Full wwPDB X-ray Structure Validation Report (i)

Oct 18, 2023 – 01:07 PM EDT

PDB ID	:	2EWJ
Title	:	Escherichia Coli Replication Terminator Protein (Tus) Complexed With DNA-Locked form
Authors	:	Oakley, A.J.; Mulcair, M.D.; Schaeffer, P.M.; Dixon, N.E.
Deposited on	:	2005-11-03
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 (1)) were used in the production of this report:

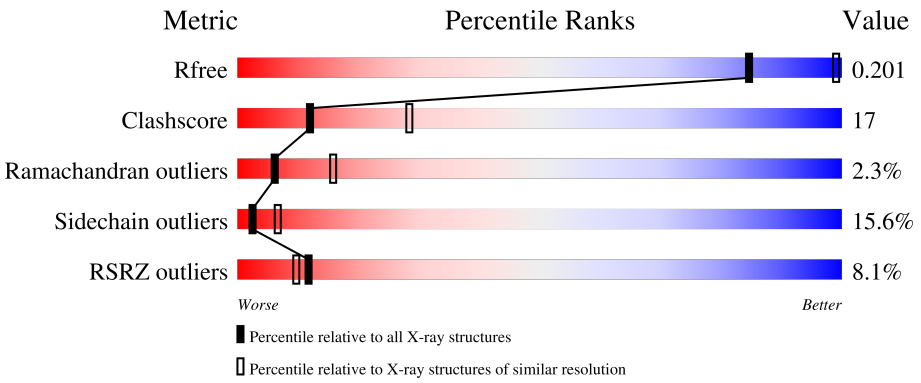
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (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))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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% 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	B	16	19% 38% 38% 6%
2	C	16	19% 12% 62% 12% 12%
3	A	309	8% 55% 36% 7% ••

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
4	IOD	A	1003	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3062 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 5'-D(*T*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	286	137	52	83	14	0	0	0

- Molecule 2 is a DNA chain called 5'-D(*TP*G*AP*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	14	251	119	40	79	13	0	0	1

- Molecule 3 is a protein called DNA replication terminus site-binding 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 IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	I		
4	A	3	3	3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	B	3	3	3	0	0
5	C	5	Total	O	0	0
			5	5		
5	A	19	Total	O	0	0
			19	19		

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 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: 5'-D(*T*TP*AP*GP*TP*TP*TP*AP*CP*AP*AP*CP*AP*TP*AP*CP*T)-3'

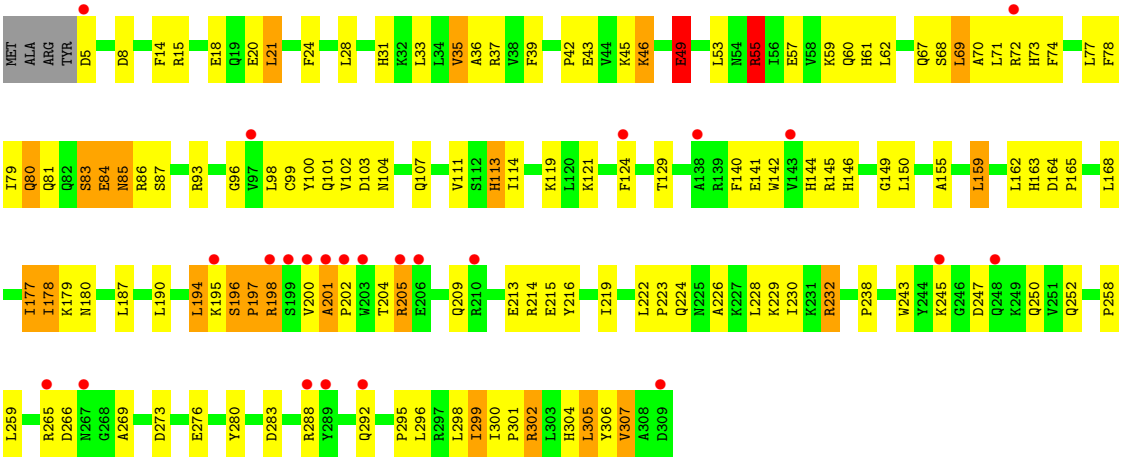
Chain B:

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

Chain C:

• Molecule 3: DNA replication terminus site-binding protein

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	62.68Å 62.68Å 251.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 20.93 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.9 (50.00-2.70) 98.2 (20.93-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.219 , 0.303 0.221 , 0.201	Depositor DCC
R_{free} test set	720 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	47.3	Xtriage
Anisotropy	0.620	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 49.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	3062	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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	1.45	1/320 (0.3%)	2.63	33/492 (6.7%)
2	C	1.55	0/279	2.64	25/431 (5.8%)
3	A	0.81	0/2553	0.97	6/3465 (0.2%)
All	All	0.98	1/3152 (0.0%)	1.49	64/4388 (1.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	321	DA	N9-C4	5.16	1.41	1.37

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	318	DA	O4'-C1'-N9	17.82	120.47	108.00
2	C	338	DA	O4'-C1'-N9	12.35	116.64	108.00
2	C	333	DG	O4'-C1'-N9	11.73	116.21	108.00
2	C	332	DT	P-O3'-C3'	9.93	131.62	119.70
1	B	323	DA	O4'-C1'-N9	-9.47	101.37	108.00
1	B	311	DT	C4-C5-C7	9.03	124.42	119.00
1	B	311	DT	C6-C5-C7	-8.86	117.58	122.90
2	C	334	DT	C4-C5-C7	8.38	124.03	119.00
2	C	336	DG	C1'-O4'-C4'	-8.16	101.94	110.10
1	B	315	DT	O4'-C4'-C3'	-8.12	101.13	106.00
2	C	332	DT	N3-C4-O4	7.95	124.67	119.90
2	C	338	DA	C1'-O4'-C4'	-7.75	102.35	110.10
1	B	319	DA	O4'-C1'-N9	7.56	113.29	108.00
2	C	339	DA	O4'-C1'-N9	7.54	113.28	108.00
1	B	320	DC	C4'-C3'-C2'	-7.49	96.36	103.10
1	B	319	DA	N1-C2-N3	-7.48	125.56	129.30
2	C	337	DT	C6-C5-C7	-7.24	118.56	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	336	DG	C4'-C3'-C2'	-7.13	96.69	103.10
1	B	316	DA	O4'-C1'-N9	6.98	112.89	108.00
1	B	311	DT	C3'-C2'-C1'	-6.89	94.23	102.50
2	C	331	DA	N9-C4-C5	-6.75	103.10	105.80
2	C	331	DA	C8-N9-C4	6.67	108.47	105.80
2	C	331	DA	C1'-O4'-C4'	-6.65	103.45	110.10
2	C	334	DT	C6-C5-C7	-6.64	118.92	122.90
2	C	335	DT	O4'-C1'-N1	6.59	112.61	108.00
1	B	321	DA	C4'-C3'-C2'	-6.43	97.32	103.10
1	B	321	DA	O4'-C4'-C3'	-6.24	102.00	104.50
2	C	338	DA	C3'-C2'-C1'	-6.21	95.05	102.50
1	B	320	DC	O5'-P-OP1	6.20	118.14	110.70
1	B	315	DT	N3-C2-O2	-6.18	118.59	122.30
1	B	317	DC	O4'-C1'-N1	6.17	112.32	108.00
1	B	319	DA	O4'-C1'-C2'	6.11	110.78	105.90
2	C	337	DT	N3-C4-O4	6.10	123.56	119.90
2	C	339	DA	N1-C2-N3	-6.01	126.30	129.30
1	B	321	DA	C2-N3-C4	5.97	113.58	110.60
1	B	311	DT	O4'-C1'-C2'	-5.94	101.15	105.90
1	B	320	DC	N3-C4-N4	-5.93	113.84	118.00
1	B	313	DG	N1-C6-O6	-5.89	116.36	119.90
3	A	247	ASP	CB-CG-OD2	5.86	123.58	118.30
2	C	341	DT	P-O3'-C3'	5.86	126.73	119.70
1	B	314	DT	C5-C4-O4	-5.80	120.84	124.90
1	B	317	DC	C1'-O4'-C4'	-5.78	104.32	110.10
2	C	335	DT	N3-C2-O2	-5.69	118.89	122.30
1	B	320	DC	C1'-O4'-C4'	-5.59	104.51	110.10
2	C	337	DT	P-O3'-C3'	-5.58	113.00	119.70
2	C	337	DT	C4-C5-C7	5.57	122.34	119.00
3	A	283	ASP	CB-CG-OD2	5.57	123.31	118.30
3	A	266	ASP	CB-CG-OD2	5.56	123.30	118.30
1	B	323	DA	O4'-C4'-C3'	-5.55	102.28	104.50
2	C	338	DA	OP1-P-OP2	5.50	127.85	119.60
1	B	323	DA	C8-N9-C4	5.49	108.00	105.80
1	B	320	DC	O5'-P-OP2	-5.46	100.79	105.70
3	A	55	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	B	320	DC	O4'-C4'-C3'	-5.43	102.33	104.50
1	B	319	DA	N9-C4-C5	-5.41	103.64	105.80
1	B	313	DG	C5-C6-N1	5.38	114.19	111.50
2	C	335	DT	P-O5'-C5'	-5.28	112.45	120.90
3	A	21	LEU	CA-CB-CG	5.26	127.39	115.30
3	A	69	LEU	CB-CG-CD1	-5.19	102.17	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	314	DT	O4'-C1'-N1	5.18	111.63	108.00
1	B	323	DA	C3'-C2'-C1'	-5.12	96.35	102.50
2	C	340	DC	O4'-C1'-N1	5.11	111.57	108.00
1	B	320	DC	C4-C5-C6	-5.09	114.85	117.40
1	B	311	DT	O4'-C4'-C3'	-5.03	102.49	104.50

There are no chirality outliers.

There are no planarity outliers.

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	286	0	159	5	0
2	C	251	0	138	3	0
3	A	2495	0	2533	98	0
4	A	3	0	0	3	0
5	A	19	0	0	2	0
5	B	3	0	0	0	0
5	C	5	0	0	0	0
All	All	3062	0	2830	101	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 17.

All (101) 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)
3:A:219:ILE:CD1	3:A:299:ILE:HD11	1.97	0.93
3:A:196:SER:HB2	3:A:197:PRO:HD3	1.52	0.92
3:A:177:ILE:HD11	4:A:1003:IOD:I	2.41	0.90
3:A:201:ALA:HB3	3:A:202:PRO:HD3	1.54	0.87
3:A:144:HIS:HE1	3:A:150:LEU:O	1.63	0.80
3:A:219:ILE:HD13	3:A:299:ILE:HD11	1.64	0.77
3:A:39:PHE:CE1	3:A:60:GLN:HG3	2.21	0.76
3:A:200:VAL:HG13	3:A:201:ALA:N	2.03	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:DA:H2"	1:B:324:DC:H5'	1.73	0.71
3:A:232:ARG:NH1	4:A:1003:IOD:I	2.95	0.70
3:A:37:ARG:HH11	3:A:60:GLN:NE2	1.89	0.70
3:A:42:PRO:HD3	3:A:57:GLU:O	1.93	0.69
3:A:200:VAL:HG13	3:A:201:ALA:H	1.57	0.69
1:B:311:DT:O2	3:A:288:ARG:HD2	1.93	0.68
3:A:177:ILE:CD1	4:A:1003:IOD:I	3.12	0.67
1:B:320:DC:H5"	3:A:129:THR:HG21	1.75	0.66
3:A:201:ALA:CB	3:A:202:PRO:HD3	2.25	0.66
3:A:78:PHE:HB3	3:A:80:GLN:NE2	2.11	0.66
3:A:20:GLU:OE2	3:A:113:HIS:HE1	1.80	0.65
3:A:219:ILE:HD11	3:A:299:ILE:HD11	1.77	0.64
3:A:24:PHE:CZ	3:A:114:ILE:HD11	2.32	0.64
3:A:35:VAL:HG23	3:A:99:CYS:HB2	1.80	0.64
3:A:46:LYS:O	3:A:49:GLU:HB2	1.97	0.64
3:A:141:GLU:HB3	3:A:145:ARG:HH21	1.64	0.63
3:A:200:VAL:CG1	3:A:201:ALA:N	2.62	0.63
3:A:55:ARG:NH1	3:A:57:GLU:HG3	2.14	0.62
3:A:215:GLU:OE1	3:A:302:ARG:NH1	2.33	0.61
3:A:55:ARG:HH11	3:A:55:ARG:HG3	1.66	0.60
3:A:39:PHE:HE1	3:A:60:GLN:HG3	1.66	0.60
3:A:55:ARG:HH12	3:A:57:GLU:HG3	1.66	0.60
3:A:37:ARG:NH1	3:A:276:GLU:HB3	2.17	0.59
3:A:144:HIS:CE1	3:A:150:LEU:O	2.52	0.58
3:A:180:ASN:ND2	3:A:229:LYS:HE2	2.19	0.58
3:A:196:SER:CB	3:A:197:PRO:HD3	2.31	0.57
3:A:83:SER:C	3:A:85:ASN:H	2.07	0.56
3:A:55:ARG:HH11	3:A:55:ARG:CG	2.17	0.56
3:A:140:PHE:O	3:A:144:HIS:HD2	1.89	0.56
3:A:113:HIS:HD2	5:A:1008:HOH:O	1.89	0.56
1:B:319:DA:H62	3:A:177:ILE:HD12	1.71	0.55
3:A:194:LEU:HD21	3:A:213:GLU:HG3	1.89	0.54
3:A:24:PHE:CZ	3:A:114:ILE:CD1	2.92	0.53
3:A:80:GLN:HE21	3:A:80:GLN:H	1.55	0.53
3:A:5:ASP:O	3:A:8:ASP:HB3	2.09	0.52
3:A:194:LEU:C	3:A:196:SER:H	2.14	0.51
3:A:68:SER:O	3:A:72:ARG:HB2	2.11	0.49
3:A:78:PHE:H	3:A:81:GLN:HE21	1.61	0.49
3:A:78:PHE:HB3	3:A:80:GLN:HE21	1.76	0.49
3:A:37:ARG:HH11	3:A:60:GLN:HE22	1.59	0.49
2:C:330:DT:H5"	3:A:200:VAL:CG2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:299:ILE:HG21	3:A:307:VAL:HG22	1.94	0.48
3:A:222:LEU:HD23	3:A:228:LEU:HD21	1.96	0.48
3:A:298:LEU:HD11	3:A:301:PRO:HA	1.95	0.48
3:A:24:PHE:CE1	3:A:114:ILE:CD1	2.97	0.48
3:A:43:GLU:HB2	3:A:86:ARG:NH2	2.28	0.47
3:A:177:ILE:N	3:A:232:ARG:O	2.47	0.47
3:A:180:ASN:HD21	3:A:229:LYS:HE2	1.77	0.47
3:A:142:TRP:O	3:A:146:HIS:HD2	1.98	0.47
3:A:33:LEU:HD11	3:A:36:ALA:HB2	1.96	0.47
3:A:102:VAL:HG21	3:A:107:GLN:HB2	1.96	0.47
3:A:111:VAL:HG21	3:A:163:HIS:HE1	1.80	0.47
3:A:230:ILE:HA	3:A:304:HIS:O	2.14	0.47
3:A:162:LEU:HD11	3:A:259:LEU:HD13	1.97	0.46
3:A:295:PRO:O	3:A:296:LEU:HD23	2.15	0.46
3:A:24:PHE:CE1	3:A:114:ILE:HD11	2.49	0.46
3:A:31:HIS:HD2	3:A:101:GLN:O	1.99	0.46
3:A:300:ILE:HD12	3:A:305:LEU:HD12	1.98	0.46
3:A:103:ASP:O	3:A:104:ASN:C	2.54	0.45
3:A:140:PHE:O	3:A:144:HIS:CD2	2.67	0.45
3:A:14:PHE:HB2	3:A:124:PHE:CE1	2.52	0.45
3:A:78:PHE:H	3:A:81:GLN:NE2	2.13	0.45
3:A:190:LEU:HD12	3:A:216:TYR:HA	1.98	0.45
3:A:219:ILE:O	3:A:222:LEU:HB2	2.17	0.44
3:A:55:ARG:NH1	3:A:55:ARG:CG	2.80	0.44
3:A:164:ASP:N	3:A:165:PRO:HD2	2.33	0.44
3:A:223:PRO:HG2	3:A:226:ALA:HB2	1.99	0.44
3:A:46:LYS:HE3	3:A:46:LYS:HB2	1.81	0.44
3:A:37:ARG:HD3	3:A:62:LEU:HD21	2.01	0.43
3:A:28:LEU:HD23	3:A:28:LEU:HA	1.53	0.43
3:A:74:PHE:CD1	3:A:159:LEU:HD11	2.53	0.43
3:A:59:LYS:HD3	3:A:61:HIS:CE1	2.53	0.43
3:A:121:LYS:HG2	3:A:155:ALA:O	2.18	0.43
3:A:204:THR:O	3:A:205:ARG:HB2	2.19	0.43
3:A:46:LYS:HD3	5:A:1020:HOH:O	2.19	0.43
3:A:70:ALA:O	3:A:73:HIS:HB3	2.19	0.42
1:B:314:DT:C6	1:B:315:DT:H72	2.54	0.42
2:C:336:DG:H2"	2:C:337:DT:O5'	2.19	0.42
3:A:111:VAL:CG2	3:A:163:HIS:HE1	2.32	0.42
3:A:196:SER:HB2	3:A:197:PRO:CD	2.37	0.42
3:A:243:TRP:NE1	3:A:250:GLN:HB3	2.34	0.42
3:A:67:GLN:NE2	3:A:100:TYR:OH	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:296:LEU:HB3	3:A:306:TYR:HB3	2.00	0.41
3:A:299:ILE:HG12	3:A:300:ILE:HG13	2.01	0.41
2:C:330:DT:H5'	3:A:198:ARG:HH22	1.86	0.41
3:A:55:ARG:CD	3:A:280:TYR:O	2.68	0.41
3:A:141:GLU:O	3:A:145:ARG:HB2	2.20	0.41
3:A:96:GLY:O	3:A:258:PRO:HA	2.20	0.41
3:A:37:ARG:NH1	3:A:60:GLN:HE22	2.17	0.41
3:A:55:ARG:HD2	3:A:280:TYR:O	2.21	0.41
3:A:79:ILE:HG23	3:A:149:GLY:O	2.20	0.41
3:A:178:ILE:HA	3:A:230:ILE:O	2.21	0.41
3:A:93:ARG:HD3	3:A:238:PRO:CD	2.51	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%)	279 (92%)	17 (6%)	7 (2%)	6 16

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	49	GLU
3	A	196	SER
3	A	197	PRO
3	A	201	ALA
3	A	269	ALA
3	A	84	GLU
3	A	205	ARG

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%)	228 (84%)	42 (16%)	2 7

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	15	ARG
3	A	18	GLU
3	A	21	LEU
3	A	35	VAL
3	A	45	LYS
3	A	46	LYS
3	A	49	GLU
3	A	53	LEU
3	A	55	ARG
3	A	69	LEU
3	A	71	LEU
3	A	77	LEU
3	A	80	GLN
3	A	83	SER
3	A	84	GLU
3	A	85	ASN
3	A	87	SER
3	A	98	LEU
3	A	113	HIS
3	A	119	LYS
3	A	159	LEU
3	A	168	LEU
3	A	177	ILE
3	A	178	ILE
3	A	179	LYS
3	A	187	LEU
3	A	194	LEU
3	A	195	LYS
3	A	198	ARG
3	A	209	GLN

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Mol	Chain	Res	Type
3	A	214	ARG
3	A	224	GLN
3	A	232	ARG
3	A	245	LYS
3	A	252	GLN
3	A	265	ARG
3	A	273	ASP
3	A	292	GLN
3	A	299	ILE
3	A	302	ARG
3	A	305	LEU
3	A	307	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	27	HIS
3	A	30	GLN
3	A	31	HIS
3	A	51	ASN
3	A	60	GLN
3	A	64	ASN
3	A	67	GLN
3	A	80	GLN
3	A	81	GLN
3	A	113	HIS
3	A	144	HIS
3	A	146	HIS
3	A	163	HIS
3	A	180	ASN
3	A	237	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)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	B	15/16 (93%)	-0.37	0 100 100	29, 37, 63, 72	0
2	C	14/16 (87%)	0.28	3 (21%) 0 0	32, 41, 89, 100	0
3	A	305/309 (98%)	0.19	24 (7%) 12 10	24, 39, 78, 106	0
All	All	334/341 (97%)	0.17	27 (8%) 12 10	24, 39, 81, 106	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	199	SER	6.4
3	A	201	ALA	6.2
2	C	329	DA	6.1
3	A	206	GLU	4.9
3	A	205	ARG	4.8
3	A	198	ARG	4.2
3	A	200	VAL	4.2
3	A	265	ARG	3.8
3	A	210	ARG	3.5
3	A	195	LYS	3.2
3	A	202	PRO	3.0
3	A	309	ASP	2.7
3	A	289	TYR	2.7
3	A	5	ASP	2.5
3	A	248	GLN	2.5
3	A	138	ALA	2.4
2	C	342	DA	2.4
3	A	292	GLN	2.4
3	A	97	VAL	2.3
3	A	72	ARG	2.3
3	A	267	ASN	2.2
3	A	245	LYS	2.2
3	A	288	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	330	DT	2.2
3	A	124	PHE	2.1
3	A	143	VAL	2.1
3	A	203	TRP	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	IOD	A	1003	1/1	0.94	0.09	62,62,62,62	1
4	IOD	A	1002	1/1	0.97	0.13	53,53,53,53	1
4	IOD	A	1001	1/1	0.99	0.14	29,29,29,29	1

6.5 Other polymers (i)

There are no such residues in this entry.