



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2018 – 06:22 pm GMT

PDB ID : 3JSM
Title : K65R mutant HIV-1 reverse transcriptase cross-linked to DS-DNA and complexed with tenofovir-diphosphate as the incoming nucleotide substrate
Authors : Das, K.; Arnold, E.
Deposited on : 2009-09-10
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

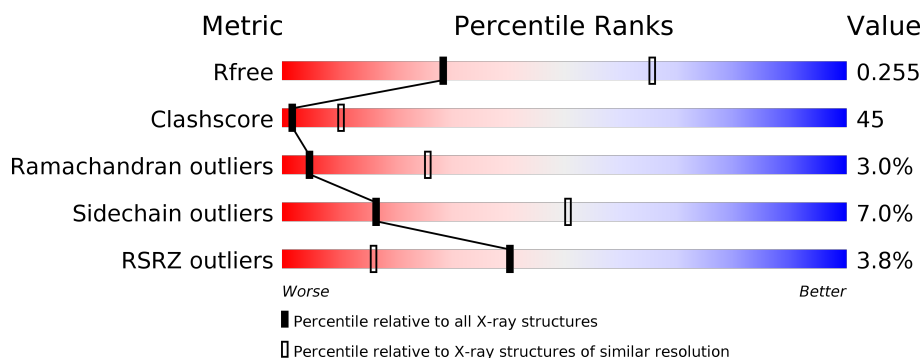
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	111664	1851 (3.00-3.00)
Clashscore	122126	2167 (3.00-3.00)
Ramachandran outliers	120053	2101 (3.00-3.00)
Sidechain outliers	120020	2104 (3.00-3.00)
RSRZ outliers	108989	1751 (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 $\leq 5\%$. 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	T	27	<div> <div>4%</div> <div> <div>15%</div> <div>52%</div> <div>22%</div> <div>11%</div> </div> </div>
2	P	21	<div> <div>19%</div> <div>48%</div> <div>29%</div> <div>5%</div> </div>
3	A	558	<div> <div>2%</div> <div> <div>38%</div> <div>58%</div> <div>• •</div> </div> </div>
4	B	437	<div> <div>6%</div> <div> <div>27%</div> <div>57%</div> <div>11%</div> <div>5%</div> </div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8854 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(*A*TP*GP*GP*TP*CP*GP*GP*CP*GP*C
P*CP*CP*GP*AP*AP*CP*AP*GP*GP*GP*AP*CP*TP*GP*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	24	Total	C	N	O	P	0	0	0
			494	233	97	141	23			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	P	20	Total	C	N	O	P	S	0	0	0
			407	195	72	120	19	1			

- Molecule 3 is a protein called HIV-1 REVERSE TRANSCRIPTASE P66 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	554	Total	C	N	O	S	0	0	0
			4508	2917	751	832	8			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	65	ARG	LYS	ENGINEERED	UNP P03366
A	258	CYS	GLN	ENGINEERED	UNP P03366
A	280	SER	CYS	ENGINEERED	UNP P03366

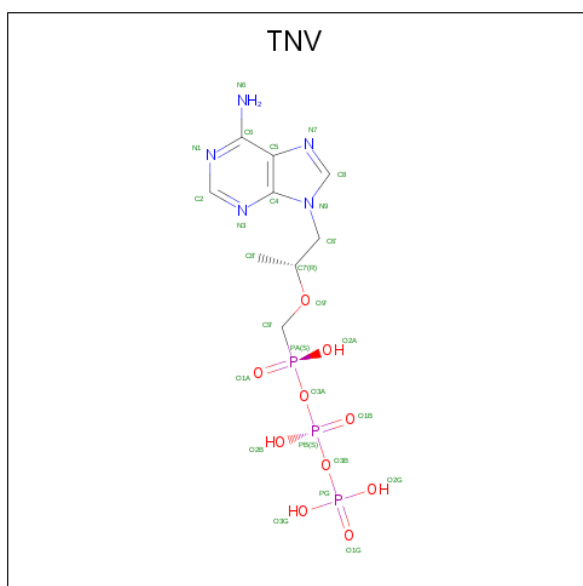
- Molecule 4 is a protein called HIV-1 REVERSE TRANSCRIPTASE P51 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	413	Total	C	N	O	S	0	0	0
			3405	2215	564	620	6			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	ENGINEERED	UNP P03366
B	430	GLY	-	EXPRESSION TAG	UNP P03366
B	431	GLY	-	EXPRESSION TAG	UNP P03366
B	432	HIS	-	EXPRESSION TAG	UNP P03366
B	433	HIS	-	EXPRESSION TAG	UNP P03366
B	434	HIS	-	EXPRESSION TAG	UNP P03366
B	435	HIS	-	EXPRESSION TAG	UNP P03366
B	436	HIS	-	EXPRESSION TAG	UNP P03366
B	437	HIS	-	EXPRESSION TAG	UNP P03366

- Molecule 5 is [2-(6-AMINO-9H-PURIN-9-YL)-1-METHYLETHOXY]METHYL-TRIPHOSPHATE (three-letter code: TNV) (formula: C₉H₁₆N₅O₁₀P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			27	9	5	10	3		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Mg	0	0
			2	2		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		

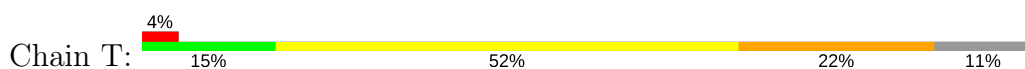
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	O	0	0
			1	1		

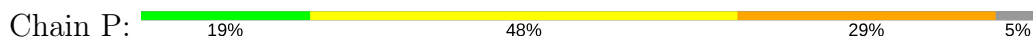
3 Residue-property plots

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

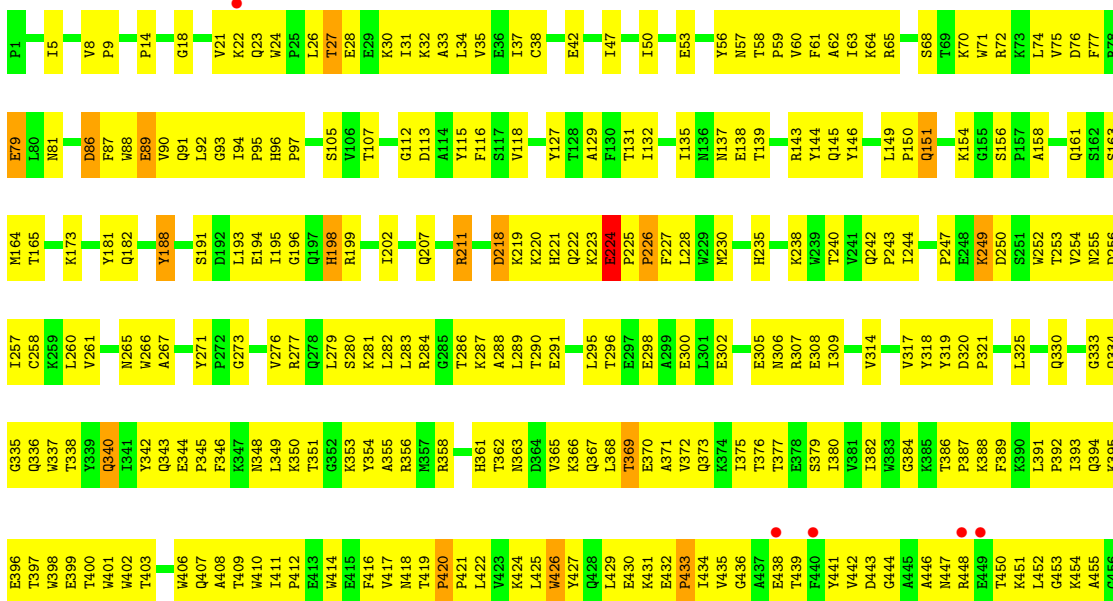
- Molecule 1: DNA (5'-D(*A*TP*GP*GP*TP*CP*GP*GP*CP*GP*CP*CP*GP*AP*AP*CP*AP*GP*GP*GP*AP*CP*TP*GP*TP*G)-3')

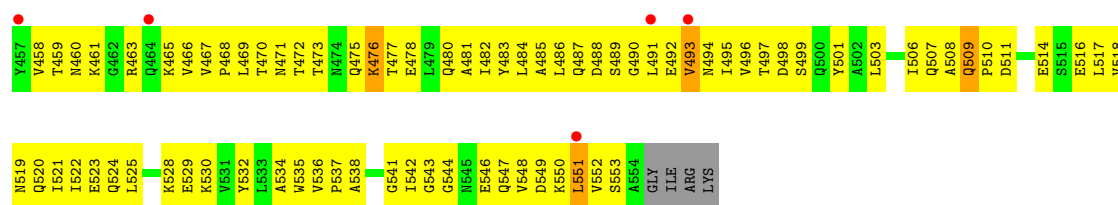


- Molecule 2: DNA (5'-D(*A*CP*AP*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*(MR G)P*CP*GP*CP*CP*(DDG))-3')

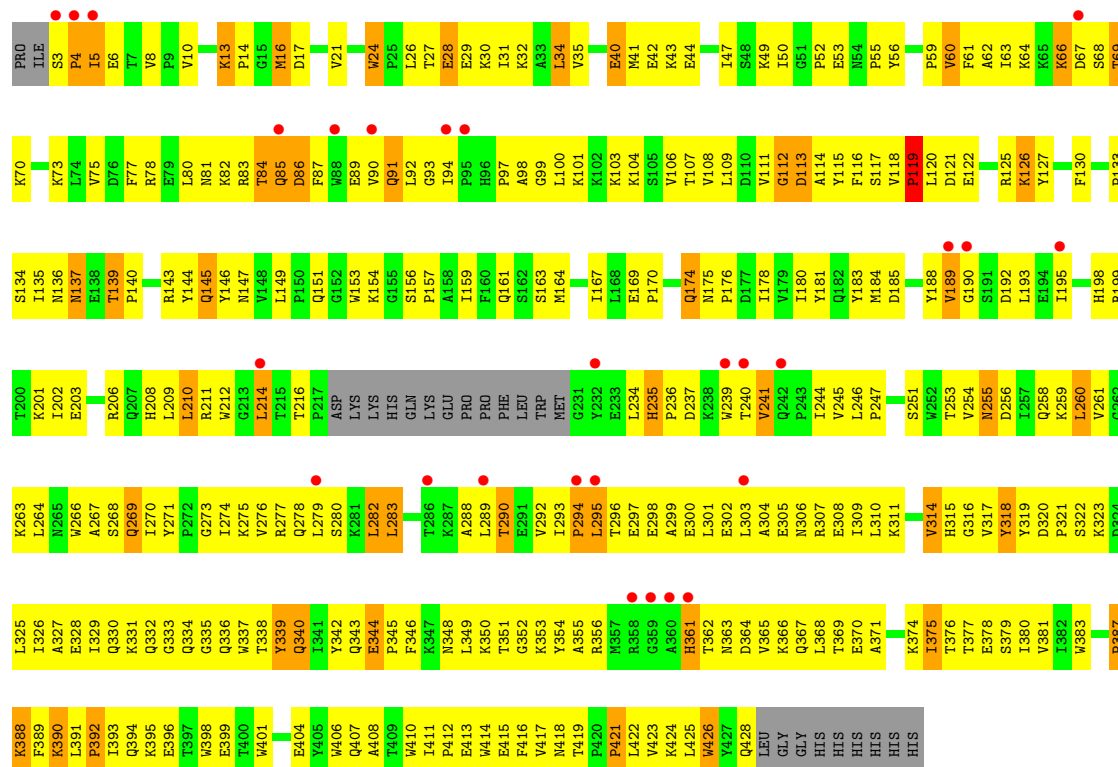


- Molecule 3: HIV-1 REVERSE TRANSCRIPTASE P66 SUBUNIT





● Molecule 4: HIV-1 REVERSE TRANSCRIPTASE P51 SUBUNIT



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, α , β , γ	170.31Å 170.31Å 155.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.17 – 3.00 49.16 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.8 (49.17-3.00) 95.9 (49.16-3.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.252 , 0.285 0.254 , 0.255	Depositor DCC
R_{free} test set	1482 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å ²)	65.5	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 71.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.059 for -h,-k,l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8854	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% 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, 0.333 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: MRG, MG, TNV, DDG, SO4

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	T	0.60	0/555	1.07	6/856 (0.7%)
2	P	1.00	2/400 (0.5%)	1.61	11/612 (1.8%)
3	A	0.46	0/4626	0.78	4/6285 (0.1%)
4	B	0.44	0/3502	0.75	7/4760 (0.1%)
All	All	0.50	2/9083 (0.0%)	0.85	28/12513 (0.2%)

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	T	0	3
2	P	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	803	DC	O3'-P	-11.40	1.47	1.61
2	P	808	DC	O3'-P	-5.19	1.54	1.61

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	806	DT	O5'-P-OP1	-25.18	80.48	110.70
1	T	718	DA	OP2-P-O3'	-9.02	85.36	105.20
1	T	717	DC	OP1-P-O3'	-8.98	85.44	105.20
2	P	805	DG	OP1-P-O3'	8.85	124.67	105.20
1	T	717	DC	P-O3'-C3'	-8.84	109.09	119.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	P	815	DG	Sidechain
1	T	703	DG	Sidechain
1	T	704	DG	Sidechain
1	T	714	DG	Sidechain

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	T	494	0	269	34	0
2	P	407	0	231	34	0
3	A	4508	0	4566	399	0
4	B	3405	0	3437	374	0
5	A	27	0	12	1	0
6	A	2	0	0	0	0
7	A	10	0	0	0	0
8	A	1	0	0	0	0
All	All	8854	0	8515	786	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 45.

The worst 5 of 786 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:195:ILE:HD11	3:A:199:ARG:HE	1.11	1.09
4:B:332:GLN:HB2	4:B:336:GLN:HB3	1.33	1.08
3:A:408:ALA:HB1	4:B:364:ASP:HB3	1.39	1.04
3:A:195:ILE:HD11	3:A:199:ARG:NE	1.76	1.01
4:B:246:LEU:HD22	4:B:260:LEU:HD11	1.47	0.97

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	552/558 (99%)	449 (81%)	92 (17%)	11 (2%)	8	37
4	B	409/437 (94%)	310 (76%)	81 (20%)	18 (4%)	3	16
All	All	961/995 (97%)	759 (79%)	173 (18%)	29 (3%)	5	26

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	98	ALA
3	A	485	ALA
3	A	541	GLY
4	B	86	ASP
4	B	112	GLY

5.3.2 Protein sidechains

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	495/498 (99%)	470 (95%)	25 (5%)	26	64
4	B	375/397 (94%)	339 (90%)	36 (10%)	9	34
All	All	870/895 (97%)	809 (93%)	61 (7%)	16	50

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	24	TRP

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Mol	Chain	Res	Type
4	B	91	GLN
4	B	375	ILE
4	B	28	GLU
4	B	34	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
3	A	494	ASN
4	B	85	GLN
4	B	340	GLN
3	A	487	GLN
4	B	348	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are 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
2	MRG	P	817	1,3,2	22,28,29	1.73	2 (9%)	24,39,42	3.14	6 (25%)
2	DDG	P	822	1,2	17,23,24	1.17	2 (11%)	15,33,36	2.99	5 (33%)

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	MRG	P	817	1,3,2	-	0/8/26/27	0/3/3/3
2	DDG	P	822	1,2	-	0/3/18/19	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	817	MRG	C21-N2	-6.85	1.31	1.45
2	P	822	DDG	C8-N7	-2.07	1.30	1.34
2	P	817	MRG	C6-N1	2.88	1.38	1.33
2	P	822	DDG	C6-N1	3.50	1.39	1.33

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	817	MRG	C21-N2-C2	-10.26	105.78	123.73
2	P	822	DDG	C5-C6-N1	-8.40	111.52	123.47
2	P	817	MRG	C5-C6-N1	-8.24	111.75	123.47
2	P	817	MRG	C2-N3-C4	-2.99	111.70	115.11
2	P	822	DDG	C2-N3-C4	-2.67	112.05	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	817	MRG	5	0
2	P	822	DDG	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	$\# Z > 2$
7	SO4	A	559	-	4,4,4	0.72	0	6,6,6	0.18	0
7	SO4	A	560	-	4,4,4	0.64	0	6,6,6	0.41	0
5	TNV	A	823	6	25,28,28	1.42	3 (12%)	18,43,43	1.45	3 (16%)

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
7	SO4	A	559	-	-	0/0/0/0	0/0/0/0
7	SO4	A	560	-	-	0/0/0/0	0/0/0/0
5	TNV	A	823	6	-	0/17/22/22	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	823	TNV	PA-O3A	-3.34	1.54	1.58
5	A	823	TNV	C6'-N9	-2.59	1.45	1.48
5	A	823	TNV	C2-N3	2.96	1.37	1.32

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	823	TNV	PA-C9'-O9'	-3.70	102.37	109.06
5	A	823	TNV	PB-O3B-PG	-2.40	124.57	132.63
5	A	823	TNV	O3A-PA-C9'	2.10	113.76	104.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	823	TNV	1	0

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	T	24/27 (88%)	-0.13	1 (4%) 36 14	40, 111, 138, 143	0
2	P	18/21 (85%)	-0.01	0 100 100	46, 105, 145, 150	0
3	A	554/558 (99%)	-0.16	10 (1%) 68 39	24, 70, 131, 149	0
4	B	413/437 (94%)	0.17	27 (6%) 19 6	41, 105, 147, 150	0
All	All	1009/1043 (96%)	-0.02	38 (3%) 40 16	24, 85, 141, 150	0

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	94	ILE	4.1
4	B	3	SER	4.0
4	B	295	LEU	3.9
4	B	358	ARG	3.8
3	A	448	ARG	3.5

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. 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
2	MRG	P	817	26/27	0.91	0.20	57,68,85,93	0
2	DDG	P	822	21/22	0.98	0.18	38,50,62,72	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. 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
7	SO4	A	559	5/5	0.85	0.22	131,132,136,137	0
7	SO4	A	560	5/5	0.90	0.41	113,115,119,119	0
6	MG	A	601	1/1	0.95	0.06	75,75,75,75	0
5	TNV	A	823	27/27	0.97	0.21	40,58,66,75	0
6	MG	A	600	1/1	0.98	0.23	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.