



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:41 PM GMT

PDB ID : 4MFV  
Title : Crystal structure of human CTNNBL1(residues 33 563)  
Authors : Ahn, J.W.; Kim, S.; Kim, K.J.  
Deposited on : 2013-08-28  
Resolution : 2.92 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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

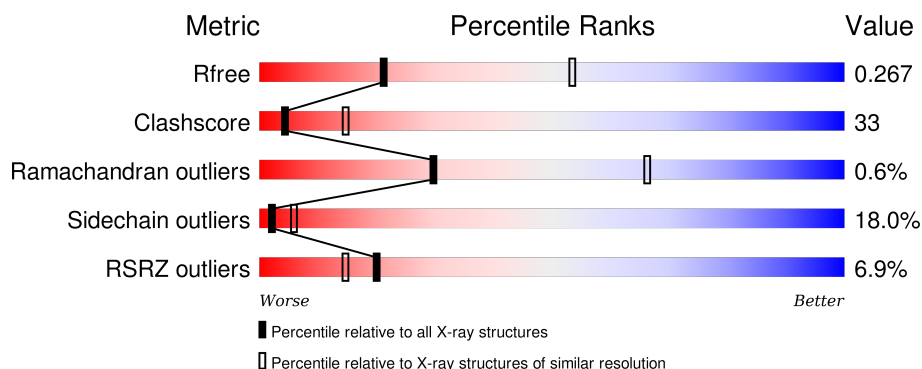
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.92 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))
$R_{free}$	91344	1643 (2.94-2.90)
Clashscore	102246	1871 (2.94-2.90)
Ramachandran outliers	100387	1824 (2.94-2.90)
Sidechain outliers	100360	1826 (2.94-2.90)
RSRZ outliers	91569	1650 (2.94-2.90)

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	534	 6% 49% 35% 8% 8%
1	B	534	 6% 45% 37% 10% 8%

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7866 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.

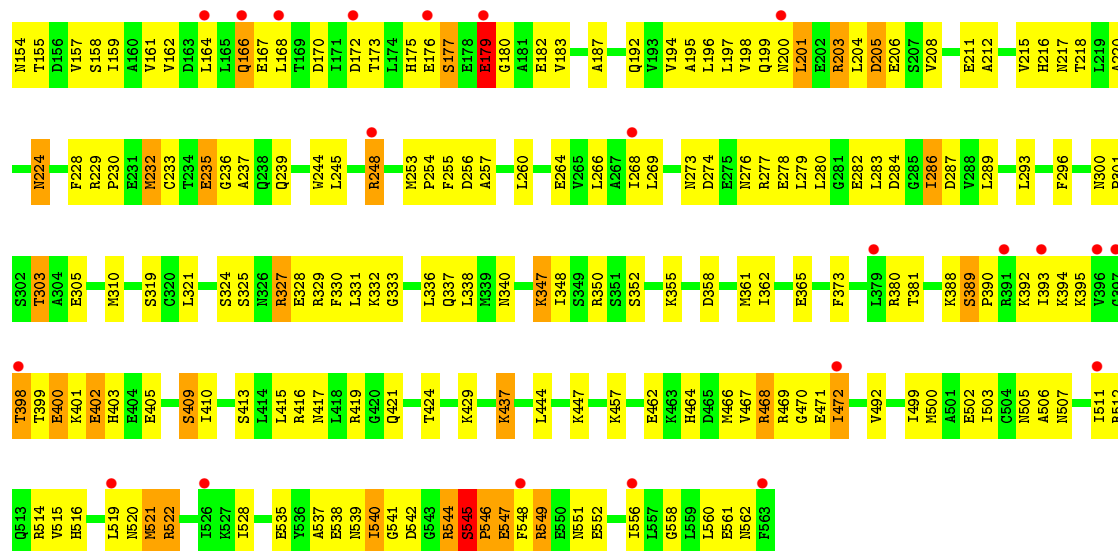
- Molecule 1 is a protein called Beta-catenin-like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	489	Total	C	N	O	S	0	0	0
			3933	2466	686	754	27			
1	B	489	Total	C	N	O	S	0	0	0
			3933	2466	686	754	27			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	GLY	-	EXPRESSION TAG	UNP Q8WYA6
A	31	HIS	-	EXPRESSION TAG	UNP Q8WYA6
A	32	MET	-	EXPRESSION TAG	UNP Q8WYA6
B	30	GLY	-	EXPRESSION TAG	UNP Q8WYA6
B	31	HIS	-	EXPRESSION TAG	UNP Q8WYA6
B	32	MET	-	EXPRESSION TAG	UNP Q8WYA6





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.04Å 90.04Å 175.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.84 – 2.92 46.84 – 2.92	Depositor EDS
% Data completeness (in resolution range)	94.1 (46.84-2.92) 94.1 (46.84-2.92)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.33 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.233 , 0.305 0.249 , 0.267	Depositor DCC
$R_{free}$ test set	1635 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	68.1	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 39.6	EDS
Estimated twinning fraction	0.048 for -h,-k,l 0.480 for h,-h-k,-l 0.054 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 32463 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7866	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.50% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.54	1/3985 (0.0%)	0.75	4/5358 (0.1%)
1	B	0.54	2/3985 (0.1%)	0.76	5/5358 (0.1%)
All	All	0.54	3/7970 (0.0%)	0.76	9/10716 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	4
All	All	0	7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	104	PRO	N-CD	5.26	1.55	1.47
1	B	546	PRO	N-CD	5.16	1.55	1.47
1	A	76	PRO	N-CD	5.09	1.54	1.47

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	300	ASN	C-N-CD	5.99	140.98	128.40
1	B	327	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	A	75	GLU	C-N-CD	5.75	140.47	128.40
1	B	103	PHE	C-N-CD	5.74	140.45	128.40
1	B	545	SER	C-N-CD	5.70	140.37	128.40
1	A	327	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	B	179	GLU	C-N-CA	-5.64	110.46	122.30
1	B	347	LYS	N-CA-C	-5.15	97.09	111.00
1	A	327	ARG	NE-CZ-NH2	-5.09	117.75	120.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	175	HIS	Peptide
1	A	254	PRO	Peptide
1	A	398	THR	Peptide
1	B	254	PRO	Peptide
1	B	256	ASP	Peptide
1	B	347	LYS	Peptide
1	B	398	THR	Peptide

## 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	3933	0	3972	258	0
1	B	3933	0	3972	266	0
All	All	7866	0	7944	520	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 33.

All (520) 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:393:ILE:CG2	1:A:399:THR:HG21	1.35	1.53
1:B:201:LEU:HD23	1:B:244:TRP:CE2	1.48	1.48
1:B:201:LEU:HD21	1:B:244:TRP:CH2	1.64	1.31
1:B:124:MET:O	1:B:127:VAL:HG23	1.34	1.27
1:B:201:LEU:HD23	1:B:244:TRP:CZ2	1.72	1.25
1:B:208:VAL:HB	1:B:211:GLU:CG	1.67	1.24
1:B:201:LEU:CD2	1:B:244:TRP:CE2	2.20	1.23
1:B:201:LEU:HD21	1:B:244:TRP:CZ3	1.73	1.22
1:B:201:LEU:CD2	1:B:244:TRP:CZ2	2.26	1.18
1:B:464:HIS:O	1:B:467:VAL:HG22	1.37	1.17
1:A:393:ILE:HG23	1:A:399:THR:HG21	1.23	1.16
1:A:204:LEU:HD23	1:A:211:GLU:HG3	1.27	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:MET:HA	1:B:114:GLU:HG3	1.30	1.13
1:A:215:VAL:HG21	1:A:248:ARG:NH2	1.64	1.10
1:A:393:ILE:CG2	1:A:399:THR:CG2	2.28	1.10
1:A:92:ARG:HB3	1:A:117:LEU:HD13	1.24	1.09
1:B:201:LEU:CD2	1:B:244:TRP:CD2	2.37	1.06
1:B:208:VAL:CB	1:B:211:GLU:HG3	1.85	1.06
1:A:208:VAL:HB	1:A:211:GLU:HB2	1.36	1.04
1:A:393:ILE:HG22	1:A:399:THR:HG21	1.40	1.04
1:A:215:VAL:CG2	1:A:248:ARG:HH22	1.70	1.04
1:B:201:LEU:CD2	1:B:244:TRP:CH2	2.40	1.03
1:A:204:LEU:CD2	1:A:211:GLU:HG3	1.88	1.03
1:B:100:ARG:O	1:B:104:PRO:HG3	1.58	1.02
1:B:279:LEU:O	1:B:283:LEU:HD12	1.62	0.99
1:B:208:VAL:HB	1:B:211:GLU:HG3	1.01	0.99
1:B:109:LYS:HE3	1:B:109:LYS:HA	1.44	0.97
1:A:215:VAL:HG21	1:A:248:ARG:HH22	0.82	0.97
1:A:237:ALA:HB2	1:A:276:ASN:OD1	1.64	0.97
1:B:237:ALA:HB2	1:B:276:ASN:OD1	1.65	0.96
1:B:537:ALA:O	1:B:540:ILE:HB	1.67	0.94
1:B:232:MET:HE2	1:B:233:CYS:HA	1.49	0.94
1:A:520:ASN:O	1:A:522:ARG:HA	1.69	0.92
1:A:393:ILE:HG21	1:A:399:THR:HG21	1.51	0.92
1:A:171:ILE:O	1:A:174:LEU:HD13	1.68	0.92
1:B:201:LEU:CD2	1:B:244:TRP:CZ3	2.53	0.91
1:B:201:LEU:CD2	1:B:244:TRP:CE3	2.54	0.91
1:B:399:THR:CB	1:B:400:GLU:HG2	2.00	0.91
1:A:232:MET:HE2	1:A:233:CYS:HA	1.52	0.91
1:B:472:ILE:H	1:B:472:ILE:HD13	1.35	0.90
1:B:117:LEU:O	1:B:120:ILE:HG22	1.71	0.90
1:B:114:GLU:HA	1:B:117:LEU:HD23	1.53	0.90
1:B:232:MET:CE	1:B:233:CYS:HA	2.02	0.90
1:A:393:ILE:HG23	1:A:399:THR:CG2	1.99	0.89
1:A:128:ALA:HB1	1:A:171:ILE:HG13	1.55	0.89
1:A:117:LEU:O	1:A:120:ILE:HG22	1.73	0.88
1:A:544:ARG:HB2	1:A:544:ARG:HH11	1.36	0.88
1:A:390:PRO:HB2	1:A:391:ARG:HG3	1.54	0.87
1:A:540:ILE:HG13	1:A:541:GLY:H	1.38	0.87
1:B:164:LEU:O	1:B:168:LEU:HD12	1.73	0.86
1:A:117:LEU:O	1:A:121:ILE:HD13	1.76	0.86
1:A:163:ASP:O	1:A:166:GLN:HG2	1.77	0.85
1:B:520:ASN:O	1:B:522:ARG:HA	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:GLN:HG3	1:A:167:GLU:N	1.91	0.85
1:B:115:LEU:HD22	1:B:115:LEU:O	1.77	0.85
1:A:169:THR:O	1:A:172:ASP:HB3	1.78	0.84
1:A:92:ARG:HB3	1:A:117:LEU:CD1	2.07	0.84
1:A:94:TYR:OH	1:B:91:LYS:HD2	1.77	0.84
1:B:540:ILE:HG13	1:B:541:GLY:H	1.41	0.84
1:B:401:LYS:O	1:B:405:GLU:HG3	1.78	0.83
1:B:149:LEU:HB3	1:B:161:VAL:HG21	1.58	0.83
1:A:398:THR:O	1:A:402:GLU:HB3	1.78	0.83
1:A:212:ALA:O	1:A:215:VAL:HG22	1.78	0.82
1:A:204:LEU:HD23	1:A:211:GLU:CG	2.07	0.82
1:B:212:ALA:O	1:B:215:VAL:HG22	1.79	0.82
1:A:279:LEU:O	1:A:283:LEU:HD12	1.78	0.82
1:A:237:ALA:CB	1:A:276:ASN:OD1	2.27	0.82
1:A:125:HIS:HA	1:A:164:LEU:HD12	1.62	0.82
1:B:120:ILE:HD13	1:B:120:ILE:O	1.80	0.82
1:B:201:LEU:HD22	1:B:244:TRP:CD2	2.12	0.81
1:B:464:HIS:O	1:B:467:VAL:CG2	2.26	0.81
1:B:398:THR:O	1:B:402:GLU:HB3	1.79	0.81
1:B:78:ASP:HB3	1:B:81:SER:HB3	1.63	0.80
1:A:228:PHE:O	1:A:230:PRO:HD3	1.82	0.80
1:A:537:ALA:O	1:A:540:ILE:HB	1.81	0.80
1:B:467:VAL:HG23	1:B:468:ARG:N	1.97	0.80
1:A:146:LEU:HD22	1:A:161:VAL:HG13	1.62	0.79
1:B:237:ALA:CB	1:B:276:ASN:OD1	2.30	0.79
1:A:78:ASP:HB2	1:A:130:MET:SD	2.22	0.79
1:A:544:ARG:HH11	1:A:544:ARG:CB	1.94	0.79
1:A:540:ILE:HD13	1:A:556:ILE:CD1	2.13	0.79
1:A:124:MET:O	1:A:127:VAL:HG23	1.83	0.78
1:A:163:ASP:O	1:A:166:GLN:CG	2.31	0.78
1:A:401:LYS:O	1:A:405:GLU:HG3	1.84	0.78
1:A:78:ASP:HB2	1:A:130:MET:HE3	1.67	0.77
1:A:120:ILE:HD13	1:A:120:ILE:O	1.84	0.77
1:A:393:ILE:HG22	1:A:399:THR:CG2	2.07	0.77
1:B:78:ASP:CB	1:B:81:SER:HB3	2.14	0.77
1:B:399:THR:OG1	1:B:400:GLU:HG2	1.84	0.77
1:A:78:ASP:HB2	1:A:130:MET:CE	2.14	0.77
1:A:399:THR:CB	1:A:400:GLU:HG2	2.15	0.76
1:B:180:GLY:HA2	1:B:183:VAL:HG22	1.67	0.76
1:B:78:ASP:HB3	1:B:81:SER:CB	2.16	0.76
1:A:115:LEU:O	1:A:115:LEU:HD22	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:LEU:O	1:B:121:ILE:HD13	1.85	0.76
1:B:109:LYS:CE	1:B:109:LYS:HA	2.16	0.76
1:A:171:ILE:O	1:A:174:LEU:CD1	2.33	0.75
1:B:147:LEU:O	1:B:150:LEU:HB2	1.86	0.75
1:B:110:PHE:O	1:B:113:SER:HB3	1.86	0.75
1:B:158:SER:HB3	1:B:200:ASN:HD21	1.51	0.75
1:B:121:ILE:HG23	1:B:164:LEU:HD13	1.69	0.75
1:A:235:GLU:O	1:A:239:GLN:HG2	1.87	0.75
1:A:155:THR:HG22	1:A:203:ARG:HD2	1.69	0.75
1:A:166:GLN:HG3	1:A:167:GLU:H	1.49	0.74
1:B:111:MET:HA	1:B:114:GLU:CG	2.14	0.74
1:A:102:LYS:C	1:A:104:PRO:HD3	2.06	0.74
1:B:170:ASP:O	1:B:173:THR:HG22	1.88	0.74
1:B:123:GLU:O	1:B:126:VAL:HG22	1.88	0.73
1:A:390:PRO:HB2	1:A:391:ARG:CG	2.17	0.73
1:A:149:LEU:HB3	1:A:161:VAL:HG21	1.69	0.73
1:B:472:ILE:HD13	1:B:472:ILE:N	2.03	0.73
1:A:228:PHE:C	1:A:230:PRO:HD3	2.08	0.73
1:B:327:ARG:NH2	1:B:362:ILE:O	2.22	0.73
1:B:235:GLU:O	1:B:239:GLN:HG2	1.88	0.72
1:B:503:ILE:HB	1:B:511:ILE:HD12	1.71	0.72
1:B:399:THR:HB	1:B:400:GLU:HG2	1.69	0.72
1:B:201:LEU:HD21	1:B:244:TRP:CE3	2.19	0.72
1:A:208:VAL:CG2	1:A:211:GLU:OE1	2.37	0.72
1:A:122:GLN:O	1:A:125:HIS:HB2	1.89	0.72
1:A:544:ARG:HB2	1:A:544:ARG:NH1	2.03	0.72
1:B:132:ASP:O	1:B:177:SER:HB3	1.89	0.72
1:B:399:THR:HB	1:B:400:GLU:OE2	1.89	0.71
1:A:150:LEU:CD1	1:A:161:VAL:HG11	2.20	0.71
1:B:134:TYR:HB2	1:B:180:GLY:HA3	1.71	0.71
1:A:327:ARG:NH2	1:A:362:ILE:O	2.22	0.71
1:B:201:LEU:HD12	1:B:218:THR:HG21	1.72	0.71
1:A:165:LEU:HA	1:A:168:LEU:HD12	1.71	0.71
1:A:125:HIS:NE2	1:A:167:GLU:HG3	2.04	0.70
1:A:503:ILE:HB	1:A:511:ILE:HD12	1.72	0.70
1:A:392:LYS:N	1:A:393:ILE:HA	2.06	0.70
1:A:155:THR:HG22	1:A:203:ARG:CD	2.22	0.70
1:A:150:LEU:CD1	1:A:161:VAL:CG1	2.70	0.70
1:A:521:MET:HA	1:A:522:ARG:HD3	1.73	0.69
1:A:232:MET:HE3	1:A:232:MET:O	1.92	0.69
1:B:149:LEU:HD22	1:B:161:VAL:CG2	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:LEU:HD23	1:B:168:LEU:HD13	1.74	0.69
1:A:173:THR:HG22	1:A:174:LEU:HD12	1.75	0.69
1:A:521:MET:HA	1:A:522:ARG:CD	2.23	0.69
1:A:544:ARG:CG	1:A:544:ARG:HH11	2.05	0.68
1:B:232:MET:HE3	1:B:232:MET:O	1.93	0.68
1:A:540:ILE:HG23	1:A:541:GLY:N	2.08	0.68
1:B:540:ILE:HG23	1:B:541:GLY:N	2.08	0.68
1:A:179:GLU:O	1:A:183:VAL:HG22	1.93	0.68
1:B:149:LEU:CD2	1:B:161:VAL:CG2	2.72	0.68
1:B:232:MET:HE2	1:B:233:CYS:CA	2.24	0.67
1:A:147:LEU:O	1:A:150:LEU:HB2	1.95	0.67
1:B:248:ARG:HH21	1:B:253:MET:CE	2.07	0.67
1:B:201:LEU:HD22	1:B:244:TRP:CE3	2.28	0.67
1:A:125:HIS:CA	1:A:164:LEU:HD12	2.24	0.67
1:A:174:LEU:H	1:A:174:LEU:HD12	1.60	0.67
1:B:337:GLN:N	1:B:337:GLN:OE1	2.27	0.67
1:A:79:GLU:HG3	1:A:79:GLU:O	1.94	0.67
1:B:164:LEU:HD23	1:B:168:LEU:CD1	2.25	0.67
1:A:77:LEU:HD23	1:A:77:LEU:H	1.60	0.67
1:B:324:SER:O	1:B:327:ARG:HB2	1.95	0.66
1:A:540:ILE:HG13	1:A:541:GLY:N	2.09	0.66
1:B:547:GLU:O	1:B:551:ASN:HB2	1.94	0.66
1:A:399:THR:HB	1:A:400:GLU:HG2	1.77	0.66
1:B:229:ARG:O	1:B:232:MET:HG2	1.95	0.66
1:A:167:GLU:O	1:A:171:ILE:HG12	1.95	0.66
1:A:174:LEU:N	1:A:174:LEU:HD12	2.11	0.66
1:B:155:THR:HG22	1:B:203:ARG:HD2	1.76	0.66
1:A:540:ILE:CD1	1:A:556:ILE:CD1	2.74	0.66
1:B:540:ILE:HD13	1:B:556:ILE:CD1	2.26	0.65
1:B:109:LYS:HD3	1:B:109:LYS:O	1.96	0.65
1:B:164:LEU:CD2	1:B:168:LEU:HD11	2.26	0.65
1:B:205:ASP:HB3	1:B:206:GLU:CD	2.17	0.64
1:B:119:ASP:O	1:B:123:GLU:HG2	1.97	0.64
1:A:464:HIS:O	1:A:467:VAL:HG22	1.97	0.64
1:B:201:LEU:CD1	1:B:218:THR:HG21	2.28	0.64
1:B:399:THR:HB	1:B:400:GLU:CD	2.17	0.64
1:B:78:ASP:OD1	1:B:78:ASP:N	2.30	0.64
1:B:399:THR:HB	1:B:400:GLU:CG	2.27	0.64
1:B:150:LEU:CD1	1:B:161:VAL:HG11	2.28	0.64
1:B:164:LEU:CD2	1:B:168:LEU:CD1	2.76	0.63
1:A:125:HIS:HA	1:A:164:LEU:CD1	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:MET:CE	1:A:233:CYS:HA	2.29	0.63
1:B:122:GLN:O	1:B:125:HIS:HB2	1.99	0.63
1:B:399:THR:C	1:B:400:GLU:HG2	2.19	0.62
1:A:415:LEU:HB3	1:A:502:GLU:HG2	1.81	0.62
1:A:93:SER:HA	1:A:117:LEU:HD22	1.82	0.62
1:B:195:ALA:O	1:B:199:GLN:HG3	2.00	0.61
1:A:75:GLU:HG3	1:A:76:PRO:HD3	1.82	0.61
1:A:83:LYS:O	1:A:87:LEU:HD12	2.01	0.61
1:B:279:LEU:O	1:B:283:LEU:CD1	2.43	0.61
1:B:540:ILE:HG13	1:B:541:GLY:N	2.13	0.61
1:A:164:LEU:HG	1:A:168:LEU:HD11	1.82	0.61
1:B:205:ASP:HB3	1:B:206:GLU:OE2	2.00	0.60
1:B:503:ILE:O	1:B:511:ILE:HD11	2.01	0.60
1:A:147:LEU:HB3	1:A:196:LEU:HD12	1.84	0.60
1:A:472:ILE:H	1:A:472:ILE:HD13	1.65	0.60
1:B:103:PHE:CE2	1:B:107:PRO:O	2.54	0.60
1:B:392:LYS:N	1:B:393:ILE:HA	2.17	0.60
1:B:115:LEU:HD22	1:B:115:LEU:C	2.21	0.59
1:A:206:GLU:OE1	1:A:206:GLU:HA	2.01	0.59
1:A:194:VAL:O	1:A:198:VAL:HG23	2.02	0.59
1:B:108:GLU:HB2	1:B:110:PHE:HE1	1.67	0.59
1:B:331:LEU:O	1:B:333:GLY:O	2.21	0.59
1:A:465:ASP:HA	1:A:468:ARG:HH22	1.67	0.59
1:B:279:LEU:HD12	1:B:283:LEU:HD11	1.84	0.59
1:B:467:VAL:HG23	1:B:468:ARG:H	1.68	0.58
1:B:398:THR:O	1:B:402:GLU:CB	2.50	0.58
1:B:152:HIS:ND1	1:B:157:VAL:HG11	2.18	0.58
1:B:176:GLU:OE1	1:B:177:SER:N	2.36	0.58
1:A:248:ARG:NH1	1:A:258:ASN:HB3	2.18	0.58
1:A:232:MET:HE2	1:A:233:CYS:CA	2.29	0.58
1:A:103:PHE:N	1:A:104:PRO:HD3	2.18	0.58
1:B:467:VAL:CG2	1:B:468:ARG:N	2.66	0.58
1:A:164:LEU:O	1:A:168:LEU:HD12	2.03	0.58
1:A:77:LEU:CD2	1:A:77:LEU:H	2.17	0.58
1:A:260:LEU:HD12	1:A:260:LEU:O	2.04	0.58
1:B:405:GLU:HG2	1:B:492:VAL:HB	1.86	0.58
1:B:176:GLU:CD	1:B:177:SER:N	2.57	0.58
1:A:159:ILE:HA	1:A:162:VAL:HG12	1.85	0.58
1:B:415:LEU:HB3	1:B:502:GLU:HG2	1.86	0.57
1:B:289:LEU:O	1:B:293:LEU:HD12	2.04	0.57
1:A:84:LYS:HA	1:A:87:LEU:HD12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:HIS:CD2	1:A:167:GLU:HG3	2.39	0.57
1:A:196:LEU:N	1:A:196:LEU:HD23	2.18	0.57
1:B:208:VAL:CG2	1:B:211:GLU:HG3	2.34	0.57
1:A:115:LEU:HD22	1:A:115:LEU:C	2.25	0.57
1:A:77:LEU:HD23	1:A:77:LEU:O	2.04	0.57
1:B:296:PHE:HB3	1:B:310:MET:CE	2.35	0.57
1:B:114:GLU:HA	1:B:117:LEU:CD2	2.31	0.56
1:A:399:THR:OG1	1:A:400:GLU:HG2	2.06	0.56
1:B:101:ILE:O	1:B:104:PRO:HD3	2.05	0.56
1:A:157:VAL:O	1:A:161:VAL:HG23	2.06	0.56
1:A:170:ASP:O	1:A:173:THR:HB	2.05	0.56
1:B:220:ALA:O	1:B:224:ASN:OD1	2.24	0.56
1:B:117:LEU:HG	1:B:118:ASN:N	2.20	0.56
1:B:146:LEU:HD22	1:B:161:VAL:HG13	1.88	0.56
1:A:331:LEU:O	1:A:331:LEU:HD23	2.06	0.56
1:A:229:ARG:O	1:A:232:MET:HG2	2.06	0.56
1:A:89:PHE:CD1	1:A:121:ILE:HD11	2.40	0.55
1:B:336:LEU:O	1:B:340:ASN:HB2	2.07	0.55
1:A:137:LEU:HD23	1:A:142:ALA:CB	2.36	0.55
1:B:521:MET:HA	1:B:522:ARG:CD	2.36	0.55
1:B:296:PHE:CB	1:B:310:MET:CE	2.85	0.55
1:B:274:ASP:HA	1:B:277:ARG:HD2	1.89	0.55
1:A:540:ILE:CD1	1:A:556:ILE:HD11	2.37	0.55
1:A:125:HIS:N	1:A:164:LEU:CD1	2.70	0.55
1:A:539:ASN:C	1:A:540:ILE:HG22	2.27	0.54
1:B:154:ASN:O	1:B:157:VAL:HG12	2.07	0.54
1:A:124:MET:O	1:A:127:VAL:N	2.33	0.54
1:A:163:ASP:O	1:A:166:GLN:HG3	2.05	0.54
1:A:324:SER:O	1:A:327:ARG:HB2	2.08	0.54
1:B:82:VAL:CG2	1:B:136:LEU:HD23	2.36	0.54
1:A:274:ASP:HA	1:A:277:ARG:HD2	1.89	0.54
1:B:358:ASP:OD1	1:B:409:SER:OG	2.26	0.54
1:A:201:LEU:HD22	1:A:218:THR:HG21	1.89	0.54
1:A:146:LEU:CD2	1:A:161:VAL:HG13	2.37	0.54
1:A:125:HIS:CA	1:A:164:LEU:CD1	2.85	0.54
1:B:248:ARG:NH2	1:B:253:MET:HE3	2.23	0.54
1:B:143:VAL:HG13	1:B:144:GLN:N	2.24	0.54
1:A:545:SER:O	1:A:547:GLU:N	2.41	0.53
1:B:146:LEU:O	1:B:149:LEU:HB2	2.08	0.53
1:B:150:LEU:CD1	1:B:161:VAL:CG1	2.86	0.53
1:B:362:ILE:HA	1:B:413:SER:OG	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:LEU:HB3	1:A:196:LEU:CD1	2.39	0.53
1:B:108:GLU:HB2	1:B:110:PHE:CE1	2.43	0.53
1:B:365:GLU:OE1	1:B:365:GLU:N	2.35	0.53
1:B:204:LEU:HD23	1:B:211:GLU:O	2.08	0.53
1:A:163:ASP:OD1	1:A:166:GLN:OE1	2.27	0.53
1:A:540:ILE:HD11	1:A:556:ILE:HD11	1.89	0.53
1:B:150:LEU:HD11	1:B:161:VAL:CG1	2.39	0.53
1:A:296:PHE:HB3	1:A:310:MET:CE	2.39	0.53
1:B:153:ASP:N	1:B:153:ASP:OD1	2.42	0.53
1:B:208:VAL:HB	1:B:211:GLU:HG2	1.79	0.53
1:A:180:GLY:O	1:A:183:VAL:HG23	2.08	0.53
1:A:143:VAL:HG13	1:A:144:GLN:N	2.24	0.53
1:B:539:ASN:C	1:B:540:ILE:HG22	2.30	0.53
1:A:155:THR:CG2	1:A:203:ARG:HD2	2.37	0.53
1:B:540:ILE:HG23	1:B:541:GLY:H	1.73	0.52
1:B:248:ARG:HD3	1:B:253:MET:HE1	1.90	0.52
1:A:133:LEU:HD12	1:A:133:LEU:H	1.73	0.52
1:B:279:LEU:CD1	1:B:283:LEU:HD11	2.38	0.52
1:B:155:THR:HG22	1:B:203:ARG:CD	2.38	0.52
1:A:188:LEU:O	1:A:193:VAL:HG12	2.08	0.52
1:A:336:LEU:O	1:A:340:ASN:HB2	2.09	0.52
1:A:540:ILE:HD13	1:A:556:ILE:HD12	1.89	0.52
1:B:521:MET:HA	1:B:522:ARG:HD3	1.90	0.52
1:A:236:GLY:HA2	1:A:239:GLN:HG3	1.90	0.52
1:A:362:ILE:HA	1:A:413:SER:OG	2.10	0.52
1:A:220:ALA:O	1:A:224:ASN:OD1	2.27	0.52
1:B:206:GLU:OE1	1:B:206:GLU:HA	2.10	0.52
1:A:296:PHE:CB	1:A:310:MET:CE	2.88	0.52
1:A:132:ASP:HB2	1:A:177:SER:HB3	1.90	0.52
1:A:208:VAL:O	1:A:211:GLU:N	2.43	0.52
1:B:546:PRO:HA	1:B:549:ARG:HB2	1.92	0.52
1:B:149:LEU:HD23	1:B:161:VAL:CG2	2.40	0.52
1:B:78:ASP:HB2	1:B:81:SER:HB3	1.90	0.52
1:A:337:GLN:OE1	1:A:337:GLN:N	2.39	0.52
1:B:208:VAL:CB	1:B:211:GLU:CG	2.60	0.51
1:B:88:THR:HG22	1:B:120:ILE:HG13	1.91	0.51
1:B:248:ARG:NH2	1:B:253:MET:CE	2.72	0.51
1:B:229:ARG:O	1:B:232:MET:CG	2.57	0.51
1:B:469:ARG:HD2	1:B:471:GLU:OE2	2.09	0.51
1:B:467:VAL:O	1:B:470:GLY:N	2.44	0.51
1:A:390:PRO:HB2	1:A:391:ARG:CA	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:LEU:HD23	1:A:280:LEU:C	2.31	0.51
1:B:121:ILE:N	1:B:121:ILE:CD1	2.73	0.51
1:A:540:ILE:CG1	1:A:541:GLY:N	2.73	0.51
1:A:244:TRP:CH2	1:A:248:ARG:HG3	2.46	0.51
1:A:544:ARG:HH11	1:A:544:ARG:HG3	1.76	0.51
1:A:204:LEU:HD22	1:A:211:GLU:HG3	1.86	0.51
1:B:416:ARG:NH2	1:B:417:ASN:OD1	2.44	0.51
1:A:174:LEU:CD1	1:A:174:LEU:H	2.23	0.51
1:B:236:GLY:HA2	1:B:239:GLN:HG3	1.91	0.51
1:A:545:SER:O	1:A:548:PHE:N	2.44	0.51
1:B:149:LEU:HD22	1:B:161:VAL:HG22	1.91	0.50
1:B:149:LEU:CD2	1:B:161:VAL:HG21	2.40	0.50
1:A:82:VAL:CG2	1:A:136:LEU:HD23	2.42	0.50
1:A:185:ILE:O	1:A:186:ASP:C	2.50	0.50
1:A:544:ARG:CG	1:A:544:ARG:NH1	2.72	0.50
1:B:180:GLY:CA	1:B:183:VAL:HG22	2.40	0.50
1:A:234:THR:HA	1:A:276:ASN:HD21	1.77	0.50
1:A:399:THR:C	1:A:400:GLU:HG2	2.31	0.50
1:B:166:GLN:CG	1:B:167:GLU:N	2.75	0.50
1:B:110:PHE:N	1:B:110:PHE:CD1	2.77	0.50
1:A:465:ASP:HA	1:A:468:ARG:NH2	2.26	0.50
1:B:78:ASP:HB3	1:B:81:SER:HB2	1.92	0.50
1:A:150:LEU:HD12	1:A:161:VAL:CG1	2.41	0.50
1:B:147:LEU:HD23	1:B:147:LEU:N	2.27	0.49
1:A:215:VAL:HG23	1:A:216:HIS:N	2.27	0.49
1:B:147:LEU:O	1:B:150:LEU:N	2.45	0.49
1:B:286:ILE:HD12	1:B:287:ASP:H	1.76	0.49
1:B:79:GLU:O	1:B:80:SER:HB2	2.11	0.49
1:A:299:HIS:ND1	1:A:299:HIS:N	2.60	0.49
1:B:137:LEU:HD23	1:B:142:ALA:CB	2.43	0.49
1:B:558:GLY:O	1:B:561:GLU:HG2	2.13	0.49
1:A:208:VAL:HG21	1:A:211:GLU:OE1	2.11	0.49
1:B:303:THR:OG1	1:B:305:GLU:HG2	2.13	0.49
1:A:540:ILE:HG23	1:A:541:GLY:H	1.77	0.49
1:B:82:VAL:HA	1:B:85:MET:HB2	1.95	0.49
1:B:462:GLU:O	1:B:466:MET:HG3	2.13	0.49
1:A:539:ASN:O	1:A:540:ILE:HG22	2.13	0.49
1:B:159:ILE:HA	1:B:162:VAL:HG12	1.94	0.49
1:B:520:ASN:C	1:B:522:ARG:HA	2.33	0.48
1:B:89:PHE:CE1	1:B:121:ILE:HD11	2.48	0.48
1:B:175:HIS:H	1:B:175:HIS:CD2	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:GLN:O	1:B:196:LEU:HG	2.13	0.48
1:A:279:LEU:O	1:A:283:LEU:CD1	2.56	0.48
1:A:244:TRP:HH2	1:A:248:ARG:NE	2.11	0.48
1:A:146:LEU:O	1:A:149:LEU:HB2	2.12	0.48
1:B:176:GLU:HG3	1:B:177:SER:HG	1.78	0.48
1:A:143:VAL:HG13	1:A:144:GLN:H	1.79	0.48
1:A:99:LEU:HD13	1:A:113:SER:OG	2.13	0.48
1:B:118:ASN:OD1	1:B:119:ASP:N	2.46	0.48
1:B:399:THR:CB	1:B:400:GLU:CG	2.82	0.48
1:B:149:LEU:HD23	1:B:157:VAL:CG2	2.44	0.48
1:B:78:ASP:O	1:B:130:MET:HE1	2.13	0.48
1:B:544:ARG:HB3	1:B:548:PHE:CD1	2.49	0.48
1:A:331:LEU:HD12	1:A:369:ASN:OD1	2.14	0.47
1:A:514:ARG:O	1:A:515:VAL:C	2.52	0.47
1:B:157:VAL:O	1:B:161:VAL:HG23	2.14	0.47
1:A:165:LEU:HB3	1:A:221:ILE:CD1	2.44	0.47
1:A:280:LEU:HD13	1:A:320:CYS:SG	2.54	0.47
1:A:358:ASP:OD1	1:A:409:SER:OG	2.30	0.47
1:B:514:ARG:O	1:B:515:VAL:C	2.51	0.47
1:B:109:LYS:CA	1:B:109:LYS:HE3	2.16	0.47
1:A:520:ASN:C	1:A:522:ARG:HA	2.32	0.47
1:B:399:THR:O	1:B:402:GLU:HB2	2.14	0.47
1:A:530:ARG:NH2	1:A:563:PHE:O	2.47	0.47
1:A:97:GLN:OE1	1:B:141:ASN:HB2	2.14	0.47
1:A:462:GLU:O	1:A:466:MET:HG3	2.15	0.47
1:A:208:VAL:HG23	1:A:211:GLU:OE1	2.14	0.47
1:B:120:ILE:HD13	1:B:120:ILE:C	2.35	0.46
1:B:147:LEU:HB3	1:B:196:LEU:CD1	2.45	0.46
1:B:215:VAL:HG23	1:B:216:HIS:N	2.30	0.46
1:A:450:GLY:O	1:A:454:VAL:HG23	2.16	0.46
1:A:244:TRP:CH2	1:A:248:ARG:NE	2.83	0.46
1:B:89:PHE:CD1	1:B:121:ILE:HD11	2.50	0.46
1:B:164:LEU:HG	1:B:168:LEU:HD11	1.96	0.46
1:A:391:ARG:HD2	1:A:394:LYS:HE2	1.97	0.46
1:B:109:LYS:CE	1:B:109:LYS:CA	2.85	0.46
1:A:150:LEU:HD12	1:A:161:VAL:HG11	1.96	0.46
1:A:289:LEU:O	1:A:293:LEU:HD12	2.14	0.46
1:A:255:PHE:HB3	1:A:259:LYS:HD3	1.98	0.46
1:B:264:GLU:O	1:B:268:ILE:HG12	2.16	0.46
1:B:472:ILE:O	1:B:472:ILE:HG12	2.16	0.46
1:A:178:GLU:O	1:A:182:GLU:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:LYS:O	1:B:437:LYS:CD	2.64	0.46
1:A:467:VAL:O	1:A:470:GLY:N	2.49	0.45
1:B:506:ALA:O	1:B:507:ASN:HB3	2.16	0.45
1:A:164:LEU:CD2	1:A:168:LEU:HD11	2.46	0.45
1:B:228:PHE:C	1:B:230:PRO:HD3	2.37	0.45
1:A:123:GLU:O	1:A:126:VAL:HG22	2.15	0.45
1:A:296:PHE:CB	1:A:310:MET:HE2	2.46	0.45
1:B:544:ARG:CZ	1:B:545:SER:OG	2.64	0.45
1:A:248:ARG:HD2	1:A:262:CYS:SG	2.55	0.45
1:B:164:LEU:O	1:B:168:LEU:CD1	2.56	0.45
1:B:539:ASN:O	1:B:540:ILE:HG22	2.15	0.45
1:A:521:MET:HA	1:A:522:ARG:HD2	1.98	0.45
1:A:350:ARG:HH22	1:A:390:PRO:HG3	1.81	0.45
1:B:103:PHE:CD2	1:B:103:PHE:O	2.70	0.45
1:B:540:ILE:CD1	1:B:556:ILE:HD11	2.47	0.45
1:B:180:GLY:O	1:B:183:VAL:HG22	2.16	0.45
1:B:358:ASP:HA	1:B:410:ILE:HG12	1.98	0.45
1:A:77:LEU:CD2	1:A:77:LEU:N	2.79	0.44
1:B:393:ILE:HG22	1:B:394:LYS:N	2.32	0.44
1:A:278:GLU:OE2	1:B:278:GLU:OE1	2.35	0.44
1:A:232:MET:CE	1:A:232:MET:C	2.85	0.44
1:B:472:ILE:N	1:B:472:ILE:CD1	2.73	0.44
1:A:165:LEU:CA	1:A:168:LEU:HD12	2.43	0.44
1:B:512:ARG:O	1:B:516:HIS:HD2	2.00	0.44
1:A:103:PHE:N	1:A:104:PRO:CD	2.79	0.44
1:B:194:VAL:O	1:B:198:VAL:HG23	2.17	0.44
1:A:97:GLN:O	1:A:101:ILE:HG13	2.18	0.44
1:A:85:MET:HE2	1:A:123:GLU:HB2	2.00	0.44
1:A:125:HIS:N	1:A:164:LEU:HD11	2.32	0.44
1:A:165:LEU:O	1:A:169:THR:HG23	2.17	0.44
1:A:171:ILE:C	1:A:174:LEU:HD13	2.37	0.44
1:A:174:LEU:CD1	1:A:174:LEU:N	2.80	0.44
1:A:358:ASP:HA	1:A:410:ILE:HG12	1.98	0.44
1:A:140:LEU:N	1:A:140:LEU:HD12	2.33	0.44
1:B:540:ILE:CD1	1:B:556:ILE:CD1	2.95	0.44
1:B:330:PHE:O	1:B:333:GLY:O	2.35	0.44
1:A:466:MET:CE	1:A:477:THR:HG21	2.47	0.44
1:A:390:PRO:HB2	1:A:391:ARG:CB	2.47	0.43
1:A:150:LEU:HD11	1:A:161:VAL:HG12	1.99	0.43
1:B:77:LEU:HG	1:B:77:LEU:O	2.17	0.43
1:B:361:MET:HE2	1:B:373:PHE:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:ILE:HG23	1:B:121:ILE:HD12	2.00	0.43
1:A:401:LYS:HE3	1:A:401:LYS:HB3	1.78	0.43
1:A:468:ARG:HB3	1:A:468:ARG:NH2	2.34	0.43
1:A:154:ASN:O	1:A:157:VAL:HG12	2.18	0.43
1:B:516:HIS:O	1:B:519:LEU:N	2.52	0.43
1:B:176:GLU:CD	1:B:177:SER:H	2.22	0.43
1:A:465:ASP:CA	1:A:468:ARG:HH22	2.32	0.43
1:A:436:GLU:O	1:A:439:ASP:HB2	2.18	0.43
1:B:467:VAL:CG2	1:B:468:ARG:H	2.30	0.43
1:B:102:LYS:C	1:B:104:PRO:HD3	2.38	0.43
1:A:351:SER:HB2	1:A:398:THR:HG21	1.99	0.43
1:B:166:GLN:NE2	1:B:217:ASN:OD1	2.52	0.43
1:B:548:PHE:CZ	1:B:552:GLU:OE2	2.71	0.43
1:A:178:GLU:H	1:A:178:GLU:HG3	1.52	0.43
1:B:278:GLU:OE2	1:B:282:GLU:OE2	2.36	0.43
1:B:180:GLY:HA2	1:B:183:VAL:CG2	2.44	0.43
1:B:511:ILE:HG13	1:B:512:ARG:N	2.33	0.43
1:B:96:ASN:HD22	1:B:117:LEU:CD2	2.31	0.43
1:A:122:GLN:O	1:A:125:HIS:CB	2.63	0.43
1:B:389:SER:HB3	1:B:403:HIS:ND1	2.34	0.43
1:A:264:GLU:O	1:A:268:ILE:HG12	2.17	0.43
1:B:400:GLU:HB2	1:B:401:LYS:H	1.56	0.43
1:B:177:SER:C	1:B:179:GLU:N	2.70	0.43
1:B:415:LEU:CD1	1:B:499:ILE:HG23	2.49	0.43
1:B:286:ILE:HD12	1:B:287:ASP:N	2.34	0.43
1:B:103:PHE:CG	1:B:103:PHE:O	2.70	0.43
1:A:229:ARG:O	1:A:232:MET:CG	2.67	0.43
1:B:150:LEU:HD11	1:B:161:VAL:HG12	1.99	0.43
1:B:248:ARG:HH21	1:B:253:MET:HE1	1.80	0.43
1:A:93:SER:HA	1:A:117:LEU:CD2	2.46	0.43
1:A:140:LEU:CD1	1:A:140:LEU:N	2.82	0.43
1:B:540:ILE:CG1	1:B:541:GLY:N	2.73	0.43
1:B:166:GLN:HG2	1:B:167:GLU:N	2.33	0.43
1:B:138:VAL:CG2	1:B:187:ALA:HB2	2.49	0.43
1:B:257:ALA:O	1:B:260:LEU:HB3	2.19	0.43
1:B:179:GLU:H	1:B:179:GLU:HG2	1.47	0.42
1:B:111:MET:O	1:B:114:GLU:N	2.52	0.42
1:A:92:ARG:CG	1:A:117:LEU:HA	2.49	0.42
1:A:150:LEU:HD13	1:A:161:VAL:HG11	2.00	0.42
1:B:505:ASN:OD1	1:B:562:ASN:HB2	2.19	0.42
1:A:215:VAL:CG2	1:A:216:HIS:N	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:MET:CE	1:B:232:MET:C	2.88	0.42
1:A:205:ASP:HB3	1:A:206:GLU:OE2	2.19	0.42
1:A:208:VAL:O	1:A:212:ALA:N	2.41	0.42
1:B:133:LEU:H	1:B:133:LEU:HD12	1.84	0.42
1:A:351:SER:OG	1:A:398:THR:HB	2.19	0.42
1:B:361:MET:HE1	1:B:373:PHE:CG	2.55	0.42
1:A:208:VAL:HB	1:A:211:GLU:OE1	2.19	0.42
1:A:273:ASN:ND2	1:A:276:ASN:HD22	2.17	0.42
1:B:176:GLU:HG3	1:B:177:SER:OG	2.20	0.42
1:B:103:PHE:CE2	1:B:107:PRO:C	2.93	0.41
1:B:134:TYR:HD1	1:B:137:LEU:HD12	1.85	0.41
1:A:278:GLU:OE1	1:B:278:GLU:OE2	2.37	0.41
1:B:104:PRO:HA	1:B:110:PHE:HE2	1.84	0.41
1:A:197:LEU:HD22	1:A:218:THR:HG23	2.01	0.41
1:B:164:LEU:CD2	1:B:168:LEU:HD13	2.45	0.41
1:A:89:PHE:HD1	1:A:121:ILE:HD11	1.80	0.41
1:B:154:ASN:O	1:B:157:VAL:CG1	2.68	0.41
1:B:296:PHE:CG	1:B:310:MET:HE2	2.56	0.41
1:A:364:PRO:HG2	1:A:548:PHE:HE2	1.84	0.41
1:A:228:PHE:O	1:A:230:PRO:CD	2.60	0.41
1:B:103:PHE:N	1:B:104:PRO:HD3	2.35	0.41
1:B:232:MET:HE3	1:B:233:CYS:HA	1.96	0.41
1:A:390:PRO:CB	1:A:391:ARG:HA	2.50	0.41
1:A:124:MET:HA	1:A:127:VAL:HG23	2.02	0.41
1:B:280:LEU:HD23	1:B:280:LEU:C	2.41	0.41
1:A:166:GLN:CG	1:A:167:GLU:N	2.73	0.41
1:A:541:GLY:C	1:A:543:GLY:HA2	2.41	0.41
1:A:260:LEU:HD13	1:A:309:MET:HB2	2.01	0.41
1:A:121:ILE:N	1:A:121:ILE:CD1	2.84	0.41
1:A:232:MET:HE3	1:A:232:MET:C	2.39	0.41
1:A:147:LEU:HD23	1:A:147:LEU:N	2.35	0.41
1:A:193:VAL:HG22	1:A:197:LEU:HD12	2.03	0.41
1:A:261:TYR:HD1	1:A:261:TYR:HA	1.77	0.41
1:A:548:PHE:CD1	1:A:548:PHE:C	2.94	0.41
1:B:286:ILE:HG12	1:B:329:ARG:HB3	2.02	0.41
1:B:541:GLY:O	1:B:549:ARG:CG	2.68	0.41
1:B:538:GLU:O	1:B:540:ILE:HG22	2.20	0.41
1:B:134:TYR:HB2	1:B:180:GLY:CA	2.44	0.41
1:A:511:ILE:HG13	1:A:512:ARG:N	2.35	0.41
1:B:83:LYS:O	1:B:87:LEU:HD22	2.20	0.41
1:B:147:LEU:HB3	1:B:196:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:VAL:O	1:B:211:GLU:N	2.54	0.40
1:A:155:THR:CG2	1:A:203:ARG:CD	2.97	0.40
1:A:118:ASN:OD1	1:A:119:ASP:N	2.54	0.40
1:A:246:LEU:HA	1:A:246:LEU:HD23	1.84	0.40
1:A:124:MET:CA	1:A:127:VAL:HG23	2.51	0.40
1:A:503:ILE:O	1:A:511:ILE:HD11	2.21	0.40
1:B:248:ARG:CD	1:B:253:MET:HE1	2.51	0.40
1:B:300:ASN:HB3	1:B:301:PRO:CD	2.51	0.40
1:B:500:MET:O	1:B:503:ILE:HG12	2.21	0.40
1:A:105:ASP:O	1:A:107:PRO:O	2.38	0.40
1:A:516:HIS:O	1:A:520:ASN:ND2	2.54	0.40
1:A:164:LEU:CG	1:A:168:LEU:HD11	2.50	0.40
1:B:472:ILE:H	1:B:472:ILE:CD1	2.12	0.40
1:A:180:GLY:HA2	1:A:183:VAL:CG2	2.50	0.40
1:A:472:ILE:O	1:A:472:ILE:HG12	2.21	0.40
1:B:197:LEU:HD23	1:B:197:LEU:HA	1.87	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	487/534 (91%)	452 (93%)	32 (7%)	3 (1%)	30	66
1	B	487/534 (91%)	444 (91%)	40 (8%)	3 (1%)	30	66
All	All	974/1068 (91%)	896 (92%)	72 (7%)	6 (1%)	30	66

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	540	ILE
1	B	540	ILE

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Mol	Chain	Res	Type
1	B	76	PRO
1	B	390	PRO
1	A	103	PHE
1	A	390	PRO

### 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	442/482 (92%)	368 (83%)	74 (17%)	3	7
1	B	442/482 (92%)	357 (81%)	85 (19%)	2	5
All	All	884/964 (92%)	725 (82%)	159 (18%)	2	6

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	GLU
1	A	77	LEU
1	A	79	GLU
1	A	81	SER
1	A	92	ARG
1	A	93	SER
1	A	99	LEU
1	A	100	ARG
1	A	108	GLU
1	A	109	LYS
1	A	110	PHE
1	A	113	SER
1	A	115	LEU
1	A	118	ASN
1	A	120	ILE
1	A	121	ILE
1	A	125	HIS
1	A	130	MET
1	A	133	LEU

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Mol	Chain	Res	Type
1	A	136	LEU
1	A	139	GLU
1	A	149	LEU
1	A	166	GLN
1	A	173	THR
1	A	178	GLU
1	A	182	GLU
1	A	201	LEU
1	A	203	ARG
1	A	205	ASP
1	A	211	GLU
1	A	232	MET
1	A	235	GLU
1	A	245	LEU
1	A	255	PHE
1	A	261	TYR
1	A	266	LEU
1	A	269	LEU
1	A	271	GLN
1	A	273	ASN
1	A	283	LEU
1	A	284	ASP
1	A	286	ILE
1	A	303	THR
1	A	319	SER
1	A	321	LEU
1	A	325	SER
1	A	328	GLU
1	A	332	LYS
1	A	348	ILE
1	A	350	ARG
1	A	355	LYS
1	A	380	ARG
1	A	388	LYS
1	A	389	SER
1	A	393	ILE
1	A	398	THR
1	A	400	GLU
1	A	402	GLU
1	A	419	ARG
1	A	421	GLN
1	A	437	LYS

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Mol	Chain	Res	Type
1	A	444	LEU
1	A	447	LYS
1	A	457	LYS
1	A	462	GLU
1	A	472	ILE
1	A	473	ILE
1	A	521	MET
1	A	522	ARG
1	A	528	ILE
1	A	535	GLU
1	A	542	ASP
1	A	544	ARG
1	A	560	LEU
1	B	77	LEU
1	B	78	ASP
1	B	79	GLU
1	B	84	LYS
1	B	85	MET
1	B	87	LEU
1	B	90	GLU
1	B	91	LYS
1	B	97	GLN
1	B	99	LEU
1	B	100	ARG
1	B	108	GLU
1	B	109	LYS
1	B	110	PHE
1	B	111	MET
1	B	112	GLU
1	B	114	GLU
1	B	115	LEU
1	B	117	LEU
1	B	120	ILE
1	B	121	ILE
1	B	124	MET
1	B	130	MET
1	B	133	LEU
1	B	136	LEU
1	B	139	GLU
1	B	149	LEU
1	B	153	ASP
1	B	166	GLN

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Mol	Chain	Res	Type
1	B	172	ASP
1	B	177	SER
1	B	179	GLU
1	B	182	GLU
1	B	201	LEU
1	B	203	ARG
1	B	205	ASP
1	B	224	ASN
1	B	232	MET
1	B	235	GLU
1	B	245	LEU
1	B	248	ARG
1	B	255	PHE
1	B	266	LEU
1	B	269	LEU
1	B	273	ASN
1	B	284	ASP
1	B	286	ILE
1	B	303	THR
1	B	319	SER
1	B	321	LEU
1	B	325	SER
1	B	328	GLU
1	B	332	LYS
1	B	338	LEU
1	B	348	ILE
1	B	350	ARG
1	B	352	SER
1	B	355	LYS
1	B	380	ARG
1	B	381	THR
1	B	388	LYS
1	B	389	SER
1	B	395	LYS
1	B	400	GLU
1	B	402	GLU
1	B	409	SER
1	B	419	ARG
1	B	421	GLN
1	B	424	THR
1	B	437	LYS
1	B	444	LEU

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Mol	Chain	Res	Type
1	B	447	LYS
1	B	457	LYS
1	B	468	ARG
1	B	472	ILE
1	B	521	MET
1	B	522	ARG
1	B	528	ILE
1	B	535	GLU
1	B	542	ASP
1	B	544	ARG
1	B	545	SER
1	B	547	GLU
1	B	549	ARG
1	B	560	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	ASN
1	A	122	GLN
1	A	166	GLN
1	A	273	ASN
1	A	326	ASN
1	A	433	ASN
1	A	510	GLN
1	A	562	ASN
1	B	122	GLN
1	B	166	GLN
1	B	175	HIS
1	B	312	ASN
1	B	326	ASN
1	B	359	HIS
1	B	433	ASN
1	B	510	GLN
1	B	513	GLN
1	B	516	HIS
1	B	539	ASN
1	B	562	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	489/534 (91%)	0.56	33 (6%)	21 15	24, 85, 128, 157	0
1	B	489/534 (91%)	0.55	34 (6%)	19 14	24, 87, 130, 158	0
All	All	978/1068 (91%)	0.55	67 (6%)	20 15	24, 86, 130, 158	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	397	GLY	11.1
1	B	398	THR	7.2
1	A	395	LYS	5.9
1	B	134	TYR	5.8
1	A	82	VAL	5.1
1	B	117	LEU	5.0
1	A	398	THR	4.8
1	A	177	SER	4.7
1	B	200	ASN	4.5
1	B	393	ILE	4.3
1	B	472	ILE	4.0
1	B	396	VAL	4.0
1	A	211	GLU	3.9
1	A	248	ARG	3.9
1	B	391	ARG	3.9
1	A	172	ASP	3.8
1	A	394	LYS	3.6
1	A	532	ILE	3.6
1	B	176	GLU	3.5
1	B	556	ILE	3.5
1	B	129	THR	3.4
1	A	396	VAL	3.4
1	B	78	ASP	3.3
1	B	526	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	168	LEU	3.3
1	B	172	ASP	3.1
1	B	133	LEU	3.0
1	B	179	GLU	2.9
1	A	130	MET	2.9
1	A	138	VAL	2.9
1	A	503	ILE	2.9
1	A	149	LEU	2.8
1	B	164	LEU	2.8
1	B	121	ILE	2.8
1	A	536	TYR	2.7
1	A	254	PRO	2.7
1	B	563	PHE	2.7
1	B	131	PRO	2.6
1	A	127	VAL	2.6
1	A	469	ARG	2.5
1	A	541	GLY	2.5
1	A	129	THR	2.4
1	A	472	ILE	2.4
1	A	171	ILE	2.4
1	A	431	THR	2.4
1	B	548	PHE	2.4
1	B	519	LEU	2.3
1	B	90	GLU	2.3
1	A	162	VAL	2.3
1	B	82	VAL	2.3
1	A	89	PHE	2.3
1	B	268	ILE	2.3
1	B	86	ILE	2.3
1	A	255	PHE	2.2
1	A	204	LEU	2.2
1	A	397	GLY	2.2
1	A	164	LEU	2.2
1	B	379	LEU	2.1
1	B	136	LEU	2.1
1	B	97	GLN	2.1
1	B	511	ILE	2.1
1	A	385	LEU	2.1
1	B	248	ARG	2.0
1	B	166	GLN	2.0
1	A	182	GLU	2.0
1	A	393	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	563	PHE	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.