



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 13, 2018 – 07:54 pm GMT

PDB ID : 3V6K
Title : Replication of N2,3-Ethenoguanine by DNA Polymerases
Authors : Zhao, L.
Deposited on : 2011-12-20
Resolution : 3.60 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	:	trunk31020
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)	:	trunk31020

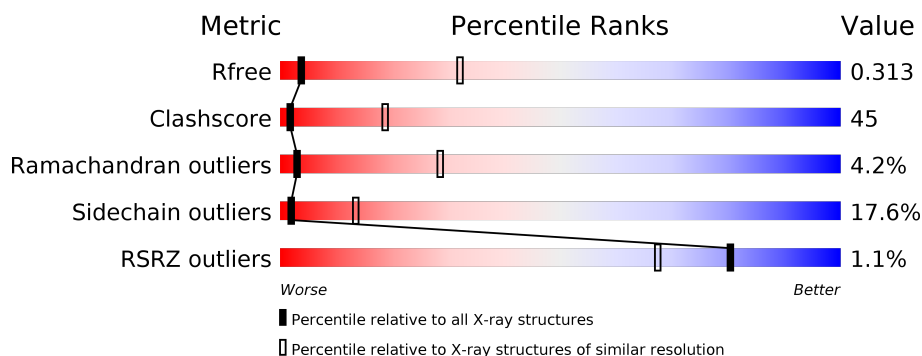
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1053 (3.70-3.50)
Clashscore	122126	1141 (3.70-3.50)
Ramachandran outliers	120053	1102 (3.70-3.50)
Sidechain outliers	120020	1102 (3.70-3.50)
RSRZ outliers	108989	1009 (3.72-3.48)

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	347	
1	J	347	
2	K	10	
2	P	10	
3	B	14	
3	M	14	

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
3	EFG	B	5	-	-	X	-
3	EFG	M	5	-	-	X	-
4	MG	A	401	-	-	-	X
4	MG	A	402	-	-	-	X
5	CA	A	403	-	-	-	X
5	CA	J	402	-	-	-	X
5	CA	J	406	-	-	-	X
6	NA	B	101	-	-	-	X
6	NA	J	407	-	-	-	X
6	NA	P	101	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6100 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 IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	0	0
			2729	1752	467	503	7			
1	J	334	Total	C	N	O	S	0	0	1
			2368	1498	412	451	7			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	HIS	-	EXPRESSION TAG	UNP Q97W02
A	-3	HIS	-	EXPRESSION TAG	UNP Q97W02
A	-2	HIS	-	EXPRESSION TAG	UNP Q97W02
A	-1	HIS	-	EXPRESSION TAG	UNP Q97W02
A	0	HIS	-	EXPRESSION TAG	UNP Q97W02
J	-4	HIS	-	EXPRESSION TAG	UNP Q97W02
J	-3	HIS	-	EXPRESSION TAG	UNP Q97W02
J	-2	HIS	-	EXPRESSION TAG	UNP Q97W02
J	-1	HIS	-	EXPRESSION TAG	UNP Q97W02
J	0	HIS	-	EXPRESSION TAG	UNP Q97W02

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	10	Total	C	N	O	P	0	0	0
			207	99	39	59	10			
2	K	10	Total	C	N	O	P	0	0	0
			207	99	39	59	10			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	B	14	Total	C	F	N	O	P	0	0	0
			282	137	1	48	83	13			
3	M	13	Total	C	F	N	O	P	0	0	0
			262	127	1	46	76	12			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	J	2	Total	Mg	0	0
			2	2		
4	A	2	Total	Mg	0	0
			2	2		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	J	4	Total	Ca	0	0
			4	4		
5	A	3	Total	Ca	0	0
			3	3		

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

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	9	Total	O	0	0
			9	9		
7	J	15	Total	O	0	0
			15	15		
7	P	2	Total	O	0	0
			2	2		

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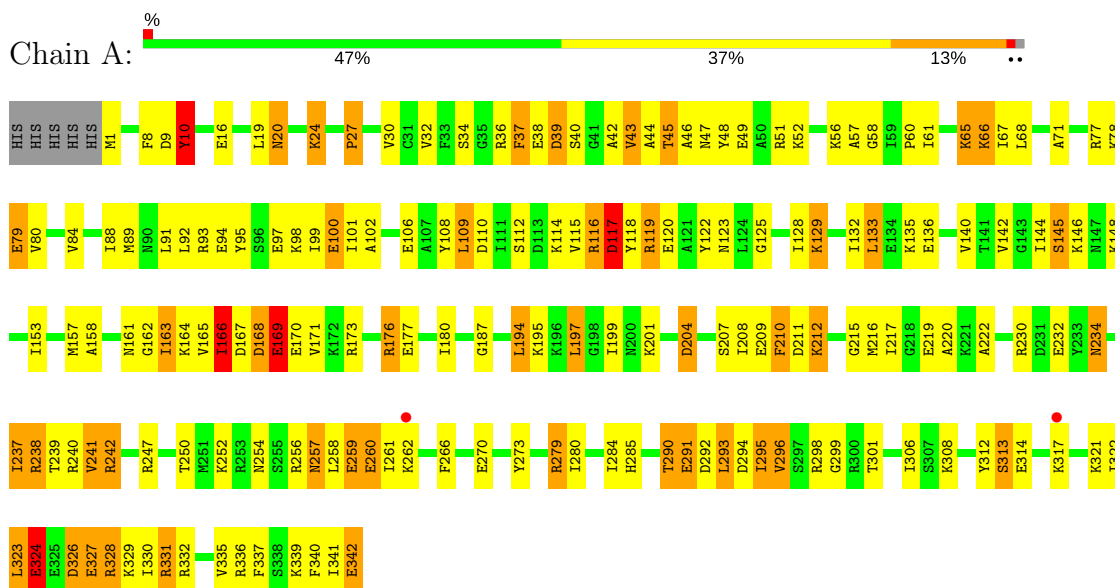
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	3	Total	O	0	0
			3	3		
7	M	1	Total	O	0	0
			1	1		

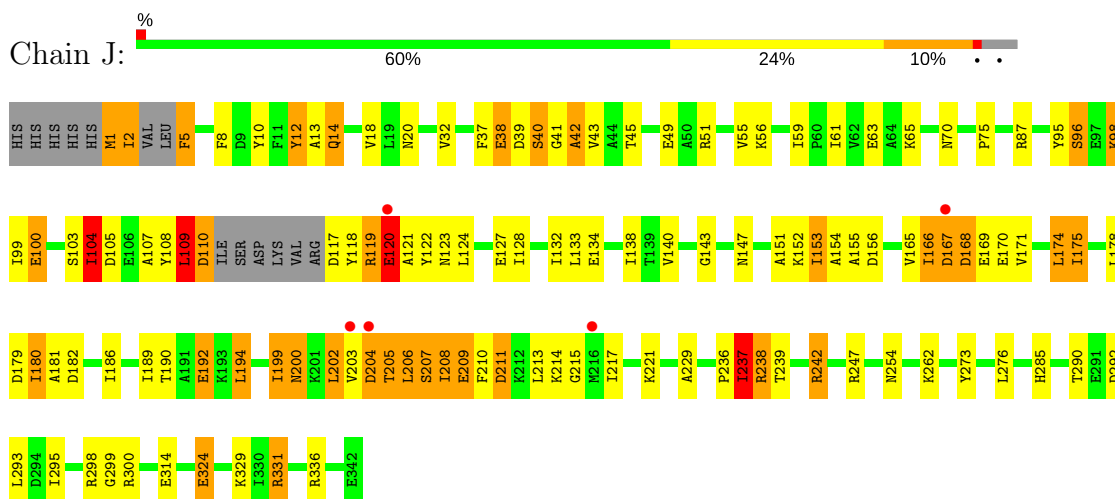
3 Residue-property plots [i](#)

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 polymerase IV

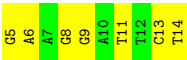


• Molecule 1: DNA polymerase IV

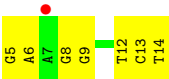


• Molecule 2: DNA (5'-D(P*GP*AP*AP*GP*GP*AP*TP*TP*CP*(2DT))-3')

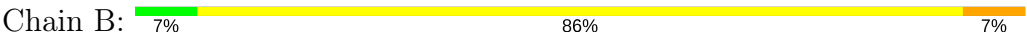




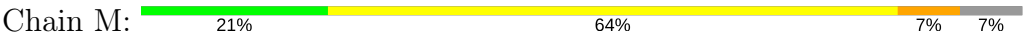
• Molecule 2: DNA (5'-D(P*GP*AP*AP*GP*GP*AP*TP*TP*CP*(2DT))-3')



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.85Å 110.95Å 100.24Å 90.00° 102.70° 90.00°	Depositor
Resolution (Å)	48.90 – 3.60 48.89 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.90-3.60) 99.9 (48.89-3.60)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.229 , 0.303 0.245 , 0.313	Depositor DCC
R_{free} test set	1026 reflections (7.93%)	wwPDB-VP
Wilson B-factor (Å ²)	89.0	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 104.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.042 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	6100	wwPDB-VP
Average B, all atoms (Å ²)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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: 2DT, MG, EFG, CA, NA

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	0.68	1/2768 (0.0%)	0.83	3/3720 (0.1%)
1	J	0.48	0/2396	0.83	9/3257 (0.3%)
2	K	0.32	0/211	0.80	0/324
2	P	0.42	0/211	0.83	1/324 (0.3%)
3	B	0.53	1/285 (0.4%)	0.88	1/434 (0.2%)
3	M	0.37	0/263	0.92	1/400 (0.2%)
All	All	0.57	2/6134 (0.0%)	0.84	15/8459 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	79	GLU	CD-OE1	5.52	1.31	1.25
3	B	3	DA	O3'-P	5.33	1.67	1.61

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	38	GLU	N-CA-CB	13.70	135.26	110.60
1	J	37	PHE	N-CA-C	9.59	136.90	111.00
1	J	38	GLU	N-CA-C	-8.03	89.31	111.00
1	J	210	PHE	N-CA-C	7.33	130.78	111.00
2	P	11	DT	P-O3'-C3'	6.83	127.90	119.70

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	2729	0	2856	228	0
1	J	2368	0	2208	220	0
2	K	207	0	114	8	0
2	P	207	0	114	9	0
3	B	282	0	159	43	0
3	M	262	0	147	42	0
4	A	2	0	0	0	0
4	J	2	0	0	0	0
5	A	3	0	0	0	0
5	J	4	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	J	1	0	0	0	0
6	P	1	0	0	0	0
7	A	9	0	0	1	0
7	B	3	0	0	0	0
7	J	15	0	0	6	0
7	M	1	0	0	0	0
7	P	2	0	0	3	0
All	All	6100	0	5598	527	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 527 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:145:SER:HB2	1:A:166:ILE:CG2	1.55	1.36
1:J:166:ILE:HD11	1:J:170:GLU:CB	1.59	1.31
1:J:205:THR:CG2	1:J:206:LEU:H	1.46	1.28
1:J:204:ASP:HA	1:J:206:LEU:N	1.50	1.25
1:J:98:LYS:HD3	1:J:110:ASP:OD2	1.33	1.23

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	
1	A	340/347 (98%)	283 (83%)	44 (13%)	13 (4%)	3	31
1	J	328/347 (94%)	267 (81%)	46 (14%)	15 (5%)	2	26
All	All	668/694 (96%)	550 (82%)	90 (14%)	28 (4%)	3	28

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	TYR
1	A	37	PHE
1	A	39	ASP
1	A	293	LEU
1	A	324	GLU

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	296/306 (97%)	242 (82%)	54 (18%)	2	12
1	J	216/306 (71%)	180 (83%)	36 (17%)	2	16
All	All	512/612 (84%)	422 (82%)	90 (18%)	2	13

5 of 90 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	260	GLU

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Mol	Chain	Res	Type
1	A	329	LYS
1	J	211	ASP
1	A	279	ARG
1	A	317	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	ASN
1	J	285	HIS
1	A	234	ASN
1	A	47	ASN
1	J	20	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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
3	EFG	B	5	3	18,28,29	1.95	7 (38%)	18,42,45	1.94	5 (27%)
2	2DT	K	14	2,4	12,20,21	0.83	0	11,28,31	2.80	2 (18%)
3	EFG	M	5	3	18,28,29	2.32	7 (38%)	18,42,45	2.63	4 (22%)
2	2DT	P	14	2	12,20,21	0.89	0	11,28,31	3.12	3 (27%)

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	EFG	B	5	3	-	0/3/25/26	0/4/4/4
2	2DT	K	14	2,4	-	0/3/18/19	0/2/2/2
3	EFG	M	5	3	-	0/3/25/26	0/4/4/4
2	2DT	P	14	2	-	0/3/18/19	0/2/2/2

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	5	EFG	C6-C5	-4.62	1.33	1.41
3	M	5	EFG	C2'-C3'	-4.11	1.46	1.52
3	M	5	EFG	C8-N9	-3.66	1.32	1.36
3	M	5	EFG	C5-C4	-3.36	1.32	1.40
3	M	5	EFG	O5'-C5'	-3.25	1.40	1.44

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	5	EFG	F-C2'-C3'	-9.67	89.02	109.13
3	B	5	EFG	F-C2'-C3'	-3.10	102.69	109.13
3	B	5	EFG	C5-C6-N1	-3.03	119.17	123.47
3	M	5	EFG	O4'-C4'-C5'	-2.10	102.40	109.39
3	M	5	EFG	C5-C6-N1	-2.08	120.51	123.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5	EFG	8	0
2	K	14	2DT	1	0
3	M	5	EFG	11	0
2	P	14	2DT	3	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 15 ligands modelled in this entry, 15 are monoatomic - leaving 0 for Mogul analysis.

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

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 [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	342/347 (98%)	-0.19	2 (0%) 89 81	43, 78, 126, 154	16 (4%)
1	J	334/347 (96%)	-0.11	5 (1%) 73 60	64, 121, 201, 254	25 (7%)
2	K	9/10 (90%)	0.35	1 (11%) 5 4	118, 158, 205, 221	1 (11%)
2	P	9/10 (90%)	0.06	0 100 100	99, 127, 193, 233	2 (22%)
3	B	13/14 (92%)	0.06	0 100 100	65, 111, 209, 221	2 (15%)
3	M	12/14 (85%)	0.31	0 100 100	86, 180, 219, 226	0
All	All	719/742 (96%)	-0.13	8 (1%) 80 67	43, 98, 193, 254	46 (6%)

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	120	GLU	3.2
1	A	262	LYS	2.7
1	A	317	LYS	2.4
1	J	167	ASP	2.4
1	J	204	ASP	2.3

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	2DT	K	14	19/20	0.76	0.30	131,150,178,178	0
3	EFG	M	5	25/26	0.81	0.20	94,110,166,171	0
2	2DT	P	14	19/20	0.87	0.22	76,96,142,152	0
3	EFG	B	5	25/26	0.97	0.15	65,70,73,75	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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
4	MG	J	401	1/1	0.30	0.37	210,210,210,210	0
6	NA	P	101	1/1	0.37	0.60	209,209,209,209	0
6	NA	J	407	1/1	0.47	0.67	209,209,209,209	0
5	CA	J	405	1/1	0.51	0.20	209,209,209,209	0
5	CA	J	406	1/1	0.53	0.90	209,209,209,209	0
4	MG	J	403	1/1	0.58	0.36	210,210,210,210	0
5	CA	A	404	1/1	0.66	0.30	209,209,209,209	0
6	NA	A	406	1/1	0.66	0.25	209,209,209,209	0
5	CA	J	402	1/1	0.67	0.69	210,210,210,210	0
4	MG	A	402	1/1	0.69	1.29	210,210,210,210	0
5	CA	A	403	1/1	0.72	0.76	210,210,210,210	0
6	NA	B	101	1/1	0.75	0.86	148,148,148,148	0
4	MG	A	401	1/1	0.78	0.99	210,210,210,210	0
5	CA	A	405	1/1	0.87	0.43	209,209,209,209	0
5	CA	J	404	1/1	0.91	0.13	209,209,209,209	0

6.5 Other polymers ⓘ

There are no such residues in this entry.