



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 04:19 pm BST

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)

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

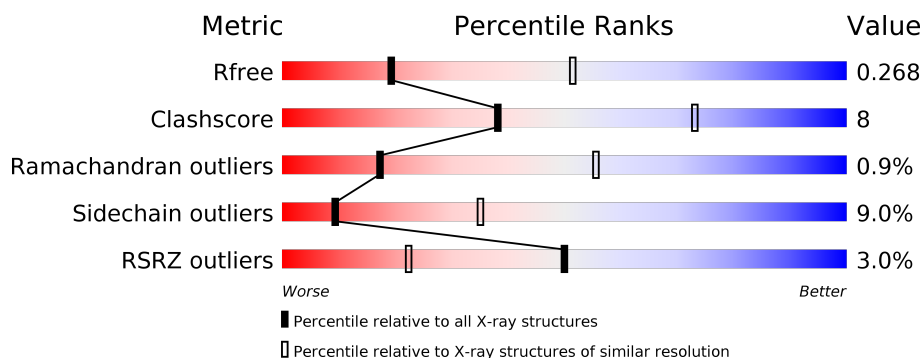
# 1 Overall quality at a glance

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 on 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	305	<div> <div>4%</div> <div> <div></div> <div>68%</div> <div>20%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	305	<div> <div>%</div> <div> <div></div> <div>70%</div> <div>15%</div> <div>•</div> <div>12%</div> </div> </div>
1	C	305	<div> <div>%</div> <div> <div></div> <div>70%</div> <div>15%</div> <div>•</div> <div>12%</div> </div> </div>
1	D	305	<div> <div>3%</div> <div> <div></div> <div>74%</div> <div>13%</div> <div>•</div> <div>10%</div> </div> </div>
1	E	305	<div> <div>2%</div> <div> <div></div> <div>69%</div> <div>19%</div> <div>•</div> <div>11%</div> </div> </div>
1	F	305	<div> <div>3%</div> <div> <div></div> <div>63%</div> <div>23%</div> <div>••</div> <div>12%</div> </div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	G	305	
1	H	305	
1	I	305	
1	J	305	
1	K	305	
1	L	305	

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

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<sub>4</sub>P).



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		

*Continued on next page...*

*Continued from previous page...*

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

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

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

- Molecule 4 is water.

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

*Continued on next page...*

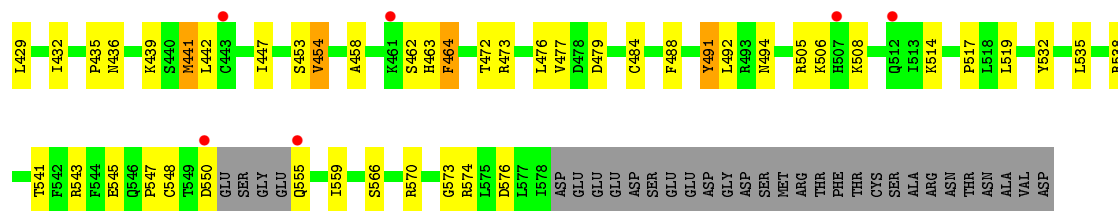
*Continued from previous page...*

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

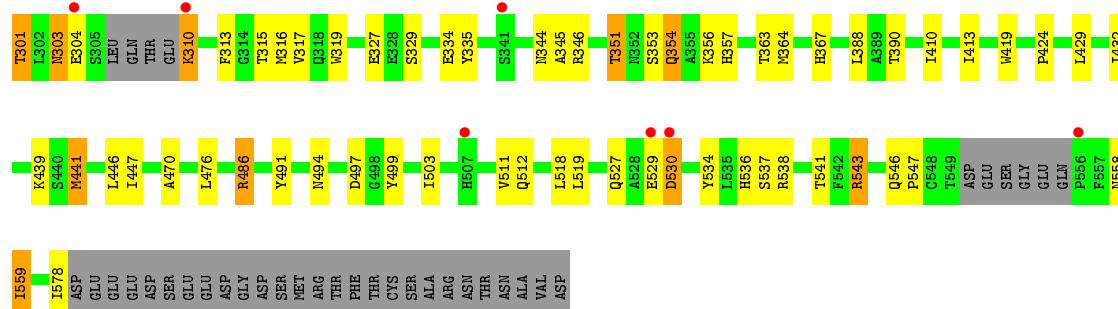




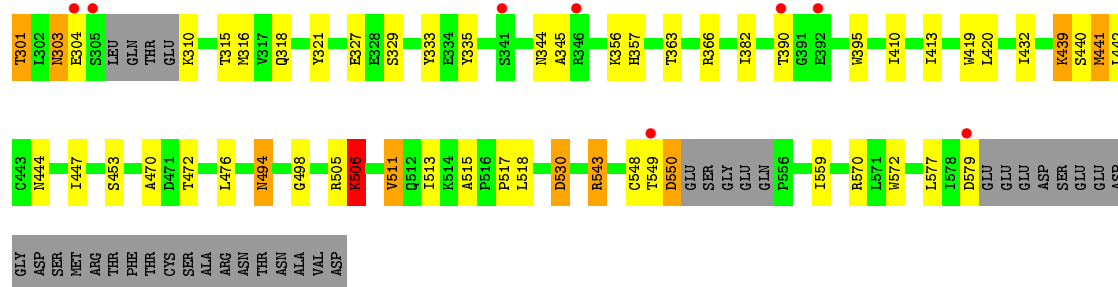
T301 T302 T303 T304 T305 T306 T307 T308 T309 T310 T311 T312 T313 T314 T315 T316 T317 T318 T319 T320 T321 T322 T323 T324 T325 T326 T327 T328 T329 T330 T331 T332 T333 T334 T335 T336 T337 T338 T339 T340 T341 T342 T343 T344 T345 T346 T347 T348 T349 T350 T351 T352 T353 T354 T355 T356 T357 T358 T359 T360 T361 T362 T363 T364 T365 T366 T367 T368 T369 T370 T371 T372 T373 T374 T375 T376 T377 T378 T379 T380 T381 T382 T383 T384 T385 T386 T387 T388 T389 T390 T391 T392 T393 T394 T395 T396 T397 T398 T399 T400 T401 T402 T403 T404 T405 T406 T407 T408 T409 T410 T411 T412 T413 T414 T415 T416 T417 T418 T419 T420 T421 T422 T423 T424 T425 T426 T427 T428 T429 T430 T431 T432 T433 T434 T435 T436 T437 T438 T439 T440 T441 T442 T443 T444 T445 T446 T447 T448 T449 T450 T451 T452 T453 T454 T455 T456 T457 T458 T459 T460 T461 T462 T463 T464 T465 T466 T467 T468 T469 T470 T471 T472 T473 T474 T475 T476 T477 T478 T479 T480 T481 T482 T483 T484 T485 T486 T487 T488 T489 T490 T491 T492 T493 T494 T495 T496 T497 T498 T499 T500



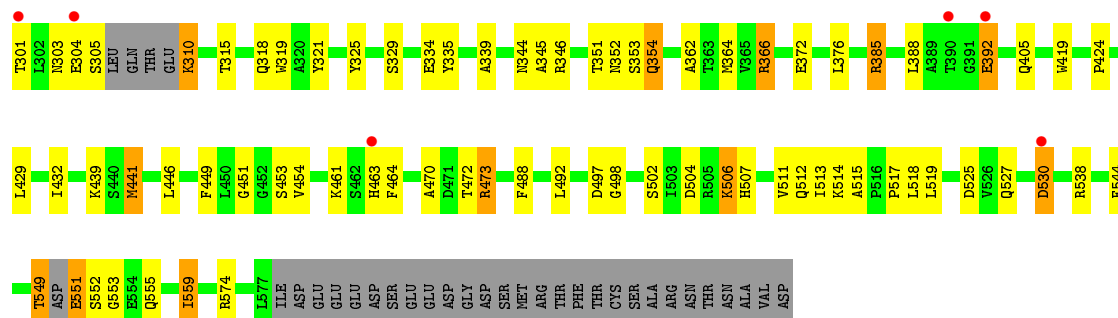
• Molecule 1: REPLICATION PROTEIN E1



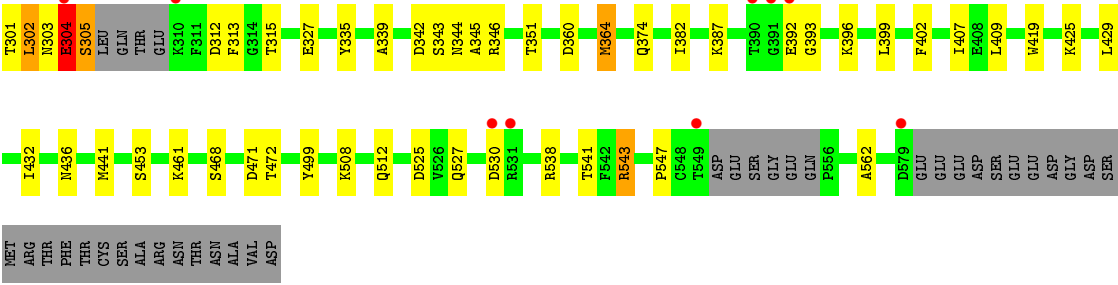
• Molecule 1: REPLICATION PROTEIN E1



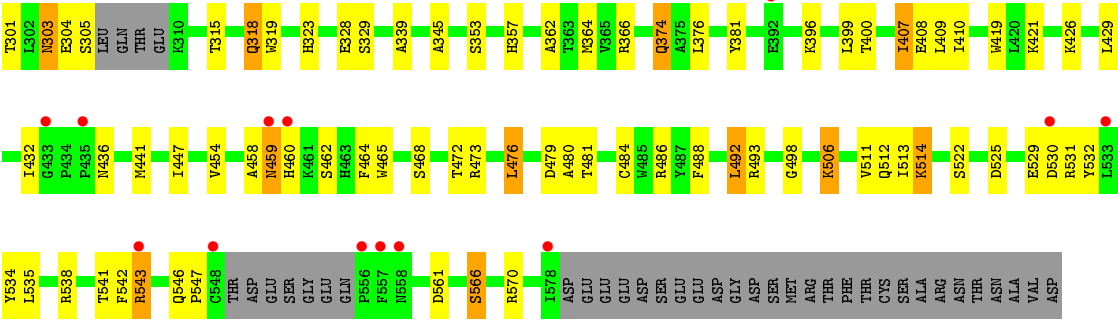
• Molecule 1: REPLICATION PROTEIN E1



• Molecule 1: REPLICATION PROTEIN E1



● Molecule 1: REPLICATION PROTEIN E1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	66.9	Xtriage
Anisotropy	0.616	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 68.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	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 <sup>2</sup> )	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.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, MG

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(°)	Ideal(°)
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

*Continued on next page...*

*Continued from previous page...*

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 [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	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 [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	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	303	ASN
1	H	329	SER
1	L	436	ASN
1	G	394	SER
1	G	514	LYS

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

Mol	Chain	Res	Type
1	G	367	HIS
1	H	344	ASN
1	L	357	HIS
1	G	436	ASN
1	H	357	HIS

### 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 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	A	1580	3	4,4,4	0.98	0	6,6,6	0.92	0
2	PO4	L	1579	-	4,4,4	0.76	0	6,6,6	0.53	0
2	PO4	G	1580	3	4,4,4	1.28	0	6,6,6	0.53	0
2	PO4	H	1580	3	4,4,4	1.04	0	6,6,6	0.76	0
2	PO4	J	1578	-	4,4,4	0.97	0	6,6,6	0.48	0
2	PO4	F	1580	-	4,4,4	0.95	0	6,6,6	0.43	0
2	PO4	I	1580	3	4,4,4	1.12	0	6,6,6	0.93	0
2	PO4	G	1579	3	4,4,4	1.10	0	6,6,6	1.04	0
2	PO4	B	1579	3	4,4,4	1.04	0	6,6,6	1.01	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	K	1580	-	4,4,4	0.83	0	6,6,6	0.55	0
2	PO4	I	1581	3	4,4,4	1.15	0	6,6,6	0.86	0
2	PO4	A	1581	3	4,4,4	1.27	0	6,6,6	0.72	0
2	PO4	B	1580	3	4,4,4	1.13	0	6,6,6	0.89	0
2	PO4	C	1580	3	4,4,4	1.70	1 (25%)	6,6,6	2.54	2 (33%)
2	PO4	H	1579	3	4,4,4	1.06	0	6,6,6	1.04	0
2	PO4	C	1579	3	4,4,4	1.81	1 (25%)	6,6,6	2.44	4 (66%)

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(°)	Ideal(°)
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	A	1580	PO4	2	0
2	G	1580	PO4	2	0
2	H	1580	PO4	1	0
2	J	1578	PO4	1	0
2	I	1580	PO4	2	0
2	G	1579	PO4	1	0
2	B	1579	PO4	1	0
2	D	1580	PO4	1	0
2	I	1581	PO4	1	0
2	A	1581	PO4	1	0
2	B	1580	PO4	1	0
2	H	1579	PO4	2	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, 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	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.

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	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	G	1579	5/5	0.90	0.19	77,79,80,82	0
2	PO4	A	1581	5/5	0.90	0.20	78,79,79,79	5
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
2	PO4	L	1579	5/5	0.93	0.17	94,95,96,97	0
3	MG	A	1582	1/1	0.93	0.14	74,74,74,74	0
3	MG	G	1581	1/1	0.93	0.17	67,67,67,67	0
2	PO4	B	1579	5/5	0.94	0.15	77,78,79,79	0
2	PO4	B	1580	5/5	0.94	0.12	80,82,83,83	0
2	PO4	D	1580	5/5	0.94	0.13	86,87,88,88	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	K	1580	5/5	0.96	0.11	87,88,89,89	0
2	PO4	A	1580	5/5	0.96	0.09	76,76,79,79	0
2	PO4	H	1580	5/5	0.96	0.11	79,80,80,82	0
2	PO4	H	1579	5/5	0.96	0.11	79,81,81,81	0
2	PO4	J	1578	5/5	0.97	0.10	82,82,83,83	0
2	PO4	C	1579	5/5	0.97	0.13	82,83,84,84	0
2	PO4	E	1579	5/5	0.98	0.12	86,86,88,88	0
2	PO4	F	1580	5/5	0.98	0.11	83,84,84,84	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.