wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 04:07 PM GMT

PDB ID	:	4E2I
Title	:	The Complex Structure of the SV40 Helicase Large T Antigen and p68 Subunit of DNA Polymerase Alpha-Primase
Authors	:	Zhou, B.; Arnett, D.R.; Yu, X.; Brewster, A.; Sowd, G.A.; Xie, C.L.; Vila, S.; Gai, D.; Fanning, E.; Chen, X.S.
Deposited on	:	2012-03-08
Resolution	:	5.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

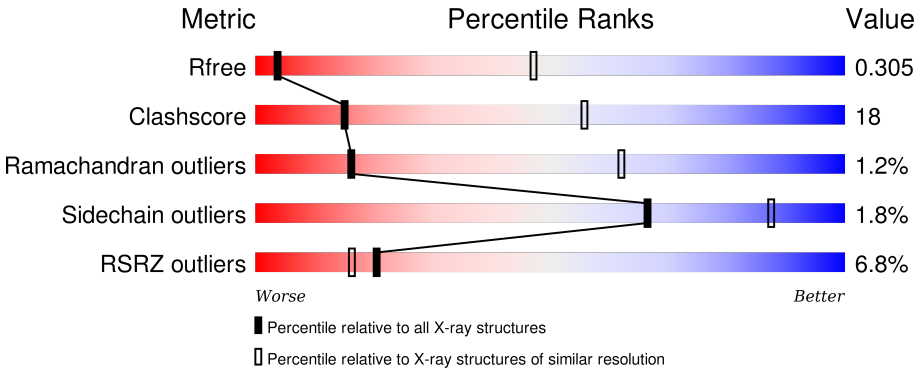
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 5.00 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	1119 (6.22-3.60)
Clashscore	102246	1019 (6.22-3.66)
Ramachandran outliers	100387	1158 (6.22-3.60)
Sidechain outliers	100360	1136 (6.22-3.60)
RSRZ outliers	91569	1122 (6.22-3.60)

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 <=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	362	6% 61% 38%
1	B	362	2% 62% 36%
1	C	362	3% 62% 37%
1	D	362	2% 59% 39%
1	E	362	3% 61% 37%

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Mol	Chain	Length	Quality of chain
1	F	362	3% 60% 38%
1	G	362	5% 61% 37%
1	H	362	3% 63% 36%
1	I	362	4% 59% 39%
1	J	362	3% 60% 38%
1	K	362	3% 60% 38%
1	L	362	4% 60% 39%
2	1	78	23% 54% 44%
2	2	78	13% 55% 44%
2	3	78	18% 54% 44%
2	4	78	32% 56% 41%
2	5	78	24% 55% 42%
2	6	78	26% 55% 42%
2	7	78	19% 55% 42%
2	8	78	37% 55% 42%
2	9	78	24% 54% 44%
2	U	78	27% 53% 45%
2	W	78	14% 55% 42%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 41874 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 Large T antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	0	0
			2933	1888	493	531	21			
1	B	362	Total	C	N	O	S	0	0	0
			2933	1888	493	531	21			
1	C	362	Total	C	N	O	S	0	0	0
			2933	1888	493	531	21			
1	D	362	Total	C	N	O	S	0	0	0
			2933	1888	493	531	21			
1	E	362	Total	C	N	O	S	0	0	0
			2933	1888	493	531	21			
1	F	362	Total	C	N	O	S	0	0	0
			2933	1888	493	531	21			
1	G	362	Total	C	N	O	S	0	0	0
			2933	1888	493	531	21			
1	H	362	Total	C	N	O	S	0	0	0
			2933	1888	493	531	21			
1	I	362	Total	C	N	O	S	0	0	0
			2933	1888	493	531	21			
1	J	362	Total	C	N	O	S	0	0	0
			2933	1888	493	531	21			
1	K	362	Total	C	N	O	S	0	0	0
			2933	1888	493	531	21			
1	L	362	Total	C	N	O	S	0	0	0
			2933	1888	493	531	21			

- Molecule 2 is a protein called DNA polymerase alpha subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	78	Total	C	N	O	S	0	0	0
			606	380	99	122	5			
2	3	78	Total	C	N	O	S	0	0	0
			606	380	99	122	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	6	78	Total	C	N	O	S	0	0	0
			606	380	99	122	5			
2	U	78	Total	C	N	O	S	0	0	0
			606	380	99	122	5			
2	W	78	Total	C	N	O	S	0	0	0
			606	380	99	122	5			
2	5	78	Total	C	N	O	S	0	0	0
			606	380	99	122	5			
2	7	78	Total	C	N	O	S	0	0	0
			606	380	99	122	5			
2	9	78	Total	C	N	O	S	0	0	0
			606	380	99	122	5			
2	1	78	Total	C	N	O	S	0	0	0
			606	380	99	122	5			
2	4	78	Total	C	N	O	S	0	0	0
			606	380	99	122	5			
2	8	78	Total	C	N	O	S	0	0	0
			606	380	99	122	5			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Zn	0	0
			1	1		
3	J	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		
3	K	1	Total	Zn	0	0
			1	1		
3	E	1	Total	Zn	0	0
			1	1		
3	H	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	I	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		

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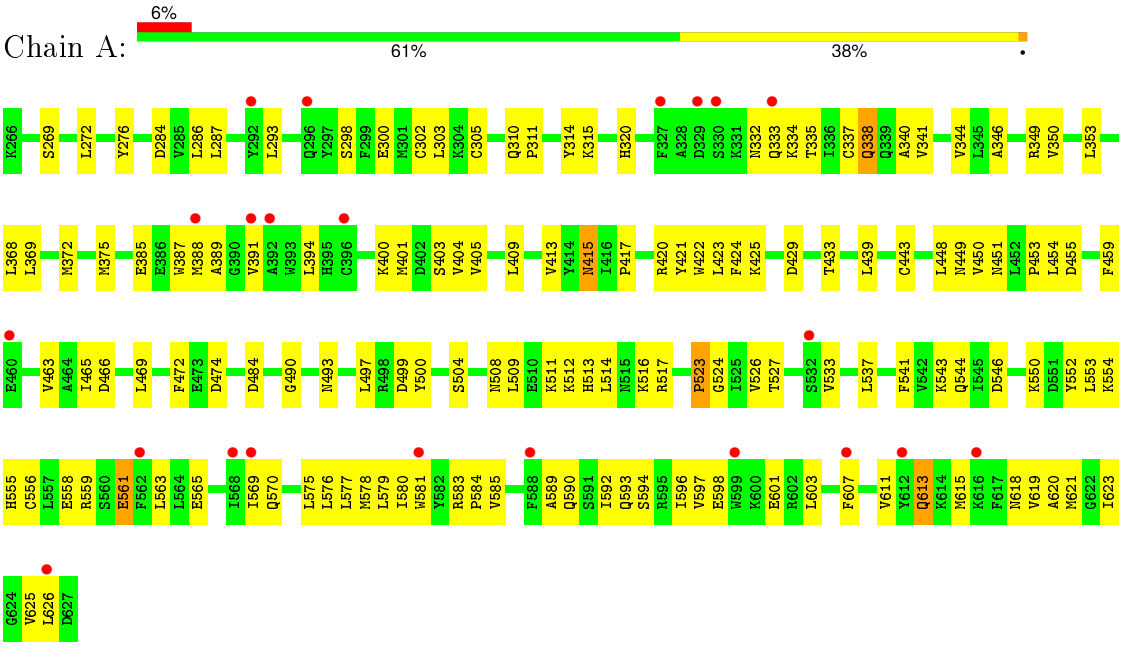
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	L	1	Total Zn 1 1	0	0
3	F	1	Total Zn 1 1	0	0

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.

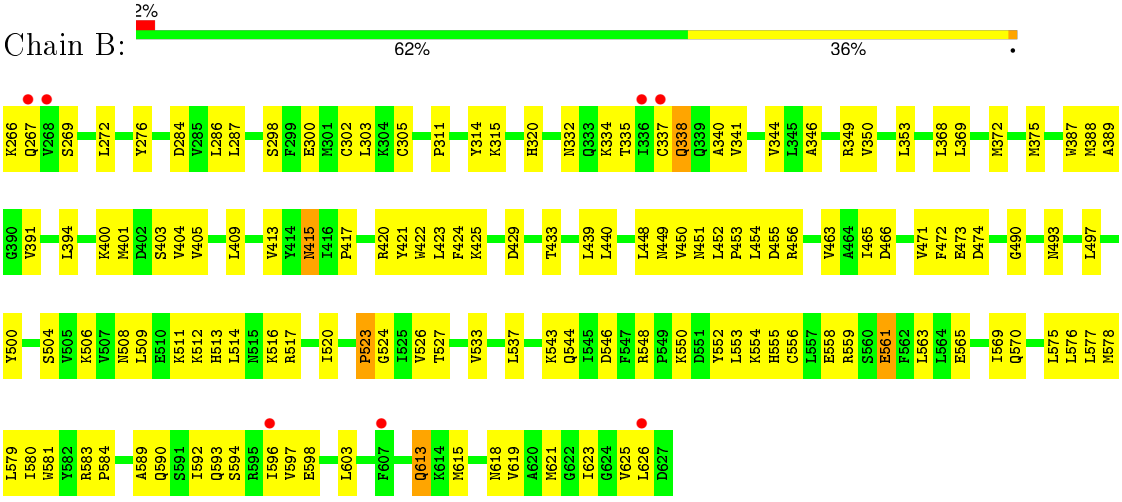
- Molecule 1: Large T antigen

Chain A:



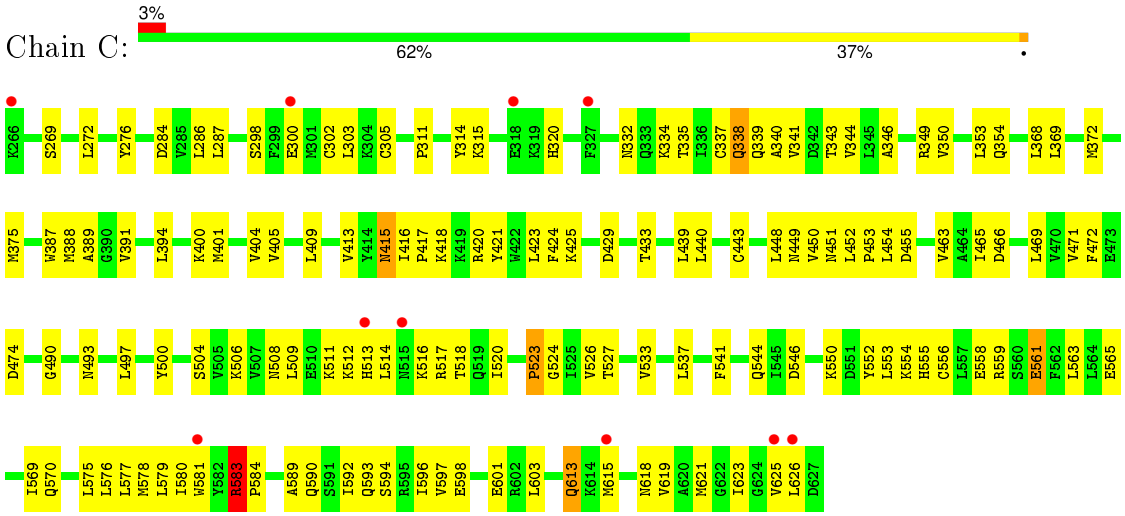
- Molecule 1: Large T antigen

Chain B:



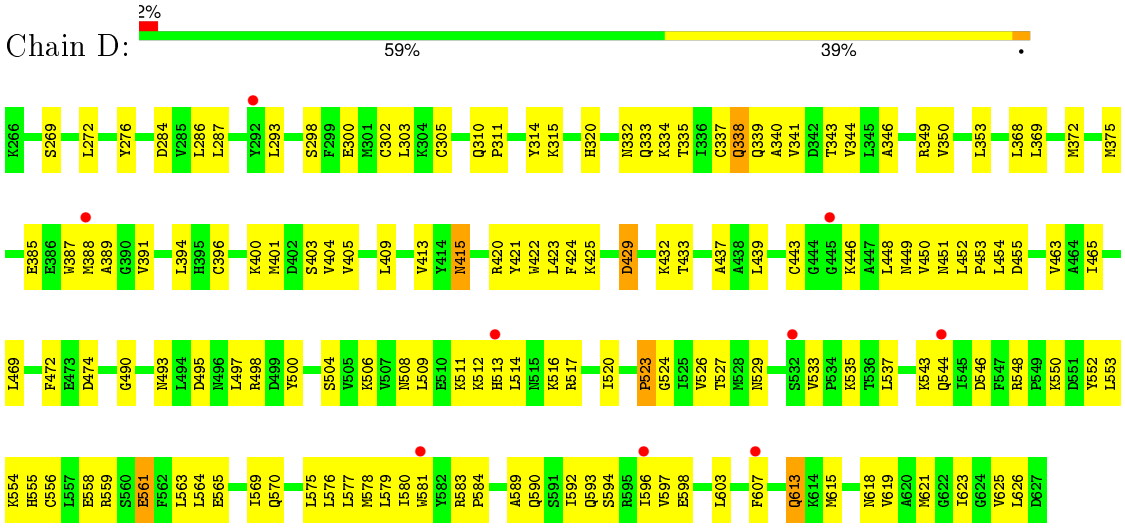
- Molecule 1: Large T antigen

Chain C:



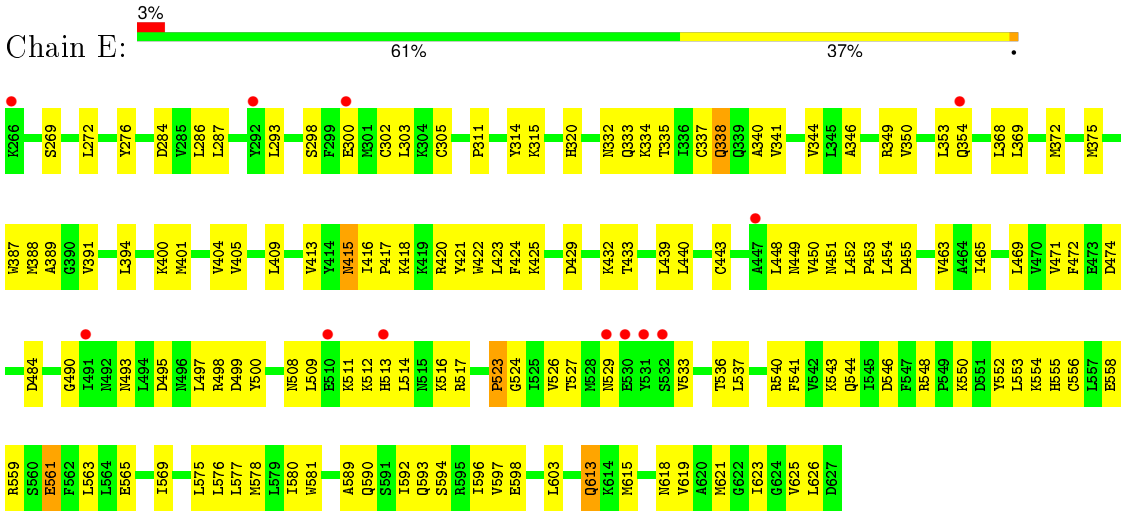
- Molecule 1: Large T antigen

Chain D:



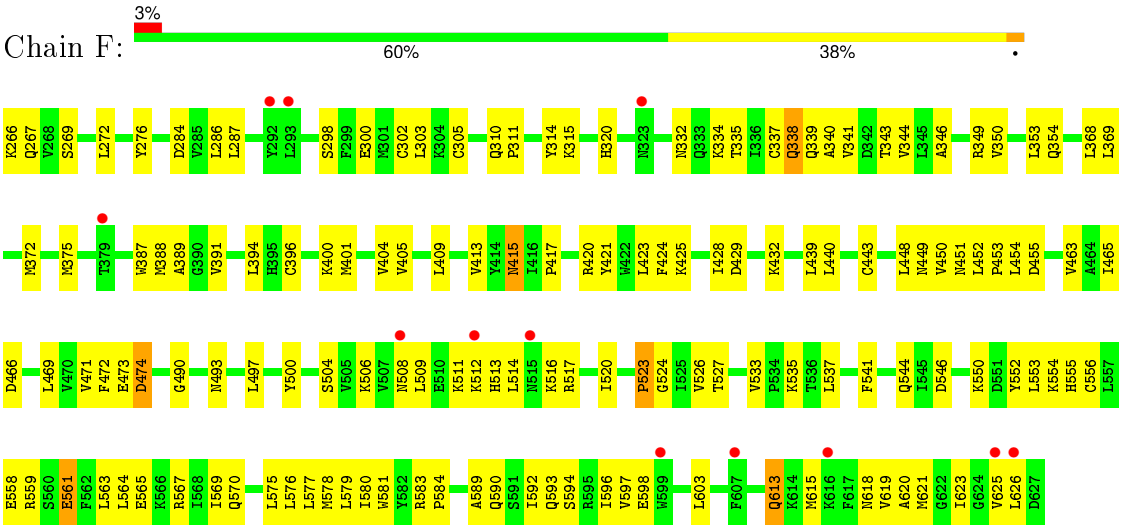
- Molecule 1: Large T antigen

Chain E:



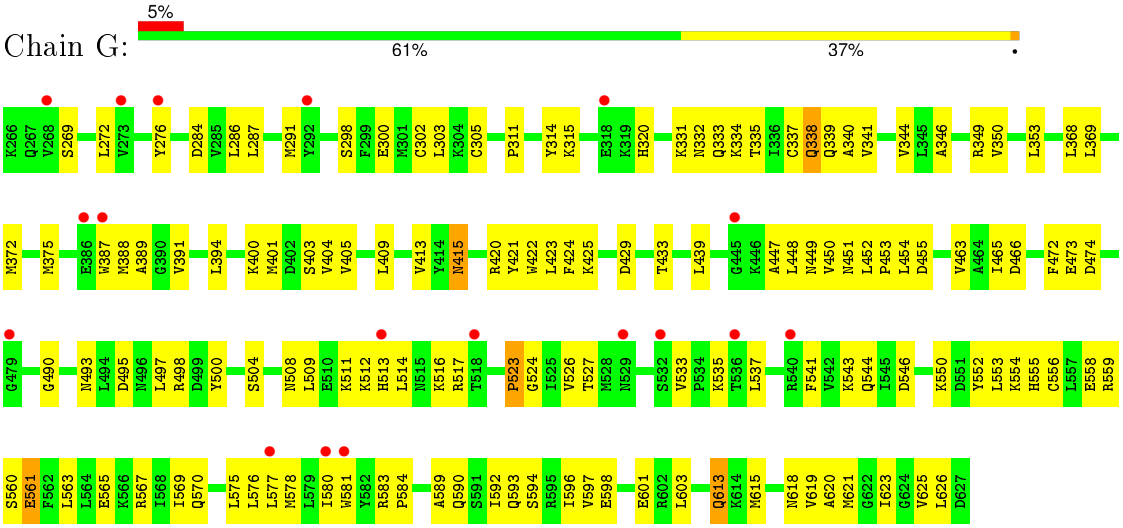
- Molecule 1: Large T antigen

Chain F:



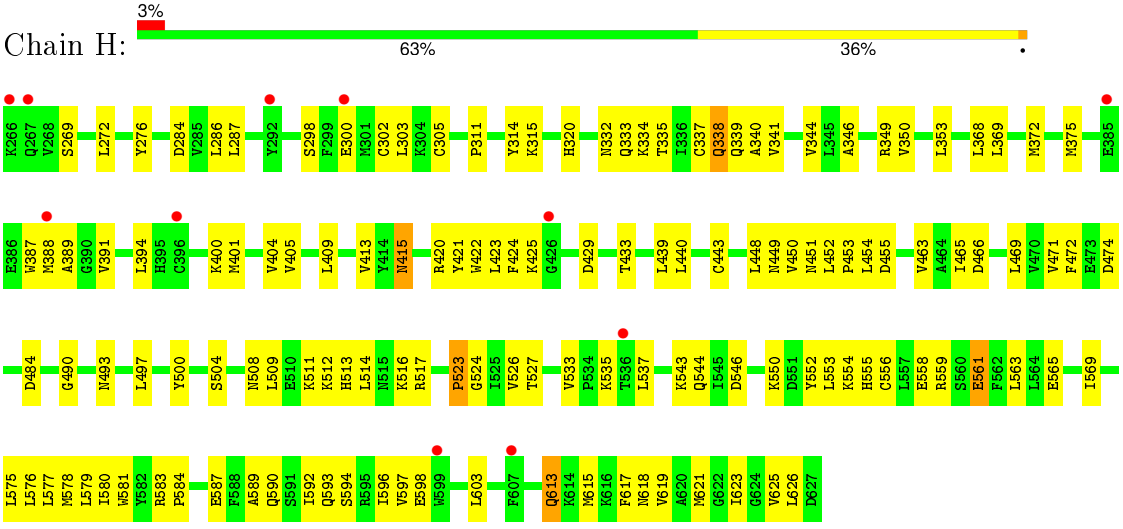
- Molecule 1: Large T antigen

Chain G:



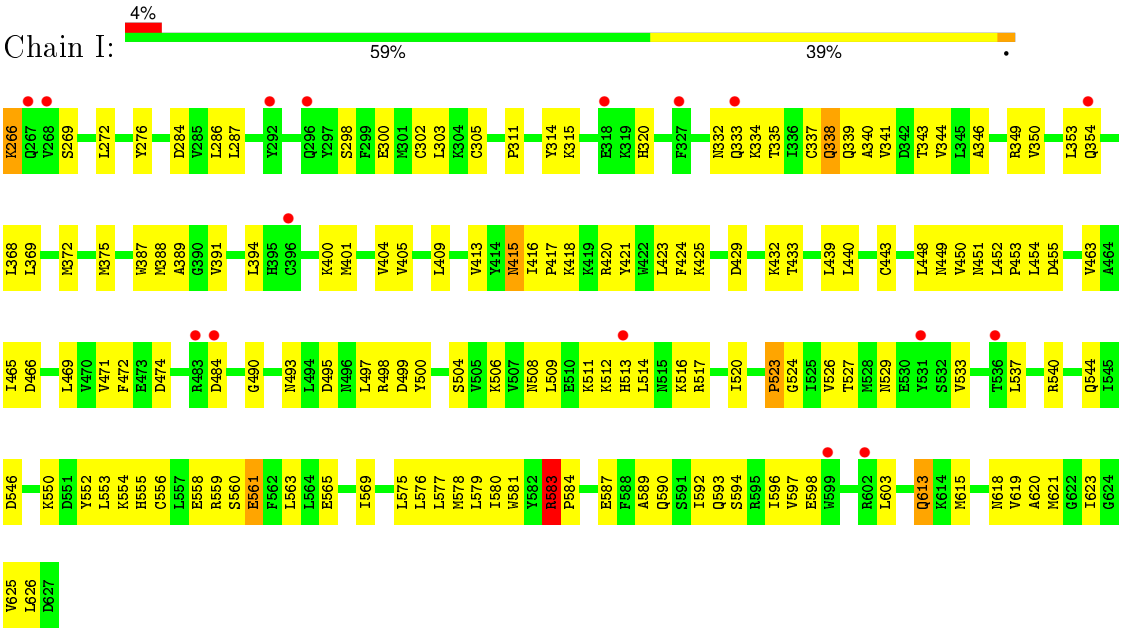
- Molecule 1: Large T antigen

Chain H:



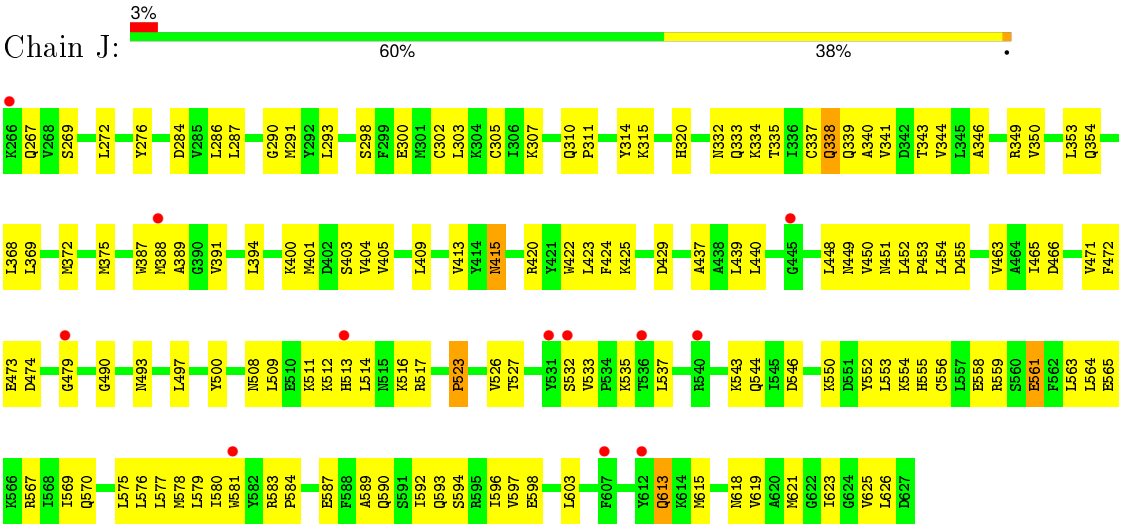
- Molecule 1: Large T antigen

Chain I:



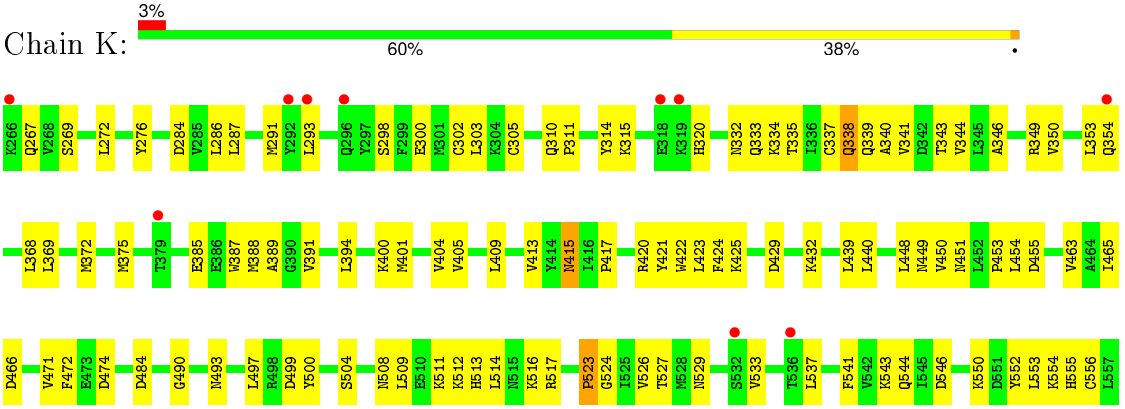
• Molecule 1: Large T antigen

Chain J:

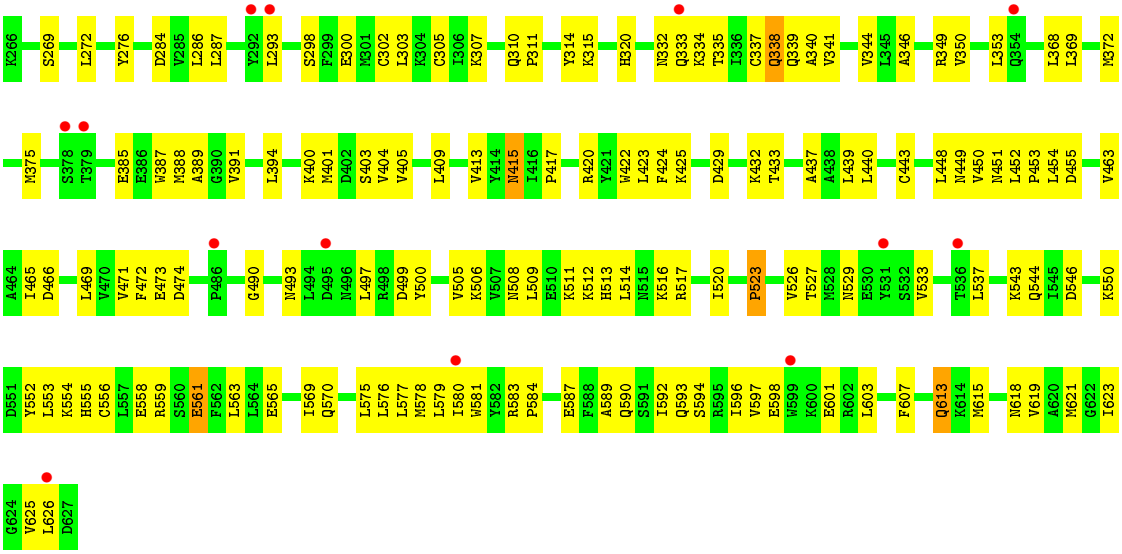


• Molecule 1: Large T antigen

Chain K:

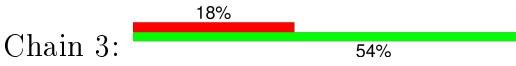


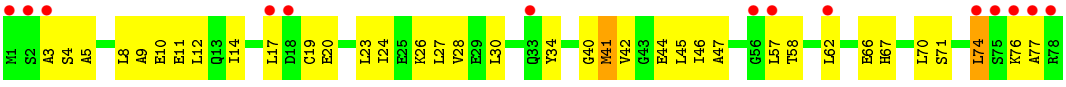
• Molecule 1: Large T antigen



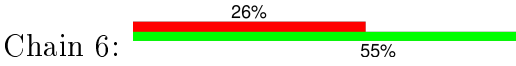
• Molecule 2: DNA polymerase alpha subunit B

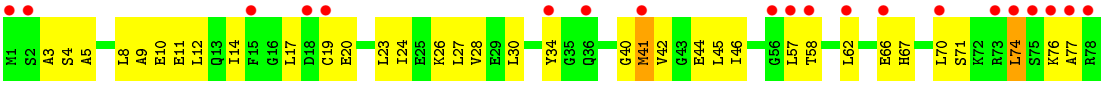
• Molecule 2: DNA polymerase alpha subunit B



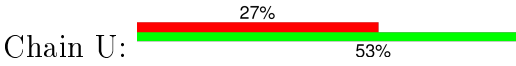


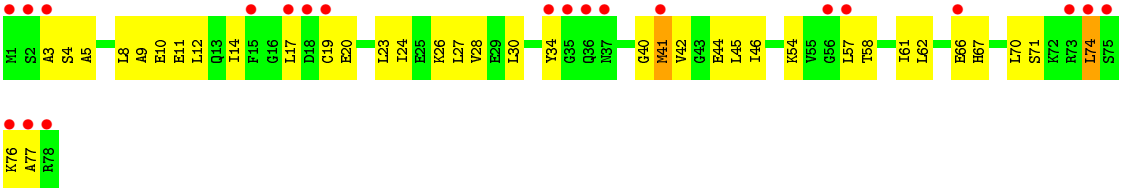
• Molecule 2: DNA polymerase alpha subunit B



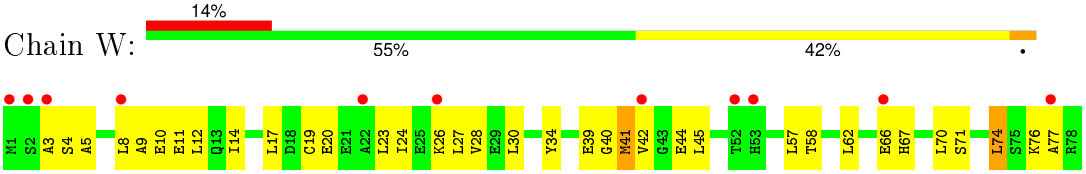


• Molecule 2: DNA polymerase alpha subunit B

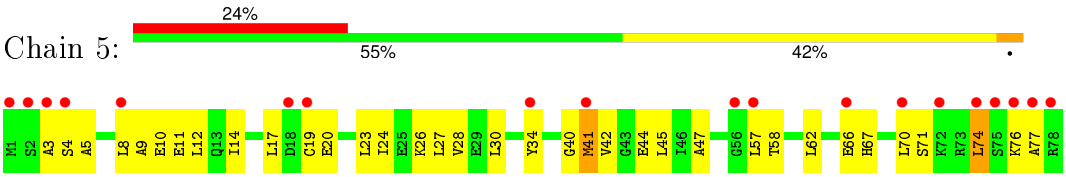




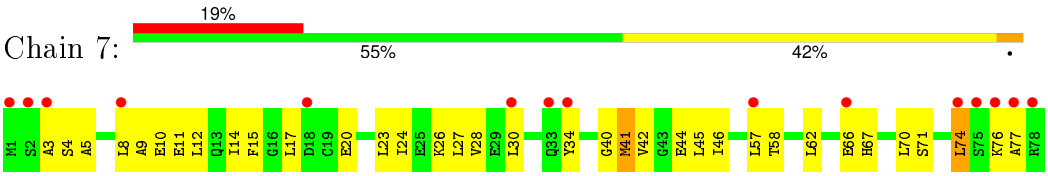
• Molecule 2: DNA polymerase alpha subunit B



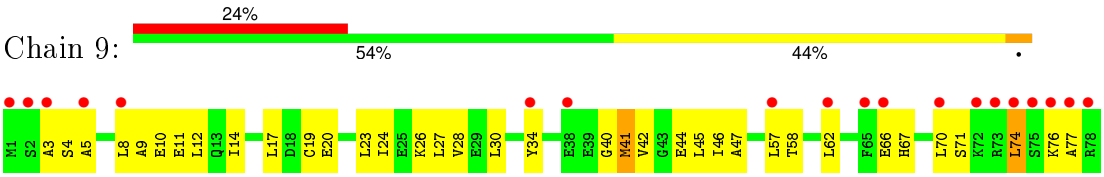
• Molecule 2: DNA polymerase alpha subunit B



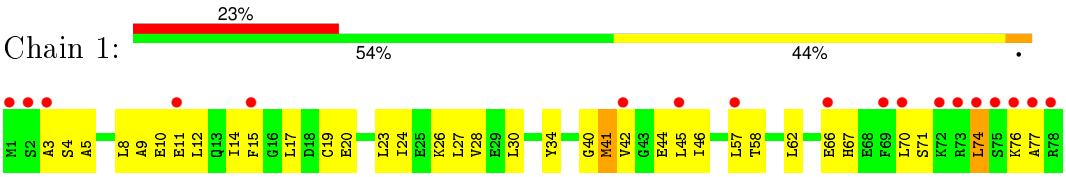
• Molecule 2: DNA polymerase alpha subunit B



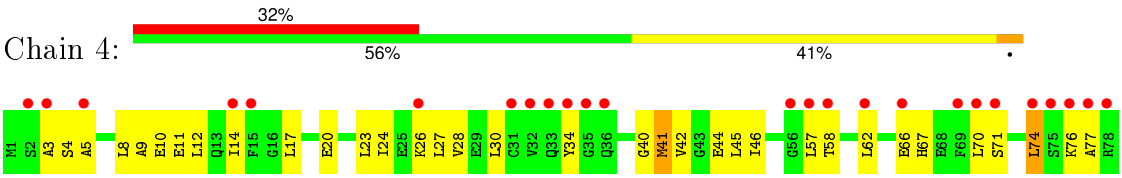
• Molecule 2: DNA polymerase alpha subunit B



• Molecule 2: DNA polymerase alpha subunit B

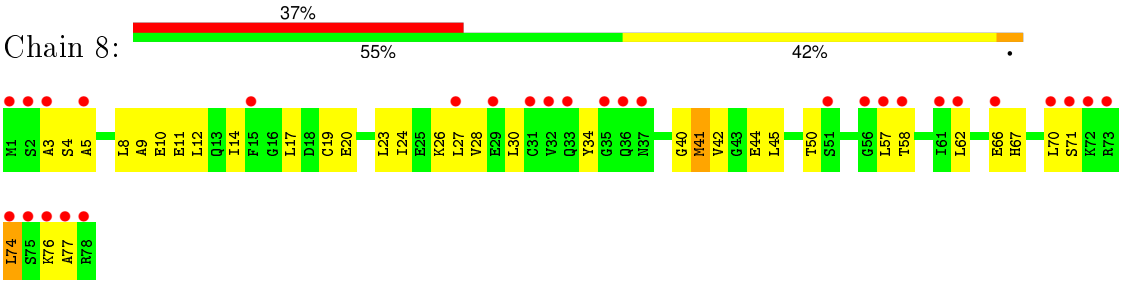


• Molecule 2: DNA polymerase alpha subunit B



• Molecule 2: DNA polymerase alpha subunit B

Chain 8:


37%
55%
42%
M1
S2
A3
S4
A5
L8
A9
E10
E11
L12
Q13
I14
F15
G16
L17
D18
C19
E20
L23
T24
E25
K26
L27
V28
E29
L30
C31
V32
Q33
Y34
G35
Q36
N37
G40
M41
V42
G43
E44
L45
T50
S51
G56
L57
T58
I61
L62
E66
H67
L70
S71
K72
R73
L74
S75
K76
A77
R78

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	249.10Å 249.10Å 387.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 5.00 49.91 – 5.01	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-5.00) 74.4 (49.91-5.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.40 (at 5.10Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.305 , 0.314 0.299 , 0.305	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	280.1	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 273.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 39655 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	41874	wwPDB-VP
Average B, all atoms (Å^2)	299.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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	0.25	0/2992	0.43	0/4030
1	B	0.25	0/2992	0.43	0/4030
1	C	0.26	0/2992	0.63	3/4030 (0.1%)
1	D	0.25	0/2992	0.43	0/4030
1	E	0.25	0/2992	0.43	0/4030
1	F	0.25	0/2992	0.43	0/4030
1	G	0.25	0/2992	0.43	0/4030
1	H	0.25	0/2992	0.43	0/4030
1	I	0.26	0/2992	0.63	3/4030 (0.1%)
1	J	0.25	0/2992	0.43	0/4030
1	K	0.25	0/2992	0.43	0/4030
1	L	0.24	0/2992	0.43	0/4030
2	1	0.25	0/612	0.43	0/820
2	2	0.26	0/612	0.44	0/820
2	3	0.25	0/612	0.43	0/820
2	4	0.25	0/612	0.44	0/820
2	5	0.26	0/612	0.43	0/820
2	6	0.26	0/612	0.44	0/820
2	7	0.25	0/612	0.43	0/820
2	8	0.25	0/612	0.43	0/820
2	9	0.26	0/612	0.43	0/820
2	U	0.25	0/612	0.43	0/820
2	W	0.26	0/612	0.44	0/820
All	All	0.25	0/42636	0.46	6/57380 (0.0%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	583	ARG	NE-CZ-NH1	-20.00	110.30	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	583	ARG	NE-CZ-NH1	-19.96	110.32	120.30
1	I	583	ARG	NE-CZ-NH2	19.44	130.02	120.30
1	C	583	ARG	NE-CZ-NH2	19.40	130.00	120.30
1	C	583	ARG	CD-NE-CZ	8.62	135.67	123.60

There are no chirality outliers.

There are no planarity outliers.

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	2933	0	2984	105	0
1	B	2933	0	2984	101	0
1	C	2933	0	2984	103	0
1	D	2933	0	2984	112	0
1	E	2933	0	2984	105	0
1	F	2933	0	2984	116	0
1	G	2933	0	2984	112	0
1	H	2933	0	2984	97	0
1	I	2933	0	2984	116	0
1	J	2933	0	2984	112	0
1	K	2933	0	2984	111	0
1	L	2933	0	2984	125	0
2	1	606	0	602	29	0
2	2	606	0	602	30	0
2	3	606	0	602	28	0
2	4	606	0	602	30	0
2	5	606	0	602	27	0
2	6	606	0	602	34	0
2	7	606	0	602	28	0
2	8	606	0	602	27	0
2	9	606	0	602	29	0
2	U	606	0	602	30	0
2	W	606	0	602	28	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
All	All	41874	0	42430	1479	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 18.

The worst 5 of 1479 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:G:286:LEU:HD12	1:L:349:ARG:HH21	1.16	1.07
1:J:349:ARG:HH21	1:K:286:LEU:HD12	1.30	0.97
1:D:349:ARG:HH21	1:E:286:LEU:HD12	1.30	0.96
1:H:349:ARG:HH21	1:I:286:LEU:HD12	1.35	0.92
1:K:349:ARG:HH21	1:L:286:LEU:HD12	1.38	0.89

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	360/362 (99%)	323 (90%)	33 (9%)	4 (1%)	17 64
1	B	360/362 (99%)	322 (89%)	34 (9%)	4 (1%)	17 64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	360/362 (99%)	323 (90%)	33 (9%)	4 (1%)	17	64
1	D	360/362 (99%)	323 (90%)	33 (9%)	4 (1%)	17	64
1	E	360/362 (99%)	323 (90%)	33 (9%)	4 (1%)	17	64
1	F	360/362 (99%)	322 (89%)	33 (9%)	5 (1%)	14	58
1	G	360/362 (99%)	323 (90%)	33 (9%)	4 (1%)	17	64
1	H	360/362 (99%)	323 (90%)	33 (9%)	4 (1%)	17	64
1	I	360/362 (99%)	323 (90%)	33 (9%)	4 (1%)	17	64
1	J	360/362 (99%)	322 (89%)	33 (9%)	5 (1%)	14	58
1	K	360/362 (99%)	322 (89%)	33 (9%)	5 (1%)	14	58
1	L	360/362 (99%)	323 (90%)	33 (9%)	4 (1%)	17	64
2	1	76/78 (97%)	68 (90%)	7 (9%)	1 (1%)	15	60
2	2	76/78 (97%)	68 (90%)	7 (9%)	1 (1%)	15	60
2	3	76/78 (97%)	68 (90%)	7 (9%)	1 (1%)	15	60
2	4	76/78 (97%)	66 (87%)	9 (12%)	1 (1%)	15	60
2	5	76/78 (97%)	68 (90%)	7 (9%)	1 (1%)	15	60
2	6	76/78 (97%)	68 (90%)	7 (9%)	1 (1%)	15	60
2	7	76/78 (97%)	68 (90%)	7 (9%)	1 (1%)	15	60
2	8	76/78 (97%)	67 (88%)	8 (10%)	1 (1%)	15	60
2	9	76/78 (97%)	68 (90%)	7 (9%)	1 (1%)	15	60
2	U	76/78 (97%)	68 (90%)	7 (9%)	1 (1%)	15	60
2	W	76/78 (97%)	68 (90%)	7 (9%)	1 (1%)	15	60
All	All	5156/5202 (99%)	4617 (90%)	477 (9%)	62 (1%)	16	62

5 of 62 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	474	ASP
1	B	474	ASP
1	C	474	ASP
1	D	474	ASP
1	E	474	ASP

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	323/323 (100%)	318 (98%)	5 (2%)	72	89
1	B	323/323 (100%)	318 (98%)	5 (2%)	72	89
1	C	323/323 (100%)	317 (98%)	6 (2%)	65	86
1	D	323/323 (100%)	318 (98%)	5 (2%)	72	89
1	E	323/323 (100%)	318 (98%)	5 (2%)	72	89
1	F	323/323 (100%)	318 (98%)	5 (2%)	72	89
1	G	323/323 (100%)	318 (98%)	5 (2%)	72	89
1	H	323/323 (100%)	318 (98%)	5 (2%)	72	89
1	I	323/323 (100%)	316 (98%)	7 (2%)	60	84
1	J	323/323 (100%)	318 (98%)	5 (2%)	72	89
1	K	323/323 (100%)	318 (98%)	5 (2%)	72	89
1	L	323/323 (100%)	318 (98%)	5 (2%)	72	89
2	1	67/67 (100%)	65 (97%)	2 (3%)	48	78
2	2	67/67 (100%)	66 (98%)	1 (2%)	72	89
2	3	67/67 (100%)	65 (97%)	2 (3%)	48	78
2	4	67/67 (100%)	65 (97%)	2 (3%)	48	78
2	5	67/67 (100%)	65 (97%)	2 (3%)	48	78
2	6	67/67 (100%)	65 (97%)	2 (3%)	48	78
2	7	67/67 (100%)	65 (97%)	2 (3%)	48	78
2	8	67/67 (100%)	65 (97%)	2 (3%)	48	78
2	9	67/67 (100%)	65 (97%)	2 (3%)	48	78
2	U	67/67 (100%)	65 (97%)	2 (3%)	48	78
2	W	67/67 (100%)	65 (97%)	2 (3%)	48	78
All	All	4613/4613 (100%)	4529 (98%)	84 (2%)	66	87

5 of 84 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	338	GLN
1	I	613	GLN
2	9	74	LEU
1	H	561	GLU
1	I	302	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 152 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	590	GLN
1	G	613	GLN
1	L	415	ASN
1	F	613	GLN
1	G	451	ASN

5.3.3 RNA

There are no RNA molecules 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 12 ligands modelled in this entry, 12 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

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^{th} 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	362/362 (100%)	0.51	22 (6%)	25	19	262, 300, 300, 300	0
1	B	362/362 (100%)	0.34	7 (1%)	70	62	260, 300, 300, 300	0
1	C	362/362 (100%)	0.41	10 (2%)	56	48	260, 300, 300, 300	0
1	D	362/362 (100%)	0.31	9 (2%)	61	52	257, 300, 300, 300	0
1	E	362/362 (100%)	0.38	12 (3%)	50	41	260, 300, 300, 300	0
1	F	362/362 (100%)	0.45	12 (3%)	50	41	258, 300, 300, 300	0
1	G	362/362 (100%)	0.48	18 (4%)	32	27	260, 300, 300, 300	0
1	H	362/362 (100%)	0.33	11 (3%)	54	44	260, 300, 300, 300	0
1	I	362/362 (100%)	0.39	16 (4%)	38	31	260, 300, 300, 300	0
1	J	362/362 (100%)	0.37	12 (3%)	50	41	261, 300, 300, 300	0
1	K	362/362 (100%)	0.35	12 (3%)	50	41	260, 300, 300, 300	0
1	L	362/362 (100%)	0.35	13 (3%)	46	39	262, 300, 300, 300	0
2	1	78/78 (100%)	1.34	18 (23%)	1	3	281, 300, 300, 300	0
2	2	78/78 (100%)	0.81	10 (12%)	5	6	278, 300, 300, 300	0
2	3	78/78 (100%)	0.99	14 (17%)	2	4	280, 300, 300, 300	0
2	4	78/78 (100%)	1.52	25 (32%)	1	2	281, 300, 300, 300	0
2	5	78/78 (100%)	1.10	19 (24%)	1	2	281, 300, 300, 300	0
2	6	78/78 (100%)	1.29	20 (25%)	1	2	281, 300, 300, 300	0
2	7	78/78 (100%)	1.02	15 (19%)	2	3	280, 300, 300, 300	0
2	8	78/78 (100%)	1.53	29 (37%)	0	2	280, 300, 300, 300	0
2	9	78/78 (100%)	1.18	19 (24%)	1	2	280, 300, 300, 300	0
2	U	78/78 (100%)	1.36	21 (26%)	1	2	280, 300, 300, 300	0
2	W	78/78 (100%)	0.92	11 (14%)	4	5	279, 300, 300, 300	0
All	All	5202/5202 (100%)	0.52	355 (6%)	20	16	257, 300, 300, 300	0

The worst 5 of 355 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	1	1	MET	9.0
2	1	2	SER	7.2
2	1	78	ARG	6.7
2	7	1	MET	6.6
2	6	57	LEU	6.5

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, 95^{th} 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
3	ZN	B	700	1/1	0.83	0.17	-0.81	300,300,300,300	0
3	ZN	E	700	1/1	0.79	0.15	-1.61	300,300,300,300	0
3	ZN	H	700	1/1	0.70	0.10	-1.63	300,300,300,300	0
3	ZN	C	700	1/1	0.46	0.16	-1.81	300,300,300,300	0
3	ZN	I	700	1/1	0.74	0.10	-1.81	300,300,300,300	0
3	ZN	F	700	1/1	0.65	0.09	-1.89	300,300,300,300	0
3	ZN	K	700	1/1	0.51	0.15	-1.92	300,300,300,300	0
3	ZN	J	700	1/1	0.94	0.09	-2.05	300,300,300,300	0
3	ZN	A	700	1/1	0.91	0.08	-2.10	300,300,300,300	0
3	ZN	G	700	1/1	0.77	0.13	-2.23	300,300,300,300	0
3	ZN	D	700	1/1	0.91	0.06	-2.31	245,245,245,245	0
3	ZN	L	700	1/1	0.97	0.04	-2.63	300,300,300,300	0

6.5 Other polymers (i)

There are no such residues in this entry.