Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 04:27 AM EDT

PDB ID	:	1ECR
Title	:	ESCHERICHIA COLI REPLICATION TERMINATOR PROTEIN (TUS) COMPLEXED WITH DNA
Authors	:	Kamada, K.; Morikawa, K.
Deposited on	:	1996-09-01
Resolution	:	2.70 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

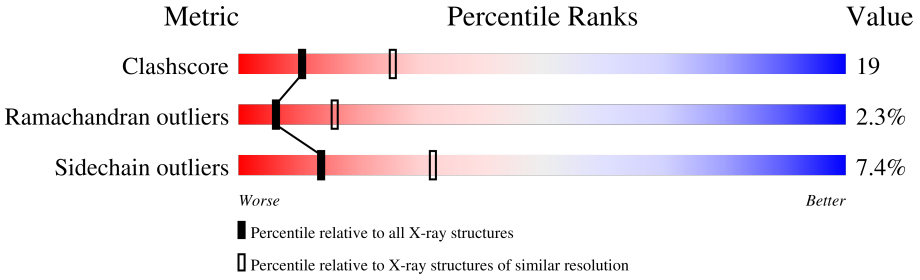
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	B	16	25% 31% 31% 6% 6%
2	C	16	6% 69% 19% 6%
3	A	309	62% 32% 5% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3152 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a DNA chain called DNA (5'-D(*TP*TP*AP*GP*TP*TP*AP*CP*AP*AP*CP*AP*TP*AP*CP*T)-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	B	15	302	147	54	87	14	0	0	0

- Molecule 2 is a DNA chain called DNA (5'-D(*TP*AP*GP*TP*AP*TP*GP*TP*TP*GP*TP*AP*AP*CP*TP*A)-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	C	15	306	149	52	91	14	0	0	0

- Molecule 3 is a protein called PROTEIN (REPLICATION-TERMINATOR PROTEIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	305	2495	1584	469	439	3	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	B	5	5	5	0	0
4	C	12	12	12	0	0
4	A	32	32	32	0	0

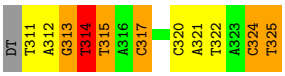
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

• Molecule 1: DNA (5'-D(*TP*TP*AP*GP*TP*TP*AP*CP*AP*AP*CP*AP*TP*AP*CP*T)-3

Chain B: 25% 31% 31% 6% 6%

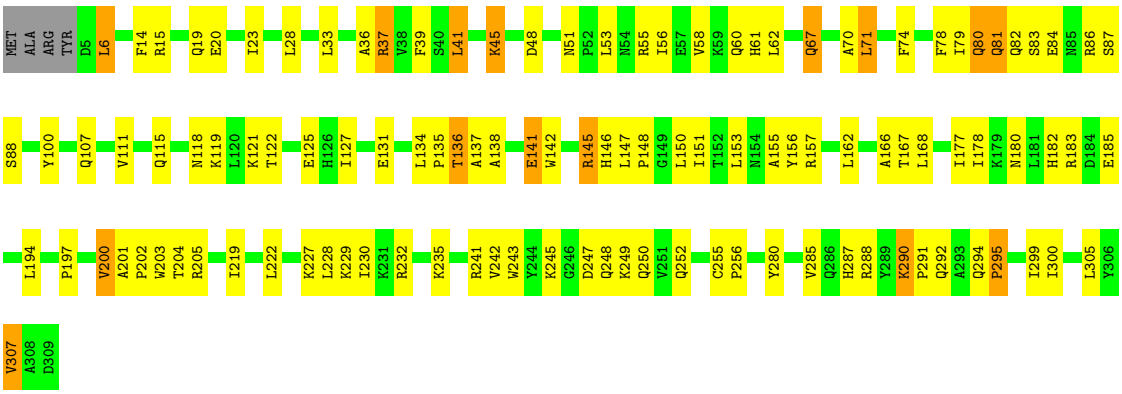


• Molecule 2: DNA (5'-D(*TP*AP*GP*TP*AP*TP*GP*TP*TP*GP*TP*AP*AP*CP*TP*A)-3

Chain C: 6% 69% 19% 6%

• Molecule 3: PROTEIN (REPLICATION-TERMINATOR PROTEIN)

Chain A: 62% 32% 5%



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	68.15Å 68.15Å 230.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.196 , 0.314	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3152	wwPDB-VP
Average B, all atoms ($Å^2$)	28.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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	B	2.37	12/338 (3.6%)	2.14	17/519 (3.3%)
2	C	2.20	9/342 (2.6%)	2.13	17/527 (3.2%)
3	A	0.58	0/2553	0.80	1/3465 (0.0%)
All	All	1.17	21/3233 (0.6%)	1.24	35/4511 (0.8%)

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	B	0	1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	314	DT	C3'-C2'	-11.84	1.38	1.52
2	C	335	DT	C2'-C1'	-10.90	1.41	1.52
2	C	335	DT	P-O5'	-9.57	1.50	1.59
1	B	315	DT	C3'-C2'	-8.50	1.42	1.52
1	B	314	DT	O4'-C1'	8.34	1.52	1.42
1	B	314	DT	C2'-C1'	-7.94	1.44	1.52
2	C	335	DT	C4'-O4'	7.63	1.52	1.45
2	C	335	DT	C3'-C2'	-7.56	1.43	1.52
1	B	320	DC	C3'-C2'	-6.96	1.43	1.52
1	B	321	DA	C3'-C2'	-6.92	1.44	1.52
2	C	333	DG	C2'-C1'	-6.83	1.45	1.52
1	B	314	DT	C4'-O4'	6.76	1.51	1.45
2	C	335	DT	O4'-C1'	6.75	1.50	1.42
2	C	334	DT	O3'-P	-6.10	1.53	1.61
1	B	311	DT	C5-C7	5.83	1.53	1.50
1	B	312	DA	C2'-C1'	-5.62	1.46	1.52
1	B	314	DT	C5'-C4'	-5.61	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	317	DC	C4'-C3'	-5.59	1.47	1.52
1	B	313	DG	P-O5'	5.42	1.65	1.59
2	C	332	DT	C2'-C1'	-5.33	1.47	1.52
2	C	338	DA	N9-C4	-5.29	1.34	1.37

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	335	DT	O4'-C1'-N1	13.46	117.42	108.00
1	B	314	DT	O4'-C4'-C3'	-10.90	99.46	106.00
2	C	335	DT	O4'-C4'-C3'	-10.33	99.80	106.00
1	B	314	DT	C4'-C3'-C2'	10.07	112.16	103.10
1	B	314	DT	P-O5'-C5'	9.33	135.83	120.90
1	B	314	DT	O4'-C1'-N1	9.16	114.41	108.00
2	C	335	DT	P-O5'-C5'	9.05	135.38	120.90
2	C	335	DT	C4'-C3'-C2'	8.22	110.50	103.10
1	B	314	DT	N1-C1'-C2'	-8.13	97.16	112.60
1	B	320	DC	O4'-C1'-N1	7.61	113.33	108.00
1	B	315	DT	O4'-C1'-N1	7.46	113.22	108.00
2	C	338	DA	O4'-C1'-N9	6.73	112.71	108.00
1	B	317	DC	O4'-C1'-N1	6.12	112.28	108.00
2	C	337	DT	O4'-C1'-N1	6.03	112.22	108.00
1	B	324	DC	O4'-C1'-N1	6.00	112.20	108.00
2	C	334	DT	C6-C5-C7	-5.96	119.32	122.90
1	B	315	DT	C6-C5-C7	-5.84	119.39	122.90
3	A	80	GLN	N-CA-C	-5.79	95.36	111.00
1	B	314	DT	C6-C5-C7	-5.74	119.45	122.90
1	B	322	DT	C6-C5-C7	-5.72	119.47	122.90
2	C	327	DT	C6-C5-C7	-5.67	119.50	122.90
2	C	336	DG	O4'-C1'-N9	5.67	111.97	108.00
2	C	330	DT	C6-C5-C7	-5.61	119.53	122.90
2	C	334	DT	P-O3'-C3'	5.58	126.40	119.70
1	B	325	DT	C6-C5-C7	-5.58	119.55	122.90
1	B	311	DT	C6-C5-C7	-5.53	119.58	122.90
1	B	314	DT	C3'-C2'-C1'	5.52	109.13	102.50
2	C	335	DT	C4-C5-C6	5.52	121.31	118.00
2	C	337	DT	C6-C5-C7	-5.46	119.63	122.90
2	C	341	DT	C6-C5-C7	-5.40	119.66	122.90
1	B	313	DG	O4'-C1'-N9	5.34	111.74	108.00
2	C	335	DT	C6-C5-C7	-5.30	119.72	122.90
2	C	339	DA	O4'-C1'-N9	5.24	111.67	108.00
1	B	322	DT	C4-C5-C6	5.21	121.12	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	327	DT	C4-C5-C6	5.16	121.10	118.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	314	DT	Sidechain

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	B	302	0	172	14	0
2	C	306	0	174	8	0
3	A	2495	0	2533	97	0
4	A	32	0	0	1	0
4	B	5	0	0	0	0
4	C	12	0	0	0	0
All	All	3152	0	2879	111	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 19.

All (111) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:327:DT:H2'	2:C:327:DT:O2	1.57	0.99
1:B:315:DT:C5'	3:A:291:PRO:HD3	1.99	0.91
3:A:145:ARG:HH11	3:A:145:ARG:HB2	1.43	0.84
1:B:315:DT:H5"	3:A:291:PRO:HD3	1.60	0.84
3:A:41:LEU:HD12	3:A:58:VAL:HG12	1.63	0.80
3:A:53:LEU:HD23	3:A:235:LYS:HE2	1.64	0.79
3:A:45:LYS:H	3:A:45:LYS:HD2	1.47	0.79
1:B:313:DG:H2"	1:B:314:DT:H72	1.67	0.77
2:C:327:DT:O2	2:C:327:DT:C2'	2.33	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:48:ASP:HA	3:A:51:ASN:OD1	1.85	0.76
3:A:182:HIS:HB2	3:A:185:GLU:HG3	1.69	0.75
1:B:313:DG:H2"	1:B:314:DT:C7	2.17	0.75
3:A:125:GLU:HA	3:A:156:TYR:CE1	2.23	0.74
3:A:55:ARG:HH11	3:A:55:ARG:HG2	1.55	0.71
1:B:315:DT:H5"	3:A:291:PRO:CD	2.21	0.70
3:A:37:ARG:NH1	3:A:60:GLN:HE22	1.90	0.69
3:A:37:ARG:HH11	3:A:60:GLN:NE2	1.91	0.67
3:A:299:ILE:HD12	3:A:307:VAL:HG21	1.76	0.66
1:B:314:DT:H2'	1:B:315:DT:H71	1.77	0.66
3:A:168:LEU:HD13	3:A:242:VAL:HG22	1.78	0.64
3:A:241:ARG:HD2	3:A:250:GLN:NE2	2.12	0.64
3:A:299:ILE:HG23	3:A:300:ILE:HG13	1.80	0.63
3:A:37:ARG:NH1	3:A:60:GLN:NE2	2.47	0.62
3:A:36:ALA:O	3:A:62:LEU:HD23	1.99	0.62
3:A:200:VAL:HG12	3:A:201:ALA:H	1.65	0.61
3:A:299:ILE:HD12	3:A:307:VAL:CG2	2.31	0.60
3:A:55:ARG:HD2	3:A:280:TYR:O	2.03	0.59
3:A:121:LYS:HE2	3:A:155:ALA:O	2.03	0.58
2:C:335:DT:H5'	3:A:256:PRO:HG3	1.85	0.57
3:A:107:GLN:O	3:A:111:VAL:HG23	2.04	0.57
3:A:118:ASN:HA	3:A:121:LYS:HG3	1.87	0.56
2:C:328:DA:C8	2:C:329:DG:N7	2.74	0.56
3:A:67:GLN:NE2	3:A:100:TYR:OH	2.38	0.56
3:A:115:GLN:O	3:A:119:LYS:HG3	2.06	0.56
3:A:222:LEU:HD11	3:A:299:ILE:HD11	1.87	0.55
1:B:313:DG:H1'	1:B:314:DT:C6	2.42	0.55
3:A:200:VAL:HG12	3:A:201:ALA:N	2.21	0.54
3:A:39:PHE:HE1	3:A:60:GLN:HE21	1.56	0.54
3:A:141:GLU:HG2	3:A:145:ARG:NH1	2.22	0.54
3:A:247:ASP:O	3:A:249:LYS:N	2.36	0.54
1:B:313:DG:H2"	1:B:314:DT:C5	2.43	0.53
3:A:178:ILE:HA	3:A:230:ILE:O	2.08	0.53
3:A:180:ASN:ND2	3:A:229:LYS:HE2	2.24	0.53
3:A:55:ARG:HG2	3:A:55:ARG:NH1	2.22	0.53
3:A:78:PHE:O	3:A:80:GLN:N	2.41	0.53
3:A:243:TRP:CZ3	3:A:245:LYS:HA	2.44	0.52
1:B:315:DT:H5'	3:A:291:PRO:HD3	1.88	0.52
1:B:317:DC:H6	3:A:178:ILE:HB	1.74	0.52
3:A:53:LEU:HD23	3:A:235:LYS:CE	2.38	0.52
3:A:150:LEU:HG	3:A:151:ILE:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:DC:C6	3:A:178:ILE:HB	2.45	0.51
3:A:125:GLU:HA	3:A:156:TYR:HE1	1.70	0.51
3:A:6:LEU:HD12	3:A:142:TRP:CH2	2.46	0.51
2:C:327:DT:C6	2:C:328:DA:C2	2.98	0.51
3:A:201:ALA:HA	3:A:203:TRP:H	1.75	0.51
3:A:167:THR:O	3:A:168:LEU:HD22	2.11	0.51
3:A:135:PRO:O	3:A:137:ALA:N	2.44	0.50
3:A:19:GLN:HE21	3:A:23:ILE:HD11	1.77	0.49
3:A:71:LEU:HA	3:A:74:PHE:HD2	1.77	0.49
3:A:145:ARG:O	3:A:146:HIS:ND1	2.45	0.49
3:A:37:ARG:HG2	3:A:62:LEU:HD23	1.94	0.49
3:A:151:ILE:HG22	3:A:151:ILE:O	2.11	0.49
3:A:147:LEU:O	3:A:150:LEU:HB2	2.13	0.49
3:A:294:GLN:OE1	3:A:295:PRO:HD2	2.12	0.49
3:A:146:HIS:O	3:A:148:PRO:HD2	2.13	0.48
3:A:86:ARG:HG2	3:A:87:SER:N	2.28	0.48
3:A:288:ARG:O	3:A:290:LYS:HG3	2.14	0.48
3:A:33:LEU:HD22	3:A:67:GLN:HG3	1.95	0.48
3:A:55:ARG:HA	3:A:280:TYR:O	2.14	0.48
3:A:41:LEU:HD12	3:A:58:VAL:CG1	2.39	0.48
3:A:145:ARG:HH11	3:A:145:ARG:CB	2.22	0.47
3:A:53:LEU:HD12	3:A:56:ILE:HG12	1.94	0.47
3:A:80:GLN:O	3:A:82:GLN:N	2.48	0.47
2:C:328:DA:H2"	2:C:329:DG:OP2	2.15	0.47
3:A:200:VAL:O	3:A:201:ALA:HB2	2.14	0.47
3:A:45:LYS:HA	3:A:86:ARG:HA	1.96	0.47
1:B:313:DG:H2"	1:B:314:DT:C6	2.50	0.46
3:A:37:ARG:HA	3:A:61:HIS:O	2.16	0.46
3:A:135:PRO:HD2	3:A:138:ALA:HB3	1.98	0.46
3:A:287:HIS:O	3:A:288:ARG:CZ	2.64	0.45
3:A:294:GLN:HA	3:A:295:PRO:HD2	1.81	0.45
3:A:115:GLN:HA	3:A:115:GLN:OE1	2.17	0.45
3:A:168:LEU:CD1	3:A:242:VAL:HG22	2.45	0.44
3:A:127:ILE:HA	3:A:131:GLU:HB2	1.99	0.44
1:B:324:DC:C2'	1:B:325:DT:H71	2.47	0.44
3:A:70:ALA:O	3:A:74:PHE:CD2	2.71	0.44
3:A:134:LEU:HA	3:A:135:PRO:HD3	1.69	0.44
2:C:327:DT:H2"	2:C:328:DA:OP2	2.17	0.43
3:A:194:LEU:HD23	3:A:194:LEU:HA	1.78	0.43
3:A:290:LYS:NZ	3:A:290:LYS:HB2	2.32	0.43
1:B:314:DT:OP1	3:A:285:VAL:HG11	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:122:THR:O	3:A:125:GLU:HB3	2.19	0.42
3:A:166:ALA:HB2	3:A:245:LYS:HB2	2.01	0.42
3:A:197:PRO:HB2	3:A:205:ARG:HG3	2.00	0.42
3:A:219:ILE:HD12	3:A:219:ILE:HG23	1.80	0.42
3:A:6:LEU:HD12	3:A:142:TRP:CZ2	2.55	0.42
3:A:183:ARG:HA	3:A:228:LEU:HD12	2.01	0.42
3:A:14:PHE:CZ	3:A:78:PHE:CE1	3.07	0.42
3:A:166:ALA:CB	3:A:245:LYS:HB2	2.49	0.42
3:A:135:PRO:O	3:A:136:THR:C	2.57	0.42
3:A:53:LEU:HD12	3:A:56:ILE:CG1	2.50	0.42
3:A:153:LEU:O	3:A:157:ARG:HG2	2.19	0.42
3:A:79:ILE:C	3:A:81:GLN:N	2.72	0.42
3:A:121:LYS:NZ	4:A:362:HOH:O	2.52	0.41
2:C:339:DA:H2"	2:C:340:DC:C6	2.56	0.41
3:A:227:LYS:HE2	3:A:227:LYS:HB3	1.71	0.41
3:A:28:LEU:HD23	3:A:28:LEU:HA	1.86	0.41
3:A:83:SER:HB3	3:A:86:ARG:HB2	2.02	0.40
3:A:141:GLU:O	3:A:145:ARG:HB2	2.22	0.40
3:A:162:LEU:HD13	3:A:242:VAL:HG11	2.03	0.40
3:A:153:LEU:HD23	3:A:153:LEU:HA	1.93	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
3	A	303/309 (98%)	273 (90%)	23 (8%)	7 (2%)	6 16

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	81	GLN

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Mol	Chain	Res	Type
3	A	136	THR
3	A	200	VAL
3	A	248	GLN
3	A	290	LYS
3	A	295	PRO
3	A	202	PRO

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
3	A	270/273 (99%)	250 (93%)	20 (7%)	13 32

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	6	LEU
3	A	15	ARG
3	A	20	GLU
3	A	37	ARG
3	A	41	LEU
3	A	45	LYS
3	A	67	GLN
3	A	71	LEU
3	A	84	GLU
3	A	88	SER
3	A	141	GLU
3	A	145	ARG
3	A	177	ILE
3	A	204	THR
3	A	232	ARG
3	A	252	GLN
3	A	255	CYS
3	A	292	GLN
3	A	305	LEU
3	A	307	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	16	GLN
3	A	19	GLN
3	A	60	GLN
3	A	176	HIS
3	A	180	ASN
3	A	248	GLN
3	A	292	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.