



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 26, 2019 – 04:23 PM EDT

PDB ID : 4A2Q  
Title : Structure of duck RIG-I tandem CARDs and helicase domain  
Authors : Kowalinski, E.; Lunardi, T.; McCarthy, A.A.; Cusack, S.  
Deposited on : 2011-09-28  
Resolution : 3.40 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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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)	:	1.13
EDS	:	rb-20031633
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20031633

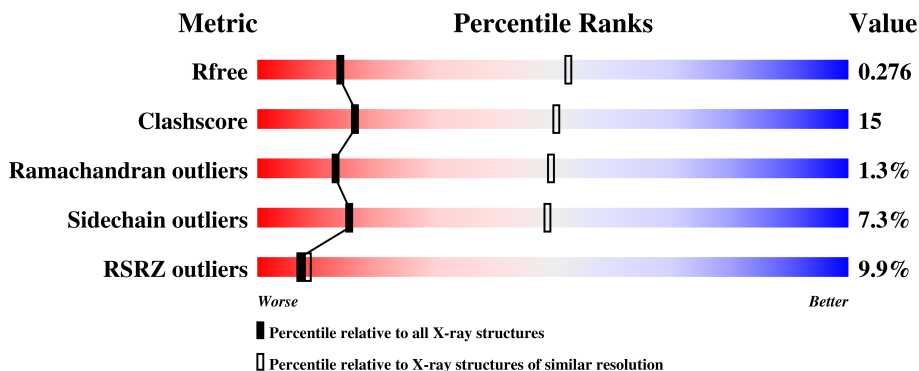
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	111664	1928 (3.50-3.30)
Clashscore	122126	2051 (3.50-3.30)
Ramachandran outliers	120053	2006 (3.50-3.30)
Sidechain outliers	120020	2006 (3.50-3.30)
RSRZ outliers	108989	1827 (3.50-3.30)

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	797	<div> <div> <div></div> <div>54%</div> <div>27%</div> <div>•</div> <div>15%</div> </div> </div>
1	B	797	<div> <div> <div>2%</div> <div>55%</div> <div>26%</div> <div>•</div> <div>15%</div> </div> </div>
1	D	797	<div> <div> <div>14%</div> <div>58%</div> <div>24%</div> <div>•</div> <div>16%</div> </div> </div>
1	E	797	<div> <div> <div>17%</div> <div>58%</div> <div>24%</div> <div>•</div> <div>16%</div> </div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 21661 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 RETINOIC ACID INDUCIBLE PROTEIN I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	674	Total	C	N	O	S	0	0	0
			5425	3430	933	1028	34			
1	B	675	Total	C	N	O	S	0	0	0
			5436	3436	937	1029	34			
1	D	671	Total	C	N	O	S	0	0	0
			5404	3417	930	1024	33			
1	E	670	Total	C	N	O	S	0	0	0
			5396	3413	929	1021	33			

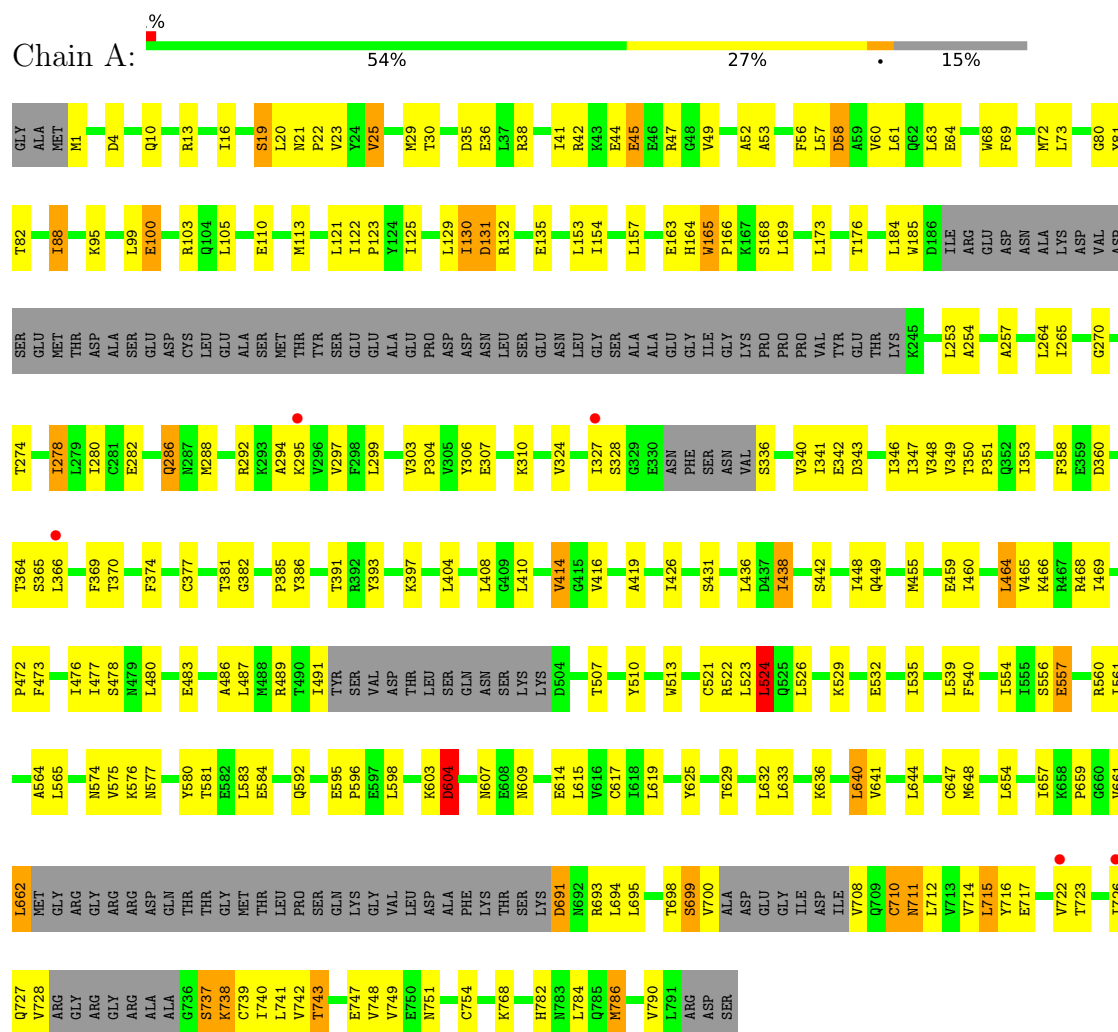
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP D3TI84
A	-1	ALA	-	expression tag	UNP D3TI84
A	0	MET	-	expression tag	UNP D3TI84
B	-2	GLY	-	expression tag	UNP D3TI84
B	-1	ALA	-	expression tag	UNP D3TI84
B	0	MET	-	expression tag	UNP D3TI84
D	-2	GLY	-	expression tag	UNP D3TI84
D	-1	ALA	-	expression tag	UNP D3TI84
D	0	MET	-	expression tag	UNP D3TI84
E	-2	GLY	-	expression tag	UNP D3TI84
E	-1	ALA	-	expression tag	UNP D3TI84
E	0	MET	-	expression tag	UNP D3TI84

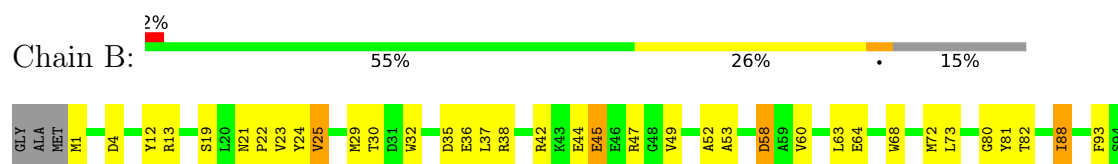
### 3 Residue-property plots

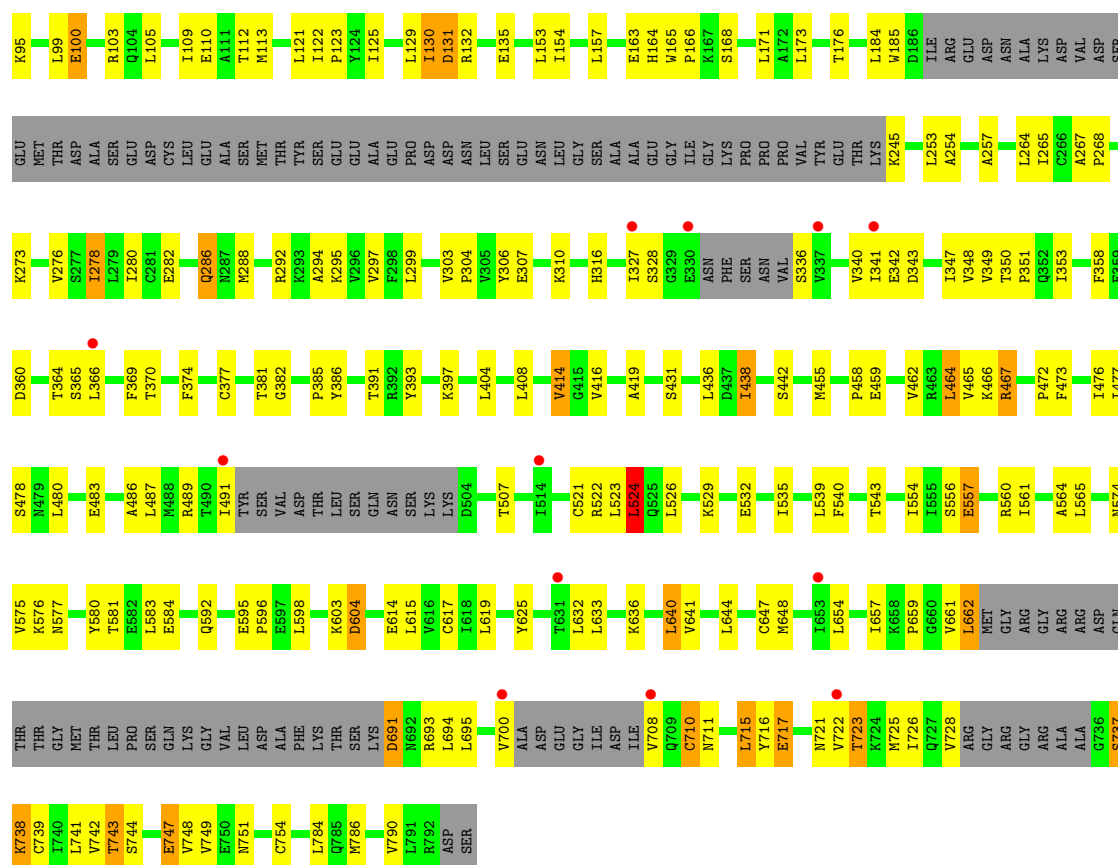
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

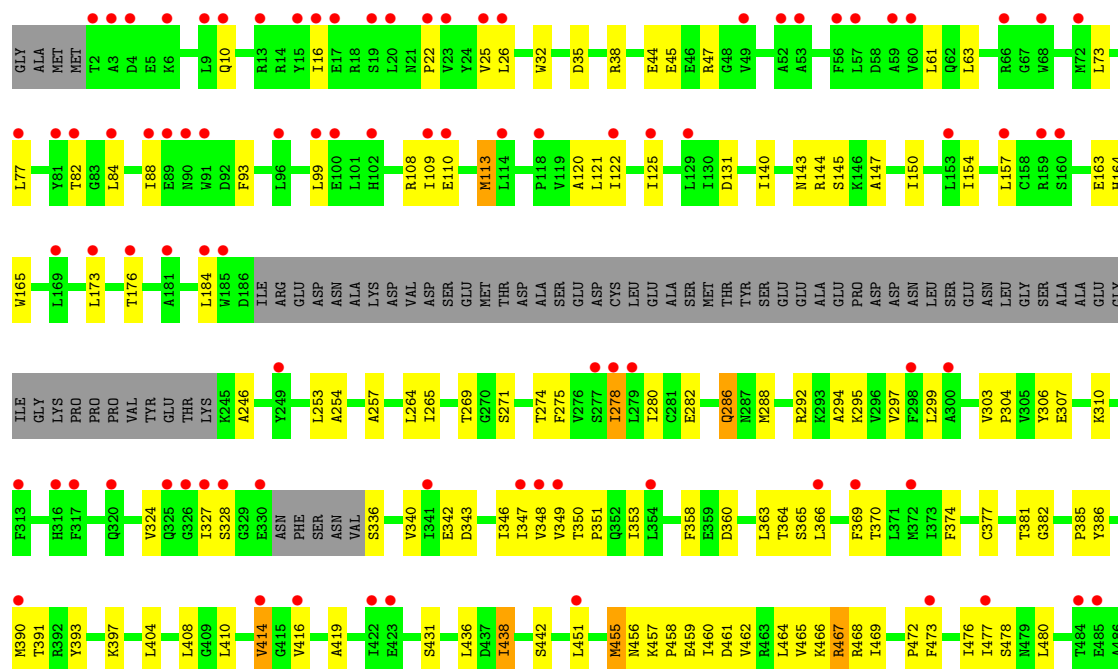


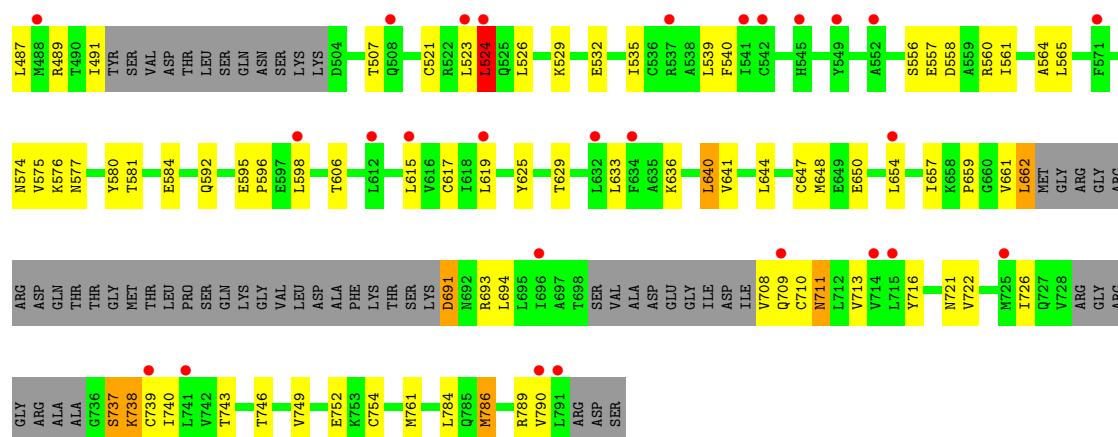
#### • Molecule 1: RETINOIC ACID INDUCIBLE PROTEIN I



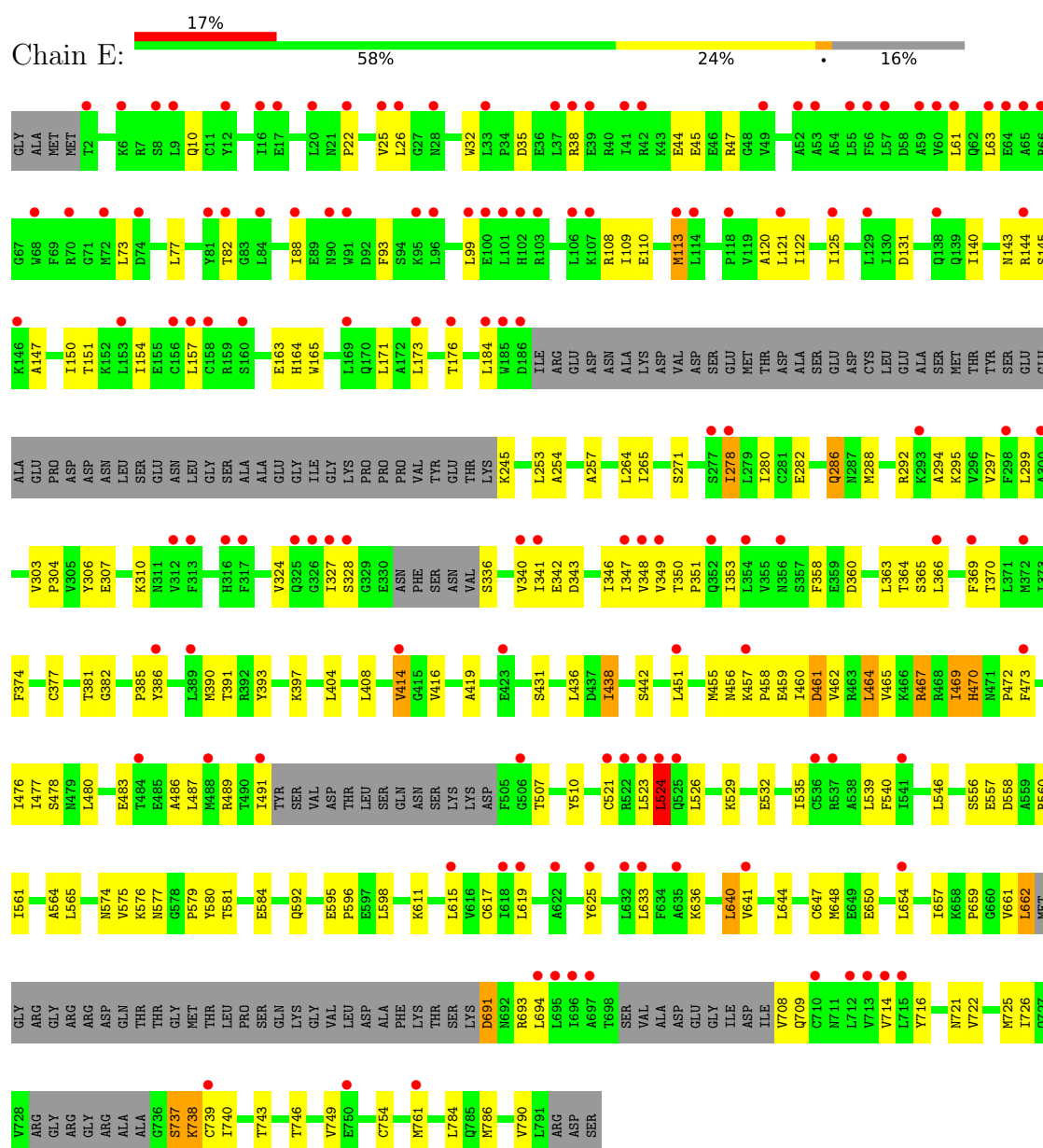


• Molecule 1: RETINOIC ACID INDUCIBLE PROTEIN I





• Molecule 1: RETINOIC ACID INDUCIBLE PROTEIN I



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	314.97Å 134.49Å 102.26Å 90.00° 92.17° 90.00°	Depositor
Resolution (Å)	157.37 – 3.40 48.06 – 3.40	Depositor EDS
% Data completeness (in resolution range)	97.6 (157.37-3.40) 97.6 (48.06-3.40)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.47 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.6.0116	Depositor
R, $R_{free}$	0.239 , 0.276 0.241 , 0.276	Depositor DCC
$R_{free}$ test set	2904 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	97.2	Xtriage
Anisotropy	0.309	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 94.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.054 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	21661	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	152.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.49	1/5510 (0.0%)	0.63	0/7434
1	B	0.49	0/5521	0.64	0/7448
1	D	0.42	0/5489	0.55	0/7406
1	E	0.43	0/5481	0.56	0/7395
All	All	0.46	1/22001 (0.0%)	0.60	0/29683

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	165	TRP	CD2-CE2	5.06	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	5425	0	5473	183	0
1	B	5436	0	5486	188	0
1	D	5404	0	5447	155	0
1	E	5396	0	5443	146	0
All	All	21661	0	21849	667	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 15.



All (667) 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:D:524:LEU:HD23	1:D:526:LEU:HD12	1.45	0.98
1:E:524:LEU:HD23	1:E:526:LEU:HD12	1.47	0.97
1:A:524:LEU:HD23	1:A:526:LEU:HD12	1.48	0.95
1:B:524:LEU:HD23	1:B:526:LEU:HD12	1.48	0.95
1:B:257:ALA:HB3	1:B:280:ILE:HD12	1.51	0.92
1:A:257:ALA:HB3	1:A:280:ILE:HD12	1.53	0.91
1:B:60:VAL:HG11	1:B:72:MET:CE	2.01	0.89
1:D:464:LEU:HD22	1:D:749:VAL:HG21	1.55	0.89
1:B:700:VAL:HG11	1:B:728:VAL:HG12	1.54	0.89
1:B:715:LEU:HD11	1:B:722:VAL:HG13	1.54	0.88
1:A:615:LEU:HD23	1:A:619:LEU:HD13	1.55	0.88
1:B:615:LEU:HD23	1:B:619:LEU:HD13	1.57	0.86
1:E:257:ALA:HB3	1:E:280:ILE:HD12	1.56	0.85
1:D:257:ALA:HB3	1:D:280:ILE:HD12	1.57	0.84
1:D:288:MET:HG3	1:D:294:ALA:HB2	1.61	0.83
1:E:327:ILE:HG22	1:E:349:VAL:HG22	1.59	0.83
1:E:288:MET:HG3	1:E:294:ALA:HB2	1.61	0.82
1:D:327:ILE:HG22	1:D:349:VAL:HG22	1.61	0.82
1:A:288:MET:HG3	1:A:294:ALA:HB2	1.62	0.81
1:A:327:ILE:HG22	1:A:349:VAL:HG22	1.63	0.81
1:B:288:MET:HG3	1:B:294:ALA:HB2	1.63	0.81
1:A:328:SER:HA	1:A:353:ILE:HD11	1.62	0.81
1:A:60:VAL:HG11	1:A:72:MET:CE	2.11	0.81
1:D:328:SER:HA	1:D:353:ILE:HD11	1.63	0.80
1:B:60:VAL:HG11	1:B:72:MET:HE1	1.63	0.80
1:B:327:ILE:HG22	1:B:349:VAL:HG22	1.63	0.79
1:A:13:ARG:NH2	1:A:58:ASP:OD1	2.15	0.79
1:E:77:LEU:HD23	1:E:82:THR:HG22	1.63	0.79
1:B:328:SER:HA	1:B:353:ILE:HD11	1.62	0.79
1:E:328:SER:HA	1:E:353:ILE:HD11	1.63	0.79
1:B:700:VAL:HG11	1:B:728:VAL:CG1	2.14	0.77
1:E:121:LEU:HD11	1:E:173:LEU:HD12	1.64	0.77
1:B:13:ARG:NH2	1:B:58:ASP:OD1	2.18	0.77
1:D:561:ILE:H	1:D:561:ILE:HD12	1.50	0.77
1:A:715:LEU:HD11	1:A:722:VAL:HG13	1.66	0.77
1:D:460:ILE:HD13	1:D:722:VAL:HG11	1.67	0.77
1:D:77:LEU:HD23	1:D:82:THR:HG22	1.64	0.77
1:D:121:LEU:HD11	1:D:173:LEU:HD12	1.67	0.77
1:D:615:LEU:HD23	1:D:619:LEU:HD13	1.67	0.76
1:B:297:VAL:HG12	1:B:299:LEU:HD23	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:615:LEU:HD23	1:E:619:LEU:HD13	1.68	0.75
1:E:561:ILE:H	1:E:561:ILE:HD12	1.52	0.75
1:B:122:ILE:HA	1:B:125:ILE:HG22	1.69	0.74
1:A:743:THR:HG21	1:A:748:VAL:HB	1.67	0.74
1:A:257:ALA:HB3	1:A:280:ILE:CD1	2.19	0.73
1:D:10:GLN:OE1	1:D:61:LEU:HD13	1.89	0.73
1:A:297:VAL:HG12	1:A:299:LEU:HD23	1.71	0.72
1:B:257:ALA:HB3	1:B:280:ILE:CD1	2.18	0.72
1:B:121:LEU:HD11	1:B:173:LEU:HD12	1.70	0.72
1:B:464:LEU:HD12	1:B:749:VAL:HG21	1.71	0.72
1:D:73:LEU:HD21	1:D:88:ILE:CD1	2.19	0.72
1:D:726:ILE:HD11	1:D:739:CYS:SG	2.30	0.72
1:A:105:LEU:HD23	1:A:185:TRP:CZ3	2.24	0.72
1:B:125:ILE:CD1	1:B:153:LEU:HD21	2.19	0.72
1:D:73:LEU:HD21	1:D:88:ILE:HD11	1.71	0.71
1:B:695:LEU:HD12	1:B:708:VAL:HG11	1.71	0.71
1:A:121:LEU:HD11	1:A:173:LEU:HD12	1.72	0.71
1:B:743:THR:HG21	1:B:748:VAL:HB	1.71	0.71
1:D:472:PRO:O	1:D:476:ILE:HD13	1.91	0.70
1:A:125:ILE:CD1	1:A:153:LEU:HD21	2.21	0.70
1:B:99:LEU:HD21	1:B:163:GLU:HA	1.73	0.70
1:E:472:PRO:O	1:E:476:ILE:HD13	1.92	0.70
1:A:122:ILE:HA	1:A:125:ILE:HG22	1.72	0.70
1:A:561:ILE:HD12	1:A:561:ILE:H	1.56	0.70
1:E:297:VAL:HG12	1:E:299:LEU:HD23	1.74	0.70
1:E:73:LEU:HD21	1:E:88:ILE:HD11	1.73	0.70
1:A:472:PRO:O	1:A:476:ILE:HD13	1.91	0.69
1:D:297:VAL:HG12	1:D:299:LEU:HD23	1.74	0.69
1:E:73:LEU:HD21	1:E:88:ILE:CD1	2.21	0.69
1:B:561:ILE:HD12	1:B:561:ILE:H	1.56	0.69
1:A:265:ILE:HD13	1:A:442:SER:HB3	1.75	0.69
1:B:105:LEU:HD23	1:B:185:TRP:CZ3	2.28	0.69
1:E:257:ALA:HB3	1:E:280:ILE:CD1	2.21	0.69
1:B:465:VAL:HG13	1:B:614:GLU:HG3	1.73	0.69
1:A:592:GLN:OE1	1:B:592:GLN:OE1	2.10	0.68
1:D:257:ALA:HB3	1:D:280:ILE:CD1	2.22	0.68
1:E:265:ILE:HD13	1:E:442:SER:HB3	1.73	0.68
1:D:265:ILE:HD13	1:D:442:SER:HB3	1.74	0.68
1:D:737:SER:O	1:D:738:LYS:HB2	1.95	0.67
1:B:737:SER:O	1:B:738:LYS:HB2	1.94	0.67
1:E:10:GLN:OE1	1:E:61:LEU:HD13	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:ILE:HD13	1:B:442:SER:HB3	1.75	0.67
1:D:73:LEU:CD2	1:D:88:ILE:HD11	2.25	0.66
1:E:654:LEU:HD22	1:E:657:ILE:HD12	1.77	0.66
1:A:737:SER:O	1:A:738:LYS:HB2	1.94	0.66
1:B:700:VAL:CG1	1:B:728:VAL:HG12	2.25	0.65
1:A:99:LEU:HD21	1:A:163:GLU:HA	1.77	0.65
1:A:722:VAL:HG21	1:A:741:LEU:HD22	1.79	0.65
1:A:60:VAL:HG11	1:A:72:MET:HE1	1.79	0.65
1:E:73:LEU:CD2	1:E:88:ILE:HD11	2.26	0.65
1:E:737:SER:O	1:E:738:LYS:HB2	1.98	0.64
1:A:125:ILE:HD11	1:A:157:LEU:CD1	2.28	0.64
1:E:288:MET:HE1	1:E:370:THR:HG21	1.79	0.64
1:D:122:ILE:HA	1:D:125:ILE:HG22	1.81	0.63
1:D:264:LEU:HD13	1:D:377:CYS:SG	2.39	0.63
1:B:25:VAL:HG13	1:B:29:MET:CE	2.29	0.63
1:E:416:VAL:HG13	1:E:419:ALA:HB3	1.81	0.63
1:B:472:PRO:O	1:B:476:ILE:HD13	1.98	0.63
1:E:122:ILE:HA	1:E:125:ILE:HG22	1.81	0.63
1:B:416:VAL:HG13	1:B:419:ALA:HB3	1.81	0.63
1:A:288:MET:HE1	1:A:370:THR:HG21	1.81	0.63
1:A:416:VAL:HG13	1:A:419:ALA:HB3	1.80	0.63
1:D:654:LEU:HD22	1:D:657:ILE:HD12	1.80	0.63
1:A:44:GLU:OE2	1:A:47:ARG:NH1	2.32	0.62
1:B:726:ILE:HD11	1:B:739:CYS:SG	2.39	0.62
1:B:654:LEU:HD22	1:B:657:ILE:HD12	1.81	0.62
1:A:715:LEU:HD12	1:A:722:VAL:HG22	1.81	0.62
1:B:153:LEU:HD23	1:B:153:LEU:C	2.19	0.62
1:D:288:MET:HE1	1:D:370:THR:HG21	1.81	0.62
1:D:416:VAL:HG13	1:D:419:ALA:HB3	1.81	0.62
1:A:153:LEU:HD23	1:A:153:LEU:C	2.20	0.62
1:A:487:LEU:O	1:A:491:ILE:HD13	1.99	0.62
1:D:108:ARG:NH2	1:D:532:GLU:OE2	2.32	0.62
1:A:654:LEU:HD22	1:A:657:ILE:HD12	1.81	0.61
1:E:726:ILE:HD11	1:E:739:CYS:SG	2.40	0.61
1:E:264:LEU:HD13	1:E:377:CYS:SG	2.40	0.61
1:B:44:GLU:OE2	1:B:47:ARG:NH1	2.34	0.61
1:A:615:LEU:HD12	1:A:716:TYR:CD1	2.36	0.61
1:A:264:LEU:HD13	1:A:377:CYS:SG	2.40	0.61
1:B:393:TYR:CD1	1:B:404:LEU:HD22	2.36	0.61
1:D:606:THR:O	1:D:606:THR:HG22	2.01	0.61
1:B:487:LEU:O	1:B:491:ILE:HD13	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:487:LEU:O	1:E:491:ILE:HD13	2.01	0.60
1:B:581:THR:HB	1:B:584:GLU:HG3	1.83	0.60
1:B:328:SER:HA	1:B:353:ILE:CD1	2.30	0.60
1:D:393:TYR:CD1	1:D:404:LEU:HD22	2.37	0.60
1:A:726:ILE:HD11	1:A:739:CYS:SG	2.42	0.59
1:B:715:LEU:HD12	1:B:722:VAL:HG22	1.83	0.59
1:E:288:MET:HE3	1:E:292:ARG:HG2	1.84	0.59
1:E:328:SER:HA	1:E:353:ILE:CD1	2.32	0.59
1:E:416:VAL:O	1:E:416:VAL:CG1	2.50	0.59
1:A:165:TRP:O	1:A:166:PRO:C	2.40	0.59
1:D:278:ILE:HD12	1:D:278:ILE:C	2.22	0.59
1:A:125:ILE:HD11	1:A:157:LEU:HD13	1.83	0.59
1:A:393:TYR:CD1	1:A:404:LEU:HD22	2.38	0.59
1:D:147:ALA:O	1:D:150:ILE:HG22	2.02	0.59
1:B:297:VAL:HG12	1:B:299:LEU:CD2	2.32	0.59
1:E:278:ILE:C	1:E:278:ILE:HD12	2.21	0.59
1:E:393:TYR:CD1	1:E:404:LEU:HD22	2.37	0.59
1:A:25:VAL:HG13	1:A:29:MET:CE	2.33	0.58
1:A:581:THR:HB	1:A:584:GLU:HG3	1.84	0.58
1:A:288:MET:HE3	1:A:292:ARG:HG2	1.85	0.58
1:D:109:ILE:O	1:D:109:ILE:HG22	2.02	0.58
1:B:165:TRP:O	1:B:166:PRO:C	2.38	0.58
1:B:615:LEU:HD12	1:B:716:TYR:CD1	2.38	0.58
1:A:615:LEU:HD12	1:A:716:TYR:CG	2.39	0.58
1:B:722:VAL:HG21	1:B:741:LEU:HD22	1.85	0.58
1:B:288:MET:HE1	1:B:370:THR:HG21	1.85	0.58
1:D:328:SER:HA	1:D:353:ILE:CD1	2.33	0.58
1:E:469:ILE:O	1:E:470:HIS:CG	2.56	0.58
1:D:416:VAL:CG1	1:D:416:VAL:O	2.51	0.58
1:A:21:ASN:OD1	1:A:23:VAL:HG23	2.04	0.58
1:A:88:ILE:HD12	1:A:88:ILE:C	2.23	0.57
1:B:21:ASN:OD1	1:B:23:VAL:HG23	2.04	0.57
1:D:487:LEU:O	1:D:491:ILE:HD13	2.04	0.57
1:D:558:ASP:HB2	1:D:640:LEU:HD11	1.86	0.57
1:E:560:ARG:HG3	1:E:647:CYS:SG	2.43	0.57
1:A:328:SER:HA	1:A:353:ILE:CD1	2.32	0.57
1:A:416:VAL:CG1	1:A:416:VAL:O	2.53	0.57
1:E:147:ALA:O	1:E:150:ILE:HG22	2.04	0.57
1:B:264:LEU:HD13	1:B:377:CYS:SG	2.44	0.57
1:D:364:THR:O	1:D:364:THR:HG22	2.04	0.57
1:E:109:ILE:O	1:E:109:ILE:HG22	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:113:MET:HE1	1:E:173:LEU:HD21	1.87	0.57
1:A:278:ILE:HD12	1:A:278:ILE:C	2.25	0.57
1:B:125:ILE:HD11	1:B:157:LEU:CD1	2.35	0.57
1:E:113:MET:CE	1:E:173:LEU:HD21	2.35	0.57
1:E:465:VAL:HG11	1:E:611:LYS:HA	1.87	0.57
1:B:184:LEU:HD12	1:B:522:ARG:HD3	1.87	0.57
1:D:26:LEU:HD22	1:D:38:ARG:HG2	1.87	0.57
1:E:26:LEU:HD22	1:E:38:ARG:HG2	1.87	0.57
1:A:184:LEU:HD12	1:A:522:ARG:HD3	1.87	0.56
1:A:603:LYS:O	1:A:604:ASP:C	2.42	0.56
1:B:364:THR:HG22	1:B:364:THR:O	2.05	0.56
1:B:88:ILE:HD12	1:B:88:ILE:C	2.26	0.56
1:A:700:VAL:HG21	1:A:728:VAL:C	2.26	0.56
1:A:60:VAL:HG11	1:A:72:MET:HE3	1.87	0.56
1:D:565:LEU:HD12	1:D:598:LEU:HB3	1.87	0.56
1:E:108:ARG:NH2	1:E:532:GLU:OE2	2.37	0.56
1:A:560:ARG:HG3	1:A:647:CYS:SG	2.45	0.56
1:A:715:LEU:CD1	1:A:722:VAL:HG22	2.36	0.56
1:B:288:MET:HE3	1:B:292:ARG:HG2	1.87	0.56
1:D:297:VAL:HG12	1:D:299:LEU:CD2	2.36	0.56
1:D:629:THR:HG23	1:D:711:ASN:OD1	2.06	0.56
1:E:364:THR:O	1:E:364:THR:HG22	2.04	0.56
1:E:297:VAL:HG12	1:E:299:LEU:CD2	2.36	0.56
1:A:297:VAL:HG12	1:A:299:LEU:CD2	2.35	0.56
1:D:560:ARG:HG3	1:D:647:CYS:SG	2.46	0.56
1:D:99:LEU:HD22	1:D:165:TRP:NE1	2.21	0.56
1:B:278:ILE:HD12	1:B:278:ILE:C	2.26	0.55
1:B:565:LEU:HD12	1:B:598:LEU:HB3	1.88	0.55
1:E:469:ILE:HD12	1:E:469:ILE:H	1.71	0.55
1:E:558:ASP:HB2	1:E:640:LEU:HD11	1.88	0.55
1:A:73:LEU:HD21	1:A:88:ILE:CG1	2.36	0.55
1:E:99:LEU:HD22	1:E:165:TRP:NE1	2.21	0.55
1:A:184:LEU:HD21	1:A:540:PHE:CE1	2.41	0.55
1:E:88:ILE:HG22	1:E:93:PHE:HZ	1.70	0.55
1:A:364:THR:O	1:A:364:THR:HG22	2.06	0.55
1:A:257:ALA:CB	1:A:280:ILE:HD12	2.33	0.55
1:D:615:LEU:HD12	1:D:716:TYR:CD1	2.40	0.55
1:E:565:LEU:HD12	1:E:598:LEU:HB3	1.87	0.55
1:D:464:LEU:CD2	1:D:749:VAL:HG21	2.34	0.55
1:A:698:THR:O	1:A:700:VAL:N	2.40	0.55
1:B:184:LEU:HD21	1:B:540:PHE:CE1	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:ILE:HG22	1:D:93:PHE:HZ	1.70	0.55
1:A:1:MET:HB2	1:A:4:ASP:HB2	1.89	0.54
1:B:130:ILE:O	1:B:131:ASP:C	2.45	0.54
1:B:22:PRO:HG3	1:B:53:ALA:HA	1.89	0.54
1:A:35:ASP:OD1	1:A:38:ARG:NH2	2.38	0.54
1:A:465:VAL:HG13	1:A:614:GLU:HG3	1.88	0.54
1:A:565:LEU:HD12	1:A:598:LEU:HB3	1.88	0.54
1:B:257:ALA:CB	1:B:280:ILE:HD12	2.32	0.54
1:B:416:VAL:O	1:B:416:VAL:CG1	2.55	0.54
1:D:288:MET:HE3	1:D:292:ARG:HG2	1.90	0.54
1:B:477:ILE:O	1:B:480:LEU:N	2.40	0.54
1:E:581:THR:HB	1:E:584:GLU:HG3	1.90	0.54
1:D:113:MET:CE	1:D:173:LEU:HD21	2.38	0.54
1:D:521:CYS:SG	1:D:539:LEU:HD13	2.48	0.53
1:D:110:GLU:HG3	1:D:154:ILE:HD11	1.91	0.53
1:B:23:VAL:HG13	1:B:42:ARG:HG2	1.90	0.53
1:D:581:THR:HB	1:D:584:GLU:HG3	1.90	0.53
1:E:633:LEU:HD12	1:E:714:VAL:HG12	1.89	0.53
1:E:461:ASP:HB3	1:E:740:ILE:HG23	1.91	0.53
1:E:464:LEU:HD12	1:E:465:VAL:N	2.24	0.53
1:B:73:LEU:HD21	1:B:88:ILE:CG1	2.39	0.53
1:D:143:ASN:CG	1:E:650:GLU:HG2	2.28	0.53
1:B:129:LEU:HD21	1:B:157:LEU:HD13	1.91	0.53
1:A:615:LEU:HD22	1:A:648:MET:HE1	1.91	0.52
1:A:73:LEU:HD21	1:A:88:ILE:HG13	1.91	0.52
1:D:710:CYS:SG	1:D:711:ASN:N	2.82	0.52
1:D:461:ASP:CB	1:D:740:ILE:HG23	2.39	0.52
1:A:130:ILE:O	1:A:131:ASP:C	2.47	0.52
1:A:129:LEU:HD21	1:A:157:LEU:HD13	1.90	0.52
1:E:140:ILE:HG23	1:E:144:ARG:HD3	1.92	0.52
1:B:125:ILE:HD11	1:B:157:LEU:HD13	1.91	0.52
1:E:349:VAL:HG12	1:E:350:THR:O	2.10	0.52
1:A:270:GLY:HA3	1:A:727:GLN:HE22	1.74	0.52
1:B:125:ILE:HD11	1:B:157:LEU:CD2	2.39	0.52
1:B:25:VAL:HG13	1:B:29:MET:HE2	1.92	0.52
1:B:790:VAL:HG12	1:B:790:VAL:O	2.10	0.52
1:E:521:CYS:SG	1:E:539:LEU:HD13	2.49	0.52
1:A:358:PHE:CZ	1:A:366:LEU:HD13	2.45	0.52
1:B:1:MET:HB2	1:B:4:ASP:HB2	1.91	0.52
1:E:310:LYS:HA	1:E:348:VAL:HG21	1.91	0.52
1:D:77:LEU:CD2	1:D:82:THR:HG22	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:77:LEU:CD2	1:E:82:THR:HG22	2.38	0.51
1:B:297:VAL:CG1	1:B:299:LEU:CD2	2.88	0.51
1:D:790:VAL:O	1:D:790:VAL:HG12	2.09	0.51
1:A:310:LYS:HA	1:A:348:VAL:HG21	1.92	0.51
1:B:358:PHE:CZ	1:B:366:LEU:HD13	2.45	0.51
1:B:73:LEU:HD21	1:B:88:ILE:HD11	1.92	0.51
1:A:110:GLU:HG3	1:A:154:ILE:HD11	1.91	0.51
1:B:615:LEU:HD11	1:B:633:LEU:HD11	1.92	0.51
1:B:632:LEU:HB2	1:B:710:CYS:SG	2.50	0.51
1:D:524:LEU:CD2	1:D:526:LEU:HD12	2.28	0.51
1:A:700:VAL:HG11	1:A:728:VAL:HG12	1.93	0.51
1:A:464:LEU:HD12	1:A:749:VAL:HG21	1.92	0.51
1:D:140:ILE:HG23	1:D:144:ARG:HD3	1.93	0.50
1:D:349:VAL:HG12	1:D:350:THR:O	2.10	0.50
1:A:349:VAL:HG12	1:A:350:THR:O	2.11	0.50
1:A:73:LEU:HD21	1:A:88:ILE:HD11	1.92	0.50
1:B:743:THR:HG21	1:B:748:VAL:CB	2.39	0.50
1:E:110:GLU:HG3	1:E:154:ILE:HD11	1.93	0.50
1:B:747:GLU:O	1:B:751:ASN:HB2	2.12	0.50
1:A:350:THR:HG23	1:A:351:PRO:HD2	1.93	0.50
1:A:615:LEU:HD22	1:A:648:MET:CE	2.41	0.50
1:A:73:LEU:HD11	1:A:88:ILE:HD11	1.94	0.50
1:B:350:THR:HG23	1:B:351:PRO:HD2	1.93	0.50
1:E:295:LYS:NZ	1:E:342:GLU:HA	2.27	0.50
1:B:310:LYS:HA	1:B:348:VAL:HG21	1.92	0.50
1:A:615:LEU:HD11	1:A:633:LEU:HD11	1.93	0.50
1:A:60:VAL:HG13	1:A:68:TRP:CZ3	2.47	0.50
1:B:381:THR:HG22	1:B:382:GLY:N	2.27	0.50
1:B:715:LEU:CD1	1:B:722:VAL:HG22	2.42	0.50
1:A:436:LEU:CB	1:A:438:ILE:HD13	2.42	0.50
1:B:110:GLU:HG3	1:B:154:ILE:HD11	1.94	0.50
1:D:464:LEU:HD13	1:D:749:VAL:CG2	2.42	0.50
1:B:661:VAL:HG12	1:B:662:LEU:N	2.27	0.50
1:B:347:ILE:HG22	1:B:349:VAL:CG2	2.42	0.50
1:B:615:LEU:HD12	1:B:716:TYR:CG	2.47	0.50
1:D:358:PHE:CZ	1:D:366:LEU:HD13	2.47	0.50
1:A:477:ILE:O	1:A:480:LEU:N	2.44	0.49
1:A:63:LEU:HD23	1:A:68:TRP:CG	2.47	0.49
1:B:483:GLU:O	1:B:486:ALA:HB3	2.12	0.49
1:A:714:VAL:HG22	1:A:740:ILE:HB	1.94	0.49
1:A:80:GLY:O	1:A:82:THR:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:LEU:HD21	1:B:88:ILE:HG13	1.93	0.49
1:B:295:LYS:NZ	1:B:342:GLU:HA	2.27	0.49
1:D:295:LYS:NZ	1:D:342:GLU:HA	2.28	0.49
1:A:110:GLU:HG3	1:A:154:ILE:CD1	2.42	0.49
1:A:465:VAL:HG21	1:A:742:VAL:HG13	1.94	0.49
1:B:328:SER:CA	1:B:353:ILE:HD11	2.37	0.49
1:D:113:MET:HE1	1:D:173:LEU:HD21	1.94	0.49
1:E:32:TRP:HB3	1:E:63:LEU:HD21	1.94	0.49
1:A:297:VAL:CG1	1:A:299:LEU:CD2	2.90	0.49
1:B:336:SER:O	1:B:340:VAL:HG23	2.13	0.49
1:A:295:LYS:NZ	1:A:342:GLU:HA	2.27	0.49
1:A:431:SER:HA	1:A:784:LEU:HD13	1.93	0.49
1:D:464:LEU:HD13	1:D:749:VAL:HG21	1.94	0.49
1:A:23:VAL:HG13	1:A:42:ARG:HG2	1.95	0.49
1:D:310:LYS:HA	1:D:348:VAL:HG21	1.94	0.49
1:D:32:TRP:HB3	1:D:63:LEU:HD21	1.94	0.49
1:A:381:THR:HG22	1:A:382:GLY:N	2.28	0.49
1:A:595:GLU:OE1	1:B:576:LYS:NZ	2.34	0.49
1:B:60:VAL:HG13	1:B:68:TRP:CZ3	2.48	0.49
1:E:328:SER:CA	1:E:353:ILE:HD11	2.38	0.49
1:E:347:ILE:HG22	1:E:349:VAL:CG2	2.43	0.49
1:A:303:VAL:N	1:A:304:PRO:HD2	2.28	0.49
1:A:629:THR:HG23	1:A:711:ASN:OD1	2.13	0.49
1:B:95:LYS:HD3	1:B:163:GLU:OE1	2.13	0.49
1:D:477:ILE:O	1:D:480:LEU:N	2.46	0.48
1:E:358:PHE:CZ	1:E:366:LEU:HD13	2.47	0.48
1:E:431:SER:HA	1:E:784:LEU:HD13	1.95	0.48
1:B:306:TYR:CZ	1:B:328:SER:HB2	2.48	0.48
1:B:35:ASP:OD1	1:B:38:ARG:NH2	2.41	0.48
1:B:595:GLU:N	1:B:596:PRO:CD	2.76	0.48
1:A:22:PRO:HG3	1:A:53:ALA:HA	1.95	0.48
1:A:615:LEU:HD23	1:A:619:LEU:CD1	2.37	0.48
1:B:303:VAL:N	1:B:304:PRO:HD2	2.28	0.48
1:B:615:LEU:HD22	1:B:648:MET:CE	2.44	0.48
1:D:615:LEU:HD22	1:D:648:MET:CE	2.44	0.48
1:D:726:ILE:CD1	1:D:739:CYS:SG	3.00	0.48
1:B:45:GLU:HG2	1:B:49:VAL:HG22	1.95	0.48
1:B:524:LEU:CD2	1:B:526:LEU:HD12	2.31	0.48
1:D:306:TYR:CZ	1:D:328:SER:HB2	2.49	0.48
1:E:615:LEU:HD22	1:E:648:MET:CE	2.44	0.48
1:A:336:SER:O	1:A:340:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:491:ILE:N	1:B:491:ILE:HD12	2.28	0.48
1:B:122:ILE:HA	1:B:125:ILE:CG2	2.40	0.48
1:B:349:VAL:HG12	1:B:350:THR:O	2.12	0.48
1:D:264:LEU:HD21	1:D:414:VAL:CG1	2.44	0.48
1:E:257:ALA:CB	1:E:280:ILE:HD12	2.36	0.48
1:A:60:VAL:CG1	1:A:68:TRP:CZ3	2.96	0.48
1:D:347:ILE:HG22	1:D:349:VAL:CG2	2.42	0.48
1:E:691:ASP:OD2	1:E:691:ASP:N	2.47	0.48
1:E:790:VAL:O	1:E:790:VAL:HG12	2.14	0.48
1:A:347:ILE:HG22	1:A:349:VAL:CG2	2.43	0.47
1:A:483:GLU:O	1:A:486:ALA:HB3	2.14	0.47
1:B:603:LYS:O	1:B:604:ASP:C	2.52	0.47
1:D:661:VAL:HG12	1:D:662:LEU:N	2.29	0.47
1:E:278:ILE:O	1:E:278:ILE:HD12	2.14	0.47
1:E:381:THR:HG22	1:E:382:GLY:N	2.29	0.47
1:E:436:LEU:CB	1:E:438:ILE:HD13	2.44	0.47
1:A:632:LEU:HB2	1:A:710:CYS:SG	2.54	0.47
1:B:523:LEU:O	1:B:524:LEU:C	2.53	0.47
1:D:431:SER:HA	1:D:784:LEU:HD13	1.96	0.47
1:A:661:VAL:HG12	1:A:662:LEU:N	2.28	0.47
1:B:465:VAL:HG12	1:B:466:LYS:N	2.29	0.47
1:D:436:LEU:CB	1:D:438:ILE:HD13	2.45	0.47
1:E:306:TYR:CZ	1:E:328:SER:HB2	2.49	0.47
1:A:521:CYS:SG	1:A:539:LEU:HD13	2.55	0.47
1:A:524:LEU:CD2	1:A:526:LEU:HD12	2.31	0.47
1:B:63:LEU:HD23	1:B:68:TRP:CG	2.50	0.47
1:D:328:SER:CA	1:D:353:ILE:HD11	2.38	0.47
1:E:125:ILE:HD11	1:E:157:LEU:CD2	2.45	0.47
1:E:524:LEU:CD2	1:E:526:LEU:HD12	2.29	0.47
1:A:328:SER:CA	1:A:353:ILE:HD11	2.39	0.47
1:E:303:VAL:N	1:E:304:PRO:HD2	2.29	0.47
1:A:306:TYR:CZ	1:A:328:SER:HB2	2.49	0.47
1:D:22:PRO:HA	1:D:25:VAL:HG12	1.97	0.47
1:E:282:GLU:O	1:E:286:GLN:HB2	2.14	0.47
1:E:299:LEU:HD12	1:E:374:PHE:CE1	2.50	0.47
1:A:523:LEU:O	1:A:524:LEU:C	2.53	0.47
1:A:722:VAL:CG2	1:A:741:LEU:HD22	2.44	0.47
1:A:790:VAL:O	1:A:790:VAL:HG12	2.14	0.47
1:D:297:VAL:CG1	1:D:299:LEU:CD2	2.93	0.47
1:D:303:VAL:N	1:D:304:PRO:HD2	2.29	0.47
1:A:554:ILE:HG22	1:A:640:LEU:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:ALA:HA	1:B:280:ILE:HD11	1.97	0.47
1:B:436:LEU:CB	1:B:438:ILE:HD13	2.45	0.47
1:B:722:VAL:O	1:B:723:THR:C	2.53	0.47
1:E:416:VAL:HG11	1:E:761:MET:CE	2.45	0.47
1:B:477:ILE:O	1:B:478:SER:C	2.52	0.47
1:D:327:ILE:HG23	1:D:353:ILE:HD13	1.97	0.47
1:E:641:VAL:HG11	1:E:661:VAL:HG13	1.97	0.47
1:A:691:ASP:OD2	1:A:691:ASP:N	2.48	0.47
1:D:257:ALA:CB	1:D:280:ILE:HD12	2.37	0.47
1:E:393:TYR:CE1	1:E:404:LEU:HD22	2.50	0.47
1:E:661:VAL:HG12	1:E:662:LEU:N	2.29	0.47
1:A:278:ILE:HD12	1:A:278:ILE:O	2.15	0.46
1:D:278:ILE:HD12	1:D:278:ILE:O	2.15	0.46
1:D:336:SER:O	1:D:340:VAL:HG23	2.16	0.46
1:E:336:SER:O	1:E:340:VAL:HG23	2.16	0.46
1:B:458:PRO:HG2	1:B:726:ILE:HD13	1.97	0.46
1:B:473:PHE:CZ	1:B:564:ALA:HB1	2.50	0.46
1:E:297:VAL:CG1	1:E:299:LEU:CD2	2.93	0.46
1:B:431:SER:HA	1:B:784:LEU:HD13	1.97	0.46
1:B:641:VAL:HG11	1:B:661:VAL:HG13	1.98	0.46
1:B:80:GLY:O	1:B:82:THR:N	2.47	0.46
1:D:184:LEU:HD21	1:D:540:PHE:CE1	2.50	0.46
1:D:282:GLU:O	1:D:286:GLN:HB2	2.14	0.46
1:D:691:ASP:N	1:D:691:ASP:OD2	2.48	0.46
1:D:561:ILE:HD12	1:D:561:ILE:N	2.25	0.46
1:D:73:LEU:CG	1:D:88:ILE:HD11	2.45	0.46
1:E:350:THR:HG23	1:E:351:PRO:HD2	1.97	0.46
1:E:477:ILE:O	1:E:480:LEU:N	2.48	0.46
1:A:125:ILE:HD11	1:A:157:LEU:CD2	2.46	0.46
1:B:722:VAL:CG2	1:B:741:LEU:HD22	2.45	0.46
1:D:641:VAL:HG11	1:D:661:VAL:HG13	1.96	0.46
1:E:99:LEU:HD21	1:E:163:GLU:HA	1.98	0.46
1:A:469:ILE:HD12	1:A:469:ILE:H	1.80	0.46
1:B:691:ASP:OD2	1:B:691:ASP:N	2.49	0.46
1:A:436:LEU:HB2	1:A:438:ILE:HD13	1.98	0.46
1:A:576:LYS:CE	1:A:592:GLN:HE22	2.28	0.46
1:A:69:PHE:CZ	1:A:88:ILE:HD13	2.51	0.46
1:A:95:LYS:HD3	1:A:163:GLU:OE1	2.16	0.46
1:B:615:LEU:HD22	1:B:648:MET:HE1	1.98	0.46
1:D:44:GLU:OE2	1:D:47:ARG:NH1	2.48	0.46
1:D:574:ASN:O	1:D:577:ASN:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:22:PRO:HA	1:E:25:VAL:HG12	1.98	0.46
1:E:523:LEU:O	1:E:524:LEU:C	2.55	0.46
1:E:708:VAL:CG1	1:E:709:GLN:N	2.79	0.46
1:E:461:ASP:CB	1:E:740:ILE:HG23	2.46	0.46
1:B:60:VAL:CG1	1:B:68:TRP:CZ3	2.99	0.46
1:D:381:THR:HG22	1:D:382:GLY:N	2.31	0.46
1:E:73:LEU:CG	1:E:88:ILE:HD11	2.46	0.46
1:A:254:ALA:HA	1:A:280:ILE:HD11	1.99	0.45
1:A:595:GLU:N	1:A:596:PRO:CD	2.78	0.45
1:B:110:GLU:HG3	1:B:154:ILE:CD1	2.46	0.45
1:E:297:VAL:CG2	1:E:369:PHE:CE2	3.00	0.45
1:B:554:ILE:HG22	1:B:640:LEU:HD12	1.97	0.45
1:B:659:PRO:HB3	1:B:694:LEU:HD23	1.98	0.45
1:D:109:ILE:O	1:D:109:ILE:CG2	2.64	0.45
1:A:132:ARG:HA	1:A:135:GLU:HG2	1.98	0.45
1:B:125:ILE:HD11	1:B:157:LEU:HD22	1.97	0.45
1:B:165:TRP:O	1:B:168:SER:N	2.50	0.45
1:B:576:LYS:CE	1:B:592:GLN:HE22	2.30	0.45
1:D:393:TYR:CE1	1:D:404:LEU:HD22	2.51	0.45
1:D:465:VAL:HG12	1:D:466:LYS:N	2.31	0.45
1:B:393:TYR:CE1	1:B:404:LEU:HD22	2.51	0.45
1:D:615:LEU:HD12	1:D:716:TYR:CG	2.52	0.45
1:A:327:ILE:HG23	1:A:353:ILE:HD13	1.98	0.45
1:A:491:ILE:HD12	1:A:491:ILE:N	2.32	0.45
1:B:467:ARG:NH1	1:B:557:GLU:OE2	2.50	0.45
1:B:560:ARG:HG3	1:B:647:CYS:SG	2.56	0.45
1:D:790:VAL:CG1	1:D:790:VAL:O	2.64	0.45
1:A:743:THR:HG21	1:A:748:VAL:CB	2.41	0.45
1:B:100:GLU:HA	1:B:103:ARG:HD3	1.99	0.45
1:B:132:ARG:HA	1:B:135:GLU:HG2	1.98	0.45
1:B:574:ASN:O	1:B:575:VAL:C	2.55	0.45
1:D:350:THR:HG23	1:D:351:PRO:HD2	1.99	0.45
1:A:529:LYS:HA	1:A:532:GLU:HB3	1.98	0.45
1:B:278:ILE:HD12	1:B:278:ILE:O	2.17	0.45
1:E:491:ILE:HD12	1:E:491:ILE:N	2.32	0.45
1:A:299:LEU:HD12	1:A:374:PHE:CE1	2.51	0.45
1:B:529:LYS:HA	1:B:532:GLU:HB3	1.99	0.45
1:B:574:ASN:O	1:B:577:ASN:N	2.50	0.45
1:B:790:VAL:O	1:B:790:VAL:CG1	2.65	0.45
1:D:327:ILE:CG2	1:D:349:VAL:HG13	2.47	0.45
1:E:109:ILE:CG2	1:E:109:ILE:O	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:ASN:O	1:A:577:ASN:N	2.50	0.45
1:D:125:ILE:HD11	1:D:157:LEU:CD2	2.46	0.45
1:E:254:ALA:HA	1:E:280:ILE:HD11	1.99	0.45
1:E:529:LYS:HA	1:E:532:GLU:HB3	1.98	0.45
1:E:615:LEU:HD12	1:E:716:TYR:CD1	2.52	0.45
1:A:100:GLU:HA	1:A:103:ARG:HD3	1.99	0.45
1:A:254:ALA:CA	1:A:280:ILE:HD11	2.47	0.45
1:A:641:VAL:HG11	1:A:661:VAL:HG13	1.97	0.45
1:D:299:LEU:HD12	1:D:374:PHE:CE1	2.52	0.45
1:B:254:ALA:CA	1:B:280:ILE:HD11	2.46	0.44
1:B:464:LEU:HD12	1:B:749:VAL:CG2	2.44	0.44
1:B:715:LEU:HD11	1:B:722:VAL:CG1	2.37	0.44
1:A:264:LEU:CD1	1:A:377:CYS:SG	3.04	0.44
1:B:700:VAL:HG21	1:B:728:VAL:C	2.38	0.44
1:D:461:ASP:HB2	1:D:740:ILE:HG23	1.99	0.44
1:E:184:LEU:HD21	1:E:540:PHE:CE1	2.51	0.44
1:D:469:ILE:O	1:D:469:ILE:HG22	2.17	0.44
1:E:254:ALA:CA	1:E:280:ILE:HD11	2.48	0.44
1:E:324:VAL:HG22	1:E:346:ILE:HB	2.00	0.44
1:E:574:ASN:O	1:E:577:ASN:N	2.49	0.44
1:A:41:ILE:HD13	1:A:56:PHE:HB2	2.00	0.44
1:B:615:LEU:CD2	1:B:619:LEU:HD13	2.39	0.44
1:D:615:LEU:HD22	1:D:648:MET:HE3	2.00	0.44
1:E:464:LEU:HD22	1:E:749:VAL:HG21	1.99	0.44
1:D:99:LEU:HD21	1:D:163:GLU:HA	1.99	0.44
1:D:416:VAL:HG11	1:D:761:MET:CE	2.47	0.44
1:E:523:LEU:HD23	1:E:524:LEU:N	2.32	0.44
1:A:487:LEU:O	1:A:491:ILE:CD1	2.63	0.44
1:A:73:LEU:HD21	1:A:88:ILE:CD1	2.47	0.44
1:B:278:ILE:HD13	1:B:316:HIS:NE2	2.32	0.44
1:B:282:GLU:O	1:B:286:GLN:HB2	2.16	0.44
1:B:45:GLU:HA	1:B:52:ALA:HB2	2.00	0.44
1:D:297:VAL:CG2	1:D:369:PHE:CE2	3.01	0.44
1:D:529:LYS:HA	1:D:532:GLU:HB3	2.00	0.44
1:E:264:LEU:HD21	1:E:414:VAL:CG1	2.48	0.44
1:A:282:GLU:O	1:A:286:GLN:HB2	2.17	0.44
1:D:254:ALA:HA	1:D:280:ILE:HD11	2.00	0.44
1:D:35:ASP:OD1	1:D:38:ARG:NH2	2.49	0.44
1:A:125:ILE:HD12	1:A:153:LEU:HD21	1.97	0.44
1:B:717:GLU:OE2	1:B:744:SER:OG	2.18	0.44
1:D:265:ILE:HG12	1:D:408:LEU:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:44:GLU:OE2	1:E:47:ARG:NH1	2.50	0.44
1:B:385:PRO:O	1:B:386:TYR:C	2.54	0.44
1:B:73:LEU:HD21	1:B:88:ILE:CD1	2.48	0.44
1:E:35:ASP:OD1	1:E:38:ARG:NH2	2.50	0.44
1:B:110:GLU:OE2	1:B:154:ILE:HD11	2.18	0.43
1:D:324:VAL:HG22	1:D:346:ILE:HB	1.99	0.43
1:E:595:GLU:N	1:E:596:PRO:CD	2.81	0.43
1:A:385:PRO:O	1:A:386:TYR:C	2.56	0.43
1:D:523:LEU:HD23	1:D:524:LEU:N	2.33	0.43
1:D:650:GLU:HG2	1:E:143:ASN:CG	2.39	0.43
1:E:436:LEU:HB2	1:E:438:ILE:HD13	1.99	0.43
1:D:436:LEU:HB2	1:D:438:ILE:HD13	2.00	0.43
1:E:469:ILE:O	1:E:470:HIS:CB	2.65	0.43
1:A:477:ILE:O	1:A:478:SER:C	2.57	0.43
1:D:491:ILE:N	1:D:491:ILE:HD12	2.33	0.43
1:D:523:LEU:O	1:D:524:LEU:C	2.56	0.43
1:E:327:ILE:CG2	1:E:349:VAL:HG13	2.49	0.43
1:B:297:VAL:CG2	1:B:369:PHE:CE2	3.02	0.43
1:D:143:ASN:HB3	1:E:650:GLU:CD	2.38	0.43
1:A:25:VAL:HG13	1:A:29:MET:HE2	1.99	0.43
1:A:297:VAL:CG2	1:A:369:PHE:CE2	3.02	0.43
1:A:393:TYR:CE1	1:A:404:LEU:HD22	2.53	0.43
1:A:460:ILE:HG22	1:A:460:ILE:O	2.17	0.43
1:B:122:ILE:O	1:B:125:ILE:HG22	2.17	0.43
1:B:297:VAL:HG11	1:B:299:LEU:HD21	2.00	0.43
1:D:461:ASP:HB3	1:D:740:ILE:HG23	1.99	0.43
1:E:458:PRO:HG2	1:E:726:ILE:HG21	2.00	0.43
1:E:487:LEU:O	1:E:491:ILE:CD1	2.67	0.43
1:B:436:LEU:HB2	1:B:438:ILE:HD13	2.01	0.43
1:B:747:GLU:O	1:B:751:ASN:CB	2.67	0.43
1:D:264:LEU:CD1	1:D:377:CYS:SG	3.06	0.43
1:E:271:SER:HB3	1:E:451:LEU:HD11	2.00	0.43
1:D:254:ALA:CA	1:D:280:ILE:HD11	2.49	0.43
1:A:341:ILE:HG23	1:A:347:ILE:CD1	2.48	0.43
1:B:521:CYS:SG	1:B:539:LEU:HD13	2.59	0.43
1:B:523:LEU:HD23	1:B:524:LEU:N	2.33	0.43
1:B:583:LEU:O	1:B:583:LEU:HD12	2.18	0.43
1:B:327:ILE:HG23	1:B:353:ILE:HD13	2.01	0.42
1:D:595:GLU:N	1:D:596:PRO:CD	2.82	0.42
1:E:708:VAL:HG12	1:E:709:GLN:N	2.34	0.42
1:A:473:PHE:CZ	1:A:564:ALA:HB1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:LEU:HG	1:A:165:TRP:CE3	2.54	0.42
1:A:45:GLU:HG2	1:A:49:VAL:HG22	1.99	0.42
1:A:523:LEU:HD23	1:A:524:LEU:N	2.34	0.42
1:B:397:LYS:HB2	1:B:404:LEU:HD11	2.02	0.42
1:D:456:ASN:O	1:D:458:PRO:N	2.53	0.42
1:D:576:LYS:CE	1:D:592:GLN:HE22	2.33	0.42
1:D:713:VAL:HG23	1:D:738:LYS:O	2.19	0.42
1:D:73:LEU:HD21	1:D:88:ILE:CG1	2.49	0.42
1:E:265:ILE:HG12	1:E:408:LEU:HD11	2.01	0.42
1:E:327:ILE:HG23	1:E:353:ILE:HD13	2.01	0.42
1:A:583:LEU:HD12	1:A:583:LEU:O	2.19	0.42
1:B:184:LEU:O	1:B:522:ARG:HD2	2.20	0.42
1:A:122:ILE:HA	1:A:125:ILE:CG2	2.45	0.42
1:A:659:PRO:HB3	1:A:694:LEU:HD23	2.01	0.42
1:B:299:LEU:HD12	1:B:374:PHE:CE1	2.55	0.42
1:D:574:ASN:O	1:D:575:VAL:C	2.56	0.42
1:E:477:ILE:O	1:E:478:SER:C	2.57	0.42
1:A:265:ILE:HG12	1:A:408:LEU:HD11	2.00	0.42
1:A:465:VAL:HG12	1:A:466:LYS:N	2.35	0.42
1:A:695:LEU:HD12	1:A:708:VAL:HG11	2.00	0.42
1:E:615:LEU:HD11	1:E:633:LEU:HD11	2.02	0.42
1:A:16:ILE:HG21	1:A:57:LEU:HD13	2.01	0.42
1:A:661:VAL:CG1	1:A:662:LEU:N	2.83	0.42
1:B:539:LEU:O	1:B:543:THR:HG23	2.20	0.42
1:B:632:LEU:CB	1:B:710:CYS:SG	3.08	0.42
1:E:264:LEU:CD1	1:E:377:CYS:SG	3.06	0.42
1:A:10:GLN:OE1	1:A:61:LEU:CD1	2.68	0.42
1:A:165:TRP:O	1:A:168:SER:N	2.52	0.42
1:A:297:VAL:HG11	1:A:299:LEU:HD21	2.01	0.42
1:A:45:GLU:HA	1:A:52:ALA:HB2	2.02	0.42
1:B:288:MET:CE	1:B:292:ARG:HG2	2.50	0.42
1:D:640:LEU:HD23	1:D:644:LEU:HG	2.01	0.42
1:D:786:MET:SD	1:D:789:ARG:NH1	2.93	0.42
1:E:473:PHE:CZ	1:E:564:ALA:HB1	2.55	0.42
1:A:712:LEU:HD12	1:A:738:LYS:HG2	2.00	0.42
1:B:32:TRP:HB3	1:B:63:LEU:HD21	2.02	0.42
1:B:465:VAL:HG21	1:B:742:VAL:HG13	2.02	0.42
1:B:73:LEU:HD11	1:B:88:ILE:HD11	2.02	0.42
1:D:468:ARG:NH1	1:D:606:THR:O	2.52	0.42
1:A:574:ASN:O	1:A:575:VAL:C	2.58	0.41
1:B:273:LYS:O	1:B:276:VAL:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:ALA:HB1	1:D:176:THR:HG21	2.01	0.41
1:D:288:MET:CE	1:D:292:ARG:HG2	2.50	0.41
1:D:385:PRO:O	1:D:386:TYR:C	2.58	0.41
1:E:390:MET:HG3	1:E:436:LEU:HD23	2.02	0.41
1:E:416:VAL:HG13	1:E:416:VAL:O	2.20	0.41
1:E:73:LEU:HG	1:E:88:ILE:HD11	2.02	0.41
1:B:661:VAL:CG1	1:B:662:LEU:N	2.83	0.41
1:D:25:VAL:O	1:D:25:VAL:HG22	2.20	0.41
1:E:640:LEU:HD23	1:E:644:LEU:HG	2.02	0.41
1:A:264:LEU:HD21	1:A:414:VAL:CG1	2.50	0.41
1:A:274:THR:O	1:A:278:ILE:HG23	2.21	0.41
1:A:448:ILE:O	1:A:449:GLN:C	2.59	0.41
1:A:468:ARG:NH2	1:A:609:ASN:HB2	2.35	0.41
1:B:157:LEU:HD12	1:B:157:LEU:HA	1.89	0.41
1:D:708:VAL:HG12	1:D:709:GLN:N	2.35	0.41
1:E:120:ALA:HB1	1:E:176:THR:HG21	2.01	0.41
1:E:574:ASN:O	1:E:575:VAL:C	2.58	0.41
1:B:109:ILE:O	1:B:109:ILE:HG22	2.20	0.41
1:B:157:LEU:HG	1:B:165:TRP:CE3	2.55	0.41
1:D:246:ALA:HB2	1:D:275:PHE:CZ	2.55	0.41
1:E:297:VAL:CG2	1:E:369:PHE:CD2	3.04	0.41
1:A:557:GLU:O	1:A:609:ASN:ND2	2.46	0.41
1:B:12:TYR:CG	1:B:93:PHE:CE2	3.09	0.41
1:B:21:ASN:HB3	1:B:24:TYR:CD2	2.56	0.41
1:D:271:SER:HB3	1:D:451:LEU:HD11	2.02	0.41
1:D:487:LEU:O	1:D:491:ILE:CD1	2.68	0.41
1:A:19:SER:OG	1:A:20:LEU:N	2.54	0.41
1:A:727:GLN:O	1:A:728:VAL:HG23	2.19	0.41
1:B:722:VAL:O	1:B:725:MET:N	2.54	0.41
1:E:615:LEU:HD22	1:E:648:MET:HE1	2.03	0.41
1:A:782:HIS:O	1:A:786:MET:HE3	2.20	0.41
1:B:264:LEU:HD21	1:B:414:VAL:CG1	2.51	0.41
1:B:640:LEU:HD23	1:B:644:LEU:HG	2.03	0.41
1:D:390:MET:HG3	1:D:436:LEU:HD23	2.01	0.41
1:D:477:ILE:O	1:D:478:SER:C	2.58	0.41
1:E:576:LYS:CE	1:E:592:GLN:HE22	2.34	0.41
1:A:122:ILE:N	1:A:123:PRO:HD2	2.36	0.41
1:A:397:LYS:HB2	1:A:404:LEU:HD11	2.03	0.41
1:B:153:LEU:CD2	1:B:153:LEU:C	2.88	0.41
1:D:297:VAL:CG2	1:D:369:PHE:CD2	3.04	0.41
1:D:473:PHE:CZ	1:D:564:ALA:HB1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:341:ILE:HG23	1:E:347:ILE:CD1	2.51	0.41
1:A:698:THR:HG23	1:A:699:SER:N	2.36	0.41
1:B:341:ILE:HG23	1:B:347:ILE:CD1	2.50	0.41
1:B:487:LEU:O	1:B:491:ILE:CD1	2.68	0.41
1:D:469:ILE:H	1:D:469:ILE:HD12	1.85	0.41
1:D:461:ASP:HB2	1:D:740:ILE:HG12	2.02	0.41
1:A:288:MET:CE	1:A:292:ARG:HG2	2.51	0.41
1:D:16:ILE:HG12	1:D:84:LEU:HD22	2.03	0.41
1:E:73:LEU:HD21	1:E:88:ILE:CG1	2.50	0.41
1:E:790:VAL:CG1	1:E:790:VAL:O	2.68	0.41
1:A:426:ILE:HD11	1:A:768:LYS:HD3	2.02	0.41
1:A:640:LEU:HD23	1:A:644:LEU:HG	2.03	0.41
1:A:747:GLU:O	1:A:751:ASN:HB2	2.21	0.41
1:B:122:ILE:N	1:B:123:PRO:HD2	2.36	0.41
1:B:125:ILE:HD12	1:B:153:LEU:HD21	1.99	0.41
1:B:171:LEU:O	1:B:171:LEU:HD23	2.21	0.41
1:B:267:ALA:HB1	1:B:268:PRO:HD2	2.02	0.41
1:D:661:VAL:CG1	1:D:662:LEU:N	2.84	0.41
1:D:659:PRO:HB3	1:D:694:LEU:HD23	2.03	0.41
1:D:73:LEU:HG	1:D:88:ILE:HD11	2.01	0.41
1:E:25:VAL:O	1:E:25:VAL:HG22	2.21	0.41
1:B:297:VAL:CG1	1:B:299:LEU:HD21	2.51	0.40
1:B:381:THR:CG2	1:B:382:GLY:N	2.84	0.40
1:D:265:ILE:HB	1:D:410:LEU:HD23	2.03	0.40
1:D:397:LYS:HB2	1:D:404:LEU:HD11	2.04	0.40
1:D:615:LEU:HD11	1:D:633:LEU:HD11	2.02	0.40
1:E:171:LEU:HD23	1:E:171:LEU:O	2.21	0.40
1:E:288:MET:CE	1:E:292:ARG:HG2	2.49	0.40
1:E:726:ILE:CD1	1:E:739:CYS:SG	3.07	0.40
1:A:44:GLU:HA	1:A:47:ARG:NH1	2.36	0.40
1:B:109:ILE:HG22	1:B:112:THR:HB	2.03	0.40
1:B:37:LEU:O	1:B:38:ARG:C	2.59	0.40
1:E:397:LYS:HB2	1:E:404:LEU:HD11	2.03	0.40
1:E:460:ILE:HD13	1:E:722:VAL:HG11	2.03	0.40
1:E:659:PRO:HB3	1:E:694:LEU:HD23	2.03	0.40
1:A:153:LEU:CD2	1:A:153:LEU:C	2.89	0.40
1:D:462:VAL:HG21	1:D:752:GLU:OE1	2.21	0.40
1:E:151:THR:OG1	1:E:579:PRO:HD3	2.21	0.40
1:A:157:LEU:HD21	1:A:169:LEU:HD13	2.02	0.40
1:A:324:VAL:HG22	1:A:346:ILE:HB	2.04	0.40
1:A:265:ILE:HB	1:A:410:LEU:HD23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:LEU:CD1	1:B:377:CYS:SG	3.08	0.40
1:B:265:ILE:HG12	1:B:408:LEU:HD11	2.02	0.40
1:D:113:MET:HE3	1:D:173:LEU:HD21	2.03	0.40
1:E:385:PRO:O	1:E:386:TYR:C	2.59	0.40
1:E:456:ASN:O	1:E:458:PRO:N	2.54	0.40
1:E:73:LEU:HD21	1:E:88:ILE:HG13	2.03	0.40
1:A:510:TYR:O	1:A:513:TRP:HB3	2.22	0.40
1:B:327:ILE:CG2	1:B:349:VAL:HG13	2.52	0.40
1:D:274:THR:O	1:D:278:ILE:HG23	2.22	0.40
1:D:269:THR:O	1:D:455:MET:HE1	2.21	0.40
1:E:483:GLU:O	1:E:486:ALA:HB3	2.22	0.40
1:E:510:TYR:OH	1:E:546:LEU:HD22	2.22	0.40

There are no symmetry-related clashes.

## 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	660/797 (83%)	586 (89%)	64 (10%)	10 (2%)	11	46
1	B	661/797 (83%)	587 (89%)	65 (10%)	9 (1%)	12	48
1	D	657/797 (82%)	590 (90%)	60 (9%)	7 (1%)	16	54
1	E	656/797 (82%)	589 (90%)	59 (9%)	8 (1%)	14	51
All	All	2634/3188 (83%)	2352 (89%)	248 (9%)	34 (1%)	13	50

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	524	LEU
1	A	699	SER
1	B	524	LEU

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Mol	Chain	Res	Type
1	D	524	LEU
1	D	746	THR
1	E	470	HIS
1	E	524	LEU
1	A	81	TYR
1	A	131	ASP
1	A	604	ASP
1	A	717	GLU
1	A	738	LYS
1	B	81	TYR
1	B	131	ASP
1	B	717	GLU
1	B	738	LYS
1	D	738	LYS
1	E	738	LYS
1	E	746	THR
1	A	365	SER
1	A	723	THR
1	B	365	SER
1	B	723	THR
1	B	747	GLU
1	D	365	SER
1	E	365	SER
1	A	607	ASN
1	D	131	ASP
1	E	131	ASP
1	E	467	ARG
1	B	711	ASN
1	D	467	ARG
1	D	457	LYS
1	E	457	LYS

### 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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	603/704 (86%)	556 (92%)	47 (8%)	14	45
1	B	604/704 (86%)	554 (92%)	50 (8%)	12	43
1	D	600/704 (85%)	563 (94%)	37 (6%)	20	55
1	E	599/704 (85%)	557 (93%)	42 (7%)	16	51
All	All	2406/2816 (85%)	2230 (93%)	176 (7%)	15	49

All (176) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	SER
1	A	25	VAL
1	A	30	THR
1	A	36	GLU
1	A	45	GLU
1	A	58	ASP
1	A	64	GLU
1	A	88	ILE
1	A	100	GLU
1	A	113	MET
1	A	130	ILE
1	A	164	HIS
1	A	176	THR
1	A	253	LEU
1	A	278	ILE
1	A	286	GLN
1	A	307	GLU
1	A	343	ASP
1	A	360	ASP
1	A	391	THR
1	A	414	VAL
1	A	438	ILE
1	A	455	MET
1	A	459	GLU
1	A	464	LEU
1	A	489	ARG
1	A	507	THR
1	A	524	LEU
1	A	535	ILE
1	A	556	SER

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Mol	Chain	Res	Type
1	A	557	GLU
1	A	580	TYR
1	A	604	ASP
1	A	617	CYS
1	A	625	TYR
1	A	636	LYS
1	A	640	LEU
1	A	662	LEU
1	A	691	ASP
1	A	693	ARG
1	A	710	CYS
1	A	711	ASN
1	A	715	LEU
1	A	737	SER
1	A	743	THR
1	A	754	CYS
1	A	786	MET
1	B	19	SER
1	B	25	VAL
1	B	30	THR
1	B	36	GLU
1	B	45	GLU
1	B	58	ASP
1	B	64	GLU
1	B	88	ILE
1	B	100	GLU
1	B	113	MET
1	B	130	ILE
1	B	164	HIS
1	B	176	THR
1	B	245	LYS
1	B	253	LEU
1	B	278	ILE
1	B	286	GLN
1	B	307	GLU
1	B	343	ASP
1	B	360	ASP
1	B	391	THR
1	B	414	VAL
1	B	438	ILE
1	B	455	MET
1	B	459	GLU

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Mol	Chain	Res	Type
1	B	462	VAL
1	B	464	LEU
1	B	467	ARG
1	B	489	ARG
1	B	507	THR
1	B	524	LEU
1	B	535	ILE
1	B	556	SER
1	B	557	GLU
1	B	580	TYR
1	B	604	ASP
1	B	617	CYS
1	B	625	TYR
1	B	636	LYS
1	B	640	LEU
1	B	662	LEU
1	B	691	ASP
1	B	693	ARG
1	B	710	CYS
1	B	715	LEU
1	B	721	ASN
1	B	737	SER
1	B	743	THR
1	B	754	CYS
1	B	786	MET
1	D	45	GLU
1	D	113	MET
1	D	145	SER
1	D	164	HIS
1	D	253	LEU
1	D	278	ILE
1	D	286	GLN
1	D	307	GLU
1	D	343	ASP
1	D	360	ASP
1	D	363	LEU
1	D	391	THR
1	D	414	VAL
1	D	438	ILE
1	D	455	MET
1	D	459	GLU
1	D	467	ARG

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Mol	Chain	Res	Type
1	D	489	ARG
1	D	507	THR
1	D	524	LEU
1	D	535	ILE
1	D	556	SER
1	D	557	GLU
1	D	580	TYR
1	D	617	CYS
1	D	625	TYR
1	D	636	LYS
1	D	640	LEU
1	D	662	LEU
1	D	691	ASP
1	D	693	ARG
1	D	711	ASN
1	D	721	ASN
1	D	737	SER
1	D	743	THR
1	D	754	CYS
1	D	786	MET
1	E	45	GLU
1	E	113	MET
1	E	145	SER
1	E	164	HIS
1	E	245	LYS
1	E	253	LEU
1	E	278	ILE
1	E	286	GLN
1	E	307	GLU
1	E	343	ASP
1	E	360	ASP
1	E	363	LEU
1	E	391	THR
1	E	414	VAL
1	E	438	ILE
1	E	455	MET
1	E	459	GLU
1	E	461	ASP
1	E	462	VAL
1	E	464	LEU
1	E	467	ARG
1	E	469	ILE

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Mol	Chain	Res	Type
1	E	489	ARG
1	E	507	THR
1	E	524	LEU
1	E	535	ILE
1	E	556	SER
1	E	557	GLU
1	E	580	TYR
1	E	617	CYS
1	E	625	TYR
1	E	636	LYS
1	E	640	LEU
1	E	662	LEU
1	E	691	ASP
1	E	693	ARG
1	E	721	ASN
1	E	725	MET
1	E	737	SER
1	E	743	THR
1	E	754	CYS
1	E	786	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	592	GLN
1	D	592	GLN
1	D	721	ASN
1	E	592	GLN

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	674/797 (84%)	0.18	5 (0%) 87 86	52, 97, 153, 210	0
1	B	675/797 (84%)	0.20	12 (1%) 68 66	53, 96, 155, 220	0
1	D	671/797 (84%)	0.82	115 (17%) 1 2	109, 192, 271, 320	0
1	E	670/797 (84%)	0.96	135 (20%) 1 1	104, 199, 293, 359	0
All	All	2690/3188 (84%)	0.54	267 (9%) 7 8	52, 145, 273, 359	0

All (267) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	56	PHE	12.2
1	E	60	VAL	12.1
1	D	17	GLU	11.8
1	D	56	PHE	8.5
1	E	53	ALA	8.4
1	D	16	ILE	8.2
1	E	16	ILE	7.4
1	E	57	LEU	7.1
1	E	157	LEU	7.0
1	D	102	HIS	6.8
1	E	9	LEU	6.5
1	E	327	ILE	6.2
1	D	88	ILE	6.1
1	E	17	GLU	6.1
1	E	102	HIS	6.0
1	E	96	LEU	5.9
1	D	327	ILE	5.9
1	E	325	GLN	5.8
1	E	88	ILE	5.6
1	E	696	ILE	5.5
1	D	22	PRO	5.5

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Mol	Chain	Res	Type	RSRZ
1	E	42	ARG	5.4
1	D	341	ILE	5.3
1	E	341	ILE	5.2
1	D	2	THR	5.1
1	E	74	ASP	5.1
1	D	20	LEU	5.0
1	E	20	LEU	5.0
1	D	19	SER	4.9
1	D	473	PHE	4.9
1	E	750	GLU	4.7
1	D	129	LEU	4.7
1	D	84	LEU	4.6
1	D	10	GLN	4.6
1	D	423	GLU	4.5
1	D	157	LEU	4.5
1	D	317	PHE	4.4
1	E	22	PRO	4.2
1	E	185	TRP	4.2
1	E	369	PHE	4.1
1	D	541	ILE	4.1
1	E	84	LEU	4.1
1	E	715	LEU	4.1
1	D	422	ILE	4.0
1	E	41	ILE	4.0
1	D	23	VAL	4.0
1	E	366	LEU	4.0
1	D	414	VAL	4.0
1	D	347	ILE	4.0
1	D	791	LEU	3.9
1	E	488	MET	3.9
1	D	169	LEU	3.8
1	E	316	HIS	3.8
1	E	347	ILE	3.8
1	E	525	GLN	3.8
1	E	300	ALA	3.7
1	E	103	ARG	3.7
1	E	328	SER	3.7
1	E	125	ILE	3.7
1	E	184	LEU	3.7
1	E	106	LEU	3.7
1	E	129	LEU	3.7
1	D	91	TRP	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	348	VAL	3.7
1	E	712	LEU	3.7
1	D	715	LEU	3.6
1	D	545	HIS	3.6
1	E	49	VAL	3.6
1	E	100	GLU	3.6
1	D	654	LEU	3.6
1	D	49	VAL	3.5
1	D	114	LEU	3.5
1	E	414	VAL	3.5
1	E	356	ASN	3.5
1	D	484	THR	3.5
1	D	9	LEU	3.5
1	E	176	THR	3.4
1	E	59	ALA	3.4
1	D	181	ALA	3.4
1	D	60	VAL	3.4
1	E	91	TRP	3.4
1	E	113	MET	3.4
1	D	184	LEU	3.4
1	E	82	THR	3.3
1	E	2	THR	3.3
1	D	125	ILE	3.3
1	E	654	LEU	3.3
1	E	52	ALA	3.3
1	E	99	LEU	3.3
1	E	313	PHE	3.2
1	D	15	TYR	3.2
1	B	330	GLU	3.2
1	E	90	ASN	3.2
1	E	95	LYS	3.1
1	D	325	GLN	3.1
1	D	6	LYS	3.1
1	D	53	ALA	3.1
1	D	313	PHE	3.1
1	D	99	LEU	3.1
1	D	82	THR	3.0
1	E	710	CYS	3.0
1	D	316	HIS	3.0
1	D	176	THR	3.0
1	D	366	LEU	3.0
1	E	372	MET	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	326	GLY	3.0
1	E	39	GLU	3.0
1	D	790	VAL	3.0
1	E	65	ALA	3.0
1	E	523	LEU	3.0
1	E	423	GLU	3.0
1	B	700	VAL	2.9
1	D	57	LEU	2.9
1	D	153	LEU	2.9
1	E	641	VAL	2.9
1	D	3	ALA	2.9
1	E	55	LEU	2.9
1	E	354	LEU	2.9
1	E	524	LEU	2.9
1	E	25	VAL	2.9
1	D	13	ARG	2.9
1	E	66	ARG	2.9
1	E	173	LEU	2.9
1	D	328	SER	2.9
1	E	28	ASN	2.8
1	E	695	LEU	2.8
1	D	739	CYS	2.8
1	E	121	LEU	2.8
1	E	144	ARG	2.8
1	D	598	LEU	2.8
1	D	619	LEU	2.8
1	E	6	LYS	2.8
1	E	8	SER	2.8
1	E	713	VAL	2.8
1	E	158	CYS	2.8
1	D	279	LEU	2.8
1	E	146	LYS	2.8
1	D	66	ARG	2.7
1	B	327	ILE	2.7
1	D	68	TRP	2.7
1	E	68	TRP	2.7
1	E	619	LEU	2.7
1	E	317	PHE	2.7
1	D	632	LEU	2.7
1	E	340	VAL	2.7
1	D	354	LEU	2.7
1	D	523	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	59	ALA	2.7
1	D	696	ILE	2.6
1	E	138	GLN	2.6
1	E	37	LEU	2.6
1	E	739	CYS	2.6
1	E	326	GLY	2.6
1	D	278	ILE	2.6
1	D	537	ARG	2.6
1	E	169	LEU	2.6
1	E	160	SER	2.6
1	A	327	ILE	2.6
1	D	185	TRP	2.5
1	D	416	VAL	2.5
1	E	484	THR	2.5
1	D	634	PHE	2.5
1	E	26	LEU	2.5
1	E	153	LEU	2.5
1	E	506	GLY	2.5
1	D	320	GLN	2.5
1	D	25	VAL	2.5
1	D	300	ALA	2.5
1	D	160	SER	2.5
1	D	451	LEU	2.4
1	D	612	LEU	2.4
1	D	26	LEU	2.4
1	E	541	ILE	2.4
1	D	77	LEU	2.4
1	D	390	MET	2.4
1	D	298	PHE	2.4
1	D	477	ILE	2.4
1	D	725	MET	2.4
1	E	12	TYR	2.4
1	E	536	CYS	2.4
1	E	107	LYS	2.4
1	D	330	GLU	2.4
1	D	109	ILE	2.4
1	D	524	LEU	2.4
1	E	349	VAL	2.3
1	D	488	MET	2.3
1	B	491	ILE	2.3
1	E	81	TYR	2.3
1	E	33	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	632	LEU	2.3
1	E	633	LEU	2.3
1	D	349	VAL	2.3
1	D	615	LEU	2.3
1	E	352	GLN	2.3
1	B	708	VAL	2.3
1	E	714	VAL	2.3
1	D	372	MET	2.3
1	D	552	ALA	2.3
1	E	537	ARG	2.3
1	D	118	PRO	2.3
1	E	457	LYS	2.3
1	E	63	LEU	2.3
1	E	72	MET	2.3
1	D	159	ARG	2.3
1	E	522	ARG	2.3
1	B	337	VAL	2.3
1	D	542	CYS	2.3
1	D	173	LEU	2.3
1	E	277	SER	2.3
1	D	485	GLU	2.2
1	D	100	GLU	2.2
1	E	38	ARG	2.2
1	E	293	LYS	2.2
1	B	341	ILE	2.2
1	E	312	VAL	2.2
1	E	491	ILE	2.2
1	E	348	VAL	2.2
1	D	122	ILE	2.2
1	E	618	ILE	2.2
1	E	761	MET	2.2
1	A	722	VAL	2.2
1	A	726	ILE	2.2
1	D	89	GLU	2.2
1	A	366	LEU	2.2
1	D	277	SER	2.2
1	D	549	TYR	2.2
1	E	70	ARG	2.2
1	E	278	ILE	2.2
1	E	61	LEU	2.2
1	E	451	LEU	2.2
1	E	625	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	722	VAL	2.2
1	D	72	MET	2.2
1	D	90	ASN	2.2
1	E	694	LEU	2.1
1	E	622	ALA	2.1
1	D	110	GLU	2.1
1	D	714	VAL	2.1
1	E	64	GLU	2.1
1	E	156	CYS	2.1
1	D	81	TYR	2.1
1	E	521	CYS	2.1
1	E	386	TYR	2.1
1	E	298	PHE	2.1
1	E	473	PHE	2.1
1	D	4	ASP	2.1
1	D	741	LEU	2.1
1	E	101	LEU	2.1
1	D	571	PHE	2.1
1	D	369	PHE	2.1
1	B	366	LEU	2.1
1	E	118	PRO	2.1
1	E	635	ALA	2.1
1	D	508	GLN	2.0
1	E	697	ALA	2.0
1	E	186	ASP	2.0
1	D	249	TYR	2.0
1	B	514	ILE	2.0
1	A	295	LYS	2.0
1	D	52	ALA	2.0
1	E	615	LEU	2.0
1	B	631	THR	2.0
1	B	653	ILE	2.0
1	D	709	GLN	2.0
1	D	96	LEU	2.0
1	E	114	LEU	2.0
1	E	389	LEU	2.0

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

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.