



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 02:39 AM GMT

PDB ID : 3O4Z  
Title : Tel2 structure and function in the Hsp90-dependent maturation of mTOR and ATR complexes  
Authors : Xie, Y.; Pavletich, N.P.  
Deposited on : 2010-07-27  
Resolution : 3.10 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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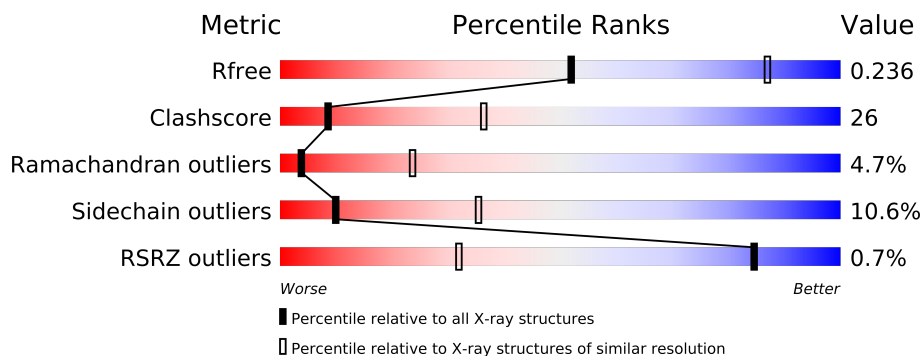
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.10 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))
$R_{free}$	66092	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	647	
1	B	647	
1	C	647	
1	D	647	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 18452 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Telomere length regulation protein TEL2.

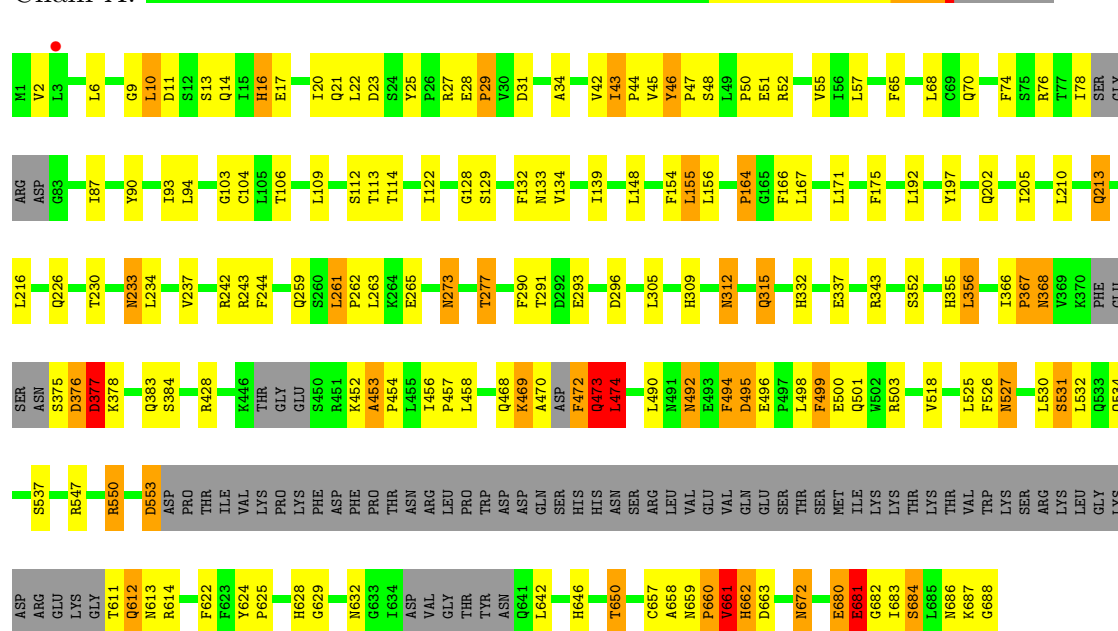
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	572	Total	C	N	O	S	0	0	0
			4613	2995	769	834	15			
1	B	572	Total	C	N	O	S	0	0	0
			4613	2995	769	834	15			
1	C	572	Total	C	N	O	S	0	0	0
			4613	2995	769	834	15			
1	D	572	Total	C	N	O	S	0	0	0
			4613	2995	769	834	15			

### 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.

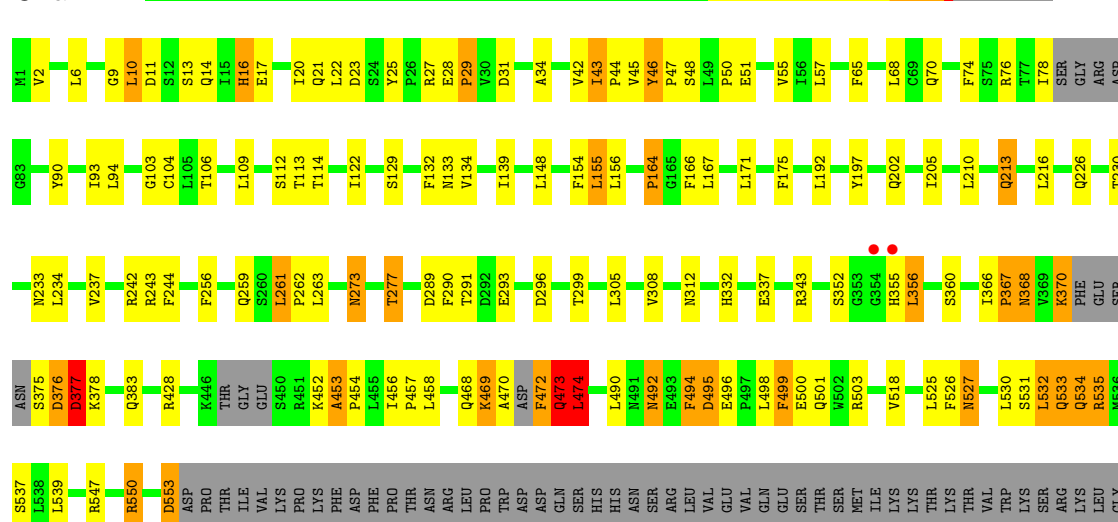
#### • Molecule 1: Telomere length regulation protein TEL2

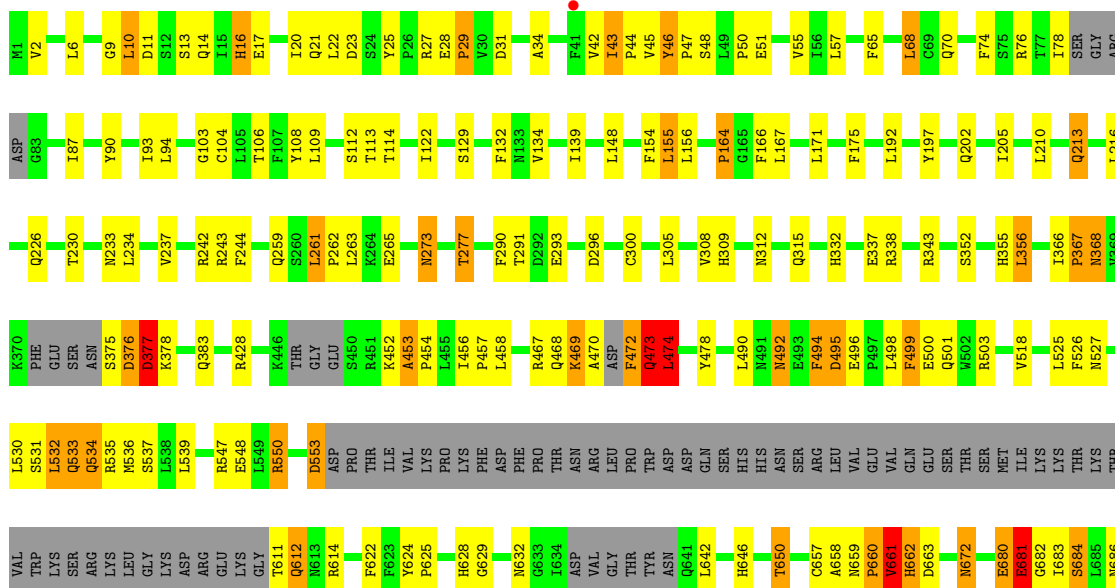
Chain A:



#### • Molecule 1: Telomere length regulation protein TEL2

Chain B:





1687  
Ge88

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.40Å 123.30Å 162.30Å 90.00° 95.17° 90.00°	Depositor
Resolution (Å)	39.20 – 3.10 39.14 – 3.09	Depositor EDS
% Data completeness (in resolution range)	96.2 (39.20-3.10) 95.8 (39.14-3.09)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.09 (at 3.06Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, $R_{free}$	0.222 , 0.239 0.222 , 0.236	Depositor DCC
$R_{free}$ test set	2541 reflections (4.19%)	DCC
Wilson B-factor (Å <sup>2</sup> )	83.7	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 52.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 65609 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	18452	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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	0.46	0/4696	0.59	1/6331 (0.0%)
1	B	0.43	0/4696	0.57	0/6331
1	C	0.43	0/4696	0.58	0/6331
1	D	0.46	1/4696 (0.0%)	0.59	0/6331
All	All	0.45	1/18784 (0.0%)	0.58	1/25324 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	300	CYS	CB-SG	-5.24	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	GLY	N-CA-C	-5.17	100.19	113.10

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4613	0	0	117	0
1	B	4613	0	0	123	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4613	0	0	121	0
1	D	4613	0	0	122	0
All	All	18452	0	0	478	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 26.

All (478) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:6:LEU:CD2	1:D:10:LEU:CD1	2.28	1.12
1:A:6:LEU:CD2	1:A:10:LEU:CD1	2.28	1.11
1:C:6:LEU:CD2	1:C:10:LEU:CD1	2.28	1.11
1:D:472:PHE:CD2	1:D:473:GLN:N	2.20	1.10
1:A:472:PHE:CD2	1:A:473:GLN:N	2.20	1.10
1:C:472:PHE:CD2	1:C:473:GLN:N	2.20	1.10
1:B:6:LEU:CD2	1:B:10:LEU:CD1	2.30	1.09
1:D:9:GLY:O	1:D:10:LEU:CG	2.01	1.08
1:A:9:GLY:O	1:A:10:LEU:CG	2.01	1.08
1:C:9:GLY:O	1:C:10:LEU:CG	2.00	1.08
1:B:9:GLY:O	1:B:10:LEU:CG	2.01	1.08
1:B:472:PHE:CD2	1:B:473:GLN:N	2.21	1.08
1:B:16:HIS:NE2	1:B:20:ILE:CD1	2.20	1.04
1:A:16:HIS:NE2	1:A:20:ILE:CD1	2.21	1.04
1:C:16:HIS:NE2	1:C:20:ILE:CD1	2.21	1.04
1:D:16:HIS:NE2	1:D:20:ILE:CD1	2.21	1.03
1:B:453:ALA:CB	1:B:454:PRO:CD	2.38	1.01
1:C:453:ALA:CB	1:C:454:PRO:CD	2.38	1.01
1:D:453:ALA:CB	1:D:454:PRO:CD	2.38	1.00
1:A:453:ALA:CB	1:A:454:PRO:CD	2.40	0.99
1:C:16:HIS:CD2	1:C:20:ILE:CD1	2.48	0.97
1:B:16:HIS:CD2	1:B:20:ILE:CD1	2.48	0.97
1:D:16:HIS:CD2	1:D:20:ILE:CD1	2.48	0.95
1:A:16:HIS:CD2	1:A:20:ILE:CD1	2.48	0.95
1:B:305:LEU:CD2	1:B:366:ILE:CD1	2.44	0.94
1:D:305:LEU:CD2	1:D:366:ILE:CD1	2.46	0.93
1:C:305:LEU:CD2	1:C:366:ILE:CD1	2.47	0.92
1:A:305:LEU:CD2	1:A:366:ILE:CD1	2.49	0.91
1:A:468:GLN:CG	1:A:468:GLN:O	2.21	0.89
1:C:468:GLN:CG	1:C:468:GLN:O	2.22	0.87
1:B:370:LYS:CD	1:B:370:LYS:N	2.36	0.86
1:B:468:GLN:CG	1:B:468:GLN:O	2.23	0.86
1:C:611:THR:O	1:C:612:GLN:CB	2.24	0.86

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:611:THR:O	1:D:612:GLN:CB	2.24	0.85
1:A:16:HIS:ND1	1:A:50:PRO:CG	2.39	0.85
1:D:468:GLN:O	1:D:468:GLN:CG	2.22	0.85
1:B:611:THR:O	1:B:612:GLN:CB	2.24	0.85
1:A:611:THR:O	1:A:612:GLN:CB	2.24	0.84
1:C:632:ASN:C	1:C:632:ASN:ND2	2.30	0.84
1:A:202:GLN:NE2	1:A:243:ARG:NH1	2.27	0.83
1:B:376:ASP:OD1	1:B:376:ASP:N	2.12	0.81
1:C:376:ASP:N	1:C:376:ASP:OD1	2.13	0.81
1:B:533:GLN:CA	1:B:533:GLN:OE1	2.30	0.80
1:D:550:ARG:CG	1:D:550:ARG:NH1	2.42	0.80
1:A:376:ASP:OD1	1:A:376:ASP:N	2.13	0.79
1:C:550:ARG:CG	1:C:550:ARG:NH1	2.45	0.79
1:A:550:ARG:NH1	1:A:550:ARG:CG	2.45	0.79
1:D:533:GLN:CA	1:D:533:GLN:OE1	2.30	0.79
1:B:531:SER:O	1:B:532:LEU:C	2.20	0.78
1:A:468:GLN:O	1:A:469:LYS:CB	2.32	0.77
1:B:550:ARG:CG	1:B:550:ARG:NH1	2.46	0.77
1:D:376:ASP:N	1:D:376:ASP:OD1	2.15	0.77
1:B:468:GLN:O	1:B:469:LYS:CB	2.33	0.77
1:B:305:LEU:CD2	1:B:366:ILE:CG1	2.63	0.77
1:C:305:LEU:CD2	1:C:366:ILE:CG1	2.64	0.75
1:B:628:HIS:O	1:B:632:ASN:ND2	2.20	0.75
1:D:305:LEU:CD2	1:D:366:ILE:CG1	2.64	0.75
1:B:202:GLN:NE2	1:B:243:ARG:NH1	2.34	0.74
1:A:74:PHE:CE1	1:A:78:ILE:CD1	2.69	0.74
1:D:74:PHE:CE1	1:D:78:ILE:CD1	2.71	0.74
1:B:16:HIS:ND1	1:B:50:PRO:CG	2.50	0.74
1:B:74:PHE:CE1	1:B:78:ILE:CD1	2.70	0.74
1:B:375:SER:C	1:B:376:ASP:OD1	2.26	0.74
1:C:658:ALA:O	1:C:661:VAL:CG2	2.36	0.74
1:C:74:PHE:CE1	1:C:78:ILE:CD1	2.70	0.74
1:C:375:SER:C	1:C:376:ASP:OD1	2.27	0.73
1:A:628:HIS:O	1:A:632:ASN:ND2	2.21	0.73
1:C:468:GLN:O	1:C:469:LYS:CB	2.34	0.73
1:A:305:LEU:CD2	1:A:366:ILE:CG1	2.66	0.73
1:D:628:HIS:O	1:D:632:ASN:ND2	2.22	0.73
1:D:468:GLN:O	1:D:469:LYS:CB	2.36	0.73
1:C:531:SER:O	1:C:533:GLN:N	2.21	0.73
1:A:155:LEU:C	1:A:155:LEU:CD2	2.58	0.73
1:D:532:LEU:O	1:D:535:ARG:N	2.22	0.72
1:B:155:LEU:C	1:B:155:LEU:CD2	2.58	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:113:THR:CG2	1:D:166:PHE:CZ	2.73	0.72
1:A:375:SER:C	1:A:376:ASP:OD1	2.28	0.72
1:D:202:GLN:NE2	1:D:243:ARG:NH1	2.37	0.72
1:C:155:LEU:C	1:C:155:LEU:CD2	2.58	0.71
1:D:155:LEU:C	1:D:155:LEU:CD2	2.58	0.71
1:B:113:THR:CG2	1:B:166:PHE:CZ	2.74	0.71
1:A:113:THR:CG2	1:A:166:PHE:CZ	2.73	0.71
1:B:658:ALA:O	1:B:661:VAL:CG2	2.38	0.71
1:D:375:SER:C	1:D:376:ASP:OD1	2.29	0.71
1:B:16:HIS:C	1:B:16:HIS:CD2	2.65	0.70
1:B:155:LEU:O	1:B:155:LEU:CD2	2.39	0.70
1:C:202:GLN:NE2	1:C:243:ARG:NH1	2.39	0.70
1:D:531:SER:O	1:D:532:LEU:C	2.30	0.70
1:D:155:LEU:O	1:D:155:LEU:CD2	2.38	0.70
1:D:16:HIS:CD2	1:D:16:HIS:C	2.65	0.70
1:D:532:LEU:O	1:D:533:GLN:C	2.29	0.70
1:C:113:THR:CG2	1:C:166:PHE:CZ	2.74	0.70
1:A:155:LEU:O	1:A:155:LEU:CD2	2.40	0.70
1:D:51:GLU:O	1:D:55:VAL:CG2	2.40	0.70
1:A:16:HIS:C	1:A:16:HIS:CD2	2.65	0.69
1:C:367:PRO:O	1:C:368:ASN:CB	2.41	0.69
1:C:16:HIS:C	1:C:16:HIS:CD2	2.65	0.69
1:B:531:SER:O	1:B:534:GLN:N	2.26	0.69
1:B:367:PRO:O	1:B:368:ASN:CB	2.40	0.69
1:A:367:PRO:O	1:A:368:ASN:CB	2.41	0.69
1:A:51:GLU:O	1:A:55:VAL:CG2	2.41	0.69
1:D:658:ALA:O	1:D:661:VAL:CG2	2.42	0.68
1:D:23:ASP:OD1	1:D:23:ASP:O	2.12	0.68
1:D:367:PRO:O	1:D:368:ASN:CB	2.41	0.68
1:C:155:LEU:O	1:C:155:LEU:CD2	2.41	0.68
1:C:51:GLU:O	1:C:55:VAL:CG2	2.42	0.68
1:C:226:GLN:NE2	1:C:259:GLN:N	2.42	0.68
1:C:23:ASP:OD1	1:C:23:ASP:O	2.11	0.67
1:B:133:ASN:ND2	1:C:478:TYR:OH	2.27	0.67
1:C:550:ARG:O	1:C:550:ARG:CD	2.43	0.67
1:A:23:ASP:OD1	1:A:23:ASP:O	2.13	0.67
1:A:226:GLN:NE2	1:A:259:GLN:N	2.43	0.67
1:B:51:GLU:O	1:B:55:VAL:CG2	2.43	0.66
1:D:16:HIS:ND1	1:D:50:PRO:CG	2.59	0.66
1:B:23:ASP:O	1:B:23:ASP:OD1	2.14	0.66
1:C:296:ASP:OD1	1:C:332:HIS:NE2	2.28	0.65
1:B:296:ASP:OD1	1:B:332:HIS:NE2	2.29	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:532:LEU:O	1:B:533:GLN:C	2.34	0.65
1:B:226:GLN:NE2	1:B:259:GLN:N	2.44	0.65
1:C:21:GLN:O	1:C:25:TYR:CD1	2.50	0.65
1:D:226:GLN:NE2	1:D:259:GLN:N	2.44	0.65
1:B:550:ARG:CD	1:B:550:ARG:O	2.45	0.65
1:B:16:HIS:CD2	1:B:16:HIS:O	2.50	0.64
1:D:550:ARG:CD	1:D:550:ARG:O	2.45	0.64
1:D:531:SER:O	1:D:533:GLN:N	2.30	0.64
1:A:550:ARG:NH2	1:A:660:PRO:CD	2.61	0.64
1:A:550:ARG:CD	1:A:550:ARG:O	2.46	0.64
1:D:78:ILE:CG2	1:D:87:ILE:CG1	2.74	0.64
1:D:550:ARG:NH2	1:D:660:PRO:CD	2.61	0.64
1:C:210:LEU:C	1:C:210:LEU:CD2	2.66	0.64
1:A:16:HIS:O	1:A:16:HIS:CD2	2.51	0.64
1:D:21:GLN:O	1:D:25:TYR:CD1	2.50	0.64
1:A:658:ALA:O	1:A:661:VAL:CG2	2.45	0.64
1:D:210:LEU:CD2	1:D:210:LEU:C	2.66	0.63
1:A:42:VAL:O	1:A:44:PRO:N	2.32	0.63
1:B:21:GLN:O	1:B:25:TYR:CD1	2.52	0.63
1:B:210:LEU:C	1:B:210:LEU:CD2	2.66	0.63
1:A:355:HIS:O	1:A:356:LEU:CB	2.46	0.63
1:D:16:HIS:O	1:D:16:HIS:CD2	2.51	0.63
1:D:2:VAL:CB	1:D:22:LEU:CD2	2.77	0.63
1:C:2:VAL:CB	1:C:22:LEU:CD2	2.76	0.63
1:A:21:GLN:O	1:A:25:TYR:CD1	2.52	0.63
1:C:16:HIS:O	1:C:16:HIS:CD2	2.51	0.62
1:B:2:VAL:CB	1:B:22:LEU:CD2	2.77	0.62
1:D:296:ASP:OD1	1:D:332:HIS:NE2	2.32	0.62
1:A:210:LEU:C	1:A:210:LEU:CD2	2.68	0.62
1:C:550:ARG:NH2	1:C:660:PRO:CD	2.62	0.62
1:C:632:ASN:ND2	1:C:633:GLY:N	2.47	0.62
1:C:355:HIS:O	1:C:356:LEU:CB	2.48	0.61
1:A:296:ASP:OD1	1:A:332:HIS:NE2	2.33	0.61
1:D:355:HIS:O	1:D:356:LEU:CB	2.47	0.61
1:A:2:VAL:CB	1:A:22:LEU:CD2	2.79	0.61
1:B:355:HIS:O	1:B:356:LEU:CB	2.48	0.61
1:C:42:VAL:O	1:C:44:PRO:N	2.34	0.60
1:C:16:HIS:ND1	1:C:50:PRO:CG	2.64	0.60
1:C:106:THR:CG2	1:C:154:PHE:CD1	2.84	0.60
1:B:106:THR:CG2	1:B:154:PHE:CD1	2.84	0.60
1:A:106:THR:CG2	1:A:154:PHE:CD1	2.85	0.60
1:D:376:ASP:O	1:D:377:ASP:C	2.40	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:156:LEU:CD2	1:D:197:TYR:CD2	2.84	0.60
1:B:42:VAL:O	1:B:44:PRO:N	2.34	0.60
1:D:106:THR:CG2	1:D:154:PHE:CD1	2.85	0.60
1:B:550:ARG:NH2	1:B:660:PRO:CD	2.64	0.60
1:A:205:ILE:CD1	1:A:244:PHE:CE1	2.84	0.59
1:D:42:VAL:O	1:D:44:PRO:N	2.35	0.59
1:D:21:GLN:O	1:D:25:TYR:CE1	2.55	0.59
1:B:612:GLN:O	1:B:614:ARG:N	2.36	0.59
1:C:21:GLN:O	1:C:25:TYR:CE1	2.55	0.59
1:B:156:LEU:CD2	1:B:197:TYR:CD2	2.86	0.59
1:C:494:PHE:O	1:C:495:ASP:C	2.41	0.59
1:C:661:VAL:O	1:C:662:HIS:CB	2.51	0.58
1:B:494:PHE:O	1:B:495:ASP:C	2.42	0.58
1:B:205:ILE:O	1:B:213:GLN:NE2	2.36	0.58
1:A:376:ASP:O	1:A:377:ASP:C	2.42	0.58
1:A:494:PHE:O	1:A:495:ASP:C	2.42	0.58
1:A:45:VAL:O	1:A:48:SER:N	2.36	0.58
1:C:45:VAL:O	1:C:48:SER:N	2.37	0.58
1:D:112:SER:OG	1:D:122:ILE:CD1	2.52	0.58
1:D:65:PHE:CZ	1:D:122:ILE:CG1	2.87	0.58
1:C:112:SER:OG	1:C:122:ILE:CD1	2.52	0.58
1:D:45:VAL:O	1:D:48:SER:N	2.36	0.58
1:C:156:LEU:CD2	1:C:197:TYR:CD2	2.86	0.58
1:C:31:ASP:OD1	1:C:34:ALA:N	2.37	0.58
1:D:661:VAL:O	1:D:662:HIS:CB	2.51	0.57
1:B:45:VAL:O	1:B:48:SER:N	2.37	0.57
1:D:494:PHE:O	1:D:495:ASP:C	2.42	0.57
1:C:376:ASP:O	1:C:377:ASP:C	2.41	0.57
1:C:531:SER:O	1:C:532:LEU:C	2.43	0.57
1:A:156:LEU:CD2	1:A:197:TYR:CD2	2.88	0.57
1:D:205:ILE:CD1	1:D:244:PHE:CE1	2.88	0.57
1:A:31:ASP:OD1	1:A:34:ALA:N	2.38	0.57
1:B:376:ASP:O	1:B:377:ASP:C	2.41	0.56
1:A:21:GLN:O	1:A:25:TYR:CE1	2.58	0.56
1:A:612:GLN:O	1:A:614:ARG:N	2.38	0.56
1:B:31:ASP:OD1	1:B:34:ALA:N	2.37	0.56
1:D:680:GLU:O	1:D:682:GLY:N	2.38	0.56
1:D:31:ASP:OD1	1:D:34:ALA:N	2.38	0.56
1:C:113:THR:CG2	1:C:113:THR:O	2.53	0.56
1:B:113:THR:O	1:B:113:THR:CG2	2.54	0.56
1:B:680:GLU:O	1:B:682:GLY:N	2.39	0.55
1:A:16:HIS:CE1	1:A:50:PRO:CG	2.89	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:661:VAL:O	1:A:662:HIS:CB	2.52	0.55
1:A:11:ASP:OD1	1:A:13:SER:N	2.39	0.55
1:A:495:ASP:OD1	1:A:495:ASP:N	2.38	0.55
1:B:661:VAL:O	1:B:662:HIS:CB	2.55	0.55
1:C:11:ASP:OD1	1:C:13:SER:N	2.40	0.55
1:B:531:SER:O	1:B:533:GLN:N	2.39	0.55
1:D:113:THR:CG2	1:D:113:THR:O	2.54	0.55
1:B:21:GLN:O	1:B:25:TYR:CE1	2.58	0.55
1:C:550:ARG:NH1	1:C:657:CYS:O	2.40	0.55
1:D:495:ASP:N	1:D:495:ASP:OD1	2.38	0.55
1:D:11:ASP:OD1	1:D:13:SER:N	2.40	0.55
1:A:680:GLU:O	1:A:682:GLY:N	2.39	0.55
1:B:112:SER:OG	1:B:122:ILE:CD1	2.54	0.55
1:B:499:PHE:CD2	1:B:500:GLU:N	2.75	0.55
1:C:612:GLN:O	1:C:614:ARG:N	2.40	0.55
1:A:492:ASN:ND2	1:A:495:ASP:CA	2.70	0.54
1:B:273:ASN:OD1	1:B:273:ASN:N	2.41	0.54
1:D:456:ILE:N	1:D:457:PRO:CD	2.70	0.54
1:C:499:PHE:CD2	1:C:500:GLU:N	2.76	0.54
1:D:273:ASN:O	1:D:277:THR:CG2	2.55	0.54
1:B:11:ASP:OD1	1:B:13:SER:N	2.41	0.54
1:A:499:PHE:CD2	1:A:500:GLU:N	2.75	0.54
1:D:492:ASN:ND2	1:D:495:ASP:CA	2.70	0.54
1:A:112:SER:OG	1:A:122:ILE:CD1	2.55	0.54
1:C:680:GLU:O	1:C:682:GLY:N	2.41	0.54
1:C:492:ASN:ND2	1:C:495:ASP:CA	2.71	0.54
1:C:78:ILE:CG2	1:C:87:ILE:CG1	2.86	0.54
1:C:273:ASN:O	1:C:277:THR:CG2	2.55	0.54
1:C:23:ASP:OD1	1:C:23:ASP:C	2.46	0.54
1:A:273:ASN:OD1	1:A:273:ASN:N	2.40	0.54
1:A:687:LYS:CE	1:C:338:ARG:NH2	2.70	0.54
1:B:205:ILE:CD1	1:B:244:PHE:CE1	2.91	0.54
1:B:492:ASN:ND2	1:B:495:ASP:CA	2.71	0.54
1:C:495:ASP:OD1	1:C:495:ASP:N	2.41	0.53
1:A:113:THR:CG2	1:A:113:THR:O	2.53	0.53
1:C:6:LEU:CD2	1:C:10:LEU:CD2	2.86	0.53
1:B:273:ASN:O	1:B:277:THR:CG2	2.56	0.53
1:C:273:ASN:N	1:C:273:ASN:OD1	2.42	0.53
1:D:612:GLN:O	1:D:614:ARG:N	2.42	0.53
1:B:256:PHE:CZ	1:B:299:THR:OG1	2.62	0.53
1:A:171:LEU:CD2	1:A:175:PHE:CE2	2.92	0.53
1:C:498:LEU:C	1:C:499:PHE:O	2.46	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:273:ASN:O	1:A:277:THR:CG2	2.57	0.53
1:A:456:ILE:N	1:A:457:PRO:CD	2.72	0.53
1:D:6:LEU:CD2	1:D:10:LEU:CD2	2.86	0.52
1:D:23:ASP:OD1	1:D:23:ASP:C	2.47	0.52
1:D:550:ARG:NH1	1:D:657:CYS:O	2.43	0.52
1:D:171:LEU:CD2	1:D:175:PHE:CE2	2.92	0.52
1:A:499:PHE:O	1:A:501:GLN:N	2.41	0.52
1:C:171:LEU:CD2	1:C:175:PHE:CE2	2.93	0.52
1:A:42:VAL:O	1:A:43:ILE:C	2.46	0.52
1:C:65:PHE:CZ	1:C:122:ILE:CG1	2.93	0.52
1:A:498:LEU:C	1:A:499:PHE:O	2.47	0.52
1:A:29:PRO:CD	1:A:29:PRO:O	2.55	0.52
1:D:265:GLU:OE2	1:D:309:HIS:CE1	2.62	0.52
1:B:646:HIS:O	1:B:650:THR:CG2	2.58	0.52
1:A:550:ARG:NH1	1:A:657:CYS:O	2.43	0.52
1:C:42:VAL:O	1:C:43:ILE:C	2.47	0.52
1:B:495:ASP:OD1	1:B:495:ASP:N	2.40	0.52
1:C:456:ILE:N	1:C:457:PRO:CD	2.73	0.52
1:D:499:PHE:CD2	1:D:500:GLU:N	2.78	0.52
1:B:456:ILE:N	1:B:457:PRO:CD	2.73	0.51
1:B:532:LEU:O	1:B:534:GLN:N	2.43	0.51
1:D:531:SER:O	1:D:534:GLN:N	2.42	0.51
1:B:499:PHE:O	1:B:501:GLN:N	2.44	0.51
1:C:499:PHE:O	1:C:501:GLN:N	2.43	0.51
1:C:500:GLU:OE1	1:C:503:ARG:NH2	2.43	0.51
1:D:29:PRO:CD	1:D:29:PRO:O	2.58	0.51
1:B:23:ASP:C	1:B:23:ASP:OD1	2.48	0.51
1:D:42:VAL:O	1:D:43:ILE:C	2.49	0.51
1:C:293:GLU:OE1	1:C:343:ARG:NH2	2.43	0.51
1:C:645:SER:OG	1:C:686:ASN:OD1	2.29	0.51
1:D:498:LEU:C	1:D:499:PHE:O	2.48	0.51
1:B:171:LEU:CD2	1:B:175:PHE:CE2	2.93	0.51
1:D:490:LEU:O	1:D:503:ARG:NH1	2.44	0.51
1:D:273:ASN:OD1	1:D:273:ASN:N	2.42	0.51
1:B:42:VAL:C	1:B:44:PRO:CD	2.79	0.51
1:A:23:ASP:C	1:A:23:ASP:OD1	2.48	0.51
1:B:500:GLU:OE1	1:B:503:ARG:NH2	2.44	0.51
1:A:490:LEU:O	1:A:503:ARG:NH1	2.44	0.51
1:A:293:GLU:OE1	1:A:343:ARG:NH2	2.44	0.51
1:C:42:VAL:C	1:C:44:PRO:CD	2.80	0.50
1:B:42:VAL:O	1:B:43:ILE:C	2.48	0.50
1:A:377:ASP:O	1:A:378:LYS:CB	2.59	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:500:GLU:OE1	1:A:503:ARG:NH2	2.45	0.50
1:B:171:LEU:CD2	1:B:216:LEU:CD2	2.89	0.50
1:D:472:PHE:O	1:D:474:LEU:N	2.45	0.50
1:B:550:ARG:NH1	1:B:657:CYS:O	2.45	0.50
1:A:42:VAL:C	1:A:44:PRO:CD	2.79	0.50
1:C:93:ILE:CG2	1:C:94:LEU:N	2.74	0.50
1:B:6:LEU:CD2	1:B:10:LEU:CD2	2.90	0.50
1:B:65:PHE:CZ	1:B:122:ILE:CG1	2.94	0.50
1:C:490:LEU:O	1:C:503:ARG:NH1	2.45	0.50
1:D:93:ILE:CG2	1:D:94:LEU:N	2.74	0.50
1:A:6:LEU:CD2	1:A:10:LEU:CD2	2.90	0.49
1:A:547:ARG:CZ	1:A:553:ASP:OD1	2.60	0.49
1:C:469:LYS:O	1:C:470:ALA:CB	2.60	0.49
1:C:29:PRO:CD	1:C:29:PRO:O	2.58	0.49
1:D:68:LEU:CD1	1:D:108:TYR:OH	2.61	0.49
1:A:65:PHE:CZ	1:A:122:ILE:CG1	2.96	0.49
1:C:205:ILE:CD1	1:C:244:PHE:CE1	2.95	0.49
1:B:498:LEU:C	1:B:499:PHE:O	2.44	0.49
1:C:129:SER:OG	1:C:132:PHE:CB	2.61	0.49
1:B:293:GLU:OE1	1:B:343:ARG:NH2	2.45	0.49
1:B:16:HIS:CE1	1:B:50:PRO:CG	2.95	0.49
1:C:624:TYR:N	1:C:625:PRO:CD	2.76	0.49
1:B:532:LEU:O	1:B:535:ARG:N	2.45	0.48
1:D:531:SER:O	1:D:531:SER:OG	2.30	0.48
1:D:646:HIS:O	1:D:650:THR:CG2	2.61	0.48
1:D:499:PHE:O	1:D:501:GLN:N	2.45	0.48
1:A:646:HIS:O	1:A:650:THR:CG2	2.61	0.48
1:B:472:PHE:O	1:B:474:LEU:N	2.46	0.48
1:A:93:ILE:CG2	1:A:94:LEU:N	2.76	0.48
1:D:103:GLY:O	1:D:104:CYS:C	2.52	0.48
1:B:93:ILE:CG2	1:B:94:LEU:N	2.77	0.48
1:D:42:VAL:C	1:D:44:PRO:CD	2.81	0.48
1:B:490:LEU:O	1:B:503:ARG:NH1	2.46	0.48
1:D:467:ARG:NH2	1:D:548:GLU:OE2	2.47	0.48
1:A:624:TYR:N	1:A:625:PRO:CD	2.76	0.48
1:A:628:HIS:C	1:A:632:ASN:ND2	2.67	0.48
1:D:686:ASN:O	1:D:687:LYS:C	2.52	0.48
1:C:472:PHE:O	1:C:474:LEU:N	2.47	0.47
1:B:360:SER:CB	1:D:687:LYS:NZ	2.76	0.47
1:A:133:ASN:ND2	1:D:478:TYR:OH	2.47	0.47
1:D:129:SER:OG	1:D:132:PHE:CB	2.62	0.47
1:D:293:GLU:OE1	1:D:343:ARG:NH2	2.47	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:9:GLY:C	1:D:10:LEU:CG	2.81	0.47
1:A:78:ILE:CG2	1:A:87:ILE:CG1	2.92	0.47
1:A:103:GLY:O	1:A:104:CYS:C	2.52	0.47
1:B:29:PRO:O	1:B:29:PRO:CD	2.58	0.47
1:B:103:GLY:O	1:B:104:CYS:C	2.53	0.47
1:B:624:TYR:N	1:B:625:PRO:CD	2.78	0.47
1:A:472:PHE:O	1:A:474:LEU:N	2.48	0.47
1:B:469:LYS:O	1:B:470:ALA:CB	2.62	0.47
1:A:45:VAL:O	1:A:46:TYR:C	2.53	0.47
1:D:45:VAL:O	1:D:46:TYR:C	2.52	0.47
1:D:500:GLU:OE1	1:D:503:ARG:NH2	2.48	0.47
1:C:90:TYR:O	1:C:93:ILE:CG2	2.63	0.47
1:C:103:GLY:O	1:C:104:CYS:C	2.52	0.47
1:D:366:ILE:O	1:D:367:PRO:O	2.33	0.47
1:D:659:ASN:CG	1:D:659:ASN:O	2.53	0.47
1:C:68:LEU:CD1	1:C:108:TYR:OH	2.63	0.47
1:A:469:LYS:O	1:A:470:ALA:CB	2.62	0.47
1:A:233:ASN:ND2	1:A:384:SER:O	2.47	0.47
1:B:628:HIS:C	1:B:632:ASN:ND2	2.68	0.47
1:D:672:ASN:ND2	1:D:672:ASN:N	2.61	0.47
1:C:377:ASP:O	1:C:378:LYS:CB	2.62	0.46
1:D:686:ASN:O	1:D:688:GLY:N	2.48	0.46
1:C:687:LYS:CG	1:C:687:LYS:O	2.62	0.46
1:D:624:TYR:N	1:D:625:PRO:CD	2.79	0.46
1:C:646:HIS:O	1:C:650:THR:CG2	2.64	0.46
1:D:628:HIS:C	1:D:632:ASN:ND2	2.68	0.46
1:A:518:VAL:CG2	1:A:622:PHE:CZ	2.99	0.46
1:A:9:GLY:C	1:A:10:LEU:CG	2.80	0.46
1:D:205:ILE:O	1:D:213:GLN:NE2	2.49	0.46
1:A:686:ASN:O	1:A:687:LYS:C	2.53	0.46
1:C:45:VAL:O	1:C:46:TYR:C	2.54	0.46
1:D:90:TYR:O	1:D:93:ILE:CG2	2.64	0.46
1:C:518:VAL:CG2	1:C:622:PHE:CZ	2.99	0.46
1:C:547:ARG:CZ	1:C:553:ASP:OD1	2.64	0.46
1:A:205:ILE:O	1:A:213:GLN:NE2	2.49	0.45
1:D:687:LYS:CG	1:D:687:LYS:O	2.65	0.45
1:B:377:ASP:O	1:B:378:LYS:CB	2.62	0.45
1:D:518:VAL:CG2	1:D:622:PHE:CZ	2.99	0.45
1:B:686:ASN:O	1:B:687:LYS:C	2.54	0.45
1:A:687:LYS:O	1:A:687:LYS:CG	2.64	0.45
1:C:261:LEU:N	1:C:262:PRO:CD	2.80	0.45
1:A:265:GLU:OE2	1:A:309:HIS:CE1	2.70	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:74:PHE:CZ	1:B:78:ILE:CD1	3.00	0.45
1:C:13:SER:O	1:C:17:GLU:CG	2.65	0.45
1:A:90:TYR:O	1:A:93:ILE:CG2	2.65	0.45
1:A:686:ASN:O	1:A:688:GLY:N	2.49	0.45
1:C:672:ASN:N	1:C:672:ASN:ND2	2.65	0.45
1:C:305:LEU:CA	1:C:366:ILE:CD1	2.94	0.45
1:C:686:ASN:O	1:C:687:LYS:C	2.55	0.45
1:B:687:LYS:O	1:B:687:LYS:CG	2.63	0.45
1:D:261:LEU:N	1:D:262:PRO:CD	2.80	0.45
1:B:547:ARG:CZ	1:B:553:ASP:OD1	2.64	0.45
1:C:659:ASN:CG	1:C:659:ASN:O	2.55	0.45
1:B:305:LEU:CA	1:B:366:ILE:CD1	2.95	0.45
1:B:45:VAL:O	1:B:46:TYR:C	2.56	0.45
1:B:672:ASN:N	1:B:672:ASN:ND2	2.65	0.45
1:A:129:SER:OG	1:A:132:PHE:CB	2.66	0.44
1:D:469:LYS:O	1:D:470:ALA:CB	2.65	0.44
1:D:114:THR:O	1:D:114:THR:CG2	2.65	0.44
1:D:547:ARG:CZ	1:D:553:ASP:OD1	2.65	0.44
1:A:20:ILE:CG2	1:A:52:ARG:NH1	2.80	0.44
1:D:305:LEU:CA	1:D:366:ILE:CD1	2.96	0.44
1:C:74:PHE:CZ	1:C:78:ILE:CD1	3.01	0.44
1:C:164:PRO:CB	1:C:166:PHE:CE1	3.00	0.44
1:B:129:SER:OG	1:B:132:PHE:CB	2.65	0.44
1:B:366:ILE:O	1:B:367:PRO:O	2.35	0.44
1:D:377:ASP:O	1:D:378:LYS:CB	2.65	0.44
1:D:171:LEU:CD2	1:D:216:LEU:CD2	2.95	0.44
1:C:205:ILE:O	1:C:213:GLN:NE2	2.50	0.44
1:C:289:ASP:O	1:C:289:ASP:CG	2.55	0.44
1:D:13:SER:O	1:D:17:GLU:CG	2.65	0.44
1:A:13:SER:O	1:A:17:GLU:CG	2.66	0.44
1:B:686:ASN:O	1:B:688:GLY:N	2.51	0.44
1:C:114:THR:CG2	1:C:114:THR:O	2.66	0.44
1:B:659:ASN:CG	1:B:659:ASN:O	2.55	0.44
1:D:11:ASP:O	1:D:14:GLN:N	2.51	0.44
1:B:499:PHE:O	1:B:500:GLU:CB	2.66	0.44
1:D:628:HIS:O	1:D:629:GLY:C	2.56	0.44
1:C:11:ASP:O	1:C:14:GLN:N	2.51	0.44
1:B:90:TYR:O	1:B:93:ILE:CG2	2.66	0.43
1:A:663:ASP:N	1:A:663:ASP:OD2	2.51	0.43
1:B:65:PHE:CE2	1:B:122:ILE:CG1	3.01	0.43
1:B:261:LEU:N	1:B:262:PRO:CD	2.81	0.43
1:D:74:PHE:CZ	1:D:78:ILE:CD1	3.01	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:13:SER:O	1:B:17:GLU:CG	2.65	0.43
1:B:680:GLU:O	1:B:681:GLU:C	2.57	0.43
1:A:499:PHE:O	1:A:500:GLU:CB	2.65	0.43
1:B:114:THR:CG2	1:B:114:THR:O	2.66	0.43
1:B:518:VAL:CG2	1:B:622:PHE:CZ	3.01	0.43
1:A:74:PHE:CZ	1:A:78:ILE:CD1	3.01	0.43
1:D:680:GLU:O	1:D:681:GLU:C	2.57	0.43
1:C:366:ILE:O	1:C:367:PRO:O	2.37	0.43
1:D:45:VAL:C	1:D:47:PRO:CD	2.87	0.43
1:B:9:GLY:C	1:B:10:LEU:CG	2.80	0.43
1:D:532:LEU:O	1:D:536:MET:N	2.52	0.43
1:A:628:HIS:O	1:A:629:GLY:C	2.58	0.43
1:D:663:ASP:OD2	1:D:663:ASP:N	2.51	0.42
1:A:659:ASN:O	1:A:659:ASN:CG	2.57	0.42
1:D:164:PRO:CB	1:D:166:PHE:CE1	3.02	0.42
1:B:164:PRO:CB	1:B:166:PHE:CE1	3.03	0.42
1:C:45:VAL:C	1:C:47:PRO:CD	2.88	0.42
1:A:261:LEU:N	1:A:262:PRO:CD	2.82	0.42
1:B:16:HIS:CD2	1:B:20:ILE:CG1	3.03	0.42
1:B:11:ASP:O	1:B:14:GLN:N	2.53	0.42
1:C:660:PRO:O	1:C:661:VAL:C	2.58	0.42
1:A:11:ASP:O	1:A:14:GLN:N	2.52	0.42
1:D:499:PHE:O	1:D:500:GLU:CB	2.66	0.42
1:A:672:ASN:ND2	1:A:672:ASN:N	2.67	0.42
1:A:45:VAL:C	1:A:47:PRO:CD	2.88	0.42
1:D:683:ILE:CG2	1:D:684:SER:N	2.82	0.42
1:B:289:ASP:O	1:B:289:ASP:CG	2.58	0.42
1:C:515:PRO:O	1:C:518:VAL:CG2	2.68	0.42
1:A:114:THR:CG2	1:A:114:THR:O	2.67	0.42
1:C:16:HIS:CD2	1:C:20:ILE:CG1	3.03	0.41
1:C:686:ASN:O	1:C:688:GLY:N	2.53	0.41
1:C:531:SER:O	1:C:534:GLN:N	2.53	0.41
1:A:42:VAL:O	1:A:44:PRO:CD	2.68	0.41
1:C:663:ASP:N	1:C:663:ASP:OD2	2.52	0.41
1:A:305:LEU:CA	1:A:366:ILE:CD1	2.99	0.41
1:B:43:ILE:N	1:B:44:PRO:CD	2.83	0.41
1:B:663:ASP:N	1:B:663:ASP:OD2	2.52	0.41
1:C:683:ILE:CG2	1:C:684:SER:N	2.84	0.41
1:B:42:VAL:O	1:B:44:PRO:CD	2.69	0.41
1:A:164:PRO:CB	1:A:166:PHE:CE1	3.04	0.41
1:C:42:VAL:O	1:C:44:PRO:CD	2.69	0.41
1:B:683:ILE:CG2	1:B:684:SER:N	2.83	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:16:HIS:CD2	1:D:20:ILE:CG1	3.03	0.41
1:B:45:VAL:C	1:B:47:PRO:CD	2.89	0.41
1:C:628:HIS:O	1:C:629:GLY:C	2.58	0.41
1:A:683:ILE:CG2	1:A:684:SER:N	2.83	0.41
1:A:680:GLU:O	1:A:681:GLU:C	2.58	0.41
1:B:660:PRO:O	1:B:661:VAL:C	2.60	0.41
1:C:680:GLU:O	1:C:681:GLU:C	2.59	0.41
1:B:687:LYS:CE	1:D:338:ARG:NH2	2.83	0.41
1:A:171:LEU:CD2	1:A:216:LEU:CD2	2.99	0.41
1:A:531:SER:O	1:A:532:LEU:C	2.59	0.41
1:C:499:PHE:O	1:C:500:GLU:CB	2.65	0.40
1:B:527:ASN:OD1	1:B:527:ASN:N	2.54	0.40
1:A:9:GLY:O	1:A:10:LEU:CD2	2.67	0.40
1:A:16:HIS:CD2	1:A:20:ILE:CG1	3.03	0.40
1:C:532:LEU:O	1:C:536:MET:N	2.55	0.40
1:C:210:LEU:O	1:C:210:LEU:CD2	2.69	0.40
1:A:43:ILE:N	1:A:44:PRO:CD	2.84	0.40
1:D:45:VAL:O	1:D:47:PRO:N	2.54	0.40
1:D:467:ARG:NH2	1:D:548:GLU:OE1	2.55	0.40
1:A:527:ASN:OD1	1:A:527:ASN:N	2.54	0.40
1:A:312:ASN:N	1:A:315:GLN:NE2	2.70	0.40
1:C:488:VAL:O	1:C:534:GLN:CG	2.70	0.40
1:C:43:ILE:N	1:C:44:PRO:CD	2.84	0.40
1:C:233:ASN:O	1:C:234:LEU:C	2.60	0.40
1:C:375:SER:CA	1:C:376:ASP:OD1	2.69	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	558/647 (86%)	486 (87%)	46 (8%)	26 (5%)	4	23
1	B	558/647 (86%)	482 (86%)	49 (9%)	27 (5%)	4	23
1	C	558/647 (86%)	485 (87%)	46 (8%)	27 (5%)	4	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	558/647 (86%)	489 (88%)	43 (8%)	26 (5%)	4	23
All	All	2232/2588 (86%)	1942 (87%)	184 (8%)	106 (5%)	4	23

All (106) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	PRO
1	A	356	LEU
1	A	367	PRO
1	A	368	ASN
1	A	473	GLN
1	A	527	ASN
1	A	612	GLN
1	A	661	VAL
1	A	681	GLU
1	B	29	PRO
1	B	356	LEU
1	B	367	PRO
1	B	368	ASN
1	B	473	GLN
1	B	527	ASN
1	B	612	GLN
1	B	661	VAL
1	B	681	GLU
1	C	29	PRO
1	C	356	LEU
1	C	367	PRO
1	C	368	ASN
1	C	473	GLN
1	C	527	ASN
1	C	532	LEU
1	C	612	GLN
1	C	661	VAL
1	C	681	GLU
1	D	29	PRO
1	D	356	LEU
1	D	367	PRO
1	D	368	ASN
1	D	377	ASP
1	D	473	GLN
1	D	527	ASN
1	D	532	LEU

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Mol	Chain	Res	Type
1	D	612	GLN
1	D	661	VAL
1	D	681	GLU
1	A	10	LEU
1	A	28	GLU
1	A	164	PRO
1	A	377	ASP
1	A	452	LYS
1	A	469	LYS
1	A	474	LEU
1	A	495	ASP
1	A	499	PHE
1	A	662	HIS
1	A	680	GLU
1	B	10	LEU
1	B	28	GLU
1	B	164	PRO
1	B	377	ASP
1	B	452	LYS
1	B	469	LYS
1	B	474	LEU
1	B	495	ASP
1	B	499	PHE
1	B	532	LEU
1	B	662	HIS
1	B	680	GLU
1	C	10	LEU
1	C	28	GLU
1	C	164	PRO
1	C	377	ASP
1	C	452	LYS
1	C	469	LYS
1	C	474	LEU
1	C	495	ASP
1	C	499	PHE
1	C	662	HIS
1	C	680	GLU
1	D	10	LEU
1	D	28	GLU
1	D	164	PRO
1	D	452	LYS
1	D	469	LYS

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Mol	Chain	Res	Type
1	D	474	LEU
1	D	495	ASP
1	D	662	HIS
1	D	680	GLU
1	A	526	PHE
1	A	613	ASN
1	A	660	PRO
1	B	526	PHE
1	B	660	PRO
1	C	526	PHE
1	D	499	PHE
1	D	526	PHE
1	D	660	PRO
1	A	453	ALA
1	B	453	ALA
1	B	613	ASN
1	C	453	ALA
1	C	613	ASN
1	C	660	PRO
1	D	453	ALA
1	A	43	ILE
1	B	43	ILE
1	C	43	ILE
1	D	43	ILE
1	D	46	TYR
1	A	46	TYR
1	B	46	TYR
1	C	46	TYR

### 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	516/590 (88%)	463 (90%)	53 (10%)	10	36
1	B	516/590 (88%)	460 (89%)	56 (11%)	9	34
1	C	516/590 (88%)	461 (89%)	55 (11%)	10	35
1	D	516/590 (88%)	461 (89%)	55 (11%)	10	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2064/2360 (88%)	1845 (89%)	219 (11%)	10	35

All (219) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	HIS
1	A	27	ARG
1	A	57	LEU
1	A	68	LEU
1	A	70	GLN
1	A	76	ARG
1	A	109	LEU
1	A	134	VAL
1	A	139	ILE
1	A	148	LEU
1	A	155	LEU
1	A	167	LEU
1	A	192	LEU
1	A	213	GLN
1	A	230	THR
1	A	233	ASN
1	A	234	LEU
1	A	237	VAL
1	A	242	ARG
1	A	261	LEU
1	A	263	LEU
1	A	273	ASN
1	A	277	THR
1	A	290	PHE
1	A	291	THR
1	A	312	ASN
1	A	315	GLN
1	A	337	GLU
1	A	352	SER
1	A	376	ASP
1	A	377	ASP
1	A	383	GLN
1	A	428	ARG
1	A	458	LEU
1	A	472	PHE
1	A	473	GLN
1	A	474	LEU

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Mol	Chain	Res	Type
1	A	492	ASN
1	A	494	PHE
1	A	496	GLU
1	A	525	LEU
1	A	530	LEU
1	A	531	SER
1	A	534	GLN
1	A	537	SER
1	A	550	ARG
1	A	553	ASP
1	A	642	LEU
1	A	650	THR
1	A	661	VAL
1	A	672	ASN
1	A	681	GLU
1	A	684	SER
1	B	16	HIS
1	B	27	ARG
1	B	57	LEU
1	B	68	LEU
1	B	70	GLN
1	B	76	ARG
1	B	109	LEU
1	B	134	VAL
1	B	139	ILE
1	B	148	LEU
1	B	155	LEU
1	B	167	LEU
1	B	192	LEU
1	B	213	GLN
1	B	230	THR
1	B	233	ASN
1	B	234	LEU
1	B	237	VAL
1	B	242	ARG
1	B	261	LEU
1	B	263	LEU
1	B	273	ASN
1	B	277	THR
1	B	290	PHE
1	B	291	THR
1	B	308	VAL

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Mol	Chain	Res	Type
1	B	312	ASN
1	B	337	GLU
1	B	352	SER
1	B	370	LYS
1	B	376	ASP
1	B	377	ASP
1	B	383	GLN
1	B	428	ARG
1	B	458	LEU
1	B	472	PHE
1	B	473	GLN
1	B	474	LEU
1	B	492	ASN
1	B	494	PHE
1	B	496	GLU
1	B	525	LEU
1	B	530	LEU
1	B	533	GLN
1	B	534	GLN
1	B	535	ARG
1	B	537	SER
1	B	539	LEU
1	B	550	ARG
1	B	553	ASP
1	B	642	LEU
1	B	650	THR
1	B	661	VAL
1	B	672	ASN
1	B	681	GLU
1	B	684	SER
1	C	16	HIS
1	C	27	ARG
1	C	57	LEU
1	C	68	LEU
1	C	70	GLN
1	C	76	ARG
1	C	109	LEU
1	C	134	VAL
1	C	139	ILE
1	C	148	LEU
1	C	155	LEU
1	C	167	LEU

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Mol	Chain	Res	Type
1	C	192	LEU
1	C	213	GLN
1	C	230	THR
1	C	233	ASN
1	C	234	LEU
1	C	237	VAL
1	C	242	ARG
1	C	261	LEU
1	C	263	LEU
1	C	273	ASN
1	C	277	THR
1	C	290	PHE
1	C	291	THR
1	C	312	ASN
1	C	315	GLN
1	C	337	GLU
1	C	352	SER
1	C	376	ASP
1	C	377	ASP
1	C	383	GLN
1	C	428	ARG
1	C	458	LEU
1	C	472	PHE
1	C	473	GLN
1	C	474	LEU
1	C	492	ASN
1	C	494	PHE
1	C	496	GLU
1	C	525	LEU
1	C	530	LEU
1	C	534	GLN
1	C	537	SER
1	C	539	LEU
1	C	550	ARG
1	C	553	ASP
1	C	632	ASN
1	C	642	LEU
1	C	650	THR
1	C	661	VAL
1	C	662	HIS
1	C	672	ASN
1	C	681	GLU

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Mol	Chain	Res	Type
1	C	684	SER
1	D	16	HIS
1	D	27	ARG
1	D	57	LEU
1	D	68	LEU
1	D	70	GLN
1	D	76	ARG
1	D	109	LEU
1	D	134	VAL
1	D	139	ILE
1	D	148	LEU
1	D	155	LEU
1	D	167	LEU
1	D	192	LEU
1	D	213	GLN
1	D	230	THR
1	D	233	ASN
1	D	234	LEU
1	D	237	VAL
1	D	242	ARG
1	D	261	LEU
1	D	263	LEU
1	D	273	ASN
1	D	277	THR
1	D	290	PHE
1	D	291	THR
1	D	308	VAL
1	D	312	ASN
1	D	315	GLN
1	D	337	GLU
1	D	352	SER
1	D	376	ASP
1	D	377	ASP
1	D	383	GLN
1	D	428	ARG
1	D	458	LEU
1	D	472	PHE
1	D	473	GLN
1	D	474	LEU
1	D	492	ASN
1	D	494	PHE
1	D	496	GLU

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Mol	Chain	Res	Type
1	D	525	LEU
1	D	530	LEU
1	D	533	GLN
1	D	534	GLN
1	D	537	SER
1	D	539	LEU
1	D	550	ARG
1	D	553	ASP
1	D	642	LEU
1	D	650	THR
1	D	661	VAL
1	D	672	ASN
1	D	681	GLU
1	D	684	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains 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	572/647 (88%)	-0.12	1 (0%)	93 61	60, 88, 144, 185	0
1	B	572/647 (88%)	-0.12	2 (0%)	91 53	64, 100, 154, 194	0
1	C	572/647 (88%)	-0.00	12 (2%)	60 11	62, 102, 210, 270	0
1	D	572/647 (88%)	-0.07	1 (0%)	93 61	52, 90, 197, 247	0
All	All	2288/2588 (88%)	-0.08	16 (0%)	84 32	52, 95, 181, 270	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	41	PHE	4.2
1	C	21	GLN	3.1
1	C	86	GLU	2.8
1	B	355	HIS	2.7
1	B	354	GLY	2.7
1	A	3	LEU	2.6
1	C	84	LEU	2.5
1	D	41	PHE	2.3
1	C	8	GLN	2.3
1	C	40	LYS	2.3
1	C	378	LYS	2.3
1	C	19	LEU	2.2
1	C	90	TYR	2.2
1	C	37	VAL	2.2
1	C	470	ALA	2.2
1	C	14	GLN	2.1

### 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 ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

There are no ligands in this entry.

### 6.5 Other polymers ⓘ

There are no such residues in this entry.