



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:44 AM UTC

PDB ID : 4IRM / pdb_00004irm
Title : Crystal structure of mntc r116a mutant exhibits flexibility in the c-terminal domain
Authors : Kanteev, M.; Adir, N.
Deposited on : 2013-01-15
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

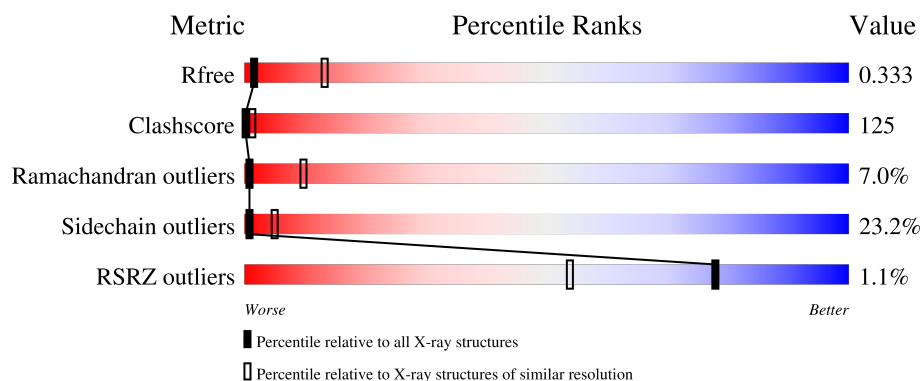
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	330	18% 38% 21% • 20%
1	B	330	16% 37% 22% • 22%
1	C	330	16% 37% 17% • 28%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5882 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 Mn transporter; MntC.

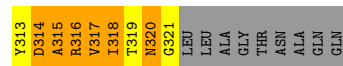
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2049	1299	338	406	6			
1	B	256	Total	C	N	O	S	0	0	0
			1992	1267	324	394	7			
1	C	236	Total	C	N	O	S	0	0	0
			1838	1174	298	360	6			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	116	ALA	ARG	engineered mutation	UNP Q79EF9
B	116	ALA	ARG	engineered mutation	UNP Q79EF9
C	116	ALA	ARG	engineered mutation	UNP Q79EF9

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	128.40Å 128.40Å 90.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.50 – 3.50 24.50 – 3.50	Depositor EDS
% Data completeness (in resolution range)	97.9 (24.50-3.50) 98.6 (24.50-3.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.77 (at 3.54Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.294 , 0.305 0.320 , 0.333	Depositor DCC
R_{free} test set	524 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	122.5	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 77.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.045 for -h,-k,l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	5882	wwPDB-VP
Average B, all atoms (Å ²)	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.46% 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: MN

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	1.24	12/2090 (0.6%)	1.21	19/2850 (0.7%)
1	B	1.40	20/2031 (1.0%)	1.47	36/2767 (1.3%)
1	C	1.32	14/1871 (0.7%)	1.37	28/2546 (1.1%)
All	All	1.32	46/5992 (0.8%)	1.35	83/8163 (1.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	190	VAL	CA-CB	-10.42	1.42	1.54
1	C	169	ILE	CA-CB	-10.06	1.43	1.54
1	C	71	VAL	CA-CB	-8.82	1.44	1.54
1	B	318	ILE	CA-CB	-7.97	1.43	1.54
1	B	266	ILE	CA-CB	-7.81	1.43	1.54
1	C	190	VAL	CA-CB	-7.77	1.45	1.54
1	A	190	VAL	CA-CB	-7.70	1.45	1.54
1	B	190	VAL	CA-C	-7.54	1.44	1.52
1	B	132	VAL	CA-CB	-7.26	1.45	1.54
1	B	137	ILE	CA-CB	-7.16	1.45	1.54
1	C	63	VAL	CA-CB	-6.99	1.46	1.54
1	A	251	VAL	CA-CB	-6.62	1.45	1.54
1	C	132	VAL	CA-CB	-6.61	1.46	1.54
1	B	107	ILE	CA-CB	-6.58	1.45	1.54
1	B	176	LEU	N-CA	-6.54	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	81	ILE	CA-CB	-6.49	1.45	1.54
1	B	217	VAL	CA-CB	-6.27	1.46	1.54
1	C	318	ILE	CA-CB	-6.25	1.45	1.54
1	A	57	VAL	CA-CB	-6.21	1.48	1.55
1	C	92	GLU	N-CA	-6.11	1.40	1.46
1	B	78	VAL	CA-CB	-6.07	1.46	1.54
1	B	177	ASP	CA-C	-6.04	1.45	1.52
1	A	190	VAL	CA-C	-5.97	1.45	1.52
1	A	108	LEU	CA-C	-5.92	1.45	1.52
1	C	132	VAL	N-CA	-5.87	1.39	1.46
1	C	99	VAL	CA-CB	-5.86	1.46	1.54
1	B	142	ILE	CA-CB	-5.70	1.46	1.54
1	A	142	ILE	CA-CB	-5.68	1.47	1.54
1	B	293	TYR	CA-C	-5.50	1.47	1.53
1	C	106	LEU	C-N	-5.45	1.26	1.33
1	B	62	THR	CA-CB	-5.43	1.45	1.53
1	A	193	GLU	CA-C	-5.42	1.46	1.52
1	B	255	ILE	CA-CB	-5.39	1.47	1.54
1	A	161	ASN	CA-C	-5.39	1.45	1.52
1	B	228	ARG	CA-C	-5.38	1.46	1.52
1	A	173	PHE	N-CA	-5.36	1.40	1.46
1	B	267	PHE	CA-C	-5.29	1.45	1.52
1	B	130	SER	C-N	5.28	1.39	1.33
1	B	266	ILE	CA-C	-5.24	1.46	1.52
1	B	107	ILE	N-CA	-5.18	1.39	1.46
1	C	66	ASP	CA-CB	-5.14	1.45	1.53
1	C	108	LEU	CA-C	-5.13	1.46	1.52
1	A	316	ARG	CA-C	-5.08	1.46	1.52
1	C	121	PHE	CA-C	-5.04	1.47	1.53
1	A	163	LEU	CA-C	-5.03	1.46	1.52
1	A	152	ASN	CA-C	-5.00	1.47	1.53

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	294	VAL	N-CA-CB	-17.16	97.57	111.64
1	C	177	ASP	CA-C-N	-12.42	104.31	119.84
1	C	177	ASP	C-N-CA	-12.42	104.31	119.84
1	B	209	VAL	CA-C-N	-12.34	106.72	119.92
1	B	209	VAL	C-N-CA	-12.34	106.72	119.92
1	B	294	VAL	N-CA-C	11.27	120.53	111.62
1	B	293	TYR	CB-CA-C	-10.91	95.74	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	LEU	N-CA-C	-10.77	99.86	113.43
1	C	106	LEU	CA-C-N	9.85	132.32	122.96
1	C	106	LEU	C-N-CA	9.85	132.32	122.96
1	B	185	ASN	N-CA-C	-9.61	101.69	113.41
1	B	293	TYR	N-CA-C	9.59	125.95	107.44
1	C	86	ALA	N-CA-CB	-9.49	93.83	111.00
1	B	177	ASP	CB-CA-C	-9.06	101.23	110.65
1	B	179	ASP	N-CA-C	-8.37	101.74	111.03
1	B	318	ILE	CB-CA-C	-8.30	101.48	111.94
1	B	125	VAL	CB-CA-C	-8.29	100.86	110.73
1	B	270	SER	CA-C-N	-8.23	109.77	122.60
1	B	270	SER	C-N-CA	-8.23	109.77	122.60
1	C	131	VAL	CA-C-N	-8.12	113.13	123.19
1	C	131	VAL	C-N-CA	-8.12	113.13	123.19
1	B	177	ASP	CA-C-N	-7.95	109.91	119.84
1	B	177	ASP	C-N-CA	-7.95	109.91	119.84
1	C	106	LEU	O-C-N	-7.76	112.26	122.59
1	C	95	PRO	CA-N-CD	-7.76	101.13	112.00
1	B	296	SER	N-CA-C	7.73	118.09	107.73
1	B	190	VAL	CB-CA-C	-7.64	102.01	111.87
1	A	127	ASP	CB-CA-C	-7.49	107.93	116.54
1	C	65	ALA	CA-C-N	-7.46	109.70	120.29
1	C	65	ALA	C-N-CA	-7.46	109.70	120.29
1	C	85	GLY	N-CA-C	7.41	130.74	113.18
1	A	296	SER	N-CA-C	7.09	119.15	107.73
1	C	181	ALA	CA-C-N	-6.84	108.89	120.58
1	C	181	ALA	C-N-CA	-6.84	108.89	120.58
1	A	114	LEU	N-CA-C	-6.80	98.61	109.76
1	B	180	ASN	N-CA-C	6.78	121.16	112.34
1	B	114	LEU	N-CA-C	-6.76	103.91	111.28
1	A	236	TYR	N-CA-C	6.72	119.54	108.99
1	A	163	LEU	N-CA-C	-6.71	103.66	110.97
1	B	125	VAL	CA-C-N	-6.68	112.12	122.87
1	B	125	VAL	C-N-CA	-6.68	112.12	122.87
1	B	109	TYR	N-CA-C	6.66	118.52	108.46
1	B	107	ILE	N-CA-CB	6.58	122.08	111.23
1	C	241	ASN	N-CA-CB	-6.47	100.38	110.55
1	C	75	LYS	N-CA-C	-6.45	105.06	113.12
1	C	311	LEU	CA-CB-CG	-6.42	93.82	116.30
1	B	284	THR	CB-CA-C	-6.38	100.84	111.23
1	C	198	ILE	N-CA-C	-6.32	104.17	110.30
1	B	271	THR	N-CA-CB	6.28	120.46	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	112	MET	O-C-N	6.24	130.55	122.19
1	C	318	ILE	CB-CA-C	-6.19	103.94	112.24
1	B	177	ASP	N-CA-CB	6.11	120.59	110.38
1	C	192	SER	CA-C-N	-6.11	110.29	121.52
1	C	192	SER	C-N-CA	-6.11	110.29	121.52
1	B	198	ILE	CA-C-N	-6.08	112.17	120.44
1	B	198	ILE	C-N-CA	-6.08	112.17	120.44
1	C	166	VAL	CA-C-N	-6.01	110.06	121.54
1	C	166	VAL	C-N-CA	-6.01	110.06	121.54
1	A	190	VAL	CB-CA-C	-5.97	104.17	111.87
1	A	261	ASN	N-CA-C	5.87	121.10	113.88
1	A	190	VAL	N-CA-C	-5.82	104.95	110.42
1	A	152	ASN	N-CA-C	-5.78	102.48	109.83
1	B	242	ALA	N-CA-C	-5.74	102.27	110.59
1	A	274	ASP	N-CA-C	-5.72	104.42	111.40
1	C	65	ALA	O-C-N	-5.70	115.56	122.11
1	A	128	VAL	CA-C-N	5.57	126.80	119.84
1	A	128	VAL	C-N-CA	5.57	126.80	119.84
1	C	184	TYR	N-CA-C	-5.55	105.14	111.14
1	A	127	ASP	O-C-N	5.52	129.90	121.23
1	A	184	TYR	N-CA-C	-5.41	105.30	111.14
1	B	176	LEU	CB-CA-C	-5.40	101.95	110.86
1	A	106	LEU	N-CA-CB	5.37	119.57	110.49
1	A	239	PRO	CA-C-N	-5.34	112.36	121.97
1	A	239	PRO	C-N-CA	-5.34	112.36	121.97
1	C	315	ALA	N-CA-C	5.26	117.09	111.36
1	B	125	VAL	N-CA-C	5.25	116.06	107.24
1	B	132	VAL	CB-CA-C	-5.25	103.71	110.84
1	A	215	PHE	N-CA-C	-5.21	99.71	110.80
1	C	77	VAL	N-CA-C	5.21	115.56	107.28
1	B	307	PHE	CA-C-N	5.12	128.87	120.63
1	B	307	PHE	C-N-CA	5.12	128.87	120.63
1	C	169	ILE	CB-CA-C	-5.10	105.29	111.87
1	B	182	LYS	N-CA-C	-5.09	102.02	109.81

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	170	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2049	0	1985	510	0
1	B	1992	0	1936	478	2
1	C	1838	0	1792	476	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
All	All	5882	0	5713	1449	2

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 125.

All (1449) 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:157:MET:HE3	1:C:225:TYR:CD1	1.29	1.66
1:A:271:THR:CG2	1:A:272:VAL:CB	1.78	1.59
1:C:106:LEU:HD11	1:C:176:LEU:CD2	1.31	1.57
1:C:57:VAL:CA	1:C:106:LEU:HB3	1.29	1.56
1:B:259:LYS:CG	1:B:260:THR:HG23	1.34	1.55
1:C:157:MET:HE3	1:C:225:TYR:CG	1.40	1.54
1:C:109:TYR:CE1	1:C:132:VAL:HG13	1.41	1.54
1:A:203:GLY:HA2	1:A:230:TYR:CE2	1.45	1.51
1:C:157:MET:SD	1:C:225:TYR:HB2	1.50	1.50
1:A:263:VAL:HG23	1:A:264:PRO:CB	1.41	1.49
1:A:263:VAL:HG23	1:A:264:PRO:CA	1.46	1.46
1:C:157:MET:CE	1:C:225:TYR:CD1	1.96	1.45
1:B:259:LYS:HB3	1:B:260:THR:CB	1.48	1.43
1:A:271:THR:HG22	1:A:272:VAL:CB	0.93	1.41
1:C:157:MET:CE	1:C:225:TYR:HD1	1.30	1.40
1:A:209:VAL:CG1	1:A:322:LEU:HD22	1.51	1.40
1:A:102:GLN:NE2	1:A:125:VAL:HG11	1.32	1.36
1:A:246:PHE:CB	1:A:250:GLN:HB2	1.55	1.36
1:C:56:LYS:NZ	1:C:58:LEU:HG	1.38	1.36
1:A:136:GLY:N	1:A:137:ILE:HB	1.35	1.35
1:B:191:TYR:CE1	1:B:308:LEU:HD11	1.59	1.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:THR:HG22	1:A:272:VAL:CA	1.57	1.33
1:B:209:VAL:CG2	1:B:214:ARG:HG2	1.59	1.33
1:C:61:PHE:CZ	1:C:64:LEU:HD13	1.61	1.33
1:B:259:LYS:CB	1:B:260:THR:HG23	1.59	1.30
1:A:60:THR:HG21	1:A:115:GLU:OE1	1.20	1.28
1:C:157:MET:HE3	1:C:225:TYR:CB	1.61	1.28
1:A:247:THR:HB	1:A:248:PRO:CD	1.64	1.27
1:C:61:PHE:CE2	1:C:64:LEU:HD13	1.69	1.27
1:C:56:LYS:O	1:C:57:VAL:HG13	1.35	1.26
1:C:105:ASP:O	1:C:106:LEU:CD2	1.82	1.25
1:A:209:VAL:HG12	1:A:322:LEU:CD2	1.67	1.25
1:C:105:ASP:O	1:C:106:LEU:HD22	1.12	1.25
1:B:183:TYR:CA	1:B:184:TYR:HB2	1.65	1.25
1:B:183:TYR:HA	1:B:184:TYR:CB	1.65	1.25
1:C:107:ILE:HD12	1:C:128:VAL:CG2	1.66	1.25
1:C:157:MET:CE	1:C:225:TYR:HB2	1.68	1.23
1:B:259:LYS:HB3	1:B:260:THR:CG2	1.67	1.23
1:B:259:LYS:HE2	1:B:260:THR:CG2	1.67	1.22
1:A:263:VAL:CG2	1:A:264:PRO:HB3	1.68	1.22
1:B:293:TYR:O	1:B:310:LEU:HD11	1.08	1.22
1:C:61:PHE:CE2	1:C:63:VAL:HG22	1.73	1.22
1:B:182:LYS:HB2	1:B:183:TYR:CD1	1.74	1.21
1:C:122:LEU:HD21	1:C:128:VAL:CG2	1.70	1.21
1:B:277:GLN:CG	1:B:288:PHE:CE2	2.23	1.21
1:C:106:LEU:CD1	1:C:176:LEU:HD22	1.70	1.21
1:B:63:VAL:HA	1:B:297:LEU:HD11	1.23	1.20
1:A:252:GLN:O	1:A:255:ILE:HG22	1.39	1.20
1:B:277:GLN:HG2	1:B:288:PHE:CE2	1.78	1.19
1:A:176:LEU:HD12	1:A:176:LEU:O	1.39	1.19
1:B:122:LEU:HD12	1:B:122:LEU:O	1.39	1.19
1:C:220:GLU:CG	1:C:241:ASN:HD21	1.57	1.18
1:B:122:LEU:O	1:B:122:LEU:CD1	1.91	1.18
1:B:275:LYS:CB	1:B:278:LYS:HZ2	1.56	1.18
1:C:57:VAL:HG23	1:C:108:LEU:HD13	1.26	1.18
1:C:154:HIS:NE2	1:C:220:GLU:OE1	1.78	1.17
1:B:223:PHE:CE2	1:B:292:LEU:HD22	1.79	1.17
1:A:263:VAL:CG2	1:A:264:PRO:CB	2.22	1.17
1:B:293:TYR:O	1:B:310:LEU:CD1	1.91	1.16
1:B:277:GLN:CG	1:B:288:PHE:HE2	1.58	1.16
1:B:209:VAL:HG21	1:B:214:ARG:CG	1.75	1.16
1:C:269:GLU:HG3	1:C:272:VAL:CG2	1.74	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:VAL:CG2	1:A:264:PRO:CA	2.24	1.15
1:C:57:VAL:HA	1:C:106:LEU:CB	1.75	1.15
1:C:303:PRO:O	1:C:304:VAL:HG12	1.46	1.15
1:A:136:GLY:H	1:A:137:ILE:CB	1.60	1.15
1:B:208:GLN:OE1	1:B:319:THR:HB	1.40	1.15
1:B:203:GLY:HA2	1:B:206:LEU:HD11	1.26	1.14
1:C:61:PHE:HE2	1:C:63:VAL:HG22	0.98	1.14
1:A:203:GLY:CA	1:A:230:TYR:CE2	2.30	1.14
1:C:57:VAL:CA	1:C:106:LEU:CB	2.26	1.14
1:B:268:CYS:SG	1:B:272:VAL:CG2	2.36	1.14
1:C:109:TYR:CE1	1:C:132:VAL:CG1	2.30	1.14
1:B:258:VAL:O	1:B:259:LYS:HG3	1.46	1.13
1:C:108:LEU:HG	1:C:131:VAL:CG1	1.79	1.13
1:A:60:THR:HG21	1:A:115:GLU:CD	1.71	1.13
1:A:246:PHE:CB	1:A:250:GLN:CB	2.25	1.12
1:B:262:ASN:O	1:B:264:PRO:HD3	1.49	1.12
1:A:242:ALA:O	1:A:243:GLU:HG3	1.43	1.12
1:B:213:GLN:CD	1:B:262:ASN:HD21	1.56	1.12
1:B:182:LYS:C	1:B:183:TYR:HD1	1.57	1.12
1:A:60:THR:CG2	1:A:115:GLU:OE1	1.96	1.12
1:B:259:LYS:CD	1:B:260:THR:HG23	1.79	1.12
1:C:140:ILE:HD12	1:C:141:PRO:HD2	1.15	1.12
1:C:154:HIS:O	1:C:157:MET:HE2	1.50	1.11
1:C:140:ILE:HD12	1:C:141:PRO:CD	1.81	1.11
1:C:269:GLU:CD	1:C:272:VAL:CG2	2.23	1.11
1:C:269:GLU:CG	1:C:272:VAL:CG2	2.28	1.11
1:B:217:VAL:HG22	1:B:266:ILE:HG23	1.33	1.11
1:B:191:TYR:CZ	1:B:308:LEU:HD11	1.86	1.10
1:C:220:GLU:HG3	1:C:241:ASN:ND2	1.65	1.10
1:C:61:PHE:CZ	1:C:64:LEU:CD1	2.34	1.10
1:B:266:ILE:HG22	1:B:267:PHE:H	1.08	1.10
1:B:268:CYS:SG	1:B:272:VAL:HG21	1.90	1.10
1:B:183:TYR:HB3	1:B:185:ASN:H	0.93	1.09
1:C:157:MET:CE	1:C:225:TYR:CB	2.26	1.09
1:B:259:LYS:CE	1:B:260:THR:CG2	2.30	1.09
1:C:56:LYS:O	1:C:57:VAL:CG1	1.99	1.09
1:B:181:ALA:O	1:B:184:TYR:CD2	2.06	1.09
1:B:314:ASP:O	1:B:318:ILE:HD12	1.51	1.08
1:C:220:GLU:HG3	1:C:241:ASN:HD21	1.09	1.08
1:A:157:MET:HB3	1:A:226:LEU:HD11	1.32	1.08
1:B:259:LYS:CG	1:B:260:THR:CG2	2.30	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:LEU:HG	1:C:131:VAL:HG11	1.29	1.08
1:A:94:THR:OG1	1:A:95:PRO:HD2	1.52	1.07
1:B:154:HIS:CG	1:B:222:ALA:HB1	1.88	1.07
1:C:57:VAL:N	1:C:106:LEU:HB3	1.69	1.07
1:A:266:ILE:CG2	1:A:267:PHE:H	1.68	1.06
1:B:150:LYS:HB3	1:B:151:PRO:HD2	1.19	1.06
1:B:259:LYS:HG2	1:B:260:THR:HG23	1.35	1.06
1:C:94:THR:HG22	1:C:96:SER:N	1.69	1.06
1:C:106:LEU:HD11	1:C:176:LEU:HD21	1.35	1.06
1:C:106:LEU:CD1	1:C:176:LEU:CD2	2.27	1.06
1:B:277:GLN:HG3	1:B:288:PHE:CE2	1.89	1.06
1:C:122:LEU:HD21	1:C:128:VAL:HG22	1.11	1.06
1:B:62:THR:CB	1:B:297:LEU:HD13	1.85	1.06
1:A:277:GLN:HG2	1:A:288:PHE:HE1	1.15	1.05
1:C:157:MET:SD	1:C:225:TYR:CB	2.44	1.05
1:A:229:ASP:OD1	1:A:230:TYR:CD1	2.10	1.05
1:B:181:ALA:O	1:B:184:TYR:CE2	2.08	1.05
1:B:275:LYS:HB3	1:B:278:LYS:HZ2	1.13	1.05
1:C:107:ILE:HD12	1:C:128:VAL:HG23	1.05	1.05
1:A:263:VAL:CB	1:A:264:PRO:HA	1.83	1.04
1:B:208:GLN:HE21	1:B:323:LEU:HD13	1.22	1.04
1:B:310:LEU:HD23	1:B:311:LEU:HD12	1.36	1.04
1:C:128:VAL:HG22	1:C:128:VAL:O	1.58	1.04
1:A:61:PHE:O	1:A:80:SER:HB2	1.57	1.03
1:A:266:ILE:HG22	1:A:267:PHE:N	1.64	1.03
1:A:247:THR:CB	1:A:248:PRO:HD2	1.89	1.03
1:A:91:TYR:C	1:A:93:PRO:HD3	1.82	1.03
1:B:275:LYS:O	1:B:278:LYS:HD2	1.58	1.03
1:A:89:HIS:ND1	1:A:241:ASN:ND2	2.06	1.03
1:A:247:THR:HB	1:A:248:PRO:HD2	1.04	1.03
1:A:263:VAL:HG23	1:A:264:PRO:HB3	1.27	1.03
1:C:61:PHE:HE2	1:C:63:VAL:CG2	1.71	1.03
1:B:154:HIS:CB	1:B:222:ALA:HB1	1.90	1.02
1:B:258:VAL:HG21	1:B:284:THR:CG2	1.89	1.01
1:B:95:PRO:HA	1:B:98:ILE:HD13	1.38	1.01
1:B:182:LYS:HZ3	1:B:183:TYR:HE1	1.05	1.01
1:C:109:TYR:HB3	1:C:118:PHE:CE2	1.96	1.01
1:C:94:THR:HG22	1:C:96:SER:H	0.86	1.00
1:C:269:GLU:CD	1:C:272:VAL:HG22	1.84	1.00
1:A:159:PRO:HG2	1:A:202:LEU:CD2	1.91	1.00
1:C:133:LEU:O	1:C:134:THR:HG23	1.60	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:LYS:H	1:C:106:LEU:HD23	1.24	1.00
1:B:122:LEU:O	1:B:122:LEU:CG	2.04	1.00
1:C:57:VAL:HA	1:C:106:LEU:O	1.59	1.00
1:A:234:GLU:O	1:A:235:ILE:HD13	1.62	0.99
1:B:183:TYR:HB3	1:B:185:ASN:N	1.77	0.99
1:B:259:LYS:HB3	1:B:260:THR:OG1	1.60	0.99
1:B:83:ARG:NH2	1:B:84:ILE:CG1	2.25	0.99
1:B:83:ARG:NH2	1:B:84:ILE:HG12	1.78	0.99
1:C:107:ILE:CD1	1:C:128:VAL:HG23	1.91	0.99
1:A:210:PRO:HA	1:A:211:ALA:O	1.60	0.99
1:B:258:VAL:HG21	1:B:284:THR:HG21	1.42	0.99
1:B:118:PHE:CE2	1:B:122:LEU:HD23	1.97	0.99
1:B:259:LYS:HB3	1:B:260:THR:CA	1.91	0.98
1:A:214:ARG:HH12	1:A:231:GLY:HA3	1.24	0.98
1:B:223:PHE:CZ	1:B:292:LEU:HD22	1.98	0.98
1:A:94:THR:CB	1:A:95:PRO:HD2	1.93	0.98
1:C:57:VAL:HG22	1:C:57:VAL:O	1.60	0.98
1:B:259:LYS:CD	1:B:260:THR:CG2	2.42	0.98
1:C:94:THR:CG2	1:C:96:SER:H	1.76	0.98
1:B:150:LYS:HB3	1:B:151:PRO:CD	1.93	0.98
1:A:59:THR:HG22	1:A:80:SER:HA	1.43	0.97
1:A:209:VAL:H	1:A:210:PRO:HD3	1.27	0.97
1:B:63:VAL:CA	1:B:297:LEU:HD11	1.94	0.97
1:A:102:GLN:NE2	1:A:125:VAL:CG1	2.27	0.97
1:A:61:PHE:HD1	1:A:61:PHE:H	1.12	0.97
1:C:149:ASP:O	1:C:151:PRO:HD3	1.64	0.97
1:B:259:LYS:HE2	1:B:260:THR:HG22	1.46	0.97
1:C:105:ASP:O	1:C:106:LEU:CG	2.12	0.97
1:C:133:LEU:O	1:C:134:THR:CG2	2.13	0.97
1:C:269:GLU:CD	1:C:272:VAL:HG21	1.87	0.97
1:B:314:ASP:O	1:B:318:ILE:CD1	2.13	0.97
1:B:258:VAL:HG23	1:B:259:LYS:H	1.29	0.97
1:C:128:VAL:CG2	1:C:128:VAL:O	2.09	0.97
1:A:263:VAL:HB	1:A:264:PRO:HA	1.44	0.96
1:B:83:ARG:NH2	1:B:84:ILE:HD11	1.79	0.96
1:C:107:ILE:CD1	1:C:128:VAL:CG2	2.44	0.96
1:C:157:MET:CG	1:C:225:TYR:HB2	1.96	0.96
1:B:277:GLN:CG	1:B:288:PHE:CD2	2.48	0.96
1:C:66:ASP:HA	1:C:69:GLN:HG2	1.48	0.96
1:A:193:GLU:HG2	1:A:194:GLN:N	1.78	0.96
1:B:259:LYS:CB	1:B:260:THR:CG2	2.30	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:GLY:HA2	1:A:230:TYR:HE2	1.20	0.96
1:B:277:GLN:HG3	1:B:288:PHE:CD2	2.01	0.95
1:C:56:LYS:CG	1:C:57:VAL:H	1.78	0.95
1:A:92:GLU:N	1:A:93:PRO:CD	2.30	0.95
1:C:154:HIS:HE1	1:C:295:ASP:OD1	1.47	0.95
1:A:266:ILE:HG22	1:A:267:PHE:H	0.81	0.95
1:C:56:LYS:NZ	1:C:58:LEU:CG	2.29	0.95
1:C:220:GLU:OE1	1:C:222:ALA:HB2	1.65	0.95
1:B:191:TYR:CE1	1:B:308:LEU:CD1	2.50	0.95
1:C:109:TYR:CB	1:C:118:PHE:CE2	2.49	0.95
1:B:266:ILE:HG22	1:B:267:PHE:N	1.74	0.95
1:B:83:ARG:NH2	1:B:84:ILE:CD1	2.30	0.95
1:C:316:ARG:HA	1:C:319:THR:HG23	1.49	0.95
1:B:258:VAL:CG2	1:B:259:LYS:N	2.30	0.94
1:C:109:TYR:HE1	1:C:132:VAL:HG13	1.13	0.94
1:C:304:VAL:HG13	1:C:304:VAL:O	1.66	0.94
1:A:220:GLU:CG	1:A:240:ILE:HD12	1.96	0.94
1:B:217:VAL:CG2	1:B:266:ILE:HG23	1.97	0.94
1:A:277:GLN:HG2	1:A:288:PHE:CE1	2.01	0.94
1:B:183:TYR:HD1	1:B:183:TYR:N	1.61	0.94
1:A:263:VAL:HG21	1:A:264:PRO:HB3	1.48	0.94
1:A:271:THR:CG2	1:A:272:VAL:CA	2.24	0.93
1:A:271:THR:CG2	1:A:272:VAL:HA	1.98	0.93
1:B:154:HIS:CG	1:B:222:ALA:CB	2.51	0.93
1:B:301:GLU:HA	1:B:301:GLU:OE1	1.67	0.93
1:C:60:THR:OG1	1:C:61:PHE:CD1	2.21	0.93
1:C:135:GLU:O	1:C:135:GLU:CD	2.10	0.93
1:A:258:VAL:O	1:A:262:ASN:O	1.85	0.93
1:C:122:LEU:CD2	1:C:128:VAL:HG22	1.99	0.93
1:A:242:ALA:C	1:A:243:GLU:HG3	1.92	0.93
1:B:213:GLN:CD	1:B:262:ASN:ND2	2.25	0.93
1:C:197:ALA:O	1:C:200:ARG:HG2	1.69	0.93
1:A:170:ARG:HH11	1:A:185:ASN:ND2	1.65	0.93
1:A:220:GLU:HG3	1:A:241:ASN:OD1	1.68	0.93
1:B:122:LEU:O	1:B:122:LEU:HG	1.69	0.93
1:B:182:LYS:C	1:B:183:TYR:CD1	2.46	0.92
1:C:57:VAL:N	1:C:106:LEU:CB	2.29	0.92
1:C:269:GLU:HG3	1:C:272:VAL:HG22	1.50	0.92
1:A:213:GLN:C	1:A:214:ARG:HG2	1.93	0.92
1:C:57:VAL:HA	1:C:106:LEU:HB3	0.93	0.92
1:C:60:THR:HG22	1:C:118:PHE:CE1	2.04	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:GLY:HA2	1:A:230:TYR:CZ	2.04	0.91
1:B:191:TYR:CE1	1:B:195:LEU:HD11	2.04	0.91
1:B:257:GLU:HG2	1:B:258:VAL:N	1.83	0.91
1:A:157:MET:CB	1:A:226:LEU:HD11	2.01	0.91
1:C:316:ARG:HA	1:C:319:THR:CG2	1.99	0.91
1:A:277:GLN:N	1:A:277:GLN:OE1	2.04	0.91
1:A:263:VAL:HG23	1:A:264:PRO:N	1.74	0.90
1:C:254:VAL:HG22	1:C:254:VAL:O	1.69	0.90
1:C:109:TYR:CD2	1:C:118:PHE:CE2	2.60	0.90
1:A:109:TYR:HB2	1:A:115:GLU:OE2	1.71	0.90
1:B:261:ASN:O	1:B:262:ASN:HB3	1.70	0.90
1:B:310:LEU:HD23	1:B:311:LEU:CD1	2.01	0.90
1:B:259:LYS:CE	1:B:260:THR:HG21	2.00	0.90
1:B:127:ASP:O	1:B:128:VAL:HG22	1.72	0.89
1:B:223:PHE:CE2	1:B:292:LEU:CD2	2.55	0.89
1:B:118:PHE:CD2	1:B:122:LEU:HD23	2.07	0.89
1:B:183:TYR:CD1	1:B:183:TYR:N	2.35	0.89
1:C:57:VAL:CB	1:C:106:LEU:HB3	2.03	0.89
1:C:248:PRO:HA	1:C:251:VAL:HG12	1.52	0.89
1:A:89:HIS:CE1	1:A:241:ASN:CG	2.50	0.89
1:B:191:TYR:HE1	1:B:308:LEU:CD1	1.83	0.89
1:A:203:GLY:CA	1:A:230:TYR:CZ	2.56	0.89
1:B:83:ARG:HH21	1:B:84:ILE:HD11	1.36	0.89
1:A:157:MET:SD	1:A:294:VAL:HG13	2.11	0.89
1:B:259:LYS:O	1:B:263:VAL:HG21	1.72	0.89
1:C:61:PHE:CE2	1:C:64:LEU:CD1	2.54	0.89
1:A:212:ASN:O	1:A:214:ARG:HG3	1.71	0.89
1:C:217:VAL:CG2	1:C:266:ILE:HD12	2.01	0.89
1:A:238:TRP:HD1	1:A:240:ILE:O	1.55	0.89
1:B:88:ILE:HG13	1:B:117:TRP:HE1	1.37	0.89
1:A:113:ASN:ND2	1:A:150:LYS:HE2	1.87	0.89
1:B:62:THR:OG1	1:B:297:LEU:CD1	2.21	0.89
1:B:191:TYR:HE1	1:B:308:LEU:HD11	1.14	0.89
1:A:246:PHE:O	1:A:250:GLN:HB3	1.73	0.88
1:C:215:PHE:O	1:C:263:VAL:HG21	1.71	0.88
1:A:220:GLU:HG2	1:A:240:ILE:CD1	2.02	0.88
1:C:269:GLU:CG	1:C:272:VAL:HG22	1.97	0.88
1:B:62:THR:HB	1:B:297:LEU:HD13	1.54	0.88
1:B:298:SER:OG	1:B:299:THR:N	2.03	0.88
1:A:229:ASP:OD1	1:A:230:TYR:CG	2.26	0.88
1:A:218:SER:HA	1:A:267:PHE:O	1.73	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:SER:OG	1:B:297:LEU:N	1.98	0.88
1:C:169:ILE:CG2	1:C:173:PHE:CE2	2.56	0.88
1:C:220:GLU:CD	1:C:241:ASN:HD21	1.83	0.87
1:A:102:GLN:HE22	1:A:125:VAL:HG11	1.32	0.87
1:C:56:LYS:C	1:C:57:VAL:CG1	2.47	0.87
1:A:159:PRO:HG2	1:A:202:LEU:HD22	1.53	0.87
1:B:111:GLY:HA2	1:B:115:GLU:OE1	1.73	0.87
1:A:59:THR:OG1	1:A:64:LEU:HD23	1.75	0.86
1:A:214:ARG:NH1	1:A:231:GLY:HA3	1.88	0.86
1:B:140:ILE:HG23	1:B:141:PRO:HD2	1.55	0.86
1:A:212:ASN:O	1:A:214:ARG:CG	2.22	0.86
1:A:256:GLU:OE2	1:A:260:THR:HG23	1.75	0.86
1:C:125:VAL:CG1	1:C:128:VAL:HG11	2.06	0.86
1:A:220:GLU:HG2	1:A:240:ILE:HD12	1.58	0.86
1:C:115:GLU:HB2	1:C:118:PHE:HB2	1.55	0.86
1:A:89:HIS:ND1	1:A:241:ASN:CG	2.34	0.85
1:A:216:LEU:HD11	1:A:223:PHE:CD2	2.11	0.85
1:B:94:THR:HB	1:B:95:PRO:HD2	1.58	0.85
1:C:56:LYS:HZ1	1:C:58:LEU:CG	1.86	0.85
1:C:268:CYS:SG	1:C:269:GLU:N	2.46	0.85
1:C:157:MET:HE1	1:C:225:TYR:HD1	1.39	0.85
1:C:56:LYS:HZ1	1:C:58:LEU:HG	0.94	0.85
1:A:213:GLN:O	1:A:214:ARG:HG2	1.77	0.85
1:B:118:PHE:CE2	1:B:122:LEU:CD2	2.59	0.85
1:B:258:VAL:CG2	1:B:284:THR:HG21	2.05	0.85
1:B:298:SER:OG	1:B:302:GLY:HA3	1.76	0.85
1:B:114:LEU:HD23	1:B:153:PRO:HB2	1.58	0.85
1:A:216:LEU:CD1	1:A:223:PHE:CD2	2.59	0.85
1:C:271:THR:HG23	1:C:272:VAL:H	1.41	0.85
1:A:220:GLU:OE1	1:A:240:ILE:HD11	1.77	0.84
1:B:111:GLY:HA2	1:B:115:GLU:CD	2.02	0.84
1:C:57:VAL:HG23	1:C:108:LEU:CD1	2.06	0.84
1:A:238:TRP:CD1	1:A:240:ILE:O	2.29	0.84
1:B:268:CYS:SG	1:B:269:GLU:N	2.46	0.84
1:B:277:GLN:HG2	1:B:288:PHE:HE2	1.16	0.84
1:C:217:VAL:HG21	1:C:266:ILE:CD1	2.07	0.84
1:A:89:HIS:CE1	1:A:241:ASN:ND2	2.45	0.84
1:B:83:ARG:HH21	1:B:84:ILE:CD1	1.88	0.84
1:B:259:LYS:O	1:B:263:VAL:CG2	2.25	0.84
1:C:169:ILE:CG2	1:C:173:PHE:HE2	1.91	0.84
1:A:102:GLN:CD	1:A:125:VAL:HG11	2.01	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:LYS:HB3	1:B:278:LYS:NZ	1.91	0.84
1:C:154:HIS:CE1	1:C:295:ASP:OD1	2.29	0.84
1:C:195:LEU:CD1	1:C:308:LEU:HD21	2.08	0.84
1:B:84:ILE:HG22	1:B:85:GLY:H	1.43	0.84
1:C:74:ASP:CG	1:C:74:ASP:O	2.20	0.84
1:C:56:LYS:HG3	1:C:57:VAL:H	1.43	0.83
1:A:206:LEU:O	1:A:209:VAL:CG2	2.26	0.83
1:B:208:GLN:CD	1:B:319:THR:HB	2.02	0.83
1:B:266:ILE:CG2	1:B:267:PHE:H	1.89	0.83
1:C:217:VAL:HG22	1:C:266:ILE:HD12	1.60	0.83
1:A:209:VAL:N	1:A:210:PRO:CD	2.42	0.83
1:C:207:GLU:HG2	1:C:207:GLU:O	1.78	0.83
1:C:271:THR:HG23	1:C:272:VAL:N	1.93	0.83
1:B:110:ASN:CG	1:B:114:LEU:HD21	2.03	0.83
1:B:259:LYS:CB	1:B:260:THR:CB	2.44	0.83
1:B:191:TYR:OH	1:B:308:LEU:CD1	2.27	0.83
1:B:215:PHE:CE1	1:B:261:ASN:ND2	2.46	0.83
1:A:203:GLY:HA3	1:A:230:TYR:OH	1.79	0.82
1:A:223:PHE:CZ	1:A:292:LEU:HD13	2.14	0.82
1:C:154:HIS:O	1:C:157:MET:CE	2.26	0.82
1:A:170:ARG:NH1	1:A:185:ASN:ND2	2.26	0.82
1:A:209:VAL:H	1:A:210:PRO:CD	1.91	0.82
1:C:106:LEU:HD21	1:C:176:LEU:HD21	1.61	0.82
1:A:261:ASN:N	1:A:262:ASN:HA	1.93	0.82
1:A:304:VAL:HG12	1:A:304:VAL:O	1.79	0.82
1:A:234:GLU:O	1:A:235:ILE:CD1	2.27	0.82
1:C:124:ASN:C	1:C:124:ASN:OD1	2.23	0.82
1:C:217:VAL:CG2	1:C:266:ILE:CD1	2.56	0.82
1:A:97:ASP:HB2	1:A:102:GLN:HB3	1.62	0.82
1:A:246:PHE:CB	1:A:250:GLN:CD	2.53	0.82
1:B:154:HIS:HB2	1:B:222:ALA:HB1	1.58	0.82
1:C:269:GLU:OE2	1:C:272:VAL:HG21	1.79	0.82
1:C:106:LEU:HD11	1:C:176:LEU:HD22	0.82	0.81
1:C:169:ILE:HG22	1:C:173:PHE:CD2	2.15	0.81
1:A:133:LEU:HA	1:A:168:ASN:HD22	1.45	0.81
1:B:63:VAL:N	1:B:297:LEU:CD1	2.43	0.81
1:A:220:GLU:CG	1:A:240:ILE:CD1	2.58	0.81
1:C:269:GLU:HG3	1:C:272:VAL:HG23	1.60	0.81
1:A:113:ASN:HD22	1:A:150:LYS:HE2	1.45	0.81
1:A:256:GLU:OE2	1:A:260:THR:CG2	2.28	0.81
1:A:261:ASN:H	1:A:262:ASN:HA	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:GLY:CA	1:A:137:ILE:HB	2.11	0.81
1:B:122:LEU:HD12	1:B:122:LEU:C	2.05	0.81
1:C:70:ASN:ND2	1:C:191:TYR:HE1	1.79	0.81
1:C:157:MET:HE2	1:C:225:TYR:CD1	2.12	0.81
1:A:263:VAL:HG23	1:A:264:PRO:CD	2.10	0.80
1:B:257:GLU:HG2	1:B:258:VAL:H	1.45	0.80
1:B:275:LYS:CG	1:B:278:LYS:HZ2	1.94	0.80
1:A:94:THR:OG1	1:A:95:PRO:CD	2.30	0.80
1:B:191:TYR:OH	1:B:308:LEU:HD11	1.80	0.80
1:C:238:TRP:HD1	1:C:240:ILE:O	1.65	0.80
1:A:244:GLN:C	1:A:244:GLN:CD	2.50	0.80
1:C:57:VAL:HA	1:C:106:LEU:C	2.07	0.80
1:C:109:TYR:HB3	1:C:118:PHE:HE2	1.46	0.80
1:C:66:ASP:O	1:C:69:GLN:HG3	1.82	0.80
1:A:269:GLU:OE1	1:A:292:LEU:HB2	1.82	0.80
1:A:234:GLU:OE1	1:A:234:GLU:N	2.15	0.79
1:B:182:LYS:CB	1:B:183:TYR:CD1	2.64	0.79
1:B:310:LEU:CD2	1:B:311:LEU:HD12	2.12	0.79
1:A:283:ALA:O	1:A:284:THR:HG23	1.81	0.79
1:B:209:VAL:CG2	1:B:214:ARG:CG	2.44	0.79
1:B:208:GLN:OE1	1:B:319:THR:CB	2.28	0.79
1:C:56:LYS:CG	1:C:57:VAL:N	2.44	0.79
1:C:109:TYR:CD2	1:C:118:PHE:HE2	2.01	0.79
1:A:89:HIS:HD2	1:A:114:LEU:HD23	1.48	0.79
1:B:259:LYS:CB	1:B:260:THR:OG1	2.30	0.79
1:A:133:LEU:HA	1:A:168:ASN:ND2	1.97	0.79
1:C:238:TRP:CD1	1:C:240:ILE:O	2.35	0.79
1:B:202:LEU:O	1:B:206:LEU:HG	1.81	0.79
1:B:223:PHE:HE2	1:B:292:LEU:HD22	1.46	0.79
1:A:60:THR:CG2	1:A:115:GLU:CD	2.50	0.79
1:A:202:LEU:HD12	1:A:203:GLY:N	1.96	0.79
1:A:213:GLN:OE1	1:A:213:GLN:HA	1.83	0.79
1:C:56:LYS:C	1:C:57:VAL:HG12	2.07	0.79
1:C:308:LEU:HA	1:C:311:LEU:HD12	1.62	0.79
1:C:315:ALA:O	1:C:318:ILE:HG13	1.83	0.78
1:A:159:PRO:HG2	1:A:202:LEU:HD21	1.63	0.78
1:C:109:TYR:CZ	1:C:132:VAL:HG13	2.16	0.78
1:A:246:PHE:CB	1:A:250:GLN:NE2	2.46	0.78
1:B:258:VAL:CG2	1:B:259:LYS:H	1.93	0.78
1:A:61:PHE:CE2	1:A:63:VAL:HB	2.19	0.78
1:A:199:ASP:O	1:A:202:LEU:CD1	2.32	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:GLY:CA	1:B:206:LEU:HD11	2.11	0.78
1:C:157:MET:CE	1:C:225:TYR:H	1.96	0.78
1:A:97:ASP:O	1:A:102:GLN:HA	1.84	0.78
1:A:263:VAL:CG2	1:A:264:PRO:N	2.45	0.78
1:C:316:ARG:CA	1:C:319:THR:HG23	2.14	0.78
1:B:195:LEU:O	1:B:198:ILE:HG22	1.83	0.78
1:B:223:PHE:HE2	1:B:292:LEU:CD2	1.95	0.78
1:A:104:ALA:O	1:A:105:ASP:HB3	1.82	0.77
1:B:258:VAL:O	1:B:259:LYS:CG	2.30	0.77
1:B:62:THR:OG1	1:B:297:LEU:HD13	1.81	0.77
1:C:57:VAL:CG2	1:C:108:LEU:HD13	2.12	0.77
1:A:136:GLY:N	1:A:137:ILE:CB	2.30	0.77
1:A:263:VAL:HG23	1:A:264:PRO:CG	2.13	0.77
1:B:261:ASN:O	1:B:262:ASN:CB	2.32	0.77
1:B:301:GLU:OE1	1:B:301:GLU:CA	2.33	0.77
1:C:249:LYS:O	1:C:253:THR:HG22	1.85	0.77
1:A:61:PHE:HD1	1:A:61:PHE:N	1.80	0.77
1:A:97:ASP:HB2	1:A:102:GLN:CB	2.15	0.77
1:B:209:VAL:HG21	1:B:214:ARG:HG2	0.80	0.77
1:B:292:LEU:C	1:B:292:LEU:HD12	2.10	0.77
1:C:70:ASN:ND2	1:C:191:TYR:CE1	2.52	0.77
1:A:242:ALA:C	1:A:243:GLU:CG	2.55	0.77
1:A:252:GLN:C	1:A:255:ILE:HG22	2.09	0.77
1:C:57:VAL:O	1:C:57:VAL:CG2	2.33	0.77
1:A:170:ARG:HH11	1:A:185:ASN:CG	1.92	0.77
1:B:236:TYR:HE2	1:B:239:PRO:HD3	1.50	0.76
1:A:63:VAL:HG11	1:A:156:TRP:NE1	1.99	0.76
1:B:58:LEU:HD23	1:B:81:ILE:HD11	1.67	0.76
1:A:176:LEU:CD1	1:A:177:ASP:OD1	2.33	0.76
1:A:199:ASP:O	1:A:202:LEU:HD12	1.84	0.76
1:C:140:ILE:O	1:C:152:ASN:HB2	1.84	0.76
1:C:169:ILE:HG22	1:C:173:PHE:CE2	2.20	0.76
1:C:306:THR:HG22	1:C:309:ASP:OD1	1.85	0.76
1:A:176:LEU:O	1:A:176:LEU:CD1	2.30	0.76
1:B:310:LEU:CD2	1:B:311:LEU:CD1	2.64	0.76
1:A:170:ARG:NH1	1:A:185:ASN:HD21	1.84	0.76
1:B:119:GLU:CG	1:B:120:GLN:N	2.48	0.76
1:B:183:TYR:CB	1:B:185:ASN:H	1.87	0.76
1:A:193:GLU:CG	1:A:194:GLN:N	2.49	0.76
1:A:199:ASP:HA	1:A:202:LEU:HD11	1.68	0.76
1:B:140:ILE:HG22	1:B:141:PRO:O	1.83	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:TYR:HE1	1:C:132:VAL:CG1	1.83	0.76
1:C:109:TYR:CD1	1:C:109:TYR:C	2.63	0.76
1:C:102:GLN:HG3	1:C:125:VAL:HG13	1.66	0.75
1:A:242:ALA:O	1:A:243:GLU:CG	2.30	0.75
1:A:64:LEU:HD11	1:A:133:LEU:HD22	1.68	0.75
1:B:182:LYS:NZ	1:B:183:TYR:CE1	2.48	0.75
1:B:182:LYS:HA	1:B:184:TYR:HB2	1.69	0.75
1:A:91:TYR:C	1:A:93:PRO:CD	2.58	0.75
1:A:116:ALA:HB1	1:A:119:GLU:CD	2.11	0.75
1:C:105:ASP:O	1:C:106:LEU:CB	2.34	0.75
1:A:202:LEU:HD12	1:A:203:GLY:H	1.50	0.75
1:C:57:VAL:H	1:C:106:LEU:CB	2.00	0.75
1:A:209:VAL:CG1	1:A:322:LEU:CD2	2.42	0.75
1:B:208:GLN:HE21	1:B:323:LEU:CD1	1.99	0.75
1:C:56:LYS:HG3	1:C:57:VAL:N	2.02	0.75
1:A:109:TYR:O	1:A:133:LEU:HD13	1.87	0.74
1:A:167:GLU:CD	1:A:167:GLU:O	2.30	0.74
1:C:303:PRO:O	1:C:304:VAL:CG1	2.30	0.74
1:C:205:ASP:OD2	1:C:319:THR:HG21	1.85	0.74
1:A:158:SER:HB3	1:A:161:ASN:OD1	1.87	0.74
1:B:268:CYS:SG	1:B:272:VAL:HG23	2.24	0.74
1:C:109:TYR:CD2	1:C:118:PHE:CD2	2.75	0.74
1:A:165:TYR:HD1	1:A:165:TYR:H	1.33	0.74
1:A:266:ILE:O	1:A:267:PHE:CD1	2.39	0.74
1:C:140:ILE:CD1	1:C:141:PRO:HD2	2.07	0.74
1:A:263:VAL:CG2	1:A:264:PRO:HA	2.04	0.74
1:B:62:THR:C	1:B:297:LEU:HD13	2.12	0.74
1:C:57:VAL:HB	1:C:106:LEU:HG	1.68	0.74
1:C:63:VAL:CG2	1:C:64:LEU:N	2.51	0.74
1:B:62:THR:OG1	1:B:297:LEU:HD12	1.86	0.73
1:C:66:ASP:HA	1:C:69:GLN:CG	2.18	0.73
1:A:94:THR:CG2	1:A:95:PRO:HD2	2.17	0.73
1:A:271:THR:HG23	1:A:272:VAL:HA	1.68	0.73
1:C:108:LEU:HA	1:C:131:VAL:CG1	2.18	0.73
1:A:177:ASP:O	1:A:177:ASP:CG	2.30	0.73
1:A:220:GLU:HG3	1:A:240:ILE:HD12	1.69	0.73
1:B:275:LYS:CB	1:B:278:LYS:NZ	2.45	0.73
1:C:157:MET:HE1	1:C:225:TYR:H	1.53	0.73
1:A:203:GLY:CA	1:A:230:TYR:HE2	1.87	0.73
1:B:216:LEU:O	1:B:216:LEU:HD12	1.87	0.73
1:C:111:GLY:N	1:C:115:GLU:OE2	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:HIS:CD2	1:A:114:LEU:HD23	2.23	0.73
1:A:200:ARG:CZ	1:B:122:LEU:HD13	2.17	0.73
1:A:63:VAL:HG11	1:A:156:TRP:CE2	2.23	0.72
1:C:56:LYS:HD3	1:C:104:ALA:HB3	1.71	0.72
1:C:83:ARG:C	1:C:84:ILE:HG12	2.14	0.72
1:C:133:LEU:C	1:C:134:THR:CG2	2.60	0.72
1:A:62:THR:O	1:A:65:ALA:N	2.22	0.72
1:A:303:PRO:O	1:A:304:VAL:CB	2.38	0.72
1:B:127:ASP:C	1:B:128:VAL:CG2	2.61	0.72
1:A:163:LEU:O	1:A:166:VAL:HG12	1.89	0.72
1:A:281:ALA:HA	1:A:286:ALA:HB3	1.70	0.72
1:B:111:GLY:CA	1:B:115:GLU:OE1	2.36	0.72
1:A:61:PHE:O	1:A:80:SER:CB	2.37	0.72
1:B:217:VAL:HG22	1:B:266:ILE:CG2	2.17	0.72
1:C:109:TYR:HD2	1:C:118:PHE:CE2	2.03	0.72
1:C:157:MET:HG3	1:C:225:TYR:CB	2.19	0.72
1:A:92:GLU:N	1:A:93:PRO:HD2	2.05	0.72
1:A:114:LEU:O	1:A:115:GLU:HG2	1.90	0.71
1:B:84:ILE:HG22	1:B:85:GLY:N	2.05	0.71
1:C:122:LEU:CD2	1:C:128:VAL:CG2	2.60	0.71
1:C:133:LEU:C	1:C:134:THR:HG22	2.14	0.71
1:A:87:GLU:O	1:A:87:GLU:HG2	1.90	0.71
1:B:83:ARG:CZ	1:B:84:ILE:HG12	2.20	0.71
1:A:303:PRO:O	1:A:304:VAL:HB	1.89	0.71
1:C:124:ASN:OD1	1:C:124:ASN:O	2.07	0.71
1:A:203:GLY:CA	1:A:230:TYR:OH	2.38	0.71
1:A:247:THR:HB	1:A:248:PRO:HD3	1.68	0.71
1:B:258:VAL:HG22	1:B:259:LYS:N	2.04	0.71
1:C:56:LYS:HZ2	1:C:58:LEU:HG	1.49	0.71
1:B:208:GLN:NE2	1:B:323:LEU:HD13	2.02	0.71
1:C:107:ILE:HD11	1:C:128:VAL:HB	1.72	0.71
1:A:61:PHE:CD2	1:A:88:ILE:HD13	2.26	0.70
1:A:217:VAL:HG11	1:A:266:ILE:HG12	1.73	0.70
1:A:220:GLU:O	1:A:221:GLY:C	2.33	0.70
1:B:95:PRO:HA	1:B:98:ILE:CD1	2.18	0.70
1:C:111:GLY:HA2	1:C:115:GLU:OE2	1.90	0.70
1:A:102:GLN:CD	1:A:102:GLN:O	2.33	0.70
1:B:111:GLY:HA2	1:B:115:GLU:OE2	1.91	0.70
1:C:106:LEU:CD1	1:C:176:LEU:HD21	2.08	0.70
1:B:115:GLU:O	1:B:115:GLU:HG2	1.91	0.70
1:A:255:ILE:CD1	1:A:284:THR:HG23	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:ARG:O	1:B:163:LEU:HD12	1.92	0.70
1:A:176:LEU:HD12	1:A:176:LEU:C	2.13	0.70
1:C:248:PRO:HA	1:C:251:VAL:CG1	2.22	0.70
1:A:255:ILE:HD11	1:A:284:THR:HG23	1.72	0.70
1:B:262:ASN:O	1:B:264:PRO:CD	2.36	0.70
1:C:56:LYS:HG2	1:C:57:VAL:H	1.54	0.70
1:A:269:GLU:O	1:A:270:SER:C	2.34	0.70
1:B:126:LYS:HE3	1:C:299:THR:HG22	1.73	0.70
1:C:111:GLY:CA	1:C:115:GLU:OE2	2.40	0.70
1:C:57:VAL:H	1:C:106:LEU:HB2	1.57	0.70
1:A:61:PHE:N	1:A:61:PHE:CD1	2.50	0.69
1:B:182:LYS:HA	1:B:184:TYR:CD2	2.27	0.69
1:A:142:ILE:HG12	1:A:150:LYS:O	1.93	0.69
1:A:271:THR:HG23	1:A:272:VAL:CB	2.16	0.69
1:C:154:HIS:CD2	1:C:220:GLU:OE1	2.45	0.69
1:B:182:LYS:HB2	1:B:183:TYR:CG	2.26	0.69
1:B:182:LYS:NZ	1:B:183:TYR:HE1	1.87	0.69
1:B:275:LYS:HA	1:B:278:LYS:HE3	1.71	0.69
1:C:271:THR:CG2	1:C:272:VAL:H	2.04	0.69
1:B:112:MET:HE3	1:B:225:TYR:OH	1.93	0.69
1:C:105:ASP:O	1:C:106:LEU:CD1	2.40	0.69
1:C:135:GLU:O	1:C:135:GLU:OE1	2.09	0.69
1:A:94:THR:HG1	1:A:95:PRO:HD2	1.58	0.69
1:A:246:PHE:H	1:A:250:GLN:HE21	1.39	0.69
1:C:109:TYR:HD2	1:C:118:PHE:HE2	1.36	0.69
1:A:154:HIS:HE1	1:A:240:ILE:HD11	1.57	0.69
1:C:107:ILE:HD12	1:C:128:VAL:HG21	1.72	0.69
1:C:269:GLU:CG	1:C:272:VAL:HG21	2.14	0.69
1:A:167:GLU:CD	1:A:167:GLU:C	2.60	0.69
1:B:257:GLU:CG	1:B:258:VAL:N	2.53	0.69
1:C:195:LEU:HD11	1:C:308:LEU:HD21	1.74	0.69
1:A:62:THR:HA	1:A:65:ALA:HB2	1.75	0.69
1:A:154:HIS:CE1	1:A:240:ILE:HD11	2.28	0.69
1:B:115:GLU:HB2	1:B:118:PHE:HB2	1.73	0.69
1:C:115:GLU:CB	1:C:118:PHE:HB2	2.22	0.69
1:B:309:ASP:O	1:B:310:LEU:C	2.32	0.69
1:A:92:GLU:N	1:A:93:PRO:HD3	2.04	0.68
1:A:274:ASP:HA	1:A:277:GLN:NE2	2.08	0.68
1:A:209:VAL:HB	1:A:214:ARG:HD2	1.76	0.68
1:C:157:MET:CG	1:C:225:TYR:CB	2.71	0.68
1:A:191:TYR:HE1	1:A:308:LEU:HD11	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:LEU:O	1:A:209:VAL:HG23	1.94	0.68
1:B:63:VAL:CA	1:B:297:LEU:CD1	2.69	0.68
1:B:171:GLN:O	1:B:173:PHE:N	2.27	0.68
1:B:157:MET:HE1	1:B:310:LEU:HD21	1.75	0.68
1:A:266:ILE:O	1:A:267:PHE:CG	2.47	0.68
1:A:303:PRO:O	1:A:304:VAL:HG23	1.94	0.68
1:A:164:VAL:HG12	1:A:165:TYR:CD1	2.29	0.68
1:C:220:GLU:CD	1:C:222:ALA:HB2	2.17	0.68
1:A:246:PHE:CB	1:A:250:GLN:CG	2.72	0.67
1:B:259:LYS:CB	1:B:260:THR:CA	2.65	0.67
1:B:259:LYS:HE2	1:B:260:THR:HG21	1.62	0.67
1:C:109:TYR:C	1:C:109:TYR:HD1	2.01	0.67
1:A:59:THR:CG2	1:A:61:PHE:O	2.42	0.67
1:A:103:ASP:CG	1:A:103:ASP:O	2.36	0.67
1:A:246:PHE:C	1:A:250:GLN:HB3	2.19	0.67
1:B:119:GLU:HG2	1:B:120:GLN:H	1.59	0.67
1:B:308:LEU:O	1:B:312:GLU:HG3	1.95	0.67
1:A:104:ALA:O	1:A:105:ASP:CB	2.43	0.67
1:A:255:ILE:CD1	1:A:284:THR:CG2	2.72	0.67
1:A:307:PHE:O	1:A:310:LEU:HB3	1.94	0.67
1:B:87:GLU:OE2	1:B:241:ASN:ND2	2.27	0.67
1:B:213:GLN:NE2	1:B:262:ASN:ND2	2.41	0.67
1:B:275:LYS:HA	1:B:278:LYS:CE	2.25	0.67
1:A:247:THR:O	1:A:248:PRO:C	2.36	0.67
1:C:108:LEU:HA	1:C:131:VAL:HG12	1.76	0.67
1:C:255:ILE:HD12	1:C:255:ILE:N	2.10	0.67
1:A:277:GLN:CG	1:A:288:PHE:HE1	1.99	0.67
1:C:57:VAL:CB	1:C:106:LEU:HG	2.24	0.67
1:C:66:ASP:OD1	1:C:67:MET:N	2.28	0.67
1:C:108:LEU:CG	1:C:131:VAL:CG1	2.68	0.67
1:C:254:VAL:O	1:C:254:VAL:CG2	2.43	0.67
1:A:193:GLU:HG2	1:A:194:GLN:H	1.55	0.67
1:B:177:ASP:HB2	1:B:184:TYR:OH	1.95	0.67
1:A:61:PHE:HD2	1:A:88:ILE:HD13	1.59	0.66
1:A:62:THR:C	1:A:64:LEU:N	2.49	0.66
1:B:182:LYS:HA	1:B:184:TYR:CB	2.25	0.66
1:C:220:GLU:CD	1:C:241:ASN:ND2	2.51	0.66
1:B:170:ARG:NH2	1:B:170:ARG:HG3	2.10	0.66
1:B:268:CYS:O	1:B:292:LEU:HG	1.95	0.66
1:A:216:LEU:HD11	1:A:223:PHE:HD2	1.58	0.66
1:B:126:LYS:HE2	1:C:299:THR:HA	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:ASP:O	1:C:106:LEU:HD13	1.94	0.66
1:A:223:PHE:CE2	1:A:292:LEU:HD13	2.31	0.66
1:C:57:VAL:CA	1:C:106:LEU:O	2.39	0.66
1:A:274:ASP:HA	1:A:277:GLN:HE22	1.61	0.66
1:C:154:HIS:CE1	1:C:220:GLU:OE1	2.49	0.66
1:B:111:GLY:N	1:B:115:GLU:OE1	2.29	0.66
1:A:271:THR:HG21	1:A:272:VAL:CB	2.14	0.65
1:C:217:VAL:HG22	1:C:266:ILE:CD1	2.26	0.65
1:B:259:LYS:HG2	1:B:260:THR:CG2	2.13	0.65
1:B:298:SER:HB3	1:B:304:VAL:O	1.96	0.65
1:C:106:LEU:CD2	1:C:176:LEU:HD21	2.26	0.65
1:B:170:ARG:O	1:B:174:VAL:HG13	1.95	0.65
1:C:109:TYR:CZ	1:C:132:VAL:HG22	2.31	0.65
1:A:62:THR:O	1:A:64:LEU:N	2.30	0.65
1:A:200:ARG:CZ	1:B:122:LEU:CD1	2.75	0.65
1:B:207:GLU:O	1:B:207:GLU:CD	2.39	0.65
1:B:223:PHE:O	1:B:226:LEU:N	2.27	0.65
1:B:275:LYS:CG	1:B:278:LYS:NZ	2.59	0.65
1:C:205:ASP:CG	1:C:319:THR:HG21	2.22	0.65
1:A:102:GLN:NE2	1:A:102:GLN:O	2.30	0.65
1:B:314:ASP:O	1:B:317:VAL:HG12	1.96	0.65
1:A:157:MET:O	1:A:226:LEU:HG	1.96	0.65
1:C:167:GLU:O	1:C:169:ILE:N	2.30	0.65
1:A:157:MET:CB	1:A:226:LEU:CD1	2.73	0.65
1:C:98:ILE:HD13	1:C:121:PHE:HE1	1.62	0.65
1:B:191:TYR:CE1	1:B:195:LEU:CD1	2.79	0.64
1:A:203:GLY:HA3	1:A:230:TYR:CZ	2.31	0.64
1:A:62:THR:C	1:A:64:LEU:H	2.05	0.64
1:A:215:PHE:CB	1:A:234:GLU:N	2.60	0.64
1:A:215:PHE:HB2	1:A:234:GLU:N	2.13	0.64
1:A:234:GLU:C	1:A:235:ILE:HG12	2.22	0.64
1:A:293:TYR:CD1	1:A:304:VAL:HG21	2.33	0.64
1:C:217:VAL:O	1:C:267:PHE:HD1	1.79	0.64
1:A:94:THR:HG23	1:A:95:PRO:HD2	1.78	0.64
1:A:170:ARG:NH1	1:A:185:ASN:CG	2.54	0.64
1:A:216:LEU:HD22	1:A:318:ILE:HD13	1.79	0.64
1:B:191:TYR:O	1:B:194:GLN:N	2.30	0.64
1:C:118:PHE:O	1:C:121:PHE:HB3	1.97	0.64
1:C:168:ASN:HD22	1:C:171:GLN:HE22	1.45	0.64
1:B:244:GLN:HG2	1:B:245:GLN:N	2.13	0.64
1:C:114:LEU:HD12	1:C:153:PRO:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:TYR:OH	1:B:308:LEU:HD13	1.98	0.64
1:C:58:LEU:N	1:C:58:LEU:HD23	2.11	0.64
1:C:115:GLU:HB2	1:C:118:PHE:CB	2.27	0.64
1:A:131:VAL:HG22	1:A:132:VAL:O	1.97	0.64
1:B:126:LYS:HE3	1:C:84:ILE:HD12	1.78	0.64
1:A:170:ARG:O	1:A:173:PHE:N	2.27	0.64
1:C:57:VAL:HB	1:C:106:LEU:CG	2.27	0.64
1:C:109:TYR:CG	1:C:118:PHE:CE2	2.85	0.64
1:C:170:ARG:HG3	1:C:171:GLN:H	1.63	0.64
1:A:144:ASP:OD1	1:A:145:GLY:N	2.31	0.64
1:A:304:VAL:H	1:A:305:PRO:CD	2.11	0.64
1:C:220:GLU:O	1:C:222:ALA:N	2.31	0.64
1:B:114:LEU:O	1:B:116:ALA:N	2.31	0.63
1:B:210:PRO:O	1:B:212:ASN:N	2.31	0.63
1:B:220:GLU:HG3	1:B:241:ASN:OD1	1.98	0.63
1:B:270:SER:HG	1:B:293:TYR:HD1	1.45	0.63
1:A:94:THR:CB	1:A:95:PRO:CD	2.75	0.63
1:C:125:VAL:CB	1:C:128:VAL:HG11	2.27	0.63
1:C:238:TRP:HE3	1:C:250:GLN:NE2	1.96	0.63
1:A:152:ASN:OD1	1:A:153:PRO:HD2	1.97	0.63
1:A:255:ILE:HG23	1:A:256:GLU:N	2.13	0.63
1:B:223:PHE:HD1	1:B:226:LEU:HD22	1.63	0.63
1:A:269:GLU:OE1	1:A:269:GLU:CA	2.47	0.63
1:B:167:GLU:O	1:B:170:ARG:HG2	1.98	0.63
1:A:159:PRO:CG	1:A:202:LEU:CD2	2.74	0.63
1:C:125:VAL:HB	1:C:128:VAL:HG11	1.79	0.63
1:C:271:THR:CG2	1:C:272:VAL:N	2.61	0.63
1:A:56:LYS:HG3	1:A:104:ALA:HA	1.80	0.63
1:A:157:MET:HB3	1:A:226:LEU:CD1	2.21	0.63
1:A:190:VAL:HG21	1:B:139:PRO:HG3	1.81	0.63
1:C:61:PHE:CZ	1:C:64:LEU:HD11	2.31	0.63
1:C:138:GLU:HG3	1:C:139:PRO:HD2	1.81	0.63
1:A:283:ALA:O	1:A:284:THR:CG2	2.47	0.63
1:B:180:ASN:OD1	1:B:180:ASN:N	2.27	0.63
1:B:201:GLN:O	1:B:202:LEU:C	2.42	0.63
1:A:304:VAL:H	1:A:305:PRO:HD3	1.64	0.62
1:B:208:GLN:NE2	1:B:319:THR:O	2.32	0.62
1:A:303:PRO:O	1:A:304:VAL:CG2	2.48	0.62
1:B:191:TYR:CD1	1:B:195:LEU:CD1	2.82	0.62
1:B:260:THR:O	1:B:261:ASN:HB3	1.98	0.62
1:B:270:SER:OG	1:B:293:TYR:HD1	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:VAL:HG12	1:B:134:THR:H	1.63	0.62
1:B:203:GLY:HA2	1:B:206:LEU:CD1	2.17	0.62
1:A:255:ILE:CG2	1:A:256:GLU:N	2.63	0.62
1:B:124:ASN:OD1	1:B:124:ASN:N	2.30	0.62
1:B:58:LEU:HD23	1:B:81:ILE:CD1	2.30	0.62
1:B:110:ASN:CB	1:B:114:LEU:HD21	2.28	0.62
1:B:283:ALA:O	1:B:284:THR:OG1	2.14	0.62
1:B:199:ASP:O	1:B:202:LEU:N	2.33	0.62
1:A:209:VAL:HG12	1:A:322:LEU:HD22	0.70	0.62
1:B:257:GLU:C	1:B:257:GLU:OE1	2.42	0.62
1:C:105:ASP:C	1:C:106:LEU:HD13	2.25	0.62
1:A:164:VAL:HG12	1:A:165:TYR:N	2.14	0.62
1:A:176:LEU:HD13	1:A:177:ASP:OD1	1.99	0.62
1:B:258:VAL:HG21	1:B:284:THR:HG22	1.77	0.62
1:C:169:ILE:HG23	1:C:173:PHE:CE2	2.35	0.61
1:A:255:ILE:HD11	1:A:283:ALA:O	2.00	0.61
1:A:268:CYS:HB2	1:A:277:GLN:HG3	1.81	0.61
1:C:57:VAL:HA	1:C:106:LEU:CA	2.28	0.61
1:A:107:ILE:HB	1:A:130:SER:OG	2.01	0.61
1:B:62:THR:OG1	1:B:63:VAL:N	2.24	0.61
1:C:304:VAL:O	1:C:304:VAL:CG1	2.40	0.61
1:C:316:ARG:C	1:C:319:THR:HG23	2.25	0.61
1:C:133:LEU:O	1:C:134:THR:HG22	1.98	0.61
1:A:89:HIS:CE1	1:A:295:ASP:OD2	2.53	0.61
1:A:236:TYR:HE1	1:A:239:PRO:HG3	1.64	0.61
1:A:269:GLU:OE1	1:A:269:GLU:HA	1.99	0.61
1:C:60:THR:OG1	1:C:61:PHE:N	2.32	0.61
1:C:198:ILE:HD11	1:C:312:GLU:OE2	2.00	0.61
1:A:247:THR:CB	1:A:248:PRO:CD	2.46	0.61
1:A:165:TYR:CD1	1:A:165:TYR:N	2.68	0.60
1:C:70:ASN:C	1:C:70:ASN:OD1	2.43	0.60
1:C:119:GLU:HG2	1:C:120:GLN:N	2.16	0.60
1:C:168:ASN:HD22	1:C:171:GLN:NE2	1.98	0.60
1:B:190:VAL:O	1:B:193:GLU:HB3	2.01	0.60
1:C:63:VAL:O	1:C:64:LEU:C	2.43	0.60
1:A:62:THR:HA	1:A:65:ALA:CB	2.31	0.60
1:A:198:ILE:O	1:A:202:LEU:HG	2.01	0.60
1:A:252:GLN:O	1:A:255:ILE:CG2	2.33	0.60
1:A:295:ASP:O	1:A:296:SER:OG	2.16	0.60
1:B:119:GLU:HG3	1:B:120:GLN:N	2.16	0.60
1:C:109:TYR:CZ	1:C:132:VAL:CG1	2.78	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:THR:O	1:C:134:THR:OG1	2.17	0.60
1:C:178:PRO:C	1:C:180:ASN:H	2.09	0.60
1:C:217:VAL:HG21	1:C:266:ILE:HD12	1.73	0.60
1:B:220:GLU:HG3	1:B:241:ASN:CG	2.26	0.60
1:B:170:ARG:HG3	1:B:170:ARG:HH21	1.65	0.60
1:B:174:VAL:O	1:B:178:PRO:HB3	2.02	0.60
1:B:150:LYS:CB	1:B:151:PRO:HD2	2.11	0.60
1:B:182:LYS:HA	1:B:184:TYR:CG	2.37	0.60
1:C:149:ASP:OD1	1:C:150:LYS:N	2.32	0.60
1:C:265:THR:HB	1:C:267:PHE:CZ	2.36	0.60
1:A:105:ASP:C	1:A:105:ASP:OD1	2.44	0.60
1:B:110:ASN:ND2	1:B:114:LEU:HD21	2.17	0.60
1:B:126:LYS:CE	1:C:299:THR:HA	2.32	0.60
1:C:98:ILE:O	1:C:101:ALA:N	2.33	0.60
1:A:161:ASN:C	1:A:163:LEU:N	2.56	0.60
1:A:220:GLU:HG2	1:A:220:GLU:O	2.01	0.60
1:B:182:LYS:HB2	1:B:183:TYR:CE1	2.35	0.60
1:B:228:ARG:O	1:B:230:TYR:N	2.35	0.60
1:C:191:TYR:O	1:C:194:GLN:N	2.35	0.60
1:C:193:GLU:O	1:C:196:LYS:N	2.35	0.60
1:A:105:ASP:CG	1:A:105:ASP:O	2.45	0.60
1:A:246:PHE:N	1:A:250:GLN:HE21	2.00	0.60
1:B:110:ASN:HB3	1:B:114:LEU:HD11	1.83	0.60
1:A:199:ASP:HA	1:A:202:LEU:CD1	2.31	0.59
1:B:176:LEU:C	1:B:178:PRO:HD3	2.27	0.59
1:C:316:ARG:HA	1:C:319:THR:HG21	1.82	0.59
1:A:273:SER:O	1:A:277:GLN:OE1	2.20	0.59
1:B:95:PRO:CA	1:B:98:ILE:HD13	2.23	0.59
1:B:127:ASP:C	1:B:128:VAL:HG22	2.24	0.59
1:C:102:GLN:CG	1:C:125:VAL:HG13	2.31	0.59
1:C:269:GLU:OE1	1:C:271:THR:HG22	2.02	0.59
1:C:170:ARG:HG3	1:C:171:GLN:N	2.17	0.59
1:B:259:LYS:O	1:B:263:VAL:HG22	2.02	0.59
1:A:212:ASN:O	1:A:214:ARG:HG2	2.00	0.59
1:B:63:VAL:HG23	1:B:297:LEU:HD12	1.85	0.59
1:B:309:ASP:O	1:B:312:GLU:N	2.35	0.59
1:B:237:MET:HE2	1:B:256:GLU:OE1	2.03	0.59
1:C:61:PHE:CD2	1:C:63:VAL:HG22	2.35	0.59
1:C:195:LEU:CD1	1:C:308:LEU:CD2	2.80	0.59
1:C:313:TYR:O	1:C:315:ALA:N	2.29	0.59
1:A:216:LEU:HD13	1:A:223:PHE:CD2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ILE:O	1:A:258:VAL:HG12	2.01	0.59
1:B:62:THR:C	1:B:297:LEU:CD1	2.74	0.59
1:B:277:GLN:CG	1:B:288:PHE:HD2	2.13	0.59
1:C:60:THR:HG22	1:C:118:PHE:CZ	2.38	0.59
1:B:215:PHE:CZ	1:B:261:ASN:ND2	2.70	0.59
1:C:56:LYS:HG2	1:C:106:LEU:HB2	1.85	0.59
1:B:266:ILE:HG21	1:B:277:GLN:OE1	2.03	0.58
1:C:60:THR:OG1	1:C:61:PHE:HD1	1.84	0.58
1:A:244:GLN:C	1:A:244:GLN:OE1	2.45	0.58
1:A:250:GLN:O	1:A:251:VAL:C	2.45	0.58
1:B:63:VAL:N	1:B:297:LEU:HD11	2.14	0.58
1:C:109:TYR:CD1	1:C:109:TYR:O	2.56	0.58
1:C:115:GLU:CG	1:C:118:PHE:HB2	2.33	0.58
1:A:198:ILE:HG13	1:A:199:ASP:N	2.18	0.58
1:C:89:HIS:ND1	1:C:241:ASN:HB2	2.19	0.58
1:C:198:ILE:HD11	1:C:312:GLU:CD	2.28	0.58
1:B:278:LYS:HG2	1:B:279:GLN:N	2.18	0.58
1:C:268:CYS:O	1:C:292:LEU:N	2.29	0.58
1:A:109:TYR:O	1:A:133:LEU:CD1	2.51	0.58
1:A:214:ARG:HH22	1:A:231:GLY:H	1.52	0.58
1:A:268:CYS:SG	1:A:269:GLU:N	2.76	0.58
1:A:102:GLN:O	1:A:102:GLN:CG	2.51	0.58
1:A:225:TYR:O	1:A:226:LEU:C	2.45	0.58
1:A:114:LEU:HD13	1:A:115:GLU:HB3	1.85	0.58
1:A:191:TYR:O	1:A:194:GLN:N	2.36	0.58
1:A:217:VAL:C	1:A:266:ILE:HG23	2.20	0.58
1:B:110:ASN:OD1	1:B:165:TYR:OH	2.21	0.58
1:B:228:ARG:C	1:B:230:TYR:H	2.11	0.58
1:C:139:PRO:HB2	1:C:151:PRO:O	2.04	0.58
1:C:306:THR:HG23	1:C:307:PHE:N	2.17	0.58
1:A:106:LEU:HD12	1:A:129:PRO:O	2.03	0.58
1:A:213:GLN:OE1	1:A:213:GLN:CA	2.51	0.58
1:B:140:ILE:CG2	1:B:141:PRO:HD2	2.30	0.58
1:B:65:ALA:O	1:B:69:GLN:HG3	2.04	0.58
1:A:216:LEU:CD1	1:A:223:PHE:HD2	2.13	0.57
1:A:249:LYS:O	1:A:253:THR:OG1	2.22	0.57
1:B:97:ASP:O	1:B:121:PHE:CE2	2.57	0.57
1:A:60:THR:HG21	1:A:115:GLU:OE2	2.02	0.57
1:A:199:ASP:HA	1:A:202:LEU:CG	2.33	0.57
1:C:195:LEU:O	1:C:198:ILE:HG22	2.04	0.57
1:A:90:GLY:O	1:A:91:TYR:HB2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:VAL:CG2	1:A:264:PRO:CD	2.82	0.57
1:C:63:VAL:HG22	1:C:64:LEU:H	1.68	0.57
1:A:190:VAL:HG21	1:B:139:PRO:CG	2.34	0.57
1:C:61:PHE:HA	1:C:82:THR:HG23	1.87	0.57
1:C:261:ASN:CG	1:C:261:ASN:O	2.47	0.57
1:B:104:ALA:C	1:B:105:ASP:OD1	2.48	0.57
1:B:218:SER:OG	1:B:219:CYS:N	2.34	0.57
1:B:269:GLU:HG2	1:B:292:LEU:HD11	1.87	0.57
1:B:300:GLU:O	1:B:301:GLU:OE1	2.23	0.57
1:B:318:ILE:O	1:B:321:GLY:N	2.37	0.57
1:A:304:VAL:N	1:A:305:PRO:CD	2.67	0.57
1:A:157:MET:HE1	1:A:310:LEU:HD21	1.87	0.57
1:B:210:PRO:C	1:B:212:ASN:H	2.12	0.57
1:A:293:TYR:O	1:A:294:VAL:HG22	2.05	0.57
1:B:61:PHE:HE2	1:B:63:VAL:HB	1.69	0.57
1:B:275:LYS:HD3	1:B:275:LYS:N	2.16	0.56
1:B:292:LEU:C	1:B:292:LEU:CD1	2.78	0.56
1:B:303:PRO:HG2	1:B:304:VAL:HG12	1.86	0.56
1:A:137:ILE:HG13	1:A:138:GLU:N	2.18	0.56
1:B:94:THR:O	1:B:98:ILE:HG23	2.04	0.56
1:C:157:MET:SD	1:C:225:TYR:N	2.78	0.56
1:A:244:GLN:OE1	1:A:244:GLN:N	2.38	0.56
1:C:109:TYR:CZ	1:C:132:VAL:CG2	2.89	0.56
1:C:240:ILE:H	1:C:240:ILE:CD1	2.19	0.56
1:C:61:PHE:CE2	1:C:63:VAL:CG2	2.60	0.56
1:A:94:THR:O	1:A:95:PRO:C	2.49	0.56
1:A:116:ALA:HA	1:A:119:GLU:HG3	1.87	0.56
1:A:137:ILE:HG13	1:A:138:GLU:H	1.69	0.56
1:A:176:LEU:CD1	1:A:176:LEU:C	2.77	0.56
1:A:225:TYR:O	1:A:228:ARG:N	2.37	0.56
1:B:61:PHE:CE2	1:B:63:VAL:HB	2.41	0.56
1:B:277:GLN:CD	1:B:277:GLN:C	2.73	0.56
1:A:116:ALA:CB	1:A:119:GLU:CD	2.78	0.56
1:B:63:VAL:HA	1:B:297:LEU:CD1	2.15	0.56
1:B:190:VAL:O	1:B:191:TYR:C	2.47	0.56
1:C:125:VAL:CG1	1:C:128:VAL:CG1	2.80	0.56
1:C:316:ARG:O	1:C:319:THR:HG23	2.05	0.56
1:A:191:TYR:CE1	1:A:308:LEU:HD11	2.40	0.56
1:B:75:LYS:O	1:B:76:LEU:HD23	2.05	0.56
1:C:109:TYR:HB3	1:C:118:PHE:CZ	2.39	0.56
1:C:190:VAL:O	1:C:191:TYR:C	2.46	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316:ARG:NH1	1:C:317:VAL:HA	2.21	0.56
1:A:113:ASN:HD22	1:A:150:LYS:CE	2.15	0.56
1:B:57:VAL:HG12	1:B:106:LEU:HB2	1.87	0.56
1:C:238:TRP:CE3	1:C:250:GLN:NE2	2.74	0.56
1:A:59:THR:HG21	1:A:61:PHE:O	2.06	0.56
1:A:190:VAL:O	1:A:191:TYR:C	2.48	0.56
1:A:255:ILE:HG13	1:A:284:THR:CG2	2.36	0.56
1:B:299:THR:OG1	1:B:300:GLU:N	2.38	0.56
1:C:157:MET:CE	1:C:225:TYR:N	2.67	0.56
1:C:169:ILE:HG22	1:C:173:PHE:HD2	1.69	0.56
1:C:308:LEU:HA	1:C:311:LEU:CD1	2.32	0.56
1:B:195:LEU:HA	1:B:198:ILE:HG22	1.86	0.56
1:C:220:GLU:CG	1:C:241:ASN:ND2	2.35	0.56
1:A:212:ASN:O	1:A:213:GLN:C	2.48	0.55
1:A:241:ASN:O	1:A:242:ALA:HB2	2.06	0.55
1:C:57:VAL:CG1	1:C:106:LEU:HG	2.36	0.55
1:A:163:LEU:O	1:A:164:VAL:C	2.49	0.55
1:A:251:VAL:O	1:A:254:VAL:N	2.35	0.55
1:B:130:SER:O	1:B:131:VAL:HG23	2.06	0.55
1:C:128:VAL:HG23	1:C:128:VAL:O	2.04	0.55
1:C:247:THR:O	1:C:250:GLN:HG2	2.06	0.55
1:C:255:ILE:HD12	1:C:255:ILE:H	1.70	0.55
1:C:314:ASP:O	1:C:317:VAL:HG22	2.06	0.55
1:A:303:PRO:C	1:A:304:VAL:HG23	2.31	0.55
1:B:62:THR:CB	1:B:297:LEU:CD1	2.70	0.55
1:C:63:VAL:HG23	1:C:64:LEU:N	2.19	0.55
1:C:65:ALA:O	1:C:66:ASP:C	2.42	0.55
1:C:165:TYR:O	1:C:169:ILE:HG13	2.06	0.55
1:A:199:ASP:CA	1:A:202:LEU:HD11	2.36	0.55
1:B:170:ARG:HH21	1:B:170:ARG:CG	2.19	0.55
1:C:109:TYR:CD1	1:C:132:VAL:HG13	2.24	0.55
1:C:118:PHE:O	1:C:121:PHE:N	2.24	0.55
1:C:125:VAL:HG12	1:C:128:VAL:CG1	2.36	0.55
1:C:220:GLU:OE1	1:C:222:ALA:CB	2.49	0.55
1:C:151:PRO:O	1:C:152:ASN:O	2.25	0.55
1:B:210:PRO:O	1:B:213:GLN:N	2.31	0.55
1:C:61:PHE:HZ	1:C:64:LEU:CD1	2.10	0.55
1:A:244:GLN:NE2	1:A:245:GLN:C	2.65	0.55
1:B:114:LEU:HD12	1:B:115:GLU:N	2.22	0.55
1:C:108:LEU:HA	1:C:131:VAL:HG13	1.86	0.55
1:C:261:ASN:HA	1:C:262:ASN:CB	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:LYS:HE2	1:C:299:THR:CA	2.37	0.55
1:A:62:THR:C	1:A:65:ALA:H	2.14	0.54
1:B:83:ARG:HH22	1:B:84:ILE:CG1	2.17	0.54
1:C:171:GLN:O	1:C:174:VAL:HG22	2.07	0.54
1:A:203:GLY:N	1:A:230:TYR:HE2	2.05	0.54
1:A:270:SER:OG	1:A:271:THR:N	2.37	0.54
1:B:61:PHE:CZ	1:B:64:LEU:HD13	2.42	0.54
1:B:259:LYS:CB	1:B:260:THR:HA	2.36	0.54
1:C:56:LYS:HA	1:C:77:VAL:O	2.07	0.54
1:C:261:ASN:HA	1:C:262:ASN:HB3	1.88	0.54
1:A:217:VAL:CG1	1:A:266:ILE:HG12	2.36	0.54
1:B:67:MET:HE1	1:B:165:TYR:CB	2.38	0.54
1:C:307:PHE:CE2	1:C:311:LEU:HD11	2.41	0.54
1:A:199:ASP:HA	1:A:202:LEU:HD21	1.90	0.54
1:A:307:PHE:CZ	1:A:311:LEU:HD11	2.43	0.54
1:C:58:LEU:N	1:C:106:LEU:O	2.41	0.54
1:B:266:ILE:C	1:B:267:PHE:CG	2.85	0.54
1:A:133:LEU:HD23	1:A:169:ILE:HG12	1.90	0.54
1:A:137:ILE:CG1	1:A:138:GLU:H	2.21	0.54
1:A:161:ASN:O	1:A:164:VAL:N	2.39	0.54
1:A:274:ASP:CA	1:A:277:GLN:HE22	2.20	0.54
1:C:56:LYS:HZ2	1:C:58:LEU:CG	2.13	0.54
1:C:198:ILE:O	1:C:201:GLN:N	2.41	0.54
1:A:263:VAL:CB	1:A:264:PRO:CA	2.55	0.54
1:B:79:GLU:CD	1:B:80:SER:O	2.51	0.54
1:B:107:ILE:HG23	1:B:130:SER:HA	1.90	0.54
1:B:183:TYR:HB3	1:B:186:ALA:H	1.72	0.54
1:B:213:GLN:OE1	1:B:262:ASN:ND2	2.32	0.54
1:A:63:VAL:HG21	1:A:294:VAL:O	2.07	0.54
1:C:307:PHE:O	1:C:310:LEU:HB3	2.08	0.54
1:A:277:GLN:O	1:A:278:LYS:C	2.50	0.54
1:A:293:TYR:C	1:A:294:VAL:CG2	2.81	0.54
1:B:109:TYR:CD2	1:B:118:PHE:CE2	2.96	0.54
1:B:292:LEU:HD12	1:B:292:LEU:O	2.07	0.54
1:C:167:GLU:C	1:C:169:ILE:N	2.66	0.53
1:B:92:GLU:CD	1:B:92:GLU:N	2.66	0.53
1:C:64:LEU:O	1:C:67:MET:HG2	2.08	0.53
1:A:144:ASP:CG	1:A:145:GLY:N	2.66	0.53
1:A:167:GLU:O	1:A:171:GLN:HG2	2.09	0.53
1:B:191:TYR:CD1	1:B:195:LEU:HD13	2.43	0.53
1:B:304:VAL:O	1:B:304:VAL:HG22	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:TYR:O	1:A:187:ASN:N	2.41	0.53
1:C:63:VAL:HG22	1:C:64:LEU:N	2.20	0.53
1:A:55:LYS:O	1:A:76:LEU:HD22	2.09	0.53
1:B:199:ASP:O	1:B:200:ARG:C	2.50	0.53
1:B:210:PRO:C	1:B:212:ASN:N	2.66	0.53
1:A:94:THR:HG23	1:A:96:SER:H	1.72	0.53
1:A:283:ALA:C	1:A:284:THR:HG23	2.34	0.53
1:A:157:MET:HB2	1:A:226:LEU:CD1	2.38	0.53
1:A:237:MET:O	1:A:250:GLN:CD	2.52	0.53
1:B:182:LYS:CA	1:B:184:TYR:HB2	2.37	0.53
1:B:277:GLN:NE2	1:B:288:PHE:HD2	2.07	0.53
1:A:206:LEU:O	1:A:209:VAL:HG21	2.07	0.52
1:A:144:ASP:CG	1:A:145:GLY:H	2.17	0.52
1:A:212:ASN:O	1:A:214:ARG:N	2.42	0.52
1:B:269:GLU:CG	1:B:292:LEU:HD11	2.39	0.52
1:C:274:ASP:OD1	1:C:278:LYS:HG3	2.09	0.52
1:A:60:THR:CB	1:A:115:GLU:CD	2.82	0.52
1:A:246:PHE:H	1:A:250:GLN:NE2	2.07	0.52
1:A:277:GLN:N	1:A:277:GLN:CD	2.67	0.52
1:B:109:TYR:CE2	1:B:118:PHE:CE2	2.97	0.52
1:C:271:THR:HG23	1:C:272:VAL:HG13	1.90	0.52
1:A:60:THR:OG1	1:A:115:GLU:CD	2.53	0.52
1:A:234:GLU:C	1:A:235:ILE:CG1	2.82	0.52
1:A:255:ILE:HD11	1:A:284:THR:CG2	2.37	0.52
1:B:66:ASP:CG	1:B:307:PHE:H	2.18	0.52
1:C:125:VAL:HG11	1:C:128:VAL:HG11	1.87	0.52
1:A:198:ILE:HD12	1:A:202:LEU:HD23	1.91	0.52
1:A:234:GLU:O	1:A:235:ILE:CG1	2.58	0.52
1:A:252:GLN:HA	1:A:255:ILE:CG2	2.40	0.52
1:B:126:LYS:CE	1:C:299:THR:HG22	2.39	0.52
1:B:275:LYS:CA	1:B:278:LYS:HZ2	2.18	0.52
1:A:170:ARG:NH1	1:A:185:ASN:OD1	2.42	0.52
1:B:63:VAL:N	1:B:297:LEU:HD13	2.22	0.52
1:B:89:HIS:NE2	1:B:295:ASP:OD1	2.37	0.52
1:B:104:ALA:O	1:B:105:ASP:OD1	2.27	0.52
1:B:217:VAL:HG22	1:B:217:VAL:O	2.09	0.52
1:B:169:ILE:CG2	1:B:173:PHE:CE2	2.92	0.52
1:B:181:ALA:O	1:B:184:TYR:HE2	1.87	0.52
1:B:258:VAL:CB	1:B:284:THR:HG21	2.40	0.52
1:B:277:GLN:C	1:B:277:GLN:NE2	2.67	0.52
1:C:119:GLU:OE1	1:C:119:GLU:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:ILE:O	1:C:170:ARG:C	2.54	0.51
1:B:263:VAL:HG23	1:B:263:VAL:O	2.10	0.51
1:A:61:PHE:CZ	1:A:63:VAL:HB	2.45	0.51
1:A:156:TRP:CD1	1:A:157:MET:SD	3.03	0.51
1:A:176:LEU:HD12	1:A:177:ASP:OD1	2.07	0.51
1:B:161:ASN:H	1:B:161:ASN:ND2	2.08	0.51
1:C:172:ALA:O	1:C:175:GLU:HG2	2.10	0.51
1:B:62:THR:O	1:B:65:ALA:HB3	2.11	0.51
1:B:119:GLU:HG2	1:B:120:GLN:N	2.17	0.51
1:B:173:PHE:O	1:B:175:GLU:N	2.44	0.51
1:B:228:ARG:C	1:B:230:TYR:N	2.68	0.51
1:C:57:VAL:CB	1:C:106:LEU:CB	2.78	0.51
1:C:57:VAL:HG12	1:C:106:LEU:HG	1.92	0.51
1:C:178:PRO:O	1:C:180:ASN:N	2.44	0.51
1:A:164:VAL:CG1	1:A:165:TYR:N	2.72	0.51
1:A:191:TYR:O	1:A:192:SER:C	2.51	0.51
1:B:180:ASN:N	1:B:181:ALA:HA	2.26	0.51
1:B:195:LEU:C	1:B:198:ILE:HG22	2.36	0.51
1:C:238:TRP:HZ2	1:C:272:VAL:HG11	1.75	0.51
1:C:109:TYR:CD1	1:C:115:GLU:OE2	2.63	0.51
1:C:298:SER:HB3	1:C:304:VAL:HG12	1.93	0.51
1:B:236:TYR:CE2	1:B:239:PRO:HD3	2.39	0.51
1:B:237:MET:HB3	1:B:238:TRP:CD1	2.45	0.51
1:C:81:ILE:HG22	1:C:82:THR:N	2.23	0.51
1:A:102:GLN:HE22	1:A:125:VAL:CG1	2.06	0.51
1:A:133:LEU:HD23	1:A:169:ILE:CG1	2.41	0.51
1:A:217:VAL:O	1:A:217:VAL:CG2	2.58	0.51
1:A:252:GLN:CA	1:A:255:ILE:HG22	2.41	0.51
1:B:110:ASN:O	1:B:134:THR:OG1	2.23	0.51
1:C:60:THR:O	1:C:82:THR:HG23	2.11	0.51
1:C:109:TYR:HB2	1:C:118:PHE:CE2	2.42	0.51
1:A:248:PRO:O	1:A:250:GLN:N	2.44	0.51
1:A:137:ILE:CG1	1:A:138:GLU:N	2.74	0.50
1:B:112:MET:O	1:B:153:PRO:HB3	2.12	0.50
1:C:187:ASN:N	1:C:187:ASN:OD1	2.36	0.50
1:A:167:GLU:OE2	1:A:171:GLN:OE1	2.30	0.50
1:B:66:ASP:OD1	1:B:307:PHE:CB	2.59	0.50
1:B:203:GLY:O	1:B:206:LEU:HD12	2.11	0.50
1:B:277:GLN:HE22	1:B:281:ALA:HB2	1.76	0.50
1:C:115:GLU:O	1:C:118:PHE:N	2.28	0.50
1:A:271:THR:HG23	1:A:272:VAL:CA	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:GLN:NE2	1:B:277:GLN:O	2.44	0.50
1:B:79:GLU:OE2	1:B:80:SER:O	2.30	0.50
1:A:105:ASP:OD1	1:A:105:ASP:O	2.30	0.50
1:A:247:THR:O	1:A:249:LYS:N	2.45	0.50
1:B:214:ARG:HB3	1:B:232:MET:HA	1.94	0.50
1:C:57:VAL:HB	1:C:106:LEU:CB	2.40	0.50
1:C:98:ILE:O	1:C:99:VAL:C	2.55	0.50
1:B:259:LYS:CD	1:B:260:THR:HG21	2.30	0.50
1:B:269:GLU:CD	1:B:292:LEU:HD11	2.37	0.50
1:C:135:GLU:CD	1:C:135:GLU:C	2.79	0.50
1:A:82:THR:C	1:A:83:ARG:HD2	2.37	0.50
1:A:133:LEU:CD2	1:A:169:ILE:HG12	2.42	0.50
1:A:187:ASN:N	1:A:187:ASN:OD1	2.37	0.50
1:A:202:LEU:HD12	1:A:230:TYR:OH	2.12	0.50
1:B:268:CYS:O	1:B:269:GLU:HG2	2.12	0.50
1:B:277:GLN:NE2	1:B:281:ALA:HB2	2.26	0.50
1:B:322:LEU:O	1:B:323:LEU:HD12	2.12	0.50
1:C:107:ILE:O	1:C:130:SER:HB2	2.12	0.50
1:C:170:ARG:O	1:C:173:PHE:HB2	2.12	0.50
1:B:176:LEU:O	1:B:178:PRO:CD	2.60	0.49
1:C:269:GLU:OE1	1:C:272:VAL:HG22	2.11	0.49
1:C:310:LEU:O	1:C:313:TYR:O	2.30	0.49
1:A:94:THR:HG23	1:A:95:PRO:CD	2.41	0.49
1:A:161:ASN:C	1:A:163:LEU:H	2.20	0.49
1:A:229:ASP:OD1	1:A:230:TYR:CE1	2.64	0.49
1:A:266:ILE:CG2	1:A:267:PHE:N	2.40	0.49
1:B:198:ILE:HD11	1:B:312:GLU:HG3	1.93	0.49
1:A:258:VAL:O	1:A:262:ASN:C	2.54	0.49
1:B:68:VAL:HG11	1:B:108:LEU:HD12	1.93	0.49
1:B:183:TYR:HA	1:B:184:TYR:HB2	0.73	0.49
1:A:316:ARG:O	1:A:320:ASN:N	2.37	0.49
1:B:237:MET:HE2	1:B:256:GLU:HG3	1.94	0.49
1:A:89:HIS:CD2	1:A:114:LEU:CD2	2.94	0.49
1:A:176:LEU:O	1:A:177:ASP:OD1	2.30	0.49
1:B:79:GLU:OE1	1:B:80:SER:O	2.30	0.49
1:B:130:SER:O	1:B:131:VAL:CG2	2.61	0.49
1:C:157:MET:HE2	1:C:225:TYR:HD1	1.51	0.49
1:C:178:PRO:C	1:C:180:ASN:N	2.68	0.49
1:B:118:PHE:CE2	1:B:122:LEU:HD22	2.46	0.49
1:C:195:LEU:HD12	1:C:308:LEU:CD2	2.43	0.49
1:A:165:TYR:HD1	1:A:165:TYR:N	2.04	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:PRO:O	1:A:249:LYS:C	2.56	0.49
1:A:304:VAL:N	1:A:305:PRO:HD3	2.27	0.49
1:B:201:GLN:O	1:B:204:ALA:N	2.44	0.49
1:B:127:ASP:C	1:B:128:VAL:HG23	2.37	0.49
1:B:223:PHE:CD1	1:B:226:LEU:HD22	2.46	0.49
1:A:106:LEU:HD23	1:A:108:LEU:HD11	1.95	0.49
1:A:245:GLN:O	1:A:246:PHE:C	2.55	0.49
1:B:66:ASP:OD1	1:B:307:PHE:HB3	2.13	0.49
1:B:68:VAL:HG11	1:B:108:LEU:CD1	2.42	0.49
1:B:115:GLU:O	1:B:115:GLU:CG	2.58	0.49
1:B:299:THR:O	1:B:305:PRO:HB3	2.13	0.49
1:C:122:LEU:HD21	1:C:128:VAL:HG21	1.85	0.49
1:C:316:ARG:NH1	1:C:320:ASN:HD21	2.10	0.49
1:B:67:MET:HE1	1:B:165:TYR:HB3	1.95	0.48
1:B:84:ILE:HD13	1:B:84:ILE:N	2.28	0.48
1:B:94:THR:HB	1:B:95:PRO:CD	2.38	0.48
1:B:154:HIS:CD2	1:B:222:ALA:CB	2.96	0.48
1:B:199:ASP:O	1:B:201:GLN:N	2.46	0.48
1:C:193:GLU:O	1:C:194:GLN:C	2.56	0.48
1:A:91:TYR:CA	1:A:93:PRO:HD3	2.40	0.48
1:A:215:PHE:HB3	1:A:234:GLU:N	2.27	0.48
1:A:237:MET:HE1	1:A:276:GLY:CA	2.42	0.48
1:B:61:PHE:HA	1:B:80:SER:OG	2.13	0.48
1:B:65:ALA:O	1:B:69:GLN:CG	2.61	0.48
1:B:206:LEU:HA	1:B:319:THR:HG22	1.94	0.48
1:A:177:ASP:O	1:A:177:ASP:OD2	2.30	0.48
1:A:245:GLN:O	1:A:245:GLN:HG3	2.13	0.48
1:A:277:GLN:CD	1:A:278:LYS:N	2.71	0.48
1:A:310:LEU:HD23	1:A:311:LEU:N	2.28	0.48
1:B:155:ALA:HA	1:B:225:TYR:CD1	2.49	0.48
1:B:213:GLN:NE2	1:B:262:ASN:HD22	2.10	0.48
1:A:60:THR:CG2	1:A:61:PHE:CD1	2.96	0.48
1:A:132:VAL:C	1:A:133:LEU:HD12	2.39	0.48
1:B:171:GLN:O	1:B:174:VAL:N	2.46	0.48
1:B:176:LEU:O	1:B:178:PRO:HD2	2.14	0.48
1:C:75:LYS:HE3	1:C:183:TYR:CD2	2.48	0.48
1:A:165:TYR:O	1:A:168:ASN:N	2.46	0.48
1:B:97:ASP:O	1:B:121:PHE:HE2	1.97	0.48
1:B:142:ILE:CG2	1:B:152:ASN:HB2	2.43	0.48
1:C:191:TYR:CZ	1:C:308:LEU:HD11	2.48	0.48
1:A:137:ILE:O	1:A:138:GLU:CG	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:ILE:C	1:A:267:PHE:CG	2.92	0.48
1:B:270:SER:OG	1:B:293:TYR:CD1	2.62	0.48
1:C:115:GLU:C	1:C:117:TRP:N	2.69	0.48
1:C:135:GLU:OE1	1:C:135:GLU:C	2.56	0.48
1:B:183:TYR:CA	1:B:184:TYR:CB	2.49	0.48
1:C:248:PRO:O	1:C:249:LYS:C	2.56	0.48
1:A:106:LEU:CD2	1:A:108:LEU:HD11	2.43	0.48
1:A:299:THR:OG1	1:A:300:GLU:N	2.45	0.48
1:B:110:ASN:HB3	1:B:114:LEU:HD21	1.96	0.48
1:C:122:LEU:HD21	1:C:128:VAL:O	2.14	0.48
1:C:226:LEU:HD12	1:C:226:LEU:HA	1.52	0.48
1:A:159:PRO:CG	1:A:202:LEU:HD22	2.36	0.48
1:C:66:ASP:CG	1:C:67:MET:N	2.72	0.48
1:C:160:ARG:NH1	1:C:199:ASP:OD2	2.47	0.48
1:C:269:GLU:OE1	1:C:271:THR:CG2	2.62	0.48
1:B:89:HIS:HE2	1:B:295:ASP:CG	2.20	0.48
1:B:318:ILE:CG2	1:B:322:LEU:HD11	2.44	0.48
1:C:107:ILE:CD1	1:C:128:VAL:CB	2.92	0.48
1:C:167:GLU:O	1:C:168:ASN:C	2.54	0.48
1:C:57:VAL:CB	1:C:106:LEU:CG	2.90	0.47
1:A:94:THR:O	1:A:96:SER:N	2.47	0.47
1:B:97:ASP:O	1:B:121:PHE:CZ	2.68	0.47
1:C:115:GLU:HG3	1:C:118:PHE:CG	2.49	0.47
1:C:306:THR:HG23	1:C:308:LEU:H	1.78	0.47
1:A:288:PHE:O	1:A:288:PHE:CD2	2.67	0.47
1:B:91:TYR:CG	1:B:92:GLU:N	2.83	0.47
1:B:94:THR:CB	1:B:95:PRO:HD2	2.34	0.47
1:C:91:TYR:HB3	1:C:117:TRP:CD1	2.49	0.47
1:A:95:PRO:O	1:A:96:SER:C	2.57	0.47
1:A:137:ILE:O	1:A:138:GLU:HG2	2.14	0.47
1:B:84:ILE:CG2	1:B:85:GLY:H	2.17	0.47
1:B:113:ASN:O	1:B:114:LEU:C	2.50	0.47
1:B:259:LYS:CE	1:B:260:THR:HG23	2.17	0.47
1:C:61:PHE:HZ	1:C:64:LEU:HD11	1.73	0.47
1:C:118:PHE:O	1:C:119:GLU:C	2.56	0.47
1:B:161:ASN:ND2	1:B:161:ASN:N	2.62	0.47
1:B:176:LEU:HD12	1:B:176:LEU:HA	1.64	0.47
1:B:199:ASP:C	1:B:201:GLN:N	2.73	0.47
1:B:208:GLN:NE2	1:B:319:THR:C	2.72	0.47
1:B:216:LEU:HD12	1:B:216:LEU:C	2.40	0.47
1:A:62:THR:O	1:A:63:VAL:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:MET:HE1	1:B:310:LEU:CD2	2.44	0.47
1:B:277:GLN:CD	1:B:288:PHE:HD2	2.22	0.47
1:C:109:TYR:CE2	1:C:132:VAL:HG22	2.49	0.47
1:C:149:ASP:CG	1:C:150:LYS:H	2.22	0.47
1:A:63:VAL:CG2	1:A:294:VAL:O	2.62	0.47
1:A:164:VAL:HG12	1:A:165:TYR:HD1	1.79	0.47
1:A:274:ASP:O	1:A:275:LYS:C	2.55	0.47
1:C:115:GLU:O	1:C:117:TRP:N	2.48	0.47
1:C:198:ILE:O	1:C:199:ASP:C	2.58	0.47
1:A:59:THR:HG22	1:A:80:SER:CA	2.30	0.47
1:A:64:LEU:HD11	1:A:133:LEU:CD2	2.41	0.47
1:B:70:ASN:N	1:B:70:ASN:HD22	2.13	0.47
1:B:75:LYS:NZ	1:B:183:TYR:O	2.48	0.47
1:C:106:LEU:CG	1:C:176:LEU:HD21	2.45	0.47
1:C:109:TYR:CE1	1:C:111:GLY:CA	2.98	0.47
1:A:107:ILE:O	1:A:130:SER:HB3	2.15	0.47
1:A:220:GLU:O	1:A:222:ALA:N	2.48	0.47
1:C:64:LEU:O	1:C:65:ALA:C	2.57	0.47
1:C:72:ALA:HB1	1:C:76:LEU:HG	1.96	0.47
1:C:137:ILE:HD12	1:C:161:ASN:HB3	1.97	0.47
1:B:109:TYR:N	1:B:109:TYR:CD1	2.83	0.46
1:B:223:PHE:HE2	1:B:292:LEU:HD21	1.75	0.46
1:C:75:LYS:HA	1:C:75:LYS:HD3	1.30	0.46
1:C:98:ILE:O	1:C:100:LYS:N	2.48	0.46
1:A:133:LEU:O	1:A:135:GLU:N	2.48	0.46
1:B:209:VAL:HG23	1:B:214:ARG:CG	2.42	0.46
1:C:56:LYS:HD3	1:C:104:ALA:CB	2.43	0.46
1:C:58:LEU:N	1:C:58:LEU:CD2	2.78	0.46
1:C:107:ILE:HG21	1:C:122:LEU:HD11	1.97	0.46
1:A:199:ASP:OD1	1:A:200:ARG:N	2.48	0.46
1:B:169:ILE:HG22	1:B:173:PHE:CE2	2.50	0.46
1:C:109:TYR:CD2	1:C:118:PHE:HD2	2.32	0.46
1:C:313:TYR:C	1:C:315:ALA:N	2.72	0.46
1:A:60:THR:HG23	1:A:61:PHE:CD1	2.50	0.46
1:B:292:LEU:HD13	1:B:294:VAL:HG12	1.98	0.46
1:C:91:TYR:HE1	1:C:93:PRO:HA	1.80	0.46
1:C:115:GLU:HG3	1:C:118:PHE:CB	2.45	0.46
1:C:154:HIS:O	1:C:157:MET:HG2	2.16	0.46
1:A:200:ARG:NH2	1:B:122:LEU:HD13	2.31	0.46
1:B:315:ALA:O	1:B:319:THR:HG23	2.15	0.46
1:C:109:TYR:CD1	1:C:111:GLY:N	2.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:TYR:HD1	1:C:111:GLY:N	2.13	0.46
1:C:139:PRO:HG2	1:C:151:PRO:HB2	1.97	0.46
1:B:92:GLU:HA	1:B:93:PRO:HD3	1.62	0.46
1:C:91:TYR:CD1	1:C:92:GLU:N	2.83	0.46
1:C:197:ALA:HA	1:C:200:ARG:HE	1.79	0.46
1:A:97:ASP:OD1	1:A:102:GLN:N	2.48	0.46
1:A:112:MET:SD	1:A:153:PRO:HA	2.56	0.46
1:B:171:GLN:C	1:B:173:PHE:N	2.71	0.46
1:C:105:ASP:O	1:C:106:LEU:HB2	2.14	0.46
1:C:154:HIS:O	1:C:225:TYR:CD1	2.69	0.46
1:B:95:PRO:O	1:B:98:ILE:HG12	2.16	0.46
1:B:259:LYS:NZ	1:B:260:THR:HG21	2.29	0.46
1:A:61:PHE:CG	1:A:62:THR:N	2.84	0.46
1:A:213:GLN:OE1	1:A:215:PHE:HE1	1.97	0.46
1:B:154:HIS:HA	1:B:156:TRP:CZ3	2.50	0.46
1:B:158:SER:HB3	1:B:161:ASN:ND2	2.30	0.46
1:B:318:ILE:O	1:B:319:THR:C	2.59	0.46
1:C:60:THR:CG2	1:C:118:PHE:CZ	2.98	0.46
1:A:170:ARG:O	1:A:171:GLN:C	2.59	0.46
1:A:209:VAL:HG11	1:A:322:LEU:HD13	1.97	0.46
1:A:213:GLN:OE1	1:A:215:PHE:CE1	2.69	0.46
1:C:82:THR:HG21	1:C:88:ILE:HD12	1.98	0.46
1:C:87:GLU:HG3	1:C:271:THR:OG1	2.15	0.46
1:C:237:MET:HG3	1:C:250:GLN:HG3	1.97	0.46
1:A:297:LEU:HD12	1:A:297:LEU:HA	1.55	0.45
1:A:105:ASP:O	1:A:106:LEU:HB2	2.16	0.45
1:A:244:GLN:OE1	1:A:244:GLN:CA	2.64	0.45
1:C:94:THR:O	1:C:97:ASP:OD1	2.33	0.45
1:C:97:ASP:HA	1:C:100:LYS:HE2	1.97	0.45
1:C:108:LEU:N	1:C:108:LEU:HD12	2.30	0.45
1:C:255:ILE:H	1:C:255:ILE:CD1	2.24	0.45
1:A:137:ILE:O	1:A:138:GLU:CD	2.58	0.45
1:A:317:VAL:HA	1:A:320:ASN:HB3	1.97	0.45
1:B:169:ILE:CG2	1:B:173:PHE:HE2	2.28	0.45
1:B:220:GLU:CG	1:B:241:ASN:OD1	2.64	0.45
1:C:60:THR:CG2	1:C:118:PHE:CE1	2.91	0.45
1:A:200:ARG:NE	1:B:122:LEU:CD1	2.79	0.45
1:C:75:LYS:HE3	1:C:183:TYR:CE2	2.52	0.45
1:A:58:LEU:HA	1:A:58:LEU:HD12	1.63	0.45
1:A:217:VAL:O	1:A:267:PHE:HB2	2.15	0.45
1:B:83:ARG:HH22	1:B:84:ILE:HD11	1.76	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:LYS:C	1:B:278:LYS:HD2	2.36	0.45
1:B:277:GLN:HG2	1:B:288:PHE:CD2	2.32	0.45
1:C:107:ILE:O	1:C:130:SER:HA	2.16	0.45
1:A:193:GLU:O	1:A:194:GLN:C	2.59	0.45
1:A:217:VAL:O	1:A:266:ILE:CG2	2.65	0.45
1:A:292:LEU:HD23	1:A:292:LEU:HA	1.63	0.45
1:B:121:PHE:C	1:B:123:GLY:HA3	2.41	0.45
1:B:196:LYS:C	1:B:198:ILE:H	2.24	0.45
1:C:119:GLU:HG2	1:C:120:GLN:H	1.81	0.45
1:C:306:THR:CG2	1:C:307:PHE:N	2.77	0.45
1:A:118:PHE:CD1	1:A:119:GLU:N	2.85	0.45
1:A:271:THR:HA	1:A:272:VAL:HA	1.84	0.45
1:B:277:GLN:CD	1:B:288:PHE:CD2	2.94	0.45
1:C:110:ASN:O	1:C:134:THR:CG2	2.65	0.45
1:C:182:LYS:O	1:C:183:TYR:C	2.59	0.45
1:C:306:THR:CG2	1:C:308:LEU:H	2.30	0.45
1:A:112:MET:HE2	1:A:139:PRO:HB3	1.99	0.45
1:A:191:TYR:O	1:A:193:GLU:N	2.50	0.45
1:B:88:ILE:O	1:B:91:TYR:N	2.45	0.45
1:B:138:GLU:HA	1:B:139:PRO:HD3	1.76	0.45
1:B:236:TYR:HE2	1:B:239:PRO:CD	2.23	0.45
1:C:70:ASN:CG	1:C:191:TYR:CE1	2.94	0.45
1:C:157:MET:SD	1:C:225:TYR:CA	3.04	0.45
1:C:237:MET:CG	1:C:250:GLN:HG3	2.47	0.45
1:C:297:LEU:HA	1:C:297:LEU:HD12	1.78	0.45
1:A:56:LYS:H	1:A:56:LYS:HG2	1.21	0.45
1:A:110:ASN:N	1:A:115:GLU:OE2	2.34	0.45
1:A:163:LEU:HD12	1:A:163:LEU:HA	1.81	0.45
1:B:67:MET:HE1	1:B:165:TYR:HB2	1.99	0.45
1:B:158:SER:HB2	1:B:225:TYR:O	2.17	0.45
1:B:190:VAL:HG12	1:B:194:GLN:OE1	2.16	0.45
1:A:89:HIS:CE1	1:A:241:ASN:OD1	2.69	0.45
1:B:214:ARG:HD3	1:B:232:MET:HG2	1.99	0.45
1:B:278:LYS:CG	1:B:279:GLN:N	2.79	0.45
1:C:60:THR:O	1:C:81:ILE:HB	2.17	0.45
1:C:94:THR:CG2	1:C:95:PRO:N	2.79	0.45
1:C:115:GLU:HG3	1:C:118:PHE:HB2	1.99	0.45
1:A:56:LYS:O	1:A:57:VAL:HG23	2.17	0.44
1:A:217:VAL:CB	1:A:266:ILE:HG12	2.37	0.44
1:B:169:ILE:HG22	1:B:173:PHE:HE2	1.81	0.44
1:C:182:LYS:HD3	1:C:182:LYS:HA	1.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:TYR:CB	1:B:186:ALA:H	2.30	0.44
1:B:223:PHE:C	1:B:225:TYR:N	2.72	0.44
1:C:201:GLN:O	1:C:204:ALA:N	2.49	0.44
1:C:209:VAL:O	1:C:209:VAL:HG12	2.16	0.44
1:A:112:MET:SD	1:A:134:THR:HG21	2.57	0.44
1:A:161:ASN:O	1:A:162:ALA:C	2.57	0.44
1:A:256:GLU:HA	1:A:256:GLU:OE1	2.16	0.44
1:B:171:GLN:O	1:B:172:ALA:C	2.60	0.44
1:C:183:TYR:HD1	1:C:183:TYR:H	1.65	0.44
1:B:258:VAL:HG23	1:B:259:LYS:N	1.97	0.44
1:C:56:LYS:HZ2	1:C:58:LEU:CD2	2.30	0.44
1:A:103:ASP:O	1:A:103:ASP:OD1	2.35	0.44
1:C:157:MET:SD	1:C:222:ALA:O	2.75	0.44
1:A:89:HIS:CG	1:A:241:ASN:HB2	2.53	0.44
1:A:152:ASN:OD1	1:A:153:PRO:CD	2.63	0.44
1:A:165:TYR:O	1:A:167:GLU:N	2.51	0.44
1:A:209:VAL:N	1:A:210:PRO:HD2	2.30	0.44
1:B:62:THR:CA	1:B:297:LEU:HD13	2.46	0.44
1:B:124:ASN:HB3	1:C:84:ILE:HB	2.00	0.44
1:A:55:LYS:HD2	1:A:55:LYS:N	2.33	0.44
1:A:157:MET:HB2	1:A:226:LEU:HD12	2.00	0.44
1:A:217:VAL:HG22	1:A:266:ILE:HA	1.41	0.44
1:A:277:GLN:CD	1:A:278:LYS:H	2.26	0.44
1:A:307:PHE:O	1:A:308:LEU:C	2.59	0.44
1:B:161:ASN:O	1:B:164:VAL:N	2.50	0.44
1:C:115:GLU:HB2	1:C:118:PHE:CG	2.52	0.44
1:A:83:ARG:O	1:A:84:ILE:C	2.60	0.44
1:A:299:THR:HG23	1:A:302:GLY:H	1.83	0.44
1:B:123:GLY:C	1:B:125:VAL:H	2.25	0.44
1:C:70:ASN:ND2	1:C:191:TYR:CD1	2.86	0.44
1:C:157:MET:O	1:C:226:LEU:HD13	2.18	0.44
1:A:64:LEU:CD1	1:A:133:LEU:HD22	2.44	0.44
1:A:102:GLN:CD	1:A:125:VAL:CG1	2.82	0.44
1:A:164:VAL:O	1:A:165:TYR:C	2.57	0.44
1:A:220:GLU:CD	1:A:240:ILE:HD11	2.41	0.44
1:B:161:ASN:H	1:B:161:ASN:HD22	1.66	0.44
1:B:181:ALA:O	1:B:184:TYR:HD2	1.82	0.44
1:C:107:ILE:HD11	1:C:128:VAL:CB	2.42	0.44
1:C:316:ARG:C	1:C:316:ARG:HE	2.26	0.44
1:A:76:LEU:HD23	1:A:76:LEU:HA	1.71	0.43
1:B:150:LYS:CB	1:B:151:PRO:CD	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:TRP:C	1:B:158:SER:H	2.25	0.43
1:B:191:TYR:CD1	1:B:195:LEU:HD11	2.45	0.43
1:B:308:LEU:O	1:B:312:GLU:CG	2.65	0.43
1:C:72:ALA:O	1:C:75:LYS:HB2	2.18	0.43
1:A:56:LYS:C	1:A:104:ALA:HB1	2.43	0.43
1:B:275:LYS:HG3	1:B:278:LYS:NZ	2.31	0.43
1:C:137:ILE:HD11	1:C:225:TYR:HE2	1.83	0.43
1:B:217:VAL:CG2	1:B:266:ILE:CG2	2.82	0.43
1:C:55:LYS:HE3	1:C:55:LYS:HB2	1.76	0.43
1:C:109:TYR:CB	1:C:118:PHE:CZ	2.99	0.43
1:C:240:ILE:HD13	1:C:240:ILE:C	2.43	0.43
1:A:66:ASP:O	1:A:67:MET:C	2.59	0.43
1:B:176:LEU:C	1:B:178:PRO:CD	2.91	0.43
1:B:318:ILE:HD12	1:B:318:ILE:H	1.83	0.43
1:C:183:TYR:CD1	1:C:183:TYR:N	2.86	0.43
1:C:240:ILE:H	1:C:240:ILE:HD13	1.81	0.43
1:A:311:LEU:O	1:A:312:GLU:C	2.61	0.43
1:B:60:THR:O	1:B:82:THR:HG23	2.18	0.43
1:B:154:HIS:ND1	1:B:222:ALA:CB	2.82	0.43
1:B:180:ASN:ND2	1:B:184:TYR:CE2	2.81	0.43
1:B:266:ILE:O	1:B:267:PHE:CD1	2.71	0.43
1:C:98:ILE:HD12	1:C:98:ILE:HG23	1.71	0.43
1:C:217:VAL:HG21	1:C:266:ILE:HD13	1.96	0.43
1:A:116:ALA:HB1	1:A:119:GLU:OE1	2.18	0.43
1:A:156:TRP:NE1	1:A:157:MET:SD	2.92	0.43
1:B:64:LEU:O	1:B:68:VAL:HG22	2.19	0.43
1:C:168:ASN:ND2	1:C:171:GLN:HE22	2.12	0.43
1:A:118:PHE:CD1	1:A:118:PHE:C	2.92	0.43
1:A:214:ARG:HH22	1:A:231:GLY:N	2.17	0.43
1:A:220:GLU:CG	1:A:241:ASN:OD1	2.54	0.43
1:A:316:ARG:O	1:A:319:THR:N	2.51	0.43
1:B:57:VAL:CG1	1:B:106:LEU:HB2	2.49	0.43
1:B:76:LEU:HD23	1:B:76:LEU:HA	1.85	0.43
1:B:220:GLU:HG3	1:B:241:ASN:ND2	2.33	0.43
1:C:239:PRO:HB2	1:C:240:ILE:H	1.72	0.43
1:A:161:ASN:O	1:A:163:LEU:N	2.51	0.43
1:A:255:ILE:CG1	1:A:284:THR:CG2	2.97	0.43
1:A:277:GLN:NE2	1:A:278:LYS:N	2.67	0.43
1:B:121:PHE:C	1:B:121:PHE:CD1	2.97	0.43
1:C:68:VAL:HG22	1:C:169:ILE:HD13	2.00	0.43
1:C:219:CYS:HB2	1:C:269:GLU:OE2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:304:VAL:N	1:C:305:PRO:CD	2.82	0.43
1:B:140:ILE:CG2	1:B:141:PRO:CD	2.97	0.43
1:B:142:ILE:HG12	1:B:150:LYS:O	2.19	0.43
1:B:292:LEU:CD1	1:B:294:VAL:HG12	2.49	0.43
1:C:133:LEU:N	1:C:133:LEU:HD12	2.33	0.43
1:A:147:TYR:O	1:A:150:LYS:HB2	2.19	0.43
1:A:248:PRO:C	1:A:250:GLN:N	2.73	0.43
1:A:252:GLN:HA	1:A:255:ILE:HG22	1.99	0.43
1:B:173:PHE:O	1:B:176:LEU:N	2.52	0.42
1:B:203:GLY:O	1:B:206:LEU:CD1	2.66	0.42
1:C:157:MET:CE	1:C:225:TYR:CG	2.37	0.42
1:C:316:ARG:HH11	1:C:320:ASN:ND2	2.17	0.42
1:A:89:HIS:ND1	1:A:241:ASN:CB	2.81	0.42
1:A:157:MET:O	1:A:226:LEU:CG	2.66	0.42
1:A:195:LEU:HA	1:A:195:LEU:HD23	1.44	0.42
1:A:293:TYR:CG	1:A:304:VAL:HG21	2.53	0.42
1:C:109:TYR:CE1	1:C:111:GLY:HA2	2.53	0.42
1:C:198:ILE:CD1	1:C:312:GLU:OE2	2.66	0.42
1:A:170:ARG:CZ	1:A:185:ASN:OD1	2.68	0.42
1:B:119:GLU:C	1:B:121:PHE:H	2.27	0.42
1:A:202:LEU:C	1:A:230:TYR:HE2	2.27	0.42
1:A:213:GLN:O	1:A:322:LEU:HD21	2.19	0.42
1:C:64:LEU:O	1:C:67:MET:N	2.53	0.42
1:C:193:GLU:C	1:C:195:LEU:N	2.76	0.42
1:A:184:TYR:O	1:A:185:ASN:C	2.63	0.42
1:B:84:ILE:CG2	1:B:85:GLY:N	2.73	0.42
1:A:199:ASP:HA	1:A:202:LEU:CD2	2.48	0.42
1:A:210:PRO:HA	1:A:211:ALA:C	2.27	0.42
1:B:266:ILE:CG2	1:B:277:GLN:OE1	2.67	0.42
1:C:303:PRO:O	1:C:304:VAL:CB	2.67	0.42
1:A:63:VAL:HG22	1:A:296:SER:HA	2.01	0.42
1:A:118:PHE:O	1:A:121:PHE:N	2.53	0.42
1:C:156:TRP:O	1:C:157:MET:C	2.63	0.42
1:C:157:MET:HG3	1:C:225:TYR:HB3	1.96	0.42
1:A:128:VAL:HG23	1:A:128:VAL:O	2.19	0.42
1:A:277:GLN:NE2	1:A:278:LYS:H	2.18	0.42
1:B:109:TYR:CE2	1:B:118:PHE:HE2	2.38	0.42
1:B:190:VAL:O	1:B:193:GLU:N	2.50	0.42
1:C:56:LYS:HB2	1:C:58:LEU:HD21	2.00	0.42
1:C:56:LYS:N	1:C:106:LEU:HD23	2.09	0.42
1:A:142:ILE:HA	1:A:142:ILE:HD13	1.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:THR:O	1:A:148:THR:HG23	2.20	0.42
1:C:168:ASN:HA	1:C:171:GLN:OE1	2.20	0.42
1:A:306:THR:OG1	1:A:307:PHE:N	2.53	0.42
1:B:122:LEU:N	1:B:123:GLY:HA3	2.35	0.42
1:B:214:ARG:O	1:B:233:GLU:N	2.49	0.42
1:B:310:LEU:CD2	1:B:311:LEU:HD13	2.48	0.42
1:C:138:GLU:HA	1:C:139:PRO:HD3	1.78	0.42
1:C:152:ASN:HD22	1:C:225:TYR:HE1	1.65	0.42
1:C:167:GLU:HA	1:C:170:ARG:HG2	2.01	0.42
1:C:298:SER:HB3	1:C:304:VAL:CG1	2.49	0.42
1:A:64:LEU:O	1:A:64:LEU:HG	2.19	0.41
1:A:137:ILE:CD1	1:A:138:GLU:H	2.33	0.41
1:B:126:LYS:HG3	1:C:299:THR:HG22	2.02	0.41
1:B:154:HIS:ND1	1:B:222:ALA:HB2	2.35	0.41
1:B:173:PHE:C	1:B:175:GLU:N	2.74	0.41
1:C:205:ASP:OD1	1:C:319:THR:HG21	2.20	0.41
1:C:272:VAL:HG22	1:C:272:VAL:H	1.62	0.41
1:C:307:PHE:O	1:C:308:LEU:C	2.61	0.41
1:C:58:LEU:HA	1:C:79:GLU:O	2.20	0.41
1:C:312:GLU:O	1:C:316:ARG:HG2	2.20	0.41
1:C:167:GLU:O	1:C:170:ARG:N	2.52	0.41
1:C:316:ARG:HH11	1:C:317:VAL:HA	1.82	0.41
1:A:294:VAL:C	1:A:296:SER:N	2.75	0.41
1:B:154:HIS:CG	1:B:222:ALA:HB2	2.51	0.41
1:C:61:PHE:HB2	1:C:62:THR:H	1.69	0.41
1:C:313:TYR:CD1	1:C:314:ASP:N	2.88	0.41
1:A:240:ILE:HG13	1:A:241:ASN:H	1.85	0.41
1:A:310:LEU:O	1:A:311:LEU:C	2.63	0.41
1:B:277:GLN:O	1:B:278:LYS:C	2.63	0.41
1:B:310:LEU:HD22	1:B:311:LEU:CD1	2.46	0.41
1:C:109:TYR:CB	1:C:118:PHE:HE2	2.12	0.41
1:C:167:GLU:O	1:C:170:ARG:HG2	2.21	0.41
1:C:304:VAL:N	1:C:305:PRO:HD3	2.36	0.41
1:A:76:LEU:HB3	1:A:77:VAL:H	1.70	0.41
1:A:243:GLU:HB2	1:A:244:GLN:H	1.54	0.41
1:C:115:GLU:O	1:C:116:ALA:C	2.63	0.41
1:C:308:LEU:O	1:C:309:ASP:C	2.63	0.41
1:A:140:ILE:HD11	1:A:224:SER:HB3	2.03	0.41
1:A:193:GLU:OE2	1:B:111:GLY:O	2.39	0.41
1:A:217:VAL:O	1:A:266:ILE:HG22	2.20	0.41
1:C:56:LYS:CD	1:C:104:ALA:HB3	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:ILE:CD1	1:C:121:PHE:HE1	2.30	0.41
1:A:293:TYR:C	1:A:294:VAL:HG23	2.45	0.41
1:B:159:PRO:O	1:B:160:ARG:C	2.63	0.41
1:C:63:VAL:H	1:C:63:VAL:HG13	1.45	0.41
1:C:97:ASP:OD1	1:C:97:ASP:N	2.33	0.41
1:B:169:ILE:HG23	1:B:173:PHE:CE2	2.55	0.41
1:B:217:VAL:HG13	1:B:266:ILE:HA	2.02	0.41
1:C:170:ARG:O	1:C:173:PHE:N	2.54	0.41
1:C:200:ARG:CG	1:C:201:GLN:N	2.83	0.41
1:C:265:THR:HB	1:C:267:PHE:CE2	2.56	0.41
1:A:88:ILE:HD12	1:A:114:LEU:HD11	2.03	0.41
1:A:159:PRO:CG	1:A:202:LEU:HD21	2.39	0.41
1:A:193:GLU:O	1:A:196:LYS:N	2.54	0.41
1:B:266:ILE:C	1:B:267:PHE:CD2	2.99	0.41
1:B:300:GLU:C	1:B:301:GLU:OE1	2.64	0.41
1:C:265:THR:HG21	1:C:321:GLY:HA3	2.02	0.41
1:A:66:ASP:CG	1:A:70:ASN:HD21	2.28	0.40
1:A:112:MET:CE	1:A:139:PRO:HB3	2.51	0.40
1:A:310:LEU:HD23	1:A:311:LEU:HG	2.03	0.40
1:B:106:LEU:HA	1:B:106:LEU:HD23	1.69	0.40
1:B:154:HIS:HD2	1:B:294:VAL:CG2	2.33	0.40
1:A:92:GLU:H	1:A:93:PRO:HD2	1.82	0.40
1:A:169:ILE:O	1:A:170:ARG:C	2.61	0.40
1:B:191:TYR:O	1:B:193:GLU:N	2.55	0.40
1:C:115:GLU:O	1:C:118:PHE:HB2	2.21	0.40
1:C:312:GLU:H	1:C:312:GLU:HG2	1.41	0.40
1:A:82:THR:HG22	1:A:83:ARG:H	1.86	0.40
1:B:267:PHE:N	1:B:267:PHE:CD2	2.89	0.40
1:C:161:ASN:N	1:C:161:ASN:OD1	2.54	0.40
1:C:206:LEU:HD13	1:C:230:TYR:HB3	2.03	0.40
1:A:63:VAL:CG2	1:A:296:SER:HA	2.52	0.40
1:C:266:ILE:C	1:C:267:PHE:CG	2.99	0.40
1:C:310:LEU:HD12	1:C:314:ASP:OD2	2.22	0.40
1:A:115:GLU:C	1:A:117:TRP:H	2.30	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:PRO:CD	1:B:300:GLU:CG[5_555]	2.09	0.11
1:B:278:LYS:CD	1:B:282:GLN:CG[6_555]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	258/330 (78%)	177 (69%)	56 (22%)	25 (10%)	0	6
1	B	250/330 (76%)	181 (72%)	56 (22%)	13 (5%)	1	14
1	C	220/330 (67%)	166 (76%)	41 (19%)	13 (6%)	1	12
All	All	728/990 (74%)	524 (72%)	153 (21%)	51 (7%)	1	10

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	92	GLU
1	A	211	ALA
1	A	248	PRO
1	A	264	PRO
1	A	270	SER
1	A	294	VAL
1	A	304	VAL
1	B	107	ILE
1	B	184	TYR
1	B	261	ASN
1	B	262	ASN
1	C	106	LEU
1	C	152	ASN
1	A	63	VAL
1	A	105	ASP
1	A	106	LEU
1	A	213	GLN
1	A	221	GLY
1	A	242	ALA
1	B	172	ALA
1	B	178	PRO
1	B	211	ALA
1	C	168	ASN
1	C	239	PRO

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Mol	Chain	Res	Type
1	A	137	ILE
1	A	139	PRO
1	A	214	ARG
1	A	249	LYS
1	A	284	THR
1	B	84	ILE
1	C	153	PRO
1	C	221	GLY
1	A	209	VAL
1	A	243	GLU
1	A	285	GLY
1	B	89	HIS
1	B	115	GLU
1	B	259	LYS
1	C	84	ILE
1	C	116	ALA
1	C	262	ASN
1	A	153	PRO
1	A	95	PRO
1	C	179	ASP
1	A	266	ILE
1	B	150	LYS
1	C	304	VAL
1	B	153	PRO
1	C	57	VAL
1	A	240	ILE
1	C	294	VAL

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	221/273 (81%)	172 (78%)	49 (22%)	1	5
1	B	215/273 (79%)	159 (74%)	56 (26%)	0	3
1	C	201/273 (74%)	158 (79%)	43 (21%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	637/819 (78%)	489 (77%)	148 (23%)	1 5

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	LYS
1	A	59	THR
1	A	61	PHE
1	A	62	THR
1	A	64	LEU
1	A	78	VAL
1	A	82	THR
1	A	94	THR
1	A	103	ASP
1	A	105	ASP
1	A	114	LEU
1	A	118	PHE
1	A	125	VAL
1	A	131	VAL
1	A	132	VAL
1	A	140	ILE
1	A	161	ASN
1	A	164	VAL
1	A	165	TYR
1	A	167	GLU
1	A	176	LEU
1	A	177	ASP
1	A	193	GLU
1	A	199	ASP
1	A	201	GLN
1	A	202	LEU
1	A	208	GLN
1	A	209	VAL
1	A	213	GLN
1	A	214	ARG
1	A	217	VAL
1	A	218	SER
1	A	219	CYS
1	A	226	LEU
1	A	240	ILE
1	A	243	GLU
1	A	244	GLN

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Mol	Chain	Res	Type
1	A	250	GLN
1	A	254	VAL
1	A	255	ILE
1	A	262	ASN
1	A	263	VAL
1	A	269	GLU
1	A	277	GLN
1	A	280	VAL
1	A	294	VAL
1	A	300	GLU
1	A	310	LEU
1	A	320	ASN
1	B	56	LYS
1	B	58	LEU
1	B	66	ASP
1	B	70	ASN
1	B	75	LYS
1	B	81	ILE
1	B	82	THR
1	B	83	ARG
1	B	88	ILE
1	B	92	GLU
1	B	98	ILE
1	B	100	LYS
1	B	107	ILE
1	B	112	MET
1	B	114	LEU
1	B	115	GLU
1	B	119	GLU
1	B	122	LEU
1	B	124	ASN
1	B	125	VAL
1	B	128	VAL
1	B	160	ARG
1	B	163	LEU
1	B	166	VAL
1	B	170	ARG
1	B	174	VAL
1	B	175	GLU
1	B	182	LYS
1	B	183	TYR
1	B	202	LEU

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Mol	Chain	Res	Type
1	B	206	LEU
1	B	217	VAL
1	B	220	GLU
1	B	237	MET
1	B	238	TRP
1	B	245	GLN
1	B	255	ILE
1	B	256	GLU
1	B	257	GLU
1	B	258	VAL
1	B	260	THR
1	B	271	THR
1	B	274	ASP
1	B	275	LYS
1	B	277	GLN
1	B	278	LYS
1	B	279	GLN
1	B	294	VAL
1	B	296	SER
1	B	299	THR
1	B	300	GLU
1	B	301	GLU
1	B	304	VAL
1	B	308	LEU
1	B	310	LEU
1	B	311	LEU
1	C	57	VAL
1	C	58	LEU
1	C	63	VAL
1	C	74	ASP
1	C	75	LYS
1	C	82	THR
1	C	84	ILE
1	C	92	GLU
1	C	94	THR
1	C	97	ASP
1	C	106	LEU
1	C	107	ILE
1	C	109	TYR
1	C	112	MET
1	C	118	PHE
1	C	122	LEU

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Mol	Chain	Res	Type
1	C	124	ASN
1	C	125	VAL
1	C	128	VAL
1	C	134	THR
1	C	137	ILE
1	C	140	ILE
1	C	157	MET
1	C	174	VAL
1	C	195	LEU
1	C	198	ILE
1	C	206	LEU
1	C	217	VAL
1	C	228	ARG
1	C	240	ILE
1	C	253	THR
1	C	255	ILE
1	C	261	ASN
1	C	265	THR
1	C	267	PHE
1	C	280	VAL
1	C	294	VAL
1	C	306	THR
1	C	312	GLU
1	C	314	ASP
1	C	316	ARG
1	C	317	VAL
1	C	320	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	GLN
1	A	113	ASN
1	A	168	ASN
1	A	171	GLN
1	A	194	GLN
1	A	201	GLN
1	A	250	GLN
1	B	70	ASN
1	B	161	ASN
1	B	208	GLN
1	B	262	ASN

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Mol	Chain	Res	Type
1	C	154	HIS
1	C	168	ASN
1	C	180	ASN
1	C	241	ASN
1	C	291	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	264/330 (80%)	0.04	3 (1%)	78 54	23, 124, 158, 180	0
1	B	256/330 (77%)	0.07	2 (0%)	82 60	76, 122, 167, 255	0
1	C	236/330 (71%)	0.13	3 (1%)	75 50	66, 140, 181, 204	0
All	All	756/990 (76%)	0.08	8 (1%)	78 54	23, 128, 171, 255	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	105	ASP	3.1
1	A	105	ASP	2.8
1	C	106	LEU	2.7
1	B	221	GLY	2.5
1	C	128	VAL	2.4
1	A	92	GLU	2.3
1	A	136	GLY	2.2
1	B	222	ALA	2.1

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(Å ²)	Q<0.9
2	MN	B	401	1/1	0.98	0.12	124,124,124,124	0
2	MN	C	900	1/1	0.98	0.07	126,126,126,126	0
2	MN	A	401	1/1	0.99	0.06	91,91,91,91	0

6.5 Other polymers [i](#)

There are no such residues in this entry.