



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 19, 2016 – 11:30 PM EDT

PDB ID : 5IIN
Title : Crystal structure of the pre-catalytic ternary extension complex of DNA polymerase lambda with an 8-oxo-dG:dC base-pair
Authors : Burak, M.J.; Guja, K.E.; Garcia-Diaz, M.
Deposited on : 2016-03-01
Resolution : 2.15 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027939
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) : rb-20027939

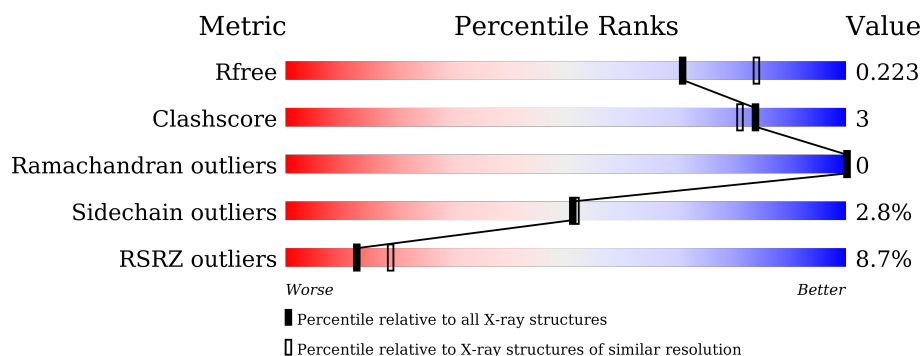
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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	334	<div> <div>9%</div> <div>89%</div> <div>8%</div> <div>..</div> </div>
2	D	4	<div> <div>75%</div> <div>25%</div> </div>
3	P	6	<div> <div>100%</div> </div>
4	T	11	<div> <div>64%</div> <div>36%</div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 3198 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 lambda.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	1	0
			2502	1572	450	468	12			

- Molecule 2 is a DNA chain called DNA (5'-D(P*GP*CP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	4	Total	C	N	O	P	0	0	0
			83	38	16	25	4			

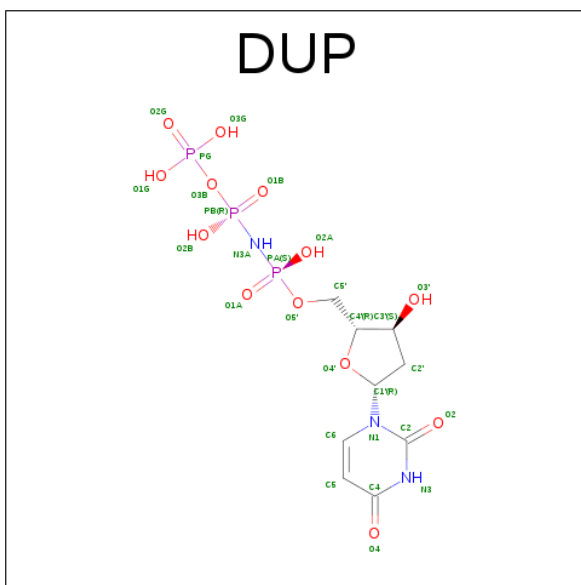
- Molecule 3 is a DNA chain called DNA (5'-D(*CP*AP*GP*TP*AP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	6	Total	C	N	O	P	0	0	0
			119	58	23	33	5			

- Molecule 4 is a DNA chain called DNA (5'-D(*CP*GP*GP*CP*AP*(8OG)P*TP*AP*CP*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	T	11	Total	C	N	O	P	0	0	0
			225	107	43	65	10			

- Molecule 5 is 2'-DEOXYURIDINE 5'-ALPHA,BETA-IMIDO-TRIPHOSPHATE (three-letter code: DUP) (formula: C₉H₁₆N₃O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			28	9	3	13	3		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Na 1 1	0	0

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Mg 1 1	0	0

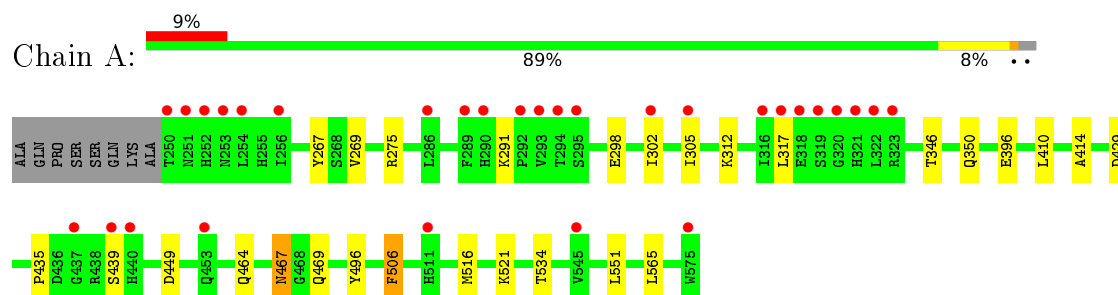
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	154	Total O 154 154	0	0
8	D	6	Total O 6 6	0	0
8	P	31	Total O 31 31	0	0
8	T	48	Total O 48 48	0	0

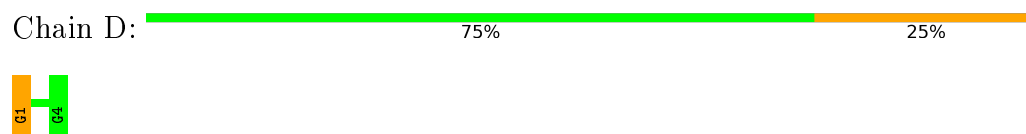
3 Residue-property plots

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: DNA polymerase lambda



- Molecule 2: DNA (5'-D(P*GP*CP*CP*G)-3')

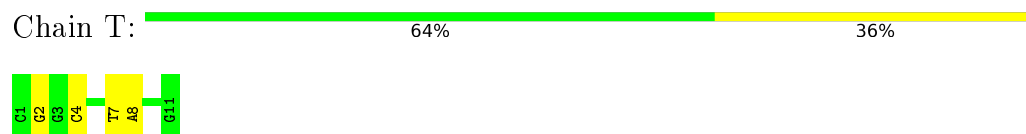


- Molecule 3: DNA (5'-D(*CP*AP*GP*TP*AP*C)-3')



There are no outlier residues recorded for this chain.

- Molecule 4: DNA (5'-D(*CP*GP*GP*CP*AP*(8OG)P*TP*AP*CP*TP*G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	56.47Å 62.72Å 140.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.36 – 2.15 31.36 – 2.03	Depositor EDS
% Data completeness (in resolution range)	97.8 (31.36-2.15) 90.4 (31.36-2.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.03Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.187 , 0.231 0.182 , 0.223	Depositor DCC
R_{free} test set	1262 reflections (4.92%)	DCC
Wilson B-factor (Å ²)	30.1	Xtriage
Anisotropy	0.556	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3198	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.30% 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: DUP, NA, MG, 8OG

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	0.38	0/2557	0.49	0/3463
2	D	1.28	1/92 (1.1%)	0.73	0/138
3	P	0.88	0/133	0.97	0/203
4	T	0.91	0/225	1.09	1/343 (0.3%)
All	All	0.52	1/3007 (0.0%)	0.61	1/4147 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	DG	OP3-P	-10.36	1.48	1.61

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	T	2	DG	O4'-C1'-N9	5.95	112.16	108.00

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	2502	0	2414	15	0
2	D	83	0	45	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	P	119	0	69	0	0
4	T	225	0	125	3	0
5	A	28	0	12	0	0
6	A	1	0	0	0	0
7	A	1	0	0	0	0
8	A	154	0	0	2	1
8	D	6	0	0	0	0
8	P	31	0	0	0	0
8	T	48	0	0	0	1
All	All	3198	0	2665	17	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 3.

All (17) 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:565:LEU:O	8:A:701:HOH:O	2.15	0.64
1:A:467:ASN:HD21	1:A:469:GLN:HB2	1.67	0.59
1:A:302:ILE:HB	1:A:305:ILE:HD13	1.85	0.58
1:A:396:GLU:HG3	1:A:414:ALA:HB2	1.93	0.50
1:A:534:THR:HB	1:A:551:LEU:HD11	1.94	0.49
1:A:291:LYS:HE3	1:A:298:GLU:OE2	2.14	0.48
4:T:7:DT:H2''	4:T:8:DA:H5'	1.97	0.46
1:A:267:TYR:CE1	1:A:275:ARG:HD2	2.51	0.46
1:A:429:ASP:HB3	1:A:506:PHE:CZ	2.51	0.45
1:A:467:ASN:ND2	8:A:713:HOH:O	2.49	0.45
1:A:521:LYS:NZ	4:T:4:DC:OP1	2.38	0.45
1:A:312:LYS:NZ	2:D:1:DG:OP3	2.43	0.44
1:A:346:THR:O	1:A:350:GLN:HG3	2.18	0.42
1:A:435:PRO:HA	1:A:496:TYR:CD1	2.55	0.42
1:A:317:LEU:HD23	1:A:317:LEU:HA	1.91	0.41
4:T:7:DT:H2'	4:T:8:DA:C8	2.55	0.41
1:A:410:LEU:HD23	1:A:410:LEU:HA	1.92	0.41

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)
8:A:728:HOH:O	8:T:110:HOH:O[4_-455]	2.19	0.01

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	
1	A	325/334 (97%)	314 (97%)	11 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	
1	A	254/280 (91%)	247 (97%)	7 (3%)	51	52

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	269	VAL
1	A	439	SER
1	A	449	ASP
1	A	464	GLN
1	A	467	ASN
1	A	506	PHE
1	A	516	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	$\# Z > 2$
4	8OG	T	6	3,4	16,25,26	5.17	10 (62%)	20,37,40	2.68	8 (40%)

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	8OG	T	6	3,4	-	0/3/21/22	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	T	6	8OG	C3'-C4'	-7.04	1.33	1.53
4	T	6	8OG	O4'-C1'	-5.09	1.30	1.42
4	T	6	8OG	O3'-C3'	2.51	1.49	1.43
4	T	6	8OG	C2-N2	3.66	1.41	1.34
4	T	6	8OG	C6-C5	4.08	1.49	1.41
4	T	6	8OG	C6-N1	4.57	1.41	1.33
4	T	6	8OG	C4-N3	4.79	1.43	1.35
4	T	6	8OG	C2-N1	4.89	1.44	1.35
4	T	6	8OG	O4'-C4'	7.48	1.62	1.45
4	T	6	8OG	C8-N7	13.72	1.49	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	T	6	8OG	N3-C2-N1	-5.92	119.51	127.56
4	T	6	8OG	C1'-N9-C4	-4.29	122.27	127.30
4	T	6	8OG	C5-C6-N1	-4.13	118.12	123.52
4	T	6	8OG	C2'-C1'-N9	-3.44	112.37	115.77
4	T	6	8OG	C4'-O4'-C1'	-2.71	102.49	109.42
4	T	6	8OG	N2-C2-N1	2.63	121.54	117.20
4	T	6	8OG	C8-N9-C1'	3.24	130.95	125.83
4	T	6	8OG	C6-N1-C2	5.17	121.94	115.88

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 3 ligands modelled in this entry, 2 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
5	DUP	A	601	7	28,29,29	3.90	15 (53%)	32,45,45	2.51	8 (25%)

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	DUP	A	601	7	-	0/18/34/34	0/2/2/2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	DUP	C6-C5	-9.21	1.36	1.52
5	A	601	DUP	C2'-C3'	-8.55	1.29	1.52
5	A	601	DUP	C6-N1	-7.85	1.37	1.47
5	A	601	DUP	C5-C4	-5.39	1.36	1.50
5	A	601	DUP	O4'-C1'	-4.59	1.31	1.42
5	A	601	DUP	PA-O2A	-3.25	1.48	1.56
5	A	601	DUP	C5'-C4'	-3.00	1.41	1.51
5	A	601	DUP	PA-O5'	2.30	1.64	1.57
5	A	601	DUP	PB-N3A	2.71	1.70	1.63
5	A	601	DUP	PA-N3A	2.80	1.70	1.63
5	A	601	DUP	O4'-C4'	3.40	1.52	1.45
5	A	601	DUP	C2'-C1'	3.75	1.63	1.52
5	A	601	DUP	O3'-C3'	3.79	1.51	1.43
5	A	601	DUP	PB-O1B	4.06	1.50	1.46
5	A	601	DUP	PA-O1A	6.68	1.53	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	DUP	C2'-C1'-N1	-6.01	108.07	115.65
5	A	601	DUP	C4-N3-C2	-3.90	122.23	125.77
5	A	601	DUP	C6-N1-C2	-2.35	118.53	122.16
5	A	601	DUP	PG-O3B-PB	-2.12	125.03	132.71
5	A	601	DUP	C5-C4-N3	2.50	119.27	116.62
5	A	601	DUP	N3-C2-N1	2.65	119.10	116.64
5	A	601	DUP	O4'-C1'-N1	2.85	112.40	108.47
5	A	601	DUP	C5-C6-N1	9.95	121.66	110.76

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	326/334 (97%)	0.37	30 (9%) 11 17	18, 34, 70, 84	0
2	D	4/4 (100%)	-0.65	0 100 100	34, 35, 37, 39	0
3	P	6/6 (100%)	0.02	0 100 100	20, 21, 23, 25	0
4	T	10/11 (90%)	-0.47	0 100 100	25, 27, 32, 34	0
All	All	346/355 (97%)	0.32	30 (8%) 13 19	18, 33, 69, 84	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	319	SER	7.0
1	A	289	PHE	4.8
1	A	440	HIS	4.8
1	A	294	THR	4.3
1	A	254	LEU	3.8
1	A	286	LEU	3.7
1	A	302	ILE	3.6
1	A	256	ILE	3.5
1	A	253	ASN	3.5
1	A	250	THR	3.4
1	A	545	VAL	3.1
1	A	321	HIS	3.1
1	A	252	HIS	2.9
1	A	439	SER	2.8
1	A	290	HIS	2.8
1	A	305	ILE	2.7
1	A	316	ILE	2.6
1	A	292	PRO	2.6
1	A	320	GLY	2.5
1	A	251	ASN	2.5
1	A	575	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	323	ARG	2.4
1	A	318	GLU	2.4
1	A	317	LEU	2.3
1	A	437	GLY	2.3
1	A	453	GLN	2.3
1	A	322	LEU	2.3
1	A	295	SER	2.3
1	A	293	VAL	2.2
1	A	511[A]	HIS	2.1

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
4	8OG	T	6	23/24	0.98	0.13	-	22,25,29,32	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	NA	A	602	1/1	0.99	0.18	1.88	20,20,20,20	0
5	DUP	A	601	28/28	0.98	0.11	-0.68	20,24,27,30	0
7	MG	A	603	1/1	0.99	0.12	-	26,26,26,26	0

6.5 Other polymers ⓘ

There are no such residues in this entry.