



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:09 PM GMT

PDB ID : 3WBK  
Title : crystal structure analysis of eukaryotic translation initiation factor 5B and 1A complex  
Authors : Zheng, A.; Yamamoto, R.; Ose, T.; Yu, J.; Tanaka, I.; Yao, M.  
Deposited on : 2013-05-20  
Resolution : 3.30 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

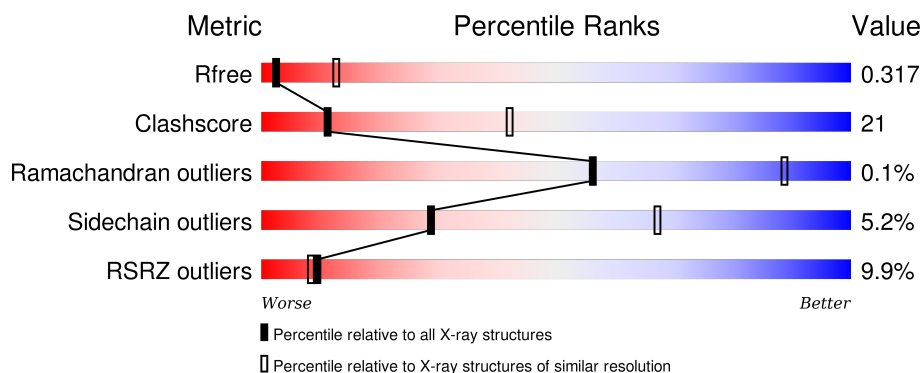
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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	606	<div> <div>7%</div> <div>65%</div> <div>30%</div> <div>• •</div> </div>
1	B	606	<div> <div>12%</div> <div>62%</div> <div>33%</div> <div>• •</div> </div>
2	C	131	<div> <div>%</div> <div>6%</div> <div>92%</div> <div>• •</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9309 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 Eukaryotic translation initiation factor 5B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	590	Total	C	N	O	S	0	0	0
			4588	2918	778	872	20			
1	B	590	Total	C	N	O	S	0	0	0
			4634	2949	785	879	21			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	EXPRESSION TAG	UNP P39730
A	-2	SER	-	EXPRESSION TAG	UNP P39730
A	-1	HIS	-	EXPRESSION TAG	UNP P39730
A	0	MET	-	EXPRESSION TAG	UNP P39730
B	-3	GLY	-	EXPRESSION TAG	UNP P39730
B	-2	SER	-	EXPRESSION TAG	UNP P39730
B	-1	HIS	-	EXPRESSION TAG	UNP P39730
B	0	MET	-	EXPRESSION TAG	UNP P39730

- Molecule 2 is a protein called Eukaryotic translation initiation factor 1A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	11	Total	C	N	O	0	0	0
			87	51	11	25			

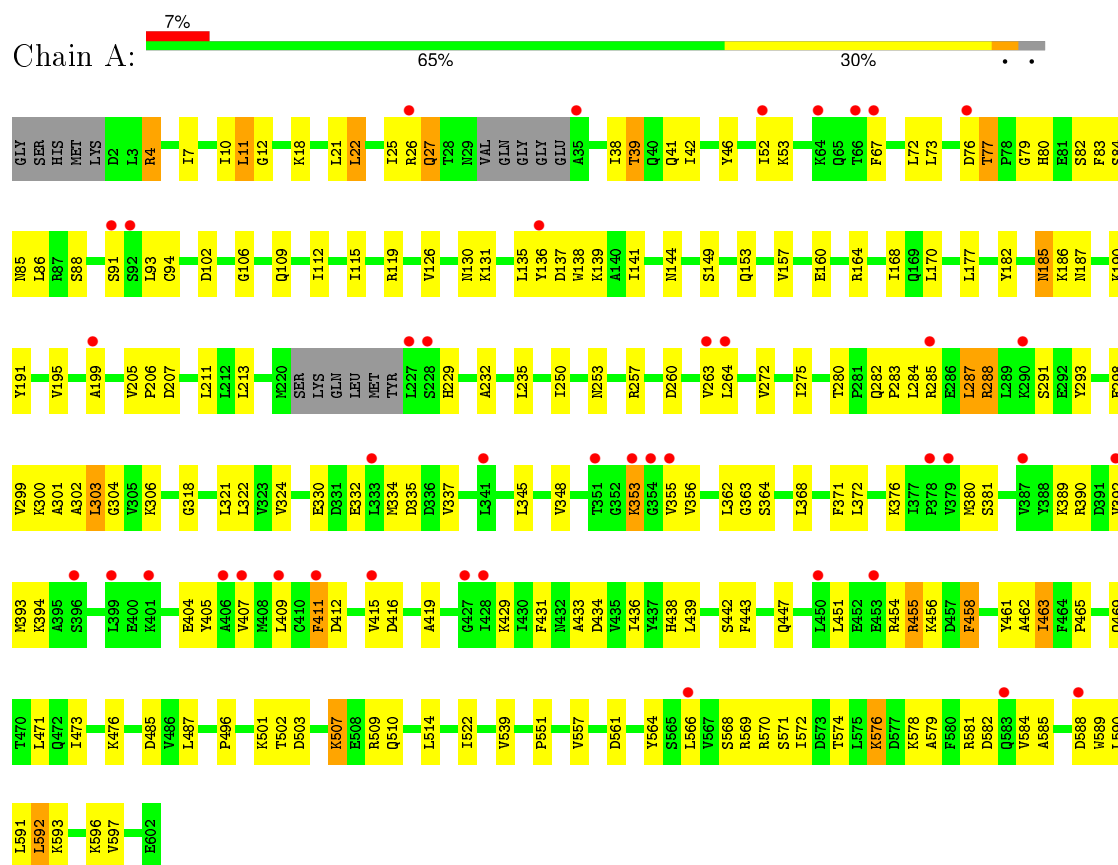
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	EXPRESSION TAG	UNP P38912
C	-2	SER	-	EXPRESSION TAG	UNP P38912
C	-1	HIS	-	EXPRESSION TAG	UNP P38912
C	0	MET	-	EXPRESSION TAG	UNP P38912

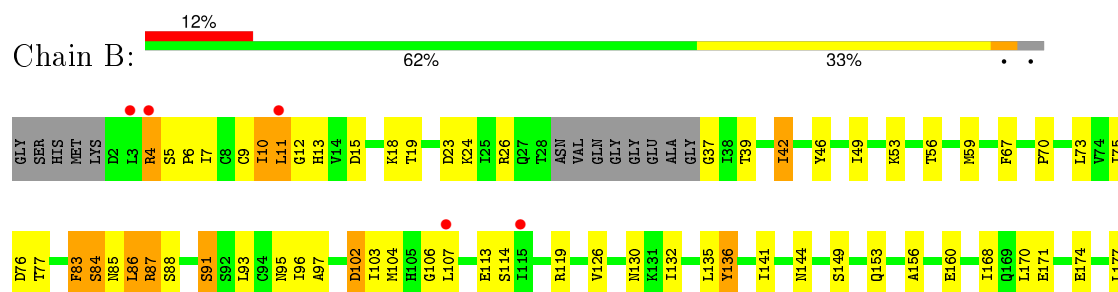
### 3 Residue-property plots

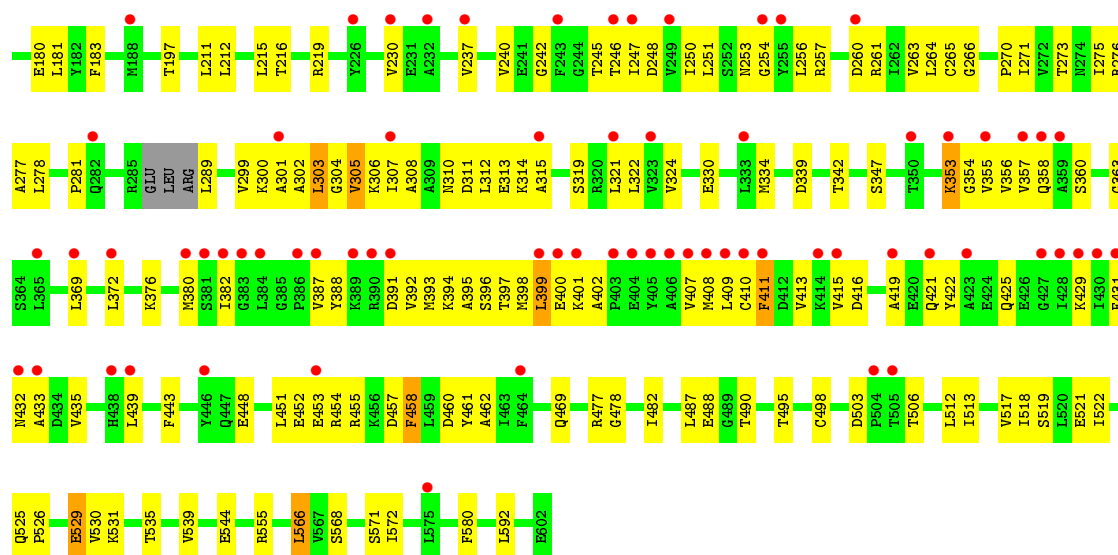
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Eukaryotic translation initiation factor 5B



- Molecule 1: Eukaryotic translation initiation factor 5B





● Molecule 2: Eukaryotic translation initiation factor 1A



GLY	ASP
SER	PHE
HIS	GLN
MET	ASP
ILE	GLP
TYR	ASP
LYS	CYS
GLU	ASP
GLY	VAL
GLN	VAL
GLY	LYS
TYR	ASN
ALA	LEU
GLN	ASP
ILE	GLU
THR	ALA
LYS	ARG
MET	THR
LEU	LEU
GLY	LEU
ASN	LYS
GLY	ASN
ARG	GLN
VAL	GLY
GLU	GLU
ALA	LEU
CYS	PRO
GLU	ASN
PHE	ALA
ASP	LYS
GLY	ILE
ASN	ASN
LYS	PHE
ARG	GLY
GLY	PHE
LYS	GLU
LEU	SER
ARG	ASP
LYS	GLU
LYS	ASP
VAL	VAL
TRP	ASN
MET	PHE
GLY	PHE
GLN	GLY
GLY	ASN
ASP	ALA
ILE	ASP
LEU	GLU
VAL	ASP
SER	ASP
LEU	LEU
ARG	GLU

G117
E118
D119
E120
E121
L122
D123
I124
D125
D126
I127

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.94Å 120.94Å 132.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.30 44.70 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.2 (40.00-3.30) 98.4 (44.70-3.30)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.84 (at 3.32Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.257 , 0.317 0.254 , 0.317	Depositor DCC
$R_{free}$ test set	1768 reflections (7.67%)	DCC
Wilson B-factor (Å <sup>2</sup> )	112.3	Xtriage
Anisotropy	0.667	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 97.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 24828 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9309	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	159.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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 [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	0.43	0/4655	0.67	0/6295
1	B	0.41	0/4704	0.65	1/6356 (0.0%)
2	C	0.34	0/86	0.55	0/115
All	All	0.42	0/9445	0.66	1/12766 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	102	ASP	CB-CG-OD1	5.05	122.85	118.30

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	4588	0	4694	175	0
1	B	4634	0	4766	207	0
2	C	87	0	69	21	0
All	All	9309	0	9529	389	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 21.

All (389) 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)
2:C:120:GLU:HB3	2:C:121:GLU:HB2	1.36	1.07
1:A:287:LEU:HD12	1:A:291:SER:HB3	1.31	1.07
1:B:9:CYS:HB3	1:B:83:PHE:CE1	1.90	1.06
1:B:11:LEU:HB3	1:B:83:PHE:CE2	1.95	1.02
1:A:86:LEU:HA	1:A:363:GLY:HA3	1.44	0.97
1:B:11:LEU:HB3	1:B:83:PHE:HE2	1.28	0.96
1:A:287:LEU:CD1	1:A:291:SER:HB3	1.96	0.95
1:B:299:VAL:HB	1:B:303:LEU:HD21	1.54	0.89
1:B:9:CYS:HB2	1:B:87:ARG:NH1	1.88	0.89
1:B:9:CYS:HB3	1:B:83:PHE:HE1	1.33	0.89
1:B:83:PHE:CE1	1:B:87:ARG:NH1	2.41	0.88
1:B:275:ILE:HG23	1:B:307:ILE:HG23	1.56	0.87
1:A:461:TYR:HB3	1:A:574:THR:HG21	1.57	0.86
2:C:120:GLU:HB3	2:C:121:GLU:CB	2.06	0.85
1:B:77:THR:HG21	1:B:83:PHE:CG	2.12	0.85
1:B:83:PHE:CZ	1:B:87:ARG:NH1	2.48	0.81
1:B:9:CYS:HB3	1:B:83:PHE:CZ	2.15	0.81
1:A:501:LYS:O	1:A:510:GLN:HB2	1.81	0.81
1:A:232:ALA:HB3	1:A:321:LEU:HB3	1.64	0.79
1:B:85:ASN:HA	1:B:363:GLY:HA3	1.64	0.79
1:B:356:VAL:HG13	1:B:408:MET:HA	1.63	0.79
1:A:42:ILE:HD13	1:A:306:LYS:HB2	1.65	0.78
1:B:245:THR:HB	1:B:312:LEU:HA	1.67	0.76
1:A:431:PHE:CZ	1:A:443:PHE:HA	2.20	0.76
1:A:455:ARG:HA	1:A:458:PHE:HD2	1.52	0.75
1:B:300:LYS:O	1:B:303:LEU:HD23	1.86	0.75
1:A:300:LYS:HG2	1:A:301:ALA:H	1.51	0.75
1:A:11:LEU:O	1:A:11:LEU:HD22	1.87	0.75
1:A:287:LEU:HD12	1:A:287:LEU:O	1.85	0.75
1:B:369:LEU:HD21	1:B:382:ILE:HG21	1.69	0.74
1:A:284:LEU:HB2	1:A:287:LEU:HB2	1.70	0.74
1:B:407:VAL:HG12	1:B:429:LYS:HB2	1.69	0.74
1:B:522:ILE:HG12	1:B:539:VAL:HG22	1.68	0.74
1:A:300:LYS:HG2	1:A:301:ALA:N	2.03	0.74
1:A:407:VAL:HG12	1:A:429:LYS:HB3	1.69	0.73
1:B:568:SER:H	1:B:571:SER:HB3	1.53	0.73
1:A:501:LYS:O	1:A:510:GLN:CB	2.37	0.73
1:A:11:LEU:HD13	1:A:11:LEU:N	2.05	0.72
1:A:431:PHE:HB3	1:A:439:LEU:HG	1.71	0.72
1:B:77:THR:HG21	1:B:83:PHE:CD1	2.25	0.71
1:B:9:CYS:CB	1:B:87:ARG:HH11	2.02	0.71
1:B:11:LEU:O	1:B:11:LEU:HD22	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:576:LYS:NZ	2:C:127:ILE:C	2.45	0.70
1:A:285:ARG:O	1:A:288:ARG:HG3	1.92	0.69
1:B:314:LYS:O	1:B:314:LYS:HD2	1.92	0.69
1:A:86:LEU:HA	1:A:363:GLY:CA	2.19	0.69
1:B:458:PHE:HA	1:B:461:TYR:HB2	1.73	0.69
1:A:42:ILE:HG22	1:A:304:GLY:O	1.92	0.69
1:B:126:VAL:HG21	1:B:211:LEU:HD23	1.73	0.69
1:A:263:VAL:HG12	1:A:272:VAL:HG12	1.74	0.69
1:A:284:LEU:HD22	1:A:287:LEU:HD22	1.74	0.68
1:A:514:LEU:HD21	1:A:557:VAL:HG21	1.75	0.68
1:A:284:LEU:HB2	1:A:287:LEU:CB	2.23	0.68
1:B:11:LEU:C	1:B:11:LEU:HD22	2.14	0.68
1:A:187:ASN:O	1:A:191:TYR:HB2	1.93	0.68
1:B:245:THR:CB	1:B:312:LEU:HA	2.23	0.67
1:B:83:PHE:O	1:B:87:ARG:HG3	1.95	0.67
2:C:124:ILE:O	2:C:124:ILE:HG12	1.94	0.67
1:B:237:VAL:HG22	1:B:247:ILE:HG22	1.75	0.67
1:B:357:VAL:HG11	1:B:372:LEU:HD11	1.77	0.67
1:B:339:ASP:HA	1:B:342:THR:HB	1.76	0.66
1:A:7:ILE:HG12	1:A:73:LEU:HD23	1.75	0.66
1:A:284:LEU:CB	1:A:287:LEU:HB2	2.25	0.66
1:A:451:LEU:HB3	1:A:578:LYS:HE2	1.77	0.66
1:A:514:LEU:HD23	1:A:551:PRO:HG2	1.78	0.66
1:B:353:LYS:HD2	1:B:402:ALA:HB2	1.78	0.66
1:B:9:CYS:CB	1:B:83:PHE:CE1	2.75	0.65
1:B:411:PHE:HB3	1:B:433:ALA:O	1.96	0.65
1:B:42:ILE:HG13	1:B:281:PRO:HD3	1.77	0.65
1:A:11:LEU:HD13	1:A:11:LEU:H	1.61	0.65
1:A:576:LYS:HG3	2:C:124:ILE:HD11	1.77	0.65
1:A:53:LYS:HG2	1:A:67:PHE:CZ	2.31	0.65
1:A:260:ASP:HB2	1:A:275:ILE:HD12	1.79	0.65
1:A:568:SER:H	1:A:571:SER:HB3	1.62	0.65
1:A:303:LEU:HD12	1:A:303:LEU:O	1.98	0.64
1:A:102:ASP:OD1	1:A:131:LYS:HD3	1.97	0.64
1:B:9:CYS:CB	1:B:87:ARG:NH1	2.58	0.64
1:B:119:ARG:HD2	1:B:177:LEU:HD21	1.80	0.64
1:A:284:LEU:HD22	1:A:287:LEU:CD2	2.28	0.64
1:A:38:ILE:O	1:A:38:ILE:HD12	1.98	0.64
1:A:85:ASN:O	1:A:88:SER:HB3	1.97	0.64
1:B:23:ASP:HA	1:B:26:ARG:NH1	2.12	0.64
1:B:11:LEU:HD13	1:B:11:LEU:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:LYS:CG	1:A:301:ALA:H	2.10	0.63
1:B:93:LEU:HD11	1:B:250:ILE:HG21	1.80	0.63
1:B:263:VAL:HG22	1:B:322:LEU:HB2	1.80	0.63
1:B:498:CYS:HB2	1:B:512:LEU:O	1.99	0.63
1:B:9:CYS:CB	1:B:83:PHE:HE1	2.09	0.62
1:A:502:THR:HG22	1:A:509:ARG:HA	1.80	0.62
1:A:318:GLY:C	1:A:362:LEU:HD12	2.19	0.62
1:B:330:GLU:O	1:B:334:MET:HG3	1.99	0.62
1:A:593:LYS:O	1:A:596:LYS:HG2	1.99	0.62
2:C:119:ASP:OD1	2:C:119:ASP:N	2.29	0.62
1:B:11:LEU:CB	1:B:83:PHE:HE2	2.08	0.62
1:B:452:GLU:O	1:B:455:ARG:HB2	1.99	0.62
1:A:79:GLY:O	1:A:82:SER:HB3	2.00	0.62
1:A:282:GLN:CD	1:A:283:PRO:HD2	2.20	0.61
1:B:39:THR:OG1	1:B:46:TYR:HB3	2.01	0.61
1:A:590:LEU:HD12	2:C:122:LEU:HD11	1.83	0.61
1:A:590:LEU:CD1	2:C:122:LEU:HD11	2.30	0.61
1:B:277:ALA:HB3	1:B:308:ALA:HB3	1.83	0.61
2:C:118:GLU:HG2	2:C:118:GLU:O	2.01	0.61
1:A:451:LEU:HG	1:A:578:LYS:HD3	1.83	0.61
1:B:522:ILE:O	1:B:525:GLN:HB2	2.01	0.60
1:B:357:VAL:CG2	1:B:382:ILE:HG22	2.31	0.60
1:A:503:ASP:HB2	1:A:507:LYS:H	1.66	0.60
1:A:588:ASP:O	1:A:592:LEU:HD12	2.02	0.60
1:A:160:GLU:O	1:A:164:ARG:HG3	2.02	0.60
1:B:271:ILE:CD1	1:B:313:GLU:HG2	2.31	0.60
1:A:149:SER:O	1:A:153:GLN:HG2	2.02	0.60
1:A:364:SER:HB2	1:A:411:PHE:CD2	2.38	0.59
1:A:280:THR:O	1:A:293:TYR:HB3	2.02	0.59
1:A:411:PHE:CE1	1:A:412:ASP:HB2	2.37	0.59
1:B:230:VAL:HA	1:B:254:GLY:HA3	1.85	0.59
1:B:462:ALA:HB2	1:B:580:PHE:CE1	2.37	0.59
1:B:360:SER:HA	1:B:413:VAL:HG13	1.84	0.59
1:A:569:ARG:HH22	2:C:127:ILE:CG1	2.16	0.59
1:A:465:PRO:HB2	1:A:591:LEU:HD23	1.83	0.59
1:A:263:VAL:HG22	1:A:322:LEU:HB2	1.84	0.58
1:A:569:ARG:HH22	2:C:127:ILE:HG12	1.68	0.58
1:A:447:GLN:O	1:A:451:LEU:HD13	2.03	0.58
1:B:113:GLU:HG3	1:B:435:VAL:HG13	1.86	0.58
1:B:247:ILE:O	1:B:306:LYS:HA	2.03	0.58
1:B:136:TYR:CE2	1:B:156:ALA:HB1	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ILE:O	1:A:10:ILE:HG23	2.04	0.58
1:B:83:PHE:O	1:B:87:ARG:CG	2.52	0.58
1:A:126:VAL:HG21	1:A:211:LEU:HD23	1.86	0.57
2:C:121:GLU:OE1	2:C:122:LEU:N	2.36	0.57
1:B:421:GLN:O	1:B:425:GLN:HG3	2.04	0.57
1:A:576:LYS:HE2	2:C:124:ILE:CG1	2.35	0.57
1:B:11:LEU:HD13	1:B:11:LEU:H	1.69	0.57
1:B:353:LYS:HB3	1:B:398:MET:SD	2.45	0.57
1:B:215:LEU:HA	1:B:219:ARG:HD2	1.85	0.57
1:B:410:CYS:O	1:B:432:ASN:HA	2.05	0.57
1:A:235:LEU:HD22	1:A:250:ILE:HD13	1.87	0.57
1:B:136:TYR:HE2	1:B:156:ALA:HB1	1.69	0.57
1:B:409:LEU:HB3	1:B:439:LEU:HD21	1.87	0.57
1:B:37:GLY:O	1:B:39:THR:HG23	2.04	0.57
1:A:503:ASP:CG	1:A:507:LYS:HB2	2.25	0.57
1:B:457:ASP:O	1:B:460:ASP:HB2	2.05	0.56
1:B:42:ILE:HD13	1:B:306:LYS:HG3	1.88	0.56
1:B:469:GLN:HB2	1:B:487:LEU:HD11	1.86	0.56
1:B:431:PHE:CZ	1:B:443:PHE:HA	2.40	0.56
1:B:358:GLN:NE2	1:B:387:VAL:HA	2.19	0.56
1:B:4:ARG:HD2	1:B:5:SER:O	2.06	0.56
1:A:301:ALA:O	1:A:302:ALA:HB3	2.05	0.56
1:A:21:LEU:O	1:A:25:ILE:HG13	2.06	0.56
1:B:12:GLY:H	1:B:18:LYS:HD3	1.70	0.56
1:A:264:LEU:HA	1:A:337:VAL:HG11	1.87	0.56
1:B:411:PHE:HE2	1:B:439:LEU:HD22	1.72	0.55
1:A:409:LEU:HD23	1:A:431:PHE:HD2	1.72	0.55
2:C:123:ASP:HB3	2:C:125:ASP:OD1	2.07	0.55
1:A:503:ASP:HB2	1:A:507:LYS:HB2	1.87	0.55
1:B:5:SER:OG	1:B:70:PRO:HG2	2.07	0.55
1:B:264:LEU:HD13	1:B:315:ALA:HB1	1.89	0.55
1:B:260:ASP:HB2	1:B:275:ILE:HD12	1.89	0.54
1:A:569:ARG:NH2	2:C:127:ILE:O	2.40	0.54
1:A:232:ALA:CB	1:A:321:LEU:HB3	2.37	0.54
1:A:83:PHE:O	1:A:86:LEU:CB	2.55	0.54
1:B:314:LYS:O	1:B:314:LYS:CD	2.55	0.54
1:A:52:ILE:HD11	1:A:72:LEU:HB2	1.90	0.54
1:A:22:LEU:HA	1:A:25:ILE:HD12	1.89	0.54
1:B:264:LEU:HB3	1:B:321:LEU:HD23	1.88	0.54
1:B:256:LEU:HD13	1:B:307:ILE:HD11	1.90	0.54
1:A:318:GLY:O	1:A:362:LEU:HD12	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:454:ARG:HA	1:B:457:ASP:HB3	1.88	0.54
1:B:240:VAL:HG12	1:B:242:GLY:H	1.73	0.54
1:A:345:LEU:O	1:A:348:VAL:HG22	2.08	0.54
2:C:117:GLY:O	2:C:118:GLU:HB3	2.08	0.54
1:B:387:VAL:CG2	1:B:416:ASP:H	2.21	0.54
1:B:10:ILE:HG23	1:B:10:ILE:O	2.08	0.53
1:A:411:PHE:CE1	1:A:434:ASP:O	2.62	0.53
1:B:458:PHE:HA	1:B:461:TYR:CB	2.37	0.53
1:B:84:SER:O	1:B:87:ARG:O	2.26	0.53
1:A:455:ARG:HG3	1:A:456:LYS:N	2.24	0.53
1:B:314:LYS:O	1:B:314:LYS:CG	2.56	0.53
1:B:95:ASN:O	1:B:96:ILE:HG13	2.09	0.53
1:A:411:PHE:CD1	1:A:412:ASP:HB2	2.44	0.53
1:B:353:LYS:HA	1:B:398:MET:CE	2.39	0.53
2:C:121:GLU:C	2:C:122:LEU:HD23	2.30	0.52
1:A:463:ILE:HD13	1:A:566:LEU:O	2.09	0.52
1:B:149:SER:O	1:B:153:GLN:HG2	2.09	0.52
1:A:42:ILE:CD1	1:A:306:LYS:HB2	2.37	0.52
1:B:251:LEU:HG	1:B:301:ALA:HA	1.92	0.52
1:A:284:LEU:HD22	1:A:287:LEU:HB2	1.92	0.52
1:B:314:LYS:C	1:B:314:LYS:HD2	2.30	0.52
1:A:299:VAL:HB	1:A:303:LEU:HD21	1.91	0.52
1:B:11:LEU:CD1	1:B:11:LEU:H	2.23	0.52
1:A:53:LYS:HG2	1:A:67:PHE:CE2	2.45	0.52
1:B:357:VAL:HG12	1:B:409:LEU:HB2	1.92	0.51
1:A:141:ILE:HG22	1:A:144:ASN:HB2	1.92	0.51
1:B:11:LEU:N	1:B:11:LEU:CD1	2.73	0.51
1:B:394:LYS:O	1:B:397:THR:HG22	2.10	0.51
1:A:353:LYS:O	1:A:353:LYS:HG2	2.10	0.51
1:A:572:ILE:HG12	1:A:592:LEU:CD2	2.41	0.51
1:A:84:SER:CB	1:A:93:LEU:HD12	2.40	0.51
1:B:392:VAL:O	1:B:396:SER:N	2.39	0.51
1:B:49:ILE:HD11	1:B:67:PHE:HD1	1.76	0.51
1:A:185:ASN:OD1	1:A:191:TYR:HB3	2.11	0.51
1:B:248:ASP:OD1	1:B:306:LYS:HG2	2.11	0.51
1:B:357:VAL:HG23	1:B:382:ILE:HG22	1.91	0.50
1:B:251:LEU:CD2	1:B:301:ALA:HA	2.41	0.50
1:B:448:GLU:O	1:B:451:LEU:HB3	2.11	0.50
1:A:330:GLU:O	1:A:334:MET:HG3	2.12	0.50
1:B:260:ASP:HB2	1:B:275:ILE:CD1	2.41	0.50
1:B:132:ILE:O	1:B:135:LEU:HG	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:PHE:O	1:A:462:ALA:N	2.43	0.50
1:A:364:SER:HB2	1:A:411:PHE:CE2	2.46	0.50
1:A:22:LEU:O	1:A:26:ARG:HG3	2.11	0.50
1:A:503:ASP:CB	1:A:507:LYS:HB2	2.42	0.50
1:B:42:ILE:HG13	1:B:281:PRO:CD	2.42	0.50
1:B:303:LEU:HD12	1:B:304:GLY:O	2.12	0.50
1:A:11:LEU:N	1:A:11:LEU:CD1	2.74	0.50
1:B:270:PRO:C	1:B:271:ILE:HD13	2.32	0.50
1:B:212:LEU:O	1:B:216:THR:HG22	2.12	0.50
1:B:13:HIS:HD2	1:B:15:ASP:H	1.60	0.50
1:B:313:GLU:O	1:B:313:GLU:HG3	2.12	0.49
1:A:522:ILE:HG12	1:A:539:VAL:HB	1.92	0.49
1:A:4:ARG:HD3	1:A:4:ARG:O	2.12	0.49
1:B:518:ILE:HD11	1:B:544:GLU:HB2	1.94	0.49
1:B:107:LEU:HD22	1:B:171:GLU:HB3	1.92	0.49
1:B:530:VAL:HG21	1:B:539:VAL:HG21	1.95	0.49
1:A:119:ARG:HH21	1:B:376:LYS:NZ	2.10	0.49
1:B:12:GLY:N	1:B:18:LYS:HD3	2.27	0.49
1:A:80:HIS:O	1:A:84:SER:N	2.34	0.49
1:B:237:VAL:HG21	1:B:315:ALA:O	2.13	0.49
1:B:477:ARG:HG2	1:B:478:GLY:N	2.27	0.49
1:A:584:VAL:HG12	1:A:585:ALA:O	2.12	0.49
1:A:404:GLU:HG2	1:A:405:TYR:N	2.27	0.49
1:A:469:GLN:HB2	1:A:487:LEU:HD11	1.95	0.49
1:A:257:ARG:HG2	1:A:298:GLU:HB2	1.95	0.49
1:A:371:PHE:CD2	1:A:436:ILE:HD13	2.48	0.49
1:B:7:ILE:HG12	1:B:73:LEU:HD23	1.94	0.49
1:B:393:MET:HA	1:B:396:SER:OG	2.13	0.48
1:A:390:ARG:O	1:A:393:MET:HB2	2.13	0.48
1:A:462:ALA:O	1:A:463:ILE:HG13	2.13	0.48
1:B:521:GLU:HA	1:B:525:GLN:O	2.13	0.48
1:B:358:GLN:CG	1:B:413:VAL:HG21	2.44	0.48
1:A:39:THR:HB	1:A:46:TYR:HB3	1.96	0.48
1:A:205:VAL:HB	1:A:206:PRO:HD3	1.95	0.48
1:B:301:ALA:O	1:B:302:ALA:HB3	2.12	0.48
1:B:358:GLN:HG3	1:B:413:VAL:HG21	1.95	0.48
1:A:409:LEU:HD23	1:A:431:PHE:CD2	2.49	0.48
1:B:132:ILE:HG12	1:B:197:THR:O	2.13	0.48
1:A:190:LYS:HE3	1:B:347:SER:HA	1.95	0.48
1:A:471:LEU:HD21	1:A:485:ASP:HB2	1.96	0.48
1:B:513:ILE:CD1	1:B:566:LEU:HG	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ASN:HD22	1:A:186:LYS:N	2.11	0.48
1:A:10:ILE:HG21	1:A:22:LEU:CD1	2.44	0.48
1:A:501:LYS:O	1:A:510:GLN:HB3	2.12	0.48
1:B:355:VAL:HG11	1:B:409:LEU:HD12	1.95	0.48
1:A:141:ILE:O	1:A:144:ASN:HB2	2.14	0.48
1:B:416:ASP:HB2	1:B:419:ALA:HB3	1.96	0.48
1:B:503:ASP:HB2	1:B:506:THR:OG1	2.13	0.48
1:B:265:CYS:HB3	1:B:319:SER:OG	2.14	0.47
1:A:576:LYS:HZ2	2:C:127:ILE:C	2.17	0.47
1:A:581:ARG:HD2	1:A:582:ASP:N	2.30	0.47
1:A:570:ARG:O	1:A:574:THR:HG23	2.14	0.47
1:A:293:TYR:N	1:A:293:TYR:CD1	2.78	0.47
1:B:273:THR:CB	1:B:311:ASP:HB3	2.45	0.47
1:B:251:LEU:HD23	1:B:301:ALA:HA	1.95	0.47
1:B:53:LYS:HG2	1:B:67:PHE:CZ	2.49	0.47
1:B:23:ASP:HA	1:B:26:ARG:HH12	1.77	0.47
1:A:411:PHE:CD1	1:A:411:PHE:C	2.87	0.47
1:B:253:ASN:C	1:B:301:ALA:HB2	2.34	0.47
1:B:181:LEU:HD13	1:B:183:PHE:CZ	2.50	0.47
1:B:9:CYS:HB2	1:B:87:ARG:HH11	1.59	0.47
1:B:42:ILE:HD13	1:B:306:LYS:N	2.30	0.47
1:B:416:ASP:HB2	1:B:419:ALA:CB	2.44	0.47
1:A:454:ARG:O	1:A:458:PHE:HB3	2.15	0.47
1:B:106:GLY:HA2	1:B:168:ILE:HG12	1.96	0.47
1:A:463:ILE:HD11	1:A:496:PRO:HG2	1.97	0.46
1:A:115:ILE:HG22	1:A:119:ARG:HH11	1.80	0.46
1:B:513:ILE:HD11	1:B:566:LEU:HG	1.96	0.46
1:A:380:MET:CE	1:A:394:LYS:HB3	2.45	0.46
1:A:284:LEU:HB2	1:A:287:LEU:HB3	1.97	0.46
1:B:355:VAL:HG11	1:B:409:LEU:CD1	2.46	0.46
1:B:141:ILE:HG22	1:B:144:ASN:HB2	1.98	0.46
1:B:360:SER:HA	1:B:413:VAL:CG1	2.46	0.46
1:A:431:PHE:HE1	1:A:442:SER:HG	1.63	0.46
1:B:398:MET:SD	1:B:401:LYS:HD3	2.56	0.46
1:B:11:LEU:HD13	1:B:11:LEU:N	2.31	0.46
1:B:42:ILE:HG13	1:B:281:PRO:CG	2.45	0.45
1:B:477:ARG:HG2	1:B:478:GLY:H	1.80	0.45
1:B:273:THR:HG21	1:B:311:ASP:OD2	2.16	0.45
1:B:399:LEU:HG	1:B:400:GLU:N	2.30	0.45
1:B:257:ARG:HA	1:B:278:LEU:HD11	1.98	0.45
1:A:288:ARG:HA	1:A:291:SER:OG	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:ILE:O	1:B:42:ILE:HG22	2.16	0.45
1:A:584:VAL:HG11	1:A:589:TRP:CE2	2.50	0.45
1:A:433:ALA:CB	1:A:438:HIS:HB3	2.46	0.45
1:A:42:ILE:HG23	1:A:42:ILE:O	2.16	0.45
1:B:572:ILE:HG12	1:B:592:LEU:HD11	1.99	0.45
1:B:9:CYS:HB3	1:B:87:ARG:HH11	1.80	0.45
1:A:288:ARG:O	1:A:288:ARG:HD2	2.17	0.45
1:B:299:VAL:HB	1:B:303:LEU:CD2	2.37	0.45
1:B:495:THR:O	1:B:517:VAL:HG23	2.17	0.45
1:A:458:PHE:CE1	1:A:579:ALA:HB2	2.52	0.45
1:A:77:THR:HB	1:A:80:HIS:H	1.81	0.45
1:A:303:LEU:HD12	1:A:303:LEU:C	2.38	0.44
1:A:41:GLN:OE1	1:A:303:LEU:HA	2.16	0.44
1:B:276:ARG:HB3	1:B:308:ALA:O	2.17	0.44
1:B:180:GLU:OE1	1:B:180:GLU:HA	2.17	0.44
1:B:305:VAL:HG23	1:B:306:LYS:N	2.32	0.44
1:A:263:VAL:HG23	1:A:337:VAL:HG21	1.99	0.44
1:A:10:ILE:CG2	1:A:76:ASP:HA	2.46	0.44
1:A:83:PHE:HA	1:A:86:LEU:CB	2.47	0.44
1:B:266:GLY:HA2	1:B:315:ALA:HA	1.99	0.44
1:A:507:LYS:HD2	1:A:507:LYS:HA	1.39	0.44
1:B:170:LEU:O	1:B:174:GLU:HG3	2.17	0.44
1:A:368:LEU:O	1:A:372:LEU:HG	2.17	0.44
1:B:518:ILE:CD1	1:B:544:GLU:HB2	2.48	0.44
1:A:356:VAL:HG13	1:A:381:SER:OG	2.17	0.44
1:B:75:ILE:HG22	1:B:76:ASP:O	2.18	0.44
1:B:85:ASN:CA	1:B:363:GLY:HA3	2.41	0.44
1:B:358:GLN:O	1:B:410:CYS:HA	2.18	0.43
1:A:12:GLY:H	1:A:18:LYS:HD3	1.83	0.43
1:A:284:LEU:CD2	1:A:287:LEU:HB2	2.48	0.43
1:B:275:ILE:HG23	1:B:307:ILE:CG2	2.40	0.43
1:B:271:ILE:HD12	1:B:313:GLU:HG2	1.99	0.43
1:A:324:VAL:HG11	1:A:330:GLU:HG2	2.00	0.43
1:A:182:TYR:CD2	1:A:195:VAL:HG22	2.52	0.43
1:B:555:ARG:HA	1:B:555:ARG:HD3	1.89	0.43
1:A:135:LEU:HB2	1:A:138:TRP:HB2	1.99	0.43
1:A:501:LYS:HD2	1:A:561:ASP:OD2	2.18	0.43
1:A:27:GLN:HA	1:A:27:GLN:OE1	2.19	0.43
1:B:88:SER:N	1:B:91:SER:O	2.51	0.43
1:B:261:ARG:O	1:B:324:VAL:HG12	2.18	0.43
1:B:387:VAL:HG21	1:B:416:ASP:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:GLY:O	1:B:18:LYS:HD3	2.19	0.43
1:B:264:LEU:HB3	1:B:321:LEU:CD2	2.49	0.43
1:B:85:ASN:HA	1:B:363:GLY:CA	2.41	0.43
1:B:86:LEU:N	1:B:86:LEU:HD13	2.34	0.43
1:A:284:LEU:HB3	1:A:287:LEU:H	1.83	0.43
1:B:357:VAL:HG23	1:B:382:ILE:HA	2.00	0.43
1:B:86:LEU:N	1:B:86:LEU:CD1	2.82	0.43
1:A:596:LYS:HG3	1:A:597:VAL:N	2.33	0.43
1:B:4:ARG:HG3	1:B:4:ARG:O	2.19	0.43
1:A:300:LYS:CG	1:A:301:ALA:N	2.67	0.43
1:A:303:LEU:C	1:A:303:LEU:CD1	2.87	0.43
1:B:250:ILE:O	1:B:250:ILE:HG22	2.18	0.43
1:B:251:LEU:CG	1:B:301:ALA:HA	2.49	0.43
1:B:487:LEU:C	1:B:488:GLU:HG2	2.40	0.43
1:A:473:ILE:HG12	1:A:476:LYS:HG2	2.01	0.43
1:A:576:LYS:HE2	2:C:124:ILE:HG13	2.00	0.42
1:B:42:ILE:CD1	1:B:306:LYS:HG3	2.49	0.42
1:A:88:SER:O	1:A:91:SER:O	2.38	0.42
1:A:137:ASP:HB3	1:A:157:VAL:HG23	2.00	0.42
1:A:455:ARG:HA	1:A:458:PHE:CD2	2.42	0.42
1:B:353:LYS:HD3	1:B:401:LYS:HG2	2.00	0.42
1:B:388:TYR:HB2	1:B:391:ASP:OD2	2.19	0.42
1:B:354:GLY:C	1:B:380:MET:HB2	2.39	0.42
1:B:353:LYS:HA	1:B:398:MET:HE3	2.01	0.42
1:B:136:TYR:HB3	1:B:160:GLU:OE2	2.19	0.42
1:A:38:ILE:C	1:A:38:ILE:HD12	2.40	0.42
1:B:254:GLY:O	1:B:301:ALA:HB2	2.19	0.42
1:A:106:GLY:HA2	1:A:168:ILE:HG12	2.00	0.42
1:B:11:LEU:HD21	1:B:114:SER:HB3	2.01	0.42
1:A:229:HIS:O	1:A:253:ASN:HB3	2.20	0.42
1:A:389:LYS:HA	1:A:392:VAL:HG12	2.02	0.42
1:B:103:ILE:HG22	1:B:130:ASN:O	2.20	0.42
1:B:357:VAL:HG11	1:B:372:LEU:CD1	2.47	0.41
1:A:119:ARG:HD2	1:A:177:LEU:HD21	2.01	0.41
1:B:525:GLN:HA	1:B:526:PRO:HD3	1.90	0.41
1:A:141:ILE:O	1:A:141:ILE:HG22	2.20	0.41
1:B:56:THR:O	1:B:59:MET:HB2	2.20	0.41
1:B:490:THR:CG2	1:B:529:GLU:HG3	2.50	0.41
1:B:356:VAL:HB	1:B:395:ALA:CB	2.51	0.41
1:B:102:ASP:OD1	1:B:104:MET:HB2	2.21	0.41
1:B:5:SER:HA	1:B:6:PRO:HD3	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:ASP:HB3	1:A:419:ALA:H	1.84	0.41
1:A:332:GLU:O	1:A:335:ASP:HB2	2.20	0.41
1:A:130:ASN:HD21	1:A:199:ALA:H	1.67	0.41
1:B:422:TYR:HA	1:B:425:GLN:OE1	2.21	0.41
1:A:355:VAL:HG12	1:A:405:TYR:HA	2.02	0.41
1:B:531:LYS:HE2	1:B:531:LYS:HB2	1.93	0.41
1:B:87:ARG:HH22	1:B:97:ALA:HB2	1.86	0.41
1:B:304:GLY:C	1:B:305:VAL:HG12	2.41	0.41
1:A:576:LYS:HE2	2:C:124:ILE:HG12	2.01	0.41
1:B:6:PRO:HG2	1:B:216:THR:HG21	2.03	0.41
1:A:52:ILE:HG21	1:A:213:LEU:HD11	2.02	0.41
1:B:264:LEU:C	1:B:264:LEU:HD12	2.41	0.41
1:A:596:LYS:HD3	2:C:127:ILE:HD12	2.03	0.40
1:B:88:SER:HB2	1:B:91:SER:O	2.20	0.40
1:A:109:GLN:O	1:A:112:ILE:HB	2.21	0.40
1:A:139:LYS:HB3	1:A:139:LYS:HE3	1.98	0.40
1:B:9:CYS:CB	1:B:83:PHE:CZ	2.96	0.40
1:B:230:VAL:HG23	1:B:251:LEU:HD11	2.02	0.40
1:B:95:ASN:C	1:B:96:ILE:HG13	2.42	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	584/606 (96%)	561 (96%)	22 (4%)	1 (0%)	52	85
1	B	584/606 (96%)	566 (97%)	18 (3%)	0	100	100
2	C	9/131 (7%)	9 (100%)	0	0	100	100
All	All	1177/1343 (88%)	1136 (96%)	40 (3%)	1 (0%)	56	89

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	463	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	506/529 (96%)	482 (95%)	24 (5%)	32	70
1	B	518/529 (98%)	490 (95%)	28 (5%)	27	66
2	C	10/113 (9%)	8 (80%)	2 (20%)	1	6
All	All	1034/1171 (88%)	980 (95%)	54 (5%)	29	67

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	11	LEU
1	A	22	LEU
1	A	27	GLN
1	A	39	THR
1	A	77	THR
1	A	94	CYS
1	A	136	TYR
1	A	170	LEU
1	A	185	ASN
1	A	207	ASP
1	A	287	LEU
1	A	288	ARG
1	A	303	LEU
1	A	353	LYS
1	A	376	LYS
1	A	411	PHE
1	A	415	VAL
1	A	455	ARG
1	A	458	PHE
1	A	507	LYS
1	A	564	TYR

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Mol	Chain	Res	Type
1	A	576	LYS
1	A	592	LEU
1	B	4	ARG
1	B	10	ILE
1	B	11	LEU
1	B	19	THR
1	B	24	LYS
1	B	42	ILE
1	B	83	PHE
1	B	84	SER
1	B	86	LEU
1	B	87	ARG
1	B	91	SER
1	B	136	TYR
1	B	246	THR
1	B	289	LEU
1	B	303	LEU
1	B	305	VAL
1	B	310	ASN
1	B	353	LYS
1	B	399	LEU
1	B	411	PHE
1	B	415	VAL
1	B	453	GLU
1	B	458	PHE
1	B	482	ILE
1	B	519	SER
1	B	529	GLU
1	B	535	THR
1	B	566	LEU
2	C	121	GLU
2	C	122	LEU

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	130	ASN
1	A	268	ASN
1	B	13	HIS
1	B	130	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	590/606 (97%)	0.45	42 (7%) 19 15	71, 144, 219, 298	0
1	B	590/606 (97%)	0.69	75 (12%) 5 4	75, 161, 262, 324	0
2	C	11/131 (8%)	0.54	1 (9%) 11 9	183, 204, 232, 238	0
All	All	1191/1343 (88%)	0.57	118 (9%) 9 8	71, 151, 246, 324	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	407	VAL	8.8
1	B	358	GLN	6.6
1	A	427	GLY	5.9
1	B	430	ILE	5.8
1	B	355	VAL	5.2
1	B	406	ALA	5.1
1	B	415	VAL	5.0
1	B	429	LYS	4.8
1	B	404	GLU	4.7
1	B	409	LEU	4.7
1	B	431	PHE	4.7
1	A	396	SER	4.6
1	B	387	VAL	4.4
1	A	66	THR	4.4
1	B	410	CYS	4.3
1	A	353	LYS	4.3
1	B	446	TYR	4.2
1	B	249	VAL	4.2
1	A	64	LYS	4.1
1	B	428	ILE	4.1
1	B	255	TYR	4.0
1	A	76	ASP	4.0
1	A	387	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	414	LYS	3.9
1	B	333	LEU	3.9
1	B	243	PHE	3.8
1	B	403	PRO	3.8
1	B	438	HIS	3.8
1	B	382	ILE	3.8
1	B	350	THR	3.7
1	B	107	LEU	3.6
1	B	230	VAL	3.6
1	B	391	ASP	3.5
1	B	423	ALA	3.4
1	B	4	ARG	3.3
1	A	392	VAL	3.3
1	B	365	LEU	3.3
1	B	260	ASP	3.3
1	A	354	GLY	3.3
1	B	307	ILE	3.2
1	B	408	MET	3.2
1	B	353	LYS	3.2
1	B	427	GLY	3.2
1	B	188	MET	3.1
1	A	409	LEU	3.1
1	B	399	LEU	3.0
1	B	389	LYS	3.0
1	A	35	ALA	3.0
1	A	26	ARG	3.0
1	B	421	GLN	3.0
1	B	381	SER	3.0
1	A	401	LYS	3.0
1	B	386	PRO	3.0
1	A	411	PHE	2.9
1	B	246	THR	2.9
1	A	583	GLN	2.9
1	A	341	LEU	2.9
1	B	432	ASN	2.9
1	B	357	VAL	2.8
1	A	52	ILE	2.8
1	A	228	SER	2.8
1	B	323	VAL	2.7
1	A	67	PHE	2.7
1	A	378	PRO	2.7
1	B	321	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	439	LEU	2.6
1	B	411	PHE	2.6
1	B	505	THR	2.5
1	B	232	ALA	2.5
1	B	359	ALA	2.5
1	B	400	GLU	2.5
1	B	575	LEU	2.4
1	A	355	VAL	2.4
1	B	380	MET	2.4
1	A	285	ARG	2.4
1	A	453	GLU	2.4
1	A	407	VAL	2.4
1	B	3	LEU	2.4
1	A	227	LEU	2.4
1	B	383	GLY	2.3
1	B	315	ALA	2.3
1	A	379	VAL	2.3
1	B	390	ARG	2.3
1	A	588	ASP	2.3
1	B	237	VAL	2.3
1	B	504	PRO	2.3
1	B	301	ALA	2.3
1	A	290	LYS	2.3
1	A	92	SER	2.2
1	B	419	ALA	2.2
1	B	453	GLU	2.2
1	B	384	LEU	2.2
1	B	433	ALA	2.2
1	A	406	ALA	2.2
1	B	372	LEU	2.2
1	B	405	TYR	2.2
1	A	333	LEU	2.2
1	B	282	GLN	2.2
1	A	136	TYR	2.2
1	B	464	PHE	2.2
1	A	263	VAL	2.2
1	A	428	ILE	2.2
1	B	369	LEU	2.2
1	A	264	LEU	2.1
1	B	254	GLY	2.1
1	B	401	LYS	2.1
1	A	415	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	226	TYR	2.1
1	B	247	ILE	2.1
1	A	351	THR	2.1
1	A	199	ALA	2.1
1	B	115	ILE	2.1
1	A	399	LEU	2.1
2	C	127	ILE	2.1
1	A	91	SER	2.1
1	A	450	LEU	2.1
1	A	566	LEU	2.1
1	B	11	LEU	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.