



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 10:33 pm GMT

PDB ID : 2B3J  
Title : Crystal Structure of Staphylococcus aureus tRNA Adenosine Deaminase, TadA, in Complex with RNA  
Authors : Losey, H.C.; Ruthenburg, A.J.; Verdine, G.L.  
Deposited on : 2005-09-20  
Resolution : 2.00 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

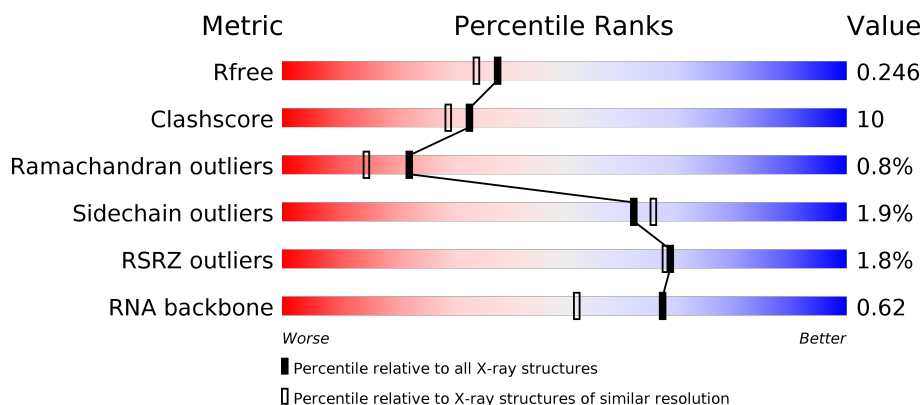
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)
RNA backbone	2435	1011 (2.66-1.34)

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  $\geq 3$ , 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	E	16	
1	F	16	
1	G	16	
1	H	16	

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Mol	Chain	Length	Quality of chain
2	A	159	
2	B	159	
2	C	159	
2	D	159	

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
1	P5P	G	34	-	-	X	-
4	GOL	A	1001	-	-	-	X
4	GOL	B	1002	-	-	-	X
4	GOL	C	1004	-	-	-	X
4	GOL	D	1003	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5991 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 RNA chain called anticodon stem-loop of t-RNA-Arg2 (nucleotides 27-42).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	15	Total	C	N	O	P	0	0	0
			315	143	56	102	14			
1	F	15	Total	C	N	O	P	0	0	0
			315	143	56	102	14			
1	G	8	Total	C	N	O	P	0	0	0
			169	77	32	53	7			
1	H	16	Total	C	N	O	P	0	0	0
			335	152	58	110	15			

- Molecule 2 is a protein called tRNA adenosine deaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	151	Total	C	N	O	S	0	0	0
			1137	715	202	211	9			
2	B	151	Total	C	N	O	S	0	0	0
			1132	712	202	208	10			
2	C	152	Total	C	N	O	S	0	0	0
			1140	718	203	209	10			
2	D	150	Total	C	N	O	S	0	0	0
			1120	702	201	208	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP Q99W51
A	-1	SER	-	EXPRESSION TAG	UNP Q99W51
A	0	HIS	-	EXPRESSION TAG	UNP Q99W51
B	-2	GLY	-	EXPRESSION TAG	UNP Q99W51
B	-1	SER	-	EXPRESSION TAG	UNP Q99W51
B	0	HIS	-	EXPRESSION TAG	UNP Q99W51
C	-2	GLY	-	EXPRESSION TAG	UNP Q99W51
C	-1	SER	-	EXPRESSION TAG	UNP Q99W51

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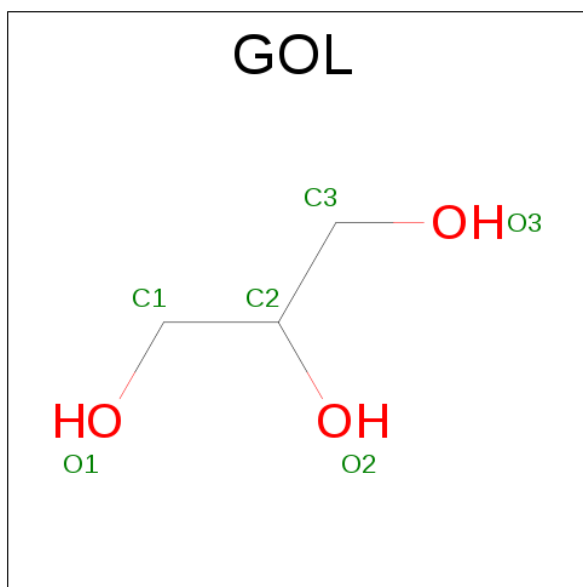
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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	EXPRESSION TAG	UNP Q99W51
D	-2	GLY	-	EXPRESSION TAG	UNP Q99W51
D	-1	SER	-	EXPRESSION TAG	UNP Q99W51
D	0	HIS	-	EXPRESSION TAG	UNP Q99W51

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Zn 1 1	0	0
3	A	1	Total Zn 1 1	0	0
3	D	1	Total Zn 1 1	0	0
3	C	1	Total Zn 1 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

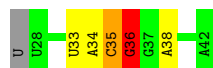
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	17	Total	O	0	0
			17	17		
5	F	10	Total	O	0	0
			10	10		
5	G	3	Total	O	0	0
			3	3		
5	H	11	Total	O	0	0
			11	11		
5	A	69	Total	O	0	0
			69	69		
5	B	53	Total	O	0	0
			53	53		
5	C	82	Total	O	0	0
			82	82		
5	D	55	Total	O	0	0
			55	55		

### 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.

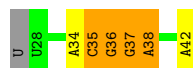
- Molecule 1: anticodon stem-loop of t-RNA-Arg2 (nucleotides 27-42)

Chain E: 




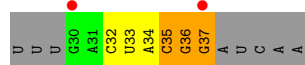
- Molecule 1: anticodon stem-loop of t-RNA-Arg2 (nucleotides 27-42)

Chain F: 



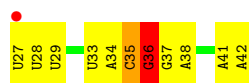
- Molecule 1: anticodon stem-loop of t-RNA-Arg2 (nucleotides 27-42)

Chain G: 




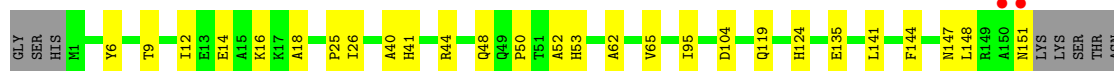
- Molecule 1: anticodon stem-loop of t-RNA-Arg2 (nucleotides 27-42)

Chain H: 




- Molecule 2: tRNA adenosine deaminase

Chain A: 

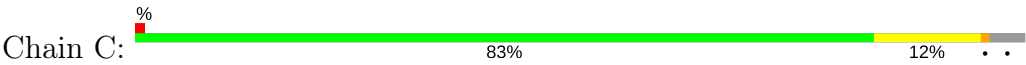


- Molecule 2: tRNA adenosine deaminase

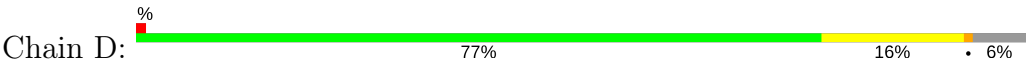
Chain B: 



● Molecule 2: tRNA adenosine deaminase



● Molecule 2: tRNA adenosine deaminase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.06Å 89.03Å 119.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.00 – 2.00 48.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.9 (48.00-2.00) 95.1 (48.00-2.00)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.32 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.215 , 0.242 0.219 , 0.246	Depositor DCC
$R_{free}$ test set	2836 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.0	Xtriage
Anisotropy	0.650	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 52.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5991	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, P5P

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	E	0.32	0/327	0.93	3/505 (0.6%)
1	F	0.26	0/327	0.99	2/505 (0.4%)
1	G	0.47	0/164	1.33	3/252 (1.2%)
1	H	0.29	0/349	0.90	2/539 (0.4%)
2	A	0.32	0/1154	0.59	0/1564
2	B	0.31	0/1149	0.58	0/1557
2	C	0.33	0/1157	0.59	0/1568
2	D	0.33	0/1137	0.56	0/1541
All	All	0.32	0/5764	0.70	10/8031 (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	G	1	0

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	37	G	C2'-C3'-O3'	9.63	130.68	109.50
1	F	37	G	C2'-C3'-O3'	8.49	128.18	109.50
1	E	35	C	N1-C1'-C2'	5.98	121.78	114.00
1	G	37	G	C5'-C4'-C3'	-5.32	107.48	116.00
1	G	37	G	C4'-C3'-C2'	5.26	107.86	102.60
1	E	35	C	O4'-C1'-N1	5.17	112.34	108.20
1	H	37	G	N9-C1'-C2'	5.17	120.73	114.00
1	E	36	G	N9-C1'-C2'	5.15	120.69	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	37	G	C4'-C3'-C2'	5.11	107.71	102.60
1	H	36	G	N9-C1'-C2'	5.09	120.62	114.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	G	37	G	C3'

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	E	315	0	162	3	0
1	F	315	0	162	10	0
1	G	169	0	88	12	0
1	H	335	0	172	18	0
2	A	1137	0	1145	23	0
2	B	1132	0	1139	23	0
2	C	1140	0	1153	19	0
2	D	1120	0	1111	18	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
4	C	6	0	8	0	0
4	D	6	0	8	2	0
5	A	69	0	0	1	0
5	B	53	0	0	2	0
5	C	82	0	0	2	0
5	D	55	0	0	1	0
5	E	17	0	0	2	0
5	F	10	0	0	3	0
5	G	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	11	0	0	1	0
All	All	5991	0	5164	106	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 10.

All (106) 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:F:42:A:H3'	1:H:27:U:H5'	1.35	1.05
2:A:48:GLN:HE21	2:B:68:SER:HA	1.42	0.83
2:D:44:ARG:HD2	2:D:53:HIS:CD2	2.15	0.82
1:F:42:A:C3'	1:H:27:U:H5'	2.13	0.79
2:B:29:ILE:HD13	2:B:39:ARG:HB3	1.68	0.73
2:C:5:ILE:HG23	2:C:133:LEU:HD11	1.70	0.73
2:A:26:ILE:HD11	2:A:141:LEU:HD21	1.69	0.73
1:G:34:P5P:O2'	1:G:35:C:OP2	2.07	0.72
1:F:34:P5P:C4	2:B:26:ILE:HD12	2.20	0.71
2:A:44:ARG:HD2	2:A:53:HIS:CD2	2.26	0.70
2:B:44:ARG:HD2	2:B:53:HIS:CD2	2.27	0.69
2:A:18:ALA:HB2	2:A:41:HIS:HB2	1.73	0.68
1:H:27:U:H3'	1:H:27:U:O2	1.92	0.68
2:D:82:PRO:HG2	2:D:110:SER:OG	1.93	0.67
2:C:91:VAL:HG12	2:C:92:MET:CE	2.25	0.67
2:D:145:PHE:O	2:D:149:ARG:HG3	1.95	0.66
1:G:33:U:H4'	1:G:34:P5P:O5'	1.98	0.64
2:C:92:MET:HE2	2:C:92:MET:HA	1.80	0.63
2:D:14:GLU:OE1	2:D:41:HIS:HD2	1.82	0.62
2:C:12:ILE:HD12	2:C:133:LEU:HD23	1.83	0.61
2:B:94:ARG:HD2	5:B:2005:HOH:O	2.01	0.61
1:G:35:C:O2'	1:G:36:G:H3'	2.01	0.60
2:B:70:ARG:NH2	5:B:2046:HOH:O	2.35	0.59
2:A:62:ALA:O	2:A:65:VAL:HG22	2.03	0.58
2:B:18:ALA:HB2	2:B:41:HIS:HB2	1.86	0.58
2:D:81:GLU:HB2	2:D:103:ASP:HA	1.86	0.57
1:G:36:G:C8	2:C:149:ARG:HG2	2.38	0.57
2:D:84:VAL:HG12	4:D:1003:GOL:H12	1.86	0.57
1:H:28:U:H2'	1:H:29:U:C6	2.40	0.57
1:F:35:C:H4'	1:F:36:G:H5'	1.86	0.57
2:C:91:VAL:HG12	2:C:92:MET:HE3	1.87	0.56
1:H:33:U:H4'	1:H:34:P5P:O5'	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:6:TYR:O	2:D:9:THR:HB	2.05	0.56
5:F:192:HOH:O	2:B:44:ARG:HD2	2.05	0.55
1:G:35:C:H6	1:G:35:C:H5'	1.73	0.54
2:A:14:GLU:HG2	2:A:40:ALA:O	2.07	0.53
1:H:27:U:H2'	1:H:28:U:H6	1.74	0.53
1:G:34:P5P:H4'	2:C:145:PHE:CZ	2.43	0.53
1:E:36:G:H5''	1:E:38:A:N7	2.24	0.53
1:F:34:P5P:H2	2:B:42:ASN:HB2	1.91	0.51
1:G:36:G:H8	2:C:149:ARG:HG2	1.75	0.51
5:H:43:HOH:O	2:C:124:HIS:HD2	1.94	0.51
2:D:44:ARG:HD2	2:D:53:HIS:HD2	1.70	0.50
1:H:27:U:H2'	1:H:28:U:C6	2.46	0.50
2:C:148:LEU:O	2:C:152:LYS:HG3	2.12	0.49
2:A:48:GLN:HE21	2:B:68:SER:CA	2.21	0.49
5:F:192:HOH:O	2:B:44:ARG:CD	2.60	0.49
2:D:78:VAL:O	2:D:100:TYR:HA	2.12	0.49
5:F:63:HOH:O	2:A:124:HIS:HD2	1.95	0.49
2:A:26:ILE:CD1	2:A:141:LEU:HD21	2.42	0.49
1:H:33:U:O3'	2:D:106:LYS:HD3	2.12	0.49
1:G:32:C:H2'	1:G:36:G:O6	2.13	0.49
1:H:28:U:H2'	1:H:29:U:H6	1.77	0.49
2:A:135:GLU:CD	2:A:135:GLU:H	2.17	0.48
1:H:27:U:O2'	1:H:28:U:H5'	2.13	0.48
1:F:37:G:O2'	1:F:38:A:H5'	2.13	0.48
2:A:14:GLU:HG3	2:A:41:HIS:HB3	1.96	0.48
5:E:56:HOH:O	2:A:44:ARG:CD	2.60	0.48
2:B:136:ALA:O	2:B:140:LEU:HD13	2.13	0.47
2:C:125:ARG:NH2	5:C:2083:HOH:O	2.46	0.47
2:C:145:PHE:O	2:C:149:ARG:HG3	2.13	0.47
1:G:34:P5P:HO2'	1:G:35:C:P	2.34	0.47
2:D:90:ILE:HG23	2:D:95:ILE:HB	1.95	0.47
1:H:27:U:C3'	1:H:27:U:O2	2.60	0.47
1:H:34:P5P:O2'	1:H:35:C:P	2.73	0.47
5:E:56:HOH:O	2:A:44:ARG:HD2	2.16	0.46
1:F:34:P5P:H2	2:B:42:ASN:CB	2.46	0.46
1:F:34:P5P:H6	2:B:55:GLU:OE1	2.16	0.45
2:D:44:ARG:HA	2:D:52:ALA:HB3	1.98	0.45
1:H:36:G:C8	2:D:149:ARG:HG2	2.52	0.45
2:C:97:ARG:NH1	2:C:129:ASP:OD2	2.50	0.45
1:G:34:P5P:O2'	1:G:35:C:P	2.75	0.45
2:A:12:ILE:O	2:A:16:LYS:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:50:PRO:HD3	2:B:69:TRP:HA	1.99	0.44
2:B:125:ARG:HG3	2:B:125:ARG:NH1	2.33	0.44
2:B:125:ARG:HH11	2:B:125:ARG:HG3	1.83	0.44
1:H:36:G:H5''	1:H:38:A:N7	2.32	0.44
1:H:34:P5P:H2	2:D:42:ASN:HB2	2.00	0.44
2:A:25:PRO:O	2:A:26:ILE:HD13	2.18	0.43
2:B:44:ARG:HD2	2:B:53:HIS:HD2	1.81	0.43
2:A:144:PHE:CE2	2:A:148:LEU:HD12	2.53	0.43
2:B:29:ILE:HD13	2:B:39:ARG:CB	2.42	0.43
2:C:92:MET:HE2	2:C:92:MET:CA	2.47	0.43
2:C:84:VAL:HG13	2:C:85:MET:N	2.33	0.43
2:B:81:GLU:HG3	2:B:110:SER:HB2	2.01	0.42
2:C:91:VAL:HG12	2:C:92:MET:HE2	2.00	0.42
2:A:95:ILE:O	2:A:124:HIS:HE1	2.02	0.42
2:A:119:GLN:NE2	5:A:2024:HOH:O	2.52	0.42
1:E:33:U:O2	2:A:104:ASP:HA	2.20	0.42
2:A:44:ARG:HD2	2:A:53:HIS:HD2	1.82	0.42
1:H:34:P5P:C4	2:D:26:ILE:HD12	2.49	0.42
2:D:44:ARG:HD2	2:D:53:HIS:NE2	2.33	0.42
1:F:34:P5P:H2	2:B:42:ASN:CG	2.40	0.42
1:F:42:A:N6	1:H:27:U:C5	2.88	0.42
2:A:6:TYR:O	2:A:9:THR:HB	2.19	0.41
1:E:33:U:H4'	1:E:34:P5P:O5'	2.19	0.41
2:D:118:GLN:NE2	5:D:2047:HOH:O	2.48	0.41
2:A:147:ASN:O	2:A:151:ASN:HB2	2.20	0.41
1:H:41:A:H2'	1:H:42:A:C8	2.56	0.41
2:C:12:ILE:CD1	2:C:133:LEU:HD23	2.48	0.41
2:B:100:TYR:CZ	2:B:130:LYS:HB3	2.56	0.41
2:B:84:VAL:HG13	2:B:85:MET:N	2.36	0.41
1:G:34:P5P:H4'	2:C:145:PHE:HZ	1.83	0.41
1:G:34:P5P:H6	5:C:2012:HOH:O	2.21	0.40
2:C:122:PHE:CG	4:D:1003:GOL:H31	2.56	0.40
2:D:94:ARG:HG3	2:D:94:ARG:HH11	1.87	0.40

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	
2	A	149/159 (94%)	143 (96%)	5 (3%)	1 (1%)	25	18
2	B	149/159 (94%)	143 (96%)	5 (3%)	1 (1%)	25	18
2	C	150/159 (94%)	143 (95%)	6 (4%)	1 (1%)	25	18
2	D	148/159 (93%)	137 (93%)	9 (6%)	2 (1%)	13	6
All	All	596/636 (94%)	566 (95%)	25 (4%)	5 (1%)	22	15

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	52	ALA
2	A	52	ALA
2	C	52	ALA
2	D	52	ALA
2	D	25	PRO

### 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	
2	A	119/131 (91%)	119 (100%)	0	100	100
2	B	117/131 (89%)	115 (98%)	2 (2%)	66	70
2	C	119/131 (91%)	115 (97%)	4 (3%)	42	40
2	D	115/131 (88%)	112 (97%)	3 (3%)	51	52
All	All	470/524 (90%)	461 (98%)	9 (2%)	62	66

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	103	ASP
2	B	148	LEU
2	C	1	MET
2	C	2	THR
2	C	33	ASP
2	C	125	ARG
2	D	39	ARG
2	D	72	GLU
2	D	152	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	48	GLN
2	A	124	HIS
2	B	3	ASN
2	B	121	ASN
2	C	3	ASN
2	C	119	GLN
2	C	124	HIS
2	D	20	GLN
2	D	41	HIS
2	D	118	GLN
2	D	151	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	E	13/16 (81%)	2 (15%)	0
1	F	13/16 (81%)	3 (23%)	0
1	G	6/16 (37%)	3 (50%)	0
1	H	14/16 (87%)	2 (14%)	0
All	All	46/64 (71%)	10 (21%)	0

All (10) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	E	35	C
1	E	36	G

*Continued on next page...*



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Mol	Chain	Res	Type
1	F	35	C
1	F	36	G
1	F	38	A
1	G	35	C
1	G	36	G
1	G	37	G
1	H	35	C
1	H	36	G

There are no RNA pucker outliers to report.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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	P5P	E	34	1	16,23,24	0.63	0	14,33,36	1.87	3 (21%)
1	P5P	F	34	1	16,23,24	0.66	0	14,33,36	1.87	3 (21%)
1	P5P	G	34	1	16,23,24	0.77	0	14,33,36	2.00	3 (21%)
1	P5P	H	34	1	16,23,24	0.55	0	14,33,36	1.86	3 (21%)

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	P5P	E	34	1	-	0/3/25/26	0/3/3/3
1	P5P	F	34	1	-	0/3/25/26	0/3/3/3
1	P5P	G	34	1	-	0/3/25/26	0/3/3/3
1	P5P	H	34	1	-	0/3/25/26	0/3/3/3

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	34	P5P	N1-C2-N3	-4.68	121.43	127.67
1	F	34	P5P	N1-C2-N3	-4.52	121.63	127.67
1	E	34	P5P	N1-C2-N3	-4.44	121.74	127.67
1	H	34	P5P	N1-C2-N3	-4.27	121.97	127.67
1	G	34	P5P	C1'-N9-C4	-3.24	121.04	126.64
1	E	34	P5P	C1'-N9-C4	-2.62	122.10	126.64
1	F	34	P5P	C1'-N9-C4	-2.48	122.35	126.64
1	H	34	P5P	O3'-C3'-C2'	2.59	120.14	111.83
1	H	34	P5P	C6-N1-C2	3.84	121.16	115.89
1	F	34	P5P	C6-N1-C2	3.93	121.27	115.89
1	E	34	P5P	C6-N1-C2	4.10	121.51	115.89
1	G	34	P5P	C6-N1-C2	4.10	121.51	115.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	34	P5P	1	0
1	F	34	P5P	5	0
1	G	34	P5P	7	0
1	H	34	P5P	4	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 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	$\# Z  > 2$
4	GOL	A	1001	-	5,5,5	0.30	0	5,5,5	0.46	0
4	GOL	B	1002	-	5,5,5	0.37	0	5,5,5	0.55	0
4	GOL	C	1004	-	5,5,5	0.30	0	5,5,5	0.54	0
4	GOL	D	1003	-	5,5,5	0.41	0	5,5,5	0.56	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
4	GOL	A	1001	-	-	0/4/4/4	0/0/0/0
4	GOL	B	1002	-	-	0/4/4/4	0/0/0/0
4	GOL	C	1004	-	-	0/4/4/4	0/0/0/0
4	GOL	D	1003	-	-	0/4/4/4	0/0/0/0

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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1003	GOL	2	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

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	E	14/16 (87%)	-0.35	0 <span>100</span> <span>100</span>	35, 45, 79, 85	0
1	F	14/16 (87%)	-0.19	0 <span>100</span> <span>100</span>	35, 43, 82, 88	0
1	G	7/16 (43%)	0.63	2 (28%) <span>1</span> <span>1</span>	36, 50, 70, 72	0
1	H	15/16 (93%)	-0.20	1 (6%) <span>19</span> <span>18</span>	35, 40, 88, 103	0
2	A	151/159 (94%)	-0.16	2 (1%) <span>77</span> <span>77</span>	19, 30, 48, 64	0
2	B	151/159 (94%)	0.01	4 (2%) <span>56</span> <span>56</span>	19, 32, 50, 62	0
2	C	152/159 (95%)	-0.15	2 (1%) <span>77</span> <span>77</span>	18, 27, 42, 63	0
2	D	150/159 (94%)	0.22	1 (0%) <span>87</span> <span>87</span>	20, 34, 49, 58	0
All	All	654/700 (93%)	-0.03	12 (1%) <span>69</span> <span>68</span>	18, 31, 54, 103	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1	MET	3.3
2	D	34	ASP	2.8
2	C	1	MET	2.8
2	B	148	LEU	2.6
2	A	151	ASN	2.6
2	A	150	ALA	2.3
2	B	147	ASN	2.3
1	H	27	U	2.3
2	B	150	ALA	2.2
2	C	2	THR	2.2
1	G	37	G	2.1
1	G	30	G	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	P5P	E	34	21/22	0.97	0.10	-	25,31,33,35	0
1	P5P	F	34	21/22	0.95	0.10	-	27,31,35,38	0
1	P5P	G	34	21/22	0.86	0.21	-	44,62,67,69	0
1	P5P	H	34	21/22	0.93	0.15	-	25,33,37,41	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	GOL	B	1002	6/6	0.89	0.19	5.47	27,32,33,35	0
4	GOL	D	1003	6/6	0.88	0.23	4.50	26,29,35,38	0
4	GOL	A	1001	6/6	0.91	0.15	4.23	27,29,33,38	0
4	GOL	C	1004	6/6	0.90	0.19	3.16	31,35,36,38	0
3	ZN	A	2001	1/1	1.00	0.11	0.57	25,25,25,25	0
3	ZN	D	2004	1/1	0.99	0.12	0.01	26,26,26,26	0
3	ZN	B	2002	1/1	1.00	0.10	-0.26	25,25,25,25	0
3	ZN	C	2003	1/1	1.00	0.10	-0.80	23,23,23,23	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.