



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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
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

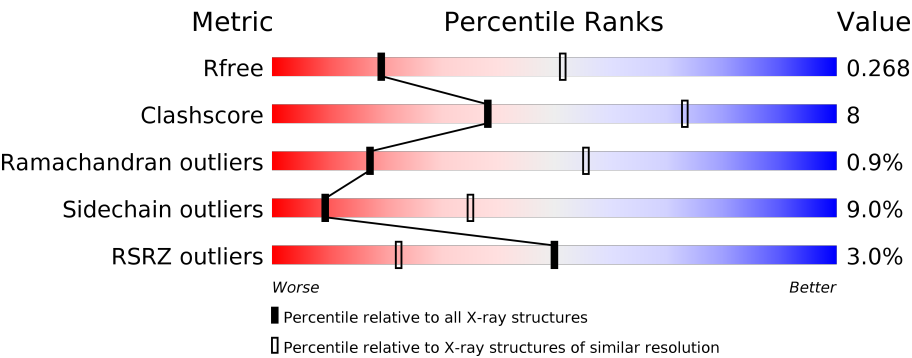
# 1 Overall quality at a glance i

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>

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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		

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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		

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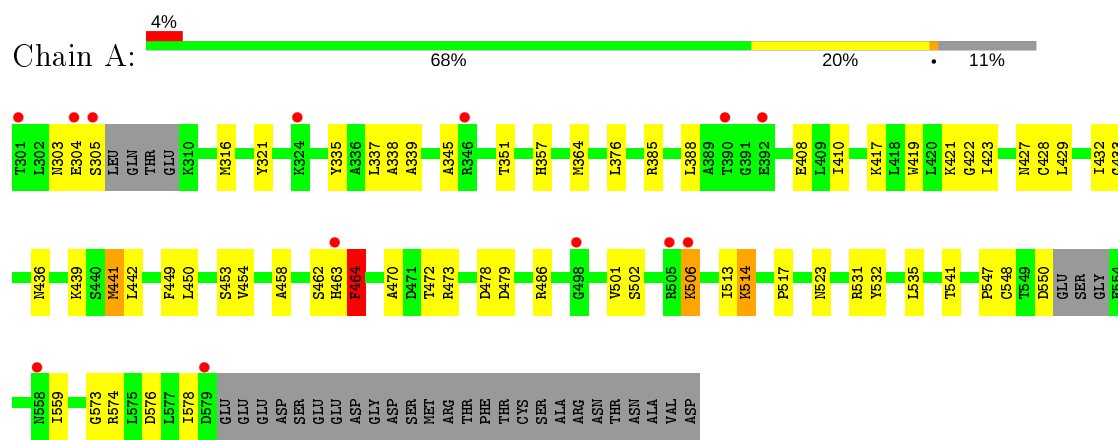
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	4	Total 4	O 4	0	0
4	I	4	Total 4	O 4	0	0
4	J	4	Total 4	O 4	0	0
4	L	1	Total 1	O 1	0	0

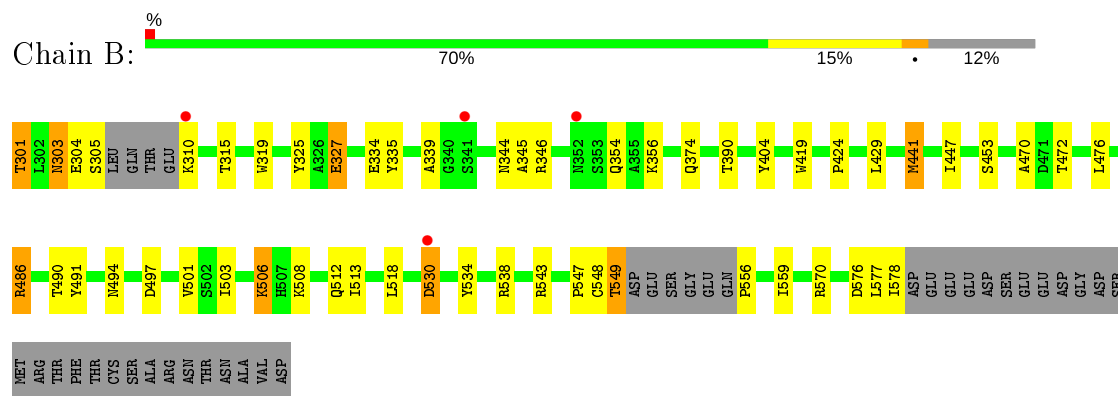
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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 ( $\text{RSRZ} > 2$ ). 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.

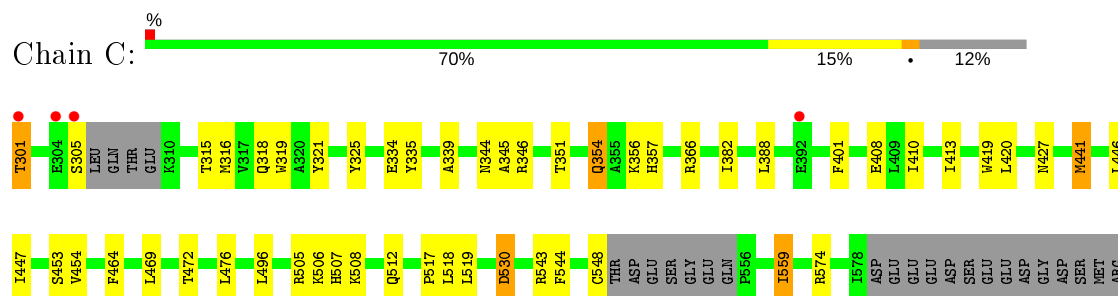
- Molecule 1: REPLICATION PROTEIN E1



- 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: 3% 74% 13% 10%

T301 E304 E305 LEU GLN THR K310 T315 Y321 Y325 S329 E334 Y335 A339 N344 A345 E346 N352 K387 L388 K389 T390 W419 G422 L423 P424 L429 K439 S440 W441 L442 Q443 L446 I447 S453 S456 F464 S468 T472

L476 D497 P500 K506 H507 Q512 I513 K514 L518 L519 Q527 D530 R531 E545 T549 ASP E551 S552 Q553 E554 Q555 T559 R570 I578 D579 GLU GLU ASP SER GLU ASP GLY SER MET ARG THR PHE THR CYS SER ALA ARG ASN THR

ASN  
ALA  
VAL  
ASP

• Molecule 1: REPLICATION PROTEIN E1

Chain E: 2% 69% 19% 11%

T301 L302 N303 E304 LEU GLN THR K310 F313 G314 T315 M316 W319 K320 E334 Y335 A345 T351 H357 S358 D360 K364 R370 Q374 K387 T390 G391 E392 G393 F402 N403 Y404 Q405 N406 I407 W419 P424 K425 K426 L429 I432

P435 N441 S443 D471 T472 D478 A479 A480 T481 A482 A483 R486 Y499 P500 Y501 S502 R505 K506 H507 A509 Q512 P517 S522 D525 D530 R531 Y532 L535 R538 R543 P544 E545 Q546 T549 D550 E551 SER GLY GLU P556

A562 R570 R574 I576 ASP GLU GLU GLU ASP ASP ASP GLU GLU ASP ASP GLY ASP SER MET ARG THR PHE THR CYS SER SER ALA ARG ASN THR ASN ALA VAL ASP

• Molecule 1: REPLICATION PROTEIN E1

Chain F: 3% 63% 23% 12%

T301 L302 N303 E304 LEU GLN THR K310 F311 T315 M316 Y321 E327 E328 Y335 G340 S343 N344 K346 T351 N352 S353 Q354 R357 A362 R366 R370 Q374 A389 T390 G391 E392 K396 S397 T398 L399 T400 E408 L409 I410 P424

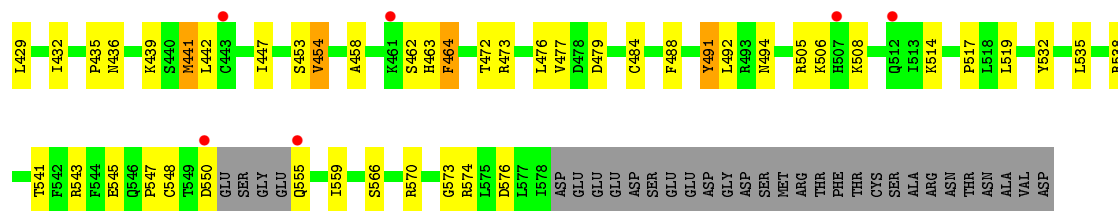
K425 L432 E434 N436 T437 G438 W441 L442 C443 A458 M459 H460 K461 S462 H463 F464 W465 S468 T472 L476 V477 D478 D479 A480 T481 H482 F488 L492 R493 W494 A495 I503 P504 R505 R506 R508 Q512 I513 K514 A515 V520 D525 V526 E529 Y532

L533 Y534 L535 R538 R543 C548 T549 ASP GLU SER GLY GLU GLN P556 T559 T560 D561 R574 I578 D579 GLU GLU GLU ASP ASP MET ARG THR PHE THR CYS SER ALA ARG ASN ASN ALA VAL ASP

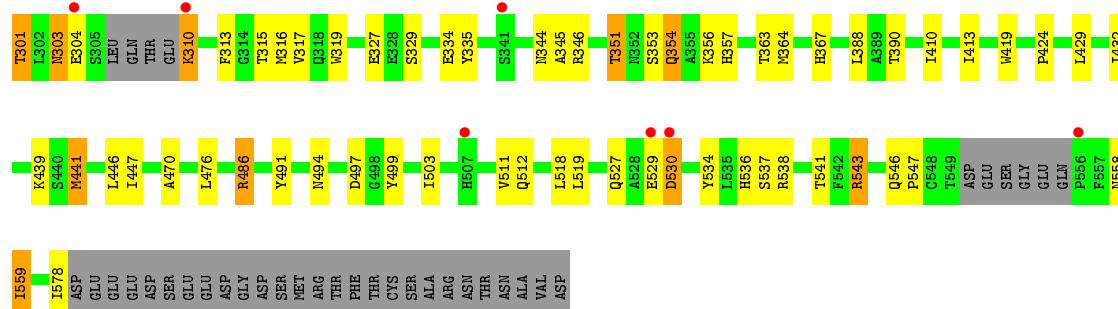
• Molecule 1: REPLICATION PROTEIN E1

Chain G: 4% 64% 23% 11%

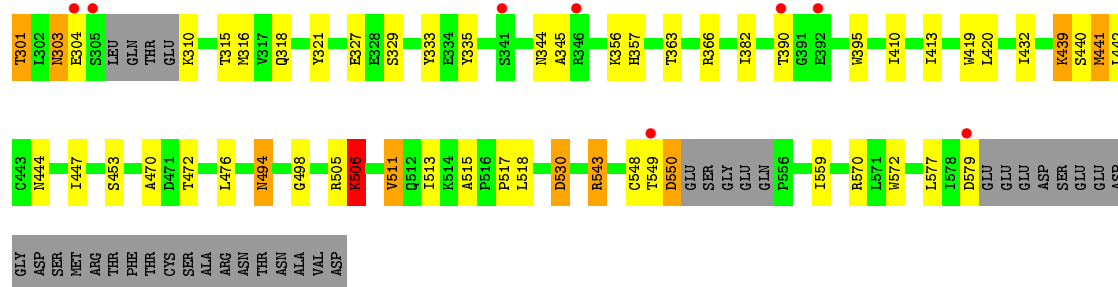
T301 L302 N303 E304 S305 LEU GLN THR K310 T315 M316 Y317 Q318 W319 A320 Y321 E328 S329 E334 L337 K338 A339 D342 S343 S344 N344 K345 K346 L349 S353 H357 A362 R366 L388 K389 T390 G391 E392 G393 S394 I410 W419 L420 K421 G422 I423



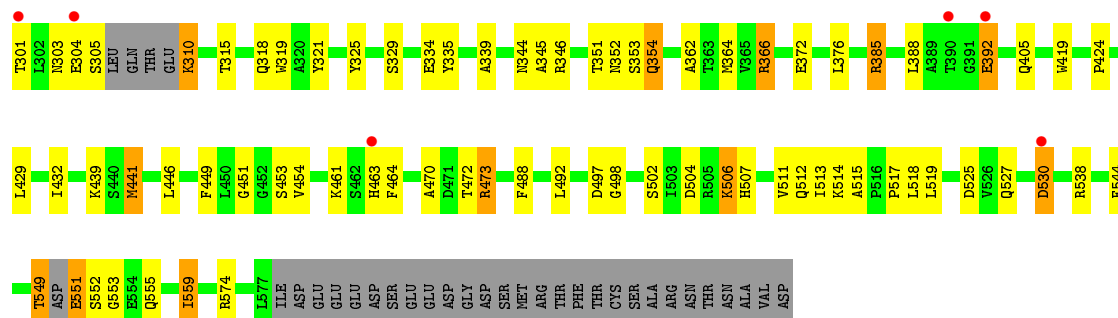
• Molecule 1: REPLICATION PROTEIN E1



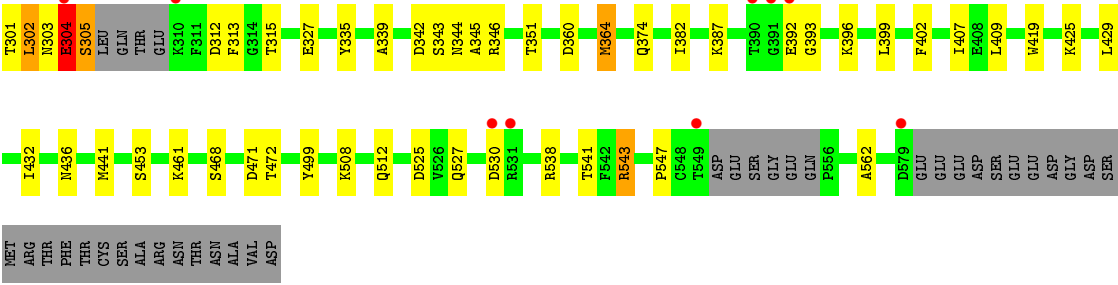
• Molecule 1: REPLICATION PROTEIN E1



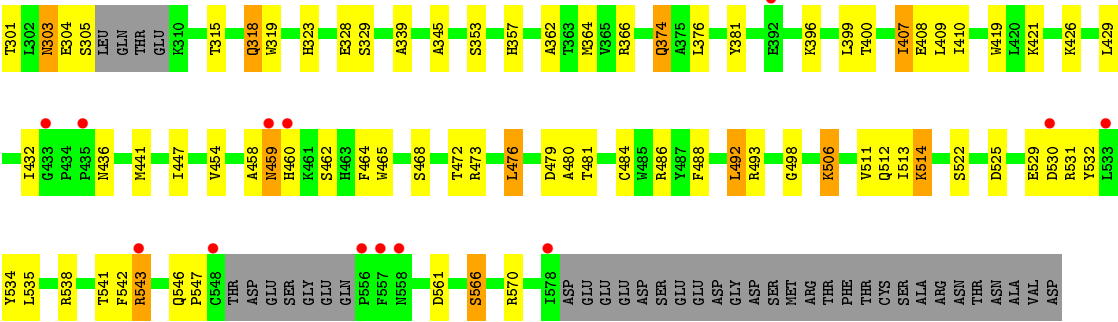
• Molecule 1: REPLICATION PROTEIN E1



• 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 [i](#)

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

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

All (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
1	D	570	ARG	NE-CZ-NH1	-5.58	117.51	120.30
1	J	473	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	H	486	ARG	NE-CZ-NH1	5.13	122.86	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 ⓘ

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	10	0	0	2	0
2	I	10	0	0	2	0
2	J	5	0	0	1	0
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.

All (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
1:J:376:LEU:O	1:J:473:ARG:NH2	2.04	0.90
1:K:312:ASP:H	1:K:344:ASN:HD21	1.17	0.90
1:G:432:ILE:HD13	1:G:541:THR:HG23	1.56	0.88
1:A:304:GLU:HG2	1:A:305:SER:H	1.41	0.85
2:A:1580:PO4:O1	2:A:1581:PO4:O2	1.97	0.82
1:G:435:PRO:HD3	1:H:534:TYR:HE2	1.46	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:363:THR:O	1:H:367:HIS:HD2	1.64	0.80
1:I:494:ASN:H	1:I:494:ASN:HD22	1.27	0.79
1:F:503:ILE:HD12	1:F:513:ILE:CD1	2.13	0.78
1:I:470:ALA:HA	1:I:513:ILE:HD11	1.66	0.77
1:L:447:ILE:HG13	1:L:476:LEU:HB2	1.68	0.76
1:J:549:THR:HG22	1:J:551:GLU:N	2.00	0.75
1:A:464:PHE:HD1	1:A:464:PHE:H	1.35	0.75
1:L:399:LEU:HD13	1:L:409:LEU:HD22	1.71	0.72
1:C:441:MET:HE3	1:C:559:ILE:H	1.54	0.72
1:D:304:GLU:HG2	1:D:305:SER:N	1.98	0.72
1:I:494:ASN:H	1:I:494:ASN:ND2	1.87	0.72
1:F:370:ARG:O	1:F:374:GLN:HG2	1.88	0.71
1:A:376:LEU:O	1:A:473:ARG:NH2	2.24	0.71
1:I:498:GLY:HA2	1:I:515:ALA:HB3	1.73	0.71
1:K:453:SER:HB3	1:K:472:THR:HG21	1.71	0.71
2:B:1579:PO4:O1	2:B:1580:PO4:O2	2.09	0.71
1:A:421:LYS:HB2	1:A:423:ILE:HD12	1.71	0.71
1:F:482:HIS:HD1	1:F:532:TYR:HH	1.36	0.70
1:D:439:LYS:NZ	2:D:1580:PO4:O4	2.24	0.70
1:A:458:ALA:HA	1:B:491:TYR:CD2	2.26	0.70
1:A:573:GLY:HA2	1:A:578:ILE:HD11	1.73	0.70
1:K:304:GLU:HG3	1:K:305:SER:H	1.55	0.69
1:B:303:ASN:HD22	1:C:318:GLN:HA	1.57	0.69
2:G:1579:PO4:O1	2:G:1580:PO4:O2	2.10	0.69
1:J:470:ALA:HA	1:J:513:ILE:CD1	2.23	0.69
2:I:1580:PO4:O1	2:I:1581:PO4:O2	2.11	0.69
1:D:352:ASN:OD1	1:E:313:PHE:HB2	1.93	0.69
1:L:462:SER:O	1:L:465:TRP:HD1	1.76	0.68
1:E:505:ARG:HH11	1:E:505:ARG:HB2	1.56	0.68
1:J:352:ASN:OD1	1:K:313:PHE:HB2	1.92	0.68
1:B:549:THR:HB	1:B:556:PRO:HD2	1.78	0.66
1:I:441:MET:HE3	1:I:559:ILE:H	1.61	0.65
1:H:363:THR:O	1:H:367:HIS:CD2	2.50	0.64
1:F:462:SER:O	1:F:465:TRP:HD1	1.81	0.63
1:K:453:SER:HB2	1:L:512:GLN:HE22	1.63	0.62
1:J:453:SER:HB3	1:J:472:THR:HG21	1.81	0.62
1:A:453:SER:HA	1:B:512:GLN:HE22	1.65	0.62
1:J:304:GLU:HG2	1:J:305:SER:H	1.64	0.62
1:G:532:TYR:HB3	1:G:535:LEU:HD12	1.81	0.61
1:L:362:ALA:O	1:L:366:ARG:HG3	2.01	0.61
1:A:385:ARG:HD3	1:A:449:PHE:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:ASN:ND2	1:C:318:GLN:HA	2.15	0.60
1:D:304:GLU:CG	1:D:305:SER:H	2.02	0.60
1:L:462:SER:O	1:L:465:TRP:CD1	2.54	0.60
1:F:503:ILE:HD12	1:F:513:ILE:HD11	1.84	0.60
1:F:362:ALA:O	1:F:366:ARG:HG2	2.02	0.59
1:I:549:THR:HG23	1:I:550:ASP:H	1.67	0.59
1:H:439:LYS:N	2:H:1579:PO4:O3	2.35	0.59
1:D:507:HIS:HE1	1:E:507:HIS:O	1.86	0.59
1:H:441:MET:HE3	1:H:559:ILE:H	1.67	0.59
1:J:439:LYS:NZ	2:J:1578:PO4:O4	2.34	0.59
1:D:441:MET:HE3	1:D:559:ILE:H	1.67	0.58
1:C:453:SER:HA	1:D:512:GLN:HE22	1.68	0.58
1:F:462:SER:O	1:F:465:TRP:CD1	2.56	0.58
1:G:435:PRO:HD3	1:H:534:TYR:CE2	2.34	0.58
1:G:494:ASN:HD21	1:L:454:VAL:HG21	1.67	0.58
1:A:532:TYR:HB3	1:A:535:LEU:HD12	1.85	0.58
1:A:432:ILE:CD1	1:A:541:THR:HG23	2.34	0.57
1:E:419:TRP:CD1	1:E:429:LEU:HG	2.39	0.57
1:L:353:SER:O	1:L:357:HIS:CD2	2.58	0.57
1:A:453:SER:HB3	1:A:472:THR:HG21	1.87	0.57
1:G:432:ILE:CD1	1:G:541:THR:HG23	2.29	0.57
1:J:441:MET:HE3	1:J:559:ILE:H	1.69	0.56
1:D:419:TRP:CD1	1:D:429:LEU:HG	2.40	0.56
1:G:419:TRP:CD1	1:G:429:LEU:HG	2.41	0.56
1:J:464:PHE:CE1	1:J:506:LYS:HA	2.40	0.56
1:D:441:MET:HA	1:E:499:TYR:OH	2.06	0.56
1:L:407:ILE:HG21	1:L:542:PHE:HD1	1.71	0.56
1:B:506:LYS:NZ	1:C:508:LYS:O	2.36	0.56
1:F:399:LEU:HD13	1:F:409:LEU:HD22	1.86	0.56
1:F:578:ILE:HG13	1:F:578:ILE:O	2.06	0.56
1:K:419:TRP:CD1	1:K:429:LEU:HG	2.40	0.56
2:H:1579:PO4:O1	2:H:1580:PO4:O2	2.24	0.56
1:J:441:MET:HA	1:K:499:TYR:OH	2.06	0.56
1:D:551:GLU:HG3	1:D:552:SER:N	2.21	0.55
1:E:453:SER:HB3	1:E:472:THR:HG21	1.88	0.55
1:H:335:TYR:OH	1:H:344:ASN:ND2	2.38	0.55
1:L:319:TRP:O	1:L:323:HIS:HD2	1.87	0.55
1:F:424:PRO:O	1:F:425:LYS:HB2	2.06	0.55
1:A:464:PHE:N	1:A:464:PHE:CD1	2.73	0.55
1:A:316:MET:HE1	1:A:357:HIS:HB3	1.89	0.55
1:H:301:THR:HG22	1:I:321:TYR:CE1	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:488:PHE:HA	1:L:492:LEU:HB2	1.88	0.55
1:E:478:ASP:OD2	1:F:494:ASN:ND2	2.40	0.55
1:H:303:ASN:HD22	1:I:318:GLN:HA	1.72	0.54
1:F:353:SER:O	1:F:357:HIS:CD2	2.61	0.54
1:G:458:ALA:HA	1:H:491:TYR:CD2	2.42	0.54
1:G:464:PHE:HD1	1:G:464:PHE:H	1.53	0.54
1:L:480:ALA:HB3	1:L:522:SER:HB2	1.90	0.54
1:B:447:ILE:HG13	1:B:476:LEU:HB2	1.89	0.54
1:K:304:GLU:HG3	1:K:305:SER:N	2.23	0.54
1:G:447:ILE:HG12	1:G:519:LEU:HD12	1.90	0.54
1:A:304:GLU:HG2	1:A:305:SER:N	2.17	0.54
1:B:453:SER:HB3	1:B:472:THR:HG21	1.90	0.54
1:B:301:THR:HG22	1:C:321:TYR:CE1	2.43	0.54
1:I:505:ARG:NH2	1:I:511:VAL:HG13	2.24	0.53
1:F:438:GLY:O	1:F:441:MET:HB3	2.07	0.53
1:H:424:PRO:HA	1:H:497:ASP:O	2.09	0.53
1:F:488:PHE:HA	1:F:492:LEU:HB2	1.89	0.53
1:H:470:ALA:HB2	1:H:503:ILE:HG21	1.91	0.53
1:A:436:ASN:O	1:A:547:PRO:HA	2.08	0.53
1:B:304:GLU:HG2	1:B:305:SER:H	1.74	0.53
1:C:453:SER:HB3	1:C:472:THR:HG21	1.91	0.53
1:J:304:GLU:HG2	1:J:305:SER:N	2.23	0.53
1:G:316:MET:HE1	1:G:357:HIS:HB3	1.91	0.53
1:A:385:ARG:HD2	1:A:450:LEU:O	2.08	0.53
1:E:319:TRP:HH2	1:E:334:GLU:HB3	1.74	0.53
1:C:325:TYR:CE1	1:C:334:GLU:HG2	2.43	0.53
1:E:505:ARG:HH11	1:E:505:ARG:CB	2.22	0.53
1:L:534:TYR:CE2	1:L:538:ARG:CZ	2.92	0.52
1:F:432:ILE:HD13	1:F:525:ASP:HA	1.90	0.52
1:H:441:MET:CE	1:H:559:ILE:H	2.21	0.52
1:A:432:ILE:HD12	1:A:541:THR:HG23	1.89	0.52
1:J:325:TYR:CE1	1:J:334:GLU:HG2	2.45	0.52
1:L:513:ILE:HG13	1:L:514:LYS:N	2.24	0.52
1:D:453:SER:HB2	1:E:512:GLN:OE1	2.10	0.52
1:E:425:LYS:HG2	1:E:538:ARG:HG3	1.92	0.52
1:H:316:MET:HE1	1:H:357:HIS:HB3	1.92	0.52
1:G:491:TYR:HD1	1:G:491:TYR:N	2.08	0.51
1:H:530:ASP:OD2	1:H:530:ASP:N	2.42	0.51
1:G:473:ARG:O	1:G:517:PRO:HD2	2.10	0.51
1:K:360:ASP:O	1:K:364:MET:HB2	2.11	0.51
1:A:486:ARG:NH1	1:A:531:ARG:HH11	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:530:ASP:OD2	1:B:530:ASP:N	2.43	0.51
1:J:339:ALA:HA	1:J:345:ALA:HB3	1.93	0.51
1:A:321:TYR:CE1	1:F:301:THR:HG22	2.46	0.51
1:B:453:SER:HA	1:C:512:GLN:HE22	1.74	0.51
1:L:566:SER:O	1:L:570:ARG:HB2	2.10	0.51
1:J:488:PHE:CE1	1:J:492:LEU:HD12	2.46	0.50
1:E:505:ARG:NH1	1:E:509:ALA:O	2.44	0.50
1:G:453:SER:HB3	1:G:472:THR:HG21	1.93	0.50
1:G:491:TYR:CD1	1:G:491:TYR:N	2.80	0.50
1:J:392:GLU:HA	1:J:392:GLU:OE2	2.10	0.50
1:J:498:GLY:HA2	1:J:515:ALA:HB3	1.94	0.50
1:K:432:ILE:HD12	1:K:541:THR:HG23	1.93	0.50
1:F:482:HIS:ND1	1:F:532:TYR:OH	2.32	0.50
1:G:318:GLN:HA	1:L:303:ASN:HD22	1.77	0.50
1:H:335:TYR:CE2	1:H:345:ALA:HA	2.47	0.50
1:I:447:ILE:HG13	1:I:476:LEU:HB2	1.94	0.49
1:C:316:MET:HE1	1:C:357:HIS:HB3	1.94	0.49
1:I:303:ASN:ND2	1:J:318:GLN:HA	2.26	0.49
1:G:441:MET:HE1	1:G:559:ILE:N	2.14	0.49
1:K:301:THR:O	1:K:302:LEU:C	2.49	0.49
1:A:513:ILE:HG22	1:A:514:LYS:O	2.12	0.49
1:C:351:THR:O	1:C:354:GLN:HG2	2.12	0.49
1:J:470:ALA:HB1	1:J:511:VAL:HG21	1.95	0.49
1:F:389:ALA:HB1	1:F:561:ASP:HB3	1.94	0.49
1:G:315:THR:HB	1:G:344:ASN:ND2	2.28	0.49
1:K:312:ASP:H	1:K:344:ASN:ND2	1.98	0.49
1:H:301:THR:HG22	1:I:321:TYR:CZ	2.48	0.49
1:L:493:ARG:HD3	1:L:534:TYR:CE2	2.48	0.49
1:A:419:TRP:CD1	1:A:429:LEU:HG	2.48	0.48
1:A:385:ARG:HD2	1:A:450:LEU:C	2.34	0.48
1:H:541:THR:HB	1:H:543:ARG:NH2	2.28	0.48
1:B:424:PRO:HA	1:B:497:ASP:O	2.14	0.48
1:G:432:ILE:HD13	1:G:541:THR:CG2	2.35	0.48
1:I:530:ASP:OD2	1:I:530:ASP:N	2.44	0.48
1:F:311:PHE:HZ	1:F:316:MET:HE1	1.78	0.48
1:D:315:THR:HB	1:D:344:ASN:ND2	2.28	0.48
1:J:454:VAL:N	1:K:512:GLN:OE1	2.43	0.48
1:E:335:TYR:CE2	1:E:345:ALA:HA	2.48	0.48
1:G:321:TYR:CZ	1:L:301:THR:HG22	2.49	0.48
1:H:527:GLN:NE2	1:H:536:HIS:HA	2.29	0.48
1:D:441:MET:CE	1:D:559:ILE:H	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:304:GLU:HG3	1:J:315:THR:HA	1.95	0.48
1:A:486:ARG:HH12	1:A:531:ARG:HH11	1.62	0.48
1:G:484:CYS:O	1:G:488:PHE:HD2	1.97	0.48
1:E:505:ARG:HH11	1:E:505:ARG:CG	2.26	0.47
1:G:338:ALA:O	1:G:342:ASP:HB3	2.14	0.47
1:I:441:MET:CE	1:I:559:ILE:H	2.27	0.47
1:B:304:GLU:HG3	1:C:315:THR:HA	1.97	0.47
1:I:363:THR:HA	1:I:366:ARG:NH1	2.29	0.47
1:K:453:SER:CB	1:K:472:THR:HG21	2.43	0.47
1:J:385:ARG:HD3	1:J:449:PHE:O	2.14	0.47
1:C:301:THR:HG22	1:D:321:TYR:CE1	2.49	0.47
1:C:446:LEU:HD23	1:C:519:LEU:HD11	1.95	0.47
1:E:393:GLY:H	1:E:562:ALA:HB1	1.79	0.47
1:B:325:TYR:CE1	1:B:334:GLU:HG2	2.49	0.47
1:E:313:PHE:CZ	1:E:360:ASP:HB3	2.49	0.47
1:J:335:TYR:CE2	1:J:345:ALA:HA	2.50	0.47
1:F:315:THR:HB	1:F:344:ASN:ND2	2.30	0.47
1:G:316:MET:CE	1:G:357:HIS:HB3	2.45	0.47
1:L:459:ASN:HB3	1:L:460:HIS:H	1.56	0.47
1:K:343:SER:HA	1:K:346:ARG:NH1	2.30	0.47
1:D:464:PHE:CE1	1:D:506:LYS:HA	2.49	0.47
1:F:351:THR:O	1:F:354:GLN:HG3	2.15	0.47
1:A:421:LYS:HB2	1:A:423:ILE:CD1	2.44	0.47
1:C:427:ASN:HB3	1:C:496:LEU:O	2.14	0.46
1:G:508:LYS:HE3	1:L:328:GLU:HB2	1.95	0.46
1:J:530:ASP:N	1:J:530:ASP:OD2	2.47	0.46
1:D:447:ILE:HG13	1:D:476:LEU:HB2	1.97	0.46
1:J:424:PRO:HA	1:J:497:ASP:O	2.15	0.46
1:L:432:ILE:HD13	1:L:525:ASP:HA	1.96	0.46
1:B:339:ALA:HA	1:B:345:ALA:HB3	1.98	0.46
1:B:441:MET:HE3	1:B:559:ILE:H	1.81	0.46
1:C:346:ARG:HE	1:C:346:ARG:HB2	1.50	0.46
1:C:447:ILE:HG13	1:C:476:LEU:HB2	1.97	0.46
1:C:530:ASP:N	1:C:530:ASP:OD2	2.44	0.46
1:F:335:TYR:CE2	1:F:345:ALA:HA	2.51	0.46
1:L:419:TRP:CD1	1:L:429:LEU:HG	2.50	0.46
1:E:532:TYR:HB3	1:E:535:LEU:HD12	1.97	0.46
1:J:352:ASN:HA	1:K:313:PHE:CB	2.46	0.46
1:G:353:SER:O	1:G:357:HIS:CD2	2.69	0.46
1:J:304:GLU:HG3	1:K:315:THR:HA	1.98	0.46
1:A:470:ALA:HA	1:A:513:ILE:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:THR:HB	1:B:344:ASN:ND2	2.30	0.46
1:D:551:GLU:CG	1:D:552:SER:N	2.79	0.46
1:G:453:SER:HA	1:H:512:GLN:HE22	1.80	0.46
1:L:534:TYR:CZ	1:L:538:ARG:NH2	2.84	0.46
1:I:301:THR:HG22	1:J:321:TYR:CE1	2.50	0.46
1:I:333:TYR:CZ	1:J:372:GLU:HB3	2.50	0.46
1:A:422:GLY:HA2	1:A:427:ASN:HD22	1.81	0.46
1:E:419:TRP:CE2	1:E:517:PRO:HB3	2.51	0.45
1:G:454:VAL:HG12	1:G:476:LEU:HD23	1.97	0.45
1:L:304:GLU:HG2	1:L:305:SER:H	1.81	0.45
1:E:480:ALA:HB3	1:E:522:SER:HB2	1.97	0.45
1:D:555:GLN:HG3	1:D:555:GLN:O	2.16	0.45
1:I:395:TRP:NE1	1:I:570:ARG:HD2	2.31	0.45
1:I:453:SER:HA	1:J:512:GLN:HE22	1.82	0.45
1:J:446:LEU:HD23	1:J:519:LEU:HD11	1.97	0.45
1:A:417:LYS:HD2	1:A:576:ASP:HB2	1.97	0.45
1:E:304:GLU:HB3	1:E:305:SER:H	1.65	0.45
1:A:441:MET:HE1	1:A:559:ILE:N	2.14	0.45
1:E:404:TYR:O	1:E:546:GLN:HG3	2.16	0.45
1:K:304:GLU:HG2	1:L:318:GLN:HG3	1.98	0.45
1:L:381:TYR:CE1	1:L:473:ARG:HG3	2.51	0.45
1:C:382:ILE:HD11	1:C:420:LEU:HD22	1.98	0.45
1:H:447:ILE:HG13	1:H:476:LEU:HB2	1.99	0.45
1:D:530:ASP:OD2	1:D:530:ASP:N	2.49	0.45
1:G:436:ASN:ND2	1:H:537:SER:HB3	2.31	0.45
1:H:546:GLN:HA	1:H:547:PRO:HD2	1.65	0.45
1:J:419:TRP:CD1	1:J:429:LEU:HG	2.52	0.45
1:B:490:THR:HB	1:B:491:TYR:CD1	2.52	0.45
1:I:440:SER:O	1:I:444:ASN:HB2	2.16	0.45
1:G:421:LYS:HB2	1:G:423:ILE:HD12	1.98	0.45
1:I:439:LYS:N	2:I:1580:PO4:O3	2.50	0.45
1:L:374:GLN:HB3	1:L:374:GLN:HE21	1.60	0.45
1:E:301:THR:O	1:E:302:LEU:C	2.55	0.44
1:B:419:TRP:CD1	1:B:429:LEU:HG	2.52	0.44
1:C:319:TRP:HH2	1:C:334:GLU:HB3	1.81	0.44
1:G:435:PRO:HA	2:G:1580:PO4:O2	2.18	0.44
1:H:446:LEU:HD23	1:H:519:LEU:HD11	1.99	0.44
1:H:541:THR:HB	1:H:543:ARG:HH21	1.83	0.44
1:I:419:TRP:CE2	1:I:517:PRO:HB3	2.52	0.44
1:F:463:HIS:HE1	1:F:504:ASP:OD2	2.00	0.44
1:H:364:MET:O	1:H:367:HIS:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:419:TRP:CE2	1:J:517:PRO:HB3	2.52	0.44
1:E:301:THR:HG22	1:F:321:TYR:CZ	2.53	0.44
1:C:419:TRP:CE2	1:C:517:PRO:HB3	2.53	0.44
1:F:503:ILE:HD12	1:F:513:ILE:HD13	1.92	0.44
1:G:328:GLU:HB3	1:H:367:HIS:HE1	1.82	0.44
1:H:419:TRP:CD1	1:H:429:LEU:HG	2.53	0.44
1:H:534:TYR:O	1:H:538:ARG:NH1	2.51	0.44
1:C:454:VAL:HG21	1:D:500:PRO:HB2	2.00	0.44
1:D:422:GLY:HA3	1:D:514:LYS:NZ	2.32	0.44
1:H:346:ARG:HE	1:H:346:ARG:HB2	1.62	0.44
1:E:370:ARG:O	1:E:374:GLN:HG2	2.17	0.44
1:L:339:ALA:HA	1:L:345:ALA:HB3	1.99	0.44
1:E:402:PHE:HD1	1:E:407:ILE:HD11	1.83	0.44
1:G:362:ALA:O	1:G:366:ARG:HG2	2.18	0.44
1:H:410:ILE:HA	1:H:413:ILE:HD12	2.00	0.44
1:D:453:SER:HB3	1:D:472:THR:HG21	1.99	0.44
1:D:339:ALA:HA	1:D:345:ALA:HB3	2.00	0.43
1:J:346:ARG:HE	1:J:346:ARG:HB2	1.55	0.43
1:C:339:ALA:HA	1:C:345:ALA:HB3	2.00	0.43
1:E:482:HIS:O	1:E:483:ALA:C	2.56	0.43
1:D:456:SER:HB2	1:E:502:SER:HB3	2.00	0.43
1:I:410:ILE:HA	1:I:413:ILE:HD12	2.00	0.43
1:J:551:GLU:HB3	1:J:552:SER:H	1.56	0.43
1:F:532:TYR:HB3	1:F:535:LEU:HD12	2.00	0.43
1:L:498:GLY:O	1:L:514:LYS:HE2	2.18	0.43
1:C:464:PHE:CE1	1:C:506:LYS:HA	2.53	0.43
1:E:330:LYS:O	1:E:334:GLU:HB2	2.18	0.43
1:F:534:TYR:CE2	1:F:538:ARG:CZ	3.02	0.43
1:J:385:ARG:NH1	1:J:451:GLY:N	2.66	0.43
1:K:512:GLN:HB3	1:K:512:GLN:HE21	1.58	0.43
1:E:435:PRO:HB3	1:F:534:TYR:CE1	2.53	0.43
1:E:432:ILE:HD13	1:E:525:ASP:HA	1.99	0.43
1:H:304:GLU:HG3	1:I:315:THR:HA	2.00	0.43
1:J:353:SER:O	1:J:354:GLN:C	2.56	0.43
1:I:506:LYS:NZ	1:J:504:ASP:OD1	2.51	0.43
1:G:304:GLU:HG2	1:G:305:SER:H	1.84	0.43
1:H:313:PHE:O	1:H:317:VAL:HG23	2.19	0.43
1:K:304:GLU:OE1	1:L:315:THR:HG23	2.19	0.43
1:A:464:PHE:HE2	1:A:506:LYS:HA	1.84	0.43
1:I:505:ARG:CZ	1:I:511:VAL:HG13	2.49	0.43
1:B:470:ALA:HB2	1:B:503:ILE:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:432:ILE:HD13	1:J:525:ASP:HA	2.00	0.43
1:K:339:ALA:HA	1:K:345:ALA:HB3	2.01	0.43
1:K:399:LEU:HD13	1:K:409:LEU:HD22	2.01	0.43
1:K:543:ARG:HG2	1:K:543:ARG:H	1.69	0.43
1:L:532:TYR:HB3	1:L:535:LEU:HD12	2.00	0.43
1:F:327:GLU:O	1:F:328:GLU:C	2.56	0.43
1:H:432:ILE:HD12	1:H:541:THR:HG23	2.00	0.43
1:I:316:MET:HE1	1:I:357:HIS:HB3	2.00	0.43
1:J:362:ALA:O	1:J:366:ARG:HG2	2.19	0.43
1:L:376:LEU:O	1:L:473:ARG:NH2	2.41	0.43
1:L:570:ARG:HD2	1:L:570:ARG:HA	1.87	0.43
1:A:432:ILE:HD13	1:A:541:THR:HG23	2.01	0.42
1:G:319:TRP:HH2	1:G:334:GLU:HB3	1.83	0.42
1:J:405:GLN:HG3	1:J:544:PHE:CD1	2.53	0.42
1:G:447:ILE:HG13	1:G:476:LEU:HB2	2.00	0.42
1:H:497:ASP:HB3	1:H:499:TYR:CD2	2.53	0.42
1:E:301:THR:HG22	1:F:321:TYR:CE1	2.55	0.42
1:F:398:ILE:HG12	1:F:559:ILE:HD12	2.02	0.42
1:F:482:HIS:CE1	1:F:532:TYR:HH	2.37	0.42
1:H:351:THR:O	1:H:354:GLN:HG2	2.20	0.42
1:L:464:PHE:CE1	1:L:506:LYS:HA	2.54	0.42
1:D:555:GLN:HE21	1:D:555:GLN:HB2	1.66	0.42
1:E:499:TYR:HB3	1:E:500:PRO:CD	2.49	0.42
1:G:337:LEU:C	1:G:339:ALA:H	2.22	0.42
1:A:478:ASP:HB3	1:B:494:ASN:HD22	1.83	0.42
1:B:374:GLN:HE22	1:B:513:ILE:HD11	1.85	0.42
1:D:424:PRO:HA	1:D:497:ASP:O	2.19	0.42
1:E:405:GLN:NE2	1:E:546:GLN:HB2	2.34	0.42
1:G:321:TYR:CE1	1:L:301:THR:HG22	2.55	0.42
1:C:410:ILE:HA	1:C:413:ILE:HD12	2.02	0.42
1:G:436:ASN:O	1:G:547:PRO:HA	2.19	0.42
1:J:315:THR:HB	1:J:344:ASN:ND2	2.34	0.42
1:K:335:TYR:CE2	1:K:345:ALA:HA	2.54	0.42
1:K:453:SER:HB3	1:K:472:THR:CG2	2.44	0.42
1:J:319:TRP:HH2	1:J:334:GLU:HB3	1.85	0.42
1:A:335:TYR:CE2	1:A:345:ALA:HA	2.55	0.41
1:D:325:TYR:CE1	1:D:334:GLU:HG2	2.54	0.41
1:K:393:GLY:H	1:K:562:ALA:HB1	1.85	0.41
1:A:439:LYS:N	2:A:1580:PO4:O3	2.53	0.41
1:E:374:GLN:HE22	1:E:471:ASP:HA	1.84	0.41
1:C:335:TYR:OH	1:C:344:ASN:ND2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:304:GLU:HG3	1:H:315:THR:HA	2.02	0.41
1:I:335:TYR:CE2	1:I:345:ALA:HA	2.54	0.41
1:C:441:MET:CE	1:C:559:ILE:H	2.29	0.41
1:K:432:ILE:HD13	1:K:525:ASP:HA	2.02	0.41
1:C:401:PHE:HE2	1:C:544:PHE:CE2	2.38	0.41
1:E:301:THR:O	1:E:301:THR:HG23	2.21	0.41
1:E:374:GLN:NE2	1:E:471:ASP:HA	2.34	0.41
1:I:442:LEU:HD12	1:I:559:ILE:HD12	2.02	0.41
1:K:402:PHE:HD1	1:K:407:ILE:HD11	1.86	0.41
1:B:441:MET:CE	1:B:559:ILE:H	2.32	0.41
1:F:477:VAL:HB	1:F:520:VAL:HG13	2.02	0.41
1:F:495:ALA:HB1	1:F:515:ALA:CB	2.50	0.41
1:G:303:ASN:HA	1:G:349:LEU:HD22	2.03	0.41
1:I:382:ILE:HD11	1:I:420:LEU:HD22	2.02	0.41
1:L:484:CYS:O	1:L:488:PHE:HD2	2.04	0.41
1:A:458:ALA:HB2	1:B:491:TYR:HB3	2.03	0.41
1:B:319:TRP:HH2	1:B:334:GLU:HB3	1.85	0.41
1:B:346:ARG:HB2	1:B:346:ARG:HE	1.59	0.41
1:F:443:CYS:HB3	1:F:476:LEU:HD22	2.03	0.41
1:A:501:VAL:HG22	1:A:502:SER:N	2.36	0.41
1:D:446:LEU:HD23	1:D:519:LEU:HD11	2.03	0.41
1:G:392:GLU:HA	1:G:392:GLU:OE1	2.21	0.41
1:H:319:TRP:HH2	1:H:334:GLU:HB3	1.86	0.41
1:I:432:ILE:O	1:I:543:ARG:HA	2.21	0.41
1:A:316:MET:CE	1:A:357:HIS:HB3	2.50	0.41
1:D:304:GLU:CG	1:D:305:SER:N	2.71	0.41
1:H:303:ASN:ND2	1:I:318:GLN:HA	2.35	0.41
1:A:337:LEU:C	1:A:339:ALA:H	2.23	0.41
1:B:404:TYR:OH	1:B:547:PRO:O	2.31	0.41
1:E:424:PRO:O	1:E:425:LYS:HB2	2.20	0.41
1:I:572:TRP:NE1	1:I:577:LEU:O	2.54	0.41
1:K:374:GLN:NE2	1:K:471:ASP:HA	2.36	0.41
1:L:541:THR:HB	1:L:543:ARG:HH21	1.86	0.41
1:J:385:ARG:HH11	1:J:451:GLY:N	2.20	0.40
1:E:316:MET:HE1	1:E:357:HIS:HB3	2.01	0.40
1:E:319:TRP:CH2	1:E:334:GLU:HB3	2.56	0.40
1:G:505:ARG:CZ	1:G:508:LYS:HD3	2.51	0.40
1:H:315:THR:HB	1:H:344:ASN:ND2	2.36	0.40
1:K:425:LYS:HG2	1:K:538:ARG:HG2	2.02	0.40
1:A:473:ARG:O	1:A:517:PRO:HD2	2.21	0.40
1:B:335:TYR:OH	1:B:344:ASN:ND2	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:577:LEU:O	1:B:578:ILE:C	2.59	0.40
1:I:453:SER:HB3	1:I:472:THR:HG21	2.03	0.40
1:K:342:ASP:HB3	1:K:345:ALA:HB3	2.04	0.40
1:K:436:ASN:O	1:K:547:PRO:HA	2.20	0.40
1:E:453:SER:HB3	1:E:472:THR:CG2	2.50	0.40
1:G:477:VAL:HG21	1:G:488:PHE:HZ	1.87	0.40
1:I:335:TYR:OH	1:I:344:ASN:ND2	2.53	0.40
1:J:405:GLN:HG3	1:J:544:PHE:CG	2.57	0.40
1:A:433:GLY:O	1:A:523:ASN:HA	2.22	0.40
1:B:534:TYR:O	1:B:538:ARG:NH1	2.54	0.40
1:D:335:TYR:OH	1:D:344:ASN:ND2	2.55	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

All (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
1	K	302	LEU
1	K	304	GLU
1	L	458	ALA
1	F	479	ASP
1	F	506	LYS
1	G	464	PHE
1	G	492	LEU
1	I	506	LYS
1	I	548	CYS
1	L	479	ASP
1	B	576	ASP
1	D	552	SER
1	F	458	ALA
1	F	578	ILE
1	G	576	ASP
1	H	558	ASN
1	A	338	ALA
1	A	464	PHE
1	F	459	ASN
1	F	462	SER
1	L	547	PRO
1	D	578	ILE
1	F	441	MET
1	J	553	GLY
1	G	573	GLY

### 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

All (245) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	303	ASN
1	A	351	THR
1	A	364	MET
1	A	388	LEU
1	A	408	GLU
1	A	410	ILE
1	A	428	CYS
1	A	441	MET
1	A	442	LEU
1	A	454	VAL
1	A	462	SER
1	A	463	HIS
1	A	464	PHE
1	A	479	ASP
1	A	506	LYS
1	A	514	LYS
1	A	548	CYS
1	A	550	ASP

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Mol	Chain	Res	Type
1	A	574	ARG
1	B	301	THR
1	B	303	ASN
1	B	310	LYS
1	B	327	GLU
1	B	354	GLN
1	B	356	LYS
1	B	390	THR
1	B	441	MET
1	B	486	ARG
1	B	501	VAL
1	B	506	LYS
1	B	508	LYS
1	B	518	LEU
1	B	530	ASP
1	B	543	ARG
1	B	548	CYS
1	B	549	THR
1	B	570	ARG
1	C	301	THR
1	C	305	SER
1	C	354	GLN
1	C	356	LYS
1	C	366	ARG
1	C	388	LEU
1	C	408	GLU
1	C	441	MET
1	C	469	LEU
1	C	505	ARG
1	C	507	HIS
1	C	518	LEU
1	C	530	ASP
1	C	543	ARG
1	C	548	CYS
1	C	559	ILE
1	C	574	ARG
1	D	310	LYS
1	D	329	SER
1	D	387	LYS
1	D	388	LEU
1	D	441	MET
1	D	468	SER

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Mol	Chain	Res	Type
1	D	514	LYS
1	D	518	LEU
1	D	527	GLN
1	D	530	ASP
1	D	531	ARG
1	D	549	THR
1	D	555	GLN
1	D	570	ARG
1	E	315	THR
1	E	334	GLU
1	E	351	THR
1	E	364	MET
1	E	387	LYS
1	E	392	GLU
1	E	426	LYS
1	E	441	MET
1	E	486	ARG
1	E	505	ARG
1	E	530	ASP
1	E	538	ARG
1	E	543	ARG
1	E	550	ASP
1	E	570	ARG
1	E	574	ARG
1	F	302	LEU
1	F	303	ASN
1	F	304	GLU
1	F	343	SER
1	F	396	LYS
1	F	400	THR
1	F	408	GLU
1	F	410	ILE
1	F	436	ASN
1	F	441	MET
1	F	468	SER
1	F	472	THR
1	F	481	THR
1	F	482	HIS
1	F	494	ASN
1	F	506	LYS
1	F	507	HIS
1	F	508	LYS

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Mol	Chain	Res	Type
1	F	513	ILE
1	F	526	VAL
1	F	529	GLU
1	F	543	ARG
1	F	548	CYS
1	F	549	THR
1	F	574	ARG
1	F	578	ILE
1	G	303	ASN
1	G	329	SER
1	G	346	ARG
1	G	388	LEU
1	G	394	SER
1	G	410	ILE
1	G	439	LYS
1	G	441	MET
1	G	442	LEU
1	G	454	VAL
1	G	462	SER
1	G	463	HIS
1	G	479	ASP
1	G	491	TYR
1	G	514	LYS
1	G	538	ARG
1	G	543	ARG
1	G	545	GLU
1	G	548	CYS
1	G	550	ASP
1	G	555	GLN
1	G	566	SER
1	G	570	ARG
1	H	301	THR
1	H	303	ASN
1	H	310	LYS
1	H	327	GLU
1	H	329	SER
1	H	351	THR
1	H	353	SER
1	H	354	GLN
1	H	356	LYS
1	H	388	LEU
1	H	390	THR

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Mol	Chain	Res	Type
1	H	441	MET
1	H	486	ARG
1	H	494	ASN
1	H	511	VAL
1	H	518	LEU
1	H	529	GLU
1	H	530	ASP
1	H	543	ARG
1	H	559	ILE
1	H	578	ILE
1	I	301	THR
1	I	303	ASN
1	I	310	LYS
1	I	327	GLU
1	I	329	SER
1	I	356	LYS
1	I	390	THR
1	I	439	LYS
1	I	441	MET
1	I	494	ASN
1	I	506	LYS
1	I	511	VAL
1	I	518	LEU
1	I	530	ASP
1	I	543	ARG
1	I	550	ASP
1	I	579	ASP
1	J	301	THR
1	J	303	ASN
1	J	310	LYS
1	J	329	SER
1	J	351	THR
1	J	354	GLN
1	J	364	MET
1	J	366	ARG
1	J	385	ARG
1	J	388	LEU
1	J	392	GLU
1	J	441	MET
1	J	461	LYS
1	J	463	HIS
1	J	502	SER

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Mol	Chain	Res	Type
1	J	507	HIS
1	J	514	LYS
1	J	518	LEU
1	J	527	GLN
1	J	530	ASP
1	J	538	ARG
1	J	549	THR
1	J	551	GLU
1	J	555	GLN
1	J	559	ILE
1	J	574	ARG
1	K	303	ASN
1	K	304	GLU
1	K	305	SER
1	K	327	GLU
1	K	351	THR
1	K	364	MET
1	K	382	ILE
1	K	387	LYS
1	K	392	GLU
1	K	396	LYS
1	K	441	MET
1	K	461	LYS
1	K	468	SER
1	K	508	LYS
1	K	527	GLN
1	K	530	ASP
1	K	543	ARG
1	L	303	ASN
1	L	318	GLN
1	L	329	SER
1	L	364	MET
1	L	374	GLN
1	L	396	LYS
1	L	400	THR
1	L	407	ILE
1	L	408	GLU
1	L	410	ILE
1	L	421	LYS
1	L	426	LYS
1	L	436	ASN
1	L	441	MET

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Mol	Chain	Res	Type
1	L	459	ASN
1	L	468	SER
1	L	472	THR
1	L	476	LEU
1	L	481	THR
1	L	486	ARG
1	L	492	LEU
1	L	506	LYS
1	L	511	VAL
1	L	514	LYS
1	L	529	GLU
1	L	530	ASP
1	L	531	ARG
1	L	543	ARG
1	L	546	GLN
1	L	561	ASP
1	L	566	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	427	ASN
1	A	463	HIS
1	A	512	GLN
1	A	527	GLN
1	B	374	GLN
1	B	527	GLN
1	C	427	ASN
1	C	459	ASN
1	D	507	HIS
1	D	527	GLN
1	D	555	GLN
1	E	494	ASN
1	E	523	ASN
1	F	323	HIS
1	F	427	ASN
1	F	463	HIS
1	F	512	GLN
1	F	546	GLN
1	G	318	GLN
1	G	323	HIS
1	G	367	HIS

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Mol	Chain	Res	Type
1	G	427	ASN
1	G	436	ASN
1	G	463	HIS
1	G	494	ASN
1	H	344	ASN
1	H	357	HIS
1	H	367	HIS
1	H	527	GLN
1	H	546	GLN
1	I	427	ASN
1	I	494	ASN
1	J	444	ASN
1	J	527	GLN
1	J	555	GLN
1	K	344	ASN
1	K	374	GLN
1	K	414	ASN
1	K	494	ASN
1	K	523	ASN
1	L	323	HIS
1	L	357	HIS
1	L	374	GLN
1	L	427	ASN
1	L	444	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 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

All (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
2	C	1580	PO4	O4-P-O3	2.16	114.89	107.97

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%)

All (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
1	F	579	ASP	4.3
1	L	460	HIS	4.1
1	I	392	GLU	4.0
1	L	558	ASN	4.0
1	A	390	THR	3.7
1	I	579	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	G	507	HIS	3.6
1	F	346	ARG	3.6
1	I	305	SER	3.5
1	B	530	ASP	3.4
1	G	461	LYS	3.4
1	H	341	SER	3.4
1	G	310	LYS	3.4
1	E	549	THR	3.3
1	D	443	CYS	3.3
1	F	305	SER	3.3
1	A	305	SER	3.3
1	D	310	LYS	3.2
1	A	506	LYS	3.1
1	E	391	GLY	3.1
1	I	304	GLU	3.1
1	E	530	ASP	3.0
1	F	460	HIS	3.0
1	A	579	ASP	2.9
1	K	390	THR	2.9
1	D	530	ASP	2.9
1	A	498	GLY	2.9
1	D	346	ARG	2.9
1	F	392	GLU	2.9
1	C	304	GLU	2.8
1	L	548	CYS	2.8
1	L	530	ASP	2.8
1	E	390	THR	2.8
1	H	310	LYS	2.7
1	D	390	THR	2.7
1	K	391	GLY	2.7
1	L	578	ILE	2.7
1	D	305	SER	2.7
1	B	310	LYS	2.7
1	C	392	GLU	2.7
1	I	549	THR	2.6
1	H	530	ASP	2.6
1	K	531	ARG	2.6
1	A	463	HIS	2.6
1	H	556	PRO	2.5
1	L	556	PRO	2.5
1	K	392	GLU	2.5
1	L	543	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	L	459	ASN	2.5
1	L	392	GLU	2.5
1	F	390	THR	2.5
1	A	346	ARG	2.5
1	A	324	LYS	2.5
1	J	304	GLU	2.4
1	B	341	SER	2.4
1	K	549	THR	2.4
1	C	305	SER	2.4
1	D	570	ARG	2.4
1	J	301	THR	2.4
1	F	343	SER	2.3
1	I	341	SER	2.3
1	G	391	GLY	2.3
1	G	550	ASP	2.3
1	A	392	GLU	2.3
1	L	533	LEU	2.3
1	D	545	GLU	2.3
1	F	396	LYS	2.3
1	B	352	ASN	2.3
1	H	529	GLU	2.2
1	K	310	LYS	2.2
1	A	301	THR	2.2
1	E	545	GLU	2.2
1	A	505	ARG	2.2
1	G	392	GLU	2.2
1	I	346	ARG	2.2
1	K	304	GLU	2.2
1	G	555	GLN	2.2
1	C	301	THR	2.2
1	L	435	PRO	2.1
1	H	507	HIS	2.1
1	K	530	ASP	2.1
1	A	558	ASN	2.1
1	G	443	CYS	2.1
1	K	579	ASP	2.1
1	G	512	GLN	2.1
1	I	390	THR	2.1
1	J	390	THR	2.1
1	F	578	ILE	2.1
1	J	530	ASP	2.1
1	H	304	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	L	557	PHE	2.0
1	J	463	HIS	2.0
1	G	301	THR	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no 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, 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( $\text{\AA}^2$ )	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	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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
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 [i](#)

There are no such residues in this entry.