:VAL:HG12	1.88	0.73
1:C:61:SER:O	1:C:65:PRO:CG	2.36	0.73
1:C:124:THR:HG23	1:C:395:ARG:HH21	1.51	0.73
1:A:527:THR:CG2	1:A:528:PRO:HD3	2.18	0.73
1:B:121:LYS:NZ	1:B:550:TYR:HD1	1.86	0.73
1:B:186:MET:HG2	1:B:190:THR:CG2	2.19	0.73
1:B:128:GLY:HA3	1:B:390:ARG:NH1	2.03	0.73
1:B:142:ILE:HA	1:B:145:MET:SD	2.27	0.73
1:B:237:LEU:O	1:B:241:LEU:HG	1.89	0.73
1:C:144:MET:SD	1:C:388:ILE:HG12	2.29	0.73
1:B:316:LEU:HD22	1:B:460:LEU:HD12	1.70	0.73
1:B:346:GLN:HG3	1:B:347:MET:N	2.04	0.73
1:C:209:PHE:CE1	1:C:390:ARG:HB2	2.24	0.73
1:A:302:ILE:CG1	1:A:303:GLN:H	2.00	0.73
1:A:309:ASN:OD1	1:A:464:PHE:HE1	1.70	0.73
1:B:470:ASP:O	1:B:474:THR:HG23	1.89	0.73
1:B:539:ALA:O	1:B:543:ASP:HB3	1.88	0.73
1:C:144:MET:SD	1:C:388:ILE:CD1	2.77	0.73
1:A:112:PHE:O	1:A:116:VAL:CG1	2.36	0.72
1:B:175:GLU:O	1:B:176:HIS:HB2	1.87	0.72
1:B:197:TYR:HH	1:B:374:TRP:HE3	1.36	0.72
1:C:248:PHE:HB3	1:C:522:THR:HG22	1.70	0.72
1:B:104:ILE:HD12	1:B:105:LEU:N	2.04	0.72
1:B:456:ILE:O	1:B:460:LEU:HG	1.88	0.72
1:C:76:TRP:CE2	1:C:85:THR:HA	2.23	0.72
1:C:264:GLY:CA	1:C:441:PHE:CZ	2.72	0.72
1:A:66:ALA:O	1:A:70:VAL:HG23	1.89	0.72
1:A:183:SER:OG	1:A:339:ASN:HB3	1.88	0.72
1:C:134:PRO:CG	1:C:391:GLY:O	2.37	0.72
1:B:95:VAL:HG21	1:B:527:THR:HG21	1.70	0.72
1:B:373:TRP:C	1:B:373:TRP:HD1	1.97	0.72
1:A:197:TYR:CE1	1:A:381:VAL:HG21	2.25	0.72
1:B:78:ILE:CG2	1:B:79:GLY:H	2.02	0.72
1:B:177:ASN:C	1:B:177:ASN:OD1	2.30	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:PHE:CD1	1:C:544:LEU:HB3	2.25	0.72
1:C:416:PHE:CE1	1:C:440:LEU:HD11	2.25	0.72
1:B:135:GLU:HG2	1:B:136:PHE:CD2	2.25	0.71
1:C:230:ALA:O	1:C:231:GLU:CB	2.38	0.71
1:A:387:ARG:HB3	1:A:387:ARG:HH11	1.54	0.71
1:A:154:LEU:O	1:A:158:GLY:HA3	1.90	0.71
1:B:312:LEU:CB	1:B:460:LEU:HD21	2.07	0.71
1:A:136:PHE:CE1	1:A:144:MET:HE3	2.26	0.71
1:C:433:ASP:C	1:C:433:ASP:OD1	2.31	0.71
1:C:108:THR:CA	1:C:192:HIS:CE1	2.72	0.71
1:C:148:ALA:HB2	1:C:384:PHE:CE2	2.26	0.71
1:A:161:GLU:HG3	1:A:366:TRP:HZ3	1.56	0.71
1:B:343:ASN:O	1:B:347:MET:CG	2.36	0.71
1:B:110:PHE:CD1	1:B:196:ILE:CG2	2.73	0.71
1:A:106:PHE:HB3	1:A:534:ILE:HD11	1.73	0.70
1:A:72:ALA:O	1:A:76:TRP:HB2	1.91	0.70
1:A:245:ALA:HB2	1:A:526:ALA:HB2	1.73	0.70
1:B:110:PHE:HD1	1:B:196:ILE:CG2	2.04	0.70
1:B:283:VAL:HA	1:B:286:LEU:HG	1.71	0.70
1:B:464:PHE:O	1:B:468:SER:N	2.23	0.70
1:C:305:LEU:HA	1:C:308:ALA:HB3	1.73	0.70
1:A:302:ILE:HG13	1:A:303:GLN:H	1.54	0.70
1:A:329:ILE:HG23	1:A:414:SER:O	1.91	0.70
1:B:177:ASN:HD21	1:B:180:VAL:HG23	1.56	0.70
1:C:224:LEU:CD1	1:C:539:ALA:HB2	2.20	0.70
1:B:365:SER:CB	1:B:366:TRP:CD1	2.73	0.70
1:A:235:GLY:H	1:A:238:ILE:HD13	1.56	0.70
1:B:476:MET:HB3	1:B:495:TRP:CE3	2.27	0.70
1:C:281:GLY:O	1:C:285:VAL:HG22	1.91	0.70
1:C:379:PRO:HD3	1:C:529:PHE:CE2	2.26	0.70
1:A:209:PHE:CE2	1:A:390:ARG:HG2	2.26	0.70
1:C:414:SER:O	1:C:418:GLY:HA3	1.90	0.70
1:B:144:MET:HE3	1:B:388:ILE:HD11	1.73	0.70
1:C:456:ILE:O	1:C:459:ILE:HG22	1.90	0.70
1:B:114:ILE:HD12	1:B:402:LEU:HD21	1.74	0.70
1:B:92:LEU:HD12	1:B:524:VAL:HG13	1.74	0.69
1:B:95:VAL:HG21	1:B:527:THR:HG23	1.74	0.69
1:A:63:ILE:O	1:A:66:ALA:HB3	1.93	0.69
1:A:412:TRP:CD2	1:A:416:PHE:HE2	2.09	0.69
1:B:435:ALA:O	1:B:438:GLU:HG2	1.92	0.69
1:A:112:PHE:O	1:A:116:VAL:HG13	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ILE:O	1:A:145:MET:HE3	1.92	0.69
1:A:344:PHE:CD2	1:A:344:PHE:O	2.44	0.69
1:B:270:ILE:HD12	1:B:270:ILE:H	1.57	0.69
1:A:114:ILE:HD13	1:A:195:ALA:CB	2.22	0.69
1:A:412:TRP:CH2	1:A:416:PHE:CZ	2.81	0.69
1:C:134:PRO:HD3	1:C:391:GLY:O	1.93	0.69
1:A:473:SER:HA	1:A:476:MET:HG2	1.75	0.69
1:B:225:ILE:HG21	1:B:230:ALA:HA	1.73	0.69
1:C:401:VAL:O	1:C:405:PRO:HD2	1.91	0.69
1:A:101:TRP:CZ2	1:C:330:LEU:HD13	2.27	0.69
1:A:444:LEU:CD1	1:A:450:GLY:O	2.41	0.69
1:B:189:TRP:CH2	1:B:370:TYR:OH	2.44	0.69
1:C:76:TRP:CZ2	1:C:85:THR:HA	2.28	0.69
1:C:303:GLN:O	1:C:304:TYR:HB3	1.92	0.69
1:A:206:TYR:HE2	1:A:543:ASP:CG	2.00	0.69
1:B:464:PHE:HA	1:B:467:THR:CG2	2.22	0.68
1:A:222:VAL:HA	1:A:226:GLY:O	1.93	0.68
1:A:353:MET:HE2	1:A:353:MET:HA	1.74	0.68
1:C:416:PHE:HE1	1:C:440:LEU:HD11	1.58	0.68
1:B:320:VAL:HG11	1:B:416:PHE:CE1	2.28	0.68
1:C:64:VAL:O	1:C:68:VAL:HG23	1.93	0.68
1:C:354:SER:O	1:C:359:ALA:HB3	1.93	0.68
1:B:476:MET:HE2	1:B:495:TRP:HE3	1.59	0.68
1:C:66:ALA:N	1:C:240:ILE:HD11	2.09	0.68
1:C:224:LEU:CD1	1:C:539:ALA:CA	2.67	0.68
1:A:369:PHE:CE1	1:A:519:GLN:CB	2.65	0.68
1:B:369:PHE:HA	1:B:523:ILE:HD12	1.76	0.68
1:C:380:PHE:C	1:C:380:PHE:CD1	2.70	0.68
1:A:243:ILE:HD12	1:A:244:ILE:N	2.09	0.68
1:B:540:LEU:O	1:B:544:LEU:HG	1.93	0.68
1:C:121:LYS:HD3	1:C:121:LYS:N	2.05	0.68
1:A:412:TRP:CD2	1:A:416:PHE:CE2	2.82	0.68
1:A:114:ILE:HD13	1:A:195:ALA:HB1	1.76	0.68
1:A:309:ASN:ND2	1:A:464:PHE:HE1	1.91	0.68
1:A:379:PRO:HG3	1:A:529:PHE:CE2	2.29	0.68
1:C:103:PHE:CE2	1:C:530:LEU:HD23	2.28	0.68
1:C:520:ASN:O	1:C:524:VAL:HG23	1.93	0.67
1:A:199:ILE:HG22	1:A:536:LEU:HD23	1.76	0.67
1:A:412:TRP:CH2	1:A:416:PHE:CE2	2.81	0.67
1:C:267:ALA:HB1	1:C:451:GLN:CD	2.19	0.67
1:C:506:LEU:HD23	1:C:518:LEU:HD12	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:VAL:HG21	1:B:98:ASN:OD1	1.94	0.67
1:A:404:VAL:O	1:A:408:VAL:HG13	1.94	0.67
1:C:156:PHE:CE1	1:C:256:LEU:HB2	2.29	0.67
1:C:270:ILE:HA	1:C:271:ILE:HG12	1.75	0.67
1:C:371:TRP:HE3	1:C:371:TRP:N	1.91	0.67
1:B:213:ARG:NH1	1:B:222:VAL:HB	2.10	0.67
1:B:398:ILE:O	1:B:402:LEU:CD1	2.35	0.67
1:C:76:TRP:NE1	1:C:85:THR:CB	2.54	0.67
1:A:476:MET:SD	1:A:495:TRP:HB3	2.35	0.67
1:C:304:TYR:CE1	1:C:305:LEU:CG	2.76	0.67
1:B:186:MET:CE	1:B:336:SER:HB3	2.25	0.67
1:C:319:PHE:CG	1:C:453:MET:HE3	2.30	0.67
1:A:71:LEU:HA	1:A:74:VAL:HB	1.77	0.67
1:A:351:THR:HG22	1:C:331:ASN:HB3	1.76	0.67
1:C:134:PRO:CA	1:C:391:GLY:HA3	2.18	0.67
1:A:478:THR:HA	1:A:481:GLN:HE21	1.60	0.67
1:C:103:PHE:CD2	1:C:530:LEU:CD2	2.76	0.67
1:C:329:ILE:CG2	1:C:415:ILE:HG12	2.25	0.67
1:A:158:GLY:HA2	1:A:413:PHE:HE1	1.60	0.66
1:C:193:PRO:HB3	1:C:374:TRP:NE1	2.11	0.66
1:C:230:ALA:O	1:C:231:GLU:HB3	1.95	0.66
1:C:431:TRP:NE1	1:C:434:GLY:HA2	2.09	0.66
1:B:423:PHE:HB3	1:B:428:GLU:O	1.95	0.66
1:C:264:GLY:CA	1:C:441:PHE:CE1	2.77	0.66
1:C:389:SER:OG	1:C:397:PHE:CD1	2.48	0.66
1:B:327:VAL:O	1:B:331:ASN:N	2.29	0.66
1:C:95:VAL:HG21	1:C:527:THR:CG2	2.25	0.66
1:C:454:GLY:O	1:C:458:MET:HE3	1.96	0.66
1:C:163:LEU:CG	1:C:431:TRP:HZ3	2.04	0.66
1:C:561:ALA:O	1:C:565:ARG:HG3	1.94	0.66
1:A:136:PHE:HE2	1:A:388:ILE:HG23	1.59	0.66
1:B:341:LEU:HB3	1:C:345:PHE:CD2	2.30	0.66
1:B:365:SER:C	1:B:366:TRP:CD1	2.74	0.66
1:B:158:GLY:HA2	1:B:413:PHE:HE1	1.54	0.66
1:B:329:ILE:HG21	1:B:415:ILE:HG13	1.77	0.66
1:C:67:LEU:O	1:C:70:VAL:HG12	1.94	0.66
1:C:106:PHE:HA	1:C:109:VAL:CG2	2.26	0.66
1:C:144:MET:CB	1:C:388:ILE:HD13	2.26	0.66
1:A:137:ARG:HD3	1:A:138:THR:N	2.10	0.66
1:C:164:THR:HG21	1:C:366:TRP:HZ2	1.60	0.66
1:C:208:THR:HG21	1:C:215:GLN:HG3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:TRP:HZ3	1:C:385:LEU:HD11	1.61	0.66
1:C:253:SER:OG	1:C:377:TRP:CH2	2.47	0.66
1:A:215:GLN:CD	1:A:387:ARG:NH2	2.54	0.66
1:B:79:GLY:O	1:B:80:PHE:HB3	1.96	0.66
1:B:384:PHE:CZ	1:B:471:SER:HB2	2.31	0.66
1:C:76:TRP:HZ2	1:C:84:PHE:O	1.79	0.66
1:C:353:MET:O	1:C:357:GLY:N	2.29	0.66
1:A:449:GLY:O	1:A:452:ILE:HG12	1.95	0.65
1:B:59:ASN:HB3	1:B:480:SER:O	1.97	0.65
1:C:192:HIS:N	1:C:193:PRO:CD	2.59	0.65
1:B:200:VAL:HG12	1:B:382:GLY:HA3	1.79	0.65
1:B:372:ALA:HB3	1:B:523:ILE:HG23	1.77	0.65
1:B:145:MET:HE3	1:B:404:VAL:HG21	1.78	0.65
1:B:186:MET:HE1	1:B:336:SER:HB3	1.78	0.65
1:A:152:ILE:HD12	1:A:152:ILE:H	1.61	0.65
1:B:279:ILE:HA	1:B:282:ILE:HG23	1.78	0.65
1:C:148:ALA:C	2:C:2486:CHT:H62	2.18	0.65
1:B:305:LEU:HB3	1:B:467:THR:CG2	2.27	0.65
1:A:113:PHE:CZ	1:A:117:ILE:HD12	2.31	0.65
1:A:92:LEU:O	1:A:95:VAL:CG2	2.44	0.65
1:C:225:ILE:HG22	1:C:226:GLY:O	1.96	0.65
1:C:226:GLY:CA	1:C:227:GLU:HB2	2.17	0.65
1:B:157:TYR:HA	1:B:160:THR:HG22	1.79	0.65
1:B:117:ILE:HG23	1:B:398:ILE:CD1	2.27	0.64
1:A:150:MET:SD	1:A:309:ASN:HB3	2.36	0.64
1:B:185:THR:O	1:B:189:TRP:HE3	1.80	0.64
1:B:404:VAL:HB	1:B:405:PRO:HD3	1.79	0.64
1:C:173:HIS:CG	1:C:180:VAL:HG21	2.32	0.64
1:C:186:MET:HE3	1:C:190:THR:HG21	1.78	0.64
1:C:426:ASN:HB2	1:C:428:GLU:OE1	1.98	0.64
1:A:329:ILE:HD11	1:A:419:THR:HG23	1.78	0.64
1:A:182:MET:HE2	1:A:332:LEU:HD21	1.80	0.64
1:B:418:GLY:O	1:B:422:VAL:HG23	1.98	0.64
1:C:113:PHE:CD2	1:C:199:ILE:HD11	2.32	0.64
1:C:312:LEU:HD12	1:C:312:LEU:N	2.12	0.64
1:A:163:LEU:HD21	1:A:424:GLU:OE2	1.97	0.64
1:A:283:VAL:HA	1:A:286:LEU:HD12	1.79	0.64
1:A:453:MET:O	1:A:456:ILE:HG12	1.98	0.64
1:A:246:THR:O	1:A:250:THR:HG23	1.97	0.64
1:B:167:ARG:HH11	1:B:424:GLU:CD	2.05	0.64
1:B:291:ILE:HA	1:B:466:ILE:CD1	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:404:VAL:HB	1:C:405:PRO:HD3	1.78	0.64
1:A:222:VAL:CG2	1:A:227:GLU:HG2	2.28	0.64
1:A:223:PRO:CG	1:A:543:ASP:HB2	2.28	0.64
1:B:231:GLU:HG3	1:B:236:LYS:HE3	1.80	0.64
1:B:267:ALA:HB1	1:B:445:HIS:HE1	1.62	0.64
1:C:76:TRP:HE1	1:C:85:THR:HB	1.58	0.64
1:A:369:PHE:CZ	1:A:519:GLN:CB	2.74	0.64
1:B:208:THR:O	1:B:212:GLY:CA	2.41	0.64
1:C:432:GLY:O	1:C:433:ASP:CG	2.41	0.64
1:A:295:ILE:HG21	1:A:492:THR:HG21	1.80	0.63
1:B:312:LEU:CB	1:B:460:LEU:CD2	2.70	0.63
1:C:464:PHE:O	1:C:468:SER:HB2	1.97	0.63
1:B:455:ILE:HG13	1:B:456:ILE:N	2.13	0.63
1:C:292:PHE:O	1:C:296:SER:N	2.30	0.63
1:C:319:PHE:O	1:C:323:VAL:HG12	1.98	0.63
1:B:267:ALA:HB1	1:B:445:HIS:CE1	2.33	0.63
1:C:503:GLY:O	1:C:507:LEU:HD13	1.99	0.63
1:B:135:GLU:HG2	1:B:136:PHE:CE2	2.33	0.63
1:B:197:TYR:OH	1:B:374:TRP:CE3	2.51	0.63
1:A:183:SER:C	1:A:347:MET:HE1	2.23	0.63
1:B:145:MET:HE3	1:B:404:VAL:HG22	1.80	0.63
1:B:243:ILE:O	1:B:246:THR:HG22	1.99	0.63
1:B:320:VAL:CG2	1:B:415:ILE:HG22	2.29	0.63
1:C:60:TRP:O	1:C:64:VAL:HG12	1.99	0.63
1:C:202:LEU:HD23	1:C:540:LEU:HD21	1.80	0.63
1:B:365:SER:CB	1:B:366:TRP:HD1	2.12	0.63
1:C:488:ASN:O	1:C:491:VAL:HG12	1.99	0.63
1:C:95:VAL:HG21	1:C:527:THR:HG21	1.80	0.62
1:C:370:TYR:C	1:C:371:TRP:HE3	2.07	0.62
1:C:465:PHE:C	1:C:465:PHE:CD2	2.76	0.62
1:A:404:VAL:HB	1:A:405:PRO:HD3	1.81	0.62
1:B:380:PHE:HE1	1:B:384:PHE:CZ	2.16	0.62
1:C:164:THR:HG21	1:C:366:TRP:CZ2	2.34	0.62
1:C:371:TRP:N	1:C:371:TRP:CE3	2.67	0.62
1:C:431:TRP:CD1	1:C:434:GLY:HA2	2.34	0.62
1:B:366:TRP:O	1:B:370:TYR:HD2	1.80	0.62
1:C:167:ARG:HH12	1:C:431:TRP:CG	2.17	0.62
1:A:318:ILE:O	1:A:322:VAL:HG22	1.98	0.62
1:B:544:LEU:C	1:B:546:ASN:H	2.07	0.62
1:C:155:MET:HB3	1:C:260:GLN:HE22	1.64	0.62
1:C:267:ALA:HB1	1:C:451:GLN:NE2	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ASP:O	1:C:327:VAL:HG11	1.99	0.62
1:A:129:ARG:NH2	1:A:212:GLY:HA3	2.14	0.62
1:A:579:ALA:O	1:A:582:ARG:HG2	2.00	0.62
1:B:192:HIS:HB2	1:B:193:PRO:HD3	1.82	0.62
1:A:378:SER:HA	1:A:381:VAL:CG2	2.30	0.62
1:A:526:ALA:C	1:A:528:PRO:HD2	2.23	0.62
1:C:259:LEU:HD23	1:C:507:LEU:HG	1.81	0.62
1:C:304:TYR:HE1	1:C:305:LEU:HG	1.57	0.62
1:A:170:VAL:HG13	1:A:171:PRO:HD2	1.80	0.62
1:A:175:GLU:O	1:A:176:HIS:HB2	1.99	0.62
1:A:323:VAL:HG12	1:A:447:LEU:HD22	1.82	0.62
1:A:295:ILE:HD13	1:A:492:THR:CG2	2.30	0.62
1:C:304:TYR:HD1	1:C:304:TYR:C	2.08	0.62
1:A:478:THR:O	1:A:481:GLN:HG2	2.00	0.62
1:B:103:PHE:HB3	1:B:371:TRP:CD1	2.35	0.62
1:B:161:GLU:CD	1:B:189:TRP:HZ3	2.07	0.62
1:B:203:ALA:HB2	1:B:540:LEU:HD22	1.82	0.62
1:C:65:PRO:O	1:C:69:ILE:HD13	1.99	0.62
1:C:105:LEU:O	1:C:109:VAL:CG2	2.40	0.62
1:C:279:ILE:O	1:C:283:VAL:HG23	2.00	0.62
1:C:333:LEU:O	1:C:337:ILE:HG12	1.99	0.62
1:A:137:ARG:HH11	1:A:139:VAL:HG22	1.65	0.61
1:A:451:GLN:O	1:A:455:ILE:HG13	2.00	0.61
1:B:366:TRP:N	1:B:366:TRP:HD1	1.97	0.61
1:B:78:ILE:CG2	1:B:79:GLY:N	2.57	0.61
1:B:161:GLU:CD	1:B:189:TRP:CZ3	2.78	0.61
1:C:188:HIS:HB3	1:C:370:TYR:CD2	2.35	0.61
1:A:562:ARG:O	1:A:565:ARG:HB2	2.00	0.61
1:B:144:MET:HB2	1:B:388:ILE:HD11	1.82	0.61
1:B:323:VAL:HG23	1:B:447:LEU:HD22	1.82	0.61
1:A:490:TRP:CD1	1:A:491:VAL:HG13	2.31	0.61
1:B:172:GLY:O	1:B:173:HIS:CD2	2.54	0.61
1:B:533:VAL:O	1:B:536:LEU:HB3	2.01	0.61
1:C:473:SER:HB3	1:C:492:THR:O	2.00	0.61
1:A:122:PHE:HE1	1:A:545:SER:HA	1.66	0.61
1:B:194:TRP:CE2	1:B:405:PRO:HB3	2.36	0.61
1:B:282:ILE:O	1:B:285:VAL:HG12	2.01	0.61
1:A:170:VAL:HG22	1:A:362:TRP:CZ2	2.36	0.61
1:A:223:PRO:HG2	1:A:543:ASP:HB2	1.82	0.61
1:A:392:ARG:HD2	1:A:396:GLU:HG3	1.83	0.61
1:A:481:GLN:O	1:A:482:HIS:CB	2.41	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:ALA:O	1:C:91:ALA:HB3	2.01	0.61
1:A:97:ASP:O	1:C:327:VAL:CG1	2.48	0.61
1:A:167:ARG:HG2	1:A:168:ASN:OD1	2.00	0.61
1:B:223:PRO:HG3	1:B:543:ASP:HB2	1.83	0.61
1:B:372:ALA:HB2	1:B:523:ILE:HG23	1.83	0.61
1:C:465:PHE:C	1:C:465:PHE:HD2	2.09	0.61
1:A:327:VAL:CG1	1:B:97:ASP:O	2.46	0.60
1:B:476:MET:HB3	1:B:495:TRP:HE3	1.64	0.60
1:C:165:PHE:CE1	1:C:362:TRP:HZ2	2.19	0.60
1:B:110:PHE:CE1	1:B:196:ILE:HG22	2.35	0.60
1:B:365:SER:HB2	1:B:366:TRP:CD1	2.36	0.60
1:B:375:ILE:HG23	1:B:526:ALA:HB1	1.82	0.60
1:A:64:VAL:HG23	1:A:65:PRO:CD	2.28	0.60
1:C:325:PRO:O	1:C:329:ILE:HG13	2.01	0.60
1:C:375:ILE:HD12	1:C:530:LEU:HB2	1.83	0.60
1:C:488:ASN:HB3	1:C:491:VAL:HG12	1.83	0.60
1:C:524:VAL:HA	1:C:527:THR:HG23	1.84	0.60
1:A:311:VAL:O	1:A:315:LEU:HB2	2.02	0.60
1:B:312:LEU:HD13	1:B:460:LEU:HD23	1.82	0.60
1:C:375:ILE:HD13	1:C:530:LEU:CA	2.23	0.60
1:A:222:VAL:HB	1:A:227:GLU:HG2	1.83	0.60
1:C:144:MET:HB3	1:C:388:ILE:HD13	1.84	0.60
1:C:163:LEU:CD1	1:C:424:GLU:HG3	2.31	0.60
1:A:369:PHE:HZ	1:A:519:GLN:HB2	1.60	0.60
1:B:197:TYR:OH	1:B:374:TRP:HE3	1.84	0.60
1:B:417:GLY:O	1:B:421:ILE:HG12	2.02	0.60
1:C:152:ILE:HG12	1:C:464:PHE:HB3	1.84	0.60
1:A:88:ALA:HA	1:A:91:ALA:HB3	1.84	0.60
1:A:243:ILE:HD12	1:A:244:ILE:HG13	1.84	0.60
1:A:309:ASN:O	1:A:313:ALA:HB3	2.01	0.60
1:C:91:ALA:O	1:C:94:ALA:CB	2.46	0.60
1:A:149:GLY:HA2	1:A:194:TRP:HH2	1.66	0.60
1:B:114:ILE:CD1	1:B:402:LEU:HD21	2.32	0.60
1:B:365:SER:HB2	1:B:366:TRP:HD1	1.67	0.60
1:C:230:ALA:O	1:C:231:GLU:CG	2.49	0.60
1:C:304:TYR:CD1	1:C:304:TYR:C	2.80	0.60
1:C:375:ILE:CD1	1:C:530:LEU:HA	2.25	0.60
1:A:161:GLU:HG3	1:A:366:TRP:CZ3	2.34	0.60
1:B:208:THR:HG1	1:B:209:PHE:HD1	1.50	0.60
1:B:411:VAL:CG1	1:B:415:ILE:CD1	2.76	0.60
1:B:453:MET:CE	1:B:456:ILE:HD11	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:ILE:CG1	1:C:398:ILE:HG12	2.32	0.60
1:A:412:TRP:CE3	1:A:416:PHE:HE2	2.20	0.60
1:C:114:ILE:CD1	1:C:117:ILE:HD11	2.29	0.60
1:C:260:GLN:CD	1:C:461:LEU:CD2	2.71	0.60
1:A:225:ILE:HG22	1:A:225:ILE:O	2.00	0.59
1:A:329:ILE:HG21	1:A:415:ILE:CG2	2.31	0.59
1:B:321:PHE:HA	1:B:329:ILE:HD12	1.84	0.59
1:C:454:GLY:O	1:C:457:ALA:HB3	2.01	0.59
1:A:380:PHE:HA	1:A:475:VAL:HG11	1.85	0.59
1:B:117:ILE:HG23	1:B:118:ALA:N	2.17	0.59
1:B:123:GLY:HA2	1:B:394:ILE:CD1	2.31	0.59
1:C:78:ILE:HG13	1:C:79:GLY:N	2.17	0.59
1:C:128:GLY:HA2	1:C:209:PHE:O	2.02	0.59
1:C:312:LEU:H	1:C:312:LEU:CD1	2.14	0.59
1:C:161:GLU:HG3	1:C:185:THR:HG22	1.83	0.59
1:C:188:HIS:CB	1:C:370:TYR:CD2	2.85	0.59
1:C:380:PHE:CE2	2:C:2486:CHT:H82	2.38	0.59
1:A:331:ASN:OD1	1:B:101:TRP:HB3	2.02	0.59
1:A:463:THR:O	1:A:466:ILE:HG13	2.02	0.59
1:C:323:VAL:HG13	1:C:324:GLY:N	2.16	0.59
1:B:100:GLY:O	1:B:104:ILE:HG13	2.02	0.59
1:A:113:PHE:CZ	1:A:117:ILE:CD1	2.85	0.59
1:A:166:TYR:CE2	1:A:176:HIS:CD2	2.90	0.59
1:A:550:TYR:CE1	1:A:554:ARG:NH1	2.71	0.59
1:B:463:THR:O	1:B:464:PHE:CG	2.56	0.59
1:C:65:PRO:HB2	1:C:240:ILE:CD1	2.33	0.59
1:A:101:TRP:CG	1:A:102:ALA:N	2.71	0.59
1:A:370:TYR:HB3	1:A:374:TRP:NE1	2.18	0.59
1:B:359:ALA:O	1:B:360:GLY:C	2.46	0.59
1:B:463:THR:HG23	1:B:464:PHE:CD2	2.37	0.59
1:C:363:LEU:CA	1:C:367:THR:HG22	2.26	0.59
1:A:484:GLN:HB2	1:A:486:GLU:OE1	2.02	0.59
1:A:542:LYS:O	1:A:545:SER:OG	2.20	0.59
1:B:74:VAL:O	1:B:78:ILE:CG1	2.49	0.59
1:B:401:VAL:O	1:B:401:VAL:HG22	2.03	0.59
1:A:379:PRO:HG3	1:A:529:PHE:CZ	2.38	0.58
1:B:257:GLY:O	1:B:261:ILE:HG12	2.03	0.58
1:C:106:PHE:HA	1:C:109:VAL:HG23	1.85	0.58
1:C:159:THR:HA	1:C:417:GLY:HA2	1.85	0.58
1:A:222:VAL:CA	1:A:226:GLY:O	2.50	0.58
1:B:75:VAL:O	1:B:78:ILE:N	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:LEU:HD23	1:B:540:LEU:HD21	1.84	0.58
1:B:365:SER:HB3	1:B:366:TRP:CD1	2.37	0.58
1:B:372:ALA:HB1	1:B:523:ILE:HA	1.85	0.58
1:C:184:THR:O	1:C:187:PHE:HB3	2.03	0.58
1:C:481:GLN:O	1:C:482:HIS:HB2	2.03	0.58
1:B:207:SER:O	1:B:213:ARG:N	2.35	0.58
1:B:300:LYS:O	1:B:300:LYS:CG	2.51	0.58
1:B:471:SER:HA	1:B:474:THR:HG23	1.84	0.58
1:C:526:ALA:C	1:C:528:PRO:HD2	2.27	0.58
1:A:222:VAL:O	1:A:226:GLY:C	2.46	0.58
1:B:213:ARG:HH11	1:B:222:VAL:HB	1.68	0.58
1:C:430:ILE:HD13	1:C:443:LEU:HB3	1.84	0.58
1:C:564:ALA:O	1:C:568:ARG:HG2	2.03	0.58
1:A:568:ARG:HE	1:C:548:VAL:CG1	2.16	0.58
1:B:334:PRO:HG2	1:C:351:THR:HG21	1.85	0.58
1:C:148:ALA:HB2	1:C:384:PHE:HE2	1.69	0.58
1:A:330:LEU:HG	1:B:101:TRP:CD2	2.38	0.58
1:A:388:ILE:HG22	1:A:388:ILE:O	2.02	0.58
1:A:458:MET:O	1:A:461:LEU:HG	2.02	0.58
1:C:304:TYR:HE1	1:C:305:LEU:CG	2.15	0.58
1:B:316:LEU:O	1:B:320:VAL:HG13	2.03	0.58
1:C:112:PHE:O	1:C:113:PHE:C	2.47	0.58
1:A:302:ILE:HG12	1:A:303:GLN:N	2.16	0.58
1:A:378:SER:HA	1:A:381:VAL:HG22	1.86	0.58
1:B:152:ILE:HB	1:B:464:PHE:CE1	2.35	0.58
1:C:76:TRP:CZ2	1:C:84:PHE:O	2.56	0.57
1:C:138:THR:HA	1:C:392:ARG:HH22	1.68	0.57
1:C:389:SER:OG	1:C:397:PHE:HD1	1.87	0.57
1:A:222:VAL:HG23	1:A:227:GLU:HG2	1.86	0.57
1:A:258:ALA:HB1	1:A:280:VAL:HG23	1.86	0.57
1:B:283:VAL:HA	1:B:286:LEU:CG	2.34	0.57
1:C:114:ILE:HD11	1:C:398:ILE:CG1	2.35	0.57
1:B:95:VAL:CG2	1:B:527:THR:HG21	2.34	0.57
1:B:320:VAL:HG23	1:B:415:ILE:HG21	1.75	0.57
1:C:188:HIS:ND1	1:C:370:TYR:CE2	2.72	0.57
1:A:402:LEU:O	1:A:404:VAL:N	2.37	0.57
1:C:164:THR:HA	1:C:431:TRP:HH2	1.69	0.57
1:C:298:VAL:HG23	1:C:302:ILE:CD1	2.30	0.57
1:A:305:LEU:HD12	1:A:306:SER:N	2.19	0.57
1:A:477:GLY:O	1:A:481:GLN:NE2	2.32	0.57
1:A:568:ARG:HE	1:C:548:VAL:HG13	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:LEU:HD12	1:B:191:LEU:N	2.20	0.57
1:B:369:PHE:HD1	1:B:523:ILE:HD11	1.59	0.57
1:B:384:PHE:CE2	1:B:471:SER:HB2	2.39	0.57
1:C:112:PHE:O	1:C:116:VAL:HG13	2.05	0.57
1:C:267:ALA:HB1	1:C:451:GLN:HE22	1.69	0.57
1:B:544:LEU:O	1:B:547:ASP:HB2	2.05	0.57
1:C:224:LEU:CD1	1:C:539:ALA:CB	2.83	0.57
1:A:424:GLU:OE1	1:A:424:GLU:N	2.38	0.57
1:A:449:GLY:HA2	1:A:452:ILE:HG23	1.86	0.57
1:B:399:LEU:HB2	1:B:403:LEU:HD13	1.87	0.57
1:C:144:MET:SD	1:C:388:ILE:CG1	2.93	0.57
1:A:449:GLY:CA	1:A:452:ILE:HG23	2.34	0.57
1:B:108:THR:OG1	1:B:192:HIS:HE1	1.87	0.57
1:C:76:TRP:NE1	1:C:85:THR:HB	2.17	0.57
1:C:114:ILE:HD11	1:C:398:ILE:HG12	1.85	0.57
1:C:303:GLN:OE1	1:C:306:SER:HB3	2.05	0.57
1:A:235:GLY:N	1:A:238:ILE:HD13	2.20	0.56
1:A:519:GLN:O	1:A:519:GLN:HG3	2.04	0.56
1:B:327:VAL:CG2	1:B:328:SER:N	2.53	0.56
1:C:144:MET:SD	1:C:388:ILE:HD13	2.45	0.56
1:C:304:TYR:HD1	1:C:305:LEU:H	1.33	0.56
1:B:103:PHE:CD1	1:B:371:TRP:CB	2.85	0.56
1:C:69:ILE:HD12	1:C:69:ILE:N	2.20	0.56
1:C:380:PHE:CZ	2:C:2486:CHT:H82	2.40	0.56
1:A:330:LEU:HD21	1:B:101:TRP:CE2	2.40	0.56
1:A:527:THR:CG2	1:A:528:PRO:CD	2.83	0.56
1:A:574:ARG:HD3	1:A:574:ARG:N	2.17	0.56
1:B:156:PHE:O	1:B:160:THR:HG22	2.05	0.56
1:B:217:LEU:HD12	1:B:217:LEU:H	1.68	0.56
1:A:204:ILE:HD11	1:A:217:LEU:HD12	1.86	0.56
1:A:460:LEU:HD11	1:A:464:PHE:CZ	2.40	0.56
1:A:485:LEU:O	1:A:486:GLU:C	2.48	0.56
1:B:320:VAL:HG21	1:B:415:ILE:HG22	1.86	0.56
1:B:352:ALA:HB2	1:B:363:LEU:HD12	1.87	0.56
1:C:394:ILE:HG22	1:C:398:ILE:HD12	1.87	0.56
1:A:106:PHE:CD1	1:A:534:ILE:HD12	2.40	0.56
1:A:309:ASN:O	1:A:313:ALA:CB	2.54	0.56
1:C:530:LEU:O	1:C:534:ILE:HG13	2.06	0.56
1:C:92:LEU:HD13	1:C:520:ASN:CB	2.36	0.56
1:C:197:TYR:HE1	1:C:374:TRP:O	1.88	0.56
1:C:250:THR:CG2	1:C:377:TRP:HE1	2.13	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:530:LEU:C	1:B:530:LEU:HD23	2.30	0.56
1:A:215:GLN:HB2	1:A:483:GLY:O	2.04	0.56
1:A:351:THR:C	1:A:353:MET:N	2.60	0.56
1:B:161:GLU:HG3	1:B:165:PHE:CE2	2.40	0.56
1:B:288:LEU:O	1:B:291:ILE:HG22	2.06	0.56
1:B:463:THR:C	1:B:465:PHE:H	2.14	0.56
1:A:161:GLU:HA	1:A:164:THR:HG22	1.88	0.56
1:A:261:ILE:CD1	1:A:461:LEU:HD21	2.34	0.56
1:B:309:ASN:HD21	1:B:464:PHE:HD2	0.67	0.56
1:B:352:ALA:C	1:B:354:SER:H	2.14	0.56
1:C:163:LEU:HD21	1:C:431:TRP:HE3	1.71	0.56
1:A:159:THR:HG21	1:A:440:LEU:HA	1.88	0.56
1:B:352:ALA:C	1:B:354:SER:N	2.64	0.56
1:C:152:ILE:HD13	1:C:461:LEU:HG	1.87	0.56
1:A:206:TYR:CE2	1:A:543:ASP:OD2	2.59	0.55
1:A:548:VAL:HG23	1:A:549:ILE:N	2.20	0.55
1:C:321:PHE:CE1	1:C:326:THR:HG23	2.41	0.55
1:C:430:ILE:CD1	1:C:443:LEU:HB3	2.36	0.55
1:A:94:ALA:O	1:A:98:ASN:ND2	2.37	0.55
1:A:344:PHE:HD2	1:A:344:PHE:O	1.86	0.55
1:B:95:VAL:CG2	1:B:527:THR:CG2	2.84	0.55
1:B:309:ASN:ND2	1:B:464:PHE:HB3	2.20	0.55
1:C:92:LEU:O	1:C:95:VAL:HG12	2.06	0.55
1:A:246:THR:HG21	1:A:476:MET:HB3	1.89	0.55
1:A:443:LEU:HD12	1:A:443:LEU:C	2.31	0.55
1:B:103:PHE:HB3	1:B:371:TRP:HD1	1.72	0.55
1:B:251:ALA:HA	1:B:254:LEU:HG	1.88	0.55
1:B:475:VAL:CG2	1:B:479:MET:HE3	2.36	0.55
1:A:92:LEU:HD13	1:A:96:VAL:CG2	2.35	0.55
1:A:106:PHE:CB	1:A:534:ILE:HD11	2.35	0.55
1:A:121:LYS:HD2	1:A:553:TYR:CZ	2.41	0.55
1:A:408:VAL:HG23	1:A:409:SER:N	2.21	0.55
1:B:153:ASP:CG	1:B:154:LEU:HD23	2.31	0.55
1:B:202:LEU:HD23	1:B:540:LEU:CD2	2.35	0.55
1:B:373:TRP:CD1	1:B:374:TRP:N	2.74	0.55
1:C:224:LEU:CD1	1:C:539:ALA:HA	2.34	0.55
1:C:291:ILE:HD12	1:C:469:ALA:CB	2.36	0.55
1:B:305:LEU:HB3	1:B:467:THR:HG22	1.89	0.55
1:C:218:SER:C	1:C:220:ALA:H	2.15	0.55
1:B:92:LEU:HD21	1:B:523:ILE:HG13	1.87	0.55
1:B:167:ARG:NH1	1:B:424:GLU:OE2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:PHE:CD1	1:C:256:LEU:HD13	2.41	0.55
1:A:60:TRP:CA	1:A:63:ILE:HG22	2.19	0.55
1:A:70:VAL:O	1:A:74:VAL:HG23	2.07	0.55
1:A:114:ILE:HG13	1:A:115:VAL:N	2.22	0.55
1:C:270:ILE:HA	1:C:271:ILE:CG1	2.36	0.55
1:A:113:PHE:HE1	1:A:117:ILE:HD11	1.67	0.55
1:C:292:PHE:O	1:C:296:SER:CB	2.53	0.55
1:C:435:ALA:O	1:C:439:GLN:OE1	2.24	0.55
1:C:477:GLY:O	1:C:481:GLN:HG3	2.07	0.55
1:A:112:PHE:O	1:A:116:VAL:HG12	2.06	0.55
1:B:475:VAL:HG22	1:B:479:MET:HE3	1.90	0.55
1:C:63:ILE:HG12	1:C:480:SER:HB2	1.88	0.55
1:A:92:LEU:HD23	1:A:520:ASN:CG	2.32	0.54
1:A:463:THR:O	1:A:467:THR:HG23	2.07	0.54
1:A:574:ARG:HD3	1:A:574:ARG:H	1.72	0.54
1:B:286:LEU:HD12	1:B:287:THR:HG23	1.88	0.54
1:C:114:ILE:HG13	1:C:398:ILE:HG12	1.89	0.54
1:C:398:ILE:HG22	1:C:399:LEU:N	2.21	0.54
1:C:491:VAL:O	1:C:494:ALA:HB3	2.07	0.54
1:A:227:GLU:O	1:A:228:LYS:HB2	2.06	0.54
1:B:167:ARG:NH1	1:B:424:GLU:OE1	2.36	0.54
1:B:186:MET:CG	1:B:190:THR:HG21	2.32	0.54
1:B:366:TRP:C	1:B:370:TYR:HD2	2.14	0.54
1:B:463:THR:O	1:B:465:PHE:N	2.33	0.54
1:C:72:ALA:O	1:C:76:TRP:HB3	2.07	0.54
1:A:149:GLY:HA2	1:A:194:TRP:CH2	2.41	0.54
1:B:426:ASN:HB3	1:B:428:GLU:OE1	2.06	0.54
1:C:375:ILE:CD1	1:C:530:LEU:HB2	2.36	0.54
1:A:460:LEU:HD12	1:A:460:LEU:O	2.07	0.54
1:C:166:TYR:CE2	1:C:176:HIS:HD2	2.25	0.54
1:C:230:ALA:O	1:C:231:GLU:HG2	2.06	0.54
1:A:123:GLY:HA2	1:A:394:ILE:CG2	2.37	0.54
1:B:162:PRO:HG3	1:B:185:THR:HG21	1.90	0.54
1:C:298:VAL:CG2	1:C:302:ILE:HD13	2.34	0.54
1:B:103:PHE:HE1	1:B:372:ALA:HA	1.72	0.54
1:B:138:THR:O	1:B:142:ILE:HG23	2.07	0.54
1:B:200:VAL:CG1	1:B:382:GLY:HA3	2.37	0.54
1:B:327:VAL:O	1:B:330:LEU:N	2.41	0.54
1:C:190:THR:O	1:C:193:PRO:CG	2.56	0.54
1:B:186:MET:HE1	1:B:336:SER:CB	2.38	0.54
1:C:428:GLU:OE1	1:C:428:GLU:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:THR:OG1	1:A:443:LEU:HD21	2.08	0.54
1:B:191:LEU:N	1:B:191:LEU:CD1	2.71	0.54
1:B:305:LEU:HB3	1:B:467:THR:HG21	1.89	0.54
1:C:65:PRO:HB2	1:C:240:ILE:HD11	1.90	0.54
1:C:163:LEU:HD21	1:C:431:TRP:CE3	2.42	0.54
1:A:73:THR:HA	1:A:76:TRP:HB3	1.88	0.54
1:A:92:LEU:HD22	1:A:523:ILE:HD11	1.88	0.54
1:C:92:LEU:CD1	1:C:520:ASN:HA	2.32	0.54
1:A:172:GLY:C	1:A:173:HIS:CG	2.86	0.54
1:C:430:ILE:HG21	1:C:443:LEU:HA	1.90	0.54
1:A:66:ALA:HB3	1:A:67:LEU:HD12	1.90	0.53
1:B:366:TRP:O	1:B:370:TYR:CG	2.61	0.53
1:B:411:VAL:O	1:B:414:SER:HB2	2.07	0.53
1:C:473:SER:HA	1:C:476:MET:HE3	1.88	0.53
1:A:123:GLY:O	1:A:394:ILE:HB	2.08	0.53
1:A:344:PHE:HD2	1:A:345:PHE:N	2.05	0.53
1:B:106:PHE:O	1:B:107:GLY:C	2.51	0.53
1:B:279:ILE:O	1:B:282:ILE:HG12	2.07	0.53
1:B:307:ASN:HA	1:B:310:MET:HE2	1.89	0.53
1:B:401:VAL:HG13	1:B:402:LEU:HD12	1.90	0.53
1:C:81:LYS:HD3	1:C:84:PHE:CE2	2.44	0.53
1:C:82:ASP:O	1:C:85:THR:HG22	2.07	0.53
1:A:206:TYR:CD2	1:A:544:LEU:CD1	2.92	0.53
1:B:156:PHE:HB3	1:B:260:GLN:OE1	2.09	0.53
1:C:106:PHE:CD1	1:C:534:ILE:HD13	2.43	0.53
1:C:167:ARG:HH21	1:C:424:GLU:CD	2.16	0.53
1:A:538:PHE:HA	1:A:541:VAL:HG12	1.91	0.53
1:C:363:LEU:HD23	1:C:367:THR:CG2	2.30	0.53
1:A:101:TRP:CD2	1:A:102:ALA:N	2.76	0.53
1:A:377:TRP:O	1:A:381:VAL:HG22	2.08	0.53
1:B:103:PHE:CD1	1:B:371:TRP:HB2	2.43	0.53
1:C:208:THR:HG21	1:C:215:GLN:CG	2.37	0.53
1:C:472:ALA:C	1:C:476:MET:HE2	2.34	0.53
1:A:105:LEU:O	1:A:109:VAL:HG23	2.09	0.53
1:A:345:PHE:CZ	1:C:341:LEU:HD13	2.44	0.53
1:A:412:TRP:CE2	1:A:416:PHE:CD2	2.97	0.53
1:B:103:PHE:HD1	1:B:371:TRP:HB2	1.71	0.53
1:B:186:MET:CG	1:B:190:THR:CG2	2.87	0.53
1:B:395:ARG:O	1:B:399:LEU:HG	2.07	0.53
1:B:103:PHE:H	1:B:103:PHE:HD2	1.57	0.53
1:A:95:VAL:O	1:A:99:LEU:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:545:SER:O	1:B:550:TYR:HD2	1.91	0.53
1:C:76:TRP:CZ2	1:C:84:PHE:C	2.87	0.53
1:C:339:ASN:O	1:C:343:ASN:N	2.35	0.53
1:A:178:VAL:O	1:A:182:MET:HG2	2.08	0.53
1:B:83:SER:O	1:B:86:ASN:HB2	2.09	0.53
1:C:314:ALA:O	1:C:318:ILE:HG13	2.09	0.53
1:C:323:VAL:HG13	1:C:324:GLY:H	1.74	0.53
1:A:369:PHE:HE1	1:A:519:GLN:CB	2.11	0.52
1:A:370:TYR:HB3	1:A:374:TRP:HE1	1.74	0.52
1:A:563:LEU:HD23	1:A:563:LEU:C	2.33	0.52
1:B:167:ARG:NH1	1:B:424:GLU:CD	2.67	0.52
1:C:188:HIS:HB3	1:C:370:TYR:CG	2.44	0.52
1:C:527:THR:N	1:C:528:PRO:CD	2.72	0.52
1:A:202:LEU:HD21	1:A:394:ILE:HD13	1.90	0.52
1:B:201:GLY:HA2	1:B:382:GLY:O	2.09	0.52
1:B:208:THR:HG21	1:B:215:GLN:CA	2.39	0.52
1:B:464:PHE:CA	1:B:467:THR:HG23	2.36	0.52
1:C:134:PRO:CG	1:C:392:ARG:HD3	2.38	0.52
1:C:156:PHE:CG	1:C:256:LEU:HD13	2.44	0.52
1:A:165:PHE:CE1	1:A:362:TRP:HZ2	2.28	0.52
1:A:188:HIS:HA	1:A:371:TRP:CH2	2.44	0.52
1:A:222:VAL:O	1:A:226:GLY:O	2.27	0.52
1:A:222:VAL:N	1:A:223:PRO:CD	2.72	0.52
1:A:437:GLU:O	1:A:441:PHE:CE1	2.63	0.52
1:B:299:GLY:O	1:B:300:LYS:HB3	2.08	0.52
1:C:286:LEU:O	1:C:290:PHE:HD2	1.92	0.52
1:C:291:ILE:HG13	1:C:470:ASP:OD1	2.10	0.52
1:A:332:LEU:O	1:A:332:LEU:HD23	2.09	0.52
1:A:343:ASN:C	1:A:347:MET:HG3	2.29	0.52
1:B:544:LEU:C	1:B:546:ASN:N	2.67	0.52
1:C:209:PHE:CE2	1:C:390:ARG:HB2	2.43	0.52
1:A:248:PHE:N	1:A:248:PHE:CD2	2.77	0.52
1:A:330:LEU:HD21	1:B:101:TRP:CZ2	2.45	0.52
1:B:375:ILE:CG2	1:B:526:ALA:HB1	2.38	0.52
1:B:426:ASN:CB	1:B:428:GLU:OE1	2.57	0.52
1:B:430:ILE:C	1:B:430:ILE:HD12	2.35	0.52
1:C:77:GLY:O	1:C:82:ASP:HA	2.09	0.52
1:C:553:TYR:CD2	1:C:554:ARG:N	2.77	0.52
1:A:81:LYS:HB2	1:A:84:PHE:CB	2.31	0.52
1:A:351:THR:CG2	1:C:331:ASN:CB	2.75	0.52
1:C:231:GLU:HA	1:C:235:GLY:HA3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:451:GLN:O	1:C:455:ILE:HG13	2.10	0.52
1:C:475:VAL:HG12	1:C:479:MET:CE	2.40	0.52
1:A:572:GLU:HA	1:A:575:LYS:HG2	1.92	0.52
1:C:231:GLU:HA	1:C:234:LEU:O	2.10	0.52
1:A:80:PHE:CG	1:A:81:LYS:N	2.78	0.52
1:A:176:HIS:HB3	1:B:356:ASP:OD1	2.09	0.52
1:B:123:GLY:HA2	1:B:394:ILE:CG1	2.40	0.52
1:B:127:LEU:HD11	1:B:205:ALA:CB	2.38	0.52
1:B:145:MET:HG3	1:B:404:VAL:HG11	1.91	0.52
1:C:70:VAL:CG1	1:C:71:LEU:N	2.73	0.52
1:A:188:HIS:HA	1:A:371:TRP:HH2	1.76	0.51
1:B:157:TYR:HA	1:B:160:THR:CG2	2.40	0.51
1:C:114:ILE:CD1	1:C:398:ILE:HG12	2.40	0.51
1:A:154:LEU:O	1:A:158:GLY:CA	2.57	0.51
1:A:334:PRO:HG3	1:B:104:ILE:CD1	2.39	0.51
1:B:309:ASN:CG	1:B:463:THR:CG2	2.82	0.51
1:C:184:THR:HG22	1:C:188:HIS:CE1	2.44	0.51
1:C:320:VAL:HA	1:C:323:VAL:CG1	2.41	0.51
1:A:543:ASP:OD1	1:A:543:ASP:C	2.53	0.51
1:B:401:VAL:C	1:B:402:LEU:HD12	2.35	0.51
1:C:153:ASP:OD2	2:C:2486:CHT:O6	2.26	0.51
1:C:269:ASN:C	1:C:270:ILE:HD12	2.35	0.51
1:A:392:ARG:HD2	1:A:396:GLU:CG	2.40	0.51
1:B:291:ILE:HA	1:B:466:ILE:HD11	1.92	0.51
1:A:110:PHE:CE1	1:A:534:ILE:HD13	2.46	0.51
1:A:309:ASN:ND2	1:A:464:PHE:CE1	2.76	0.51
1:A:423:PHE:HB3	1:A:428:GLU:O	2.10	0.51
1:B:230:ALA:O	1:B:232:GLY:N	2.43	0.51
1:B:231:GLU:HG3	1:B:236:LYS:CE	2.40	0.51
1:C:183:SER:HB3	1:C:339:ASN:HB3	1.92	0.51
1:C:526:ALA:C	1:C:528:PRO:CD	2.84	0.51
1:A:80:PHE:CE2	1:A:81:LYS:HG2	2.45	0.51
1:A:160:THR:HG22	1:A:439:GLN:HB2	1.92	0.51
1:B:329:ILE:HD11	1:B:415:ILE:HG23	1.91	0.51
1:C:121:LYS:CD	1:C:121:LYS:N	2.56	0.51
1:C:253:SER:OG	1:C:377:TRP:HH2	1.92	0.51
1:C:320:VAL:HA	1:C:323:VAL:HG12	1.93	0.51
1:A:282:ILE:O	1:A:285:VAL:HG22	2.10	0.51
1:B:265:LEU:HB3	1:B:269:ASN:HD21	1.76	0.51
1:B:320:VAL:HG21	1:B:415:ILE:CG2	2.39	0.51
1:B:372:ALA:O	1:B:375:ILE:HG22	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:TYR:CD2	1:A:544:LEU:HD12	2.46	0.51
1:A:351:THR:HG21	1:C:331:ASN:CB	2.30	0.51
1:B:399:LEU:O	1:B:400:GLY:C	2.53	0.51
1:B:431:TRP:O	1:B:432:GLY:O	2.28	0.51
1:C:523:ILE:O	1:C:527:THR:HG23	2.10	0.51
1:A:351:THR:O	1:A:354:SER:N	2.32	0.51
1:A:379:PRO:O	1:A:383:MET:HG2	2.10	0.51
1:B:136:PHE:CE2	1:B:144:MET:SD	3.04	0.51
1:B:153:ASP:HA	1:B:156:PHE:CE2	2.46	0.51
1:B:206:TYR:HE2	1:B:543:ASP:OD2	1.91	0.51
1:C:364:GLY:HA2	1:C:368:ILE:HG21	1.93	0.51
1:A:136:PHE:CD1	1:A:144:MET:HE3	2.46	0.51
1:A:164:THR:HG21	1:A:366:TRP:CH2	2.46	0.51
1:A:350:ARG:CD	1:A:363:LEU:HD21	2.40	0.51
1:A:430:ILE:HG21	1:A:443:LEU:HB3	1.92	0.51
1:A:197:TYR:CD1	1:A:381:VAL:HG21	2.46	0.50
1:A:252:CYS:HB2	1:A:522:THR:HG21	1.93	0.50
1:A:415:ILE:O	1:A:419:THR:HG23	2.11	0.50
1:B:92:LEU:HD12	1:B:524:VAL:CG1	2.40	0.50
1:B:116:VAL:HG12	1:B:116:VAL:O	2.09	0.50
1:B:208:THR:OG1	1:B:209:PHE:HD1	1.94	0.50
1:C:252:CYS:HA	1:C:518:LEU:HD11	1.92	0.50
1:A:540:LEU:HD23	1:A:540:LEU:C	2.35	0.50
1:B:177:ASN:OD1	1:B:177:ASN:O	2.29	0.50
1:B:206:TYR:CE1	1:B:210:ARG:HG2	2.46	0.50
1:A:222:VAL:CB	1:A:227:GLU:HG2	2.41	0.50
1:A:293:SER:O	1:A:298:VAL:N	2.42	0.50
1:C:161:GLU:HG3	1:C:185:THR:CG2	2.41	0.50
1:C:167:ARG:NH1	1:C:431:TRP:CG	2.78	0.50
1:A:206:TYR:HE2	1:A:543:ASP:OD1	1.93	0.50
1:A:334:PRO:HB3	1:B:105:LEU:HD13	1.93	0.50
1:B:126:ARG:HA	1:B:393:SER:HA	1.92	0.50
1:B:136:PHE:CZ	1:B:144:MET:SD	3.05	0.50
1:B:216:LEU:HD23	1:B:218:SER:H	1.77	0.50
1:B:404:VAL:N	1:B:405:PRO:CD	2.74	0.50
1:C:121:LYS:O	1:C:122:PHE:C	2.54	0.50
1:A:351:THR:HG21	1:C:331:ASN:O	2.12	0.50
1:A:381:VAL:O	1:A:385:LEU:HD12	2.11	0.50
1:B:172:GLY:C	1:B:173:HIS:CD2	2.89	0.50
1:B:283:VAL:HG13	1:B:286:LEU:HD11	1.93	0.50
1:C:165:PHE:CE1	1:C:362:TRP:CZ2	2.99	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:GLN:HA	1:A:437:GLU:CG	2.35	0.50
1:B:341:LEU:HD23	1:C:345:PHE:CZ	2.47	0.50
1:C:141:TRP:HD1	1:C:388:ILE:CG2	2.25	0.50
1:C:159:THR:HG21	1:C:443:LEU:CD2	2.41	0.50
1:A:321:PHE:CZ	1:A:326:THR:CG2	2.95	0.50
1:B:106:PHE:HB3	1:B:110:PHE:CZ	2.47	0.50
1:B:329:ILE:CG2	1:B:415:ILE:HG13	2.41	0.50
1:C:116:VAL:HA	1:C:119:ALA:HB3	1.94	0.50
1:A:206:TYR:HE2	1:A:543:ASP:OD2	1.93	0.50
1:A:380:PHE:CD1	1:A:472:ALA:HA	2.46	0.50
1:B:67:LEU:O	1:B:70:VAL:HG12	2.11	0.50
1:C:92:LEU:HA	1:C:95:VAL:HG12	1.93	0.50
1:C:163:LEU:CD2	1:C:431:TRP:CZ3	2.95	0.50
1:C:282:ILE:O	1:C:286:LEU:HD23	2.12	0.50
1:A:137:ARG:HD3	1:A:138:THR:H	1.76	0.50
1:A:207:SER:O	1:A:213:ARG:HG2	2.12	0.50
1:A:247:VAL:HG22	1:A:476:MET:HE1	1.94	0.50
1:A:548:VAL:HG23	1:A:549:ILE:H	1.75	0.50
1:B:538:PHE:HA	1:B:541:VAL:HG12	1.94	0.50
1:A:329:ILE:HG23	1:A:414:SER:C	2.36	0.49
1:B:318:ILE:O	1:B:322:VAL:HG22	2.12	0.49
1:A:276:ASP:N	1:A:279:ILE:HG13	2.27	0.49
1:B:103:PHE:N	1:B:103:PHE:CD2	2.79	0.49
1:B:379:PRO:O	1:B:383:MET:SD	2.71	0.49
1:A:99:LEU:O	1:A:100:GLY:C	2.55	0.49
1:B:210:ARG:NH2	1:B:547:ASP:OD1	2.45	0.49
1:B:323:VAL:HG23	1:B:324:GLY:N	2.26	0.49
1:A:412:TRP:O	1:A:416:PHE:HD2	1.95	0.49
1:A:574:ARG:CD	1:A:574:ARG:H	2.22	0.49
1:A:577:GLU:HG3	1:A:578:LEU:N	2.27	0.49
1:B:213:ARG:HH12	1:B:223:PRO:HD3	1.78	0.49
1:B:544:LEU:O	1:B:547:ASP:N	2.39	0.49
1:C:103:PHE:CZ	1:C:530:LEU:HD22	2.47	0.49
1:C:173:HIS:CD2	1:C:180:VAL:CB	2.95	0.49
1:C:181:ALA:O	1:C:185:THR:HG23	2.12	0.49
1:C:337:ILE:CD1	1:C:410:THR:HG21	2.36	0.49
1:A:194:TRP:CE3	1:A:401:VAL:HG13	2.47	0.49
1:A:206:TYR:CE1	1:A:210:ARG:HG2	2.47	0.49
1:A:378:SER:N	1:A:379:PRO:CD	2.76	0.49
1:B:117:ILE:HG23	1:B:398:ILE:HD13	1.94	0.49
1:B:193:PRO:HB3	1:B:374:TRP:CD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:ALA:O	1:B:354:SER:N	2.46	0.49
1:A:466:ILE:HD12	1:A:467:THR:N	2.28	0.49
1:B:77:GLY:O	1:B:82:ASP:OD1	2.30	0.49
1:B:112:PHE:O	1:B:116:VAL:HG23	2.13	0.49
1:B:163:LEU:HD11	1:B:167:ARG:HD2	1.94	0.49
1:B:205:ALA:HB2	1:B:386:ALA:CB	2.37	0.49
1:C:67:LEU:HD23	1:C:70:VAL:HG11	1.94	0.49
1:C:191:LEU:C	1:C:193:PRO:HD2	2.38	0.49
1:C:401:VAL:O	1:C:405:PRO:CD	2.58	0.49
1:C:452:ILE:HA	1:C:455:ILE:HD12	1.95	0.49
1:A:562:ARG:O	1:A:565:ARG:CB	2.60	0.49
1:C:67:LEU:HA	1:C:70:VAL:HG12	1.94	0.49
1:A:432:GLY:H	1:A:439:GLN:HE21	1.59	0.49
1:A:559:PHE:C	1:A:559:PHE:CD2	2.91	0.49
1:B:103:PHE:CE2	1:B:530:LEU:HD12	2.47	0.49
1:B:365:SER:C	1:B:366:TRP:HD1	2.18	0.49
1:C:114:ILE:HD12	1:C:117:ILE:CD1	2.37	0.49
1:C:154:LEU:O	1:C:155:MET:C	2.55	0.49
1:C:161:GLU:HB3	1:C:162:PRO:CD	2.43	0.49
1:A:219:SER:C	1:A:221:PHE:H	2.21	0.49
1:A:345:PHE:CE1	1:C:341:LEU:CD1	2.93	0.49
1:A:402:LEU:O	1:A:403:LEU:C	2.56	0.49
1:A:558:ARG:O	1:A:562:ARG:HG2	2.12	0.49
1:B:307:ASN:O	1:B:311:VAL:HG23	2.12	0.49
1:C:141:TRP:CD1	1:C:388:ILE:CG2	2.96	0.49
1:A:215:GLN:NE2	1:A:387:ARG:NH2	2.61	0.48
1:A:562:ARG:O	1:A:565:ARG:N	2.44	0.48
1:C:163:LEU:CD2	1:C:431:TRP:CE3	2.96	0.48
1:C:251:ALA:O	1:C:255:GLY:N	2.37	0.48
1:C:311:VAL:O	1:C:315:LEU:HD13	2.13	0.48
1:A:114:ILE:HD11	1:A:402:LEU:HD11	1.94	0.48
1:A:408:VAL:CG2	1:A:409:SER:N	2.76	0.48
1:B:541:VAL:HG13	1:B:542:LYS:N	2.28	0.48
1:C:64:VAL:N	1:C:65:PRO:CD	2.76	0.48
1:C:224:LEU:HD11	1:C:538:PHE:C	2.37	0.48
1:A:444:LEU:C	1:A:446:ALA:H	2.19	0.48
1:B:132:GLU:OE1	1:B:390:ARG:CZ	2.61	0.48
1:C:155:MET:SD	1:C:461:LEU:HD11	2.54	0.48
1:C:459:ILE:O	1:C:463:THR:HG23	2.13	0.48
1:A:60:TRP:CE3	1:A:63:ILE:HG21	2.48	0.48
1:A:219:SER:O	1:A:222:VAL:HG13	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:MET:HE1	1:C:328:SER:OG	2.13	0.48
1:A:565:ARG:HG2	1:C:130:ILE:HG21	1.95	0.48
1:B:309:ASN:HD22	1:B:464:PHE:HB3	1.79	0.48
1:B:463:THR:O	1:B:464:PHE:CD1	2.67	0.48
1:B:464:PHE:CD1	1:B:465:PHE:N	2.81	0.48
1:C:167:ARG:HH22	1:C:431:TRP:HB2	1.78	0.48
1:C:291:ILE:HD12	1:C:469:ALA:HB3	1.95	0.48
1:C:466:ILE:H	1:C:466:ILE:HD12	1.79	0.48
1:A:137:ARG:CD	1:A:139:VAL:HG22	2.40	0.48
1:B:58:LEU:O	1:B:60:TRP:HD1	1.96	0.48
1:B:453:MET:O	1:B:456:ILE:CG1	2.61	0.48
1:C:232:GLY:O	1:C:233:TRP:C	2.55	0.48
1:C:546:ASN:O	1:C:551:LEU:HD12	2.13	0.48
1:A:355:ALA:O	1:A:356:ASP:CB	2.61	0.48
1:B:80:PHE:CG	1:B:80:PHE:O	2.67	0.48
1:B:333:LEU:HB2	1:B:334:PRO:CD	2.43	0.48
1:B:372:ALA:CB	1:B:523:ILE:CG2	2.88	0.48
1:C:178:VAL:HG23	1:C:179:GLY:N	2.28	0.48
1:B:118:ALA:HB2	1:B:398:ILE:HD12	1.96	0.48
1:B:127:LEU:HD23	1:B:127:LEU:C	2.39	0.48
1:B:222:VAL:O	1:B:223:PRO:C	2.54	0.48
1:B:463:THR:C	1:B:465:PHE:N	2.72	0.48
1:C:58:LEU:HD12	1:C:58:LEU:H	1.79	0.48
1:C:70:VAL:HG13	1:C:71:LEU:N	2.27	0.48
1:C:74:VAL:HG23	1:C:75:VAL:N	2.29	0.48
1:A:288:LEU:C	1:A:288:LEU:HD12	2.39	0.48
1:C:123:GLY:HA3	1:C:395:ARG:HB2	1.95	0.48
1:C:132:GLU:OE2	1:C:390:ARG:NE	2.45	0.48
1:C:264:GLY:HA2	1:C:441:PHE:CE1	2.48	0.48
1:C:303:GLN:O	1:C:304:TYR:CB	2.59	0.48
1:C:497:VAL:HG23	1:C:498:ALA:N	2.29	0.48
1:A:124:THR:O	1:A:125:ILE:C	2.57	0.48
1:A:265:LEU:HA	1:A:458:MET:HE1	1.95	0.48
1:A:371:TRP:CE3	1:A:371:TRP:CA	2.96	0.48
1:B:321:PHE:HA	1:B:329:ILE:CD1	2.43	0.48
1:B:114:ILE:HG13	1:B:115:VAL:H	1.78	0.48
1:B:125:ILE:CG2	1:B:210:ARG:NH2	2.67	0.48
1:C:189:TRP:C	1:C:193:PRO:HG3	2.39	0.48
1:C:305:LEU:HA	1:C:308:ALA:CB	2.43	0.48
1:C:379:PRO:HD3	1:C:529:PHE:HE2	1.77	0.48
1:A:106:PHE:HB3	1:A:534:ILE:CD1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:LEU:O	1:A:547:ASP:N	2.31	0.47
1:B:77:GLY:O	1:B:78:ILE:HD13	2.14	0.47
1:B:309:ASN:CG	1:B:463:THR:HG23	2.39	0.47
1:C:172:GLY:O	1:C:173:HIS:ND1	2.42	0.47
1:C:259:LEU:HD13	1:C:437:GLU:OE1	2.14	0.47
1:C:443:LEU:HG	1:C:444:LEU:N	2.29	0.47
1:A:121:LYS:HD2	1:A:553:TYR:CE2	2.49	0.47
1:A:136:PHE:CE2	1:A:388:ILE:HG23	2.46	0.47
1:A:405:PRO:O	1:A:408:VAL:HG22	2.14	0.47
1:B:58:LEU:HA	1:B:481:GLN:HG2	1.96	0.47
1:B:192:HIS:CB	1:B:193:PRO:HD3	2.44	0.47
1:B:208:THR:HG21	1:B:215:GLN:HB2	1.96	0.47
1:B:305:LEU:HD12	1:B:305:LEU:HA	1.72	0.47
1:B:379:PRO:HD3	1:B:529:PHE:CE2	2.48	0.47
1:C:186:MET:CE	1:C:190:THR:HG21	2.42	0.47
1:A:72:ALA:O	1:A:76:TRP:CB	2.61	0.47
1:A:158:GLY:HA2	1:A:413:PHE:CE1	2.46	0.47
1:A:473:SER:HA	1:A:476:MET:CG	2.43	0.47
1:A:565:ARG:HG2	1:C:130:ILE:CG2	2.44	0.47
1:B:224:LEU:HD11	1:B:538:PHE:HB2	1.97	0.47
1:B:259:LEU:CD1	1:B:437:GLU:HG2	2.43	0.47
1:B:316:LEU:HD22	1:B:460:LEU:HD11	1.93	0.47
1:B:545:SER:O	1:B:550:TYR:CD2	2.67	0.47
1:C:190:THR:C	1:C:193:PRO:HD2	2.40	0.47
1:C:267:ALA:CB	1:C:451:GLN:HE22	2.27	0.47
1:C:378:SER:N	1:C:379:PRO:HD2	2.28	0.47
1:A:101:TRP:CG	1:A:102:ALA:H	2.31	0.47
1:B:145:MET:CE	1:B:404:VAL:HG21	2.43	0.47
1:B:371:TRP:HE3	1:B:371:TRP:HA	1.80	0.47
1:B:385:LEU:C	1:B:385:LEU:HD12	2.39	0.47
1:B:464:PHE:HA	1:B:467:THR:OG1	2.15	0.47
1:A:423:PHE:HD2	1:A:430:ILE:HD11	1.80	0.47
1:A:562:ARG:HA	1:A:565:ARG:HB2	1.96	0.47
1:A:574:ARG:HA	1:A:577:GLU:HG2	1.96	0.47
1:C:75:VAL:HG12	1:C:76:TRP:N	2.29	0.47
1:C:123:GLY:CA	1:C:395:ARG:HB2	2.44	0.47
1:C:325:PRO:HB2	1:C:328:SER:HB2	1.97	0.47
1:C:392:ARG:HD2	1:C:396:GLU:CD	2.39	0.47
1:A:213:ARG:NH1	1:A:219:SER:HB3	2.29	0.47
1:A:232:GLY:O	1:A:233:TRP:C	2.57	0.47
1:A:478:THR:CA	1:A:481:GLN:NE2	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:CYS:SG	1:C:518:LEU:HG	2.54	0.47
1:A:317:ALA:O	1:A:320:VAL:HG22	2.14	0.47
1:A:392:ARG:HD3	1:A:392:ARG:HA	1.52	0.47
1:B:92:LEU:O	1:B:93:SER:C	2.57	0.47
1:B:132:GLU:OE2	1:B:390:ARG:HG3	2.15	0.47
1:B:191:LEU:CD1	1:B:191:LEU:H	2.27	0.47
1:B:247:VAL:HG12	1:B:248:PHE:HD1	1.80	0.47
1:B:378:SER:HB2	1:B:379:PRO:HD3	1.96	0.47
1:B:411:VAL:HG13	1:B:415:ILE:HD12	1.91	0.47
1:C:209:PHE:CD2	1:C:390:ARG:HD2	2.50	0.47
1:C:318:ILE:O	1:C:322:VAL:HG22	2.15	0.47
1:C:340:TYR:O	1:C:344:PHE:N	2.48	0.47
1:C:418:GLY:O	1:C:422:VAL:HG23	2.14	0.47
1:A:519:GLN:O	1:A:520:ASN:HB2	2.14	0.47
1:B:135:GLU:OE2	1:B:136:PHE:HD2	1.98	0.47
1:B:159:THR:HG23	1:B:443:LEU:HD23	1.97	0.47
1:B:189:TRP:CE3	1:B:413:PHE:CZ	3.03	0.47
1:B:379:PRO:CG	1:B:529:PHE:CZ	2.94	0.47
1:B:437:GLU:CD	1:B:437:GLU:H	2.21	0.47
1:B:453:MET:O	1:B:456:ILE:HG12	2.15	0.47
1:C:316:LEU:HB3	1:C:416:PHE:HZ	1.79	0.47
1:A:76:TRP:HZ2	1:A:84:PHE:CD2	2.32	0.47
1:B:371:TRP:HA	1:B:371:TRP:CE3	2.50	0.47
1:C:492:THR:HG22	1:C:493:ALA:N	2.30	0.47
1:A:148:ALA:HB2	1:A:384:PHE:CE2	2.50	0.47
1:A:243:ILE:HD12	1:A:244:ILE:H	1.80	0.47
1:A:371:TRP:CE3	1:A:371:TRP:N	2.82	0.47
1:B:295:ILE:N	1:B:295:ILE:HD12	2.30	0.47
1:B:322:VAL:HG23	1:B:323:VAL:N	2.29	0.47
1:B:474:THR:O	1:B:478:THR:HG23	2.14	0.47
1:C:152:ILE:HG21	1:C:257:GLY:HA3	1.97	0.47
1:C:161:GLU:HB3	1:C:162:PRO:HD3	1.97	0.47
1:C:163:LEU:CG	1:C:431:TRP:CZ3	2.89	0.47
1:C:227:GLU:O	1:C:228:LYS:C	2.58	0.47
1:C:316:LEU:HB3	1:C:416:PHE:CZ	2.50	0.47
1:A:145:MET:SD	1:A:405:PRO:HD3	2.55	0.46
1:B:128:GLY:HA3	1:B:390:ARG:HH11	1.79	0.46
1:C:256:LEU:HD12	1:C:257:GLY:N	2.29	0.46
1:A:544:LEU:C	1:A:546:ASN:H	2.23	0.46
1:A:551:LEU:HD23	1:A:551:LEU:HA	1.75	0.46
1:B:269:ASN:OD1	1:B:269:ASN:O	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:ILE:O	1:C:145:MET:N	2.47	0.46
1:C:374:TRP:HA	1:C:374:TRP:CE3	2.50	0.46
1:A:213:ARG:HH12	1:A:219:SER:C	2.23	0.46
1:A:331:ASN:C	1:A:333:LEU:H	2.24	0.46
1:A:353:MET:HG2	1:C:332:LEU:HD21	1.97	0.46
1:B:146:PHE:CB	1:B:310:MET:SD	2.99	0.46
1:B:186:MET:HE2	1:B:336:SER:HB3	1.98	0.46
1:C:159:THR:HG22	1:C:416:PHE:O	2.16	0.46
1:C:374:TRP:CE3	1:C:374:TRP:CA	2.99	0.46
1:A:93:SER:O	1:A:97:ASP:OD1	2.34	0.46
1:B:109:VAL:O	1:B:110:PHE:C	2.59	0.46
1:C:141:TRP:HA	1:C:144:MET:HE3	1.98	0.46
1:A:204:ILE:O	1:A:208:THR:HG23	2.15	0.46
1:B:411:VAL:HA	1:B:414:SER:HB2	1.98	0.46
1:C:134:PRO:HG3	1:C:391:GLY:C	2.39	0.46
1:C:559:PHE:HA	1:C:562:ARG:CG	2.43	0.46
1:A:184:THR:N	1:A:347:MET:HE1	2.31	0.46
1:A:302:ILE:HG13	1:A:303:GLN:N	2.18	0.46
1:C:367:THR:HG23	1:C:368:ILE:N	2.30	0.46
1:C:475:VAL:C	1:C:479:MET:HE2	2.41	0.46
1:A:404:VAL:HB	1:A:405:PRO:CD	2.45	0.46
1:A:412:TRP:CZ3	1:A:416:PHE:HE2	2.33	0.46
1:B:105:LEU:HD23	1:B:106:PHE:CE2	2.51	0.46
1:C:81:LYS:O	1:C:82:ASP:HB3	2.15	0.46
1:C:167:ARG:HH12	1:C:431:TRP:CD1	2.34	0.46
1:C:222:VAL:N	1:C:223:PRO:CD	2.79	0.46
1:C:559:PHE:C	1:C:561:ALA:H	2.23	0.46
1:A:64:VAL:O	1:A:68:VAL:HG12	2.16	0.46
1:A:302:ILE:O	1:A:303:GLN:HB2	2.16	0.46
1:B:346:GLN:HG3	1:B:347:MET:H	1.80	0.46
1:A:353:MET:C	1:A:357:GLY:HA2	2.40	0.46
1:A:355:ALA:O	1:A:356:ASP:HB2	2.16	0.46
1:B:95:VAL:HG13	1:B:96:VAL:N	2.31	0.46
1:B:132:GLU:OE1	1:B:390:ARG:NH1	2.49	0.46
1:C:186:MET:HE3	1:C:190:THR:CG2	2.44	0.46
1:A:371:TRP:CE3	1:A:371:TRP:HA	2.50	0.45
1:A:407:GLY:HA2	1:A:410:THR:HG22	1.98	0.45
1:B:58:LEU:HG	1:B:481:GLN:HE21	1.81	0.45
1:B:216:LEU:HD23	1:B:216:LEU:C	2.40	0.45
1:B:238:ILE:HG22	1:B:239:ASP:N	2.30	0.45
1:B:372:ALA:O	1:B:375:ILE:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:554:ARG:NH1	1:C:557:GLN:NE2	2.64	0.45
1:A:302:ILE:HG12	1:A:303:GLN:HG3	1.98	0.45
1:B:145:MET:SD	1:B:404:VAL:HG21	2.57	0.45
1:C:141:TRP:CD1	1:C:388:ILE:HG22	2.51	0.45
1:C:145:MET:SD	1:C:404:VAL:HB	2.56	0.45
1:C:224:LEU:HD11	1:C:539:ALA:CB	2.44	0.45
1:C:506:LEU:HD21	1:C:521:VAL:HG21	1.97	0.45
1:A:101:TRP:HB3	1:C:331:ASN:OD1	2.16	0.45
1:B:231:GLU:O	1:B:236:LYS:HG2	2.16	0.45
1:A:59:ASN:OD1	1:A:482:HIS:NE2	2.49	0.45
1:A:67:LEU:HD12	1:A:67:LEU:N	2.32	0.45
1:A:252:CYS:HB2	1:A:522:THR:CG2	2.46	0.45
1:B:117:ILE:CG2	1:B:118:ALA:N	2.80	0.45
1:B:187:PHE:CD1	1:B:347:MET:SD	3.09	0.45
1:B:211:VAL:CG1	1:B:213:ARG:HE	2.23	0.45
1:B:372:ALA:O	1:B:373:TRP:C	2.57	0.45
1:C:120:SER:OG	1:C:122:PHE:CD2	2.52	0.45
1:C:125:ILE:HD12	1:C:544:LEU:HD22	1.99	0.45
1:A:163:LEU:HD11	1:A:420:ALA:O	2.17	0.45
1:A:208:THR:O	1:A:212:GLY:HA2	2.16	0.45
1:A:543:ASP:OD1	1:A:543:ASP:O	2.33	0.45
1:C:316:LEU:N	1:C:316:LEU:CD1	2.78	0.45
1:A:542:LYS:HD2	1:A:542:LYS:HA	1.65	0.45
1:B:113:PHE:CZ	1:B:537:MET:HG3	2.52	0.45
1:B:118:ALA:HB2	1:B:398:ILE:HG21	1.98	0.45
1:B:234:LEU:N	1:B:234:LEU:HD12	2.32	0.45
1:C:167:ARG:NH1	1:C:431:TRP:CD2	2.84	0.45
1:C:213:ARG:HD2	1:C:219:SER:O	2.15	0.45
1:C:243:ILE:HG21	1:C:495:TRP:CH2	2.52	0.45
1:C:319:PHE:CD2	1:C:453:MET:HE3	2.50	0.45
1:C:488:ASN:HB3	1:C:491:VAL:CG1	2.44	0.45
1:A:113:PHE:HA	1:A:116:VAL:HG13	1.98	0.45
1:A:189:TRP:CH2	1:A:370:TYR:OH	2.70	0.45
1:A:215:GLN:NE2	1:A:387:ARG:HH21	2.14	0.45
1:A:264:GLY:C	1:A:458:MET:HE1	2.42	0.45
1:A:288:LEU:HD12	1:A:289:ALA:N	2.31	0.45
1:A:376:SER:O	1:A:377:TRP:HB2	2.17	0.45
1:A:387:ARG:HB3	1:A:387:ARG:NH1	2.29	0.45
1:B:216:LEU:HD21	1:B:239:ASP:OD1	2.17	0.45
1:B:331:ASN:O	1:C:351:THR:HG21	2.17	0.45
1:B:455:ILE:O	1:B:458:MET:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:ILE:HD13	1:C:383:MET:CG	2.39	0.45
1:C:295:ILE:HD12	1:C:295:ILE:C	2.42	0.45
1:C:537:MET:O	1:C:541:VAL:HG23	2.15	0.45
1:A:204:ILE:HD13	1:A:383:MET:SD	2.56	0.45
1:A:94:ALA:O	1:A:98:ASN:HB2	2.17	0.45
1:A:439:GLN:O	1:A:440:LEU:C	2.60	0.45
1:B:355:ALA:O	1:B:356:ASP:CB	2.63	0.45
1:C:191:LEU:O	1:C:195:ALA:N	2.49	0.45
1:C:193:PRO:CB	1:C:374:TRP:CD1	2.96	0.45
1:C:423:PHE:C	1:C:425:GLN:H	2.25	0.45
1:A:330:LEU:HG	1:B:101:TRP:CG	2.52	0.45
1:A:330:LEU:CD2	1:B:101:TRP:CE2	2.99	0.45
1:A:478:THR:CA	1:A:481:GLN:HE21	2.29	0.45
1:B:358:THR:O	1:B:360:GLY:N	2.50	0.45
1:B:373:TRP:HD1	1:B:373:TRP:O	2.00	0.45
1:C:92:LEU:HD22	1:C:520:ASN:CG	2.42	0.45
1:A:110:PHE:CZ	1:A:534:ILE:HD13	2.52	0.44
1:A:352:ALA:O	1:A:357:GLY:CA	2.58	0.44
1:B:103:PHE:HE1	1:B:372:ALA:CA	2.31	0.44
1:B:145:MET:HG2	1:B:146:PHE:N	2.32	0.44
1:B:216:LEU:HD23	1:B:218:SER:N	2.32	0.44
1:B:270:ILE:HA	1:B:271:ILE:HA	1.72	0.44
1:B:320:VAL:HG23	1:B:321:PHE:N	2.32	0.44
1:B:326:THR:O	1:B:330:LEU:HB2	2.17	0.44
1:C:170:VAL:HG11	1:C:350:ARG:NH2	2.33	0.44
1:C:187:PHE:CD1	1:C:347:MET:HG3	2.52	0.44
1:C:211:VAL:HG12	1:C:211:VAL:O	2.17	0.44
1:C:523:ILE:O	1:C:527:THR:CG2	2.66	0.44
1:A:182:MET:SD	1:A:332:LEU:HD11	2.57	0.44
1:A:285:VAL:HA	1:A:288:LEU:CG	2.40	0.44
1:A:407:GLY:C	1:A:410:THR:HG22	2.42	0.44
1:A:578:LEU:O	1:A:581:LYS:HB3	2.17	0.44
1:B:70:VAL:HG13	1:B:71:LEU:N	2.31	0.44
1:B:152:ILE:HD11	1:B:257:GLY:HA3	1.99	0.44
1:B:188:HIS:NE2	1:B:367:THR:OG1	2.33	0.44
1:B:362:TRP:HZ3	1:B:367:THR:HG1	1.63	0.44
1:B:468:SER:O	1:B:472:ALA:HB2	2.17	0.44
1:B:534:ILE:O	1:B:537:MET:HB3	2.16	0.44
1:A:222:VAL:HB	1:A:227:GLU:CA	2.37	0.44
1:B:328:SER:O	1:B:329:ILE:C	2.57	0.44
1:C:152:ILE:CD1	1:C:461:LEU:HG	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:392:ARG:NH1	1:C:396:GLU:OE2	2.44	0.44
1:C:452:ILE:HG13	1:C:453:MET:N	2.33	0.44
1:A:154:LEU:O	1:A:158:GLY:N	2.50	0.44
1:A:402:LEU:O	1:A:405:PRO:HD2	2.16	0.44
1:A:571:ASN:HB3	1:A:575:LYS:HE3	2.00	0.44
1:B:131:ASP:OD2	1:C:565:ARG:CZ	2.64	0.44
1:B:378:SER:HB2	1:B:529:PHE:HE2	1.82	0.44
1:B:455:ILE:CG1	1:B:456:ILE:N	2.80	0.44
1:A:579:ALA:C	1:A:581:LYS:H	2.25	0.44
1:B:65:PRO:HB2	1:B:240:ILE:HD13	2.00	0.44
1:B:152:ILE:HD13	1:B:253:SER:O	2.17	0.44
1:B:158:GLY:O	1:B:162:PRO:HD2	2.17	0.44
1:C:374:TRP:HA	1:C:374:TRP:HE3	1.82	0.44
1:A:88:ALA:HA	1:A:91:ALA:CB	2.47	0.44
1:A:155:MET:HB3	1:A:440:LEU:HD11	2.00	0.44
1:A:319:PHE:CD1	1:A:453:MET:HE2	2.53	0.44
1:A:370:TYR:O	1:A:374:TRP:CD1	2.71	0.44
1:A:544:LEU:C	1:A:546:ASN:N	2.73	0.44
1:B:86:ASN:O	1:B:89:SER:HB2	2.17	0.44
1:B:159:THR:HG23	1:B:443:LEU:CD2	2.48	0.44
1:B:206:TYR:CD2	1:B:206:TYR:C	2.96	0.44
1:B:354:SER:HA	1:B:355:ALA:HA	1.51	0.44
1:B:530:LEU:C	1:B:530:LEU:CD2	2.90	0.44
1:C:156:PHE:CD1	1:C:256:LEU:HB2	2.52	0.44
1:C:256:LEU:HD12	1:C:256:LEU:C	2.42	0.44
1:C:319:PHE:CD2	1:C:453:MET:HG3	2.53	0.44
1:C:493:ALA:O	1:C:496:GLY:N	2.51	0.44
1:B:79:GLY:O	1:B:80:PHE:CB	2.65	0.44
1:B:305:LEU:CD2	1:B:467:THR:HG22	2.40	0.44
1:B:402:LEU:C	1:B:405:PRO:HD2	2.42	0.44
1:C:341:LEU:HD23	1:C:341:LEU:HA	1.72	0.44
1:A:65:PRO:HA	1:A:68:VAL:CG1	2.48	0.44
1:A:410:THR:HG23	1:A:411:VAL:N	2.32	0.44
1:A:444:LEU:HD13	1:A:450:GLY:O	2.17	0.44
1:A:477:GLY:C	1:A:481:GLN:HE21	2.21	0.44
1:B:322:VAL:HG23	1:B:323:VAL:H	1.82	0.44
1:B:327:VAL:O	1:B:328:SER:C	2.61	0.44
1:C:187:PHE:HA	1:C:340:TYR:HE1	1.83	0.44
1:C:260:GLN:OE1	1:C:461:LEU:CD2	2.59	0.44
1:C:269:ASN:C	1:C:270:ILE:CG1	2.90	0.44
1:C:452:ILE:O	1:C:456:ILE:HG13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:PHE:CE1	1:A:347:MET:HB2	2.53	0.44
1:B:82:ASP:O	1:B:86:ASN:OD1	2.35	0.44
1:B:324:GLY:O	1:B:325:PRO:C	2.59	0.44
1:C:502:ILE:O	1:C:506:LEU:HD13	2.18	0.44
1:A:444:LEU:C	1:A:446:ALA:N	2.75	0.43
1:B:188:HIS:CD2	1:B:367:THR:HA	2.53	0.43
1:B:399:LEU:HD12	1:B:400:GLY:N	2.33	0.43
1:C:271:ILE:HD13	1:C:276:ASP:OD2	2.18	0.43
1:C:491:VAL:HG13	1:C:492:THR:N	2.33	0.43
1:B:99:LEU:O	1:B:102:ALA:HB3	2.19	0.43
1:B:248:PHE:HA	1:B:251:ALA:HB3	2.00	0.43
1:C:70:VAL:HG13	1:C:71:LEU:HD23	1.99	0.43
1:A:214:LYS:HG3	1:A:219:SER:OG	2.17	0.43
1:B:110:PHE:O	1:B:114:ILE:HG12	2.17	0.43
1:B:166:TYR:CD1	1:B:421:ILE:HG23	2.54	0.43
1:B:222:VAL:HB	1:B:223:PRO:HD3	2.00	0.43
1:B:284:SER:O	1:B:288:LEU:HB2	2.18	0.43
1:C:242:ALA:O	1:C:243:ILE:C	2.60	0.43
1:B:189:TRP:CZ2	1:B:370:TYR:OH	2.68	0.43
1:B:432:GLY:O	1:B:434:GLY:N	2.47	0.43
1:C:154:LEU:HB3	1:C:412:TRP:CD1	2.54	0.43
1:C:159:THR:HG21	1:C:443:LEU:HD21	1.99	0.43
1:C:174:ASP:O	1:C:174:ASP:OD1	2.37	0.43
1:C:189:TRP:CD2	1:C:413:PHE:CZ	3.06	0.43
1:A:92:LEU:CD1	1:A:96:VAL:HG21	2.44	0.43
1:A:130:ILE:O	1:A:131:ASP:HB3	2.17	0.43
1:A:137:ARG:HD2	1:A:139:VAL:CG2	2.40	0.43
1:A:209:PHE:HZ	1:A:387:ARG:HH12	1.64	0.43
1:A:243:ILE:H	1:A:243:ILE:HG13	1.71	0.43
1:A:466:ILE:HD12	1:A:466:ILE:C	2.44	0.43
1:C:96:VAL:O	1:C:100:GLY:HA3	2.18	0.43
1:C:157:TYR:OH	1:C:519:GLN:NE2	2.51	0.43
1:C:187:PHE:CE1	1:C:347:MET:HG3	2.53	0.43
1:C:484:GLN:HB3	1:C:486:GLU:HG2	2.00	0.43
1:A:155:MET:SD	1:A:460:LEU:HG	2.59	0.43
1:A:163:LEU:HD12	1:A:163:LEU:HA	1.75	0.43
1:A:256:LEU:C	1:A:256:LEU:HD23	2.44	0.43
1:B:106:PHE:O	1:B:109:VAL:N	2.49	0.43
1:B:125:ILE:H	1:B:125:ILE:HG13	1.69	0.43
1:B:153:ASP:C	1:B:155:MET:H	2.25	0.43
1:B:159:THR:CG2	1:B:443:LEU:HD23	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:554:ARG:HD2	1:B:558:ARG:NH2	2.34	0.43
1:C:564:ALA:HA	1:C:567:ARG:HH11	1.83	0.43
1:A:163:LEU:HD22	1:A:420:ALA:HB1	2.00	0.43
1:A:190:THR:OG1	1:A:191:LEU:N	2.50	0.43
1:A:375:ILE:CG2	1:A:529:PHE:HB3	2.49	0.43
1:A:393:SER:OG	1:A:394:ILE:N	2.52	0.43
1:A:558:ARG:HH11	1:A:558:ARG:HA	1.84	0.43
1:B:208:THR:HG21	1:B:215:GLN:HA	2.01	0.43
1:B:220:ALA:O	1:B:223:PRO:HD2	2.18	0.43
1:B:320:VAL:CG2	1:B:321:PHE:N	2.81	0.43
1:B:451:GLN:CD	1:B:451:GLN:N	2.72	0.43
1:C:92:LEU:O	1:C:95:VAL:CG1	2.67	0.43
1:C:257:GLY:O	1:C:261:ILE:HG12	2.18	0.43
1:C:389:SER:O	1:C:390:ARG:O	2.36	0.43
1:A:141:TRP:O	1:A:144:MET:HB2	2.19	0.43
1:A:153:ASP:CA	1:A:156:PHE:CE2	2.74	0.43
1:A:379:PRO:O	1:A:380:PHE:C	2.61	0.43
1:A:481:GLN:HG3	1:A:484:GLN:HG3	2.00	0.43
1:A:485:LEU:O	1:A:486:GLU:O	2.36	0.43
1:A:562:ARG:O	1:A:563:LEU:C	2.62	0.43
1:B:142:ILE:O	1:B:145:MET:HE2	2.18	0.43
1:B:375:ILE:CG2	1:B:526:ALA:CB	2.96	0.43
1:C:69:ILE:N	1:C:69:ILE:CD1	2.82	0.43
1:C:154:LEU:HB3	1:C:412:TRP:NE1	2.33	0.43
1:C:178:VAL:HG23	1:C:179:GLY:H	1.84	0.43
1:A:182:MET:O	1:A:186:MET:HG3	2.19	0.43
1:A:442:GLY:HA2	1:A:445:HIS:CD2	2.54	0.43
1:A:442:GLY:HA2	1:A:445:HIS:NE2	2.34	0.43
1:A:527:THR:HG23	1:A:528:PRO:N	2.33	0.43
1:A:532:VAL:O	1:A:536:LEU:HB2	2.19	0.43
1:B:319:PHE:CE2	1:B:453:MET:HG3	2.54	0.43
1:C:167:ARG:NH2	1:C:424:GLU:OE2	2.52	0.43
1:A:92:LEU:HA	1:A:95:VAL:HG22	1.99	0.43
1:A:453:MET:O	1:A:456:ILE:N	2.52	0.43
1:A:59:ASN:HD21	1:A:482:HIS:HA	1.84	0.42
1:A:170:VAL:HG13	1:A:171:PRO:CD	2.49	0.42
1:A:206:TYR:CE2	1:A:543:ASP:CG	2.89	0.42
1:A:209:PHE:HE2	1:A:386:ALA:O	2.02	0.42
1:A:397:PHE:CD2	1:A:397:PHE:C	2.97	0.42
1:B:123:GLY:O	1:B:394:ILE:HG13	2.18	0.42
1:B:291:ILE:HA	1:B:466:ILE:HD13	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:ASP:OD1	1:C:253:SER:OG	2.37	0.42
1:C:291:ILE:HD12	1:C:469:ALA:HB1	2.00	0.42
1:A:97:ASP:O	1:C:327:VAL:HG13	2.18	0.42
1:A:333:LEU:HB3	1:A:334:PRO:HD3	2.01	0.42
1:A:351:THR:C	1:A:353:MET:H	2.26	0.42
1:A:353:MET:O	1:A:357:GLY:N	2.52	0.42
1:A:371:TRP:N	1:A:371:TRP:HE3	2.18	0.42
1:B:96:VAL:O	1:B:96:VAL:HG12	2.19	0.42
1:B:321:PHE:CZ	1:B:326:THR:HG23	2.54	0.42
1:C:170:VAL:HG13	1:C:171:PRO:CD	2.35	0.42
1:C:414:SER:O	1:C:418:GLY:CA	2.63	0.42
1:C:417:GLY:O	1:C:421:ILE:HG12	2.19	0.42
1:A:202:LEU:HD23	1:A:202:LEU:HA	1.85	0.42
1:A:563:LEU:HD23	1:A:563:LEU:O	2.18	0.42
1:C:78:ILE:HG13	1:C:79:GLY:H	1.84	0.42
1:C:269:ASN:C	1:C:270:ILE:HG13	2.42	0.42
1:C:359:ALA:O	1:C:360:GLY:C	2.61	0.42
1:A:122:PHE:O	1:A:125:ILE:HB	2.19	0.42
1:A:353:MET:O	1:C:178:VAL:HG21	2.20	0.42
1:C:193:PRO:HA	1:C:374:TRP:CD1	2.54	0.42
1:C:323:VAL:CG1	1:C:324:GLY:N	2.81	0.42
1:C:371:TRP:CE3	1:C:371:TRP:CA	3.01	0.42
1:C:383:MET:SD	1:C:475:VAL:HG13	2.59	0.42
1:A:152:ILE:CD1	1:A:464:PHE:HB3	2.49	0.42
1:A:157:TYR:HB3	1:A:189:TRP:CH2	2.53	0.42
1:A:194:TRP:CZ2	1:A:405:PRO:HB3	2.54	0.42
1:B:395:ARG:C	1:B:397:PHE:H	2.28	0.42
1:C:154:LEU:N	1:C:154:LEU:HD12	2.34	0.42
1:C:160:THR:HG21	1:C:436:ALA:HB1	2.00	0.42
1:C:166:TYR:OH	1:C:425:GLN:HG2	2.19	0.42
1:C:186:MET:CE	1:C:410:THR:HG1	2.32	0.42
1:A:129:ARG:O	1:A:130:ILE:C	2.62	0.42
1:A:152:ILE:HD12	1:A:152:ILE:N	2.33	0.42
1:B:122:PHE:CD1	1:B:544:LEU:HD13	2.55	0.42
1:B:204:ILE:HD11	1:B:217:LEU:HA	2.02	0.42
1:C:77:GLY:HA2	1:C:85:THR:HB	2.01	0.42
1:C:122:PHE:O	1:C:124:THR:N	2.53	0.42
1:C:163:LEU:O	1:C:164:THR:C	2.62	0.42
1:C:210:ARG:NH2	1:C:549:ILE:HD12	2.14	0.42
1:A:371:TRP:O	1:A:372:ALA:C	2.63	0.42
1:B:114:ILE:O	1:B:115:VAL:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:LEU:HD21	1:B:458:MET:HE2	2.02	0.42
1:C:134:PRO:HA	1:C:391:GLY:CA	2.22	0.42
1:C:155:MET:HE1	1:C:460:LEU:HD23	2.02	0.42
1:C:337:ILE:O	1:C:340:TYR:HB3	2.20	0.42
1:C:559:PHE:C	1:C:561:ALA:N	2.77	0.42
1:A:123:GLY:C	1:A:394:ILE:HB	2.44	0.42
1:A:206:TYR:CE2	1:A:544:LEU:HD12	2.54	0.42
1:A:351:THR:O	1:A:352:ALA:C	2.63	0.42
1:A:380:PHE:CD2	1:A:381:VAL:HG13	2.55	0.42
1:B:152:ILE:HG21	1:B:253:SER:O	2.19	0.42
1:B:265:LEU:HB3	1:B:269:ASN:ND2	2.35	0.42
1:B:441:PHE:HA	1:B:444:LEU:HB2	2.01	0.42
1:A:186:MET:HE3	1:A:410:THR:HB	2.01	0.42
1:A:219:SER:O	1:A:221:PHE:N	2.53	0.42
1:B:323:VAL:CG2	1:B:324:GLY:N	2.83	0.42
1:B:380:PHE:CE1	1:B:471:SER:O	2.73	0.42
1:C:258:ALA:O	1:C:261:ILE:HB	2.19	0.42
1:C:447:LEU:HB3	1:C:448:PRO:HD2	2.02	0.42
1:A:123:GLY:O	1:A:393:SER:OG	2.38	0.42
1:A:354:SER:HA	1:A:355:ALA:HA	1.59	0.42
1:A:408:VAL:O	1:A:409:SER:C	2.63	0.42
1:A:461:LEU:O	1:A:461:LEU:HD12	2.20	0.42
1:C:92:LEU:HD12	1:C:523:ILE:HG21	2.02	0.42
1:C:292:PHE:C	1:C:296:SER:HB3	2.45	0.42
1:C:312:LEU:N	1:C:312:LEU:CD1	2.80	0.42
1:C:332:LEU:HA	1:C:332:LEU:HD23	1.81	0.42
1:A:99:LEU:O	1:A:102:ALA:N	2.54	0.41
1:A:110:PHE:HD2	1:A:196:ILE:CD1	2.33	0.41
1:A:256:LEU:HD12	1:A:518:LEU:HD21	2.02	0.41
1:B:352:ALA:HB1	1:B:360:GLY:HA2	2.02	0.41
1:C:521:VAL:O	1:C:524:VAL:N	2.53	0.41
1:A:217:LEU:C	1:A:217:LEU:HD23	2.44	0.41
1:A:373:TRP:C	1:A:373:TRP:CD1	2.98	0.41
1:B:114:ILE:HG13	1:B:115:VAL:N	2.36	0.41
1:B:209:PHE:CD2	1:B:390:ARG:HD3	2.55	0.41
1:B:406:ALA:O	1:B:410:THR:HB	2.18	0.41
1:C:372:ALA:CB	1:C:523:ILE:HG12	2.50	0.41
1:A:216:LEU:HD11	1:A:239:ASP:OD2	2.21	0.41
1:B:137:ARG:HG3	1:B:138:THR:H	1.85	0.41
1:B:371:TRP:O	1:B:375:ILE:N	2.46	0.41
1:B:385:LEU:HD13	1:B:397:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:557:GLN:HG2	1:B:558:ARG:N	2.35	0.41
1:C:423:PHE:C	1:C:425:GLN:N	2.78	0.41
1:A:423:PHE:O	1:A:428:GLU:N	2.53	0.41
1:C:76:TRP:O	1:C:80:PHE:O	2.39	0.41
1:C:175:GLU:O	1:C:176:HIS:C	2.63	0.41
1:C:234:LEU:HA	1:C:234:LEU:HD23	1.87	0.41
1:C:312:LEU:HB3	1:C:460:LEU:HD22	2.02	0.41
1:C:368:ILE:HG23	1:C:369:PHE:N	2.36	0.41
1:C:401:VAL:O	1:C:405:PRO:HG2	2.19	0.41
1:C:559:PHE:HB2	1:C:562:ARG:HE	1.84	0.41
1:A:239:ASP:O	1:A:242:ALA:HB3	2.20	0.41
1:B:152:ILE:HG23	1:B:153:ASP:N	2.35	0.41
1:C:76:TRP:HD1	1:C:77:GLY:CA	2.33	0.41
1:C:202:LEU:HA	1:C:202:LEU:HD12	1.77	0.41
1:C:203:ALA:HB1	1:C:536:LEU:HD11	2.03	0.41
1:C:302:ILE:HG23	1:C:303:GLN:N	2.35	0.41
1:A:156:PHE:CD1	1:A:157:TYR:N	2.89	0.41
1:B:92:LEU:HD11	1:B:523:ILE:CG2	2.51	0.41
1:B:117:ILE:CG2	1:B:398:ILE:HD13	2.50	0.41
1:B:444:LEU:HA	1:B:444:LEU:HD23	1.38	0.41
1:B:524:VAL:HA	1:B:527:THR:HG1	1.76	0.41
1:C:354:SER:HA	1:C:355:ALA:HA	1.73	0.41
1:C:453:MET:SD	1:C:456:ILE:HD12	2.61	0.41
1:A:88:ALA:C	1:A:91:ALA:H	2.28	0.41
1:A:122:PHE:CE1	1:A:545:SER:HA	2.50	0.41
1:A:155:MET:HE1	1:A:457:ALA:HB1	2.03	0.41
1:A:161:GLU:CD	1:A:189:TRP:HZ3	2.29	0.41
1:B:305:LEU:HD23	1:B:467:THR:CG2	2.42	0.41
1:B:491:VAL:HG13	1:B:492:THR:N	2.35	0.41
1:C:60:TRP:O	1:C:61:SER:C	2.64	0.41
1:C:108:THR:N	1:C:192:HIS:HE1	2.19	0.41
1:A:98:ASN:O	1:A:101:TRP:NE1	2.49	0.41
1:A:114:ILE:CD1	1:A:402:LEU:HD11	2.51	0.41
1:B:372:ALA:CB	1:B:523:ILE:HA	2.50	0.41
1:B:410:THR:HG22	1:B:411:VAL:N	2.35	0.41
1:A:116:VAL:HG22	1:A:117:ILE:N	2.36	0.41
1:A:135:GLU:OE1	1:A:136:PHE:CE2	2.74	0.41
1:A:337:ILE:O	1:A:338:GLY:C	2.62	0.41
1:A:435:ALA:HB3	1:A:438:GLU:CD	2.46	0.41
1:A:437:GLU:O	1:A:441:PHE:CD1	2.74	0.41
1:B:67:LEU:C	1:B:67:LEU:HD23	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:LYS:C	1:B:123:GLY:N	2.78	0.41
1:B:189:TRP:CD2	1:B:413:PHE:CZ	3.09	0.41
1:B:209:PHE:N	1:B:209:PHE:CD1	2.89	0.41
1:B:254:LEU:HD12	1:B:255:GLY:N	2.35	0.41
1:B:411:VAL:HG12	1:B:412:TRP:N	2.33	0.41
1:C:59:ASN:ND2	1:C:62:VAL:CG2	2.84	0.41
1:C:74:VAL:HG13	1:C:502:ILE:HG22	2.02	0.41
1:C:81:LYS:CD	1:C:84:PHE:CD2	2.98	0.41
1:C:180:VAL:O	1:C:181:ALA:C	2.64	0.41
1:C:209:PHE:CE1	1:C:390:ARG:CB	3.01	0.41
1:C:463:THR:O	1:C:467:THR:HG23	2.21	0.41
1:A:92:LEU:C	1:A:95:VAL:HG22	2.45	0.41
1:A:208:THR:HG21	1:A:215:GLN:CD	2.46	0.41
1:A:383:MET:O	1:A:387:ARG:NE	2.54	0.41
1:A:449:GLY:O	1:A:452:ILE:N	2.54	0.41
1:A:559:PHE:CE2	1:A:563:LEU:CD1	2.72	0.41
1:B:74:VAL:HG13	1:B:75:VAL:N	2.36	0.41
1:B:352:ALA:CB	1:B:363:LEU:HD12	2.51	0.41
1:A:334:PRO:HB3	1:B:105:LEU:CD1	2.51	0.40
1:B:154:LEU:N	1:B:154:LEU:HD23	2.35	0.40
1:B:460:LEU:HA	1:B:463:THR:HG22	2.03	0.40
1:C:281:GLY:O	1:C:285:VAL:CG2	2.64	0.40
1:A:200:VAL:HG12	1:A:382:GLY:HA3	2.03	0.40
1:A:307:ASN:O	1:A:311:VAL:HG23	2.22	0.40
1:B:95:VAL:CG2	1:B:527:THR:HG23	2.48	0.40
1:B:173:HIS:ND1	1:B:180:VAL:HG21	2.37	0.40
1:A:471:SER:O	1:A:472:ALA:C	2.63	0.40
1:A:581:LYS:O	1:A:581:LYS:HG2	2.22	0.40
1:B:92:LEU:HD13	1:B:523:ILE:HB	1.95	0.40
1:B:103:PHE:CD1	1:B:371:TRP:HB3	2.38	0.40
1:B:170:VAL:HG11	1:B:184:THR:HG21	2.02	0.40
1:B:190:THR:O	1:B:193:PRO:HD2	2.21	0.40
1:B:471:SER:HA	1:B:474:THR:CG2	2.52	0.40
1:C:136:PHE:CD2	1:C:144:MET:HE1	2.56	0.40
1:C:139:VAL:HG13	1:C:140:SER:N	2.37	0.40
1:C:264:GLY:HA2	1:C:441:PHE:CD1	2.57	0.40
1:C:515:LEU:O	1:C:518:LEU:HB3	2.21	0.40
1:A:104:ILE:O	1:A:105:LEU:C	2.64	0.40
1:A:191:LEU:HD12	1:A:191:LEU:HA	1.73	0.40
1:B:167:ARG:NH2	1:B:431:TRP:CD1	2.90	0.40
1:B:214:LYS:HB3	1:B:214:LYS:HE2	1.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:ILE:HG13	1:B:283:VAL:N	2.36	0.40
1:B:294:ALA:C	1:B:295:ILE:HD12	2.46	0.40
1:C:163:LEU:C	1:C:165:PHE:N	2.79	0.40
1:C:173:HIS:NE2	1:C:180:VAL:HG22	2.36	0.40
1:A:316:LEU:CD1	1:A:416:PHE:HZ	2.34	0.40
1:A:544:LEU:O	1:A:547:ASP:CB	2.70	0.40
1:B:385:LEU:O	1:B:388:ILE:HG22	2.22	0.40
1:C:366:TRP:O	1:C:369:PHE:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	498/566 (88%)	426 (86%)	62 (12%)	10 (2%)	6	24
1	B	470/566 (83%)	403 (86%)	61 (13%)	6 (1%)	9	32
1	C	504/566 (89%)	435 (86%)	60 (12%)	9 (2%)	6	26
All	All	1472/1698 (87%)	1264 (86%)	183 (12%)	25 (2%)	7	27

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	377	TRP
1	A	403	LEU
1	B	231	GLU
1	B	432	GLY
1	C	231	GLU
1	C	304	TYR
1	A	431	TRP
1	A	486	GLU
1	A	520	ASN

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Mol	Chain	Res	Type
1	C	227	GLU
1	C	232	GLY
1	C	270	ILE
1	A	220	ALA
1	A	302	ILE
1	B	232	GLY
1	B	464	PHE
1	C	429	SER
1	A	388	ILE
1	B	154	LEU
1	C	164	THR
1	A	482	HIS
1	B	545	SER
1	C	325	PRO
1	C	548	VAL
1	A	125	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	396/440 (90%)	367 (93%)	29 (7%)	13	39
1	B	371/440 (84%)	345 (93%)	26 (7%)	14	40
1	C	396/440 (90%)	354 (89%)	42 (11%)	6	23
All	All	1163/1320 (88%)	1066 (92%)	97 (8%)	10	35

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	VAL
1	A	68	VAL
1	A	108	THR
1	A	116	VAL
1	A	144	MET
1	A	157	TYR

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Mol	Chain	Res	Type
1	A	173	HIS
1	A	189	TRP
1	A	192	HIS
1	A	204	ILE
1	A	211	VAL
1	A	243	ILE
1	A	246	THR
1	A	302	ILE
1	A	344	PHE
1	A	371	TRP
1	A	387	ARG
1	A	392	ARG
1	A	396	GLU
1	A	398	ILE
1	A	424	GLU
1	A	443	LEU
1	A	461	LEU
1	A	484	GLN
1	A	529	PHE
1	A	542	LYS
1	A	565	ARG
1	A	573	HIS
1	A	574	ARG
1	B	82	ASP
1	B	125	ILE
1	B	154	LEU
1	B	177	ASN
1	B	185	THR
1	B	191	LEU
1	B	271	ILE
1	B	280	VAL
1	B	305	LEU
1	B	310	MET
1	B	311	VAL
1	B	319	PHE
1	B	347	MET
1	B	366	TRP
1	B	369	PHE
1	B	371	TRP
1	B	373	TRP
1	B	375	ILE
1	B	383	MET

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Mol	Chain	Res	Type
1	B	388	ILE
1	B	410	THR
1	B	411	VAL
1	B	444	LEU
1	B	466	ILE
1	B	530	LEU
1	B	543	ASP
1	C	75	VAL
1	C	76	TRP
1	C	92	LEU
1	C	104	ILE
1	C	116	VAL
1	C	121	LYS
1	C	124	THR
1	C	136	PHE
1	C	144	MET
1	C	153	ASP
1	C	186	MET
1	C	189	TRP
1	C	215	GLN
1	C	218	SER
1	C	222	VAL
1	C	224	LEU
1	C	259	LEU
1	C	286	LEU
1	C	304	TYR
1	C	316	LEU
1	C	347	MET
1	C	371	TRP
1	C	374	TRP
1	C	375	ILE
1	C	377	TRP
1	C	380	PHE
1	C	389	SER
1	C	398	ILE
1	C	415	ILE
1	C	433	ASP
1	C	437	GLU
1	C	439	GLN
1	C	443	LEU
1	C	465	PHE
1	C	468	SER

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Mol	Chain	Res	Type
1	C	481	GLN
1	C	492	THR
1	C	507	LEU
1	C	523	ILE
1	C	530	LEU
1	C	551	LEU
1	C	553	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	173	HIS
1	A	176	HIS
1	A	343	ASN
1	A	346	GLN
1	A	439	GLN
1	A	520	ASN
1	B	192	HIS
1	B	215	GLN
1	B	269	ASN
1	B	339	ASN
1	B	343	ASN
1	B	426	ASN
1	B	445	HIS
1	B	482	HIS
1	C	59	ASN
1	C	176	HIS
1	C	192	HIS
1	C	260	GLN
1	C	307	ASN
1	C	339	ASN
1	C	346	GLN
1	C	484	GLN
1	C	517	ASN
1	C	520	ASN
1	C	557	GLN

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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	CHT	C	2486	-	6,6,6	0.81	0	8,8,8	0.28	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CHT	C	2486	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2486	CHT	C4-C5-N1-C6
2	C	2486	CHT	C4-C5-N1-C8
2	C	2486	CHT	C4-C5-N1-C7
2	C	2486	CHT	O6-C4-C5-N1

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2486	CHT	6	0

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	504/566 (89%)	1.42	143 (28%) ⓘ ⓘ	28, 107, 309, 534	0
1	B	476/566 (84%)	1.59	147 (30%) ⓘ ⓘ	14, 97, 292, 557	0
1	C	508/566 (89%)	0.77	75 (14%) ⓘ ⓘ	7, 62, 194, 353	0
All	All	1488/1698 (87%)	1.25	365 (24%) ⓘ ⓘ	7, 86, 284, 557	0

All (365) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	496	GLY	11.2
1	A	296	SER	10.3
1	B	500	ALA	10.3
1	B	499	THR	9.7
1	A	490	TRP	9.0
1	B	153	ASP	9.0
1	B	492	THR	7.7
1	B	150	MET	7.4
1	A	466	ILE	7.2
1	B	234	LEU	7.2
1	A	64	VAL	7.2
1	A	150	MET	7.0
1	B	295	ILE	6.9
1	B	493	ALA	6.9
1	B	253	SER	6.8
1	C	302	ILE	6.7
1	B	469	ALA	6.4
1	B	252	CYS	6.3
1	B	270	ILE	6.1
1	A	493	ALA	6.1
1	B	296	SER	6.0
1	B	373	TRP	6.0
1	B	396	GLU	6.0

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Mol	Chain	Res	Type	RSRZ
1	A	279	ILE	5.9
1	A	292	PHE	5.9
1	C	568	ARG	5.9
1	A	491	VAL	5.8
1	A	388	ILE	5.7
1	A	459	ILE	5.7
1	B	250	THR	5.7
1	B	130	ILE	5.6
1	A	145	MET	5.6
1	B	548	VAL	5.6
1	A	323	VAL	5.5
1	A	60	TRP	5.4
1	A	174	ASP	5.4
1	A	325	PRO	5.4
1	B	246	THR	5.3
1	A	253	SER	5.3
1	C	173	HIS	5.3
1	B	76	TRP	5.2
1	A	227	GLU	5.2
1	C	391	GLY	5.2
1	C	174	ASP	5.2
1	B	551	LEU	5.1
1	B	248	PHE	5.1
1	B	147	ALA	5.1
1	B	366	TRP	5.1
1	B	521	VAL	5.0
1	B	145	MET	5.0
1	A	147	ALA	5.0
1	A	462	GLY	4.9
1	A	498	ALA	4.9
1	C	317	ALA	4.9
1	B	254	LEU	4.9
1	B	495	TRP	4.8
1	A	252	CYS	4.8
1	B	125	ILE	4.8
1	B	231	GLU	4.8
1	B	325	PRO	4.8
1	B	482	HIS	4.8
1	B	550	TYR	4.8
1	B	228	LYS	4.8
1	C	416	PHE	4.8
1	A	282	ILE	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	301	GLY	4.7
1	A	148	ALA	4.7
1	B	380	PHE	4.7
1	B	152	ILE	4.6
1	C	298	VAL	4.6
1	B	387	ARG	4.6
1	B	256	LEU	4.6
1	A	228	LYS	4.6
1	A	142	ILE	4.6
1	C	85	THR	4.6
1	C	303	GLN	4.6
1	B	497	VAL	4.5
1	C	80	PHE	4.5
1	A	141	TRP	4.5
1	B	249	GLY	4.4
1	A	280	VAL	4.4
1	B	251	ALA	4.4
1	B	393	SER	4.4
1	B	148	ALA	4.3
1	B	466	ILE	4.3
1	C	84	PHE	4.3
1	B	255	GLY	4.2
1	A	73	THR	4.2
1	A	492	THR	4.2
1	A	75	VAL	4.2
1	A	295	ILE	4.2
1	C	88	ALA	4.2
1	A	357	GLY	4.2
1	A	418	GLY	4.2
1	A	287	THR	4.1
1	B	85	THR	4.1
1	A	256	LEU	4.1
1	A	84	PHE	4.1
1	A	497	VAL	4.0
1	A	62	VAL	4.0
1	B	490	TRP	4.0
1	A	291	ILE	4.0
1	B	403	LEU	4.0
1	B	142	ILE	3.9
1	C	147	ALA	3.9
1	B	354	SER	3.9
1	B	470	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	133	ALA	3.9
1	A	525	ALA	3.8
1	B	404	VAL	3.8
1	A	519	GLN	3.8
1	C	278	THR	3.8
1	A	523	ILE	3.8
1	C	231	GLU	3.8
1	A	234	LEU	3.8
1	A	260	GLN	3.8
1	A	303	GLN	3.8
1	B	233	TRP	3.8
1	C	83	SER	3.8
1	B	377	TRP	3.7
1	A	299	GLY	3.7
1	C	301	GLY	3.7
1	B	139	VAL	3.7
1	B	389	SER	3.7
1	A	156	PHE	3.7
1	B	292	PHE	3.7
1	B	245	ALA	3.6
1	A	146	PHE	3.6
1	A	297	GLY	3.6
1	B	146	PHE	3.6
1	A	155	MET	3.6
1	A	496	GLY	3.6
1	A	57	SER	3.6
1	B	542	LYS	3.6
1	B	400	GLY	3.6
1	B	75	VAL	3.6
1	B	73	THR	3.6
1	C	299	GLY	3.6
1	A	243	ILE	3.6
1	C	79	GLY	3.5
1	B	491	VAL	3.5
1	A	87	PHE	3.5
1	C	304	TYR	3.5
1	A	364	GLY	3.5
1	B	298	VAL	3.5
1	A	88	ALA	3.5
1	B	374	TRP	3.5
1	B	144	MET	3.4
1	A	351	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	357	GLY	3.4
1	C	356	ASP	3.3
1	A	170	VAL	3.3
1	B	523	ILE	3.3
1	C	271	ILE	3.3
1	B	214	LYS	3.3
1	C	270	ILE	3.3
1	C	127	LEU	3.3
1	A	517	ASN	3.3
1	C	370	TYR	3.2
1	B	294	ALA	3.2
1	B	472	ALA	3.2
1	A	582	ARG	3.2
1	B	227	GLU	3.2
1	B	156	PHE	3.2
1	B	352	ALA	3.2
1	B	304	TYR	3.2
1	A	455	ILE	3.2
1	C	267	ALA	3.2
1	B	399	LEU	3.1
1	C	233	TRP	3.1
1	B	364	GLY	3.1
1	B	347	MET	3.1
1	A	355	ALA	3.1
1	A	447	LEU	3.1
1	C	509	SER	3.1
1	C	555	GLU	3.1
1	A	300	LYS	3.1
1	A	518	LEU	3.1
1	C	558	ARG	3.1
1	A	445	HIS	3.1
1	B	240	ILE	3.1
1	A	220	ALA	3.0
1	B	309	ASN	3.0
1	B	488	ASN	3.0
1	A	257	GLY	3.0
1	C	61	SER	3.0
1	A	83	SER	3.0
1	B	90	SER	3.0
1	A	94	ALA	3.0
1	A	255	GLY	3.0
1	B	391	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	477	GLY	3.0
1	A	468	SER	3.0
1	C	230	ALA	3.0
1	A	149	GLY	3.0
1	B	360	GLY	3.0
1	A	85	THR	3.0
1	B	486	GLU	2.9
1	A	343	ASN	2.9
1	A	520	ASN	2.9
1	A	245	ALA	2.9
1	A	311	VAL	2.9
1	C	344	PHE	2.9
1	B	60	TRP	2.9
1	A	416	PHE	2.9
1	B	384	PHE	2.9
1	B	244	ILE	2.9
1	B	302	ILE	2.9
1	A	153	ASP	2.9
1	A	79	GLY	2.9
1	B	194	TRP	2.8
1	C	297	GLY	2.8
1	B	388	ILE	2.8
1	C	514	ALA	2.8
1	A	522	THR	2.8
1	C	81	LYS	2.8
1	A	544	LEU	2.8
1	B	369	PHE	2.8
1	A	144	MET	2.8
1	A	469	ALA	2.8
1	A	495	TRP	2.8
1	A	360	GLY	2.8
1	C	436	ALA	2.8
1	B	408	VAL	2.8
1	A	259	LEU	2.8
1	A	358	THR	2.8
1	A	380	PHE	2.7
1	C	87	PHE	2.7
1	C	277	TRP	2.7
1	A	137	ARG	2.7
1	B	268	ALA	2.7
1	C	488	ASN	2.7
1	B	386	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	494	ALA	2.7
1	A	277	TRP	2.7
1	C	433	ASP	2.7
1	A	90	SER	2.7
1	B	62	VAL	2.7
1	B	84	PHE	2.7
1	A	294	ALA	2.7
1	A	154	LEU	2.7
1	B	71	LEU	2.6
1	B	429	SER	2.6
1	A	130	ILE	2.6
1	C	226	GLY	2.6
1	B	217	LEU	2.6
1	A	573	HIS	2.6
1	A	465	PHE	2.6
1	B	80	PHE	2.6
1	B	136	PHE	2.6
1	B	407	GLY	2.6
1	C	554	ARG	2.6
1	A	114	ILE	2.6
1	A	276	ASP	2.6
1	B	186	MET	2.5
1	A	328	SER	2.5
1	C	293	SER	2.5
1	A	263	ALA	2.5
1	B	549	ILE	2.5
1	A	80	PHE	2.5
1	B	128	GLY	2.5
1	B	541	VAL	2.5
1	B	220	ALA	2.5
1	A	249	GLY	2.5
1	C	64	VAL	2.5
1	C	487	ALA	2.5
1	B	78	ILE	2.5
1	B	104	ILE	2.5
1	A	419	THR	2.5
1	B	385	LEU	2.5
1	B	528	PRO	2.5
1	C	93	SER	2.4
1	C	566	GLU	2.4
1	C	300	LYS	2.4
1	B	381	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	352	ALA	2.4
1	A	78	ILE	2.4
1	C	389	SER	2.4
1	B	81	LYS	2.4
1	A	444	LEU	2.4
1	A	487	ALA	2.4
1	B	66	ALA	2.4
1	A	480	SER	2.4
1	C	365	SER	2.4
1	A	157	TYR	2.4
1	C	227	GLU	2.4
1	C	282	ILE	2.4
1	B	552	GLU	2.4
1	A	298	VAL	2.4
1	B	74	VAL	2.4
1	B	88	ALA	2.3
1	C	415	ILE	2.3
1	C	261	ILE	2.3
1	C	470	ASP	2.3
1	B	428	GLU	2.3
1	B	226	GLY	2.3
1	B	278	THR	2.3
1	B	557	GLN	2.3
1	A	574	ARG	2.3
1	B	289	ALA	2.3
1	A	488	ASN	2.3
1	A	123	GLY	2.3
1	B	406	ALA	2.3
1	C	76	TRP	2.3
1	B	326	THR	2.3
1	A	226	GLY	2.2
1	C	432	GLY	2.2
1	A	76	TRP	2.2
1	A	414	SER	2.2
1	C	57	SER	2.2
1	A	152	ILE	2.2
1	C	66	ALA	2.2
1	A	554	ARG	2.2
1	C	152	ILE	2.2
1	A	258	ALA	2.2
1	C	58	LEU	2.2
1	A	344	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	565	ARG	2.2
1	A	516	SER	2.2
1	B	282	ILE	2.2
1	C	260	GLN	2.2
1	B	287	THR	2.1
1	A	553	TYR	2.1
1	B	279	ILE	2.1
1	B	346	GLN	2.1
1	A	306	SER	2.1
1	A	561	ALA	2.1
1	B	361	GLU	2.1
1	C	481	GLN	2.1
1	A	251	ALA	2.1
1	A	231	GLU	2.1
1	A	391	GLY	2.1
1	A	173	HIS	2.1
1	A	63	ILE	2.1
1	A	489	LYS	2.1
1	A	133	ALA	2.1
1	A	486	GLU	2.1
1	C	306	SER	2.1
1	A	269	ASN	2.1
1	A	460	LEU	2.1
1	B	99	LEU	2.1
1	B	239	ASP	2.1
1	C	507	LEU	2.1
1	A	381	VAL	2.1
1	C	228	LYS	2.1
1	A	151	GLY	2.1
1	B	556	GLN	2.1
1	C	77	GLY	2.1
1	A	283	VAL	2.0
1	C	280	VAL	2.0
1	A	82	ASP	2.0
1	B	197	TYR	2.0
1	B	498	ALA	2.0
1	B	215	GLN	2.0
1	B	299	GLY	2.0
1	C	134	PRO	2.0
1	B	117	ILE	2.0
1	A	326	THR	2.0
1	B	230	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	417	GLY	2.0
1	C	292	PHE	2.0
1	B	134	PRO	2.0
1	B	303	GLN	2.0
1	B	524	VAL	2.0
1	C	562	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CHT	C	2486	7/7	0.76	0.36	85,89,97,97	0

6.5 Other polymers [i](#)

There are no such residues in this entry.