Full wwPDB X-ray Structure Validation Report (i)

Feb 28, 2014 – 02:27 AM GMT

PDB ID : 3Q8P
Title : Human DNA polymerase iota incorporating dCTP opposite 8-oxo-guanine
Authors : Kirouac, K.N.; Ling, H.
Deposited on : 2011-01-06
Resolution : 1.95 Å(reported)

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

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance ⓘ

The reported resolution of this entry is 1.95 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	Percentile Ranks	Value
Rfree		0.253
Clashscore		10
Ramachandran outliers		0.3%
Sidechain outliers		8.1%
RSRZ outliers		10.8%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
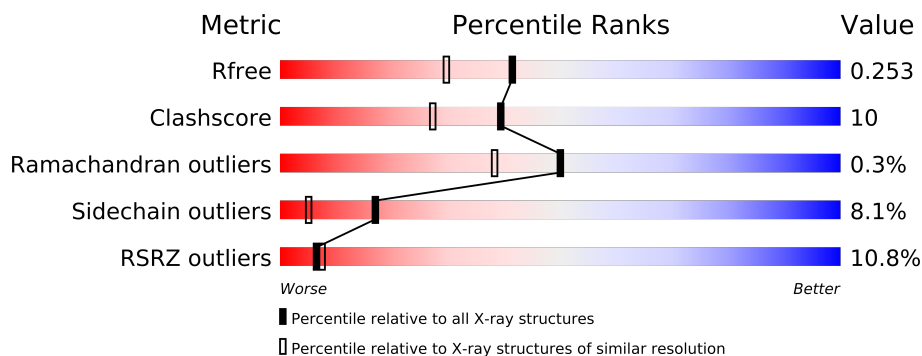
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1321 (1.96-1.96)
Clashscore	79885	1488 (1.96-1.96)
Ramachandran outliers	78287	1475 (1.96-1.96)
Sidechain outliers	78261	1475 (1.96-1.96)
RSRZ outliers	66119	1321 (1.96-1.96)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	B	420	
2	T	11	
3	P	7	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 3743 atoms, of which 0 are hydrogen and 0 are deuterium.

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 iota.

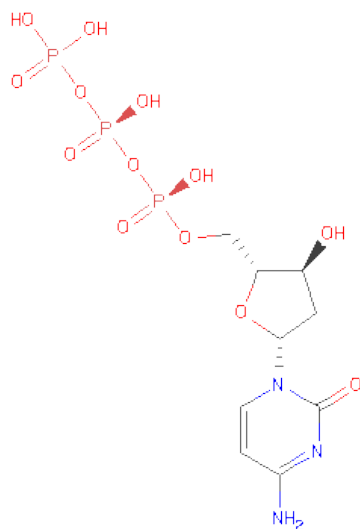| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	380	Total	C	N	O	S	0	3	0
			2983	1888	522	551	22			

- Molecule 2 is a DNA chain called DNA (5'-D(*TP*CP*AP*(8OG)P*GP*GP*GP*TP*CP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	8	Total	C	N	O	P	0	1	0
			190	88	35	58	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	7	Total	C	N	O	P	0	0	0
			142	67	29	39	7			

- Molecule 4 is 2'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (three-letter code: DCP) (formula: $C_9H_{16}N_3O_{13}P_3$).

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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
5	B	2	2	2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	367	Total 367	O 367	0	0
6	T	20	Total 20	O 20	0	0
6	P	11	Total 11	O 11	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.
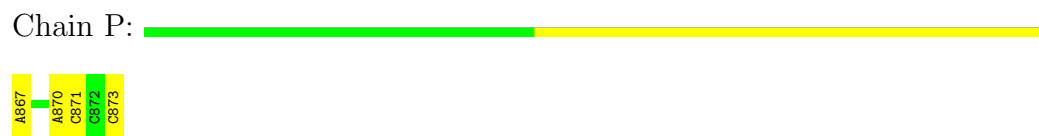
• Molecule 1: DNA polymerase iota

Chain B:
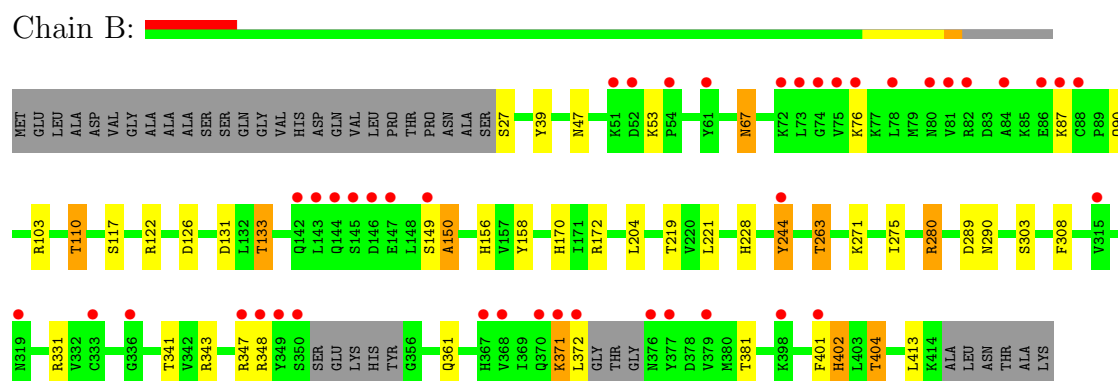
• Molecule 2: DNA (5'-D(*TP*CP*AP*(8OG)P*GP*GP*GP*TP*CP*CP*T)-3')

Chain T:

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

Chain P:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	99.16Å 99.16Å 202.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	32.73 – 1.95 32.73 – 1.95	Depositor EDS
% Data completeness (in resolution range)	95.3 (32.73-1.95) 94.2 (32.73-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.43 (at 1.95Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.225 , 0.257 0.217 , 0.253	Depositor DCC
R_{free} test set	1445 reflections (3.52%)	DCC
Wilson B-factor (Å^2)	30.8	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 47.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$<|L|> = 0.49, <L^2> = 0.33$	Xtriage
Outliers	1 of 43205 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3743	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 8OG, MG, DCP

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	B	0.33	0/3027	0.52	0/4088
2	T	0.74	0/160	1.61	5/245 (2.0%)
3	P	0.60	0/159	1.33	0/242
All	All	0.38	0/3346	0.69	5/4575 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	T	843	DG	O4'-C1'-N9	7.51	113.26	108.00
2	T	847	DT	O4'-C1'-N1	-6.50	103.45	108.00
2	T	843	DG	O4'-C4'-C3'	-6.09	102.06	104.50
2	T	841	DG	O4'-C1'-N9	5.55	111.88	108.00
2	T	843	DG	O5'-P-OP2	-5.53	100.72	105.70

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2983	0	0	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	T	190	0	99	4	1
3	P	142	0	76	7	1
4	B	28	0	11	10	0
5	B	2	0	0	0	0
6	B	367	0	0	6	0
6	P	11	0	0	0	0
6	T	20	0	0	0	0
All	All	3743	0	186	34	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (34) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:B:421[A]:DCP:H5'1	3:P:873:DC:C3'	2.05	0.87
4:B:421[A]:DCP:H5'1	3:P:873:DC:C2'	2.05	0.87
4:B:421[A]:DCP:H5'2	4:B:421[A]:DCP:H6	1.56	0.86
4:B:421[A]:DCP:C5'	3:P:873:DC:C2'	2.64	0.76
4:B:421[A]:DCP:C5'	3:P:873:DC:H2'	2.16	0.75
1:B:401[B]:PHE:CD2	1:B:402:HIS:N	2.63	0.67
1:B:149:SER:N	1:B:150:ALA:CB	2.62	0.62
4:B:421[A]:DCP:C5'	3:P:873:DC:C3'	2.81	0.58
4:B:421[A]:DCP:O2A	6:B:436:HOH:O	2.17	0.58
2:T:840[B]:8OG:H5'	2:T:840[B]:8OG:O8	2.05	0.57
1:B:131:ASP:OD2	1:B:133:THR:CG2	2.52	0.56
4:B:421[A]:DCP:H5'2	3:P:873:DC:H2'	1.86	0.55
4:B:421[A]:DCP:C4	2:T:840[A]:8OG:H7	2.20	0.54
1:B:39:TYR:N	6:B:632:HOH:O	2.41	0.54
3:P:870:DA:H2'	3:P:871:DC:C6	2.46	0.51
1:B:27:SER:O	1:B:172:ARG:NH2	2.43	0.51
1:B:149:SER:CA	1:B:150:ALA:CB	2.89	0.51
2:T:844:DT:H2'	2:T:845:DC:C6	2.47	0.49
4:B:421[A]:DCP:N3	2:T:840[A]:8OG:N7	2.58	0.48
1:B:371:LYS:O	1:B:372:LEU:C	2.51	0.48
1:B:103:ARG:NH2	6:B:767:HOH:O	2.47	0.47
1:B:244:TYR:C	1:B:244:TYR:CD2	2.87	0.47
1:B:303:SER:O	1:B:331:ARG:NH2	2.47	0.47
1:B:343:ARG:CZ	1:B:361:GLN:NE2	2.77	0.47
1:B:331:ARG:CD	6:B:757:HOH:O	2.64	0.46
1:B:156:HIS:CD2	6:B:776:HOH:O	2.70	0.44
1:B:280:ARG:NH2	1:B:289:ASP:OD1	2.53	0.42
1:B:67:ASN:C	1:B:67:ASN:ND2	2.74	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:117:SER:OG	6:B:508:HOH:O	2.22	0.41
1:B:149:SER:CB	1:B:150:ALA:CB	2.98	0.41
1:B:158:TYR:OH	1:B:228:HIS:CD2	2.74	0.41
1:B:347:ARG:NE	1:B:404:THR:CG2	2.84	0.40
1:B:110:THR:CG2	1:B:122:ARG:NH1	2.84	0.40
1:B:263:THR:O	1:B:263:THR:CG2	2.67	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	Distance(Å)	Clash(Å)
2:T:847:DT:O3'	3:P:867:DA:P[12_544]	2.06	0.14

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	B	377/420 (90%)	360 (96%)	16 (4%)	1 (0%)	50	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	150	ALA

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	B	336/376 (89%)	308 (92%)	28 (8%)	16	5

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	47	ASN
1	B	53	LYS
1	B	67	ASN
1	B	76	LYS
1	B	87	LYS
1	B	90	GLN
1	B	110	THR
1	B	126	ASP
1	B	133	THR
1	B	170	HIS
1	B	204	LEU
1	B	219	THR
1	B	221	LEU
1	B	244	TYR
1	B	263	THR
1	B	271	LYS
1	B	275	ILE
1	B	280	ARG
1	B	290[A]	ASN
1	B	290[B]	ASN
1	B	308	PHE
1	B	341	THR
1	B	348	ARG
1	B	371	LYS
1	B	381	THR
1	B	402	HIS
1	B	404	THR
1	B	413	LEU

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 chains 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	8OG	T	840[A]	2	23,25,26	1.94	6 (26%)	27,37,40	2.04	9 (33%)
2	8OG	T	840[B]	2	23,25,26	1.99	6 (26%)	27,37,40	2.10	5 (18%)

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	8OG	T	840[A]	2	-	0/6/21/22	0/1/3/3
2	8OG	T	840[B]	2	-	0/6/21/22	0/1/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	840[A]	8OG	C5-C4	5.39	1.48	1.40
2	T	840[B]	8OG	C5-C4	5.36	1.48	1.40
2	T	840[B]	8OG	C6-C5	4.64	1.48	1.41
2	T	840[A]	8OG	C6-C5	4.25	1.48	1.41
2	T	840[B]	8OG	P-OP1	4.17	1.51	1.46
2	T	840[A]	8OG	P-OP1	3.58	1.50	1.46
2	T	840[A]	8OG	C2-N2	2.73	1.36	1.32
2	T	840[A]	8OG	C4-N9	-2.55	1.34	1.37
2	T	840[B]	8OG	C2-N2	2.29	1.36	1.32
2	T	840[A]	8OG	C2-N3	2.24	1.36	1.33
2	T	840[B]	8OG	C2-N3	2.15	1.36	1.33
2	T	840[B]	8OG	C4-N9	-2.08	1.34	1.37

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	T	840[A]	8OG	N3-C4-N9	5.32	135.17	127.09
2	T	840[B]	8OG	N3-C4-N9	5.23	135.03	127.09
2	T	840[B]	8OG	C8-N9-C1'	5.10	128.00	125.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	T	840[B]	8OG	C2-N3-C4	4.49	121.39	115.09
2	T	840[A]	8OG	C2-N3-C4	4.37	121.22	115.09
2	T	840[A]	8OG	C8-N7-C5	-3.84	103.59	107.48
2	T	840[B]	8OG	C5-C4-N3	-3.50	118.09	125.70
2	T	840[B]	8OG	C8-N7-C5	-3.39	104.04	107.48
2	T	840[A]	8OG	C5-C4-N3	-3.30	118.52	125.70
2	T	840[A]	8OG	O4'-C1'-N9	2.67	110.65	108.15
2	T	840[A]	8OG	C4-C5-N7	2.38	108.13	106.14
2	T	840[A]	8OG	C8-N9-C1'	-2.34	123.88	125.17
2	T	840[A]	8OG	C1'-N9-C4	2.30	131.26	126.99
2	T	840[A]	8OG	C2'-C1'-N9	-2.01	113.75	115.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	#$|Z| > 2$
4	DCP	B	421[A]	5	29,29,29	0.81	0	42,45,45	1.46	7 (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
4	DCP	B	421[A]	5	-	0/19/34/34	0/2/2/2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	421[A]	DCP	C2-N1-C1'	-4.32	114.20	119.25
4	B	421[A]	DCP	C2-N3-C4	3.37	120.44	115.57
4	B	421[A]	DCP	PB-O3B-PG	-3.24	122.17	131.68
4	B	421[A]	DCP	C6-C5-C4	3.03	118.73	117.47
4	B	421[A]	DCP	C6-N1-C1'	2.60	125.37	119.35
4	B	421[A]	DCP	PB-O3A-PA	-2.35	124.79	131.68
4	B	421[A]	DCP	O4'-C1'-N1	2.30	112.00	107.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers (i)

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	B	380/420 (90%)	0.61	43 (11%)	6	6	17, 43, 106, 152	0
2	T	8/11 (72%)	-0.12	0	100	100	27, 33, 37, 46	0
3	P	7/7 (100%)	-0.37	0	100	100	25, 30, 40, 44	0
All	All	395/438 (90%)	0.58	43 (10%)	6	7	17, 42, 106, 152	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	349	TYR	7.2
1	B	333	CYS	6.9
1	B	86	GLU	6.3
1	B	146	ASP	6.0
1	B	372	LEU	6.0
1	B	73	LEU	5.7
1	B	74	GLY	5.5
1	B	377	TYR	5.2
1	B	84	ALA	5.2
1	B	350	SER	5.1
1	B	244	TYR	4.6
1	B	149	SER	4.6
1	B	82	ARG	4.5
1	B	376	ASN	4.4
1	B	401[A]	PHE	3.9
1	B	145	SER	3.8
1	B	147	GLU	3.7
1	B	51	LYS	3.7
1	B	367	HIS	3.5
1	B	348	ARG	3.4
1	B	61	TYR	3.1
1	B	72	LYS	2.8
1	B	80	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	398	LYS	2.7
1	B	52	ASP	2.6
1	B	368	VAL	2.6
1	B	75	VAL	2.5
1	B	81	VAL	2.5
1	B	336	GLY	2.5
1	B	88	CYS	2.4
1	B	379	VAL	2.4
1	B	87	LYS	2.4
1	B	144	GLN	2.4
1	B	76	LYS	2.3
1	B	54	PRO	2.2
1	B	370	GLN	2.2
1	B	143	LEU	2.2
1	B	315	VAL	2.1
1	B	319	ASN	2.1
1	B	347	ARG	2.1
1	B	78	LEU	2.1
1	B	142	GLN	2.1
1	B	371	LYS	2.0

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

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	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	8OG	T	840[A]	23/24	0.23	1.07	40,44,51,56	23
2	8OG	T	840[B]	23/24	0.23	1.07	37,43,50,54	23

6.3 Carbohydrates ⓘ

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	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	DCP	B	421[A]	28/28	0.18	1.17	24,36,41,43	28
5	MG	B	423	1/1	0.07	-1.76	27,27,27,27	0
5	MG	B	422	1/1	0.05	-2.00	21,21,21,21	0

6.5 Other polymers (i)

There are no such residues in this entry.