Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:02 PM GMT

PDB ID	:	4E3S
Title	:	RB69 DNA Polymerase Ternary Complex with dQTP Opposite dT
Authors	:	Xia, S.; Wang, J.; Konigsberg, W.H.
Deposited on	:	2012-03-10
Resolution	:	2.04 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:

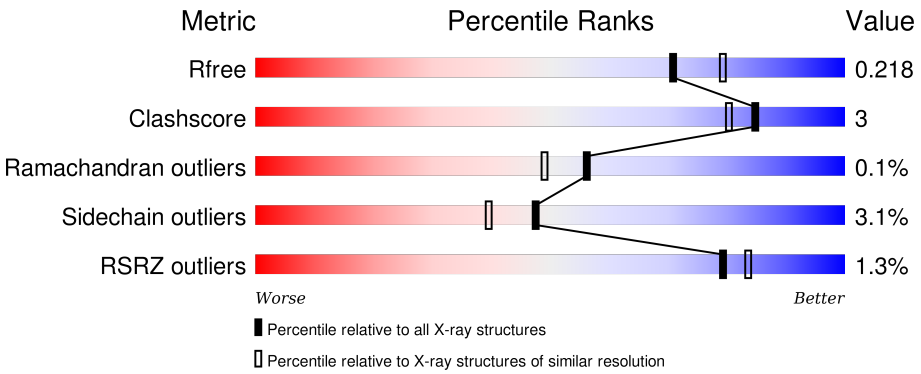
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.04 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	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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	903	% 92% 7% •
2	T	17	6% 59% 41%
3	P	13	69% 23% 8%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8523 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 DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	903	7368	4731	1226	1378	33	0	1	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	222	ALA	ASP	CONFLICT	UNP Q38087
A	327	ALA	ASP	CONFLICT	UNP Q38087
A	561	ALA	LEU	ENGINEERED MUTATION	UNP Q38087
A	565	GLY	SER	ENGINEERED MUTATION	UNP Q38087
A	567	ALA	TYR	ENGINEERED MUTATION	UNP Q38087

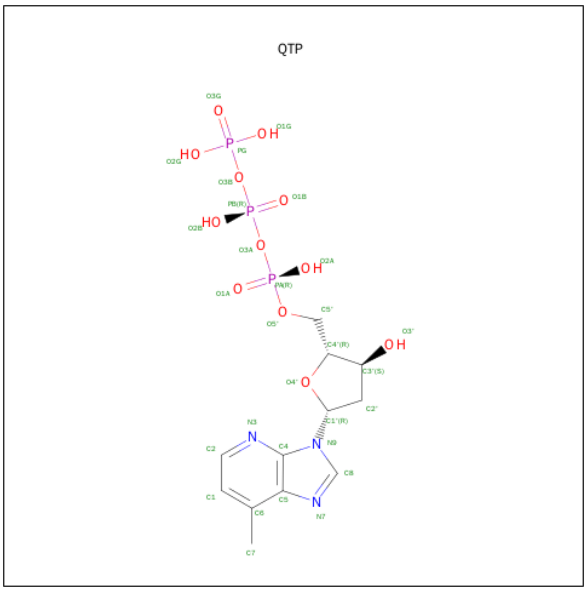
- Molecule 2 is a DNA chain called DNA template.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	T	17	349	165	66	101	17	0	0	0

- Molecule 3 is a DNA chain called DNA primer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	P	13	262	126	48	76	12	0	0	0

- Molecule 4 is 3-{2-DEOXY-5-O-[(R)-HYDROXY{[(R)-HYDROXY(PHOSPHONOOXY)PHOSPHORYL]OXY}PHOSPHORYL]-BETA-D-ERYTHRO-PENTOFURANOSYL}-7-METHYL-3H-IMIDAZO[4,5-B]PYRIDINE (three-letter code: QTP) (formula: $C_{12}H_{18}N_3O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	30	12	3	12	3	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
5	A	5	5	5	0	0

- Molecule 6 is water.

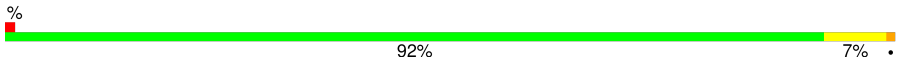
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	458	462	462	0	4
			Total	O		
6	T	35	35	35	0	0
			Total	O		
6	P	11	12	12	0	1

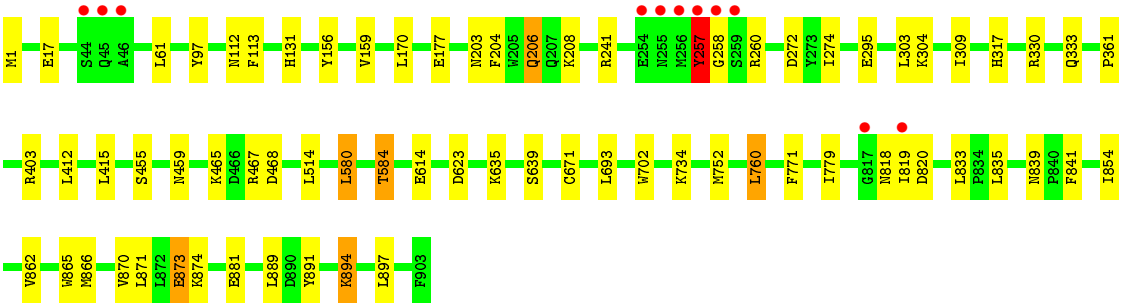
3 Residue-property plots (i)

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: DNA polymerase

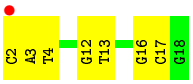
Chain A:





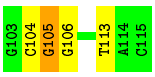
- Molecule 2: DNA template

Chain T:



- Molecule 3: DNA primer

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	78.17Å 118.51Å 130.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.22 – 2.04 47.22 – 2.03	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.22-2.04) 99.5 (47.22-2.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.69 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.180 , 0.219 0.180 , 0.218	Depositor DCC
R_{free} test set	3923 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	35.8	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 46.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 78391 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	8523	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: DOC, CA, QTP

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	0.49	2/7551 (0.0%)	0.56	0/10203
2	T	0.36	0/391	0.85	1/601 (0.2%)
3	P	0.33	0/273	0.89	1/420 (0.2%)
All	All	0.48	2/8215 (0.0%)	0.60	2/11224 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	865	TRP	CD2-CE2	5.05	1.47	1.41
1	A	702	TRP	CD2-CE2	5.04	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	P	105	DG	P-O3'-C3'	6.60	127.62	119.70
2	T	2	DC	P-O3'-C3'	5.88	126.76	119.70

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	A	7368	0	7261	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	T	349	0	191	6	0
3	P	262	0	148	3	0
4	A	30	0	15	0	0
5	A	5	0	0	0	0
6	A	462	0	0	7	0
6	P	12	0	0	0	0
6	T	35	0	0	0	0
All	All	8523	0	7615	45	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 3.

All (45) 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:A:459:ASN:HD22	1:A:584:THR:HG22	1.33	0.92
1:A:580:LEU:O	1:A:584:THR:HB	1.77	0.85
2:T:16:DG:H2"	2:T:17:DC:H5"	1.63	0.78
1:A:459:ASN:ND2	1:A:584:THR:HG22	1.99	0.77
1:A:112:ASN:HB2	6:A:1357:HOH:O	1.83	0.76
1:A:459:ASN:HD22	1:A:584:THR:CG2	1.98	0.75
1:A:170:LEU:HA	1:A:177:GLU:HG3	1.77	0.65
1:A:206:GLN:HE22	1:A:241:ARG:HE	1.42	0.65
1:A:671:CYS:SG	6:A:1554:HOH:O	2.55	0.65
1:A:131:HIS:HD2	1:A:156:TYR:OH	1.80	0.65
1:A:818:ASN:HB3	6:A:1113:HOH:O	1.96	0.63
2:T:3:DA:H2"	2:T:4:DT:OP2	1.98	0.63
1:A:403:ARG:NH2	1:A:889:LEU:HD13	2.14	0.62
1:A:881:GLU:HG3	6:A:1529:HOH:O	2.00	0.60
1:A:272:ASP:OD1	1:A:274:ILE:HG22	2.03	0.58
2:T:16:DG:C2'	2:T:17:DC:H5"	2.33	0.56
1:A:862:VAL:O	1:A:866:MET:HG3	2.05	0.55
1:A:779:ILE:O	1:A:871:LEU:HD21	2.06	0.55
2:T:16:DG:H2"	2:T:17:DC:C5'	2.35	0.55
1:A:455:SER:HB2	1:A:465:LYS:HG2	1.89	0.54
1:A:330:ARG:HA	1:A:333:GLN:HE21	1.72	0.54
1:A:206:GLN:NE2	1:A:241:ARG:HE	2.05	0.54
1:A:203:ASN:ND2	1:A:241:ARG:HH22	2.06	0.53
1:A:873:GLU:HG3	6:A:1170:HOH:O	2.07	0.53
3:P:105:DG:H2"	3:P:106:DG:OP2	2.08	0.53
1:A:771:PHE:HZ	1:A:871:LEU:HD22	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:LEU:HD22	1:A:623:ASP:HB3	1.91	0.52
1:A:734:LYS:HG2	3:P:113:DT:H5'	1.95	0.48
1:A:412:LEU:HD13	1:A:415:LEU:HD13	1.96	0.48
1:A:1:MET:HE3	6:A:1531:HOH:O	2.13	0.48
1:A:839:ASN:OD1	1:A:841:PHE:HB2	2.14	0.47
1:A:760:LEU:HD13	1:A:891:TYR:HA	1.97	0.47
1:A:204:PHE:CE1	1:A:208:LYS:HD2	2.51	0.46
1:A:833:LEU:HD13	1:A:866:MET:HG2	1.99	0.45
2:T:12:DG:H2'	2:T:13:DT:H72	1.98	0.45
1:A:870:VAL:HG13	1:A:874:LYS:HD3	1.99	0.43
1:A:752:MET:HG3	1:A:760:LEU:HG	2.01	0.42
1:A:361:PRO:HG2	2:T:4:DT:C6	2.55	0.42
1:A:257:TYR:HB3	1:A:258:GLY:H	1.51	0.41
1:A:17:GLU:OE1	1:A:97:TYR:OH	2.33	0.41
1:A:159:VAL:HG21	1:A:317:HIS:CD2	2.55	0.41
1:A:854:ILE:HD13	1:A:862:VAL:HG21	2.02	0.41
1:A:734:LYS:NZ	6:A:1465:HOH:O	2.53	0.41
1:A:894:LYS:HE3	1:A:894:LYS:H	1.86	0.40
3:P:104:DC:H2"	3:P:105:DG:C8	2.57	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	902/903 (100%)	883 (98%)	18 (2%)	1 (0%)	56 49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	257	TYR

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	798/797 (100%)	773 (97%)	25 (3%)	47 39

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	LEU
1	A	113	PHE
1	A	206	GLN
1	A	257	TYR
1	A	260	ARG
1	A	295	GLU
1	A	303	LEU
1	A	304	LYS
1	A	309	ILE
1	A	467	ARG
1	A	468	ASP
1	A	514	LEU
1	A	580	LEU
1	A	584	THR
1	A	614	GLU
1	A	635	LYS
1	A	639	SER
1	A	693	LEU
1	A	760	LEU
1	A	819	ILE
1	A	820	ASP
1	A	835	LEU
1	A	873	GLU
1	A	894	LYS
1	A	897	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	HIS
1	A	153	ASN
1	A	203	ASN
1	A	206	GLN
1	A	333	GLN
1	A	339	GLN
1	A	354	GLN
1	A	459	ASN
1	A	546	GLN
1	A	761	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)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	$\#\|Z\| > 2$
3	DOC	P	115	3,2	11,19,20	0.61	0	14,26,29	1.96	4 (28%)

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
3	DOC	P	115	3,2	-	0/3/18/19	0/2/2/2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	P	115	DOC	C5-C4-N3	-2.03	119.24	121.80
3	P	115	DOC	O4'-C1'-N1	2.09	111.33	107.72
3	P	115	DOC	C2-N3-C4	4.28	121.65	115.61
3	P	115	DOC	O4'-C4'-C5'	4.40	116.03	109.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 5 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
4	QTP	A	1001	5	25,32,32	1.79	3 (12%)	35,50,50	1.36	4 (11%)

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
4	QTP	A	1001	5	-	0/18/34/34	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	QTP	C7-C6	-7.09	1.37	1.51
4	A	1001	QTP	C6-C5	2.74	1.48	1.42
4	A	1001	QTP	C5-C4	3.07	1.47	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1001	QTP	C4-C5-N7	-2.76	106.94	109.48
4	A	1001	QTP	C2'-C1'-N9	-2.55	107.97	114.16
4	A	1001	QTP	C2-N3-C4	2.91	120.54	116.93
4	A	1001	QTP	C2-C1-C6	3.01	122.44	120.13

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	A	903/903 (100%)	-0.44	11 (1%) 81 84	25, 37, 66, 131	0
2	T	17/17 (100%)	-0.04	1 (5%) 26 29	30, 46, 115, 170	0
3	P	12/13 (92%)	0.02	0 100 100	31, 67, 91, 91	0
All	All	932/933 (99%)	-0.43	12 (1%) 79 83	25, 37, 67, 170	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	256	MET	10.0
1	A	257	TYR	9.1
1	A	44	SER	7.2
2	T	2	DC	6.6
1	A	258	GLY	6.5
1	A	819	ILE	4.7
1	A	817	GLY	3.9
1	A	45	GLN	3.4
1	A	255	ASN	3.1
1	A	46	ALA	2.6
1	A	259	SER	2.3
1	A	254	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 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	LLDF	B-factors(Å^2)	Q<0.9
3	DOC	P	115	18/19	0.98	0.14	-	28,31,38,43	0

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, 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	LLDF	B-factors(Å^2)	Q<0.9
4	QTP	A	1001	30/30	0.98	0.14	0.90	26,30,33,35	0
5	CA	A	1002	1/1	0.99	0.10	-1.01	32,32,32,32	0
5	CA	A	1005	1/1	0.81	0.08	-1.94	79,79,79,79	0
5	CA	A	1004	1/1	0.99	0.04	-2.38	60,60,60,60	0
5	CA	A	1003	1/1	0.98	0.07	-	62,62,62,62	0
5	CA	A	1006	1/1	0.97	0.07	-	54,54,54,54	0

6.5 Other polymers (i)

There are no such residues in this entry.