



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:26 AM GMT

PDB ID : 3IGC
Title : Smallpox virus topoisomerase-DNA transition state
Authors : Perry, K.; Hwang, Y.; Bushman, F.D.; Van Duyne, G.D.
Deposited on : 2009-07-27
Resolution : 2.10 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

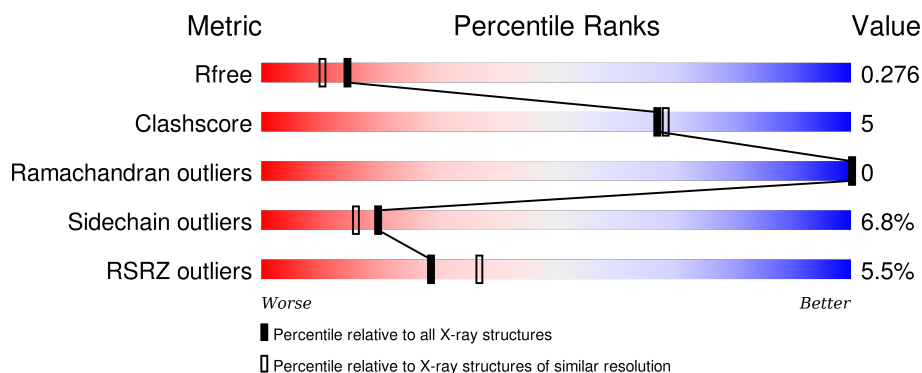
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	314	<div> <div>6%</div> <div>84%</div> <div>13%</div> <div>.</div> </div>
2	B	11	<div> <div>18%</div> <div>82%</div> </div>
3	C	5	<div> <div>40%</div> <div>60%</div> </div>
4	D	16	<div> <div>38%</div> <div>50%</div> <div>13%</div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3663 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 topoisomerase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	0	1	0
			2587	1676	439	463	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	SER	CYS	ENGINEERED	UNP P32989
A	211	SER	CYS	ENGINEERED	UNP P32989

- Molecule 2 is a DNA chain called 5'-D(*GP*TP*GP*TP*CP*GP*CP*CP*CP*TP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	11	Total	C	N	O	P	0	0	0
			219	106	35	68	10			

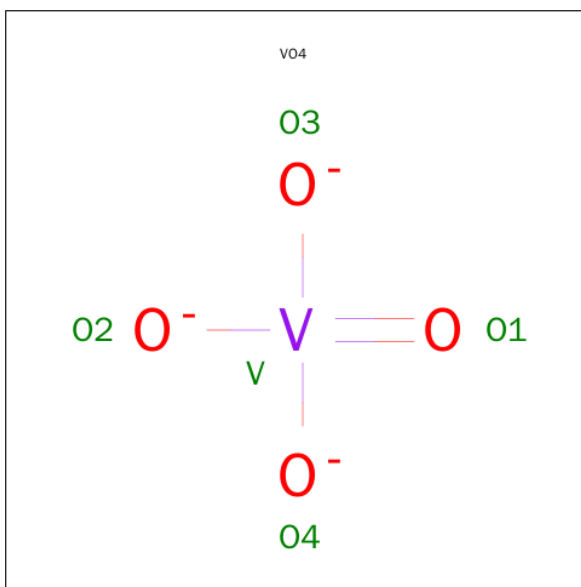
- Molecule 3 is a DNA chain called 5'-D(*AP*TP*TP*CP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	5	Total	C	N	O	P	0	0	0
			96	48	15	29	4			

- Molecule 4 is a DNA chain called 5'-D(*CP*GP*GP*AP*AP*TP*AP*AP*GP*GP*GP*CP*GP*AP*CP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	16	Total	C	N	O	P	0	0	0
			332	157	71	89	15			

- Molecule 5 is VANADATE ION (three-letter code: VO4) (formula: O₄V).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	V	0	0
			3	2	1		

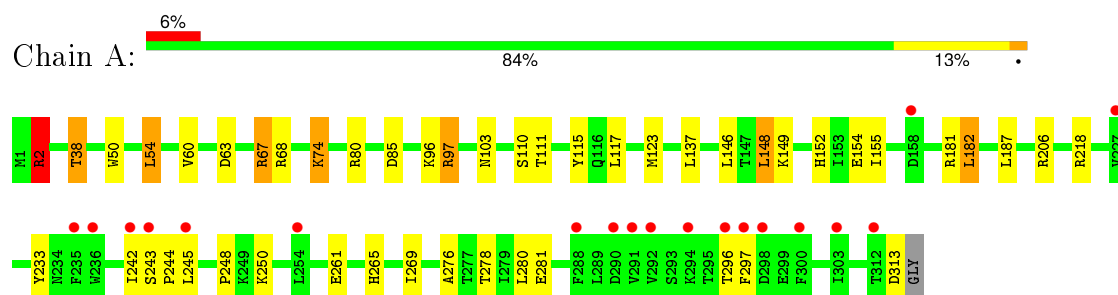
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	316	Total	O	0	0
			316	316		
6	B	31	Total	O	0	0
			31	31		
6	C	11	Total	O	0	0
			11	11		
6	D	68	Total	O	0	0
			68	68		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

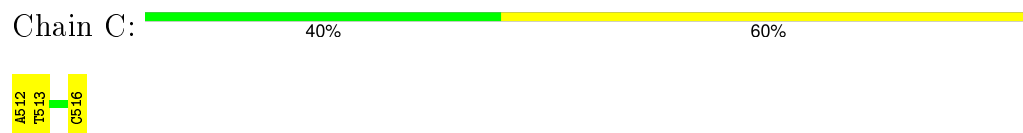
- Molecule 1: DNA topoisomerase 1



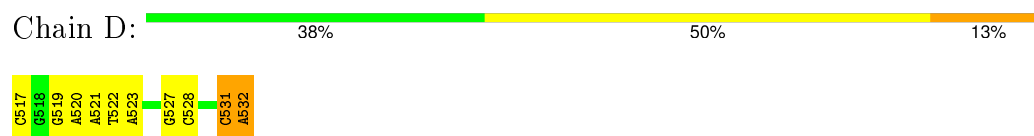
- Molecule 2: 5'-D(*GP*TP*GP*TP*CP*GP*CP*CP*CP*TP*T)-3'



- Molecule 3: 5'-D(*AP*TP*TP*CP*C)-3'



- Molecule 4: 5'-D(*CP*GP*GP*AP*AP*TP*AP*AP*GP*GP*GP*CP*GP*AP*CP*A)-3',



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	104.00 Å 104.00 Å 93.01 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 41.60 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.0 (50.00-2.10) 96.3 (41.60-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.00 Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.177 , 0.244 0.230 , 0.276	Depositor DCC
R_{free} test set	1490 reflections (5.11%)	DCC
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 36.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 33627 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3663	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 3.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: VO4

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	0.76	0/2644	0.81	6/3562 (0.2%)
2	B	1.46	0/243	2.04	9/373 (2.4%)
3	C	1.23	0/106	1.75	2/161 (1.2%)
4	D	1.61	5/375 (1.3%)	2.00	15/578 (2.6%)
All	All	0.97	5/3368 (0.1%)	1.20	32/4674 (0.7%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	517	DC	N1-C6	11.62	1.44	1.37
4	D	517	DC	C2-O2	6.44	1.30	1.24
4	D	517	DC	N3-C4	5.80	1.38	1.33
4	D	517	DC	C4-C5	5.63	1.47	1.43
4	D	528	DC	C3'-O3'	-5.42	1.36	1.44

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	505	DC	O4'-C1'-N1	-11.59	99.89	108.00
1	A	67	ARG	NE-CZ-NH2	-10.06	115.27	120.30
4	D	531	DC	O4'-C1'-N1	-9.55	101.32	108.00
4	D	517	DC	O4'-C1'-N1	8.74	114.12	108.00
1	A	2	ARG	NE-CZ-NH2	-8.09	116.25	120.30
2	B	501	DG	O4'-C1'-N9	7.50	113.25	108.00
1	A	2	ARG	NE-CZ-NH1	7.43	124.02	120.30
4	D	520	DA	O4'-C1'-N9	-7.42	102.81	108.00
4	D	519	DG	O4'-C1'-N9	7.40	113.18	108.00
4	D	532	DA	O4'-C1'-N9	-7.15	102.99	108.00
4	D	519	DG	P-O3'-C3'	7.08	128.19	119.70
2	B	504	DT	O4'-C1'-N1	-6.91	103.17	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	522	DT	P-O3'-C3'	6.72	127.76	119.70
4	D	522	DT	O3'-P-O5'	-6.63	91.39	104.00
4	D	523	DA	O4'-C1'-N9	-6.53	103.43	108.00
2	B	502	DT	O4'-C4'-C3'	6.45	109.87	106.00
2	B	507	DC	C1'-O4'-C4'	-6.36	103.74	110.10
4	D	527	DG	O4'-C1'-N9	-6.29	103.60	108.00
4	D	522	DT	O4'-C1'-C2'	-6.08	101.04	105.90
2	B	511	DT	C3'-C2'-C1'	-6.05	95.24	102.50
1	A	80	ARG	NE-CZ-NH1	5.87	123.23	120.30
2	B	511	DT	N3-C4-O4	5.77	123.36	119.90
4	D	522	DT	C6-C5-C7	-5.67	119.50	122.90
3	C	512	DA	C5-C6-N1	5.65	120.53	117.70
4	D	523	DA	N1-C2-N3	-5.48	126.56	129.30
1	A	80	ARG	NE-CZ-NH2	-5.43	117.59	120.30
2	B	509	DC	P-O3'-C3'	5.37	126.14	119.70
1	A	148	LEU	CB-CG-CD1	5.35	120.09	111.00
2	B	506	DG	O4'-C1'-N9	-5.26	104.32	108.00
3	C	513	DT	C5-C4-O4	-5.21	121.25	124.90
4	D	521	DA	O5'-P-OP2	-5.19	101.03	105.70
4	D	527	DG	C2-N3-C4	5.04	114.42	111.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2587	0	2653	28	0
2	B	219	0	126	1	0
3	C	96	0	58	1	0
4	D	332	0	179	1	0
5	A	3	0	0	0	0
6	A	316	0	0	7	1
6	B	31	0	0	0	0
6	C	11	0	0	1	0
6	D	68	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3663	0	3016	30	1

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 5.

All (30) 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:74:LYS:H	1:A:74:LYS:CD	1.57	1.18
1:A:74:LYS:HD2	1:A:74:LYS:N	1.49	1.17
1:A:74:LYS:H	1:A:74:LYS:HD2	0.82	0.97
1:A:111:THR:HG23	6:A:403:HOH:O	1.66	0.96
1:A:149:LYS:H	1:A:152:HIS:HD2	1.20	0.88
3:C:516:DC:OP2	6:C:332:HOH:O	1.91	0.87
1:A:248:PRO:HA	6:A:421:HOH:O	1.82	0.80
1:A:74:LYS:HG2	6:A:471:HOH:O	1.82	0.79
1:A:206:ARG:NH2	2:B:503:DG:N7	2.34	0.75
1:A:2:ARG:HD2	6:A:442:HOH:O	1.85	0.74
1:A:123:MET:HG2	1:A:182:LEU:HD11	1.84	0.59
1:A:38:THR:HG21	6:A:607:HOH:O	2.05	0.55
1:A:149:LYS:H	1:A:152:HIS:CD2	2.12	0.52
1:A:110:SER:HA	1:A:115:TYR:CD1	2.44	0.52
1:A:97:ARG:NH1	6:A:545:HOH:O	2.40	0.49
1:A:155:ILE:HD13	1:A:187:LEU:HD12	1.95	0.48
1:A:233:TYR:HA	1:A:297:PHE:CE1	2.48	0.48
1:A:60:VAL:HG22	1:A:68:ARG:NH2	2.31	0.46
1:A:38:THR:HG23	6:A:366:HOH:O	2.16	0.45
1:A:74:LYS:N	1:A:74:LYS:CD	2.32	0.45
1:A:103:ASN:ND2	1:A:181:ARG:HH21	2.16	0.44
1:A:243:SER:HB3	1:A:244:PRO:HD3	2.00	0.44
1:A:296:THR:HG22	1:A:297:PHE:N	2.33	0.43
1:A:54:LEU:HD12	1:A:74:LYS:HD3	2.00	0.43
1:A:63:ASP:OD2	1:A:67:ARG:HD3	2.18	0.42
4:D:531:DC:H2"	4:D:532:DA:C8	2.54	0.42
1:A:50:TRP:CH2	1:A:74:LYS:HE2	2.55	0.42
1:A:269:ILE:HA	1:A:269:ILE:HD12	1.96	0.41
1:A:85:ASP:OD1	1:A:276:ALA:HB1	2.21	0.41
1:A:278:THR:HA	1:A:281:GLU:HG2	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:326:HOH:O	6:A:582:HOH:O[8_555]	0.77	1.43

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	312/314 (99%)	304 (97%)	8 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	294/293 (100%)	274 (93%)	20 (7%)	20	16

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

Mol	Chain	Res	Type
1	A	2	ARG
1	A	38	THR
1	A	54	LEU
1	A	74	LYS
1	A	96	LYS
1	A	97	ARG
1	A	117	LEU
1	A	137	LEU

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Mol	Chain	Res	Type
1	A	146	LEU
1	A	148	LEU
1	A	154	GLU
1	A	182	LEU
1	A	218	ARG
1	A	242	ILE
1	A	245	LEU
1	A	250	LYS
1	A	261	GLU
1	A	265	HIS
1	A	280	LEU
1	A	313	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	ASN
1	A	93	ASN
1	A	103	ASN
1	A	152	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand 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	$\# Z > 2$
5	VO4	A	600	3,2	0,2,4	0.00	-	0,1,6	0.00	-

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
5	VO4	A	600	3,2	-	0/0/0/0	0/0/0/0

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

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, 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	313/314 (99%)	0.54	19 (6%) 25 33	24, 41, 96, 120	0
2	B	11/11 (100%)	0.08	0 100 100	26, 39, 77, 94	0
3	C	5/5 (100%)	-0.16	0 100 100	27, 32, 58, 75	0
4	D	16/16 (100%)	-0.08	0 100 100	23, 39, 71, 73	0
All	All	345/346 (99%)	0.48	19 (5%) 29 37	23, 41, 95, 120	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	288	PHE	6.4
1	A	312	THR	4.4
1	A	236	TRP	4.3
1	A	291	VAL	3.8
1	A	245	LEU	3.8
1	A	242	ILE	3.7
1	A	300	PHE	3.1
1	A	296	THR	3.0
1	A	297	PHE	3.0
1	A	294	LYS	2.8
1	A	292	VAL	2.7
1	A	303	ILE	2.6
1	A	243	SER	2.5
1	A	290	ASP	2.5
1	A	254	LEU	2.4
1	A	235	PHE	2.2
1	A	298	ASP	2.1
1	A	158	ASP	2.1
1	A	227	VAL	2.1

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, 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(\AA^2)	Q<0.9
5	VO4	A	600	3/5	0.99	0.15	-0.54	23,23,23,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.