



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 11:34 am GMT

PDB ID : 4IRM  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

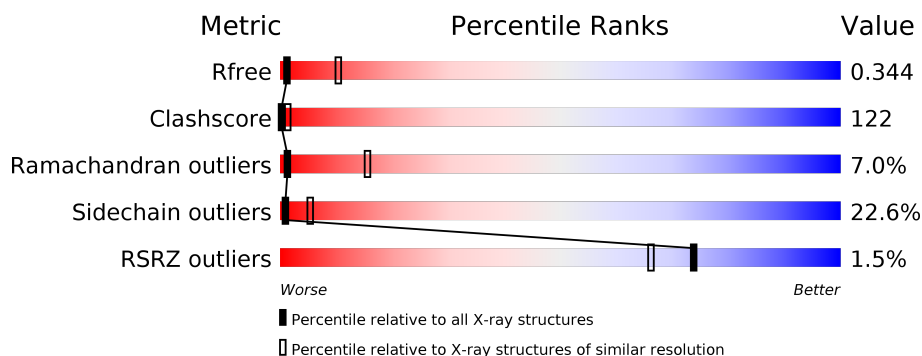
# 1 Overall quality at a glance

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))
$R_{free}$	100719	1195 (3.60-3.40)
Clashscore	112137	1322 (3.60-3.40)
Ramachandran outliers	110173	1283 (3.60-3.40)
Sidechain outliers	110143	1284 (3.60-3.40)
RSRZ outliers	101464	1226 (3.60-3.40)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>%</div> <div> <div></div> <div>20%</div> <div>41%</div> <div>17%</div> <div>•</div> <div>20%</div> </div> </div>
1	B	330	<div> <div>2%</div> <div> <div></div> <div>19%</div> <div>39%</div> <div>18%</div> <div>•</div> <div>22%</div> </div> </div>
1	C	330	<div> <div>%</div> <div> <div></div> <div>17%</div> <div>37%</div> <div>16%</div> <div>•</div> <div>28%</div> </div> </div>

## 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

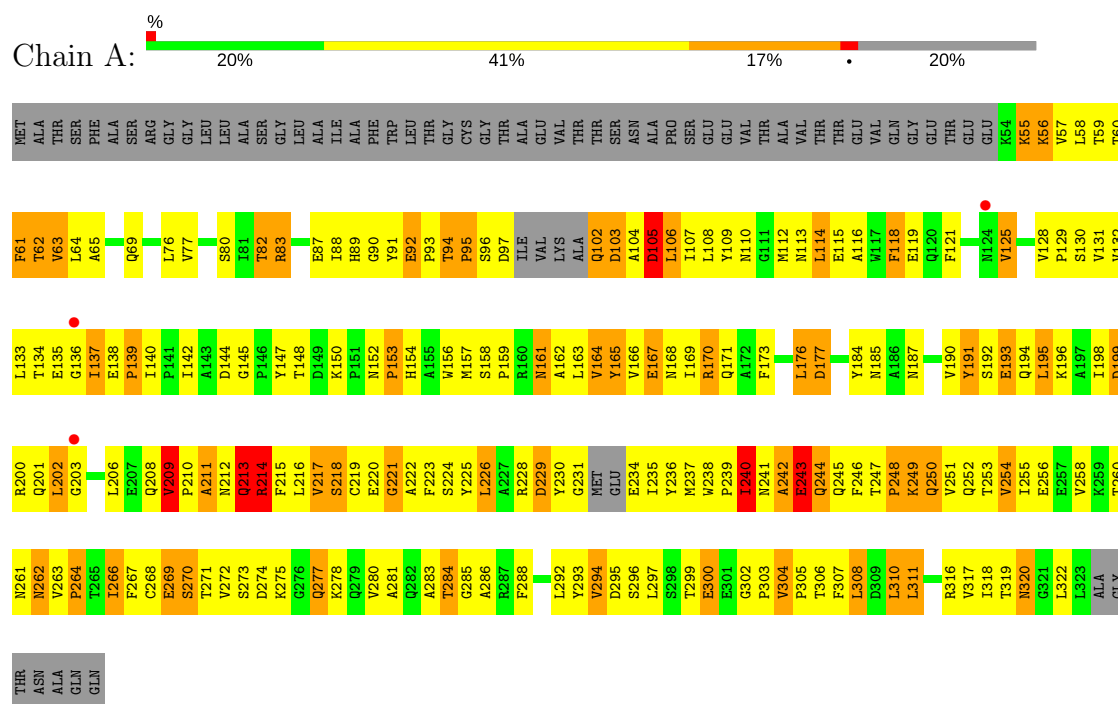
- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

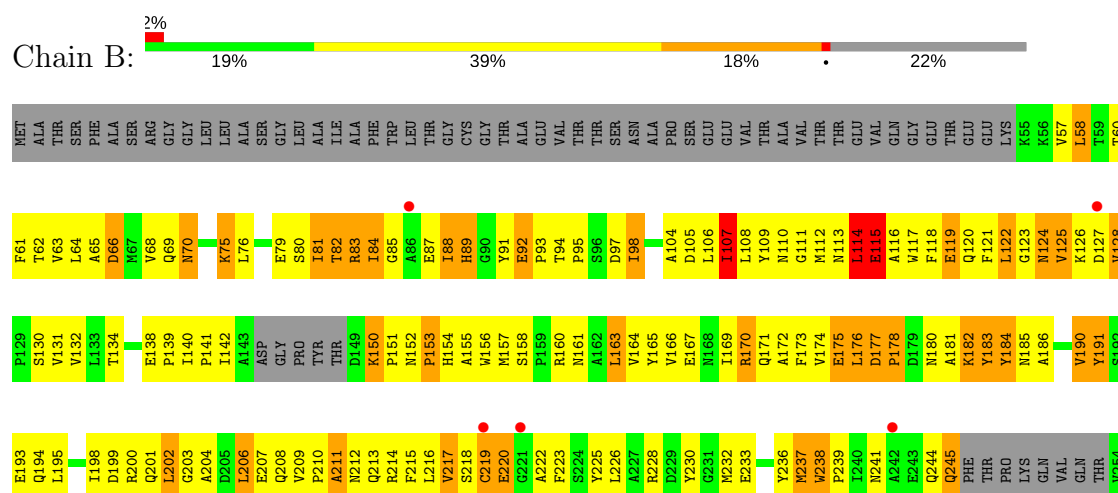
### 3 Residue-property plots

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

- Molecule 1: Mn transporter; MntC

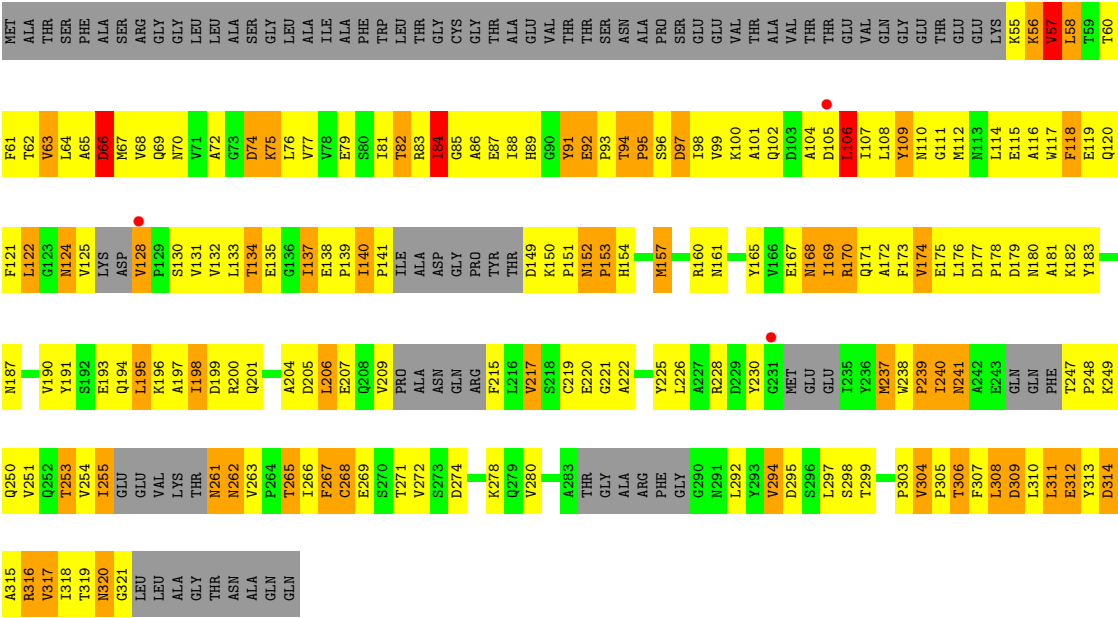


- Molecule 1: Mn transporter; MntC





● Molecule 1: Mn transporter; MntC



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	128.40Å 128.40Å 90.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.50 – 3.50 24.55 – 3.50	Depositor EDS
% Data completeness (in resolution range)	97.9 (24.50-3.50) 99.0 (24.55-3.50)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.77 (at 3.54Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.3_928)	Depositor
R, $R_{free}$	0.294 , 0.305 0.327 , 0.344	Depositor DCC
$R_{free}$ test set	524 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	122.5	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 81.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.045 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	5882	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.95	0/2090	0.87	3/2850 (0.1%)
1	B	1.04	3/2031 (0.1%)	0.96	10/2767 (0.4%)
1	C	1.03	3/1871 (0.2%)	0.98	9/2546 (0.4%)
All	All	1.00	6/5992 (0.1%)	0.93	22/8163 (0.3%)

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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	190	VAL	CA-CB	-5.80	1.42	1.54
1	C	91	TYR	CD1-CE1	-5.51	1.31	1.39
1	C	66	ASP	CB-CG	-5.42	1.40	1.51
1	B	267	PHE	CB-CG	-5.37	1.42	1.51
1	C	169	ILE	CA-CB	-5.16	1.43	1.54
1	B	318	ILE	CA-CB	-5.15	1.43	1.54

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	86	ALA	N-CA-CB	-11.62	93.83	110.10
1	C	311	LEU	CA-CB-CG	-9.34	93.82	115.30
1	C	95	PRO	CA-N-CD	-7.41	101.13	111.50
1	B	293	TYR	CB-CA-C	-7.33	95.74	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	85	GLY	N-CA-C	7.05	130.74	113.10
1	C	106	LEU	O-C-N	-6.52	112.26	122.70
1	B	294	VAL	N-CA-CB	-6.33	97.57	111.50
1	C	177	ASP	C-N-CD	6.28	141.58	128.40
1	B	114	LEU	CB-CG-CD2	-5.74	101.25	111.00
1	B	211	ALA	CB-CA-C	5.73	118.70	110.10
1	C	241	ASN	N-CA-CB	-5.68	100.38	110.60
1	B	177	ASP	N-CA-CB	5.55	120.59	110.60
1	B	125	VAL	CB-CA-C	-5.54	100.86	111.40
1	A	308	LEU	CA-CB-CG	-5.54	102.55	115.30
1	B	293	TYR	N-CA-C	5.54	125.95	111.00
1	C	308	LEU	CA-CB-CG	-5.49	102.67	115.30
1	B	271	THR	N-CA-CB	5.35	120.46	110.30
1	C	181	ALA	C-N-CA	-5.13	108.89	121.70
1	A	311	LEU	CA-CB-CG	-5.11	103.54	115.30
1	B	176	LEU	CB-CG-CD2	-5.07	102.39	111.00
1	B	318	ILE	CB-CA-C	-5.06	101.48	111.60
1	A	195	LEU	CA-CB-CG	-5.05	103.68	115.30

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 [i](#)

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	489	0
1	B	1992	0	1936	466	2
1	C	1838	0	1792	471	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	1411	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 122.

All (1411) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:THR:CG2	1:A:272:VAL:CB	1.78	1.59
1:C:157:MET:HE3	1:C:225:TYR:CD1	1.38	1.58
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: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
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:C:157:MET:HE3	1:C:225:TYR:CG	1.64	1.31
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: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:C:107:ILE:HD12	1:C:128:VAL:CG2	1.66	1.25
1:B:183:TYR:HA	1:B:184:TYR:CB	1.65	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:A:176:LEU:HD12	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:CD1	1:B:122:LEU:O	1.91	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:C:269:GLU:HG3	1:C:272:VAL:CG2	1.74	1.16
1:B:209:VAL:HG21	1:B:214:ARG:CG	1.75	1.16
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:B:208:GLN:OE1	1:B:319:THR:HB	1.40	1.15
1:A:136:GLY:H	1:A:137:ILE:CB	1.60	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:C:109:TYR:CE1	1:C:132:VAL:CG1	2.30	1.14
1:B:268:CYS:SG	1:B:272:VAL:CG2	2.36	1.14
1:B:258:VAL:O	1:B:259:LYS:HG3	1.46	1.13
1:C:157:MET:CE	1:C:225:TYR:CB	2.26	1.13
1:C:108:LEU:HG	1:C:131:VAL:CG1	1.79	1.13
1:B:262:ASN:O	1:B:264:PRO:HD3	1.49	1.12
1:A:246:PHE:CB	1:A:250:GLN:CB	2.25	1.12
1:A:242:ALA:O	1:A:243:GLU:HG3	1.43	1.12
1:B:259:LYS:CD	1:B:260:THR:HG23	1.79	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:ILE:HD12	1:C:141:PRO:HD2	1.15	1.12
1:A:60:THR:CG2	1:A:115:GLU:OE1	1.96	1.12
1:C:140:ILE:HD12	1:C:141:PRO:CD	1.81	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:C:220:GLU:HG3	1:C:241:ASN:ND2	1.65	1.10
1:B:191:TYR:CZ	1:B:308:LEU:HD11	1.86	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: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:275:LYS:HB3	1:B:278:LYS:HZ2	1.06	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
1:A:60:THR:HG21	1:A:115:GLU:CD	1.71	1.08
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:213:GLN:CD	1:B:262:ASN:HD21	1.56	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:B:182:LYS:C	1:B:183:TYR:HD1	1.57	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:C:269:GLU:CD	1:C:272:VAL:CG2	2.23	1.06
1:C:94:THR:HG22	1:C:96:SER:N	1.69	1.06
1:B:259:LYS:HG2	1:B:260:THR:HG23	1.35	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:B:181:ALA:O	1:B:184:TYR:CE2	2.08	1.05
1:C:107:ILE:HD12	1:C:128:VAL:HG23	1.05	1.05
1:A:229:ASP:OD1	1:A:230:TYR:CD1	2.10	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:266:ILE:HG22	1:A:267:PHE:N	1.64	1.03
1:A:61:PHE:O	1:A:80:SER:HB2	1.57	1.03
1:B:275:LYS:CB	1:B:278:LYS:HZ2	1.70	1.03
1:A:247:THR:CB	1:A:248:PRO:HD2	1.89	1.03
1:B:275:LYS:O	1:B:278:LYS:HD2	1.58	1.03
1:A:263:VAL:HG23	1:A:264:PRO:HB3	1.27	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: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:C:157:MET:HE1	1:C:225:TYR:CD1	1.94	1.01
1:B:182:LYS:HZ3	1:B:183:TYR:HE1	1.05	1.01
1:B:95:PRO:HA	1:B:98:ILE:HD13	1.38	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:133:LEU:O	1:C:134:THR:HG23	1.60	1.00
1:A:159:PRO:HG2	1:A:202:LEU:CD2	1.91	1.00
1:C:56:LYS:H	1:C:106:LEU:HD23	1.24	1.00
1:B:122:LEU:CG	1:B:122:LEU:O	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:A:91:TYR:C	1:A:93:PRO:HD3	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:209:VAL:H	1:A:210:PRO:HD3	1.27	0.97
1:A:59:THR:HG22	1:A:80:SER:HA	1.43	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:H	1:A:61:PHE:HD1	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: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:O	1:C:128:VAL:CG2	2.09	0.97
1:C:157:MET:HE1	1:C:225:TYR:HD1	1.25	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:C:269:GLU:CD	1:C:272:VAL:HG22	1.84	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
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:269:GLU:CG	1:C:272:VAL:HG22	1.97	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:O	1:C:304:VAL:HG13	1.66	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:GLU:CG	1:A:240:ILE:HD12	1.96	0.94
1:C:269:GLU:CD	1:C:272:VAL:HG21	1.87	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:C:157:MET:HE1	1:C:225:TYR:H	1.31	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: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: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:HG	1:B:122:LEU:O	1.69	0.93
1:C:56:LYS:HZ1	1:C:58:LEU:CG	1.81	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: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
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:213:GLN:CD	1:B:262:ASN:ND2	2.25	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:C:135:GLU:O	1:C:135:GLU:CD	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:157:MET:HE3	1:C:225:TYR:CB	1.97	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:157:MET:CE	1:C:225:TYR:CG	2.37	0.88
1:A:242:ALA:C	1:A:243:GLU:HG3	1.92	0.88
1:B:182:LYS:C	1:B:183:TYR:CD1	2.46	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: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
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:A:213:GLN:C	1:A:214:ARG:HG2	1.93	0.87
1:A:102:GLN:HE22	1:A:125:VAL:HG11	1.32	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:214:ARG:NH1	1:A:231:GLY:HA3	1.88	0.86
1:A:59:THR:OG1	1:A:64:LEU:HD23	1.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:268:CYS:SG	1:C:269:GLU:N	2.46	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:A:89:HIS:CE1	1:A:241:ASN:CG	2.50	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:259:LYS:O	1:B:263:VAL:CG2	2.25	0.84
1:B:83:ARG:HH21	1:B:84:ILE:CD1	1.88	0.84
1:C:169:ILE:CG2	1:C:173:PHE:HE2	1.91	0.84
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:154:HIS:O	1:C:157:MET:CE	2.26	0.83
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: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:259:LYS:CB	1:B:260:THR:CB	2.44	0.83
1:C:220:GLU:CD	1:C:241:ASN:HD21	1.83	0.83
1:B:215:PHE:CE1	1:B:261:ASN:ND2	2.46	0.83
1:B:191:TYR:OH	1:B:308:LEU:CD1	2.27	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:89:HIS:ND1	1:A:241:ASN:CG	2.34	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
1:A:136:GLY:CA	1:A:137:ILE:HB	2.11	0.81
1:C:70:ASN:ND2	1:C:191:TYR:HE1	1.79	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: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:B:111:GLY:HA2	1:B:115:GLU:CD	2.02	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:275:LYS:CB	1:B:278:LYS:NZ	2.45	0.79
1:B:208:GLN:OE1	1:B:319:THR:CB	2.28	0.79
1:C:109:TYR:CD2	1:C:118:PHE:HE2	2.01	0.79
1:C:56:LYS:CG	1:C:57:VAL:N	2.44	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:102:GLN:CD	1:A:125:VAL:HG11	2.01	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:74:ASP:CG	1:C:74:ASP:O	2.20	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:308:LEU:HA	1:C:311:LEU:HD12	1.62	0.79
1:B:208:GLN:CD	1:B:319:THR:HB	2.02	0.78
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:110:ASN:CG	1:B:114:LEU:HD21	2.03	0.78
1:B:258:VAL:CG2	1:B:259:LYS:H	1.93	0.78
1:C:157:MET:HE1	1:C:225:TYR:N	1.98	0.78
1:A:199:ASP:O	1:A:202:LEU:CD1	2.32	0.78
1:A:61:PHE:CE2	1:A:63:VAL:HB	2.19	0.78
1:B:203:GLY:CA	1:B:206:LEU:HD11	2.11	0.78
1:A:97:ASP:O	1:A:102:GLN:HA	1.84	0.78
1:C:157:MET:CE	1:C:225:TYR:H	1.96	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:C:56:LYS:C	1:C:57:VAL:CG1	2.47	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:C:154:HIS:O	1:C:157:MET:HE3	1.84	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:CA	1:B:301:GLU:OE1	2.33	0.77
1:C:124:ASN:C	1:C:124:ASN:OD1	2.23	0.77
1:C:249:LYS:O	1:C:253:THR:HG22	1.85	0.77
1:A:97:ASP:HB2	1:A:102:GLN:CB	2.15	0.77
1:A:246:PHE:CB	1:A:250:GLN:CD	2.53	0.77
1:A:61:PHE:N	1:A:61:PHE:HD1	1.80	0.77
1:B:209:VAL:HG21	1:B:214:ARG:HG2	0.80	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:ASN:ND2	1:C:191:TYR:CE1	2.52	0.77
1:C:57:VAL:CG2	1:C:57:VAL:O	2.33	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:C:56:LYS:HZ1	1:C:58:LEU:HG	0.92	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:122:LEU:HD12	1:B:122:LEU:C	2.05	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
1:C:109:TYR:HE1	1:C:132:VAL:CG1	1.83	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:C:57:VAL:HA	1:C:106:LEU:C	2.07	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:242:ALA:C	1:A:243:GLU:CG	2.55	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:C:56:LYS:C	1:C:57:VAL:HG12	2.07	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: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:A:60:THR:CG2	1:A:115:GLU:CD	2.50	0.74
1:B:268:CYS:SG	1:B:272:VAL:HG23	2.24	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:220:GLU:HG3	1:A:240:ILE:HD12	1.69	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
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:B:292:LEU:HD12	1:B:292:LEU:C	2.10	0.72
1:C:56:LYS:HD3	1:C:104:ALA:HB3	1.71	0.72
1:A:303:PRO:O	1:A:304:VAL:CB	2.38	0.72
1:A:62:THR:O	1:A:65:ALA:N	2.22	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:A:170:ARG:HH11	1:A:185:ASN:CG	1.92	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:252:GLN:C	1:A:255:ILE:HG22	2.09	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: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:O	1:C:124:ASN:OD1	2.07	0.71
1:A:203:GLY:CA	1:A:230:TYR:OH	2.38	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:244:GLN:CD	1:A:244:GLN:C	2.50	0.71
1:B:208:GLN:NE2	1:B:323:LEU:HD13	2.02	0.71
1:C:109:TYR:C	1:C:109:TYR:CD1	2.63	0.71
1:C:107:ILE:HD11	1:C:128:VAL:HB	1.72	0.71
1:A:217:VAL:HG11	1:A:266:ILE:HG12	1.73	0.70
1:A:61:PHE:CD2	1:A:88:ILE:HD13	2.26	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: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:A:116:ALA:HB1	1:A:119:GLU:CD	2.11	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
1:B:160:ARG:O	1:B:163:LEU:HD12	1.92	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:167:GLU:O	1:A:167:GLU:CD	2.30	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:C:105:ASP:O	1:C:106:LEU:CD1	2.40	0.69
1:C:135:GLU:OE1	1:C:135:GLU:O	2.09	0.69
1:A:246:PHE:H	1:A:250:GLN:HE21	1.39	0.69
1:A:94:THR:HG1	1:A:95:PRO:HD2	1.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:154:HIS:CE1	1:A:240:ILE:HD11	2.28	0.69
1:A:62:THR:HA	1:A:65:ALA:HB2	1.75	0.69
1:B:115:GLU:HB2	1:B:118:PHE:HB2	1.73	0.69
1:B:62:THR:C	1:B:297:LEU:HD13	2.12	0.69
1:C:115:GLU:CB	1:C:118:PHE:HB2	2.22	0.69
1:A:274:ASP:HA	1:A:277:GLN:NE2	2.08	0.68
1:A:91:TYR:C	1:A:93:PRO:CD	2.58	0.68
1:A:92:GLU:N	1:A:93:PRO:HD3	2.04	0.68
1:B:127:ASP:C	1:B:128:VAL:CG2	2.61	0.68
1:A:177:ASP:CG	1:A:177:ASP:O	2.30	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:206:LEU:O	1:A:209:VAL:HG23	1.94	0.68
1:A:191:TYR:HE1	1:A:308:LEU:HD11	1.58	0.68
1:B:171:GLN:O	1:B:173:PHE:N	2.27	0.68
1:B:63:VAL:CA	1:B:297:LEU:CD1	2.69	0.68
1:C:133:LEU:C	1:C:134:THR:CG2	2.60	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:C:83:ARG:C	1:C:84:ILE:HG12	2.14	0.68
1:A:164:VAL:HG12	1:A:165:TYR:CD1	2.29	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:A:59:THR:CG2	1:A:61:PHE:O	2.42	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:213:GLN:NE2	1:B:262:ASN:ND2	2.41	0.67
1:B:87:GLU:OE2	1:B:241:ASN:ND2	2.27	0.67
1:B:275:LYS:HA	1:B:278:LYS:CE	2.25	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:ASP:OD1	1:C:67:MET:N	2.28	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:C:133:LEU:C	1:C:134:THR:HG22	2.14	0.67
1:A:61:PHE:HD2	1:A:88:ILE:HD13	1.59	0.66
1:B:182:LYS:HA	1:B:184:TYR:CB	2.25	0.66
1:B:170:ARG:HG3	1:B:170:ARG:NH2	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:C:105:ASP:O	1:C:106:LEU:HD13	1.94	0.66
1:B:126:LYS:HE2	1:C:299:THR:HA	1.76	0.66
1:A:223:PHE:CE2	1:A:292:LEU:HD13	2.31	0.66
1:A:220:GLU:O	1:A:221:GLY:C	2.33	0.66
1:C:57:VAL:CA	1:C:106:LEU:O	2.39	0.66
1:A:102:GLN:O	1:A:102:GLN:CD	2.33	0.66
1:A:274:ASP:HA	1:A:277:GLN:HE22	1.61	0.66
1:B:275:LYS:CG	1:B:278:LYS:NZ	2.59	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:A:176:LEU:C	1:A:176:LEU:HD12	2.13	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:A:269:GLU:O	1:A:270:SER:C	2.34	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:200:ARG:CZ	1:B:122:LEU:CD1	2.75	0.65
1:A:62:THR:O	1:A:64:LEU:N	2.30	0.65
1:B:270:SER:HG	1:B:293:TYR:HD1	1.43	0.65
1:B:223:PHE:O	1:B:226:LEU:N	2.27	0.65
1:C:220:GLU:CG	1:C:241:ASN:ND2	2.35	0.65
1:A:102:GLN:O	1:A:102:GLN:NE2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:110:ASN:CB	1:B:114:LEU:HD21	2.28	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
1:B:191:TYR:OH	1:B:308:LEU:HD13	1.98	0.64
1:B:309:ASP:O	1:B:310:LEU:C	2.32	0.64
1:C:115:GLU:HB2	1:C:118:PHE:CB	2.27	0.64
1:C:58:LEU:HD23	1:C:58:LEU:N	2.11	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: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:CA	1:A:269:GLU:OE1	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:C:220:GLU:CD	1:C:222:ALA:HB2	2.17	0.63
1:A:157:MET:HB3	1:A:226:LEU:CD1	2.21	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:LYS:HG3	1:A:104:ALA:HA	1.80	0.63
1:A:190:VAL:HG21	1:B:139:PRO:HG3	1.81	0.63
1:C:138:GLU:HG3	1:C:139:PRO:HD2	1.81	0.63
1:C:61:PHE:CZ	1:C:64:LEU:HD11	2.31	0.63
1:A:283:ALA:O	1:A:284:THR:CG2	2.47	0.63
1:B:180:ASN:N	1:B:180:ASN:OD1	2.27	0.63
1:C:109:TYR:HD1	1:C:109:TYR:C	2.01	0.63
1:C:220:GLU:CD	1:C:241:ASN:ND2	2.51	0.63
1:A:103:ASP:CG	1:A:103:ASP:O	2.36	0.62
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:246:PHE:C	1:A:250:GLN:HB3	2.19	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
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:N	1:B:124:ASN:OD1	2.30	0.62
1:A:247:THR:O	1:A:248:PRO:C	2.36	0.62
1:B:58:LEU:HD23	1:B:81:ILE:CD1	2.30	0.62
1:B:199:ASP:O	1:B:202:LEU:N	2.33	0.62
1:C:56:LYS:HZ2	1:C:58:LEU:HG	1.56	0.62
1:A:209:VAL:HG12	1:A:322:LEU:HD22	0.70	0.62
1:A:62:THR:C	1:A:64:LEU:N	2.49	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:B:275:LYS:CG	1:B:278:LYS:HZ1	2.13	0.62
1:C:169:ILE:HG23	1:C:173:PHE:CE2	2.35	0.61
1:A:268:CYS:HB2	1:A:277:GLN:HG3	1.81	0.61
1:A:255:ILE:HD11	1:A:283:ALA:O	2.00	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:B:283:ALA:O	1:B:284:THR:OG1	2.14	0.61
1:C:133:LEU:O	1:C:134:THR:HG22	1.98	0.61
1:A:236:TYR:HE1	1:A:239:PRO:HG3	1.64	0.61
1:A:269:GLU:HA	1:A:269:GLU:OE1	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:HIS:CE1	1:A:295:ASP:OD2	2.53	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: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:B:207:GLU:O	1:B:207:GLU:CD	2.39	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:A:62:THR:HA	1:A:65:ALA:CB	2.31	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
1:C:134:THR:OG1	1:C:134:THR:O	2.17	0.60
1:C:217:VAL:HG21	1:C:266:ILE:HD12	1.73	0.60
1:B:170:ARG:HH21	1:B:170:ARG:HG3	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: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: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:246:PHE:N	1:A:250:GLN:HE21	2.00	0.60
1:A:62:THR:C	1:A:64:LEU:H	2.05	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:C:205:ASP:CG	1:C:319:THR:HG21	2.22	0.59
1:C:316:ARG:HA	1:C:319:THR:HG21	1.82	0.59
1:A:167:GLU:C	1:A:167:GLU:CD	2.60	0.59
1:A:170:ARG:NH1	1:A:185:ASN:CG	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:234:GLU:C	1:A:235:ILE:HG12	2.22	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: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:C:61:PHE:CD2	1:C:63:VAL:HG22	2.35	0.59
1:A:216:LEU:HD13	1:A:223:PHE:CD2	2.38	0.59
1:A:255:ILE:O	1:A:258:VAL:HG12	2.01	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:127:ASP:O	1:B:128:VAL:CG2	2.50	0.58
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:198:ILE:HG13	1:A:199:ASP:N	2.18	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:C:89:HIS:ND1	1:C:241:ASN:HB2	2.19	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: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:B:110:ASN:OD1	1:B:165:TYR:OH	2.21	0.58
1:B:201:GLN:O	1:B:202:LEU:C	2.42	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:161:ASN:C	1:A:163:LEU:N	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:ASP:C	1:C:106:LEU:HD13	2.25	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:199:ASP:HA	1:A:202:LEU:CG	2.33	0.57
1:A:60:THR:HG21	1:A:115:GLU:OE2	2.02	0.57
1:C:195:LEU:O	1:C:198:ILE:HG22	2.04	0.57
1:A:263:VAL:CG2	1:A:264:PRO:CD	2.82	0.57
1:A:90:GLY:O	1:A:91:TYR:HB2	2.03	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:B:257:GLU:C	1:B:257:GLU:OE1	2.42	0.57
1:C:61:PHE:HA	1:C:82:THR:HG23	1.87	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:C:157:MET:HE1	1:C:225:TYR:CB	2.29	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:N	1:B:275:LYS:HD3	2.16	0.56
1:B:303:PRO:HG2	1:B:304:VAL:HG12	1.86	0.56
1:C:316:ARG:C	1:C:319:THR:HG23	2.25	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:154:HIS:O	1:C:157:MET:HE2	2.05	0.56
1:C:61:PHE:CE2	1:C:63:VAL:CG2	2.60	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: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:63:VAL:HA	1:B:297:LEU:CD1	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:GLU:HG3	1:B:241:ASN:CG	2.26	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: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:C:63:VAL:O	1:C:64:LEU:C	2.43	0.56
1:C:70:ASN:OD1	1:C:70:ASN:C	2.43	0.56
1:A:255:ILE:HG13	1:A:284:THR:CG2	2.36	0.56
1:A:59:THR:HG21	1:A:61:PHE:O	2.06	0.56
1:B:299:THR:OG1	1:B:300:GLU:N	2.38	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: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: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:H	1:C:255:ILE:HD12	1.70	0.55
1:C:314:ASP:O	1:C:317:VAL:HG22	2.06	0.55
1:A:105:ASP:C	1:A:105:ASP:OD1	2.44	0.55
1:B:62:THR:CB	1:B:297:LEU:CD1	2.70	0.55
1:C:165:TYR:O	1:C:169:ILE:HG13	2.06	0.55
1:C:157:MET:HE3	1:C:225:TYR:HB2	1.62	0.55
1:C:63:VAL:HG23	1:C:64:LEU:N	2.19	0.55
1:A:105:ASP:O	1:A:105:ASP:CG	2.45	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:A:187:ASN:N	1:A:187:ASN:OD1	2.37	0.55
1:B:292:LEU:O	1:B:292:LEU:HD12	2.07	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:109:TYR:CD1	1:C:132:VAL:HG13	2.24	0.55
1:C:220:GLU:OE1	1:C:222:ALA:CB	2.49	0.55
1:B:275:LYS:HG3	1:B:278:LYS:HZ1	1.72	0.55
1:C:151:PRO:O	1:C:152:ASN:O	2.25	0.55
1:B:176:LEU:C	1:B:178:PRO:HD3	2.27	0.55
1:B:210:PRO:O	1:B:213:GLN:N	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:PHE:HZ	1:C:64:LEU:CD1	2.10	0.55
1:B:114:LEU:HD12	1:B:115:GLU:N	2.22	0.55
1:B:127:ASP:C	1:B:128:VAL:HG22	2.24	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
1:B:126:LYS:HE2	1:C:299:THR:CA	2.37	0.55
1:C:178:PRO:C	1:C:180:ASN:H	2.09	0.55
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:259:LYS:CB	1:B:260:THR:HA	2.36	0.54
1:B:61:PHE:CZ	1:B:64:LEU:HD13	2.42	0.54
1:C:261:ASN:HA	1:C:262:ASN:HB3	1.88	0.54
1:C:56:LYS:HA	1:C:77:VAL:O	2.07	0.54
1:A:217:VAL:CG1	1:A:266:ILE:HG12	2.36	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:B:62:THR:C	1:B:297:LEU:CD1	2.74	0.54
1:C:58:LEU:N	1:C:106:LEU:O	2.41	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:133:LEU:HD23	1:A:169:ILE:HG12	1.90	0.54
1:A:274:ASP:CA	1:A:277:GLN:HE22	2.20	0.54
1:C:198:ILE:O	1:C:201:GLN:N	2.41	0.54
1:A:244:GLN:OE1	1:A:244:GLN:C	2.45	0.54
1:A:250:GLN:O	1:A:251:VAL:C	2.45	0.54
1:A:263:VAL:CB	1:A:264:PRO:CA	2.55	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:C:198:ILE:HD11	1:C:312:GLU:CD	2.28	0.54
1:B:109:TYR:CD2	1:B:118:PHE:CE2	2.96	0.54
1:B:210:PRO:C	1:B:212:ASN:H	2.12	0.53
1:C:81:ILE:HG22	1:C:82:THR:N	2.23	0.53
1:A:225:TYR:O	1:A:226:LEU:C	2.45	0.53
1:C:64:LEU:O	1:C:67:MET:HG2	2.08	0.53
1:A:167:GLU:O	1:A:171:GLN:HG2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:VAL:C	1:A:266:ILE:HG23	2.20	0.53
1:B:191:TYR:CD1	1:B:195:LEU:HD13	2.43	0.53
1:B:228:ARG:C	1:B:230:TYR:H	2.11	0.53
1:B:304:VAL:HG22	1:B:304:VAL:O	2.08	0.53
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:A:94:THR:HG23	1:A:96:SER:H	1.72	0.53
1:A:157:MET:HB2	1:A:226:LEU:CD1	2.38	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:C:261:ASN:O	1:C:261:ASN:CG	2.47	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:B:104:ALA:C	1:B:105:ASP:OD1	2.48	0.52
1:A:246:PHE:H	1:A:250:GLN:NE2	2.07	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:255:ILE:HD11	1:A:284:THR:CG2	2.37	0.52
1:C:154:HIS:HE1	1:C:295:ASP:CG	2.00	0.52
1:B:292:LEU:C	1:B:292:LEU:CD1	2.78	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:A:164:VAL:CG1	1:A:165:TYR:N	2.72	0.52
1:B:126:LYS:CE	1:C:299:THR:HG22	2.39	0.52
1:A:170:ARG:NH1	1:A:185:ASN:OD1	2.42	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:89:HIS:NE2	1:B:295:ASP:OD1	2.37	0.52
1:B:63:VAL:N	1:B:297:LEU:HD13	2.22	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:C:119:GLU:N	1:C:119:GLU:OE1	2.43	0.51
1:A:176:LEU:C	1:A:176:LEU:CD1	2.77	0.51
1:A:94:THR:O	1:A:95:PRO:C	2.49	0.51
1:B:190:VAL:O	1:B:191:TYR:C	2.47	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:VAL:O	1:B:263:VAL:HG23	2.10	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:A:61:PHE:CZ	1:A:63:VAL:HB	2.45	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: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:62:THR:O	1:B:65:ALA:HB3	2.11	0.51
1:C:178:PRO:O	1:C:180:ASN:N	2.44	0.51
1:C:190:VAL:O	1:C:191:TYR:C	2.46	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:B:180:ASN:N	1:B:181:ALA:HA	2.26	0.51
1:C:238:TRP:HZ2	1:C:272:VAL:HG11	1.75	0.51
1:A:116:ALA:CB	1:A:119:GLU:CD	2.78	0.51
1:A:190:VAL:O	1:A:191:TYR:C	2.48	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:A:212:ASN:O	1:A:213:GLN:C	2.48	0.51
1:B:237:MET:HB3	1:B:238:TRP:CD1	2.45	0.51
1:B:236:TYR:CE2	1:B:239:PRO:HD3	2.39	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:CG2	1:A:217:VAL:O	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:109:TYR:HB2	1:C:118:PHE:CE2	2.42	0.51
1:C:60:THR:O	1:C:82:THR:HG23	2.11	0.51
1:A:248:PRO:O	1:A:250:GLN:N	2.44	0.51
1:A:163:LEU:O	1:A:164:VAL:C	2.49	0.50
1:A:303:PRO:C	1:A:304:VAL:HG23	2.31	0.50
1:B:283:ALA:C	1:B:284:THR:HG1	2.11	0.50
1:C:65:ALA:O	1:C:66:ASP:C	2.42	0.50
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: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:B:66:ASP:OD1	1:B:307:PHE:CB	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:GLU:O	1:C:118:PHE:N	2.28	0.50
1:A:244:GLN:NE2	1:A:245:GLN:C	2.65	0.50
1:A:271:THR:HG23	1:A:272:VAL:CA	2.26	0.50
1:B:277:GLN:O	1:B:277:GLN:NE2	2.44	0.50
1:B:79:GLU:OE2	1:B:80:SER:O	2.30	0.50
1:A:105:ASP:O	1:A:105:ASP:OD1	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:A:299:THR:OG1	1:A:300:GLU:N	2.45	0.50
1:A:62:THR:C	1:A:65:ALA:H	2.14	0.50
1:B:237:MET:HE2	1:B:256:GLU:HG3	1.93	0.50
1:B:259:LYS:CD	1:B:260:THR:HG21	2.30	0.50
1:A:133:LEU:CD2	1:A:169:ILE:HG12	2.42	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: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:A:94:THR:HG23	1:A:95:PRO:CD	2.41	0.49
1:B:198:ILE:HD11	1:B:312:GLU:HG3	1.93	0.49
1:B:266:ILE:C	1:B:267:PHE:CG	2.85	0.49
1:A:293:TYR:C	1:A:294:VAL:CG2	2.81	0.49
1:B:183:TYR:HA	1:B:184:TYR:HB2	0.73	0.49
1:B:68:VAL:HG11	1:B:108:LEU:HD12	1.93	0.49
1:A:316:ARG:O	1:A:320:ASN:N	2.37	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:130:SER:O	1:B:131:VAL:CG2	2.61	0.49
1:B:237:MET:HE2	1:B:256:GLU:HA	1.93	0.49
1:B:79:GLU:CD	1:B:80:SER:O	2.51	0.49
1:B:79:GLU:OE1	1:B:80:SER:O	2.30	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:277:GLN:O	1:A:278:LYS:C	2.50	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:223:PHE:CD1	1:B:226:LEU:HD22	2.46	0.49
1:C:167:GLU:C	1:C:169:ILE:N	2.66	0.49
1:A:106:LEU:HD23	1:A:108:LEU:HD11	1.95	0.49
1:A:144:ASP:CG	1:A:145:GLY:N	2.66	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:275:LYS:HD2	1:B:278:LYS:HZ1	1.78	0.49
1:B:299:THR:O	1:B:305:PRO:HB3	2.13	0.49
1:B:66:ASP:OD1	1:B:307:PHE:HB3	2.13	0.49
1:B:92:GLU:CD	1:B:92:GLU:N	2.66	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:199:ASP:O	1:B:201:GLN:N	2.46	0.48
1:B:154:HIS:CD2	1:B:222:ALA:CB	2.96	0.48
1:B:84:ILE:N	1:B:84:ILE:HD13	2.28	0.48
1:B:94:THR:HB	1:B:95:PRO:CD	2.38	0.48
1:A:215:PHE:HB3	1:A:234:GLU:N	2.27	0.48
1:A:91:TYR:CA	1:A:93:PRO:HD3	2.40	0.48
1:B:206:LEU:HA	1:B:319:THR:HG22	1.94	0.48
1:B:65:ALA:O	1:B:69:GLN:CG	2.61	0.48
1:B:61:PHE:HA	1:B:80:SER:OG	2.13	0.48
1:A:177:ASP:OD2	1:A:177:ASP:O	2.30	0.48
1:A:245:GLN:O	1:A:245:GLN:HG3	2.13	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:C:157:MET:CE	1:C:225:TYR:N	2.67	0.48
1:A:60:THR:CG2	1:A:61:PHE:CD1	2.96	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:A:283:ALA:C	1:A:284:THR:HG23	2.34	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:B:199:ASP:O	1:B:200:ARG:C	2.50	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:B:270:SER:OG	1:B:293:TYR:CD1	2.62	0.48
1:A:237:MET:O	1:A:250:GLN:CD	2.52	0.48
1:B:183:TYR:CA	1:B:184:TYR:CB	2.49	0.48
1:A:106:LEU:CD2	1:A:108:LEU:HD11	2.43	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: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: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:A:60:THR:CB	1:A:115:GLU:CD	2.82	0.47
1:A:144:ASP:CG	1:A:145:GLY:H	2.17	0.47
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:277:GLN:N	1:A:277:GLN:CD	2.67	0.47
1:A:288:PHE:O	1:A:288:PHE:CD2	2.67	0.47
1:A:60:THR:OG1	1:A:115:GLU:CD	2.53	0.47
1:B:66:ASP:CG	1:B:307:PHE:H	2.18	0.47
1:A:234:GLU:C	1:A:235:ILE:CG1	2.82	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:137:ILE:O	1:A:138:GLU:HG2	2.14	0.47
1:B:259:LYS:CE	1:B:260:THR:HG23	2.17	0.47
1:B:84:ILE:CG2	1:B:85:GLY:H	2.17	0.47
1:C:61:PHE:HZ	1:C:64:LEU:HD11	1.73	0.47
1:A:218:SER:HG	1:A:223:PHE:HE2	1.59	0.47
1:B:161:ASN:N	1:B:161:ASN:ND2	2.62	0.47
1:B:176:LEU:HA	1:B:176:LEU:HD12	1.64	0.47
1:C:109:TYR:CE2	1:C:132:VAL:HG22	2.49	0.47
1:B:277:GLN:CD	1:B:277:GLN:C	2.73	0.47
1:B:277:GLN:C	1:B:277:GLN:NE2	2.67	0.47
1:C:56:LYS:HZ2	1:C:58:LEU:CG	2.20	0.47
1:A:164:VAL:HG12	1:A:165:TYR:HD1	1.79	0.47
1:A:191:TYR:O	1:A:192:SER:C	2.51	0.47
1:A:63:VAL:CG2	1:A:294:VAL:O	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:PRO:C	1:B:212:ASN:N	2.66	0.47
1:C:115:GLU:O	1:C:117:TRP:N	2.48	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:75:LYS:NZ	1:B:183:TYR:O	2.48	0.47
1:B:70:ASN:HD22	1:B:70:ASN:N	2.13	0.47
1:C:109:TYR:CE1	1:C:111:GLY:CA	2.98	0.47
1:C:169:ILE:O	1:C:170:ARG:C	2.54	0.47
1:C:106:LEU:CG	1:C:176:LEU:HD21	2.45	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:137:ILE:HD12	1:C:161:ASN:HB3	1.97	0.47
1:C:72:ALA:HB1	1:C:76:LEU:HG	1.96	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:178:PRO:C	1:C:180:ASN:N	2.68	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:107:ILE:HG21	1:C:122:LEU:HD11	1.97	0.46
1:C:56:LYS:HD3	1:C:104:ALA:CB	2.43	0.46
1:C:56:LYS:HZ3	1:C:58:LEU:HG	1.62	0.46
1:C:58:LEU:CD2	1:C:58:LEU:N	2.78	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:B:195:LEU:C	1:B:198:ILE:HG22	2.36	0.46
1:C:109:TYR:CD2	1:C:118:PHE:HD2	2.32	0.46
1:C:157:MET:HE2	1:C:225:TYR:HD1	1.55	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: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:C:91:TYR:HE1	1:C:93:PRO:HA	1.80	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
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:197:ALA:HA	1:C:200:ARG:HE	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:TYR:CD1	1:C:92:GLU:N	2.83	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: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:259:LYS:NZ	1:B:260:THR:HG21	2.29	0.46
1:B:95:PRO:O	1:B:98:ILE:HG12	2.16	0.46
1:A:213:GLN:OE1	1:A:215:PHE:HE1	1.97	0.46
1:A:61:PHE:CG	1:A:62:THR:N	2.84	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:C:60:THR:CG2	1:C:118:PHE:CZ	2.98	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:237:MET:HG3	1:C:250:GLN:HG3	1.97	0.46
1:C:87:GLU:HG3	1:C:271:THR:OG1	2.15	0.46
1:C:82:THR:HG21	1:C:88:ILE:HD12	1.98	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:CA	1:A:244:GLN:OE1	2.64	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:C:94:THR:O	1:C:97:ASP:OD1	2.33	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:C:98:ILE:O	1:C:99:VAL:C	2.55	0.45
1:A:217:VAL:O	1:A:267:PHE:HB2	2.15	0.45
1:A:58:LEU:HD12	1:A:58:LEU:HA	1.63	0.45
1:B:228:ARG:C	1:B:230:TYR:N	2.68	0.45
1:B:277:GLN:HG2	1:B:288:PHE:CD2	2.32	0.45
1:B:83:ARG:HH22	1:B:84:ILE:HD11	1.76	0.45
1:C:107:ILE:O	1:C:130:SER:HA	2.16	0.45
1:A:217:VAL:O	1:A:266:ILE:CG2	2.65	0.45
1:A:292:LEU:HA	1:A:292:LEU:HD23	1.63	0.45
1:A:82:THR:C	1:A:83:ARG:HD2	2.37	0.45
1:B:269:GLU:CD	1:B:292:LEU:HD11	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:GLU:C	1:C:117:TRP:N	2.69	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:C:110:ASN:O	1:C:134:THR:CG2	2.65	0.45
1:C:306:THR:CG2	1:C:308:LEU:H	2.30	0.45
1:A:191:TYR:O	1:A:193:GLU:N	2.50	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:B:88:ILE:O	1:B:91:TYR:N	2.45	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:HD12	1:C:297:LEU:HA	1.78	0.45
1:A:110:ASN:N	1:A:115:GLU:OE2	2.34	0.45
1:A:163:LEU:HA	1:A:163:LEU:HD12	1.81	0.45
1:A:56:LYS:H	1:A:56:LYS:HG2	1.21	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:115:GLU:HG3	1:C:118:PHE:HB2	1.99	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:A:217:VAL:CB	1:A:266:ILE:HG12	2.37	0.44
1:A:56:LYS:O	1:A:57:VAL:HG23	2.17	0.44
1:B:169:ILE:HG22	1:B:173:PHE:HE2	1.81	0.44
1:C:182:LYS:HA	1:C:182:LYS:HD3	1.70	0.44
1:B:183:TYR:CB	1:B:186:ALA:H	2.30	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:C	1:A:163:LEU:H	2.20	0.44
1:A:256:GLU:HA	1:A:256:GLU:OE1	2.16	0.44
1:C:183:TYR:HD1	1:C:183:TYR:H	1.65	0.44
1:A:248:PRO:O	1:A:249:LYS:C	2.56	0.44
1:B:258:VAL:HG23	1:B:259:LYS:N	1.97	0.44
1:A:103:ASP:OD1	1:A:103:ASP:O	2.35	0.44
1:C:157:MET:SD	1:C:222:ALA:O	2.75	0.44
1:A:152:ASN:OD1	1:A:153:PRO:CD	2.63	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:89:HIS:CG	1:A:241:ASN:HB2	2.53	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: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:245:GLN:O	1:A:246:PHE:C	2.55	0.44
1:A:55:LYS:N	1:A:55:LYS:HD2	2.33	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:C:193:GLU:O	1:C:194:GLN:C	2.56	0.44
1:A:299:THR:HG23	1:A:302:GLY:H	1.83	0.44
1:B:275:LYS:CA	1:B:278:LYS:HZ2	2.29	0.44
1:C:157:MET:O	1:C:226:LEU:HD13	2.18	0.44
1:C:70:ASN:ND2	1:C:191:TYR:CD1	2.86	0.44
1:A:64:LEU:CD1	1:A:133:LEU:HD22	2.44	0.44
1:A:277:GLN:CD	1:A:278:LYS:N	2.71	0.44
1:B:161:ASN:HD22	1:B:161:ASN:H	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:A:132:VAL:C	1:A:133:LEU:HD12	2.39	0.43
1:A:76:LEU:HA	1:A:76:LEU:HD23	1.71	0.43
1:B:113:ASN:O	1:B:114:LEU:C	2.50	0.43
1:B:150:LYS:CB	1:B:151:PRO:CD	2.72	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:C:137:ILE:HD11	1:C:225:TYR:HE2	1.83	0.43
1:A:266:ILE:C	1:A:267:PHE:CG	2.92	0.43
1:B:217:VAL:CG2	1:B:266:ILE:CG2	2.82	0.43
1:C:109:TYR:CB	1:C:118:PHE:CZ	2.99	0.43
1:C:135:GLU:OE1	1:C:135:GLU:C	2.56	0.43
1:C:55:LYS:HB2	1:C:55:LYS:HE3	1.76	0.43
1:B:223:PHE:C	1:B:225:TYR:N	2.72	0.43
1:B:275:LYS:CD	1:B:278:LYS:HZ1	2.30	0.43
1:B:318:ILE:H	1:B:318:ILE:HD12	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:C:248:PRO:O	1:C:249:LYS:C	2.56	0.43
1:C:313:TYR:C	1:C:315:ALA:N	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:ASN:ND2	1:B:184:TYR:CE2	2.81	0.43
1:B:154:HIS:ND1	1:B:222:ALA:CB	2.82	0.43
1:B:266:ILE:O	1:B:267:PHE:CD1	2.71	0.43
1:B:60:THR:O	1:B:82:THR:HG23	2.18	0.43
1:C:217:VAL:HG21	1:C:266:ILE:HD13	1.96	0.43
1:C:98:ILE:HD12	1:C:98:ILE:HG23	1.71	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:C:66:ASP:CG	1:C:67:MET:N	2.72	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:220:GLU:HG3	1:B:241:ASN:ND2	2.33	0.43
1:B:76:LEU:HA	1:B:76:LEU:HD23	1.85	0.43
1:B:89:HIS:HE2	1:B:295:ASP:CG	2.20	0.43
1:C:167:GLU:O	1:C:168:ASN:C	2.54	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:277:GLN:NE2	1:A:278:LYS:N	2.67	0.43
1:A:255:ILE:CG1	1:A:284:THR:CG2	2.97	0.43
1:C:219:CYS:HB2	1:C:269:GLU:OE2	2.19	0.43
1:C:304:VAL:N	1:C:305:PRO:CD	2.82	0.43
1:C:68:VAL:HG22	1:C:169:ILE:HD13	2.00	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:HD12	1:C:133:LEU:N	2.33	0.43
1:A:147:TYR:O	1:A:150:LYS:HB2	2.19	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:316:ARG:HH11	1:C:320:ASN:ND2	2.17	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:A:89:HIS:ND1	1:A:241:ASN:CB	2.81	0.42
1:A:95:PRO:O	1:A:96:SER:C	2.57	0.42
1:C:109:TYR:CE1	1:C:111:GLY:HA2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:199:ASP:C	1:B:201:GLN:N	2.73	0.42
1:B:216:LEU:C	1:B:216:LEU:HD12	2.40	0.42
1:C:118:PHE:O	1:C:119:GLU:C	2.56	0.42
1:A:258:VAL:O	1:A:262:ASN:C	2.54	0.42
1:A:213:GLN:O	1:A:322:LEU:HD21	2.19	0.42
1:B:277:GLN:CD	1:B:288:PHE:HD2	2.22	0.42
1:B:208:GLN:NE2	1:B:319:THR:C	2.72	0.42
1:C:64:LEU:O	1:C:67:MET:N	2.53	0.42
1:A:62:THR:O	1:A:63:VAL:C	2.57	0.42
1:A:64:LEU:O	1:A:64:LEU:HG	2.19	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:274:ASP:O	1:A:275:LYS:C	2.55	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:118:PHE:O	1:A:121:PHE:N	2.53	0.42
1:A:63:VAL:HG22	1:A:296:SER:HA	2.01	0.42
1:B:127:ASP:C	1:B:128:VAL:HG23	2.37	0.42
1:C:157:MET:HG3	1:C:225:TYR:HB3	1.96	0.42
1:C:198:ILE:O	1:C:199:ASP:C	2.58	0.42
1:A:128:VAL:O	1:A:128:VAL:HG23	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:N	1:C:106:LEU:HD23	2.09	0.42
1:C:56:LYS:HB2	1:C:58:LEU:HD21	2.00	0.42
1:C:64:LEU:O	1:C:65:ALA:C	2.57	0.42
1:A:142:ILE:HD13	1:A:142:ILE:HA	1.73	0.42
1:A:148:THR:HG23	1:A:148:THR:O	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:137:ILE:CD1	1:A:138:GLU:H	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:272:VAL:H	1:C:272:VAL:HG22	1.62	0.41
1:C:205:ASP:OD1	1:C:319:THR:HG21	2.20	0.41
1:A:102:GLN:CD	1:A:125:VAL:CG1	2.82	0.41
1:B:275:LYS:HG3	1:B:278:LYS:NZ	2.31	0.41
1:C:312:GLU:O	1:C:316:ARG:HG2	2.20	0.41
1:C:58:LEU:HA	1:C:79:GLU:O	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:B:154:HIS:CG	1:B:222:ALA:HB2	2.51	0.41
1:C:313:TYR:CD1	1:C:314:ASP:N	2.88	0.41
1:C:61:PHE:HB2	1:C:62:THR:H	1.69	0.41
1:A:240:ILE:HG13	1:A:241:ASN:H	1.85	0.41
1:B:171:GLN:C	1:B:173:PHE:N	2.71	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:161:ASN:O	1:A:162:ALA:C	2.57	0.41
1:A:243:GLU:HB2	1:A:244:GLN:H	1.54	0.41
1:A:76:LEU:HB3	1:A:77:VAL:H	1.70	0.41
1:A:140:ILE:HD11	1:A:224:SER:HB3	2.03	0.41
1:A:217:VAL:O	1:A:266:ILE:HG22	2.20	0.41
1:A:193:GLU:OE2	1:B:111:GLY:O	2.39	0.41
1:B:318:ILE:O	1:B:319:THR:C	2.59	0.41
1:C:56:LYS:CD	1:C:104:ALA:HB3	2.46	0.41
1:C:98:ILE:CD1	1:C:121:PHE:HE1	2.30	0.41
1:A:170:ARG:O	1:A:171:GLN:C	2.59	0.41
1:C:63:VAL:HG13	1:C:63:VAL:H	1.45	0.41
1:C:97:ASP:OD1	1:C:97:ASP:N	2.33	0.41
1:B:121:PHE:C	1:B:123:GLY:HA3	2.41	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:137:ILE:O	1:A:138:GLU:CD	2.58	0.41
1:B:169:ILE:HG23	1:B:173:PHE:CE2	2.55	0.41
1:A:88:ILE:HD12	1:A:114:LEU:HD11	2.03	0.41
1:A:193:GLU:O	1:A:196:LYS:N	2.54	0.41
1:A:159:PRO:CG	1:A:202:LEU:HD21	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:THR:HG21	1:C:321:GLY:HA3	2.02	0.41
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:C:135:GLU:C	1:C:135:GLU:CD	2.79	0.40
1:A:92:GLU:H	1:A:93:PRO:HD2	1.82	0.40
1:B:173:PHE:C	1:B:175:GLU:N	2.74	0.40
1:B:191:TYR:O	1:B:193:GLU:N	2.55	0.40
1:B:275:LYS:C	1:B:278:LYS:HD2	2.36	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:193:GLU:O	1:A:194:GLN:C	2.59	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:OD1	1:C:161:ASN:N	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:B:157:MET:CE	1:B:310:LEU:HD21	2.51	0.40
1:C:182:LYS:O	1:C:183:TYR:C	2.59	0.40
1:C:310:LEU:HD12	1:C:314:ASP:OD2	2.22	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%)	1	9
1	B	250/330 (76%)	181 (72%)	56 (22%)	13 (5%)	2	23
1	C	220/330 (67%)	166 (76%)	41 (19%)	13 (6%)	2	20
All	All	728/990 (74%)	524 (72%)	153 (21%)	51 (7%)	1	15

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
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

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Mol	Chain	Res	Type
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%)	175 (79%)	46 (21%)	1	7
1	B	215/273 (79%)	164 (76%)	51 (24%)	1	4
1	C	201/273 (74%)	154 (77%)	47 (23%)	1	4
All	All	637/819 (78%)	493 (77%)	144 (23%)	1	5

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	LYS
1	A	56	LYS
1	A	61	PHE
1	A	62	THR
1	A	69	GLN

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Mol	Chain	Res	Type
1	A	82	THR
1	A	83	ARG
1	A	94	THR
1	A	102	GLN
1	A	103	ASP
1	A	105	ASP
1	A	114	LEU
1	A	118	PHE
1	A	125	VAL
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	191	TYR
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	229	ASP
1	A	240	ILE
1	A	243	GLU
1	A	244	GLN
1	A	250	GLN
1	A	254	VAL
1	A	262	ASN
1	A	269	GLU
1	A	277	GLN
1	A	280	VAL
1	A	300	GLU
1	A	310	LEU
1	A	320	ASN
1	B	58	LEU

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Mol	Chain	Res	Type
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	107	ILE
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	163	LEU
1	B	166	VAL
1	B	170	ARG
1	B	175	GLU
1	B	182	LYS
1	B	183	TYR
1	B	191	TYR
1	B	202	LEU
1	B	206	LEU
1	B	217	VAL
1	B	219	CYS
1	B	220	GLU
1	B	237	MET
1	B	238	TRP
1	B	245	GLN
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	278	LYS
1	B	279	GLN
1	B	294	VAL

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Mol	Chain	Res	Type
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	56	LYS
1	C	57	VAL
1	C	58	LEU
1	C	63	VAL
1	C	66	ASP
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	109	TYR
1	C	112	MET
1	C	118	PHE
1	C	122	LEU
1	C	124	ASN
1	C	128	VAL
1	C	134	THR
1	C	137	ILE
1	C	140	ILE
1	C	157	MET
1	C	170	ARG
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	237	MET
1	C	240	ILE
1	C	253	THR
1	C	255	ILE

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Mol	Chain	Res	Type
1	C	261	ASN
1	C	265	THR
1	C	267	PHE
1	C	268	CYS
1	C	280	VAL
1	C	294	VAL
1	C	306	THR
1	C	309	ASP
1	C	312	GLU
1	C	314	ASP
1	C	316	ARG
1	C	317	VAL
1	C	320	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) 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	250	GLN
1	B	70	ASN
1	B	161	ASN
1	B	208	GLN
1	B	262	ASN
1	C	154	HIS
1	C	168	ASN
1	C	180	ASN
1	C	241	ASN
1	C	291	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	264/330 (80%)	-0.19	3 (1%) 80 72	23, 124, 158, 180	0
1	B	256/330 (77%)	-0.14	5 (1%) 65 57	76, 122, 167, 255	0
1	C	236/330 (71%)	-0.06	3 (1%) 77 69	66, 140, 181, 204	0
All	All	756/990 (76%)	-0.13	11 (1%) 74 66	23, 128, 171, 255	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	231	GLY	4.2
1	B	127	ASP	3.1
1	B	242	ALA	2.8
1	B	219	CYS	2.5
1	A	203	GLY	2.3
1	B	221	GLY	2.3
1	C	128	VAL	2.3
1	B	86	ALA	2.1
1	A	124	ASN	2.0
1	C	105	ASP	2.0
1	A	136	GLY	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	MN	B	401	1/1	0.94	0.26	-0.36	124,124,124,124	0
2	MN	A	401	1/1	0.98	0.17	-1.70	91,91,91,91	0
2	MN	C	900	1/1	0.97	0.19	-2.62	126,126,126,126	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.