W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:01 AM GMT

PDB ID : 3KK1
Title : HIV-1 reverse transcriptase-DNA complex with nuceotide inhibitor GS-9148-diphosphate bound in nucleotide site
Authors : Lansdon, E.B.
Deposited on : 2009-11-04
Resolution : 2.70 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:
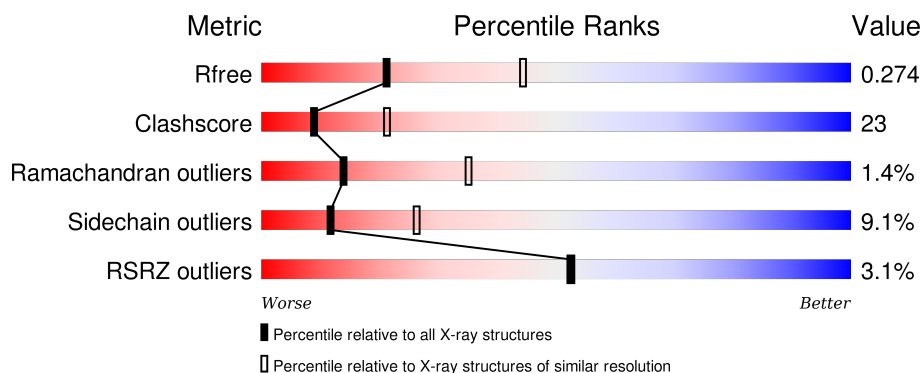
1   Overall quality at a glance (i)

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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (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 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	560	
2	B	452	
3	P	21	
4	T	27	

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
5	SO4	P	2	-	-	-	X
6	MG	A	600	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 8968 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 Reverse transcriptase p66 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total 4514	C 2917	N 753	O 836	S 8	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	258	CYS	GLN	ENGINEERED	UNP P04585
A	280	SER	CYS	ENGINEERED	UNP P04585

- Molecule 2 is a protein called Reverse transcriptase p51 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	412	Total 3396	C 2210	N 565	O 614	S 7	0	0	0

There are 13 discrepancies between the modelled and reference sequences:

| Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	MET	-	EXPRESSION TAG	UNP P04585
B	-10	GLY	-	EXPRESSION TAG	UNP P04585
B	-9	SER	-	EXPRESSION TAG	UNP P04585
B	-8	SER	-	EXPRESSION TAG	UNP P04585
B	-7	HIS	-	EXPRESSION TAG	UNP P04585
B	-6	HIS	-	EXPRESSION TAG	UNP P04585
B	-5	HIS	-	EXPRESSION TAG	UNP P04585
B	-4	HIS	-	EXPRESSION TAG	UNP P04585
B	-3	HIS	-	EXPRESSION TAG	UNP P04585
B	-2	HIS	-	EXPRESSION TAG	UNP P04585
B	-1	SER	-	EXPRESSION TAG	UNP P04585
B	0	SER	-	EXPRESSION TAG	UNP P04585
B	280	SER	CYS	ENGINEERED	UNP P04585

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	18	Total 360	C 172	N 62	O 109	P 17	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	T	24	Total 497	C 234	N 99	O 141	P 23	0	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
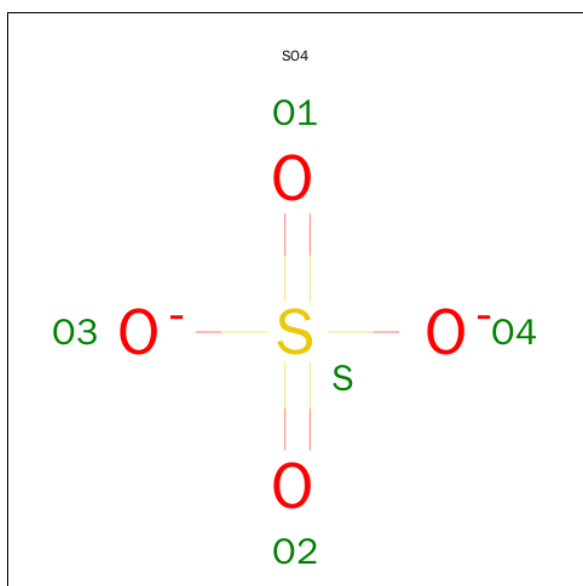
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 5	O 4	S 1	0	0
5	A	1	Total 5	O 4	S 1	0	0
5	P	1	Total 5	O 4	S 1	0	0

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

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

- Molecule 7 is [(2R,5R)-5-(6-AMINOPURIN-9-YL)-4-FLUORO-2,5-DIHYDROFURAN-2-YL]OXYMETHYL-[HYDROXY(PHOSPHONOOXY)PHOSPHORYL]OXY-PHOSPHINIC ACID (three-letter code: 914) (formula: $C_{10}H_{13}FN_5O_{11}P_3$).
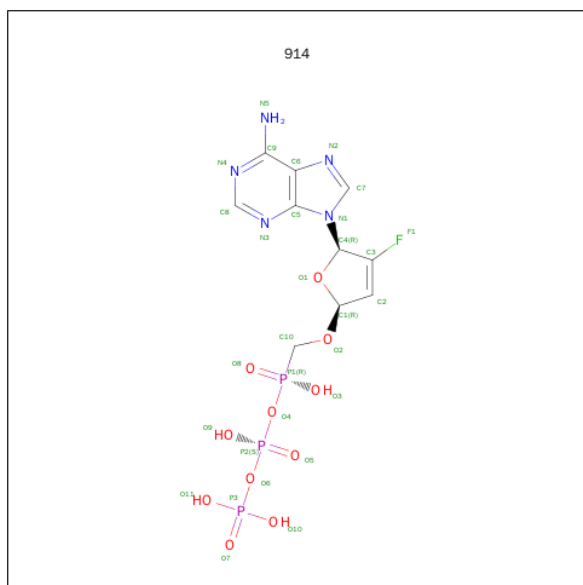
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	F	N	O	P		
7	A	1	30	10	1	5	11	3	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	76	Total 76	O 76	0	0
8	B	54	Total 54	O 54	0	0
8	P	10	Total 10	O 10	0	0
8	T	14	Total 14	O 14	0	0

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: Reverse transcriptase p66 subunit
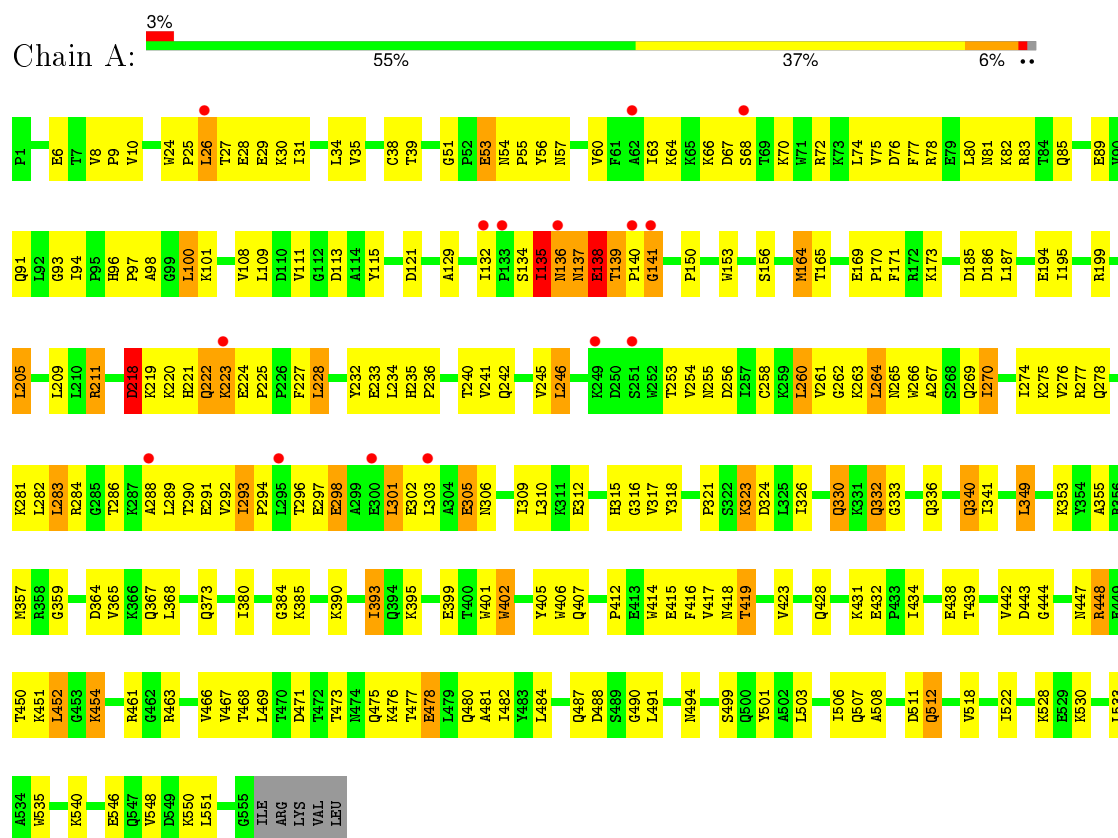
• Molecule 2: Reverse transcriptase p51 subunit
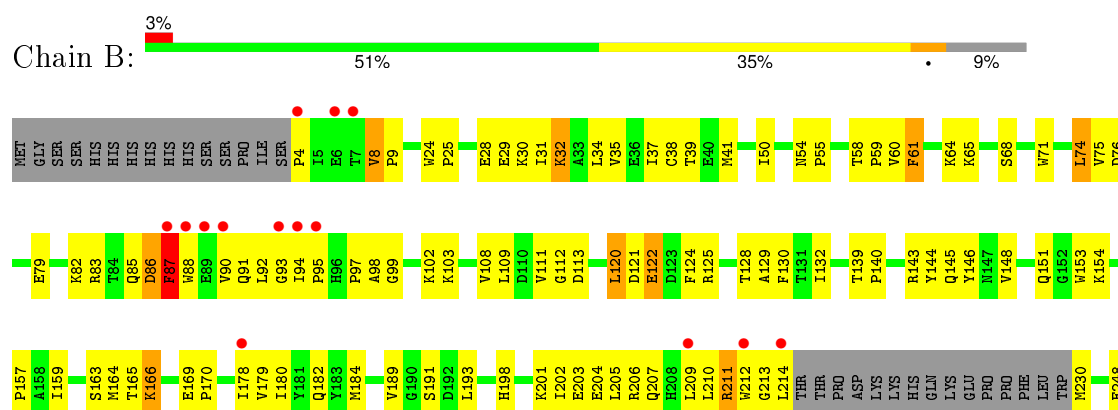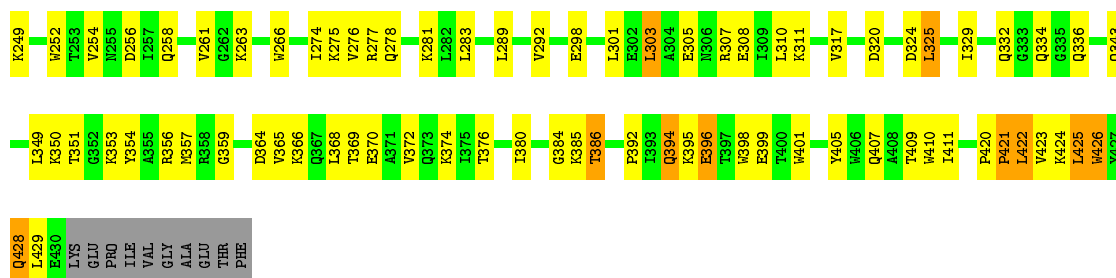
• Molecule 3: 5'-D(*AP*CP*A*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*GP*CP*GP*CP*CP*(DOC))-3'

Chain P:

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

Chain T:

4 Data and refinement statistics (i)

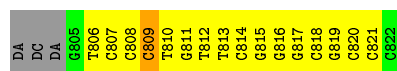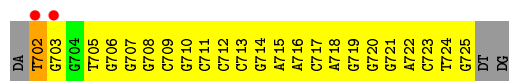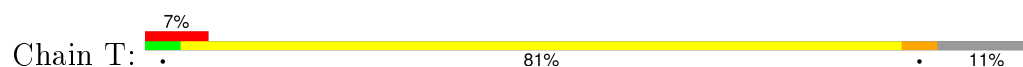| Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	165.75Å 169.24Å 103.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.71 – 2.70 47.41 – 2.70	Depositor EDS
% Data completeness (in resolution range)	91.6 (29.71-2.70) 91.7 (47.41-2.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.32 (at 2.69Å)	Xtriage
Refinement program	CNX 2005	Depositor
R, R_{free}	0.204 , 0.274 0.203 , 0.274	Depositor DCC
R_{free} test set	1837 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	55.1	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 54.9	EDS
Estimated twinning fraction	0.020 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Outliers	0 of 39358 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8968	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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, MG, SO4, 914

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	0.40	1/4631 (0.0%)	0.55	1/6292 (0.0%)
2	B	0.35	0/3491	0.52	1/4742 (0.0%)
3	P	0.46	0/381	1.10	1/586 (0.2%)
4	T	0.58	1/559 (0.2%)	1.08	4/863 (0.5%)
All	All	0.40	2/9062 (0.0%)	0.63	7/12483 (0.1%)

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	A	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	T	702	DT	C3'-O3'	-6.08	1.36	1.44
1	A	138	GLU	CD-OE1	5.71	1.31	1.25

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	T	702	DT	O4'-C4'-C3'	-11.83	98.90	106.00
4	T	702	DT	OP1-P-O3'	-5.78	92.49	105.20
4	T	702	DT	O3'-P-O5'	5.71	114.85	104.00
4	T	702	DT	C4'-C3'-O3'	5.42	123.26	109.70
2	B	4	PRO	N-CA-CB	5.30	109.66	103.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	135	ILE	Peptide
1	A	218	ASP	Peptide

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	4514	0	4563	208	0
2	B	3396	0	3426	159	0
3	P	360	0	204	20	0
4	T	497	0	269	31	0
5	A	10	0	0	0	0
5	P	5	0	0	0	0
6	A	2	0	0	0	0
7	A	30	0	9	1	0
8	A	76	0	0	1	0
8	B	54	0	0	1	0
8	P	10	0	0	0	0
8	T	14	0	0	0	0
All	All	8968	0	8471	403	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 23.

The worst 5 of 403 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:B:425:LEU:HD22	2:B:428:GLN:HG3	1.46	0.96
1:A:511:ASP:OD1	1:A:512:GLN:HG3	1.69	0.91
1:A:288:ALA:HB3	1:A:291:GLU:HG3	1.56	0.88
1:A:135:ILE:HG21	1:A:138:GLU:OE2	1.74	0.87
1:A:246:LEU:HD12	1:A:246:LEU:H	1.41	0.86

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	553/560 (99%)	508 (92%)	37 (7%)	8 (1%)	14	35
2	B	408/452 (90%)	373 (91%)	30 (7%)	5 (1%)	16	39
All	All	961/1012 (95%)	881 (92%)	67 (7%)	13 (1%)	14	35

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	THR
2	B	87	PHE
1	A	85	GLN
1	A	286	THR
1	A	355	ALA

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	495/500 (99%)	441 (89%)	54 (11%)	8	18
2	B	371/411 (90%)	346 (93%)	25 (7%)	20	44
All	All	866/911 (95%)	787 (91%)	79 (9%)	12	26

5 of 79 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	353	LYS

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Mol	Chain	Res	Type
1	A	452	LEU
2	B	394	GLN
1	A	368	LEU
1	A	402	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	407	GLN
1	A	464	GLN
2	B	343	GLN
1	A	418	ASN
1	A	428	GLN

5.3.3　RNA ⓘ

There are no RNA molecules in this entry.

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

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	822	3,4	11,19,20	0.74	0	14,26,29	1.07	1 (7%)

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	822	3,4	-	0/3/18/19	0/2/2/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	P	822	DOC	C2-N3-C4	3.06	119.93	115.61

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, 2 are monoatomic - leaving 4 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	#$|Z| > 2$
5	SO4	A	561	-	4,4,4	0.26	0	6,6,6	0.10	0
5	SO4	A	562	-	4,4,4	0.26	0	6,6,6	0.08	0
7	914	A	825	6	20,32,32	2.37	8 (40%)	23,50,50	1.80	7 (30%)
5	SO4	P	2	-	4,4,4	0.25	0	6,6,6	0.13	0

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	SO4	A	561	-	-	0/0/0/0	0/0/0/0
5	SO4	A	562	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	914	A	825	6	-	1/13/34/34	0/3/3/3
5	SO4	P	2	-	-	0/0/0/0	0/0/0/0

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	825	914	P1-O3	-2.76	1.49	1.56
7	A	825	914	C7-N2	-2.45	1.29	1.34
7	A	825	914	O1-C4	-2.10	1.39	1.43
7	A	825	914	C6-C5	2.10	1.45	1.40
7	A	825	914	C8-N3	2.54	1.36	1.32

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	825	914	C3-C4-N1	-2.60	110.43	113.42
7	A	825	914	N3-C8-N4	-2.28	127.15	128.89
7	A	825	914	C1-C2-C3	-2.16	107.83	110.11
7	A	825	914	O4-P1-C10	-2.14	96.68	104.16
7	A	825	914	O3-P1-O8	2.90	119.25	110.12

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	825	914	C10-O2-C1-O1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	825	914	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	A	555/560 (99%)	0.02	15 (2%)	58	58	22, 47, 89, 109	0
2	B	412/452 (91%)	0.04	14 (3%)	49	49	27, 57, 94, 121	0
3	P	17/21 (80%)	-0.76	0	100	100	38, 60, 78, 80	0
4	T	24/27 (88%)	-0.20	2 (8%)	14	11	37, 75, 95, 120	0
All	All	1008/1060 (95%)	0.01	31 (3%)	52	52	22, 52, 91, 121	0

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	88	TRP	7.0
2	B	4	PRO	6.4
2	B	89	GLU	5.5
2	B	87	PHE	5.4
1	A	288	ALA	4.0

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	822	18/19	0.98	0.14	-	35,39,40,41	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
6	MG	A	600	1/1	0.99	0.21	3.23	15,15,15,15	0
5	SO4	P	2	5/5	0.88	0.19	2.91	115,115,116,116	0
5	SO4	A	562	5/5	0.86	0.18	0.45	115,116,117,117	0
7	914	A	825	30/30	0.96	0.17	0.08	46,51,53,56	0
5	SO4	A	561	5/5	0.98	0.12	-0.98	66,67,67,67	0
6	MG	A	601	1/1	0.95	0.23	-	13,13,13,13	0

6.5 Other polymers (i)

There are no such residues in this entry.