



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:35 AM GMT

PDB ID : 2ASD
Title : oxoG-modified Insertion Ternary Complex
Authors : Rechkoblit, O.; Malinina, L.; Cheng, Y.; Kuryavyi, V.; Broyde, S.; Geacintov, N.E.; Patel, D.J.
Deposited on : 2005-08-23
Resolution : 1.95 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

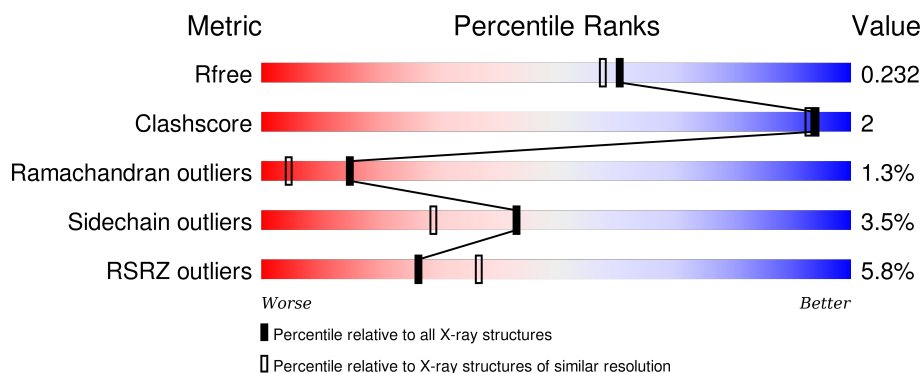
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (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. 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	D	13	<div> <div>8%</div> <div>92%</div> <div>8%</div> </div>
1	H	13	<div> <div>8%</div> <div>69%</div> <div>31%</div> </div>
2	E	19	<div> <div>11%</div> <div>79%</div> <div>11%</div> <div>11%</div> </div>
2	J	19	<div> <div>16%</div> <div>68%</div> <div>26%</div> <div>5%</div> </div>
3	A	360	<div> <div>3%</div> <div>89%</div> <div>5%</div> <div>5%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	B	360	<div><div></div><div>7%</div><div>85%</div><div>8%</div><div>5%</div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7301 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 5'-D(*GP*GP*TP*TP*GP*GP*AP*TP*GP*GP*TP*AP*(DDG))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	13	Total	C	N	O	P	0	0	0
			272	130	53	77	12			
1	H	13	Total	C	N	O	P	0	0	0
			272	130	53	77	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	17	Total	C	N	O	P	0	0	0
			338	162	63	97	16			
2	J	19	Total	C	N	O	P	0	0	0
			377	181	68	110	18			

- Molecule 3 is a protein called DNA polymerase IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	341	Total	C	N	O	S	0	0	0
			2739	1757	472	504	6			
3	B	341	Total	C	N	O	S	0	0	0
			2739	1757	472	504	6			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	CLONING ARTIFACT	UNP Q97W02
A	-6	SER	-	CLONING ARTIFACT	UNP Q97W02
A	-5	HIS	-	CLONING ARTIFACT	UNP Q97W02
A	-4	MET	-	CLONING ARTIFACT	UNP Q97W02
A	-3	GLY	-	CLONING ARTIFACT	UNP Q97W02
A	-2	GLY	-	CLONING ARTIFACT	UNP Q97W02

Continued on next page...

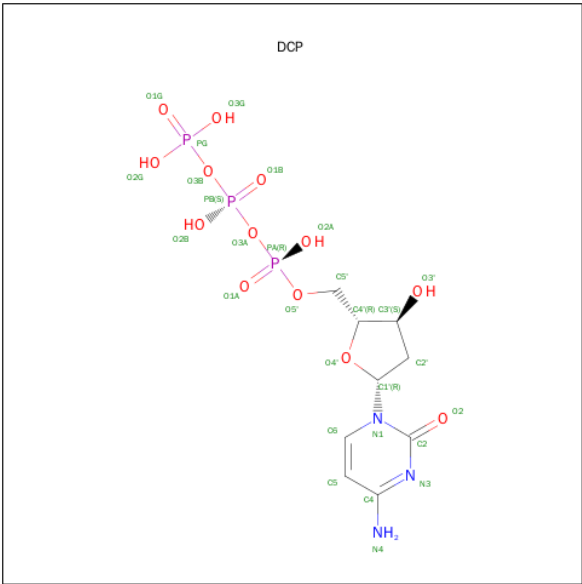
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	CLONING ARTIFACT	UNP Q97W02
A	0	GLY	-	CLONING ARTIFACT	UNP Q97W02
A	1	GLY	-	CLONING ARTIFACT	UNP Q97W02
B	-7	GLY	-	CLONING ARTIFACT	UNP Q97W02
B	-6	SER	-	CLONING ARTIFACT	UNP Q97W02
B	-5	HIS	-	CLONING ARTIFACT	UNP Q97W02
B	-4	MET	-	CLONING ARTIFACT	UNP Q97W02
B	-3	GLY	-	CLONING ARTIFACT	UNP Q97W02
B	-2	GLY	-	CLONING ARTIFACT	UNP Q97W02
B	-1	GLY	-	CLONING ARTIFACT	UNP Q97W02
B	0	GLY	-	CLONING ARTIFACT	UNP Q97W02
B	1001	GLY	-	CLONING ARTIFACT	UNP Q97W02

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	3	Total Ca 3 3	0	0
4	A	3	Total Ca 3 3	0	0
4	D	1	Total Ca 1 1	0	0

- Molecule 5 is 2'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (three-letter code: DCP) (formula: C₉H₁₆N₃O₁₃P₃).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	211	Total	O	2	0
			211	211		
6	B	164	Total	O	0	0
			164	164		
6	D	42	Total	O	1	0
			42	42		
6	E	37	Total	O	0	0
			37	37		
6	H	21	Total	O	0	0
			21	21		
6	J	26	Total	O	0	0
			26	26		

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 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: 5'-D(*GP*GP*TP*TP*GP*GP*AP*TP*GP*GP*TP*AP*(DDG))-3'

Chain D: 




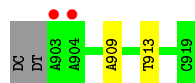
- Molecule 1: 5'-D(*GP*GP*TP*TP*GP*GP*AP*TP*GP*GP*TP*AP*(DDG))-3'

Chain H: 



- Molecule 2: 5'-D(*CP*T*AP*AP*CP*(8OG)P*CP*TP*AP*CP*CP*AP*TP*CP*CP*AP*AP*CP*C)-3'

Chain E: 




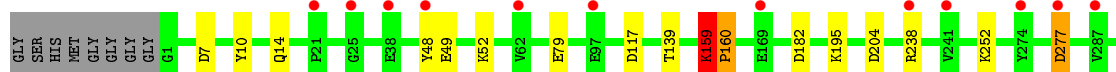
- Molecule 2: 5'-D(*CP*T*AP*AP*CP*(8OG)P*CP*TP*AP*CP*CP*AP*TP*CP*CP*AP*AP*CP*C)-3'

Chain J: 



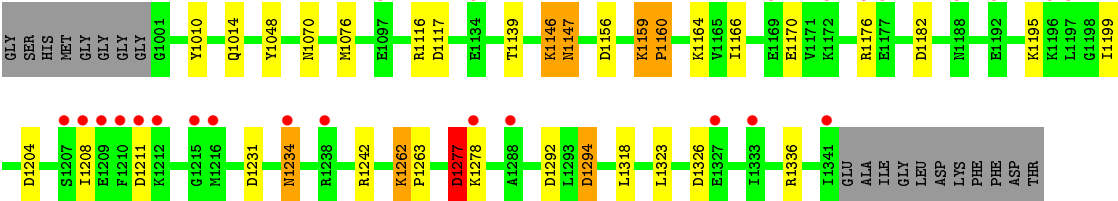
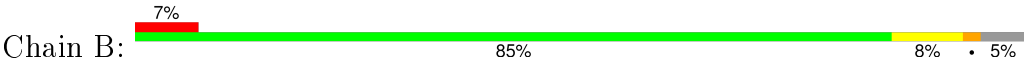
- Molecule 3: DNA polymerase IV

Chain A: 





● Molecule 3: DNA polymerase IV



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.95Å 101.11Å 84.12Å 90.00° 97.14° 90.00°	Depositor
Resolution (Å)	20.00 – 1.95 32.19 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (20.00-1.95) 99.0 (32.19-1.90)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.225 , 0.253 0.231 , 0.232	Depositor DCC
R_{free} test set	4575 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	0.494	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 98410 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7301	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.00 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.5173e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: 8OG, CA, DDG, 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	D	0.68	0/282	1.24	0/436
1	H	0.82	0/282	1.37	1/436 (0.2%)
2	E	0.65	0/351	1.26	3/534 (0.6%)
2	J	1.12	4/394 (1.0%)	1.45	2/600 (0.3%)
3	A	0.34	0/2778	0.69	6/3731 (0.2%)
3	B	0.33	0/2778	0.66	9/3731 (0.2%)
All	All	0.48	4/6865 (0.1%)	0.86	21/9468 (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
3	A	0	1
3	B	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	1919	DC	C4-C5	7.31	1.48	1.43
2	J	1916	DA	N9-C4	5.67	1.41	1.37
2	J	1919	DC	N1-C6	5.61	1.40	1.37
2	J	1919	DC	N1-C2	5.43	1.45	1.40

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1909	DA	O4'-C1'-N9	6.53	112.57	108.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	277	ASP	CB-CG-OD2	6.20	123.88	118.30
3	A	117	ASP	CB-CG-OD2	6.17	123.85	118.30
2	E	913	DT	O4'-C1'-N1	-5.95	103.84	108.00
3	A	292	ASP	CB-CG-OD2	5.85	123.56	118.30
3	A	182	ASP	CB-CG-OD2	5.82	123.54	118.30
2	E	909	DA	O4'-C1'-N9	5.76	112.03	108.00
2	J	1901	DC	O4'-C1'-N1	5.59	111.92	108.00
3	B	1277	ASP	CB-CG-OD2	5.56	123.30	118.30
3	B	1204	ASP	CB-CG-OD2	5.52	123.27	118.30
3	B	1156	ASP	CB-CG-OD2	5.39	123.15	118.30
3	A	7	ASP	CB-CG-OD2	5.31	123.08	118.30
3	A	204	ASP	CB-CG-OD2	5.25	123.02	118.30
3	B	1117	ASP	CB-CG-OD2	5.23	123.01	118.30
3	B	1211	ASP	CB-CG-OD2	5.18	122.96	118.30
3	B	1294	ASP	CB-CG-OD2	5.12	122.91	118.30
3	B	1182	ASP	CB-CG-OD2	5.11	122.90	118.30
2	E	909	DA	C1'-O4'-C4'	-5.09	105.01	110.10
1	H	1801	DG	C4-C5-N7	-5.08	108.77	110.80
3	B	1292	ASP	CB-CG-OD2	5.05	122.85	118.30
3	B	1326	ASP	CB-CG-OD2	5.04	122.84	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	159	LYS	Peptide
3	B	1159	LYS	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	D	272	0	149	1	0
1	H	272	0	149	2	0
2	E	338	0	189	0	0
2	J	377	0	212	2	0
3	A	2739	0	2883	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2739	0	2880	12	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	D	1	0	0	0	0
5	A	28	0	12	0	0
5	B	28	0	12	0	0
6	A	211	0	0	0	0
6	B	164	0	0	1	0
6	D	42	0	0	1	0
6	E	37	0	0	0	0
6	H	21	0	0	1	0
6	J	26	0	0	0	0
All	All	7301	0	6486	24	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 2.

All (24) 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:D:810:DG:OP2	6:D:713:HOH:O	1.80	0.97
3:A:14:GLN:HE22	3:A:139:THR:H	1.12	0.90
3:B:1014:GLN:HE22	3:B:1139:THR:H	1.23	0.82
3:B:1048:TYR:CZ	3:B:1160:PRO:HD3	2.26	0.70
3:B:1277:ASP:O	6:B:1778:HOH:O	2.15	0.64
3:B:1048:TYR:OH	3:B:1160:PRO:HD3	1.99	0.62
3:B:1166:ILE:HG23	3:B:1170:GLU:HB3	1.85	0.59
3:B:1234:ASN:N	3:B:1234:ASN:HD22	2.03	0.57
1:H:1808:DT:OP2	6:H:1789:HOH:O	2.17	0.54
3:B:1147:ASN:HD22	3:B:1147:ASN:C	2.11	0.54
3:B:1048:TYR:CZ	3:B:1160:PRO:CD	2.91	0.53
3:A:48:TYR:OH	3:A:160:PRO:HD3	2.10	0.52
3:B:1014:GLN:NE2	3:B:1139:THR:H	2.00	0.48
3:A:48:TYR:CZ	3:A:160:PRO:HD3	2.49	0.48
3:A:159:LYS:HB3	3:A:160:PRO:CD	2.46	0.46
3:A:79:GLU:H	3:A:79:GLU:CD	2.19	0.46
3:A:14:GLN:NE2	3:A:139:THR:H	1.95	0.45
2:J:1915:DC:C4	2:J:1916:DA:N6	2.84	0.45
3:B:1199:ILE:HD11	3:B:1208:ILE:HG21	2.00	0.43
2:J:1914:DC:C4	2:J:1915:DC:N4	2.87	0.42
3:B:1262:LYS:N	3:B:1263:PRO:HD2	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1146:LYS:HE2	3:B:1231:ASP:OD1	2.19	0.42
3:A:49:GLU:HA	3:A:52:LYS:HE2	2.01	0.42
1:H:1812:DA:H2"	1:H:1813:DDG:H8	2.02	0.41

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	
3	A	339/360 (94%)	328 (97%)	7 (2%)	4 (1%)	16	5
3	B	339/360 (94%)	328 (97%)	6 (2%)	5 (2%)	13	3
All	All	678/720 (94%)	656 (97%)	13 (2%)	9 (1%)	15	4

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	160	PRO
3	B	1160	PRO
3	A	10	TYR
3	B	1010	TYR
3	B	1277	ASP
3	B	1278	LYS
3	A	277	ASP
3	A	159	LYS
3	B	1159	LYS

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	
3	A	299/311 (96%)	293 (98%)	6 (2%)	63	55
3	B	299/311 (96%)	284 (95%)	15 (5%)	30	14
All	All	598/622 (96%)	577 (96%)	21 (4%)	43	29

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	195	LYS
3	A	238	ARG
3	A	252	LYS
3	A	297	SER
3	A	323	LEU
3	A	327	GLU
3	B	1070	ASN
3	B	1076	MET
3	B	1116	ARG
3	B	1146	LYS
3	B	1147	ASN
3	B	1164	LYS
3	B	1176	ARG
3	B	1195	LYS
3	B	1234	ASN
3	B	1242	ARG
3	B	1262	LYS
3	B	1294	ASP
3	B	1318	LEU
3	B	1323	LEU
3	B	1336	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	14	GLN
3	A	285	HIS
3	B	1014	GLN
3	B	1083	GLN
3	B	1147	ASN
3	B	1234	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$
1	DDG	D	813	1,2,4	15,23,24	1.21	1 (6%)	16,33,36	2.66	5 (31%)
2	8OG	E	906	2	16,25,26	3.14	4 (25%)	21,37,40	4.33	11 (52%)
1	DDG	H	1813	1,2,4	15,23,24	1.25	1 (6%)	16,33,36	2.73	4 (25%)
2	8OG	J	1906	2	16,25,26	3.11	4 (25%)	21,37,40	4.24	11 (52%)

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
1	DDG	D	813	1,2,4	-	0/3/18/19	0/3/3/3
2	8OG	E	906	2	-	0/3/21/22	0/3/3/3
1	DDG	H	1813	1,2,4	-	0/3/18/19	0/3/3/3
2	8OG	J	1906	2	-	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)
2	E	906	8OG	O3'-C3'	-8.62	1.24	1.43
2	J	1906	8OG	O3'-C3'	-8.43	1.24	1.43
2	J	1906	8OG	C3'-C4'	-7.32	1.32	1.53
2	E	906	8OG	C3'-C4'	-7.29	1.32	1.53
2	E	906	8OG	C6-C5	3.10	1.47	1.41
2	J	1906	8OG	C6-C5	3.31	1.47	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	1906	8OG	C5-C4	3.37	1.48	1.40
2	E	906	8OG	C5-C4	3.63	1.48	1.40
1	D	813	DDG	C6-N1	3.65	1.39	1.33
1	H	1813	DDG	C6-N1	3.77	1.40	1.33

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	1813	DDG	C5-C6-N1	-7.81	112.91	123.59
1	D	813	DDG	C5-C6-N1	-7.69	113.08	123.59
2	E	906	8OG	C4'-O4'-C1'	-4.82	97.27	109.47
2	J	1906	8OG	C5-C6-N1	-4.48	117.47	123.59
2	E	906	8OG	C6-C5-C4	-4.38	115.66	120.90
2	E	906	8OG	C5-C6-N1	-4.28	117.73	123.59
2	J	1906	8OG	C4'-O4'-C1'	-4.28	98.65	109.47
2	J	1906	8OG	C6-C5-C4	-4.11	115.99	120.90
2	E	906	8OG	N3-C2-N1	-3.51	122.10	127.44
2	J	1906	8OG	N3-C2-N1	-3.07	122.77	127.44
2	J	1906	8OG	C8-N9-C1'	-2.91	120.69	125.97
2	E	906	8OG	C3'-C2'-C1'	-2.41	96.60	102.40
2	J	1906	8OG	C3'-C2'-C1'	-2.36	96.72	102.40
2	E	906	8OG	C8-N9-C1'	-2.25	121.90	125.97
1	H	1813	DDG	N3-C2-N1	-2.19	124.11	127.44
1	D	813	DDG	C6-C5-C4	-2.01	118.50	120.90
1	H	1813	DDG	C2'-C1'-N9	2.00	116.55	112.49
1	D	813	DDG	C3'-C2'-C1'	2.05	105.00	102.71
1	D	813	DDG	C4-C5-N7	2.20	111.50	109.48
2	J	1906	8OG	O4'-C1'-C2'	2.73	111.72	106.27
2	J	1906	8OG	O3'-C3'-C2'	2.77	119.93	110.74
2	E	906	8OG	O3'-C3'-C2'	2.85	120.17	110.74
2	E	906	8OG	O4'-C1'-C2'	2.90	112.05	106.27
2	J	1906	8OG	O4'-C1'-N9	4.49	112.02	108.22
2	J	1906	8OG	C6-N1-C2	5.11	123.03	115.94
2	E	906	8OG	C6-N1-C2	5.40	123.44	115.94
1	D	813	DDG	C6-N1-C2	5.43	123.48	115.94
2	E	906	8OG	O4'-C1'-N9	5.62	112.97	108.22
1	H	1813	DDG	C6-N1-C2	5.66	123.80	115.94
2	E	906	8OG	C2'-C1'-N9	14.69	130.56	115.83
2	J	1906	8OG	C2'-C1'-N9	14.79	130.66	115.83

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
1	H	1813	DDG	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 7 are monoatomic - leaving 2 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	DCP	A	414	4	21,29,29	0.71	0	33,45,45	1.40	4 (12%)
5	DCP	B	1414	4	21,29,29	0.82	0	33,45,45	1.37	4 (12%)

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	DCP	A	414	4	-	0/18/34/34	0/2/2/2
5	DCP	B	1414	4	-	0/18/34/34	0/2/2/2

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	414	DCP	C2'-C1'-N1	-2.68	107.64	114.16
5	B	1414	DCP	C2'-C1'-N1	-2.59	107.86	114.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	414	DCP	O4'-C1'-N1	2.24	111.60	107.72
5	B	1414	DCP	O3A-PA-O5'	2.51	109.60	102.94
5	A	414	DCP	O3A-PA-O5'	2.59	109.81	102.94
5	B	1414	DCP	O4'-C1'-N1	2.92	112.78	107.72
5	B	1414	DCP	C2-N3-C4	4.05	121.32	115.61
5	A	414	DCP	C2-N3-C4	4.10	121.39	115.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 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

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	D	12/13 (92%)	-0.28	0 100 100	12, 16, 24, 26	0
1	H	12/13 (92%)	0.35	1 (8%) 14 22	15, 17, 23, 26	0
2	E	16/19 (84%)	0.27	2 (12%) 5 9	10, 19, 43, 47	0
2	J	18/19 (94%)	1.20	3 (16%) 2 3	11, 18, 48, 52	0
3	A	341/360 (94%)	0.26	12 (3%) 48 58	8, 14, 24, 29	0
3	B	341/360 (94%)	0.50	25 (7%) 18 28	9, 16, 23, 27	0
All	All	740/784 (94%)	0.39	43 (5%) 26 37	8, 15, 24, 52	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	1901	DC	8.4
2	J	1902	DT	5.9
3	B	1196	LYS	4.4
3	B	1169	GLU	4.3
3	B	1234	ASN	4.2
2	E	903	DA	4.2
3	A	25	GLY	4.2
3	B	1210	PHE	3.7
2	E	904	DA	3.4
3	B	1188	ASN	3.3
3	B	1197	LEU	3.2
1	H	1801	DG	3.1
3	A	21	PRO	3.1
3	B	1216	MET	3.0
3	A	97	GLU	2.9
3	A	38	GLU	2.8
3	B	1172	LYS	2.8
3	B	1208	ILE	2.8
3	A	287	VAL	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	B	1215	GLY	2.7
3	A	238	ARG	2.7
3	B	1176	ARG	2.7
3	B	1212	LYS	2.6
2	J	1903	DA	2.6
3	A	48	TYR	2.6
3	A	277	ASP	2.5
3	A	274	TYR	2.5
3	B	1211	ASP	2.5
3	B	1288	ALA	2.4
3	A	169	GLU	2.4
3	B	1097	GLU	2.3
3	B	1278	LYS	2.3
3	B	1327	GLU	2.3
3	A	241	VAL	2.3
3	B	1134	GLU	2.3
3	B	1177	GLU	2.3
3	B	1207	SER	2.2
3	B	1209	GLU	2.2
3	B	1333	ILE	2.1
3	B	1341	ILE	2.1
3	B	1238	ARG	2.1
3	A	62	VAL	2.0
3	B	1192	GLU	2.0

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
1	DDG	D	813	21/22	0.97	0.11	-	12,14,16,17	0
1	DDG	H	1813	21/22	0.96	0.10	-	10,12,20,20	0
2	8OG	E	906	23/24	0.96	0.09	-	9,11,16,17	0
2	8OG	J	1906	23/24	0.97	0.10	-	7,9,11,12	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(\AA^2)	Q<0.9
5	DCP	B	1414	28/28	0.95	0.11	-0.19	7,10,14,20	0
5	DCP	A	414	28/28	0.94	0.11	-0.47	7,10,16,21	0
4	CA	B	1416	1/1	0.99	0.11	-0.56	11,11,11,11	0
4	CA	A	417	1/1	0.98	0.05	-1.96	14,14,14,14	0
4	CA	A	416	1/1	0.99	0.09	-2.93	12,12,12,12	0
4	CA	B	1417	1/1	0.99	0.06	-3.64	25,25,25,25	0
4	CA	A	415	1/1	1.00	0.08	-4.82	17,17,17,17	0
4	CA	B	1415	1/1	0.99	0.04	-5.81	22,22,22,22	0
4	CA	D	418	1/1	0.96	0.19	-	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.