



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2018 – 12:14 pm GMT

PDB ID : 2GXA
Title : Crystal structure of papillomavirus E1 hexameric helicase with ssDNA and MgADP
Authors : Enemark, E.J.; Joshua-Tor, L.
Deposited on : 2006-05-08
Resolution : 3.15 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

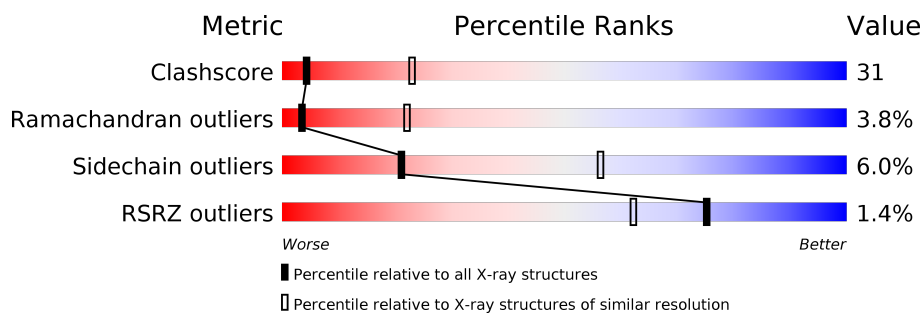
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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))
Clashscore	122126	1522 (3.20-3.12)
Ramachandran outliers	120053	1493 (3.20-3.12)
Sidechain outliers	120020	1492 (3.20-3.12)
RSRZ outliers	108989	1344 (3.20-3.12)

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	M	13	<div> <div>8%</div> <div>38%</div> <div>54%</div> </div>
1	N	13	<div> <div>8%</div> <div>38%</div> <div>8%</div> <div>46%</div> </div>
2	A	274	<div> <div>%</div> <div>49%</div> <div>44%</div> <div>5%</div> </div>
2	B	274	<div> <div>52%</div> <div>41%</div> <div>5%</div> </div>
2	C	274	<div> <div>3%</div> <div>60%</div> <div>35%</div> <div>.</div> </div>
2	D	274	<div> <div>%</div> <div>49%</div> <div>43%</div> <div>6%</div> </div>
2	E	274	<div> <div>53%</div> <div>41%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	274	
2	G	274	
2	H	274	
2	I	274	
2	J	274	
2	K	274	
2	L	274	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CL	B	42	-	-	X	-
5	ADP	F	6	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 26374 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 DNA chain called 5'-D(*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	M	6	Total	C	N	O	P	0	0	0
			121	60	12	43	6			
1	N	7	Total	C	N	O	P	0	0	0
			141	70	14	50	7			

- Molecule 2 is a protein called Replication protein E1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	270	Total	C	N	O	S	0	0	0
			2140	1380	371	379	10			
2	B	270	Total	C	N	O	S	0	0	0
			2140	1380	371	379	10			
2	C	270	Total	C	N	O	S	0	0	0
			2140	1380	371	379	10			
2	D	270	Total	C	N	O	S	0	0	0
			2140	1380	371	379	10			
2	E	274	Total	C	N	O	S	0	0	0
			2177	1402	377	388	10			
2	F	270	Total	C	N	O	S	0	0	0
			2140	1380	371	379	10			
2	G	270	Total	C	N	O	S	0	0	0
			2140	1380	371	379	10			
2	H	274	Total	C	N	O	S	0	0	0
			2177	1402	377	388	10			
2	I	270	Total	C	N	O	S	0	0	0
			2140	1380	371	379	10			
2	J	270	Total	C	N	O	S	0	0	0
			2140	1380	371	379	10			
2	K	273	Total	C	N	O	S	0	0	0
			2173	1400	376	387	10			
2	L	270	Total	C	N	O	S	0	0	0
			2140	1380	371	379	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	304	GLY	-	cloning artifact	UNP P03116
B	304	GLY	-	cloning artifact	UNP P03116
C	304	GLY	-	cloning artifact	UNP P03116
D	304	GLY	-	cloning artifact	UNP P03116
E	304	GLY	-	cloning artifact	UNP P03116
F	304	GLY	-	cloning artifact	UNP P03116
G	304	GLY	-	cloning artifact	UNP P03116
H	304	GLY	-	cloning artifact	UNP P03116
I	304	GLY	-	cloning artifact	UNP P03116
J	304	GLY	-	cloning artifact	UNP P03116
K	304	GLY	-	cloning artifact	UNP P03116
L	304	GLY	-	cloning artifact	UNP P03116

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

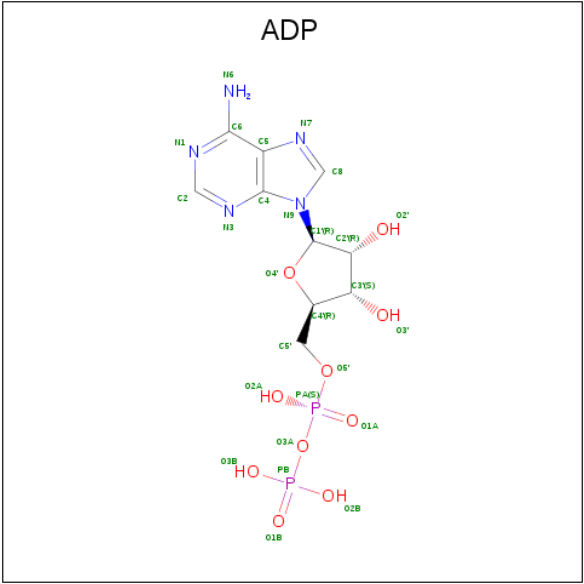
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		
4	A	1	Total	Cl	0	0
			1	1		

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	D	1	Total	C	N	O	P	10	0
			27	10	5	10	2		
5	E	1	Total	C	N	O	P	10	0
			27	10	5	10	2		
5	F	1	Total	C	N	O	P	10	0
			27	10	5	10	2		
5	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	J	1	Total	C	N	O	P	10	0
			27	10	5	10	2		

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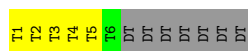
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	K	1	Total	C	N	O	P	10	0
			27	10	5	10	2		
5	L	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	O	0	0
			2	2		
6	B	3	Total	O	0	0
			3	3		
6	C	3	Total	O	0	0
			3	3		
6	D	1	Total	O	0	0
			1	1		
6	G	3	Total	O	0	0
			3	3		
6	H	2	Total	O	0	0
			2	2		
6	I	1	Total	O	0	0
			1	1		

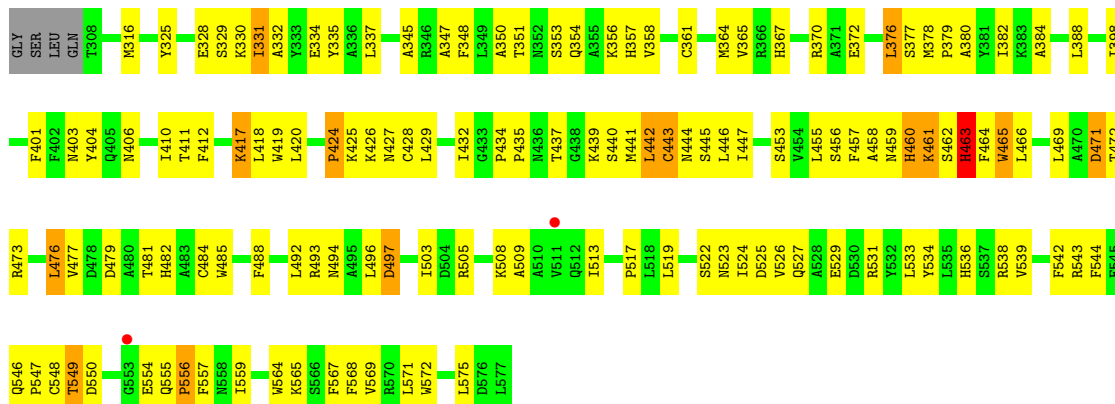
● Molecule 1: 5'-D(*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*T)-3'



Chain N: 

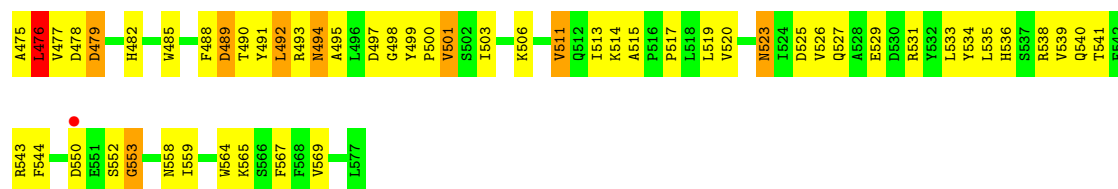


Chain A:  49% 44% 5%

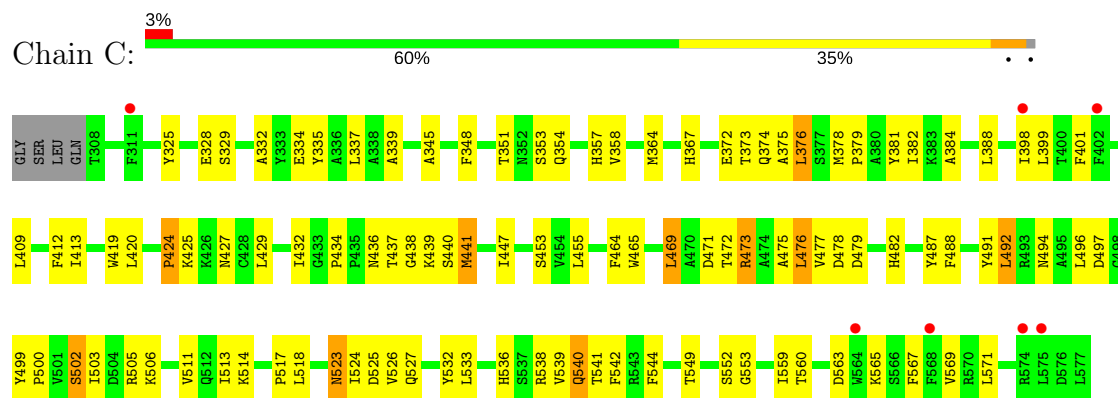


Chain B: 52% 41% 5%

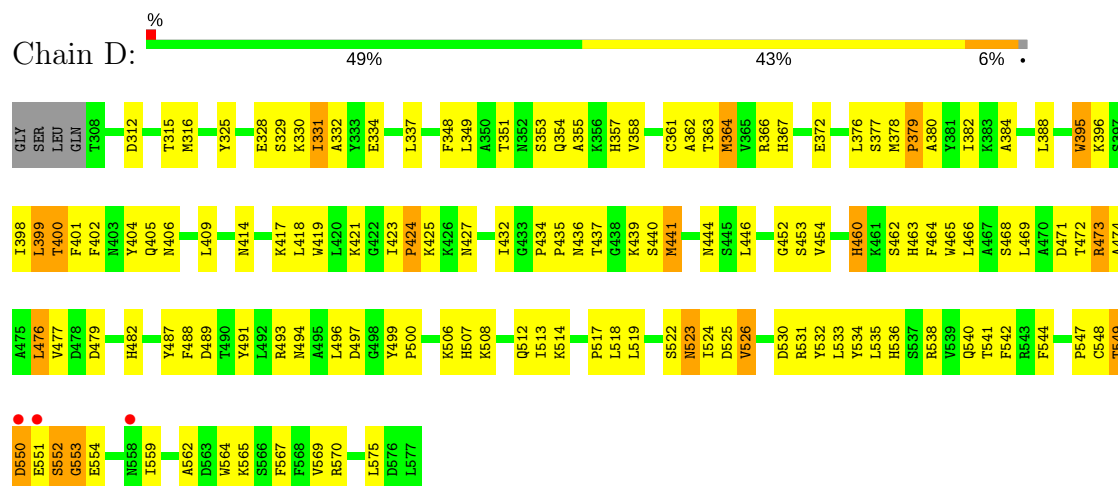




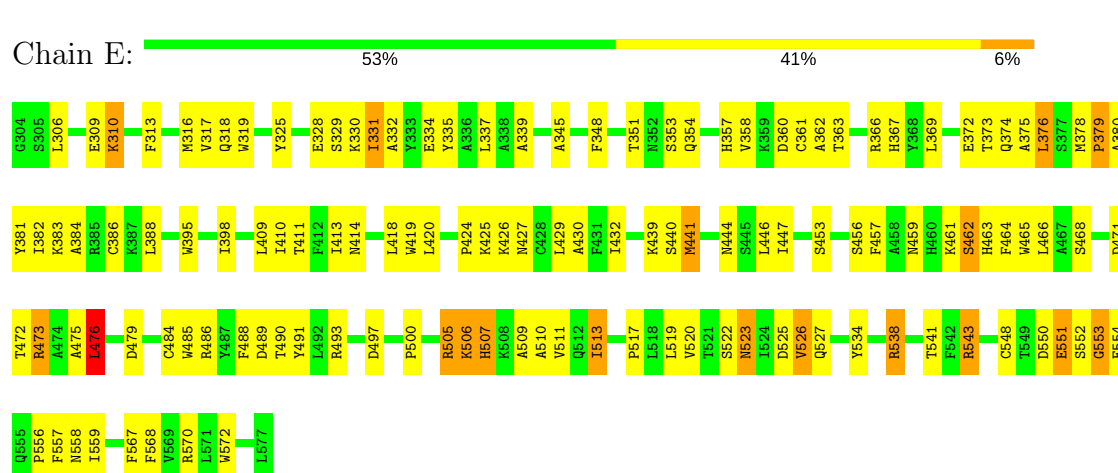
• Molecule 2: Replication protein E1



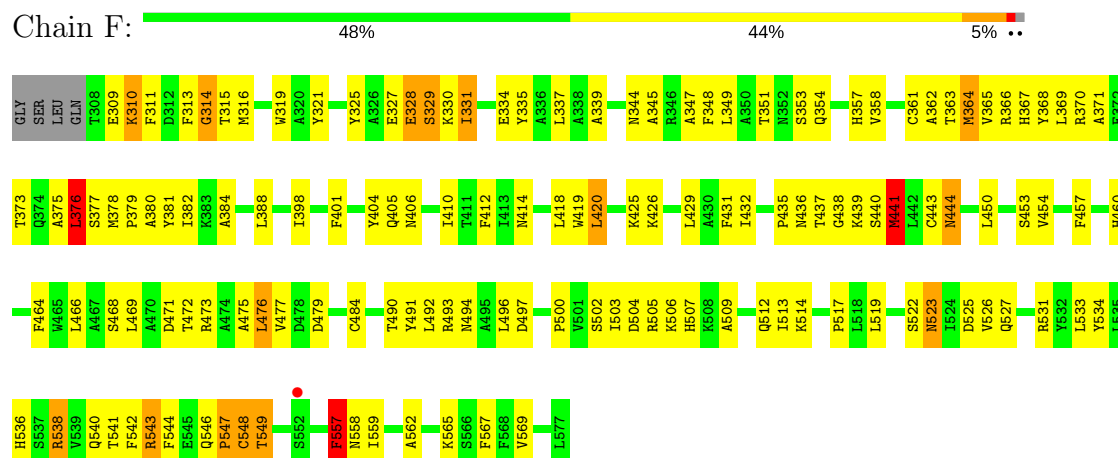
• Molecule 2: Replication protein E1



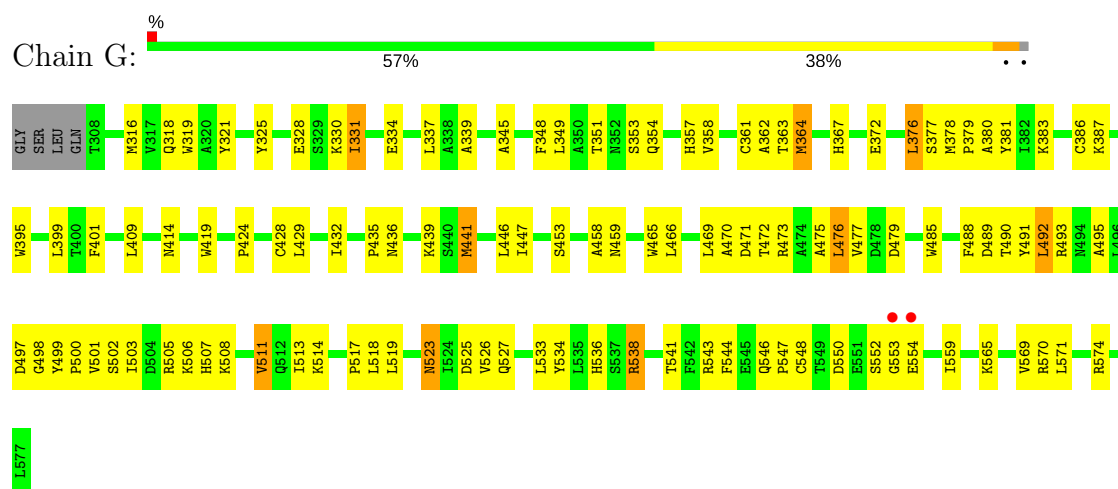
• Molecule 2: Replication protein E1



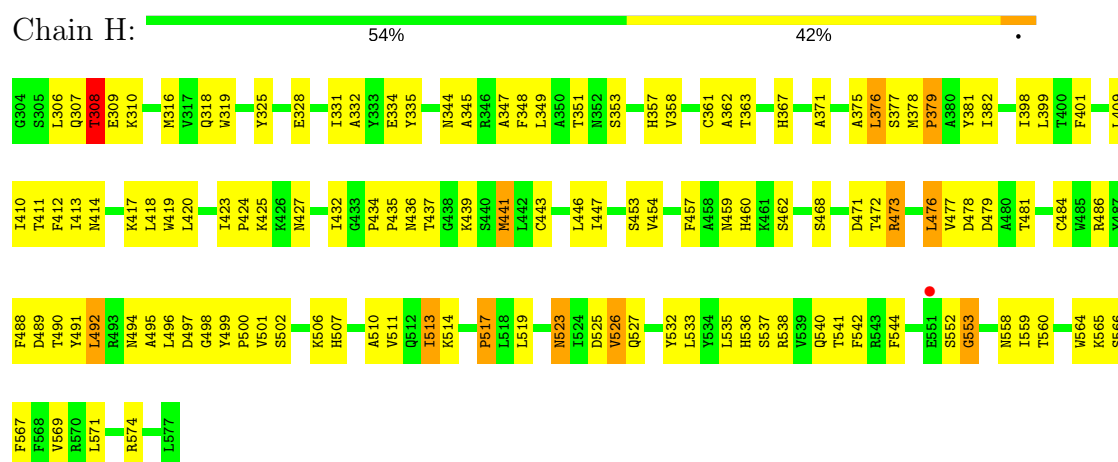
- Molecule 2: Replication protein E1



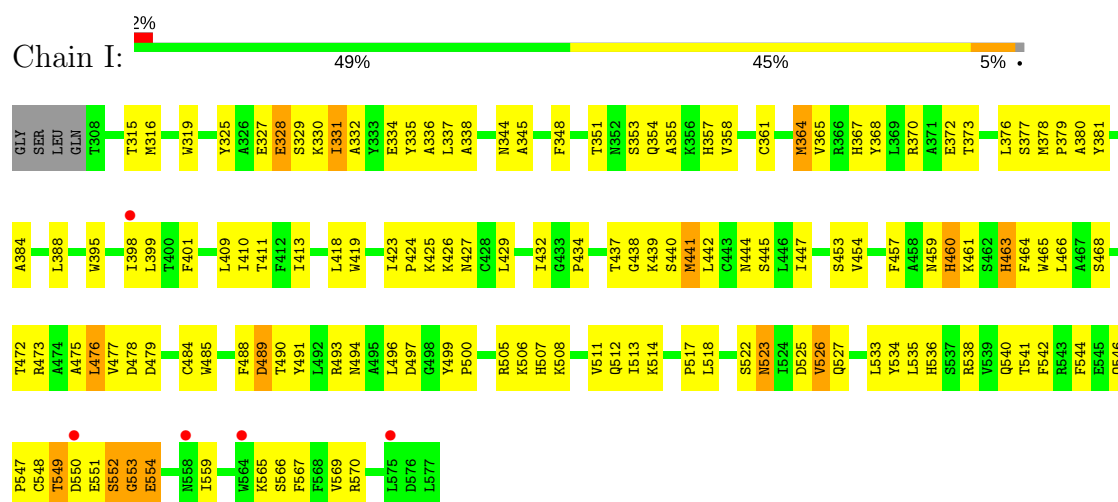
- Molecule 2: Replication protein E1



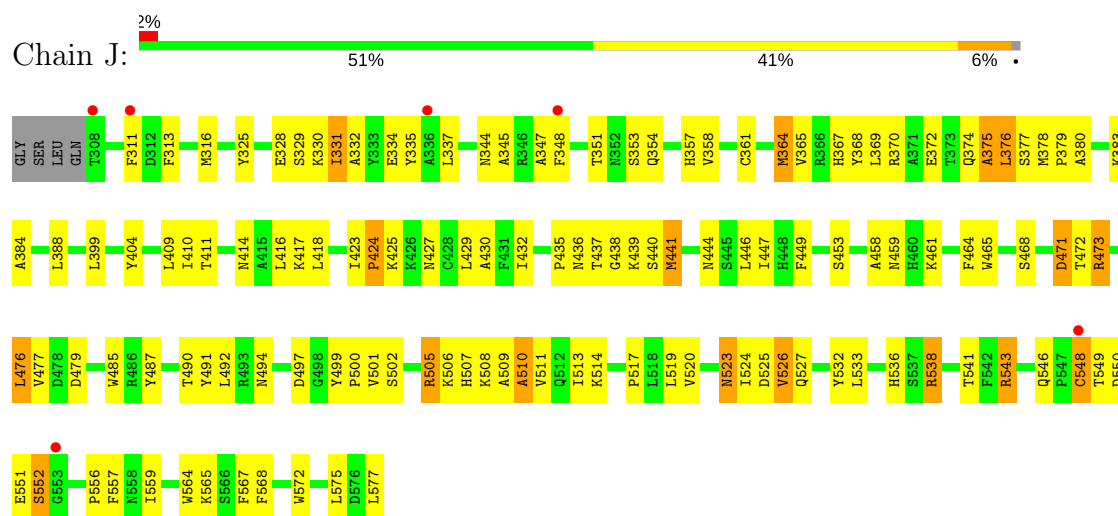
- Molecule 2: Replication protein E1



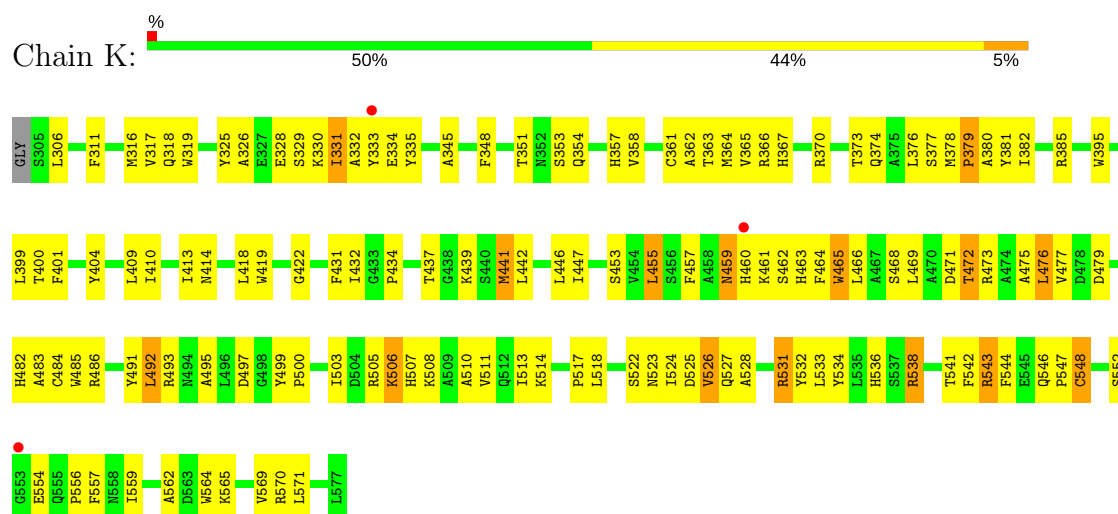
- Molecule 2: Replication protein E1



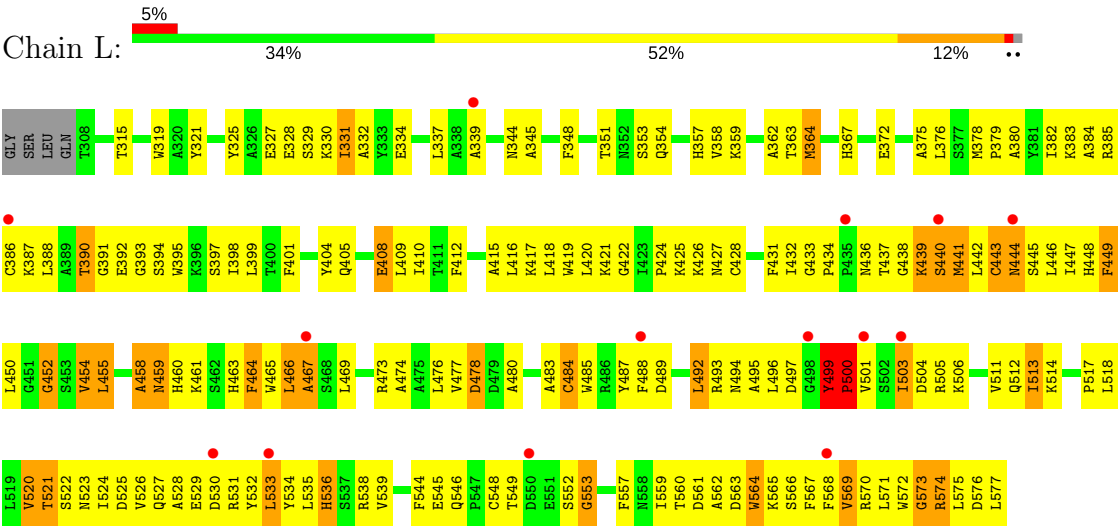
• Molecule 2: Replication protein E1



• Molecule 2: Replication protein E1



• Molecule 2: Replication protein E1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	100.51Å 100.88Å 125.02Å 92.60° 111.46° 106.01°	Depositor
Resolution (Å)	44.65 – 3.15 44.65 – 3.11	Depositor EDS
% Data completeness (in resolution range)	91.9 (44.65-3.15) 92.0 (44.65-3.11)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 3.12Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.239 , 0.298 0.212 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	74.0	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 34.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	26374	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: MG, ADP, CL

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	M	0.83	1/132 (0.8%)	0.93	0/200
1	N	0.76	1/154 (0.6%)	0.82	0/234
2	A	0.71	4/2199 (0.2%)	0.89	6/2985 (0.2%)
2	B	0.48	0/2199	0.69	1/2985 (0.0%)
2	C	0.43	0/2199	0.62	0/2985
2	D	0.41	0/2199	0.61	0/2985
2	E	0.42	0/2236	0.64	2/3033 (0.1%)
2	F	0.42	0/2199	0.64	0/2985
2	G	0.43	0/2199	0.61	0/2985
2	H	0.44	0/2236	0.64	0/3033
2	I	0.41	0/2199	0.62	0/2985
2	J	0.42	0/2199	0.63	0/2985
2	K	0.44	0/2232	0.65	0/3028
2	L	0.39	0/2199	0.73	3/2985 (0.1%)
All	All	0.46	6/26781 (0.0%)	0.67	12/36393 (0.0%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	497	ASP	CB-CG	-10.66	1.29	1.51
2	A	484	CYS	CB-SG	-7.33	1.69	1.82
1	M	1	DT	OP3-P	-6.40	1.53	1.61
1	N	1	DT	OP3-P	-6.28	1.53	1.61
2	A	464	PHE	CB-CG	-5.80	1.41	1.51

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	497	ASP	CB-CG-OD1	-15.82	104.06	118.30
2	L	500	PRO	CA-N-CD	-10.02	97.47	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	499	TYR	C-N-CD	-7.52	104.06	120.60
2	A	497	ASP	OD1-CG-OD2	7.47	137.50	123.30
2	E	476	LEU	CA-CB-CG	6.49	130.22	115.30

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	M	121	0	73	15	0
1	N	141	0	85	19	0
2	A	2140	0	2078	161	0
2	B	2140	0	2078	127	0
2	C	2140	0	2078	92	0
2	D	2140	0	2078	122	0
2	E	2177	0	2124	113	0
2	F	2140	0	2078	134	0
2	G	2140	0	2078	99	0
2	H	2177	0	2125	127	0
2	I	2140	0	2077	132	0
2	J	2140	0	2078	118	0
2	K	2173	0	2121	139	0
2	L	2140	0	2078	279	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	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
4	A	1	0	0	0	0
4	B	1	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	1	0	0	0	0
5	A	27	0	12	4	0
5	B	27	0	12	5	0
5	C	27	0	12	4	0
5	D	27	0	12	2	0
5	E	27	0	12	2	0
5	F	27	0	12	11	0
5	G	27	0	12	3	0
5	H	27	0	12	5	0
5	J	27	0	12	1	0
5	K	27	0	12	1	0
5	L	27	0	12	3	0
6	A	2	0	0	0	0
6	B	3	0	0	0	0
6	C	3	0	0	0	0
6	D	1	0	0	0	0
6	G	3	0	0	0	0
6	H	2	0	0	0	0
6	I	1	0	0	0	0
All	All	26374	0	25361	1595	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 31.

The worst 5 of 1595 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:A:534:TYR:HE2	2:A:538:ARG:NH1	1.19	1.34
2:A:534:TYR:CE2	2:A:538:ARG:NH1	1.95	1.33
2:L:444:ASN:HD21	2:L:521:THR:HG21	1.05	1.15
2:L:505:ARG:HH21	2:L:511:VAL:HB	1.08	1.10
2:L:512:GLN:O	2:L:513:ILE:HG13	1.51	1.10

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	
2	A	268/274 (98%)	212 (79%)	48 (18%)	8 (3%)	5	28
2	B	268/274 (98%)	221 (82%)	40 (15%)	7 (3%)	6	31
2	C	268/274 (98%)	232 (87%)	32 (12%)	4 (2%)	11	46
2	D	268/274 (98%)	224 (84%)	31 (12%)	13 (5%)	2	17
2	E	272/274 (99%)	229 (84%)	34 (12%)	9 (3%)	4	25
2	F	268/274 (98%)	215 (80%)	40 (15%)	13 (5%)	2	17
2	G	268/274 (98%)	225 (84%)	37 (14%)	6 (2%)	7	36
2	H	272/274 (99%)	227 (84%)	38 (14%)	7 (3%)	6	31
2	I	268/274 (98%)	220 (82%)	39 (15%)	9 (3%)	4	24
2	J	268/274 (98%)	218 (81%)	42 (16%)	8 (3%)	5	28
2	K	271/274 (99%)	219 (81%)	42 (16%)	10 (4%)	4	22
2	L	268/274 (98%)	180 (67%)	60 (22%)	28 (10%)	0	3
All	All	3227/3288 (98%)	2622 (81%)	483 (15%)	122 (4%)	3	22

5 of 122 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	376	LEU
2	A	549	THR
2	A	556	PRO
2	B	376	LEU
2	C	376	LEU

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	
2	A	218/230 (95%)	210 (96%)	8 (4%)	37	71
2	B	218/230 (95%)	207 (95%)	11 (5%)	27	63
2	C	218/230 (95%)	207 (95%)	11 (5%)	27	63
2	D	218/230 (95%)	207 (95%)	11 (5%)	27	63
2	E	224/230 (97%)	208 (93%)	16 (7%)	16	49
2	F	218/230 (95%)	202 (93%)	16 (7%)	15	48
2	G	218/230 (95%)	205 (94%)	13 (6%)	21	56
2	H	224/230 (97%)	209 (93%)	15 (7%)	18	52
2	I	218/230 (95%)	208 (95%)	10 (5%)	29	66
2	J	218/230 (95%)	204 (94%)	14 (6%)	19	54
2	K	224/230 (97%)	208 (93%)	16 (7%)	16	49
2	L	218/230 (95%)	201 (92%)	17 (8%)	14	45
All	All	2634/2760 (95%)	2476 (94%)	158 (6%)	21	56

5 of 158 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	543	ARG
2	H	318	GLN
2	L	473	ARG
2	G	318	GLN
2	G	476	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	523	ASN
2	H	427	ASN
2	L	427	ASN
2	G	318	GLN
2	G	444	ASN

5.3.3 RNA ⓘ

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 24 ligands modelled in this entry, 13 are monoatomic - leaving 11 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	ADP	A	1	3	25,29,29	1.46	3 (12%)	25,45,45	2.51	5 (20%)
5	ADP	B	2	3	25,29,29	1.27	2 (8%)	25,45,45	2.53	5 (20%)
5	ADP	C	3	3	25,29,29	1.29	2 (8%)	25,45,45	2.56	5 (20%)
5	ADP	D	4	3	25,29,29	1.23	2 (8%)	25,45,45	2.52	4 (16%)
5	ADP	E	5	3	25,29,29	1.23	2 (8%)	25,45,45	2.44	4 (16%)
5	ADP	F	6	-	25,29,29	1.19	3 (12%)	25,45,45	2.57	4 (16%)
5	ADP	G	7	3	25,29,29	1.52	3 (12%)	25,45,45	2.57	4 (16%)
5	ADP	H	8	3	25,29,29	1.20	2 (8%)	25,45,45	2.63	4 (16%)
5	ADP	J	9	3	25,29,29	1.26	2 (8%)	25,45,45	2.47	5 (20%)
5	ADP	K	10	3	25,29,29	1.28	3 (12%)	25,45,45	2.38	5 (20%)
5	ADP	L	11	3	25,29,29	1.89	5 (20%)	25,45,45	3.58	10 (40%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ADP	A	1	3	-	0/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ADP	B	2	3	-	0/12/32/32	0/3/3/3
5	ADP	C	3	3	-	0/12/32/32	0/3/3/3
5	ADP	D	4	3	-	0/12/32/32	0/3/3/3
5	ADP	E	5	3	-	0/12/32/32	0/3/3/3
5	ADP	F	6	-	-	0/12/32/32	0/3/3/3
5	ADP	G	7	3	-	0/12/32/32	0/3/3/3
5	ADP	H	8	3	-	0/12/32/32	0/3/3/3
5	ADP	J	9	3	-	0/12/32/32	0/3/3/3
5	ADP	K	10	3	-	0/12/32/32	0/3/3/3
5	ADP	L	11	3	-	0/12/32/32	0/3/3/3

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	11	ADP	C5'-C4'	-2.66	1.43	1.51
5	J	9	ADP	C8-N7	-2.38	1.30	1.34
5	A	1	ADP	C8-N7	-2.36	1.30	1.34
5	D	4	ADP	C8-N7	-2.34	1.30	1.34
5	H	8	ADP	C8-N7	-2.34	1.30	1.34

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	11	ADP	C4'-O4'-C1'	-10.80	98.57	109.83
5	G	7	ADP	N3-C2-N1	-9.28	120.92	128.86
5	E	5	ADP	N3-C2-N1	-9.07	121.10	128.86
5	B	2	ADP	N3-C2-N1	-9.00	121.16	128.86
5	J	9	ADP	N3-C2-N1	-8.94	121.21	128.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1	ADP	4	0
5	B	2	ADP	5	0
5	C	3	ADP	4	0
5	D	4	ADP	2	0
5	E	5	ADP	2	0
5	F	6	ADP	11	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	7	ADP	3	0
5	H	8	ADP	5	0
5	J	9	ADP	1	0
5	K	10	ADP	1	0
5	L	11	ADP	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	M	6/13 (46%)	-0.64	0 100 100	60, 67, 70, 143	0
1	N	7/13 (53%)	-0.83	0 100 100	53, 64, 110, 140	0
2	A	270/274 (98%)	-0.52	2 (0%) 87 81	25, 55, 147, 188	0
2	B	270/274 (98%)	-0.55	1 (0%) 92 89	25, 49, 123, 195	0
2	C	270/274 (98%)	-0.23	7 (2%) 56 40	27, 67, 154, 200	0
2	D	270/274 (98%)	-0.43	3 (1%) 80 69	32, 69, 151, 194	0
2	E	274/274 (100%)	-0.49	0 100 100	25, 64, 131, 205	0
2	F	270/274 (98%)	-0.49	1 (0%) 92 89	26, 60, 131, 202	0
2	G	270/274 (98%)	-0.44	2 (0%) 87 81	25, 63, 129, 192	0
2	H	274/274 (100%)	-0.44	1 (0%) 92 89	26, 60, 135, 205	0
2	I	270/274 (98%)	-0.31	5 (1%) 66 51	25, 69, 153, 192	0
2	J	270/274 (98%)	-0.42	6 (2%) 62 46	27, 63, 136, 205	0
2	K	273/274 (99%)	-0.50	3 (1%) 80 69	25, 59, 150, 198	0
2	L	270/274 (98%)	0.10	14 (5%) 27 14	38, 119, 186, 205	0
All	All	3264/3314 (98%)	-0.39	45 (1%) 75 62	25, 64, 154, 205	0

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	550	ASP	5.3
2	J	308	THR	4.9
2	I	550	ASP	4.6
2	L	386	CYS	4.3
2	L	444	ASN	4.2

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. 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	B-factors(Å ²)	Q<0.9
3	MG	I	29	1/1	0.73	0.15	55,55,55,55	0
4	CL	H	48	1/1	0.82	0.07	80,80,80,80	0
3	MG	E	25	1/1	0.83	0.18	30,30,30,30	0
5	ADP	D	4	27/27	0.86	0.23	81,119,162,162	10
3	MG	G	27	1/1	0.88	0.17	33,33,33,33	0
4	CL	B	42	1/1	0.89	0.13	73,73,73,73	0
5	ADP	L	11	27/27	0.89	0.24	84,142,198,198	0
5	ADP	C	3	27/27	0.90	0.19	70,80,100,100	0
5	ADP	H	8	27/27	0.91	0.22	70,94,123,123	0
5	ADP	G	7	27/27	0.92	0.18	58,70,90,90	0
5	ADP	B	2	27/27	0.92	0.23	55,69,88,88	0
5	ADP	A	1	27/27	0.92	0.18	31,65,66,66	0
5	ADP	E	5	27/27	0.92	0.19	77,105,195,195	10
5	ADP	F	6	27/27	0.92	0.19	65,130,198,198	10
4	CL	A	41	1/1	0.93	0.22	70,70,70,70	0
5	ADP	J	9	27/27	0.94	0.17	89,126,182,182	10
3	MG	K	31	1/1	0.95	0.10	51,51,51,51	0
5	ADP	K	10	27/27	0.95	0.22	67,74,133,133	10
3	MG	B	22	1/1	0.96	0.17	25,25,25,25	0
3	MG	C	23	1/1	0.97	0.08	25,25,25,25	0
3	MG	H	28	1/1	0.97	0.16	25,25,25,25	0
3	MG	J	30	1/1	0.98	0.33	36,36,36,36	0
3	MG	D	24	1/1	0.98	0.14	50,50,50,50	0
3	MG	A	21	1/1	0.98	0.17	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.