Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:57 AM 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)

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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

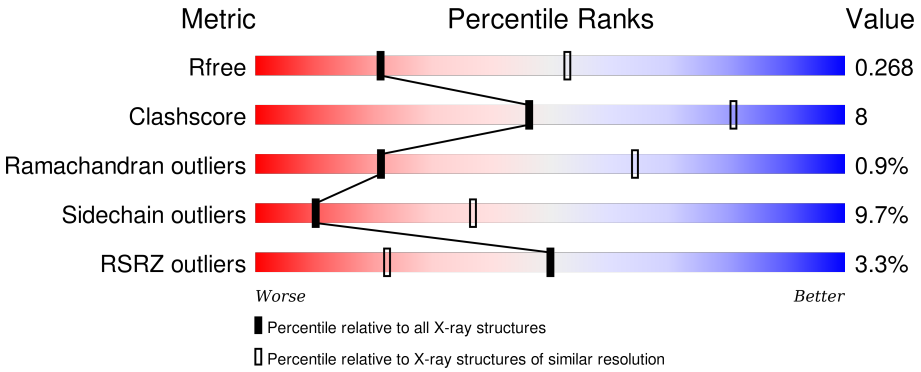
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (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 >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	305	5% 68% 20% • 11%
1	B	305	2% 70% 15% • 12%
1	C	305	2% 71% 15% • 12%
1	D	305	3% 73% 13% • 10%
1	E	305	2% 68% 20% • 11%

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Mol	Chain	Length	Quality of chain
1	F	305	4% 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% 64% 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	G	1580	-	-	X	X
2	PO4	H	1579	-	-	X	-
2	PO4	I	1580	-	-	X	-

2 Entry composition (i)

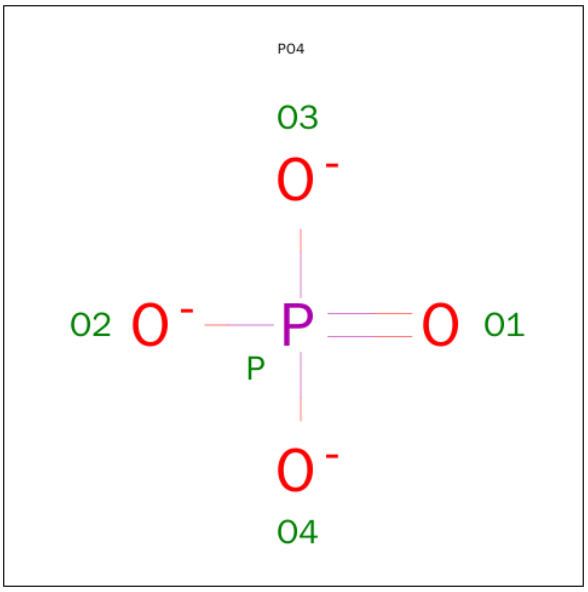
There are 4 unique types of molecules in this entry. The entry contains 26079 atoms, of which 0 are hydrogens and 0 are deuteriums.

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).



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

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

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

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

- Molecule 4 is water.

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

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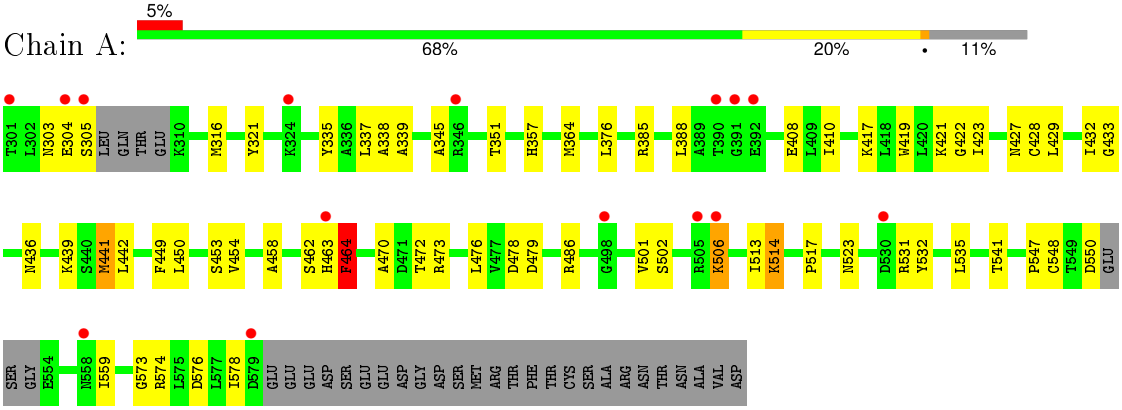
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	4	Total O 4 4	0	0
4	I	4	Total O 4 4	0	0
4	J	4	Total O 4 4	0	0
4	L	1	Total O 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

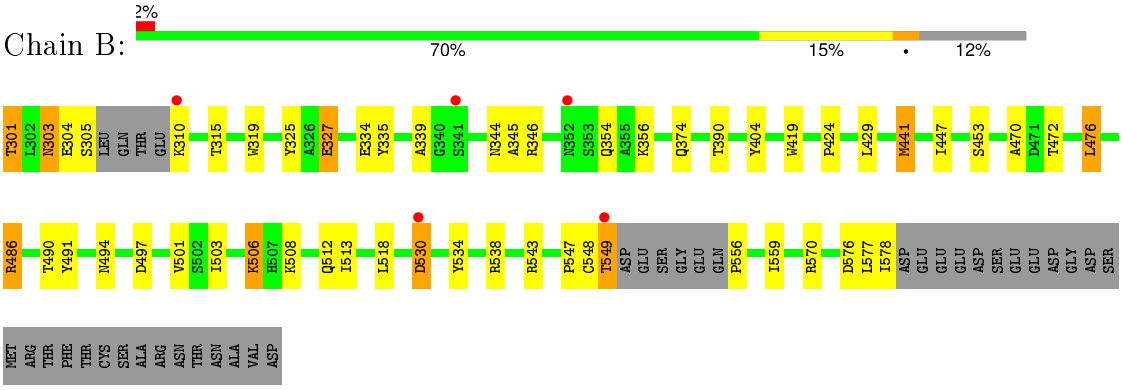
- Molecule 1: REPLICATION PROTEIN E1

Chain A:



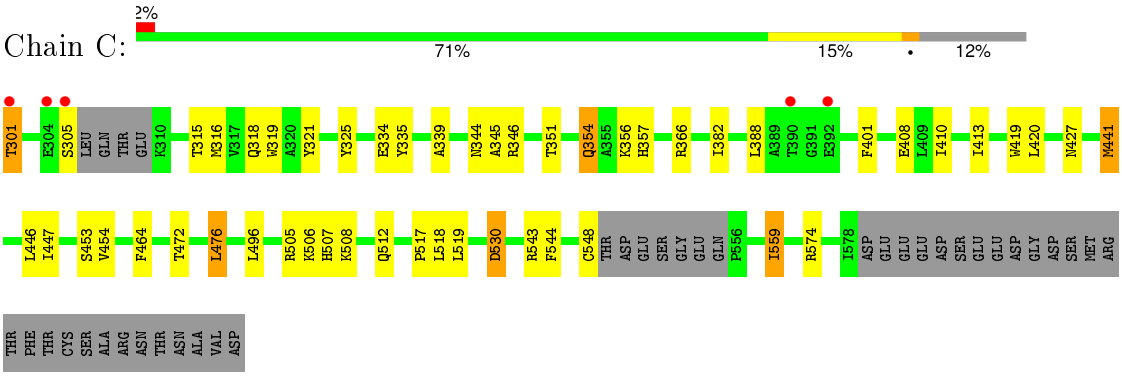
- Molecule 1: REPLICATION PROTEIN E1

Chain B:



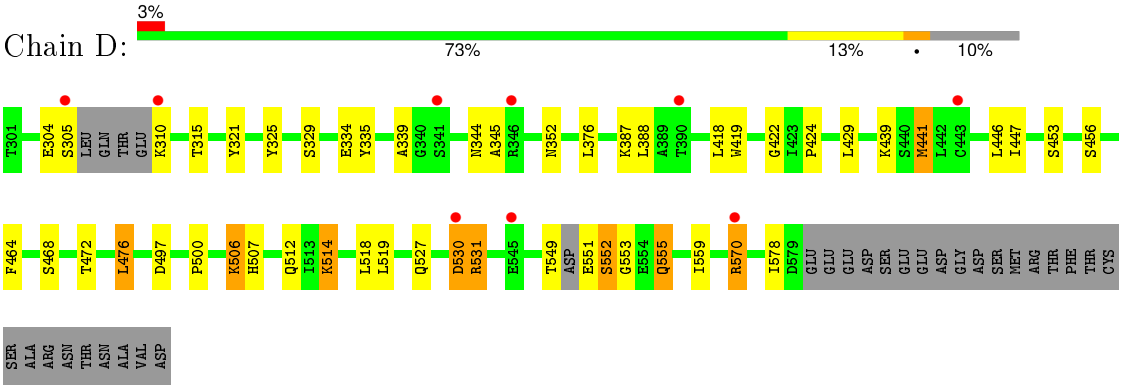
- Molecule 1: REPLICATION PROTEIN E1

Chain C:



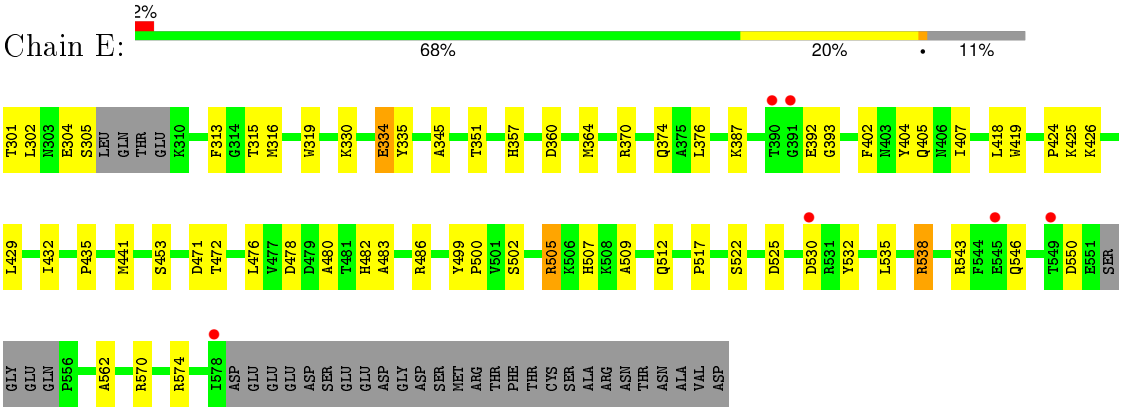
• Molecule 1: REPLICATION PROTEIN E1

Chain D:



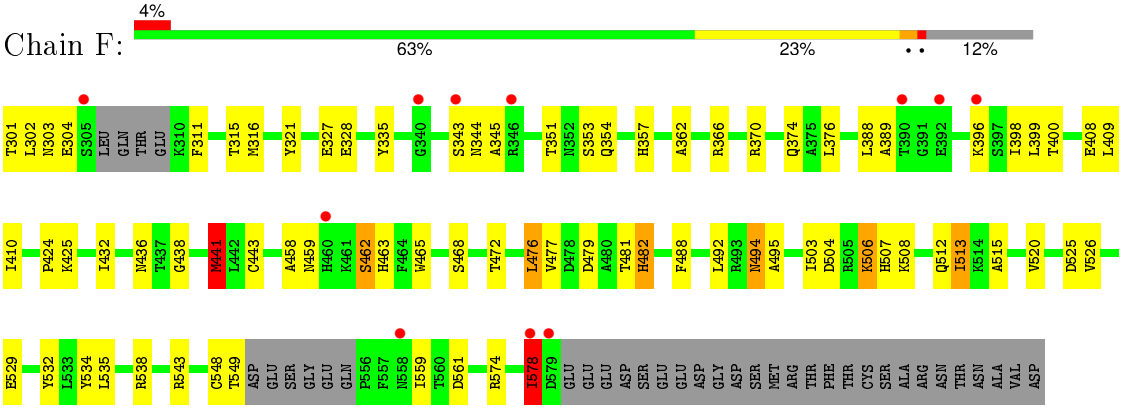
• Molecule 1: REPLICATION PROTEIN E1

Chain E:



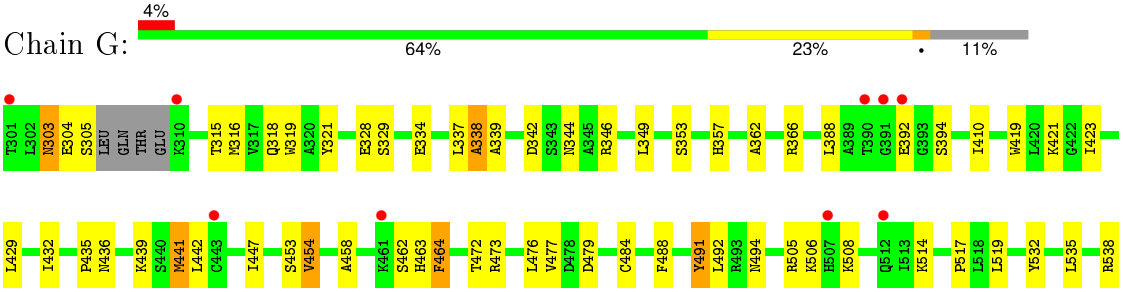
• Molecule 1: REPLICATION PROTEIN E1

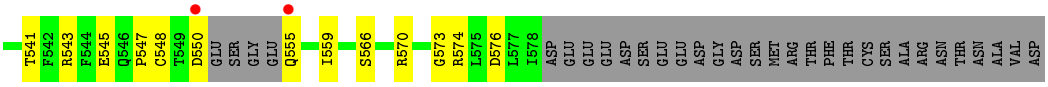
Chain F:



• Molecule 1: REPLICATION PROTEIN E1

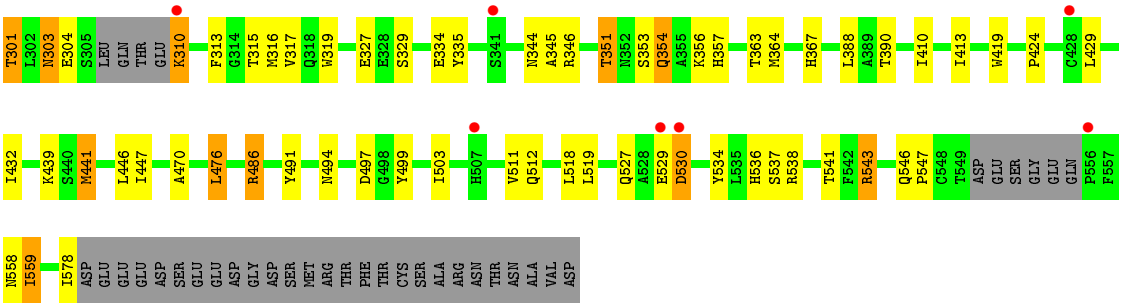
Chain G:





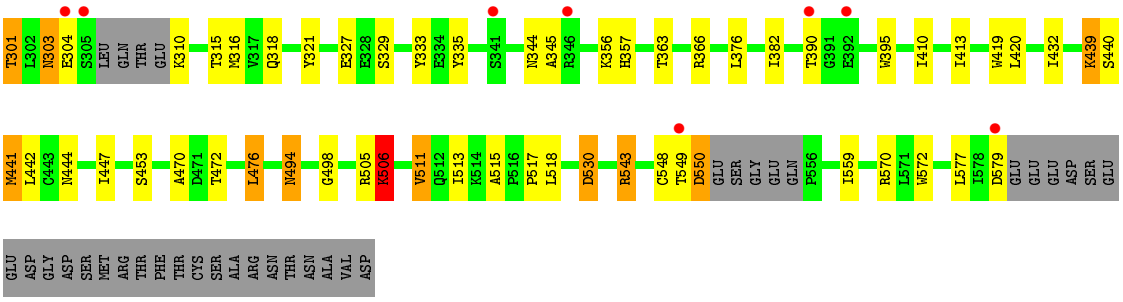
- Molecule 1: REPLICATION PROTEIN E1

Chain H:



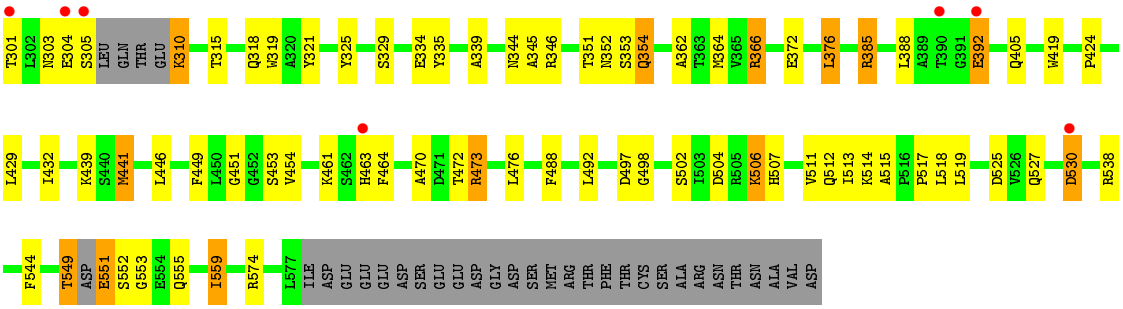
- Molecule 1: REPLICATION PROTEIN E1

Chain I:



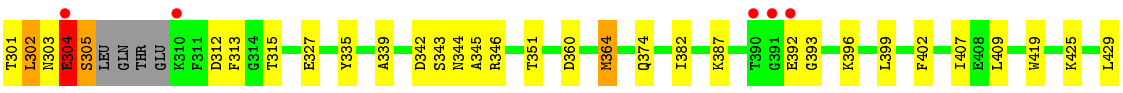
- Molecule 1: REPLICATION PROTEIN E1

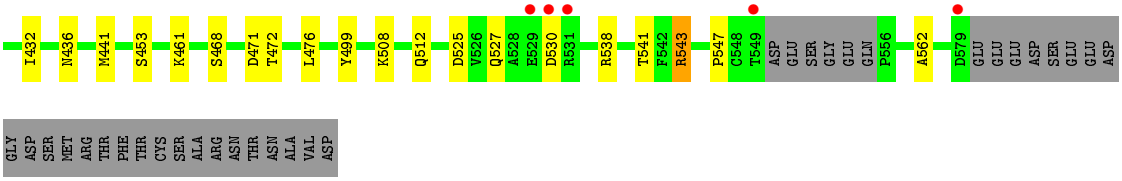
Chain J:



- Molecule 1: REPLICATION PROTEIN E1

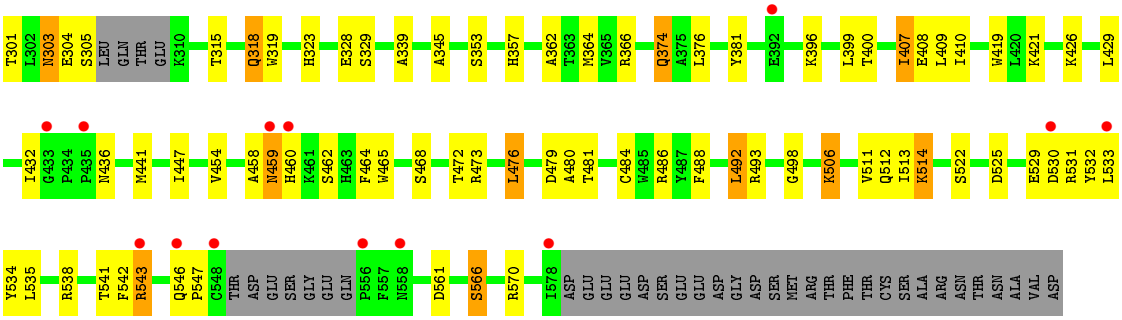
Chain K:





- Molecule 1: REPLICATION PROTEIN E1

Chain L:



4 Data and refinement statistics (i)

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 (1.00%)	DCC
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
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	2 of 86043 reflections (0.002%)	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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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(^{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
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 (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

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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:K:453:SER:HB3	1:K:472:THR:HG21	1.71	0.71
1:I:498:GLY:HA2	1:I:515:ALA:HB3	1.73	0.71
1:A:376:LEU:O	1:A:473:ARG:NH2	2.24	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
2:G:1579:PO4:O1	2:G:1580:PO4:O2	2.10	0.69
1:B:303:ASN:HD22	1:C:318:GLN:HA	1.57	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:D:304:GLU:CG	1:D:305:SER:H	2.02	0.60
1:B:303:ASN:ND2	1:C:318:GLN:HA	2.15	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:K:419:TRP:CD1	1:K:429:LEU:HG	2.40	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
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:E:453:SER:HB3	1:E:472:THR:HG21	1.88	0.55
1:D:551:GLU:HG3	1:D:552:SER:N	2.21	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:K:304:GLU:HG3	1:K:305:SER:N	2.23	0.54
1:B:447:ILE:HG13	1:B:476:LEU:HB2	1.89	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:H:424:PRO:HA	1:H:497:ASP:O	2.09	0.53
1:F:438:GLY:O	1:F:441:MET:HB3	2.07	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:J:304:GLU:HG2	1:J:305:SER:N	2.23	0.53
1:C:453:SER:HB3	1:C:472:THR: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: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:E:505:ARG:HH11	1:E:505:ARG:CB	2.22	0.53
1:C:325:TYR:CE1	1:C:334:GLU:HG2	2.43	0.53
1:L:534:TYR:CE2	1:L:538:ARG:CZ	2.92	0.52
1:H:441:MET:CE	1:H:559:ILE:H	2.21	0.52
1:F:432:ILE:HD13	1:F:525:ASP:HA	1.90	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:H:316:MET:HE1	1:H:357:HIS:HB3	1.92	0.52
1:E:425:LYS:HG2	1:E:538:ARG:HG3	1.92	0.52
1:D:453:SER:HB2	1:E:512:GLN:OE1	2.10	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:K:360:ASP:O	1:K:364:MET:HB2	2.11	0.51
1:G:473:ARG:O	1:G:517:PRO:HD2	2.10	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:J:339:ALA:HA	1:J:345:ALA:HB3	1.93	0.51
1:B:530:ASP:N	1:B:530:ASP:OD2	2.43	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:A:321:TYR:CE1	1:F:301:THR:HG22	2.46	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:C:351:THR:O	1:C:354:GLN:HG2	2.12	0.49
1:A:513:ILE:HG22	1:A:514:LYS:O	2.12	0.49
1:J:470:ALA:HB1	1:J:511:VAL:HG21	1.95	0.49
1:K:312:ASP:H	1:K:344:ASN:ND2	1.98	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: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: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:B:424:PRO:HA	1:B:497:ASP:O	2.14	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:H:527:GLN:NE2	1:H:536:HIS:HA	2.29	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: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:I:441:MET:CE	1:I:559:ILE:H	2.27	0.47
1:G:338:ALA:O	1:G:342:ASP:HB3	2.14	0.47
1:B:304:GLU:HG3	1:C:315:THR:HA	1.97	0.47
1:K:453:SER:CB	1:K:472:THR:HG21	2.43	0.47
1:I:363:THR:HA	1:I:366:ARG:NH1	2.29	0.47
1:J:385:ARG:HD3	1:J:449:PHE:O	2.14	0.47
1:E:393:GLY:H	1:E:562:ALA:HB1	1.79	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:313:PHE:CZ	1:E:360:ASP:HB3	2.49	0.47
1:G:316:MET:CE	1:G:357:HIS:HB3	2.45	0.47
1:J:335:TYR:CE2	1:J:345:ALA:HA	2.50	0.47
1:B:325:TYR:CE1	1:B:334:GLU:HG2	2.49	0.47
1:L:459:ASN:HB3	1:L:460:HIS:H	1.56	0.47
1:F:315:THR:HB	1:F:344:ASN:ND2	2.30	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:J:530:ASP:N	1:J:530:ASP:OD2	2.47	0.46
1:G:508:LYS:HE3	1:L:328:GLU:HB2	1.95	0.46
1:C:427:ASN:HB3	1:C:496:LEU:O	2.14	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:530:ASP:N	1:C:530:ASP:OD2	2.44	0.46
1:C:447:ILE:HG13	1:C:476:LEU:HB2	1.97	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:J:352:ASN:HA	1:K:313:PHE:CB	2.46	0.46
1:E:532:TYR:HB3	1:E:535:LEU:HD12	1.97	0.46
1:J:304:GLU:HG3	1:K:315:THR:HA	1.98	0.46
1:G:353:SER:O	1:G:357:HIS:CD2	2.69	0.46
1:D:551:GLU:CG	1:D:552:SER:N	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:534:TYR:CZ	1:L:538:ARG:NH2	2.84	0.46
1:G:453:SER:HA	1:H:512:GLN:HE22	1.80	0.46
1:A:470:ALA:HA	1:A:513:ILE:HD12	1.97	0.46
1:B:315:THR:HB	1:B:344:ASN:ND2	2.30	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:J:446:LEU:HD23	1:J:519:LEU:HD11	1.97	0.45
1:I:453:SER:HA	1:J:512:GLN:HE22	1.82	0.45
1:I:395:TRP:NE1	1:I:570:ARG:HD2	2.31	0.45
1:E:304:GLU:HB3	1:E:305:SER:H	1.65	0.45
1:A:417:LYS:HD2	1:A:576:ASP:HB2	1.97	0.45
1:A:441:MET:HE1	1:A:559:ILE:N	2.14	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:E:404:TYR:O	1:E:546:GLN:HG3	2.16	0.45
1:H:447:ILE:HG13	1:H:476:LEU:HB2	1.99	0.45
1:C:382:ILE:HD11	1:C:420:LEU:HD22	1.98	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:D:530:ASP:OD2	1:D:530:ASP:N	2.49	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: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:G:421:LYS:HB2	1:G:423:ILE:HD12	1.98	0.45
1:E:301:THR:O	1:E:302:LEU:C	2.55	0.44
1:G:435:PRO:HA	2:G:1580:PO4:O2	2.18	0.44
1:C:319:TRP:HH2	1:C:334:GLU:HB3	1.81	0.44
1:H:541:THR:HB	1:H:543:ARG:HH21	1.83	0.44
1:H:446:LEU:HD23	1:H:519:LEU:HD11	1.99	0.44
1:I:419:TRP:CE2	1:I:517:PRO:HB3	2.52	0.44
1:B:419:TRP:CD1	1:B:429:LEU:HG	2.52	0.44
1:H:364:MET:O	1:H:367:HIS:HB2	2.18	0.44
1:J:419:TRP:CE2	1:J:517:PRO:HB3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:463:HIS:HE1	1:F:504:ASP:OD2	2.00	0.44
1:E:301:THR:HG22	1:F:321:TYR:CZ	2.53	0.44
1:H:534:TYR:O	1:H:538:ARG:NH1	2.51	0.44
1:G:328:GLU:HB3	1:H:367:HIS:HE1	1.82	0.44
1:F:503:ILE:HD12	1:F:513:ILE:HD13	1.92	0.44
1:C:419:TRP:CE2	1:C:517:PRO:HB3	2.53	0.44
1:H:419:TRP:CD1	1:H:429:LEU:HG	2.53	0.44
1:D:422:GLY:HA3	1:D:514:LYS:NZ	2.32	0.44
1:C:454:VAL:HG21	1:D:500:PRO:HB2	2.00	0.44
1:H:346:ARG:HE	1:H:346:ARG:HB2	1.62	0.44
1:L:339:ALA:HA	1:L:345:ALA:HB3	1.99	0.44
1:E:370:ARG:O	1:E:374:GLN:HG2	2.17	0.44
1:G:362:ALA:O	1:G:366:ARG:HG2	2.18	0.44
1:E:402:PHE:HD1	1:E:407:ILE:HD11	1.83	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:J:551:GLU:HB3	1:J:552:SER:H	1.56	0.43
1:I:410:ILE:HA	1:I:413:ILE:HD12	2.00	0.43
1:E:482:HIS:O	1:E:483:ALA:C	2.56	0.43
1:C:339:ALA:HA	1:C:345:ALA:HB3	2.00	0.43
1:D:456:SER:HB2	1:E:502:SER:HB3	2.00	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:E:330:LYS:O	1:E:334:GLU:HB2	2.18	0.43
1:K:512:GLN:HB3	1:K:512:GLN:HE21	1.58	0.43
1:J:385:ARG:NH1	1:J:451:GLY:N	2.66	0.43
1:C:464:PHE:CE1	1:C:506:LYS:HA	2.53	0.43
1:F:534:TYR:CE2	1:F:538:ARG:CZ	3.02	0.43
1:E:435:PRO:HB3	1:F:534:TYR:CE1	2.53	0.43
1:H:304:GLU:HG3	1:I:315:THR:HA	2.00	0.43
1:I:506:LYS:NZ	1:J:504:ASP:OD1	2.51	0.43
1:E:432:ILE:HD13	1:E:525:ASP:HA	1.99	0.43
1:J:353:SER:O	1:J:354:GLN:C	2.56	0.43
1:K:304:GLU:OE1	1:L:315:THR:HG23	2.19	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: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:K:399:LEU:HD13	1:K:409:LEU:HD22	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:B:470:ALA:HB2	1:B:503:ILE:HG21	2.01	0.43
1:K:339:ALA:HA	1:K:345:ALA:HB3	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:L:570:ARG:HD2	1:L:570:ARG:HA	1.87	0.43
1:H:432:ILE:HD12	1:H:541:THR:HG23	2.00	0.43
1:L:376:LEU:O	1:L:473:ARG:NH2	2.41	0.43
1:F:327:GLU:O	1:F:328:GLU:C	2.56	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:A:432:ILE:HD13	1:A:541:THR:HG23	2.01	0.42
1:J:405:GLN:HG3	1:J:544:PHE:CD1	2.53	0.42
1:G:319:TRP:HH2	1:G:334:GLU:HB3	1.83	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:F:482:HIS:CE1	1:F:532:TYR:HH	2.37	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: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:G:321:TYR:CE1	1:L:301:THR:HG22	2.55	0.42
1:E:405:GLN:NE2	1:E:546:GLN:HB2	2.34	0.42
1:A:478:ASP:HB3	1:B:494:ASN:HD22	1.83	0.42
1:D:424:PRO:HA	1:D:497:ASP:O	2.19	0.42
1:B:374:GLN:HE22	1:B:513:ILE:HD11	1.85	0.42
1:C:410:ILE:HA	1:C:413:ILE:HD12	2.02	0.42
1:K:453:SER:HB3	1:K:472:THR:CG2	2.44	0.42
1:J:315:THR:HB	1:J:344:ASN:ND2	2.34	0.42
1:G:436:ASN:O	1:G:547:PRO:HA	2.19	0.42
1:K:335:TYR:CE2	1:K:345:ALA:HA	2.54	0.42
1:J:319:TRP:HH2	1:J:334:GLU:HB3	1.85	0.42
1:K:393:GLY:H	1:K:562:ALA:HB1	1.85	0.41
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: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:G:304:GLU:HG3	1:H:315:THR:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:335:TYR:CE2	1:I:345:ALA:HA	2.54	0.41
1:C:335:TYR:OH	1:C:344:ASN:ND2	2.52	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:I:442:LEU:HD12	1:I:559:ILE:HD12	2.02	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:K:402:PHE:HD1	1:K:407:ILE:HD11	1.86	0.41
1:C:401:PHE:HE2	1:C:544:PHE:CE2	2.38	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:L:484:CYS:O	1:L:488:PHE:HD2	2.04	0.41
1:I:382:ILE:HD11	1:I:420:LEU:HD22	2.02	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:F:443:CYS:HB3	1:F:476:LEU:HD12	2.03	0.41
1:B:346:ARG:HB2	1:B:346:ARG:HE	1.59	0.41
1:D:304:GLU:CG	1:D:305:SER:N	2.71	0.41
1:A:316:MET:CE	1:A:357:HIS:HB3	2.50	0.41
1:H:303:ASN:ND2	1:I:318:GLN:HA	2.35	0.41
1:I:432:ILE:O	1:I:543:ARG:HA	2.21	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:A:501:VAL:HG22	1:A:502:SER:N	2.36	0.41
1:H:319:TRP:HH2	1:H:334:GLU:HB3	1.86	0.41
1:E:424:PRO:O	1:E:425:LYS:HB2	2.20	0.41
1:K:374:GLN:NE2	1:K:471:ASP:HA	2.36	0.41
1:B:404:TYR:OH	1:B:547:PRO:O	2.31	0.41
1:I:572:TRP:NE1	1:I:577:LEU:O	2.54	0.41
1:A:337:LEU:C	1:A:339:ALA:H	2.23	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:H:315:THR:HB	1:H:344:ASN:ND2	2.36	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:K:425:LYS:HG2	1:K:538:ARG:HG2	2.02	0.40
1:E:316:MET:HE1	1:E:357:HIS:HB3	2.01	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: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:B:577:LEU:O	1:B:578:ILE:C	2.59	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:J:405:GLN:HG3	1:J:544:PHE:CG	2.57	0.40
1:I:335:TYR:OH	1:I:344:ASN:ND2	2.53	0.40
1:D:335:TYR:OH	1:D:344:ASN:ND2	2.55	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

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%)	24 66
1	B	262/305 (86%)	251 (96%)	10 (4%)	1 (0%)	39 80
1	C	261/305 (86%)	252 (97%)	9 (3%)	0	100 100
1	D	268/305 (88%)	256 (96%)	8 (3%)	4 (2%)	13 50
1	E	264/305 (87%)	246 (93%)	18 (7%)	0	100 100
1	F	263/305 (86%)	239 (91%)	17 (6%)	7 (3%)	6 32
1	G	264/305 (87%)	241 (91%)	17 (6%)	6 (2%)	8 36
1	H	262/305 (86%)	249 (95%)	12 (5%)	1 (0%)	39 80
1	I	264/305 (87%)	250 (95%)	12 (4%)	2 (1%)	24 66
1	J	266/305 (87%)	252 (95%)	12 (4%)	2 (1%)	24 66
1	K	263/305 (86%)	251 (95%)	10 (4%)	2 (1%)	24 66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	261/305 (86%)	236 (90%)	22 (8%)	3 (1%)	17	58
All	All	3164/3660 (86%)	2968 (94%)	166 (5%)	30 (1%)	21	64

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 (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%)	209 (91%)	20 (9%)	13 43
1	B	225/259 (87%)	206 (92%)	19 (8%)	14 45
1	C	224/259 (86%)	207 (92%)	17 (8%)	16 51
1	D	229/259 (88%)	212 (93%)	17 (7%)	17 52
1	E	228/259 (88%)	209 (92%)	19 (8%)	14 46
1	F	226/259 (87%)	197 (87%)	29 (13%)	5 23
1	G	226/259 (87%)	203 (90%)	23 (10%)	9 33
1	H	225/259 (87%)	203 (90%)	22 (10%)	10 36
1	I	227/259 (88%)	208 (92%)	19 (8%)	14 45
1	J	228/259 (88%)	200 (88%)	28 (12%)	6 25
1	K	226/259 (87%)	208 (92%)	18 (8%)	15 47
1	L	224/259 (86%)	192 (86%)	32 (14%)	4 19
All	All	2717/3108 (87%)	2454 (90%)	263 (10%)	10 37

All (263) 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	476	LEU
1	A	479	ASP
1	A	506	LYS
1	A	514	LYS
1	A	548	CYS

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Mol	Chain	Res	Type
1	A	550	ASP
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	476	LEU
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	476	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	376	LEU
1	D	387	LYS

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Mol	Chain	Res	Type
1	D	388	LEU
1	D	418	LEU
1	D	441	MET
1	D	468	SER
1	D	476	LEU
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	376	LEU
1	E	387	LYS
1	E	392	GLU
1	E	418	LEU
1	E	426	LYS
1	E	441	MET
1	E	476	LEU
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	376	LEU
1	F	388	LEU
1	F	396	LYS
1	F	400	THR
1	F	408	GLU
1	F	410	ILE

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Mol	Chain	Res	Type
1	F	436	ASN
1	F	441	MET
1	F	468	SER
1	F	472	THR
1	F	476	LEU
1	F	481	THR
1	F	482	HIS
1	F	494	ASN
1	F	506	LYS
1	F	507	HIS
1	F	508	LYS
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

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Mol	Chain	Res	Type
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
1	H	441	MET
1	H	476	LEU
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	376	LEU
1	I	390	THR
1	I	439	LYS
1	I	441	MET
1	I	476	LEU
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

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Mol	Chain	Res	Type
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	376	LEU
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	476	LEU
1	J	502	SER
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	476	LEU
1	K	508	LYS

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Mol	Chain	Res	Type
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
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	533	LEU
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

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Mol	Chain	Res	Type
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
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	0.56	0	6,6,6	0.28	0
2	PO4	A	1581	3	4,4,4	0.81	0	6,6,6	0.29	0
2	PO4	B	1579	3	4,4,4	0.63	0	6,6,6	0.31	0
2	PO4	B	1580	3	4,4,4	0.70	0	6,6,6	0.30	0
2	PO4	C	1579	3	4,4,4	1.27	1 (25%)	6,6,6	0.43	0
2	PO4	C	1580	3	4,4,4	1.20	1 (25%)	6,6,6	0.48	0
2	PO4	D	1580	-	4,4,4	0.50	0	6,6,6	0.28	0
2	PO4	E	1579	-	4,4,4	0.36	0	6,6,6	0.27	0
2	PO4	F	1580	-	4,4,4	0.51	0	6,6,6	0.27	0
2	PO4	G	1579	3	4,4,4	0.69	0	6,6,6	0.31	0
2	PO4	G	1580	3	4,4,4	0.80	0	6,6,6	0.27	0
2	PO4	H	1579	3	4,4,4	0.66	0	6,6,6	0.31	0
2	PO4	H	1580	3	4,4,4	0.62	0	6,6,6	0.29	0
2	PO4	I	1580	3	4,4,4	0.70	0	6,6,6	0.31	0
2	PO4	I	1581	3	4,4,4	0.72	0	6,6,6	0.30	0
2	PO4	J	1578	-	4,4,4	0.52	0	6,6,6	0.27	0
2	PO4	K	1580	-	4,4,4	0.43	0	6,6,6	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	PO4	L	1579	-	4,4,4	0.32	0	6,6,6	0.28	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PO4	A	1580	3	-	0/0/0/0	0/0/0/0
2	PO4	A	1581	3	-	0/0/0/0	0/0/0/0
2	PO4	B	1579	3	-	0/0/0/0	0/0/0/0
2	PO4	B	1580	3	-	0/0/0/0	0/0/0/0
2	PO4	C	1579	3	-	0/0/0/0	0/0/0/0
2	PO4	C	1580	3	-	0/0/0/0	0/0/0/0
2	PO4	D	1580	-	-	0/0/0/0	0/0/0/0
2	PO4	E	1579	-	-	0/0/0/0	0/0/0/0
2	PO4	F	1580	-	-	0/0/0/0	0/0/0/0
2	PO4	G	1579	3	-	0/0/0/0	0/0/0/0
2	PO4	G	1580	3	-	0/0/0/0	0/0/0/0
2	PO4	H	1579	3	-	0/0/0/0	0/0/0/0
2	PO4	H	1580	3	-	0/0/0/0	0/0/0/0
2	PO4	I	1580	3	-	0/0/0/0	0/0/0/0
2	PO4	I	1581	3	-	0/0/0/0	0/0/0/0
2	PO4	J	1578	-	-	0/0/0/0	0/0/0/0
2	PO4	K	1580	-	-	0/0/0/0	0/0/0/0
2	PO4	L	1579	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1579	PO4	P-O3	-2.05	1.46	1.53
2	C	1580	PO4	P-O2	-2.03	1.46	1.53

There are no bond angle outliers.

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	A	1581	PO4	1	0
2	B	1579	PO4	1	0
2	B	1580	PO4	1	0
2	D	1580	PO4	1	0
2	G	1579	PO4	1	0
2	G	1580	PO4	2	0
2	H	1579	PO4	2	0
2	H	1580	PO4	1	0
2	I	1580	PO4	2	0
2	I	1581	PO4	1	0
2	J	1578	PO4	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	272/305 (89%)	0.03	15 (5%)	29	11	65, 76, 100, 124	0
1	B	268/305 (87%)	-0.09	5 (1%)	70	41	67, 76, 86, 95	0
1	C	267/305 (87%)	-0.23	5 (1%)	70	41	70, 76, 87, 98	0
1	D	274/305 (89%)	0.03	9 (3%)	50	22	70, 76, 87, 97	0
1	E	270/305 (88%)	-0.05	6 (2%)	65	35	63, 76, 91, 104	0
1	F	269/305 (88%)	0.05	11 (4%)	41	16	60, 77, 92, 104	1 (0%)
1	G	270/305 (88%)	0.05	11 (4%)	41	16	64, 76, 99, 121	0
1	H	268/305 (87%)	-0.03	7 (2%)	59	29	68, 76, 87, 94	0
1	I	270/305 (88%)	-0.17	8 (2%)	54	25	67, 76, 88, 102	0
1	J	272/305 (89%)	-0.05	7 (2%)	59	29	69, 76, 85, 102	0
1	K	269/305 (88%)	-0.10	10 (3%)	45	19	62, 76, 90, 98	0
1	L	267/305 (87%)	0.16	13 (4%)	33	13	63, 77, 90, 102	1 (0%)
All	All	3236/3660 (88%)	-0.03	107 (3%)	50	22	60, 76, 90, 124	2 (0%)

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	433	GLY	5.5
1	J	392	GLU	4.6
1	F	340	GLY	4.4
1	G	390	THR	4.4
1	A	304	GLU	4.4
1	F	579	ASP	4.3
1	L	558	ASN	4.1
1	L	460	HIS	4.1
1	I	392	GLU	4.0
1	I	579	ASP	3.7
1	A	390	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	F	346	ARG	3.7
1	G	507	HIS	3.7
1	B	530	ASP	3.6
1	I	305	SER	3.6
1	A	305	SER	3.5
1	G	461	LYS	3.5
1	E	549	THR	3.5
1	F	305	SER	3.5
1	D	443	CYS	3.4
1	G	310	LYS	3.4
1	H	341	SER	3.4
1	D	310	LYS	3.2
1	A	506	LYS	3.2
1	E	530	ASP	3.2
1	E	391	GLY	3.1
1	I	304	GLU	3.1
1	A	579	ASP	3.0
1	D	530	ASP	3.0
1	D	346	ARG	3.0
1	F	460	HIS	3.0
1	F	392	GLU	2.9
1	K	390	THR	2.9
1	I	549	THR	2.9
1	H	310	LYS	2.9
1	L	530	ASP	2.9
1	C	304	GLU	2.8
1	L	548	CYS	2.8
1	E	390	THR	2.8
1	L	578	ILE	2.8
1	A	498	GLY	2.7
1	D	390	THR	2.7
1	K	391	GLY	2.7
1	B	310	LYS	2.7
1	C	392	GLU	2.7
1	D	305	SER	2.6
1	J	301	THR	2.6
1	A	346	ARG	2.6
1	L	392	GLU	2.6
1	F	390	THR	2.6
1	K	392	GLU	2.6
1	H	530	ASP	2.6
1	K	531	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	556	PRO	2.6
1	L	556	PRO	2.6
1	L	543	ARG	2.5
1	A	463	HIS	2.5
1	A	301	THR	2.5
1	J	304	GLU	2.5
1	C	305	SER	2.5
1	A	324	LYS	2.5
1	L	459	ASN	2.5
1	B	341	SER	2.5
1	K	549	THR	2.4
1	K	310	LYS	2.4
1	A	392	GLU	2.4
1	G	550	ASP	2.4
1	L	533	LEU	2.4
1	I	341	SER	2.3
1	D	570	ARG	2.3
1	F	343	SER	2.3
1	B	352	ASN	2.3
1	H	529	GLU	2.3
1	G	391	GLY	2.3
1	I	346	ARG	2.3
1	D	545	GLU	2.3
1	A	505	ARG	2.3
1	E	545	GLU	2.3
1	I	390	THR	2.3
1	G	392	GLU	2.3
1	A	558	ASN	2.2
1	K	304	GLU	2.2
1	L	435	PRO	2.2
1	C	301	THR	2.2
1	F	396	LYS	2.2
1	H	507	HIS	2.2
1	G	555	GLN	2.2
1	G	443	CYS	2.1
1	K	579	ASP	2.1
1	G	512	GLN	2.1
1	A	530	ASP	2.1
1	K	530	ASP	2.1
1	J	305	SER	2.1
1	J	463	HIS	2.1
1	F	578	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	578	ILE	2.1
1	J	530	ASP	2.1
1	J	390	THR	2.1
1	D	341	SER	2.0
1	B	549	THR	2.0
1	K	529	GLU	2.0
1	L	546	GLN	2.0
1	F	558	ASN	2.0
1	G	301	THR	2.0
1	H	428	CYS	2.0
1	C	390	THR	2.0
1	A	391	GLY	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	PO4	G	1580	5/5	0.73	0.43	3.57	77,79,80,81	5
2	PO4	A	1581	5/5	0.90	0.20	-0.33	78,79,79,79	5
2	PO4	C	1580	5/5	0.91	0.15	-0.75	82,84,85,86	0
2	PO4	G	1579	5/5	0.90	0.18	-0.76	77,79,80,82	0
3	MG	H	1581	1/1	0.90	0.16	-1.19	64,64,64,64	0
2	PO4	B	1579	5/5	0.94	0.15	-1.33	77,78,79,79	0
3	MG	B	1581	1/1	0.94	0.15	-1.38	54,54,54,54	0
2	PO4	I	1581	5/5	0.92	0.13	-1.45	78,79,80,82	0
2	PO4	D	1580	5/5	0.94	0.13	-1.46	86,87,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	PO4	I	1580	5/5	0.96	0.14	-1.51	76,77,78,78	0
3	MG	G	1581	1/1	0.93	0.17	-1.53	67,67,67,67	0
2	PO4	L	1579	5/5	0.94	0.17	-1.58	94,95,96,97	0
2	PO4	C	1579	5/5	0.96	0.13	-1.66	82,83,84,84	0
2	PO4	H	1579	5/5	0.96	0.11	-1.71	79,81,81,81	0
2	PO4	B	1580	5/5	0.94	0.11	-1.77	80,82,83,83	0
3	MG	I	1582	1/1	0.86	0.16	-1.98	64,64,64,64	0
2	PO4	E	1579	5/5	0.98	0.12	-2.09	86,86,88,88	0
2	PO4	J	1578	5/5	0.97	0.10	-2.10	82,82,83,83	0
2	PO4	H	1580	5/5	0.96	0.11	-2.14	79,80,80,82	0
3	MG	C	1581	1/1	0.83	0.13	-2.36	68,68,68,68	0
3	MG	A	1582	1/1	0.93	0.14	-2.40	74,74,74,74	0
2	PO4	K	1580	5/5	0.96	0.11	-2.72	87,88,89,89	0
2	PO4	F	1580	5/5	0.98	0.11	-2.87	83,84,84,84	0
2	PO4	A	1580	5/5	0.96	0.10	-3.23	76,76,79,79	0

6.5 Other polymers (i)

There are no such residues in this entry.