



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:47 AM 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 X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at 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.

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

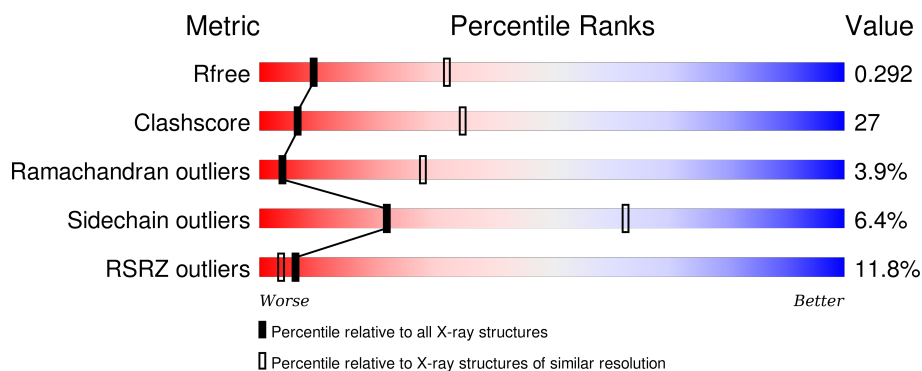
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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 ≥ 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	231	<div> <div>6%</div> <div>56%</div> <div>39%</div> <div>5%</div> </div>
1	B	231	<div> <div>26%</div> <div>42%</div> <div>49%</div> <div>9%</div> </div>
1	C	231	<div> <div>52%</div> <div>43%</div> <div>5%</div> </div>
1	D	231	<div> <div>16%</div> <div>55%</div> <div>40%</div> <div>5%</div> </div>
2	K	26	<div> <div>4%</div> <div>15%</div> <div>81%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
3	L	26	<div><div></div><div>8%</div><div>42%</div><div>58%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8456 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 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			

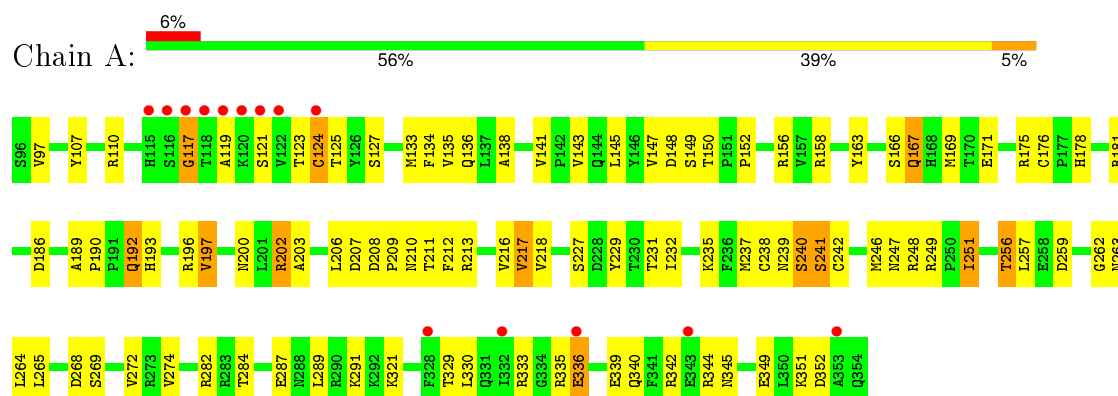
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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		

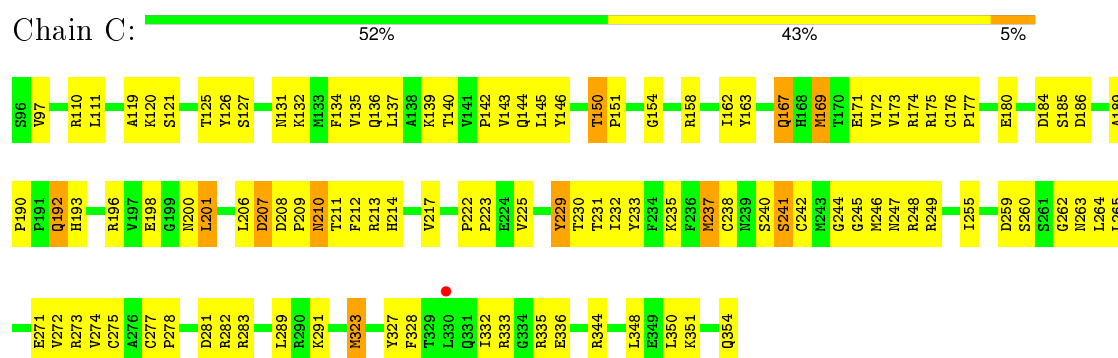
3 Residue-property plots [i](#)

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.

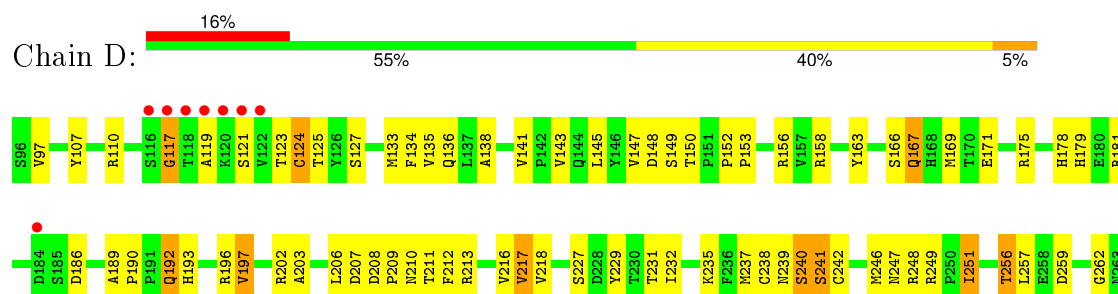
• Molecule 1: Cellular tumor antigen p53

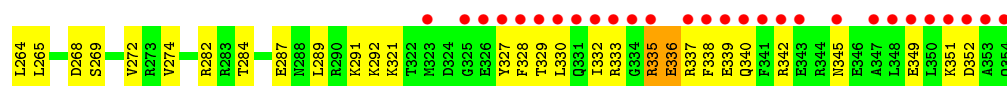


• Molecule 1: Cellular tumor antigen p53

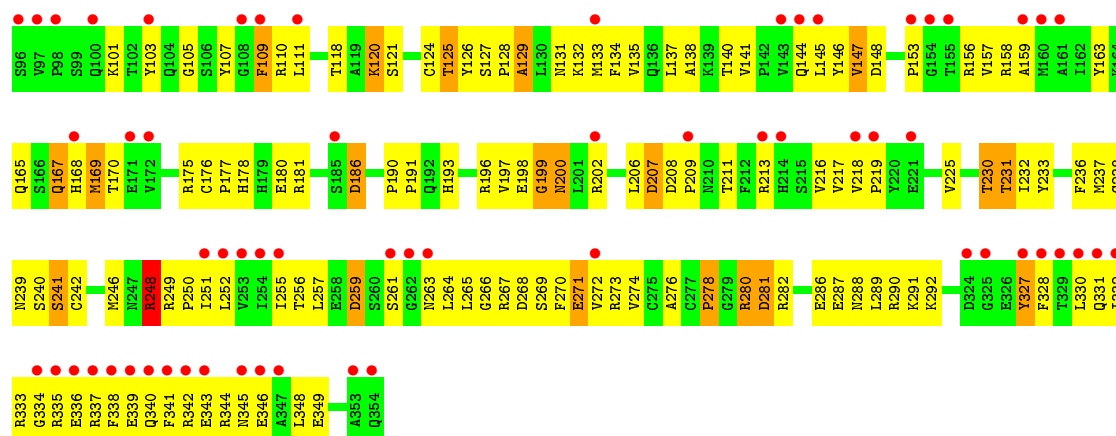
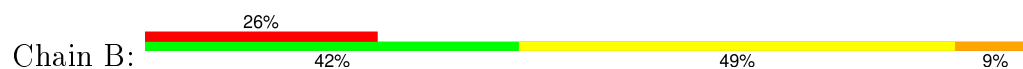


• Molecule 1: Cellular tumor antigen p53





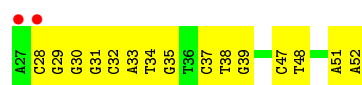
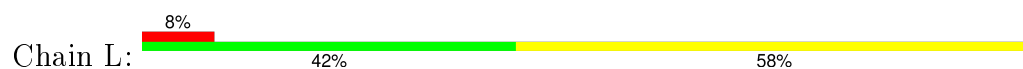
• Molecule 1: Cellular tumor antigen p53



• Molecule 2: DNA (26-MER)



• Molecule 3: DNA (26-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 3.19Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.258 , 0.314 0.243 , 0.292	Depositor DCC
R_{free} test set	1296 reflections (4.98%)	DCC
Wilson B-factor (Å ²)	58.0	Xtriage
Anisotropy	0.579	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 56.2	EDS
Estimated twinning fraction	0.029 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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](#)

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 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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

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 27.

All (440) 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: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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:21:DG:H2''	2:K:22:DC:C5'	2.20	0.67
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	229/231 (99%)	193 (84%)	30 (13%)	6 (3%)	7	40
1	B	229/231 (99%)	164 (72%)	48 (21%)	17 (7%)	1	9
1	C	229/231 (99%)	187 (82%)	35 (15%)	7 (3%)	5	34
1	D	229/231 (99%)	193 (84%)	30 (13%)	6 (3%)	7	40
All	All	916/924 (99%)	737 (80%)	143 (16%)	36 (4%)	4	28

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
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 [i](#)

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%)	14	49
1	B	206/206 (100%)	197 (96%)	9 (4%)	35	74
1	C	206/206 (100%)	195 (95%)	11 (5%)	28	69
1	D	206/206 (100%)	190 (92%)	16 (8%)	16	53
All	All	824/824 (100%)	771 (94%)	53 (6%)	22	62

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

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Mol	Chain	Res	Type
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
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

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

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](#)

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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

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, 95th 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 ²)	Q<0.9
1	A	231/231 (100%)	0.29	14 (6%) 25 13	7, 33, 117, 126	0
1	B	231/231 (100%)	1.30	61 (26%) 1 0	42, 90, 128, 134	0
1	C	231/231 (100%)	-0.33	1 (0%) 93 90	5, 17, 73, 112	0
1	D	231/231 (100%)	0.61	36 (15%) 3 2	6, 31, 118, 127	0
2	K	26/26 (100%)	0.19	1 (3%) 44 29	10, 46, 102, 114	0
3	L	26/26 (100%)	0.38	2 (7%) 16 9	12, 49, 113, 120	0
All	All	976/976 (100%)	0.46	115 (11%) 6 4	5, 38, 120, 134	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	116	SER	14.7
1	A	121	SER	12.3
1	A	118	THR	11.8
1	A	117	GLY	11.3
1	D	117	GLY	10.9
1	B	331	GLN	9.8
1	A	119	ALA	8.8
1	B	340	GLN	8.3
1	D	330	LEU	8.3
1	D	329	THR	8.3
1	B	347	ALA	8.1
1	B	329	THR	8.0
1	D	328	PHE	7.8
1	D	332	ILE	7.8
1	A	122	VAL	7.3
1	D	325	GLY	7.0
1	D	339	GLU	6.2
1	D	119	ALA	6.1
1	D	326	GLU	6.0

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Mol	Chain	Res	Type	RSRZ
1	D	348	LEU	5.9
1	B	145	LEU	5.8
1	D	118	THR	5.8
1	B	343	GLU	5.8
1	D	121	SER	5.7
1	B	109	PHE	5.5
1	A	120	LYS	5.5
1	B	330	LEU	5.4
1	A	115	HIS	5.3
1	B	353	ALA	5.2
1	D	353	ALA	5.2
1	D	352	ASP	5.1
1	B	332	ILE	5.1
1	D	350	LEU	4.9
1	D	340	GLN	4.6
1	D	341	PHE	4.6
1	D	347	ALA	4.4
1	B	354	GLN	4.4
1	B	253	VAL	4.3
1	D	327	TYR	4.3
1	B	336	GLU	4.0
1	B	328	PHE	4.0
1	B	155	THR	4.0
1	D	120	LYS	4.0
1	B	346	GLU	3.9
1	B	218	VAL	3.9
1	D	351	LYS	3.9
1	B	111	LEU	3.9
1	B	262	GLY	3.9
1	B	153	PRO	3.9
1	D	354	GLN	3.8
1	B	108	GLY	3.8
1	B	338	PHE	3.7
1	B	334	GLY	3.7
1	D	334	GLY	3.6
1	B	96	SER	3.6
1	B	272	VAL	3.6
1	D	331	GLN	3.5
1	B	342	ARG	3.5
1	B	254	ILE	3.5
1	D	349	GLU	3.5
1	A	336	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	116	SER	3.3
1	D	343	GLU	3.3
1	B	339	GLU	3.3
1	B	133	MET	3.2
1	B	98	PRO	3.2
1	A	343	GLU	3.2
1	B	154	GLY	3.2
1	B	185	SER	3.1
3	L	28	DC	3.1
1	B	251	ILE	3.1
1	B	255	ILE	3.1
1	B	345	ASN	3.0
1	A	332	ILE	3.0
1	C	330	LEU	3.0
1	B	160	MET	3.0
1	B	171	GLU	2.9
1	B	261	SER	2.8
1	B	161	ALA	2.8
1	B	324	ASP	2.8
1	B	143	VAL	2.8
1	D	338	PHE	2.7
1	D	335	ARG	2.7
1	D	337	ARG	2.7
1	D	333	ARG	2.6
1	B	213	ARG	2.6
1	B	327	TYR	2.6
1	B	252	LEU	2.6
1	B	219	PRO	2.6
3	L	27	DA	2.6
1	D	323	MET	2.5
1	B	100	GLN	2.5
1	D	345	ASN	2.5
1	B	325	GLY	2.4
1	B	214	HIS	2.4
1	B	341	PHE	2.4
1	D	342	ARG	2.4
1	D	184	ASP	2.3
1	D	122	VAL	2.3
1	B	144	GLN	2.3
1	B	97	VAL	2.3
1	B	337	ARG	2.3
1	B	221	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	159	ALA	2.2
1	B	168	HIS	2.2
1	B	209	PRO	2.2
1	B	335	ARG	2.1
1	A	353	ALA	2.1
2	K	3	DT	2.1
1	B	263	ASN	2.1
1	A	328	PHE	2.1
1	A	124	CYS	2.1
1	B	103	TYR	2.1
1	B	202	ARG	2.0
1	B	172	VAL	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](#)

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, 95th 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	ZN	C	1	1/1	0.99	0.18	1.11	18,18,18,18	0
4	ZN	B	1	1/1	0.96	0.15	-0.93	64,64,64,64	0
4	ZN	A	1	1/1	0.97	0.10	-2.29	17,17,17,17	0
4	ZN	D	1	1/1	1.00	0.13	-2.70	12,12,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.