W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Dec 7, 2023 – 01:10 pm GMT

PDB ID	:	2V9P
Title	:	Crystal structure of papillomavirus E1 hexameric helicase DNA-free form
Authors	:	Sanders, C.M.; Kovalevskiy, O.V.; Sizov, D.; Lebedev, A.A.; Isupov, M.N.; Antson, A.A.
Deposited on	:	2007-08-24
Resolution	:	3.00 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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)	:	2.36

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 3.00 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.
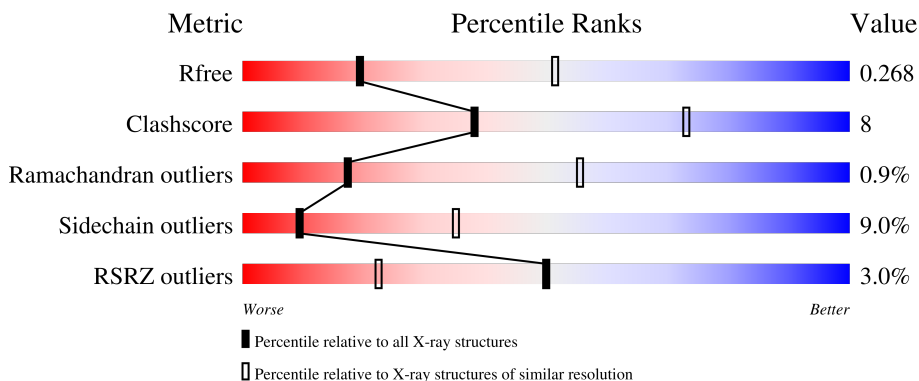
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 >=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 <=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	305	
1	B	305	
1	C	305	
1	D	305	
1	E	305	

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Mol	Chain	Length	Quality of chain
1	F	305	3% 63% 23% •• 12%
1	G	305	4% 64% 23% • 11%
1	H	305	2% 68% 17% • 12%
1	I	305	3% 70% 15% • 11%
1	J	305	2% 65% 21% • 11%
1	K	305	3% 71% 15% • 12%
1	L	305	4% 62% 22% • 12%

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
2	PO4	A	1580	-	-	X	-
2	PO4	C	1579	-	X	-	-
2	PO4	G	1580	-	-	X	X
2	PO4	H	1579	-	-	X	-
2	PO4	I	1580	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 26079 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 REPLICATION PROTEIN E1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	0	0
			2183	1404	375	394	10			
1	B	268	Total	C	N	O	S	0	0	0
			2149	1386	370	383	10			
1	C	267	Total	C	N	O	S	0	0	0
			2142	1382	369	381	10			
1	D	274	Total	C	N	O	S	0	0	0
			2191	1409	377	395	10			
1	E	270	Total	C	N	O	S	0	0	0
			2170	1398	373	389	10			
1	F	269	Total	C	N	O	S	0	0	0
			2158	1392	372	384	10			
1	G	270	Total	C	N	O	S	0	0	0
			2163	1392	373	388	10			
1	H	268	Total	C	N	O	S	0	0	0
			2149	1386	370	383	10			
1	I	270	Total	C	N	O	S	0	0	0
			2165	1394	372	389	10			
1	J	272	Total	C	N	O	S	0	0	0
			2178	1400	375	393	10			
1	K	269	Total	C	N	O	S	0	0	0
			2158	1392	372	384	10			
1	L	267	Total	C	N	O	S	0	0	0
			2142	1382	369	381	10			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

PO4

O3

O⁻

O2 O⁻ — P ═══ O O1

P

O⁻

O4

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	G	1	Total	O	P	0	0
			5	4	1		
2	G	1	Total	O	P	0	0
			5	4	1		
2	H	1	Total	O	P	0	0
			5	4	1		
2	H	1	Total	O	P	0	0
			5	4	1		
2	I	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	I	1	Total 5	O 4	P 1	0	0
2	J	1	Total 5	O 4	P 1	0	0
2	K	1	Total 5	O 4	P 1	0	0
2	L	1	Total 5	O 4	P 1	0	0

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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total 3	O 3	0	0
4	B	3	Total 3	O 3	0	0
4	C	3	Total 3	O 3	0	0
4	D	4	Total 4	O 4	0	0
4	E	2	Total 2	O 2	0	0
4	F	3	Total 3	O 3	0	0
4	G	4	Total 4	O 4	0	0

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| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	4	Total 4	O 4	0	0
4	I	4	Total 4	O 4	0	0
4	J	4	Total 4	O 4	0	0
4	L	1	Total 1	O 1	0	0

3 Residue-property plots ⓘ

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.
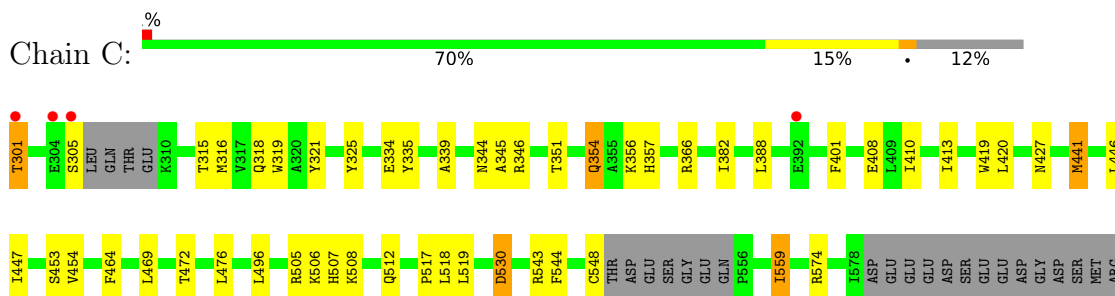
• Molecule 1: REPLICATION PROTEIN E1
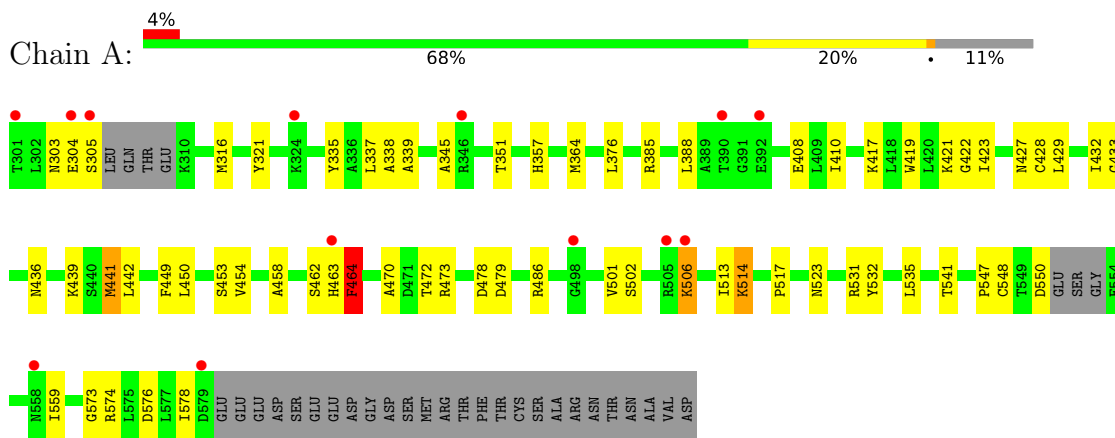
• Molecule 1: REPLICATION PROTEIN E1
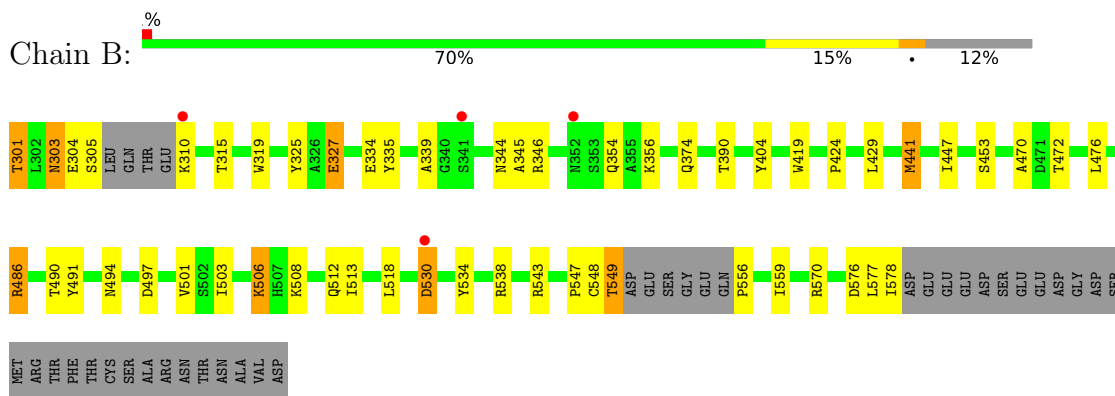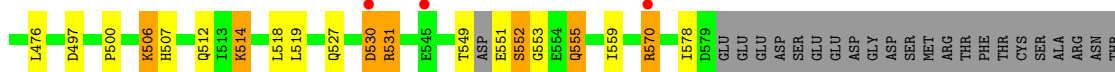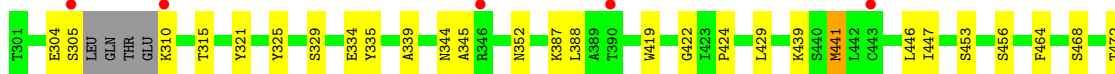

• Molecule 1: REPLICATION PROTEIN E1

THR PHE THR CYS SER ALA ARG ASN THR ASN ALA VAL ASP
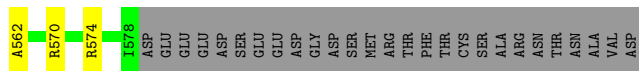
● Molecule 1: REPLICATION PROTEIN E1

Chain D:

● Molecule 1: REPLICATION PROTEIN E1

Chain E:
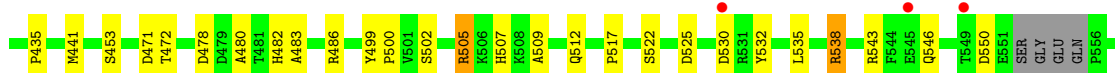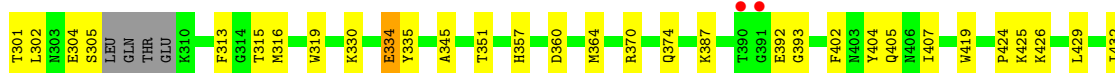
● Molecule 1: REPLICATION PROTEIN E1
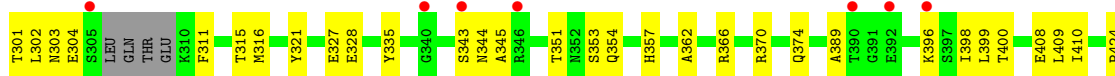
Chain F:

● Molecule 1: REPLICATION PROTEIN E1

Chain G:

• Molecule 1: REPLICATION PROTEIN E1

• Molecule 1: REPLICATION PROTEIN E1

• Molecule 1: REPLICATION PROTEIN E1

• Molecule 1: REPLICATION PROTEIN E1

Chain K:

• Molecule 1: REPLICATION PROTEIN E1

Chain L:
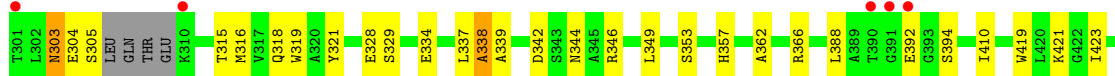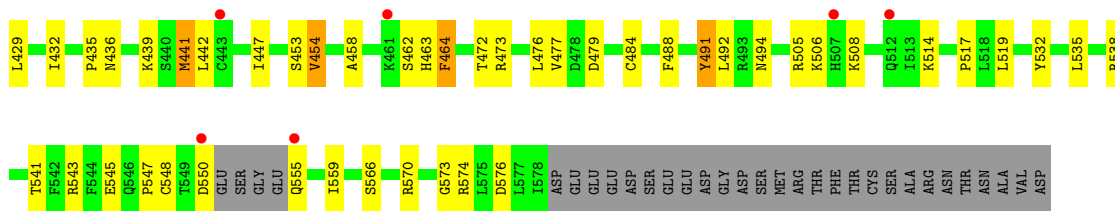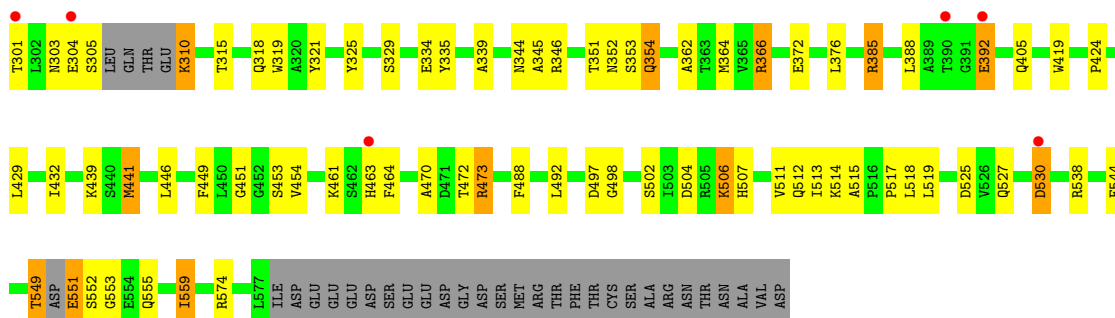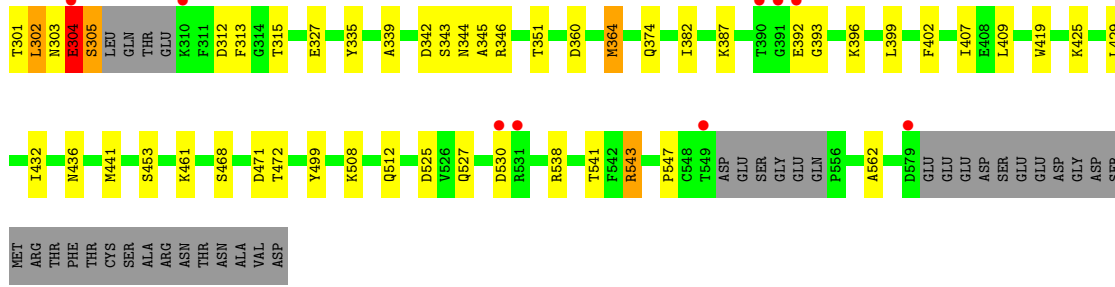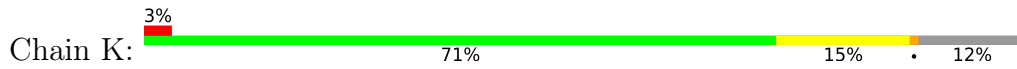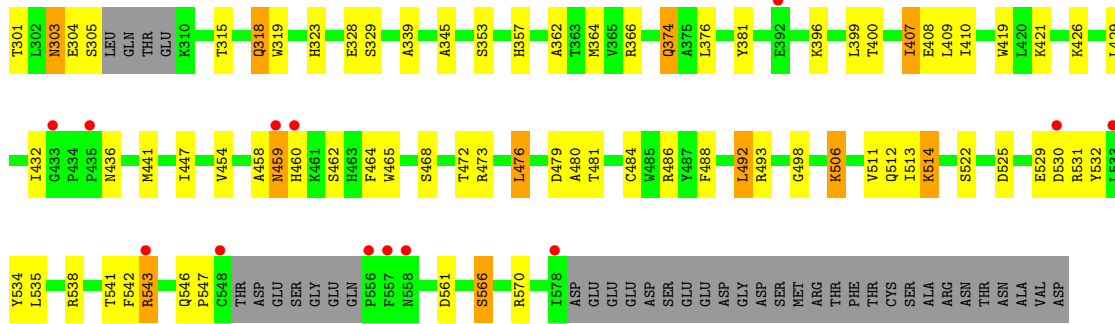
4 Data and refinement statistics ⓘ

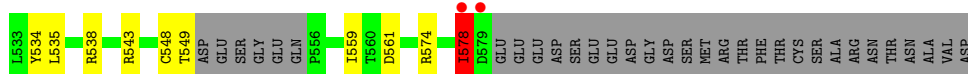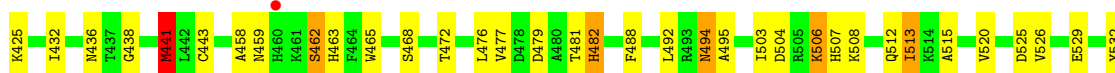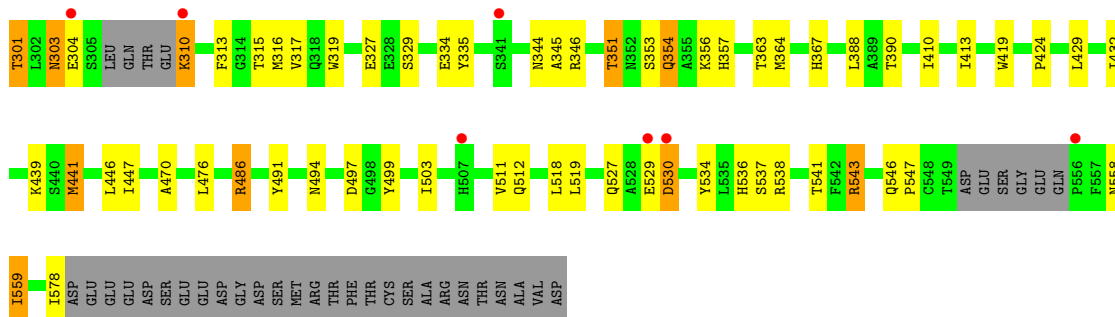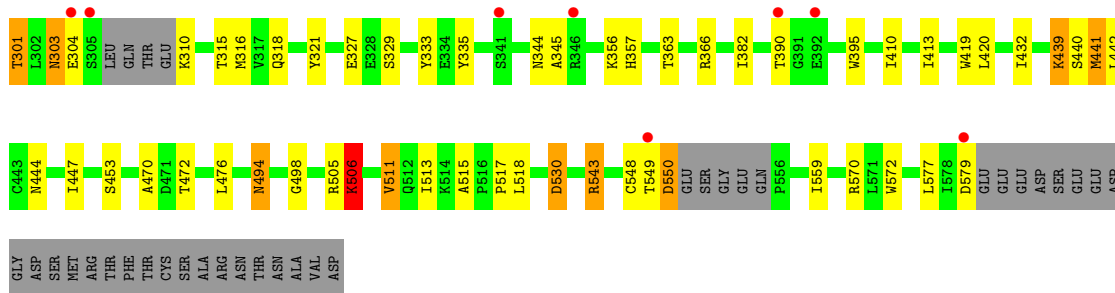| Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	135.11Å　180.65Å　187.53Å 90.00°　　90.00°　　90.00°	Depositor
Resolution (Å)	24.95　–　3.00 24.95　–　3.00	Depositor EDS
% Data completeness (in resolution range)	93.4 (24.95-3.00) 93.4 (24.95-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.47 (at 2.99Å)	Xtriage
Refinement program	REFMAC 5.3.0037	Depositor
R, R_{free}	0.219　,　0.271 0.216　,　0.268	Depositor DCC
R_{free} test set	853 reflections (0.99%)	wwPDB-VP
Wilson B-factor (Å^2)	66.9	Xtriage
Anisotropy	0.616	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 68.6	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	26079	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.95 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.4003e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: MG, PO4

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	0.48	0/2240	0.59	0/3037
1	B	0.50	1/2206 (0.0%)	0.61	2/2990 (0.1%)
1	C	0.48	0/2199	0.61	0/2980
1	D	0.46	0/2248	0.64	4/3047 (0.1%)
1	E	0.48	0/2227	0.59	0/3017
1	F	0.49	0/2215	0.61	0/3001
1	G	0.49	0/2220	0.59	0/3010
1	H	0.50	1/2206 (0.0%)	0.64	1/2990 (0.0%)
1	I	0.52	0/2222	0.62	0/3012
1	J	0.53	1/2235 (0.0%)	0.65	1/3029 (0.0%)
1	K	0.48	0/2215	0.60	0/3001
1	L	0.47	0/2199	0.62	0/2980
All	All	0.49	3/26632 (0.0%)	0.61	8/36094 (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
1	G	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	310	LYS	CE-NZ	6.77	1.66	1.49
1	B	327	GLU	CD-OE1	5.93	1.32	1.25
1	H	310	LYS	CE-NZ	5.70	1.63	1.49

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	486	ARG	NE-CZ-NH1	-7.24	116.68	120.30
1	D	531	ARG	NE-CZ-NH1	-6.25	117.18	120.30
1	B	486	ARG	NE-CZ-NH2	6.04	123.32	120.30
1	D	531	ARG	NE-CZ-NH2	6.02	123.31	120.30
1	D	570	ARG	NE-CZ-NH2	5.83	123.21	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	574	ARG	Peptide

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	2183	0	2132	40	0
1	B	2149	0	2110	31	0
1	C	2142	0	2103	28	0
1	D	2191	0	2140	31	0
1	E	2170	0	2132	41	0
1	F	2158	0	2124	36	0
1	G	2163	0	2112	44	0
1	H	2149	0	2110	40	0
1	I	2165	0	2119	36	0
1	J	2178	0	2127	45	0
1	K	2158	0	2124	32	0
1	L	2142	0	2104	37	0
2	A	10	0	0	2	0
2	B	10	0	0	1	0
2	C	10	0	0	0	0
2	D	5	0	0	1	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	G	10	0	0	2	0
2	H	10	0	0	2	0
2	I	10	0	0	2	0
2	J	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	5	0	0	0	0
2	L	5	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	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
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	C	3	0	0	0	0
4	D	4	0	0	0	0
4	E	2	0	0	0	0
4	F	3	0	0	0	0
4	G	4	0	0	0	0
4	H	4	0	0	0	0
4	I	4	0	0	0	0
4	J	4	0	0	0	0
4	L	1	0	0	0	0
All	All	26079	0	25437	391	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 8.

The worst 5 of 391 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:D:304:GLU:HG2	1:D:305:SER:H	1.18	1.08
1:J:470:ALA:HA	1:J:513:ILE:HD11	1.47	0.95
1:G:441:MET:HE1	1:G:559:ILE:H	1.32	0.95
1:A:441:MET:HE1	1:A:559:ILE:H	1.31	0.94
1:E:453:SER:HB2	1:F:512:GLN:HE22	1.32	0.90

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	266/305 (87%)	245 (92%)	19 (7%)	2 (1%)	19	57
1	B	262/305 (86%)	251 (96%)	10 (4%)	1 (0%)	34	72
1	C	261/305 (86%)	252 (97%)	9 (3%)	0	100	100
1	D	268/305 (88%)	256 (96%)	8 (3%)	4 (2%)	10	42
1	E	264/305 (87%)	246 (93%)	18 (7%)	0	100	100
1	F	263/305 (86%)	239 (91%)	17 (6%)	7 (3%)	5	26
1	G	264/305 (87%)	241 (91%)	17 (6%)	6 (2%)	6	30
1	H	262/305 (86%)	249 (95%)	12 (5%)	1 (0%)	34	72
1	I	264/305 (87%)	250 (95%)	12 (4%)	2 (1%)	19	57
1	J	266/305 (87%)	252 (95%)	12 (4%)	2 (1%)	19	57
1	K	263/305 (86%)	251 (95%)	10 (4%)	2 (1%)	19	57
1	L	261/305 (86%)	236 (90%)	22 (8%)	3 (1%)	14	50
All	All	3164/3660 (86%)	2968 (94%)	166 (5%)	30 (1%)	17	55

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	506	LYS
1	D	506	LYS
1	D	553	GLY
1	G	338	ALA
1	G	506	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	229/259 (88%)	210 (92%)	19 (8%)	11	39
1	B	225/259 (87%)	207 (92%)	18 (8%)	12	40
1	C	224/259 (86%)	207 (92%)	17 (8%)	13	43
1	D	229/259 (88%)	215 (94%)	14 (6%)	18	53
1	E	228/259 (88%)	212 (93%)	16 (7%)	15	47
1	F	226/259 (87%)	200 (88%)	26 (12%)	5	24
1	G	226/259 (87%)	203 (90%)	23 (10%)	7	28
1	H	225/259 (87%)	204 (91%)	21 (9%)	9	33
1	I	227/259 (88%)	210 (92%)	17 (8%)	13	43
1	J	228/259 (88%)	202 (89%)	26 (11%)	5	24
1	K	226/259 (87%)	209 (92%)	17 (8%)	13	43
1	L	224/259 (86%)	193 (86%)	31 (14%)	3	17
All	All	2717/3108 (87%)	2472 (91%)	245 (9%)	9	35

5 of 245 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	410	ILE
1	L	407	ILE
1	H	390	THR
1	L	396	LYS
1	L	511	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	527	GLN
1	K	344	ASN
1	H	546	GLN
1	J	444	ASN
1	K	414	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 6 are monoatomic - leaving 18 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
2	PO4	H	1579	3	4,4,4	1.06	0	6,6,6	1.04	0
2	PO4	G	1579	3	4,4,4	1.10	0	6,6,6	1.04	0
2	PO4	B	1580	3	4,4,4	1.13	0	6,6,6	0.89	0
2	PO4	I	1580	3	4,4,4	1.12	0	6,6,6	0.93	0
2	PO4	A	1580	3	4,4,4	0.98	0	6,6,6	0.92	0
2	PO4	C	1579	3	4,4,4	1.81	1 (25%)	6,6,6	2.44	4 (66%)
2	PO4	K	1580	-	4,4,4	0.83	0	6,6,6	0.55	0
2	PO4	H	1580	3	4,4,4	1.04	0	6,6,6	0.76	0
2	PO4	A	1581	3	4,4,4	1.27	0	6,6,6	0.72	0
2	PO4	I	1581	3	4,4,4	1.15	0	6,6,6	0.86	0
2	PO4	G	1580	3	4,4,4	1.28	0	6,6,6	0.53	0
2	PO4	J	1578	-	4,4,4	0.97	0	6,6,6	0.48	0
2	PO4	C	1580	3	4,4,4	1.70	1 (25%)	6,6,6	2.54	2 (33%)
2	PO4	B	1579	3	4,4,4	1.04	0	6,6,6	1.01	0
2	PO4	F	1580	-	4,4,4	0.95	0	6,6,6	0.43	0
2	PO4	E	1579	-	4,4,4	0.81	0	6,6,6	0.46	0
2	PO4	D	1580	-	4,4,4	0.91	0	6,6,6	0.62	0
2	PO4	L	1579	-	4,4,4	0.76	0	6,6,6	0.53	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1579	PO4	P-O3	-2.85	1.46	1.54
2	C	1580	PO4	P-O2	-2.83	1.46	1.54

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1580	PO4	O2-P-O1	-5.54	90.63	110.89
2	C	1579	PO4	O3-P-O1	-3.75	97.19	110.89
2	C	1579	PO4	O4-P-O3	-2.73	99.21	107.97
2	C	1579	PO4	O3-P-O2	2.62	116.37	107.97
2	C	1579	PO4	O4-P-O1	2.53	120.17	110.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1579	PO4	2	0
2	G	1579	PO4	1	0
2	B	1580	PO4	1	0
2	I	1580	PO4	2	0
2	A	1580	PO4	2	0
2	H	1580	PO4	1	0
2	A	1581	PO4	1	0
2	I	1581	PO4	1	0
2	G	1580	PO4	2	0
2	J	1578	PO4	1	0
2	B	1579	PO4	1	0
2	D	1580	PO4	1	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	A	272/305 (89%)	0.01	13 (4%)	30	11	65, 76, 100, 124	0
1	B	268/305 (87%)	-0.10	4 (1%)	73	46	67, 76, 86, 95	0
1	C	267/305 (87%)	-0.24	4 (1%)	73	46	70, 76, 87, 98	0
1	D	274/305 (89%)	0.01	8 (2%)	51	23	70, 76, 87, 97	0
1	E	270/305 (88%)	-0.07	5 (1%)	66	37	63, 76, 91, 104	0
1	F	269/305 (88%)	0.03	10 (3%)	41	17	60, 77, 92, 104	1 (0%)
1	G	270/305 (88%)	0.03	11 (4%)	37	14	64, 76, 99, 121	0
1	H	268/305 (87%)	-0.05	7 (2%)	56	27	68, 76, 87, 94	0
1	I	270/305 (88%)	-0.18	8 (2%)	50	22	67, 76, 88, 102	0
1	J	272/305 (89%)	-0.07	6 (2%)	62	33	69, 76, 85, 102	0
1	K	269/305 (88%)	-0.12	9 (3%)	46	20	62, 76, 90, 98	0
1	L	267/305 (87%)	0.13	13 (4%)	29	11	63, 77, 90, 102	1 (0%)
All	All	3236/3660 (88%)	-0.05	98 (3%)	50	22	60, 76, 90, 124	2 (0%)

The worst 5 of 98 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	433	GLY	5.2
1	J	392	GLU	4.6
1	F	340	GLY	4.5
1	A	304	GLU	4.3
1	G	390	THR	4.3

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

WORLDWIDE
wwPDB
PROTEIN DATA BANK

6.3 Carbohydrates (i)

There are no monosaccharides 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
2	PO4	G	1580	5/5	0.74	0.43	77,79,80,81	5
3	MG	C	1581	1/1	0.83	0.13	68,68,68,68	0
3	MG	I	1582	1/1	0.86	0.17	64,64,64,64	0
3	MG	H	1581	1/1	0.89	0.16	64,64,64,64	0
2	PO4	A	1581	5/5	0.90	0.20	78,79,79,79	5
2	PO4	G	1579	5/5	0.90	0.19	77,79,80,82	0
2	PO4	C	1580	5/5	0.91	0.15	82,84,85,86	0
2	PO4	I	1581	5/5	0.92	0.13	78,79,80,82	0
3	MG	G	1581	1/1	0.93	0.17	67,67,67,67	0
3	MG	A	1582	1/1	0.93	0.14	74,74,74,74	0
2	PO4	L	1579	5/5	0.93	0.17	94,95,96,97	0
2	PO4	D	1580	5/5	0.94	0.13	86,87,88,88	0
2	PO4	B	1580	5/5	0.94	0.12	80,82,83,83	0
2	PO4	B	1579	5/5	0.94	0.15	77,78,79,79	0
3	MG	B	1581	1/1	0.94	0.15	54,54,54,54	0
2	PO4	I	1580	5/5	0.96	0.14	76,77,78,78	0
2	PO4	A	1580	5/5	0.96	0.09	76,76,79,79	0
2	PO4	K	1580	5/5	0.96	0.11	87,88,89,89	0
2	PO4	H	1579	5/5	0.96	0.11	79,81,81,81	0
2	PO4	H	1580	5/5	0.96	0.11	79,80,80,82	0
2	PO4	C	1579	5/5	0.97	0.13	82,83,84,84	0
2	PO4	J	1578	5/5	0.97	0.10	82,82,83,83	0
2	PO4	F	1580	5/5	0.98	0.11	83,84,84,84	0
2	PO4	E	1579	5/5	0.98	0.12	86,86,88,88	0

6.5 Other polymers (i)

There are no such residues in this entry.