



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2023 – 12:38 PM EDT

PDB ID : 3K4X  
Title : Eukaryotic Sliding Clamp PCNA Bound to DNA  
Authors : McNally, R.; Kuriyan, J.  
Deposited on : 2009-10-06  
Resolution : 2.98 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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  
Xtrriage (Phenix) : 1.13  
EDS : 2.35  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

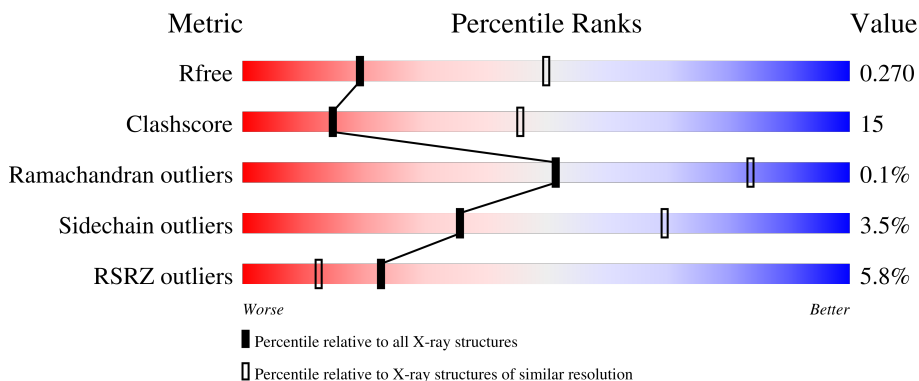
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.98 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))
$R_{free}$	130704	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	798	
2	B	10	
3	C	14	

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 6354 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 Proliferating cell nuclear antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	758	5947	3802	939	1179	27	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP P15873
A	-4	PRO	-	expression tag	UNP P15873
A	-3	HIS	-	expression tag	UNP P15873
A	-2	MET	-	expression tag	UNP P15873
A	-1	ALA	-	expression tag	UNP P15873
A	0	SER	-	expression tag	UNP P15873
A	258	GLY	-	linker	UNP P15873
A	259	SER	-	linker	UNP P15873
A	260	ASN	-	linker	UNP P15873
A	261	SER	-	linker	UNP P15873
A	262	GLN	-	linker	UNP P15873
A	263	SER	-	linker	UNP P15873
A	264	ASN	-	linker	UNP P15873
A	265	GLY	-	linker	UNP P15873
A	266	SER	-	linker	UNP P15873
A	267	GLY	-	linker	UNP P15873
A	268	ALA	-	linker	UNP P15873
A	258	GLY	-	linker	UNP P15873
A	259	SER	-	linker	UNP P15873
A	260	ASN	-	linker	UNP P15873
A	261	SER	-	linker	UNP P15873
A	262	GLN	-	linker	UNP P15873
A	263	SER	-	linker	UNP P15873
A	264	ASN	-	linker	UNP P15873
A	265	GLY	-	linker	UNP P15873
A	266	SER	-	linker	UNP P15873
A	267	GLY	-	linker	UNP P15873

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Chain	Residue	Modelled	Actual	Comment	Reference
A	268	ALA	-	linker	UNP P15873

- Molecule 2 is a DNA chain called DNA (5'-D(\*CP\*CP\*CP\*AP\*TP\*CP\*GP\*TP\*AP\*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	10	197	96	33	59	9	0	0	0

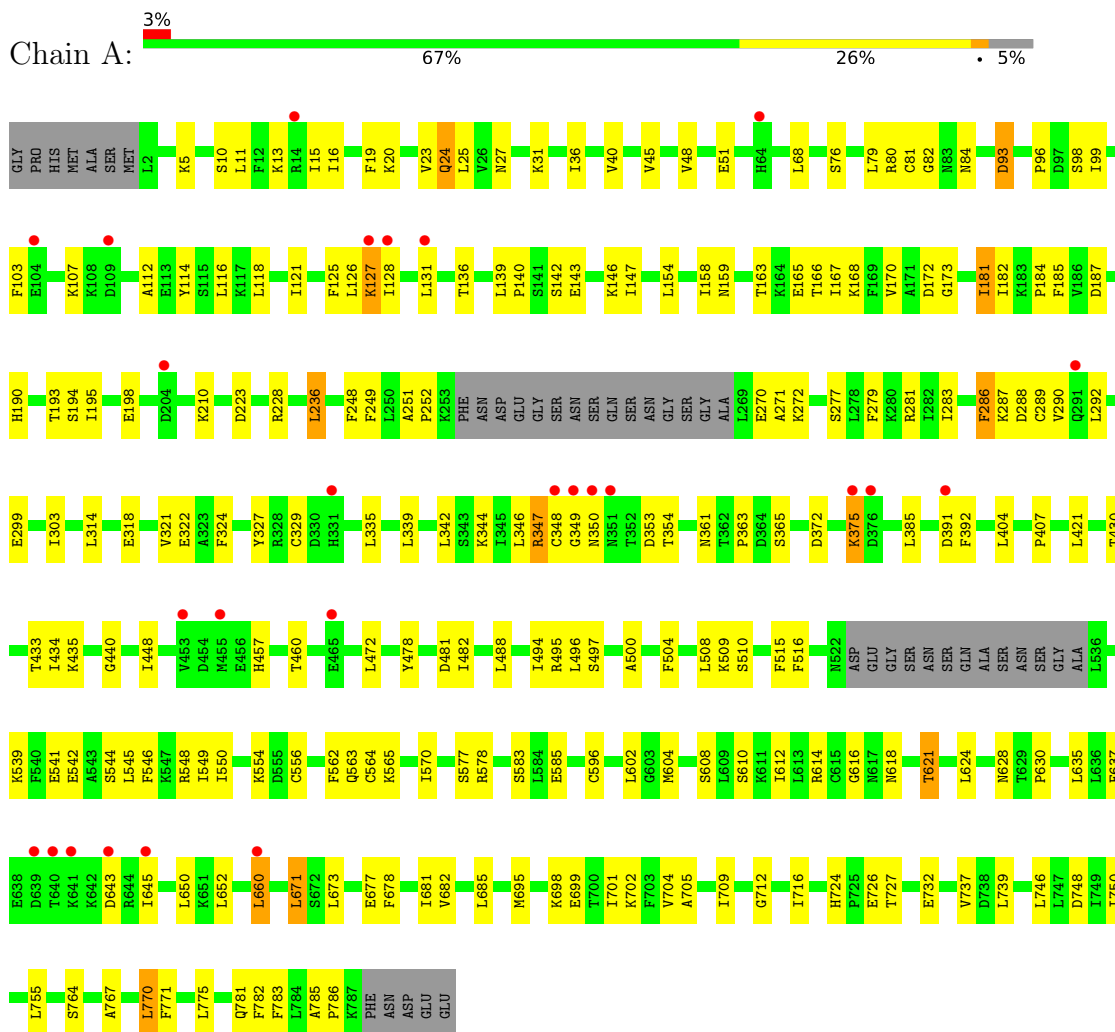
- Molecule 3 is a DNA chain called DNA (5'-D(\*TP\*TP\*TP\*TP\*AP\*TP\*AP\*CP\*GP\*AP\*TP\*GP\*GP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	10	210	99	42	59	10	0	0	0

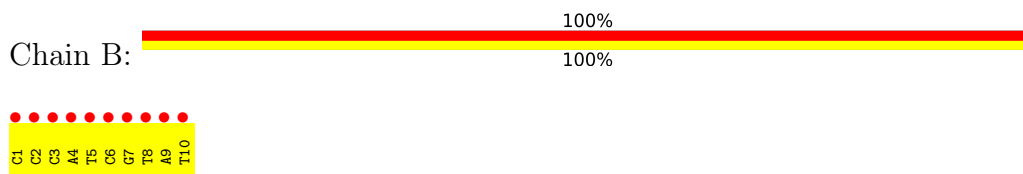
### 3 Residue-property plots i

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

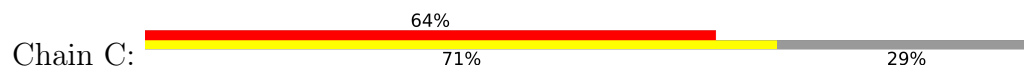
- Molecule 1: Proliferating cell nuclear antigen



- Molecule 2: DNA (5'-D(\*CP\*CP\*CP\*AP\*TP\*CP\*GP\*TP\*AP\*T)-3')



- Molecule 3: DNA (5'-D(\*TP\*TP\*TP\*TP\*AP\*TP\*AP\*CP\*GP\*AP\*TP\*GP\*GP\*G)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.94Å 93.71Å 136.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.86 – 2.98 46.86 – 2.99	Depositor EDS
% Data completeness (in resolution range)	97.6 (46.86-2.98) 97.6 (46.86-2.99)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.15 (at 3.01Å)	Xtrriage
Refinement program	PHENIX 1.4_162	Depositor
R, $R_{free}$	0.223 , 0.280 0.216 , 0.270	Depositor DCC
$R_{free}$ test set	1121 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.4	Xtrriage
Anisotropy	0.275	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 55.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	6354	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.22	0/6035	0.38	0/8142
2	B	0.86	0/219	1.32	0/335
3	C	0.86	0/236	1.29	0/363
All	All	0.31	0/6490	0.52	0/8840

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5947	0	6009	155	0
2	B	197	0	115	20	0
3	C	210	0	113	18	0
All	All	6354	0	6237	191	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (191) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:SER:HA	2:B:6:DC:OP1	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:SER:HB3	1:A:618:ASN:HB3	1.69	0.74
1:A:24:GLN:HG3	1:A:25:LEU:HG	1.71	0.73
1:A:347:ARG:HA	1:A:347:ARG:HE	1.54	0.72
1:A:190:HIS:O	1:A:193:THR:HG22	1.90	0.72
1:A:539:LYS:HE3	1:A:621:THR:HG21	1.74	0.70
1:A:10:SER:HB3	1:A:84:ASN:HB3	1.74	0.69
1:A:303:ILE:HG22	1:A:318:GLU:HG2	1.75	0.68
1:A:457:HIS:O	1:A:460:THR:HG22	1.94	0.68
1:A:272:LYS:HE3	1:A:354:THR:HG21	1.77	0.66
1:A:671:LEU:HD13	1:A:701:ILE:HD13	1.75	0.66
1:A:127:LYS:C	1:A:128:ILE:HD12	2.17	0.65
1:A:270:GLU:O	1:A:270:GLU:HG3	1.97	0.65
1:A:755:LEU:HB3	1:A:775:LEU:HD21	1.79	0.65
1:A:361:ASN:O	1:A:363:PRO:HD3	1.97	0.64
1:A:544:SER:HB2	1:A:548:ARG:HH12	1.63	0.64
1:A:563:GLN:HB3	1:A:565:LYS:NZ	2.13	0.63
1:A:182:ILE:HD12	1:A:195:ILE:HD13	1.81	0.62
1:A:724:HIS:O	1:A:727:THR:HG22	1.99	0.62
1:A:314:LEU:HB3	1:A:516:PHE:HB2	1.82	0.61
1:A:365:SER:HA	1:A:385:LEU:HG	1.83	0.60
1:A:404:LEU:HD13	1:A:434:ILE:HD13	1.82	0.60
1:A:277:SER:HB2	1:A:281:ARG:NH1	2.18	0.59
1:A:76:SER:O	1:A:80:ARG:HG3	2.02	0.59
1:A:131:LEU:H	1:A:131:LEU:HD23	1.68	0.59
1:A:286:PHE:HB3	1:A:339:LEU:HD13	1.87	0.57
1:A:287:LYS:O	1:A:288:ASP:HB2	2.04	0.57
1:A:660:LEU:H	1:A:660:LEU:HD22	1.68	0.57
3:C:8:DC:H2''	3:C:9:DG:OP2	2.05	0.57
2:B:5:DT:H2''	2:B:6:DC:OP2	2.05	0.57
2:B:8:DT:H2''	2:B:9:DA:OP2	2.05	0.56
3:C:5:DA:H2''	3:C:6:DT:OP2	2.05	0.56
2:B:7:DG:H1'	2:B:8:DT:H5'	1.88	0.56
3:C:10:DA:H2''	3:C:11:DT:OP2	2.05	0.56
3:C:10:DA:H1'	3:C:11:DT:H5'	1.88	0.56
3:C:13:DG:H1'	3:C:14:DG:H5'	1.88	0.56
2:B:4:DA:H1'	2:B:5:DT:H5'	1.88	0.56
3:C:6:DT:H1'	3:C:7:DA:H5'	1.88	0.56
2:B:1:DC:H2''	2:B:2:DC:OP2	2.05	0.56
2:B:2:DC:H1'	2:B:3:DC:H5'	1.88	0.56
3:C:7:DA:H2''	3:C:8:DC:OP2	2.05	0.56
3:C:9:DG:H1'	3:C:10:DA:H5'	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:9:DG:H2''	3:C:10:DA:OP2	2.05	0.56
2:B:4:DA:H2''	2:B:5:DT:OP2	2.05	0.56
3:C:12:DG:H2''	3:C:13:DG:OP2	2.05	0.56
3:C:13:DG:H2''	3:C:14:DG:OP2	2.05	0.56
3:C:8:DC:H1'	3:C:9:DG:H5'	1.88	0.56
2:B:1:DC:H1'	2:B:2:DC:H5'	1.88	0.56
3:C:7:DA:H1'	3:C:8:DC:H5'	1.88	0.56
1:A:136:THR:HB	1:A:198:GLU:HG2	1.88	0.56
2:B:3:DC:H1'	2:B:4:DA:H5'	1.88	0.56
3:C:5:DA:H1'	3:C:6:DT:H5'	1.88	0.56
3:C:11:DT:H1'	3:C:12:DG:H5'	1.87	0.56
1:A:68:LEU:HD23	1:A:99:ILE:HD12	1.87	0.56
2:B:5:DT:H1'	2:B:6:DC:H5'	1.88	0.56
2:B:6:DC:H2''	2:B:7:DG:OP2	2.05	0.56
1:A:570:ILE:HG22	1:A:585:GLU:HG2	1.88	0.55
1:A:610:SER:O	1:A:614:ARG:HG3	2.06	0.55
2:B:9:DA:H1'	2:B:10:DT:H5'	1.88	0.55
3:C:6:DT:H2''	3:C:7:DA:OP2	2.05	0.55
1:A:93:ASP:OD2	1:A:93:ASP:N	2.39	0.55
1:A:347:ARG:HE	1:A:347:ARG:CA	2.18	0.55
2:B:3:DC:H2''	2:B:4:DA:OP2	2.05	0.55
2:B:7:DG:H2''	2:B:8:DT:OP2	2.05	0.55
2:B:2:DC:H2''	2:B:3:DC:OP2	2.05	0.55
2:B:6:DC:H1'	2:B:7:DG:H5'	1.88	0.55
2:B:9:DA:H2''	2:B:10:DT:OP2	2.05	0.55
3:C:11:DT:H2''	3:C:12:DG:OP2	2.05	0.55
1:A:125:PHE:HE2	1:A:127:LYS:HD2	1.72	0.55
1:A:556:CYS:SG	1:A:748:ASP:HB3	2.46	0.55
2:B:8:DT:H1'	2:B:9:DA:H5'	1.88	0.55
1:A:279:PHE:HD2	1:A:346:LEU:HD11	1.72	0.55
1:A:541:GLU:HG3	1:A:542:GLU:HG2	1.88	0.55
1:A:407:PRO:HG3	1:A:460:THR:HA	1.89	0.54
1:A:286:PHE:HD2	1:A:290:VAL:HG21	1.72	0.54
3:C:12:DG:H1'	3:C:13:DG:H5'	1.88	0.54
1:A:168:LYS:HG3	1:A:181:ILE:HD13	1.88	0.54
1:A:602:LEU:HD12	1:A:652:LEU:HD11	1.89	0.54
1:A:127:LYS:N	1:A:128:ILE:HD12	2.24	0.53
1:A:549:ILE:HA	1:A:755:LEU:HD21	1.90	0.53
1:A:544:SER:O	1:A:548:ARG:HG2	2.08	0.53
1:A:612:ILE:HG21	1:A:635:LEU:HD13	1.91	0.53
1:A:272:LYS:HE3	1:A:354:THR:CG2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:746:LEU:O	1:A:750:ILE:HG23	2.09	0.52
1:A:146:LYS:HZ1	1:A:349:GLY:HA2	1.74	0.52
1:A:353:ASP:OD2	1:A:372:ASP:HA	2.10	0.52
1:A:321:VAL:HG13	1:A:327:TYR:HB3	1.91	0.51
1:A:342:LEU:O	1:A:346:LEU:HD23	2.10	0.51
1:A:168:LYS:HG3	1:A:181:ILE:CD1	2.39	0.51
1:A:27:ASN:OD1	1:A:121:ILE:HB	2.10	0.51
1:A:210:LYS:O	1:A:210:LYS:HD3	2.11	0.51
1:A:550:ILE:O	1:A:554:LYS:HB3	2.10	0.51
1:A:322:GLU:HB2	1:A:510:SER:HB2	1.92	0.51
1:A:544:SER:HB2	1:A:548:ARG:NH1	2.26	0.50
1:A:539:LYS:HE3	1:A:621:THR:CG2	2.41	0.50
1:A:628:ASN:O	1:A:630:PRO:HD3	2.11	0.50
1:A:154:LEU:O	1:A:173:GLY:HA3	2.12	0.49
1:A:116:LEU:HD12	1:A:709:ILE:O	2.13	0.49
1:A:494:ILE:HG22	1:A:496:LEU:HG	1.94	0.49
1:A:127:LYS:HA	1:A:127:LYS:HE3	1.94	0.49
1:A:478:TYR:O	1:A:482:ILE:HG13	2.13	0.49
1:A:677:GLU:O	1:A:681:ILE:HG13	2.13	0.49
1:A:185:PHE:HE1	1:A:187:ASP:HB2	1.78	0.48
1:A:771:PHE:HB2	1:A:782:PHE:HB2	1.95	0.48
1:A:114:TYR:HA	1:A:712:GLY:HA2	1.95	0.48
1:A:112:ALA:HB1	1:A:114:TYR:CE1	2.48	0.48
1:A:136:THR:HG23	1:A:228:ARG:HG2	1.96	0.48
1:A:322:GLU:HB2	1:A:510:SER:CB	2.44	0.48
1:A:314:LEU:HD23	1:A:516:PHE:CD1	2.49	0.47
1:A:13:LYS:HE2	1:A:84:ASN:HD21	1.79	0.47
1:A:93:ASP:O	1:A:96:PRO:HG3	2.14	0.47
1:A:430:THR:OG1	1:A:433:THR:HB	2.15	0.47
1:A:19:PHE:O	1:A:23:VAL:HG22	2.13	0.47
1:A:128:ILE:HD12	1:A:128:ILE:N	2.30	0.47
1:A:702:LYS:HE2	1:A:704:VAL:HG21	1.96	0.47
1:A:286:PHE:O	1:A:290:VAL:HG22	2.14	0.47
1:A:695:MET:HE3	1:A:702:LYS:HD3	1.97	0.47
1:A:724:HIS:CE1	1:A:726:GLU:HB2	2.49	0.47
1:A:142:SER:CA	2:B:6:DC:OP1	2.60	0.47
1:A:546:PHE:O	1:A:550:ILE:HG12	2.15	0.47
1:A:562:PHE:CD2	1:A:604:MET:HE2	2.49	0.46
1:A:563:GLN:NE2	1:A:570:ILE:HD11	2.30	0.46
1:A:98:SER:HB2	1:A:116:LEU:O	2.14	0.46
1:A:103:PHE:HB2	1:A:112:ALA:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ALA:HB1	1:A:114:TYR:HE1	1.80	0.46
1:A:81:CYS:HB3	1:A:114:TYR:OH	2.16	0.46
1:A:299:GLU:H	1:A:299:GLU:CD	2.19	0.46
1:A:375:LYS:HE3	1:A:375:LYS:HA	1.98	0.46
1:A:143:GLU:O	1:A:147:ILE:HG13	2.15	0.46
1:A:472:LEU:HD11	1:A:497:SER:O	2.15	0.46
1:A:770:LEU:HG	1:A:783:PHE:CE2	2.51	0.46
1:A:126:LEU:C	1:A:128:ILE:HD12	2.37	0.46
1:A:344:LYS:O	1:A:347:ARG:HB2	2.16	0.45
1:A:139:LEU:H	1:A:139:LEU:HD23	1.81	0.45
1:A:660:LEU:HD22	1:A:660:LEU:N	2.31	0.45
1:A:167:ILE:HB	1:A:182:ILE:CG1	2.47	0.45
1:A:187:ASP:OD2	1:A:190:HIS:HD2	2.00	0.45
1:A:497:SER:HB3	1:A:500:ALA:HB3	1.98	0.45
1:A:5:LYS:O	1:A:5:LYS:HG3	2.15	0.45
1:A:277:SER:HB2	1:A:281:ARG:HH11	1.81	0.45
1:A:96:PRO:HB2	1:A:118:LEU:HD12	1.99	0.45
1:A:685:LEU:HB3	1:A:705:ALA:HB2	1.98	0.45
1:A:146:LYS:NZ	1:A:349:GLY:HA2	2.31	0.44
1:A:737:VAL:HG12	1:A:739:LEU:HG	1.99	0.44
1:A:545:LEU:O	1:A:549:ILE:HG13	2.17	0.44
1:A:48:VAL:HG22	1:A:248:PHE:CD2	2.53	0.44
1:A:643:ASP:O	1:A:645:ILE:HG13	2.17	0.44
1:A:583:SER:HB3	1:A:781:GLN:HB2	1.98	0.44
1:A:125:PHE:CE2	1:A:127:LYS:HD2	2.53	0.44
1:A:163:THR:OG1	1:A:166:THR:HB	2.17	0.44
1:A:698:LYS:HG2	1:A:699:GLU:HG3	2.00	0.44
1:A:125:PHE:HE2	1:A:127:LYS:HB2	1.82	0.44
1:A:435:LYS:HG3	1:A:448:ILE:HG12	2.00	0.44
1:A:251:ALA:HA	1:A:252:PRO:HD3	1.88	0.44
1:A:509:LYS:O	1:A:510:SER:HB3	2.17	0.43
1:A:702:LYS:HE2	1:A:704:VAL:CG2	2.48	0.43
1:A:16:ILE:O	1:A:20:LYS:HB3	2.17	0.43
1:A:785:ALA:HA	1:A:786:PRO:HD3	1.87	0.43
1:A:391:ASP:HA	1:A:392:PHE:HA	1.64	0.43
1:A:289:CYS:HB3	1:A:481:ASP:HB3	2.00	0.43
1:A:624:LEU:CD2	1:A:635:LEU:HD23	2.49	0.43
1:A:36:ILE:HG22	1:A:51:GLU:HG2	2.01	0.43
1:A:125:PHE:CE2	1:A:127:LYS:HB2	2.53	0.42
1:A:488:LEU:HD13	1:A:508:LEU:HD21	2.00	0.42
1:A:107:LYS:HE2	1:A:107:LYS:HB3	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:PHE:HB2	1:A:515:PHE:HB2	2.00	0.42
1:A:11:LEU:O	1:A:15:ILE:HG13	2.19	0.42
1:A:140:PRO:HG3	1:A:193:THR:HA	2.02	0.42
1:A:271:ALA:HB1	1:A:324:PHE:CE1	2.54	0.42
1:A:347:ARG:HA	1:A:347:ARG:NE	2.30	0.42
1:A:81:CYS:HB3	1:A:114:TYR:CZ	2.55	0.42
1:A:764:SER:HB3	1:A:767:ALA:HB3	2.00	0.42
1:A:350:ASN:HB2	1:A:353:ASP:CG	2.40	0.41
1:A:165:GLU:HA	1:A:184:PRO:HG2	2.02	0.41
1:A:168:LYS:HZ3	1:A:170:VAL:HG22	1.85	0.41
1:A:350:ASN:HB2	1:A:353:ASP:OD2	2.21	0.41
1:A:187:ASP:H	1:A:194:SER:HB3	1.85	0.41
1:A:286:PHE:HB3	1:A:339:LEU:CD1	2.51	0.41
1:A:421:LEU:O	1:A:440:GLY:HA3	2.19	0.41
1:A:678:PHE:O	1:A:682:VAL:HG23	2.20	0.41
1:A:25:LEU:HB3	1:A:121:ILE:HD13	2.02	0.41
1:A:31:LYS:HB2	1:A:31:LYS:HE3	1.85	0.41
1:A:616:GLY:HA3	1:A:637:PHE:CD2	2.55	0.41
1:A:577:SER:O	1:A:578:ARG:HB2	2.20	0.41
1:A:158:ILE:HG22	1:A:159:ASN:N	2.36	0.40
1:A:279:PHE:O	1:A:283:ILE:HG12	2.21	0.40
1:A:701:ILE:HB	1:A:716:ILE:CG1	2.51	0.40
1:A:236:LEU:HG	1:A:249:PHE:CE2	2.56	0.40
1:A:608:SER:HB3	1:A:650:LEU:HD11	2.03	0.40
1:A:673:LEU:HD23	1:A:673:LEU:N	2.36	0.40
1:A:564:CYS:O	1:A:565:LYS:HD3	2.20	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	752/798 (94%)	730 (97%)	21 (3%)	1 (0%)	51 83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	GLY

### 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	683/713 (96%)	659 (96%)	24 (4%)	36 69

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	40	VAL
1	A	45	VAL
1	A	79	LEU
1	A	93	ASP
1	A	127	LYS
1	A	172	ASP
1	A	181	ILE
1	A	223	ASP
1	A	236	LEU
1	A	286	PHE
1	A	292	LEU
1	A	329	CYS
1	A	335	LEU
1	A	347	ARG
1	A	348	CYS
1	A	375	LYS
1	A	495	ARG
1	A	596	CYS
1	A	621	THR

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Mol	Chain	Res	Type
1	A	660	LEU
1	A	671	LEU
1	A	732	GLU
1	A	770	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	29	GLN
1	A	84	ASN
1	A	132	GLN
1	A	159	ASN
1	A	190	HIS
1	A	296	GLN
1	A	426	ASN
1	A	563	GLN
1	A	693	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	758/798 (94%)	0.20	26 (3%) 45 27	15, 46, 111, 210	0
2	B	10/10 (100%)	7.30	10 (100%) 0 0	179, 293, 361, 367	0
3	C	10/14 (71%)	4.92	9 (90%) 0 0	223, 275, 323, 336	0
All	All	778/822 (94%)	0.35	45 (5%) 23 12	15, 47, 131, 367	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	6	DC	13.7
3	C	5	DA	10.3
2	B	8	DT	9.7
2	B	9	DA	9.0
2	B	5	DT	8.8
1	A	643	ASP	8.0
2	B	7	DG	8.0
1	A	641	LYS	7.2
3	C	7	DA	7.0
2	B	1	DC	6.0
1	A	349	GLY	5.8
3	C	11	DT	5.3
2	B	2	DC	5.3
3	C	6	DT	4.9
2	B	4	DA	4.8
3	C	10	DA	4.7
2	B	10	DT	4.6
1	A	109	ASP	4.5
1	A	455	MET	4.2
1	A	453	VAL	4.1
3	C	12	DG	4.1
3	C	9	DG	4.0
1	A	639	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	291	GLN	3.7
3	C	8	DC	3.6
1	A	127	LYS	3.4
1	A	375	LYS	3.4
1	A	348	CYS	3.3
1	A	64	HIS	3.2
2	B	3	DC	3.2
1	A	351	ASN	3.2
3	C	14	DG	3.1
1	A	391	ASP	3.1
1	A	660	LEU	2.8
1	A	350	ASN	2.7
1	A	640	THR	2.6
1	A	104	GLU	2.6
1	A	465	GLU	2.5
1	A	645	ILE	2.5
1	A	204	ASP	2.4
1	A	131	LEU	2.3
1	A	376	ASP	2.2
1	A	331	HIS	2.1
1	A	128	ILE	2.0
1	A	14	ARG	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 monosaccharides in this entry.

## 6.4 Ligands [\(i\)](#)

There are no ligands in this entry.

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.