



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:18 PM GMT

PDB ID : 3Q06  
Title : An induced fit mechanism regulates p53 DNA binding kinetics to confer sequence specificity  
Authors : Petty, T.J.; Halazonetis, T.D.  
Deposited on : 2010-12-15  
Resolution : 3.20 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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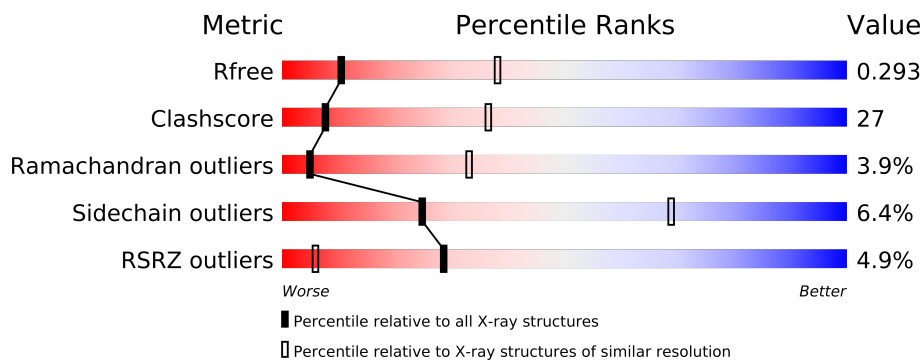
The following versions of software and data (see [references](#)) were used in the production of this report:

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


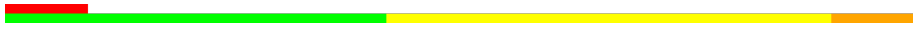


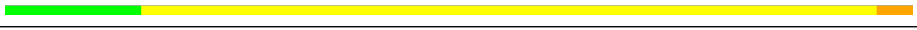
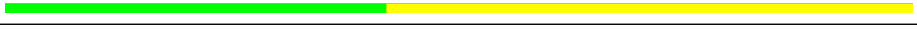
The reported resolution of this entry is 3.20 Å.

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	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)

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	231	
1	B	231	
1	C	231	
1	D	231	
2	K	26	
3	L	26	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8456 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 Cellular tumor antigen p53.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	0	0
			1848	1150	337	348	13			
1	C	231	Total	C	N	O	S	0	0	0
			1848	1150	337	348	13			
1	D	231	Total	C	N	O	S	0	0	0
			1848	1150	337	348	13			
1	B	231	Total	C	N	O	S	0	0	0
			1848	1150	337	348	13			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	135	VAL	CYS	ENGINEERED MUTATION	UNP P04637
A	141	VAL	CYS	ENGINEERED MUTATION	UNP P04637
A	146	TYR	TRP	ENGINEERED MUTATION	UNP P04637
A	182	SER	CYS	ENGINEERED MUTATION	UNP P04637
A	203	ALA	VAL	ENGINEERED MUTATION	UNP P04637
A	209	PRO	ARG	ENGINEERED MUTATION	UNP P04637
A	229	TYR	CYS	ENGINEERED MUTATION	UNP P04637
A	233	TYR	HIS	ENGINEERED MUTATION	UNP P04637
A	234	PHE	TYR	ENGINEERED MUTATION	UNP P04637
A	235	LYS	ASN	ENGINEERED MUTATION	UNP P04637
A	236	PHE	TYR	ENGINEERED MUTATION	UNP P04637
A	253	VAL	THR	ENGINEERED MUTATION	UNP P04637
A	268	ASP	ASN	ENGINEERED MUTATION	UNP P04637
A	322	THR	PRO	ENGINEERED MUTATION	UNP P04637
A	323	MET	LEU	ENGINEERED MUTATION	UNP P04637
A	340	GLN	MET	ENGINEERED MUTATION	UNP P04637
A	344	ARG	LEU	ENGINEERED MUTATION	UNP P04637
C	135	VAL	CYS	ENGINEERED MUTATION	UNP P04637
C	141	VAL	CYS	ENGINEERED MUTATION	UNP P04637
C	146	TYR	TRP	ENGINEERED MUTATION	UNP P04637
C	182	SER	CYS	ENGINEERED MUTATION	UNP P04637

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Chain	Residue	Modelled	Actual	Comment	Reference
C	203	ALA	VAL	ENGINEERED MUTATION	UNP P04637
C	209	PRO	ARG	ENGINEERED MUTATION	UNP P04637
C	229	TYR	CYS	ENGINEERED MUTATION	UNP P04637
C	233	TYR	HIS	ENGINEERED MUTATION	UNP P04637
C	234	PHE	TYR	ENGINEERED MUTATION	UNP P04637
C	235	LYS	ASN	ENGINEERED MUTATION	UNP P04637
C	236	PHE	TYR	ENGINEERED MUTATION	UNP P04637
C	253	VAL	THR	ENGINEERED MUTATION	UNP P04637
C	268	ASP	ASN	ENGINEERED MUTATION	UNP P04637
C	322	THR	PRO	ENGINEERED MUTATION	UNP P04637
C	323	MET	LEU	ENGINEERED MUTATION	UNP P04637
C	340	GLN	MET	ENGINEERED MUTATION	UNP P04637
C	344	ARG	LEU	ENGINEERED MUTATION	UNP P04637
D	135	VAL	CYS	ENGINEERED MUTATION	UNP P04637
D	141	VAL	CYS	ENGINEERED MUTATION	UNP P04637
D	146	TYR	TRP	ENGINEERED MUTATION	UNP P04637
D	182	SER	CYS	ENGINEERED MUTATION	UNP P04637
D	203	ALA	VAL	ENGINEERED MUTATION	UNP P04637
D	209	PRO	ARG	ENGINEERED MUTATION	UNP P04637
D	229	TYR	CYS	ENGINEERED MUTATION	UNP P04637
D	233	TYR	HIS	ENGINEERED MUTATION	UNP P04637
D	234	PHE	TYR	ENGINEERED MUTATION	UNP P04637
D	235	LYS	ASN	ENGINEERED MUTATION	UNP P04637
D	236	PHE	TYR	ENGINEERED MUTATION	UNP P04637
D	253	VAL	THR	ENGINEERED MUTATION	UNP P04637
D	268	ASP	ASN	ENGINEERED MUTATION	UNP P04637
D	322	THR	PRO	ENGINEERED MUTATION	UNP P04637
D	323	MET	LEU	ENGINEERED MUTATION	UNP P04637
D	340	GLN	MET	ENGINEERED MUTATION	UNP P04637
D	344	ARG	LEU	ENGINEERED MUTATION	UNP P04637
B	135	VAL	CYS	ENGINEERED MUTATION	UNP P04637
B	141	VAL	CYS	ENGINEERED MUTATION	UNP P04637
B	146	TYR	TRP	ENGINEERED MUTATION	UNP P04637
B	182	SER	CYS	ENGINEERED MUTATION	UNP P04637
B	203	ALA	VAL	ENGINEERED MUTATION	UNP P04637
B	209	PRO	ARG	ENGINEERED MUTATION	UNP P04637
B	229	TYR	CYS	ENGINEERED MUTATION	UNP P04637
B	233	TYR	HIS	ENGINEERED MUTATION	UNP P04637
B	234	PHE	TYR	ENGINEERED MUTATION	UNP P04637
B	235	LYS	ASN	ENGINEERED MUTATION	UNP P04637
B	236	PHE	TYR	ENGINEERED MUTATION	UNP P04637
B	253	VAL	THR	ENGINEERED MUTATION	UNP P04637

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Chain	Residue	Modelled	Actual	Comment	Reference
B	268	ASP	ASN	ENGINEERED MUTATION	UNP P04637
B	322	THR	PRO	ENGINEERED MUTATION	UNP P04637
B	323	MET	LEU	ENGINEERED MUTATION	UNP P04637
B	340	GLN	MET	ENGINEERED MUTATION	UNP P04637
B	344	ARG	LEU	ENGINEERED MUTATION	UNP P04637

- Molecule 2 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	26	Total	C	N	O	P	0	0	0
			527	252	96	154	25			

- Molecule 3 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	26	Total	C	N	O	P	0	0	0
			533	254	100	154	25			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	A	1	Total	Zn	0	0
			1	1		
4	D	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

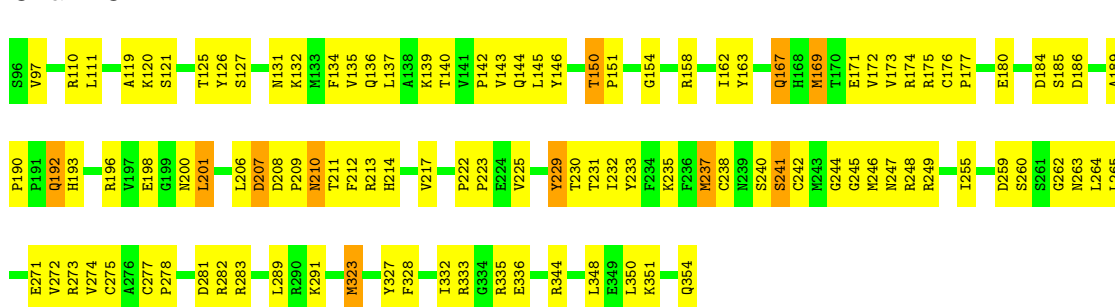
#### • Molecule 1: Cellular tumor antigen p53

Chain A:



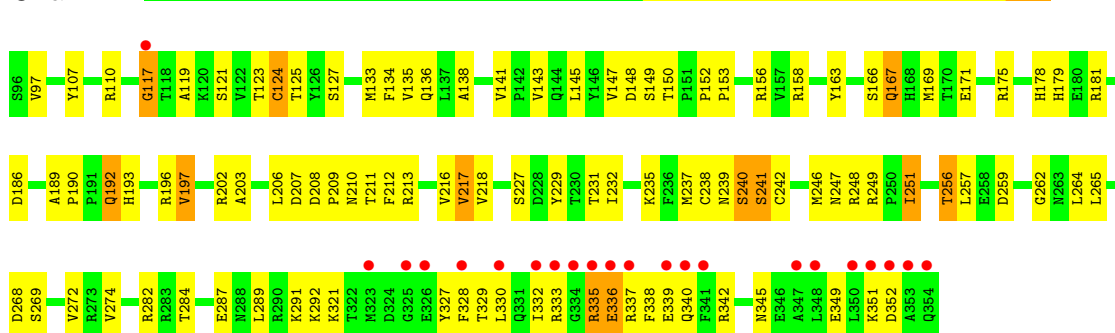
#### • Molecule 1: Cellular tumor antigen p53

Chain C:



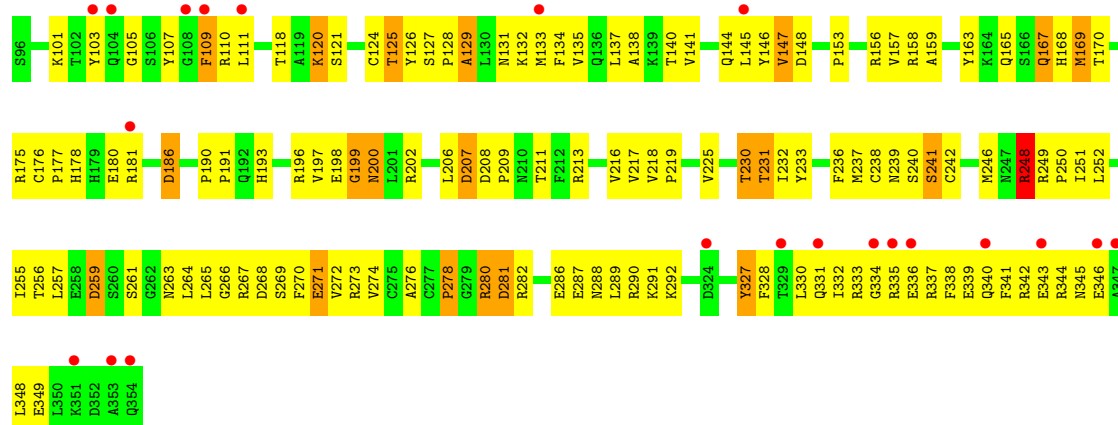
#### • Molecule 1: Cellular tumor antigen p53

Chain D:



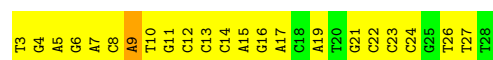
#### • Molecule 1: Cellular tumor antigen p53

Chain B: 



- Molecule 2: DNA (26-MER)

Chain K: 



- Molecule 3: DNA (26-MER)

Chain L: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	164.59Å 169.36Å 55.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.20 46.32 – 3.21	Depositor EDS
% Data completeness (in resolution range)	90.1 (50.00-3.20) 99.2 (46.32-3.21)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.18	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.39 (at 3.19Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.258 , 0.314 0.250 , 0.293	Depositor DCC
$R_{free}$ test set	1296 reflections (4.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	58.0	Xtriage
Anisotropy	0.579	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 20.1	EDS
Estimated twinning fraction	0.029 for k,h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	1 of 26029 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	8456	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.45% 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

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.36	0/1888	0.60	0/2549
1	B	0.34	0/1888	0.58	0/2549
1	C	0.46	0/1888	0.71	0/2549
1	D	0.39	0/1888	0.60	0/2549
2	K	0.45	0/590	0.80	2/908 (0.2%)
3	L	0.45	0/598	0.74	0/922
All	All	0.40	0/8740	0.65	2/12026 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	K	0	2
3	L	0	1
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	10	DT	C3'-C2'-C1'	-5.20	96.26	102.50
2	K	10	DT	C1'-O4'-C4'	-5.09	105.00	110.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	K	13	DC	Sidechain
2	K	9	DA	Sidechain
3	L	37	DC	Sidechain

## 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	1848	0	1813	76	0
1	B	1848	0	1815	166	0
1	C	1848	0	1813	92	0
1	D	1848	0	1813	93	0
2	K	527	0	294	24	0
3	L	533	0	294	16	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	8456	0	7842	440	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 27.

All (440) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:K:23:DC:H2"	2:K:24:DC:H5"	1.25	1.13
1:D:330:LEU:HD13	1:B:342:ARG:HG3	1.40	1.03
1:B:131:ASN:HD21	1:B:270:PHE:HA	1.30	0.96
2:K:21:DG:H2"	2:K:22:DC:H5"	1.46	0.93
1:B:147:VAL:HG22	1:B:148:ASP:H	1.34	0.92
1:B:131:ASN:ND2	1:B:270:PHE:HA	1.84	0.91
1:C:167:GLN:NE2	1:C:167:GLN:H	1.69	0.89
1:C:167:GLN:HE21	1:C:167:GLN:H	0.90	0.89
1:D:167:GLN:HE21	1:D:167:GLN:H	1.21	0.87
1:B:239:ASN:HB2	1:B:242:CYS:SG	2.15	0.87
1:C:241:SER:HA	1:C:248:ARG:H	1.38	0.87

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:167:GLN:HE21	1:A:167:GLN:H	1.22	0.86
1:B:127:SER:HB3	1:B:132:LYS:H	1.40	0.86
1:C:167:GLN:HE21	1:C:167:GLN:N	1.73	0.85
2:K:23:DC:C2'	2:K:24:DC:H5''	2.07	0.84
2:K:24:DC:H42	3:L:29:DG:H1	1.21	0.84
1:B:259:ASP:HB3	1:B:265:LEU:CD1	2.08	0.83
3:L:31:DG:H2''	3:L:32:DC:H5'	1.61	0.80
1:B:218:VAL:HG21	1:B:232:ILE:HD12	1.63	0.79
3:L:33:DA:H2''	3:L:34:DT:H5''	1.65	0.77
1:D:337:ARG:HD3	1:B:348:LEU:HD13	1.68	0.76
1:A:264:LEU:HD23	1:C:225:VAL:HG23	1.67	0.75
1:A:163:TYR:OH	1:A:246:MET:HA	1.87	0.74
1:D:328:PHE:O	1:B:331:GLN:HG3	1.88	0.73
1:D:333:ARG:HD3	1:B:349:GLU:HG2	1.69	0.73
1:D:163:TYR:OH	1:D:246:MET:HA	1.87	0.73
1:B:132:LYS:HE2	1:B:273:ARG:HB2	1.69	0.73
1:A:344:ARG:HG2	1:C:344:ARG:HH12	1.53	0.73
1:D:246:MET:SD	1:D:251:ILE:HG21	2.29	0.73
1:D:337:ARG:NH1	1:B:348:LEU:HB3	2.04	0.72
1:A:246:MET:SD	1:A:251:ILE:HG21	2.29	0.72
1:B:140:THR:HG23	1:B:198:GLU:OE2	1.90	0.72
1:C:134:PHE:O	1:C:278:PRO:HB3	1.90	0.72
1:C:175:ARG:NH2	1:C:237:MET:HB3	2.04	0.71
1:C:240:SER:HB2	1:C:274:VAL:H	1.55	0.71
1:C:273:ARG:NE	1:C:275:CYS:SG	2.64	0.70
1:A:175:ARG:HB2	1:A:192:GLN:O	1.91	0.70
1:B:206:LEU:HD12	1:B:207:ASP:H	1.56	0.70
1:D:167:GLN:NE2	1:D:167:GLN:H	1.89	0.70
1:A:167:GLN:NE2	1:A:167:GLN:H	1.90	0.70
3:L:33:DA:H2''	3:L:34:DT:C5'	2.21	0.70
1:D:190:PRO:HB2	1:D:193:HIS:HD2	1.56	0.69
1:D:175:ARG:HB2	1:D:192:GLN:O	1.92	0.69
1:C:240:SER:HA	1:C:246:MET:CE	2.22	0.69
1:B:261:SER:HB3	1:B:263:ASN:ND2	2.07	0.69
1:A:190:PRO:HB2	1:A:193:HIS:HD2	1.57	0.68
2:K:21:DG:C2'	2:K:22:DC:H5''	2.21	0.68
1:D:240:SER:HB2	1:D:274:VAL:H	1.57	0.68
1:B:340:GLN:HG2	1:B:344:ARG:HD3	1.76	0.68
1:B:163:TYR:HE1	1:B:246:MET:HG3	1.59	0.68
1:B:147:VAL:HG22	1:B:148:ASP:N	2.08	0.68
1:D:268:ASP:OD1	1:D:269:SER:N	2.26	0.67
2:K:21:DG:H2''	2:K:22:DC:C5'	2.20	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:268:ASP:OD1	1:A:269:SER:N	2.26	0.67
1:B:282:ARG:O	1:B:286:GLU:HB2	1.95	0.67
1:A:138:ALA:O	1:A:235:LYS:HD2	1.95	0.67
1:A:240:SER:HB2	1:A:274:VAL:H	1.59	0.66
1:B:132:LYS:HE3	1:B:271:GLU:HG2	1.75	0.66
1:B:259:ASP:HB3	1:B:265:LEU:HD12	1.76	0.66
2:K:19:DA:H2	3:L:34:DT:H3	1.44	0.66
1:C:264:LEU:O	1:C:265:LEU:HD23	1.96	0.66
1:B:127:SER:HB3	1:B:132:LYS:N	2.11	0.66
2:K:22:DC:H2"	2:K:23:DC:C6	2.31	0.65
1:C:209:PRO:HG2	1:C:210:ASN:H	1.61	0.65
1:D:138:ALA:O	1:D:235:LYS:HD2	1.96	0.64
1:B:332:ILE:HG22	1:B:333:ARG:H	1.63	0.64
1:B:287:GLU:HB2	1:B:290:ARG:HH21	1.61	0.64
1:B:338:PHE:CZ	1:B:342:ARG:HB2	2.32	0.64
1:C:272:VAL:HG12	1:C:273:ARG:N	2.14	0.63
2:K:11:DG:H2"	2:K:12:DC:H5'	1.80	0.63
1:C:289:LEU:C	1:C:291:LYS:H	2.02	0.63
1:D:123:THR:O	1:D:124:CYS:HB2	1.98	0.63
1:A:107:TYR:HB3	1:A:147:VAL:HG23	1.82	0.62
1:D:338:PHE:HE2	1:B:330:LEU:HB2	1.64	0.62
1:D:107:TYR:HB3	1:D:147:VAL:HG23	1.81	0.62
1:B:134:PHE:O	1:B:278:PRO:HB3	2.00	0.62
1:A:264:LEU:HD23	1:C:225:VAL:CG2	2.29	0.62
1:C:273:ARG:HG2	1:C:275:CYS:SG	2.40	0.62
2:K:24:DC:N4	3:L:29:DG:H1	1.97	0.61
1:B:207:ASP:HA	1:B:213:ARG:O	1.99	0.61
1:A:123:THR:O	1:A:124:CYS:HB2	1.98	0.61
2:K:7:DA:H2"	2:K:8:DC:O5'	1.99	0.61
1:D:329:THR:HG22	1:D:330:LEU:H	1.66	0.61
3:L:32:DC:H2"	3:L:33:DA:C8	2.35	0.61
1:A:167:GLN:N	1:A:167:GLN:HE21	1.96	0.60
3:L:33:DA:C2'	3:L:34:DT:H5"	2.30	0.60
1:B:339:GLU:O	1:B:343:GLU:HB2	2.01	0.60
1:B:144:GLN:C	1:B:145:LEU:HD12	2.21	0.60
1:B:175:ARG:HD3	1:B:191:PRO:O	2.02	0.59
1:B:336:GLU:HA	1:B:339:GLU:HB3	1.83	0.59
1:A:329:THR:HG22	1:A:330:LEU:H	1.66	0.59
1:A:135:VAL:HG21	1:A:141:VAL:CG2	2.33	0.59
1:D:167:GLN:HE21	1:D:167:GLN:N	1.96	0.59
1:B:141:VAL:HG21	1:B:236:PHE:CE1	2.37	0.59
1:D:329:THR:HA	1:B:331:GLN:HA	1.85	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:107:TYR:O	1:A:147:VAL:HG23	2.04	0.58
1:A:239:ASN:N	1:A:242:CYS:SG	2.77	0.58
1:D:107:TYR:O	1:D:147:VAL:HG23	2.03	0.58
1:D:135:VAL:HG21	1:D:141:VAL:CG2	2.33	0.58
1:C:348:LEU:HD23	1:C:351:LYS:HD3	1.86	0.58
1:B:135:VAL:HG11	1:B:236:PHE:HD1	1.69	0.58
1:B:168:HIS:CD2	1:B:249:ARG:HH11	2.22	0.57
1:C:323:MET:HB3	1:C:327:TYR:OH	2.04	0.57
1:B:259:ASP:HB3	1:B:265:LEU:HD11	1.86	0.57
1:A:239:ASN:O	1:A:241:SER:N	2.37	0.57
1:B:129:ALA:HB2	1:B:346:GLU:OE2	2.05	0.56
1:C:163:TYR:OH	1:C:246:MET:HA	2.05	0.56
1:B:125:THR:HG22	1:B:134:PHE:HB2	1.88	0.56
1:A:127:SER:HB2	1:A:282:ARG:NE	2.20	0.56
1:D:337:ARG:NH1	1:B:349:GLU:HG3	2.21	0.56
1:D:127:SER:HB2	1:D:282:ARG:NE	2.20	0.56
3:L:30:DG:H2"	3:L:31:DG:C8	2.40	0.56
1:B:167:GLN:H	1:B:167:GLN:NE2	2.02	0.56
1:B:158:ARG:HA	1:B:216:VAL:O	2.05	0.56
1:C:211:THR:O	1:C:212:PHE:HB2	2.05	0.56
1:C:206:LEU:HG	1:C:207:ASP:N	2.21	0.56
1:C:259:ASP:OD2	1:C:263:ASN:HB2	2.06	0.56
2:K:23:DC:H2"	2:K:24:DC:C5'	2.18	0.55
1:B:126:TYR:O	1:B:128:PRO:HD3	2.07	0.55
1:A:289:LEU:C	1:A:291:LYS:H	2.10	0.55
3:L:34:DT:H2"	3:L:35:DG:C8	2.41	0.55
1:A:197:VAL:HG21	1:A:203:ALA:HB1	1.88	0.55
1:A:197:VAL:HG22	1:A:216:VAL:HG21	1.89	0.55
1:D:289:LEU:C	1:D:291:LYS:H	2.10	0.55
1:C:132:LYS:HG3	1:C:271:GLU:HB3	1.88	0.55
1:D:239:ASN:N	1:D:242:CYS:SG	2.80	0.55
1:C:127:SER:O	1:C:131:ASN:N	2.40	0.55
1:B:145:LEU:HD11	1:B:232:ILE:HG22	1.88	0.54
2:K:5:DA:H2"	2:K:6:DG:H5"	1.88	0.54
1:B:109:PHE:CD1	1:B:257:LEU:HD22	2.42	0.54
1:B:211:THR:HB	1:B:213:ARG:HG2	1.87	0.54
1:B:110:ARG:O	1:B:111:LEU:HD23	2.07	0.54
1:C:163:TYR:CE2	1:C:173:VAL:HG22	2.41	0.54
1:C:241:SER:HA	1:C:248:ARG:N	2.17	0.54
1:C:176:CYS:HB3	1:C:242:CYS:HB3	1.88	0.54
1:C:111:LEU:HD11	1:C:255:ILE:HG13	1.90	0.54
1:C:240:SER:HA	1:C:246:MET:HE3	1.89	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:190:PRO:HB2	1:B:193:HIS:CD2	2.43	0.54
1:D:197:VAL:HG21	1:D:203:ALA:HB1	1.89	0.54
1:B:246:MET:HE1	1:B:251:ILE:HD13	1.90	0.53
1:B:167:GLN:H	1:B:167:GLN:CD	2.10	0.53
1:B:159:ALA:HB3	1:B:216:VAL:HG12	1.91	0.53
1:B:144:GLN:HG2	1:B:231:THR:HG22	1.90	0.53
1:A:333:ARG:HB3	1:C:327:TYR:CD2	2.43	0.53
1:A:127:SER:HB2	1:A:282:ARG:HE	1.73	0.53
1:B:132:LYS:HG3	1:B:271:GLU:HG2	1.89	0.53
1:B:273:ARG:HE	1:B:281:ASP:HB3	1.74	0.53
1:C:184:ASP:O	1:C:186:ASP:N	2.38	0.53
1:D:127:SER:HB2	1:D:282:ARG:HE	1.73	0.53
1:A:203:ALA:HA	1:A:218:VAL:HG12	1.91	0.53
1:B:101:LYS:NZ	1:B:103:TYR:HB2	2.24	0.53
1:B:246:MET:CE	1:B:251:ILE:HD13	2.38	0.53
1:D:197:VAL:HG22	1:D:216:VAL:HG21	1.90	0.53
1:B:280:ARG:C	1:B:282:ARG:H	2.11	0.53
1:B:259:ASP:OD2	1:B:265:LEU:HG	2.09	0.53
1:B:239:ASN:HA	1:B:274:VAL:CG1	2.39	0.52
1:D:175:ARG:NH2	1:D:237:MET:HB3	2.24	0.52
1:B:125:THR:O	1:B:125:THR:HG23	2.08	0.52
2:K:6:DG:H2''	2:K:7:DA:O5'	2.08	0.52
1:C:208:ASP:OD2	1:C:211:THR:HG23	2.10	0.52
1:D:97:VAL:HA	1:D:213:ARG:NH2	2.25	0.52
2:K:14:DC:H2''	2:K:15:DA:N7	2.24	0.52
1:B:101:LYS:HD2	1:B:103:TYR:HB2	1.91	0.52
1:B:110:ARG:NE	1:B:146:TYR:HB2	2.24	0.52
1:D:97:VAL:HA	1:D:213:ARG:HH21	1.74	0.52
1:D:239:ASN:O	1:D:241:SER:N	2.38	0.52
1:A:175:ARG:NH2	1:A:237:MET:HB3	2.25	0.52
1:D:107:TYR:HB3	1:D:147:VAL:CG2	2.40	0.51
1:A:208:ASP:OD1	1:A:209:PRO:HD2	2.11	0.51
1:C:240:SER:HA	1:C:246:MET:HE1	1.91	0.51
1:D:203:ALA:HA	1:D:218:VAL:HG12	1.93	0.51
1:D:97:VAL:HG22	1:D:213:ARG:HH22	1.74	0.51
1:B:120:LYS:HE3	2:K:15:DA:OP2	2.10	0.51
1:C:143:VAL:O	1:C:232:ILE:HG22	2.11	0.51
1:B:338:PHE:HA	1:B:341:PHE:HB2	1.92	0.51
3:L:32:DC:H2''	3:L:33:DA:N7	2.26	0.51
1:D:336:GLU:O	1:D:340:GLN:HG3	2.11	0.51
1:A:143:VAL:O	1:A:232:ILE:HG22	2.10	0.51
1:B:141:VAL:HG21	1:B:236:PHE:CD1	2.46	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:268:ASP:OD1	1:B:269:SER:N	2.44	0.51
1:A:239:ASN:HA	1:A:274:VAL:CG1	2.40	0.51
1:A:284:THR:O	1:A:287:GLU:HB3	2.11	0.51
1:A:240:SER:O	1:A:241:SER:HB3	2.11	0.51
1:C:175:ARG:HG3	1:C:192:GLN:O	2.11	0.51
1:D:143:VAL:O	1:D:232:ILE:HG22	2.10	0.51
1:C:111:LEU:HD11	1:C:255:ILE:CG1	2.40	0.50
1:B:103:TYR:CE1	1:B:105:GLY:HA2	2.46	0.50
1:B:177:PRO:HA	1:B:180:GLU:HB3	1.93	0.50
1:D:239:ASN:HA	1:D:274:VAL:CG1	2.41	0.50
1:B:335:ARG:O	1:B:339:GLU:HB2	2.11	0.50
1:A:336:GLU:O	1:A:340:GLN:HG3	2.11	0.50
3:L:51:DA:H2"	3:L:52:DA:C8	2.46	0.50
1:B:168:HIS:C	1:B:170:THR:H	2.13	0.50
1:B:103:TYR:HE2	1:B:264:LEU:HG	1.76	0.50
1:D:166:SER:HA	1:D:169:MET:HG3	1.93	0.50
1:A:206:LEU:HD12	1:A:207:ASP:H	1.76	0.50
1:D:284:THR:O	1:D:287:GLU:HB3	2.12	0.50
1:D:329:THR:HG22	1:D:330:LEU:N	2.27	0.50
1:C:229:TYR:C	1:C:229:TYR:CD1	2.85	0.50
1:D:208:ASP:OD1	1:D:209:PRO:HD2	2.12	0.50
1:B:147:VAL:CG2	1:B:148:ASP:H	2.16	0.50
1:B:109:PHE:HE1	1:B:145:LEU:HD23	1.77	0.50
1:C:125:THR:O	1:C:125:THR:HG23	2.12	0.50
1:A:97:VAL:HA	1:A:213:ARG:HH21	1.76	0.50
1:A:166:SER:HA	1:A:169:MET:HG3	1.93	0.50
1:B:252:LEU:HD12	1:B:271:GLU:CA	2.42	0.50
1:D:240:SER:O	1:D:241:SER:HB3	2.11	0.50
1:B:273:ARG:HG3	1:B:273:ARG:HH11	1.77	0.50
1:C:171:GLU:CD	1:C:249:ARG:HH12	2.15	0.50
1:C:196:ARG:NE	1:C:237:MET:HG3	2.27	0.49
1:C:135:VAL:O	1:C:274:VAL:HA	2.11	0.49
1:A:97:VAL:HG22	1:A:213:ARG:HH22	1.75	0.49
1:B:131:ASN:HD21	1:B:270:PHE:CA	2.14	0.49
1:B:127:SER:HB3	1:B:132:LYS:O	2.12	0.49
1:A:344:ARG:CG	1:C:344:ARG:HH12	2.23	0.49
1:C:283:ARG:HH11	1:C:283:ARG:HG3	1.77	0.49
1:B:248:ARG:O	1:B:250:PRO:HD3	2.12	0.49
1:A:257:LEU:O	1:A:265:LEU:HB2	2.12	0.49
1:B:126:TYR:OH	1:B:131:ASN:HA	2.12	0.49
1:B:241:SER:HA	1:B:248:ARG:H	1.77	0.49
1:C:131:ASN:CG	1:C:131:ASN:O	2.49	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:144:GLN:HG2	1:B:231:THR:CG2	2.43	0.49
1:A:107:TYR:HB3	1:A:147:VAL:CG2	2.41	0.49
1:C:335:ARG:HG3	1:C:335:ARG:NH1	2.27	0.49
1:D:206:LEU:HD12	1:D:207:ASP:H	1.78	0.49
1:C:177:PRO:HD3	1:C:244:GLY:O	2.12	0.49
1:B:107:TYR:O	1:B:148:ASP:HB2	2.11	0.49
1:B:246:MET:HE2	1:B:251:ILE:HG21	1.94	0.49
1:C:162:ILE:HG13	1:C:162:ILE:O	2.12	0.49
1:C:283:ARG:HG3	1:C:283:ARG:NH1	2.28	0.48
1:B:176:CYS:SG	1:B:178:HIS:HB3	2.53	0.48
1:B:156:ARG:HE	1:B:217:VAL:HG11	1.78	0.48
1:B:101:LYS:CD	1:B:103:TYR:HB2	2.43	0.48
1:D:337:ARG:CZ	1:B:348:LEU:HB3	2.42	0.48
1:B:190:PRO:HB2	1:B:193:HIS:HD2	1.78	0.48
1:A:97:VAL:HA	1:A:213:ARG:NH2	2.27	0.48
1:B:157:VAL:O	1:B:217:VAL:HA	2.13	0.48
1:D:264:LEU:HG	1:D:265:LEU:N	2.28	0.48
1:C:198:GLU:HG2	1:C:235:LYS:HE2	1.94	0.48
1:D:328:PHE:C	1:B:331:GLN:HG3	2.33	0.48
1:D:330:LEU:HD11	1:B:345:ASN:ND2	2.29	0.48
1:A:264:LEU:HG	1:A:265:LEU:N	2.28	0.48
1:C:273:ARG:HH21	1:C:281:ASP:CG	2.17	0.48
1:A:329:THR:HG22	1:A:330:LEU:N	2.27	0.48
1:B:252:LEU:HD12	1:B:271:GLU:HA	1.96	0.48
1:D:337:ARG:HH12	1:B:349:GLU:HG3	1.78	0.48
1:B:336:GLU:HA	1:B:339:GLU:CB	2.44	0.48
1:D:156:ARG:NH2	1:D:217:VAL:HG21	2.28	0.48
2:K:3:DT:H2"	2:K:4:DG:C8	2.48	0.47
1:B:334:GLY:O	1:B:338:PHE:HB3	2.13	0.47
1:D:330:LEU:HD11	1:B:345:ASN:CG	2.35	0.47
1:B:334:GLY:HA3	1:B:337:ARG:HB3	1.95	0.47
1:D:240:SER:HB2	1:D:274:VAL:N	2.27	0.47
1:A:197:VAL:HG21	1:A:203:ALA:CB	2.45	0.47
1:A:209:PRO:HG2	1:A:210:ASN:OD1	2.15	0.47
1:D:145:LEU:N	1:D:145:LEU:HD12	2.29	0.47
1:C:272:VAL:CG1	1:C:273:ARG:N	2.77	0.47
1:B:240:SER:N	1:B:274:VAL:HB	2.28	0.47
1:B:280:ARG:O	1:B:282:ARG:N	2.44	0.47
1:A:158:ARG:HG3	1:A:217:VAL:HG13	1.96	0.47
1:C:142:PRO:HB3	1:C:233:TYR:CE2	2.49	0.47
1:B:156:ARG:HB3	1:B:217:VAL:HG12	1.97	0.47
1:A:156:ARG:NH2	1:A:217:VAL:HG21	2.29	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:158:ARG:HB3	1:A:256:THR:HG23	1.96	0.47
1:C:169:MET:O	1:C:169:MET:HG2	2.14	0.47
1:A:145:LEU:HD12	1:A:145:LEU:N	2.29	0.47
1:B:128:PRO:HB2	1:B:346:GLU:OE1	2.15	0.47
1:B:252:LEU:HD12	1:B:271:GLU:N	2.30	0.47
1:D:158:ARG:HG3	1:D:217:VAL:HG13	1.96	0.47
1:D:197:VAL:HG21	1:D:203:ALA:CB	2.45	0.47
1:B:271:GLU:HG3	1:B:272:VAL:N	2.29	0.47
1:B:109:PHE:CZ	1:B:255:ILE:HG22	2.49	0.47
1:B:103:TYR:CZ	1:B:105:GLY:HA2	2.49	0.47
1:D:158:ARG:HB3	1:D:256:THR:HG23	1.97	0.47
1:B:282:ARG:O	1:B:282:ARG:HD3	2.15	0.46
2:K:12:DC:H6	2:K:12:DC:H5'	1.79	0.46
1:B:125:THR:CG2	1:B:134:PHE:HB2	2.45	0.46
1:D:247:ASN:O	1:D:248:ARG:HB2	2.15	0.46
1:A:196:ARG:CZ	1:A:237:MET:HG3	2.46	0.46
1:D:257:LEU:O	1:D:265:LEU:HB2	2.15	0.46
1:D:209:PRO:HG2	1:D:210:ASN:OD1	2.16	0.46
1:C:335:ARG:HG3	1:C:335:ARG:HH11	1.79	0.46
1:C:145:LEU:N	1:C:230:THR:O	2.47	0.46
1:C:140:THR:HG22	1:C:142:PRO:HD3	1.98	0.46
1:A:134:PHE:CD1	1:A:134:PHE:N	2.84	0.46
1:A:247:ASN:O	1:A:248:ARG:HB2	2.15	0.46
2:K:8:DC:H2''	2:K:9:DA:H5'	1.98	0.46
1:B:202:ARG:HB3	1:B:219:PRO:HG2	1.98	0.46
1:B:338:PHE:O	1:B:341:PHE:N	2.49	0.46
1:B:133:MET:N	1:B:271:GLU:O	2.49	0.46
1:B:175:ARG:HD2	1:B:193:HIS:O	2.16	0.46
1:C:126:TYR:OH	1:C:131:ASN:HA	2.16	0.45
1:B:163:TYR:CE1	1:B:246:MET:HG3	2.44	0.45
1:B:273:ARG:HE	1:B:281:ASP:CB	2.28	0.45
2:K:16:DG:H2''	2:K:17:DA:O5'	2.16	0.45
1:C:277:CYS:N	1:C:278:PRO:HD3	2.32	0.45
1:C:134:PHE:CE2	1:C:282:ARG:HA	2.51	0.45
1:D:196:ARG:CZ	1:D:237:MET:HG3	2.46	0.45
1:B:125:THR:O	1:B:125:THR:CG2	2.64	0.45
1:C:172:VAL:HB	1:C:174:ARG:HH12	1.82	0.45
3:L:38:DT:H2''	3:L:39:DG:N7	2.31	0.45
1:B:198:GLU:O	1:B:199:GLY:O	2.34	0.45
1:C:289:LEU:C	1:C:291:LYS:N	2.70	0.45
1:C:158:ARG:NH2	1:C:217:VAL:HG21	2.31	0.45
1:D:332:ILE:HD12	1:B:330:LEU:HD23	1.99	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:135:VAL:HG11	1:B:236:PHE:CD1	2.50	0.45
1:D:135:VAL:HG22	1:D:136:GLN:N	2.32	0.45
1:D:134:PHE:N	1:D:134:PHE:CD1	2.84	0.45
1:A:240:SER:HB2	1:A:274:VAL:N	2.28	0.45
1:D:163:TYR:HH	1:D:246:MET:HA	1.81	0.45
1:D:196:ARG:NE	1:D:237:MET:HG3	2.32	0.45
1:D:335:ARG:HA	1:B:328:PHE:CZ	2.51	0.45
1:B:199:GLY:O	1:B:200:ASN:HB2	2.18	0.45
2:K:6:DG:H2''	2:K:7:DA:C5'	2.47	0.44
1:B:145:LEU:N	1:B:145:LEU:HD12	2.32	0.44
1:C:136:GLN:HB2	1:C:139:LYS:HG3	1.98	0.44
1:D:240:SER:HA	1:D:246:MET:CE	2.47	0.44
2:K:8:DC:H2''	2:K:9:DA:C5'	2.48	0.44
1:C:111:LEU:CD1	1:C:255:ILE:HG13	2.48	0.44
1:D:339:GLU:HG3	1:D:342:ARG:CZ	2.48	0.44
1:A:240:SER:HA	1:A:246:MET:CE	2.47	0.44
1:B:287:GLU:CB	1:B:290:ARG:HH21	2.30	0.44
1:B:288:ASN:C	1:B:289:LEU:HD12	2.38	0.44
1:B:327:TYR:HB3	1:B:328:PHE:H	1.64	0.44
3:L:28:DC:H2''	3:L:29:DG:C8	2.53	0.44
1:C:241:SER:HB2	1:C:248:ARG:HG2	2.00	0.44
1:C:208:ASP:OD1	1:C:209:PRO:HD2	2.17	0.44
1:C:150:THR:HA	1:C:151:PRO:HD3	1.70	0.44
1:B:132:LYS:HG3	1:B:271:GLU:CG	2.48	0.44
1:A:135:VAL:HG22	1:A:136:GLN:N	2.32	0.44
1:B:110:ARG:HG2	1:B:146:TYR:HB2	1.99	0.44
1:D:211:THR:O	1:D:212:PHE:HB2	2.18	0.44
1:A:196:ARG:NE	1:A:237:MET:HG3	2.32	0.44
1:B:340:GLN:HE21	1:B:344:ARG:HH11	1.66	0.44
1:A:133:MET:HB3	1:A:272:VAL:HG22	2.00	0.44
1:B:196:ARG:NE	1:B:237:MET:HG3	2.33	0.44
1:A:239:ASN:HA	1:A:274:VAL:HG12	2.01	0.43
1:B:237:MET:O	1:B:238:CYS:HB2	2.17	0.43
1:B:132:LYS:CE	1:B:271:GLU:HG2	2.45	0.43
1:D:239:ASN:HA	1:D:274:VAL:HG12	2.00	0.43
1:B:251:ILE:O	1:B:271:GLU:OE1	2.35	0.43
1:B:109:PHE:HZ	1:B:255:ILE:HG22	1.84	0.43
1:D:133:MET:HB3	1:D:272:VAL:HG22	1.99	0.43
1:B:240:SER:O	1:B:241:SER:HB3	2.19	0.43
1:B:257:LEU:HB3	1:B:266:GLY:HA3	2.01	0.43
1:C:277:CYS:O	1:C:278:PRO:C	2.57	0.43
1:D:189:ALA:HA	1:D:190:PRO:HD3	1.90	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:201:LEU:CD2	1:C:201:LEU:H	2.31	0.43
1:A:339:GLU:HG3	1:A:342:ARG:CZ	2.48	0.43
1:A:259:ASP:OD1	1:A:263:ASN:N	2.52	0.43
1:A:211:THR:O	1:A:212:PHE:HB2	2.18	0.43
1:C:126:TYR:CG	1:C:127:SER:N	2.86	0.43
1:C:180:GLU:OE2	1:C:192:GLN:NE2	2.51	0.43
1:C:176:CYS:CB	1:C:242:CYS:HB3	2.48	0.43
3:L:47:DC:C2'	3:L:48:DT:H71	2.48	0.43
1:B:135:VAL:HG21	1:B:141:VAL:HG22	2.00	0.43
1:B:158:ARG:HG2	1:B:159:ALA:N	2.33	0.43
1:C:206:LEU:HG	1:C:207:ASP:H	1.84	0.43
1:D:97:VAL:HG22	1:D:213:ARG:NH2	2.33	0.43
1:A:97:VAL:HG22	1:A:213:ARG:NH2	2.34	0.43
1:C:144:GLN:HE21	1:C:146:TYR:HE1	1.66	0.43
1:B:288:ASN:O	1:B:292:LYS:HB2	2.18	0.43
1:A:345:ASN:O	1:A:349:GLU:HG2	2.19	0.43
1:A:107:TYR:OH	1:A:152:PRO:HD3	2.19	0.42
1:A:351:LYS:HG2	1:A:351:LYS:O	2.19	0.42
1:B:165:GLN:O	1:B:169:MET:HB2	2.19	0.42
1:B:335:ARG:HA	1:B:335:ARG:NE	2.34	0.42
1:D:145:LEU:N	1:D:145:LEU:CD1	2.83	0.42
1:C:184:ASP:HB2	1:C:196:ARG:HH22	1.83	0.42
1:B:278:PRO:O	1:B:282:ARG:HB2	2.19	0.42
1:B:276:ALA:C	1:B:278:PRO:HD3	2.39	0.42
1:A:259:ASP:OD1	1:A:262:GLY:N	2.50	0.42
1:D:345:ASN:O	1:D:349:GLU:HG2	2.19	0.42
1:C:200:ASN:C	1:C:200:ASN:OD1	2.58	0.42
1:A:178:HIS:O	1:A:181:ARG:HG3	2.20	0.42
1:B:118:THR:HG21	1:B:282:ARG:NH1	2.34	0.42
1:B:118:THR:HG22	1:B:125:THR:OG1	2.19	0.42
2:K:11:DG:H1'	2:K:12:DC:H5''	2.01	0.42
1:B:156:ARG:HB3	1:B:217:VAL:CG1	2.50	0.42
1:C:222:PRO:HA	1:C:223:PRO:HD3	1.90	0.42
1:B:197:VAL:CG2	1:B:232:ILE:HD11	2.50	0.42
1:B:349:GLU:CD	1:B:349:GLU:H	2.23	0.42
1:B:256:THR:HA	1:B:267:ARG:HA	2.01	0.42
1:D:125:THR:HG23	1:D:134:PHE:HB2	2.01	0.42
1:D:321:LYS:HD2	1:D:321:LYS:N	2.34	0.42
1:A:200:ASN:OD1	1:A:202:ARG:N	2.50	0.42
1:D:351:LYS:HG2	1:D:351:LYS:O	2.19	0.42
1:D:327:TYR:HB3	1:B:331:GLN:NE2	2.35	0.42
1:D:107:TYR:OH	1:D:152:PRO:HD3	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:168:HIS:O	1:B:170:THR:N	2.53	0.42
1:A:125:THR:HG23	1:A:134:PHE:HB2	2.01	0.42
1:B:181:ARG:O	1:B:181:ARG:HG2	2.20	0.42
1:B:158:ARG:HB3	1:B:256:THR:CG2	2.50	0.42
1:B:103:TYR:CD2	1:B:264:LEU:HD21	2.55	0.42
1:C:154:GLY:HA3	1:C:260:SER:OG	2.19	0.42
1:B:137:LEU:O	1:B:138:ALA:HB3	2.19	0.42
1:A:117:GLY:H	1:A:121:SER:CB	2.33	0.42
1:B:159:ALA:HB3	1:B:216:VAL:CG1	2.50	0.41
1:A:145:LEU:N	1:A:145:LEU:CD1	2.83	0.41
1:D:259:ASP:OD1	1:D:262:GLY:N	2.51	0.41
1:B:208:ASP:OD1	1:B:209:PRO:HD2	2.19	0.41
1:B:109:PHE:CE1	1:B:145:LEU:HD23	2.53	0.41
1:B:198:GLU:O	1:B:199:GLY:C	2.58	0.41
1:B:110:ARG:CG	1:B:146:TYR:HB2	2.50	0.41
1:C:245:GLY:C	1:C:247:ASN:N	2.73	0.41
2:K:26:DT:H2''	2:K:27:DT:OP2	2.20	0.41
1:C:264:LEU:HA	1:C:264:LEU:HD12	1.87	0.41
1:D:178:HIS:O	1:D:181:ARG:HG3	2.19	0.41
1:D:117:GLY:H	1:D:121:SER:CB	2.33	0.41
1:C:348:LEU:C	1:C:350:LEU:H	2.23	0.41
1:C:332:ILE:CG2	1:C:333:ARG:N	2.84	0.41
1:D:171:GLU:OE1	1:D:249:ARG:NH1	2.53	0.41
1:A:321:LYS:N	1:A:321:LYS:HD2	2.34	0.41
1:B:333:ARG:HG2	1:B:334:GLY:N	2.36	0.41
3:L:33:DA:H2''	3:L:34:DT:H5'	2.00	0.41
1:B:181:ARG:HH11	1:B:181:ARG:HG3	1.86	0.41
1:B:145:LEU:N	1:B:230:THR:O	2.53	0.41
1:A:189:ALA:HA	1:A:190:PRO:HD3	1.89	0.41
1:C:259:ASP:OD1	1:C:259:ASP:C	2.59	0.41
1:B:233:TYR:N	1:B:233:TYR:CD1	2.88	0.41
1:A:171:GLU:OE1	1:A:249:ARG:NH1	2.53	0.41
1:C:328:PHE:N	1:C:328:PHE:CD1	2.89	0.41
1:C:119:ALA:C	1:C:121:SER:H	2.22	0.41
1:C:144:GLN:C	1:C:145:LEU:HD12	2.40	0.41
1:C:97:VAL:HA	1:C:213:ARG:HH21	1.86	0.41
1:C:193:HIS:CE1	1:C:214:HIS:CG	3.08	0.41
1:C:332:ILE:HG22	1:C:333:ARG:N	2.35	0.40
1:C:189:ALA:HA	1:C:190:PRO:HD3	1.76	0.40
1:C:137:LEU:CD1	1:C:238:CYS:N	2.84	0.40
1:B:118:THR:HG21	1:B:282:ARG:CZ	2.52	0.40
1:D:338:PHE:CE2	1:B:330:LEU:HD22	2.57	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:264:LEU:HD23	1:B:225:VAL:HB	2.03	0.40
1:D:171:GLU:CD	1:D:249:ARG:HH12	2.25	0.40
1:B:186:ASP:OD1	1:B:196:ARG:NH1	2.55	0.40
1:D:179:HIS:C	1:D:181:ARG:N	2.72	0.40
1:D:292:LYS:C	1:D:321:LYS:HD2	2.42	0.40
1:A:227:SER:HB3	1:A:229:TYR:CE2	2.56	0.40
1:D:227:SER:HB3	1:D:229:TYR:CE2	2.56	0.40
1:D:152:PRO:HA	1:D:153:PRO:HD3	1.89	0.40
1:D:247:ASN:O	1:D:248:ARG:CB	2.70	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	229/231 (99%)	193 (84%)	30 (13%)	6 (3%)	8	47
1	B	229/231 (99%)	164 (72%)	48 (21%)	17 (7%)	2	12
1	C	229/231 (99%)	187 (82%)	35 (15%)	7 (3%)	7	41
1	D	229/231 (99%)	193 (84%)	30 (13%)	6 (3%)	8	47
All	All	916/924 (99%)	737 (80%)	143 (16%)	36 (4%)	5	33

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	124	CYS
1	A	241	SER
1	D	124	CYS
1	D	241	SER
1	B	109	PHE
1	B	121	SER
1	B	241	SER
1	B	259	ASP
1	A	119	ALA

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Mol	Chain	Res	Type
1	C	185	SER
1	C	241	SER
1	C	262	GLY
1	D	119	ALA
1	B	147	VAL
1	B	169	MET
1	B	199	GLY
1	B	200	ASN
1	B	291	LYS
1	A	117	GLY
1	C	169	MET
1	C	210	ASN
1	C	237	MET
1	D	117	GLY
1	B	153	PRO
1	B	186	ASP
1	B	281	ASP
1	A	148	ASP
1	D	148	ASP
1	B	129	ALA
1	B	248	ARG
1	B	327	TYR
1	A	352	ASP
1	C	120	LYS
1	D	352	ASP
1	B	280	ARG
1	B	125	THR

### 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	206/206 (100%)	189 (92%)	17 (8%)	16	55
1	B	206/206 (100%)	197 (96%)	9 (4%)	39	81
1	C	206/206 (100%)	195 (95%)	11 (5%)	32	75
1	D	206/206 (100%)	190 (92%)	16 (8%)	18	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	824/824 (100%)	771 (94%)	53 (6%)	25	69

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	ARG
1	A	149	SER
1	A	150	THR
1	A	167	GLN
1	A	176	CYS
1	A	186	ASP
1	A	192	GLN
1	A	197	VAL
1	A	202	ARG
1	A	217	VAL
1	A	231	THR
1	A	238	CYS
1	A	240	SER
1	A	251	ILE
1	A	256	THR
1	A	335	ARG
1	A	336	GLU
1	C	110	ARG
1	C	150	THR
1	C	167	GLN
1	C	192	GLN
1	C	201	LEU
1	C	207	ASP
1	C	229	TYR
1	C	231	THR
1	C	323	MET
1	C	336	GLU
1	C	354	GLN
1	D	110	ARG
1	D	149	SER
1	D	150	THR
1	D	167	GLN
1	D	186	ASP
1	D	192	GLN
1	D	197	VAL
1	D	202	ARG
1	D	217	VAL

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Mol	Chain	Res	Type
1	D	231	THR
1	D	238	CYS
1	D	240	SER
1	D	251	ILE
1	D	256	THR
1	D	335	ARG
1	D	336	GLU
1	B	120	LYS
1	B	124	CYS
1	B	167	GLN
1	B	207	ASP
1	B	230	THR
1	B	231	THR
1	B	248	ARG
1	B	271	GLU
1	B	278	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	GLN
1	A	167	GLN
1	A	192	GLN
1	A	193	HIS
1	A	214	HIS
1	C	104	GLN
1	C	144	GLN
1	C	167	GLN
1	C	192	GLN
1	C	288	ASN
1	D	104	GLN
1	D	167	GLN
1	D	192	GLN
1	D	193	HIS
1	D	214	HIS
1	B	104	GLN
1	B	131	ASN
1	B	144	GLN
1	B	167	GLN
1	B	168	HIS
1	B	192	GLN
1	B	263	ASN

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Mol	Chain	Res	Type
1	B	288	ASN
1	B	331	GLN
1	B	340	GLN

### 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 ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	231/231 (100%)	-0.07	5 (2%) 59 14	7, 33, 117, 126	0
1	B	231/231 (100%)	0.50	21 (9%) 9 2	42, 90, 128, 134	0
1	C	231/231 (100%)	-0.30	0 100 100	5, 17, 73, 112	0
1	D	231/231 (100%)	0.27	22 (9%) 8 2	6, 31, 118, 127	0
2	K	26/26 (100%)	-0.27	0 100 100	10, 46, 102, 114	0
3	L	26/26 (100%)	-0.21	0 100 100	12, 49, 113, 120	0
All	All	976/976 (100%)	0.08	48 (4%) 28 6	5, 38, 120, 134	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	340	GLN	5.2
1	D	340	GLN	5.2
1	D	339	GLU	5.1
1	B	347	ALA	4.8
1	D	332	ILE	4.7
1	D	351	LYS	4.5
1	D	354	GLN	4.3
1	D	333	ARG	4.3
1	A	116	SER	4.1
1	B	353	ALA	4.1
1	A	117	GLY	3.9
1	D	326	GLU	3.9
1	D	334	GLY	3.7
1	D	117	GLY	3.7
1	B	343	GLU	3.6
1	D	335	ARG	3.5
1	D	337	ARG	3.5
1	D	353	ALA	3.4
1	B	145	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	348	LEU	3.4
1	D	350	LEU	3.2
1	B	108	GLY	3.2
1	A	118	THR	3.1
1	B	346	GLU	3.0
1	D	352	ASP	2.9
1	B	109	PHE	2.9
1	B	181	ARG	2.9
1	D	328	PHE	2.9
1	D	323	MET	2.8
1	B	336	GLU	2.8
1	B	354	GLN	2.8
1	B	111	LEU	2.8
1	D	341	PHE	2.8
1	D	330	LEU	2.7
1	D	325	GLY	2.7
1	A	115	HIS	2.6
1	D	336	GLU	2.6
1	B	331	GLN	2.6
1	B	351	LYS	2.5
1	B	104	GLN	2.4
1	A	121	SER	2.4
1	B	335	ARG	2.4
1	B	334	GLY	2.3
1	B	324	ASP	2.3
1	B	103	TYR	2.2
1	B	329	THR	2.1
1	B	133	MET	2.1
1	D	347	ALA	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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ZN	C	1	1/1	0.16	-0.14	18,18,18,18	0
4	ZN	B	1	1/1	0.15	-1.09	64,64,64,64	0
4	ZN	A	1	1/1	0.08	-2.40	17,17,17,17	0
4	ZN	D	1	1/1	0.13	-3.66	12,12,12,12	0

## 6.5 Other polymers

There are no such residues in this entry.