



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:19 PM GMT

PDB ID : 1OB5  
Title : T. aquaticus elongation factor EF-Tu complexed with the antibiotic enacyloxin IIa, a GTP analog, and Phe-tRNA  
Authors : Dahlberg, C.; Nielsen, R.C.; Parmeggiani, A.; Nyborg, J.; Nissen, P.  
Deposited on : 2003-01-24  
Resolution : 3.10 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](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 (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

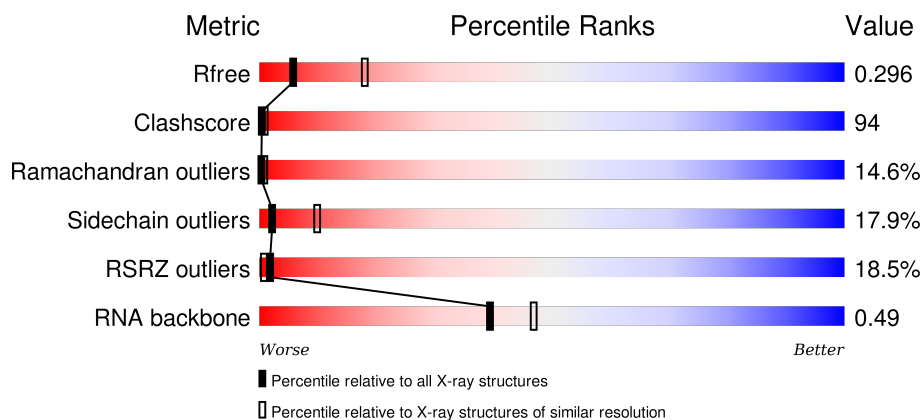
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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.



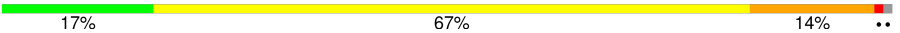
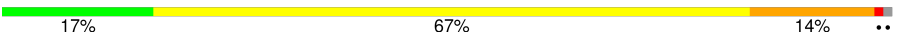
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)
RNA backbone	2183	1010 (3.52-2.68)

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	A	405	<div> <div>22%</div> <div>13% 63% 20% ..</div> </div>
1	C	405	<div> <div>21%</div> <div>12% 64% 19% ..</div> </div>
1	E	405	<div> <div>21%</div> <div>13% 63% 20% ..</div> </div>
2	B	78	<div> <div>17%</div> <div>67% 14% ..</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	78	 17% 67% 14% ..
2	F	78	 17% 67% 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
2	PHA	B	77	-	-	X	-
2	M2G	D	26	-	-	X	-
2	PHA	D	77	-	-	X	-
2	M2G	F	26	-	-	X	-
2	PHA	F	77	-	-	X	-
5	ENX	A	1408	-	-	-	X
5	ENX	C	1408	-	-	-	X
5	ENX	E	1408	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14547 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.

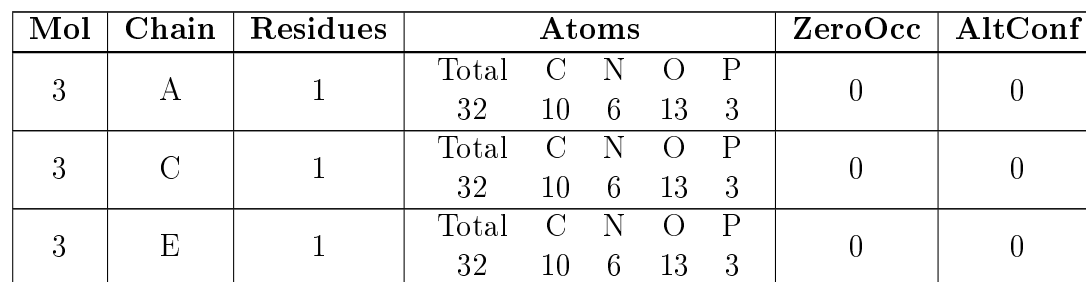
- Molecule 1 is a protein called ELONGATION FACTOR TU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	400	Total	C	N	O	S	0	0	0
			3106	1961	542	591	12			
1	C	400	Total	C	N	O	S	0	0	0
			3106	1961	542	591	12			
1	E	400	Total	C	N	O	S	0	0	0
			3106	1961	542	591	12			

- Molecule 2 is a RNA chain called TRANSFER-RNA, PHE.

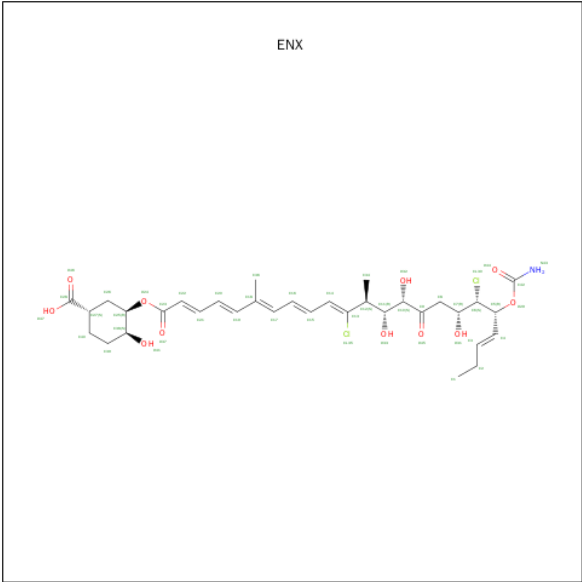
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	77	Total	C	N	O	P	0	0	0
			1663	755	295	537	76			
2	D	77	Total	C	N	O	P	0	0	0
			1663	755	295	537	76			
2	F	77	Total	C	N	O	P	0	0	0
			1663	755	295	537	76			

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>13</sub>P<sub>3</sub>).



- | Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 4   | A     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 4   | C     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 4   | E     | 1        | Total Mg<br>1 1 | 0       | 0       |

- Molecule 5 is ENACYLOXIN IIA (three-letter code: ENX) (formula:  $\text{C}_{33}\text{H}_{45}\text{Cl}_2\text{NO}_{11}$ ).

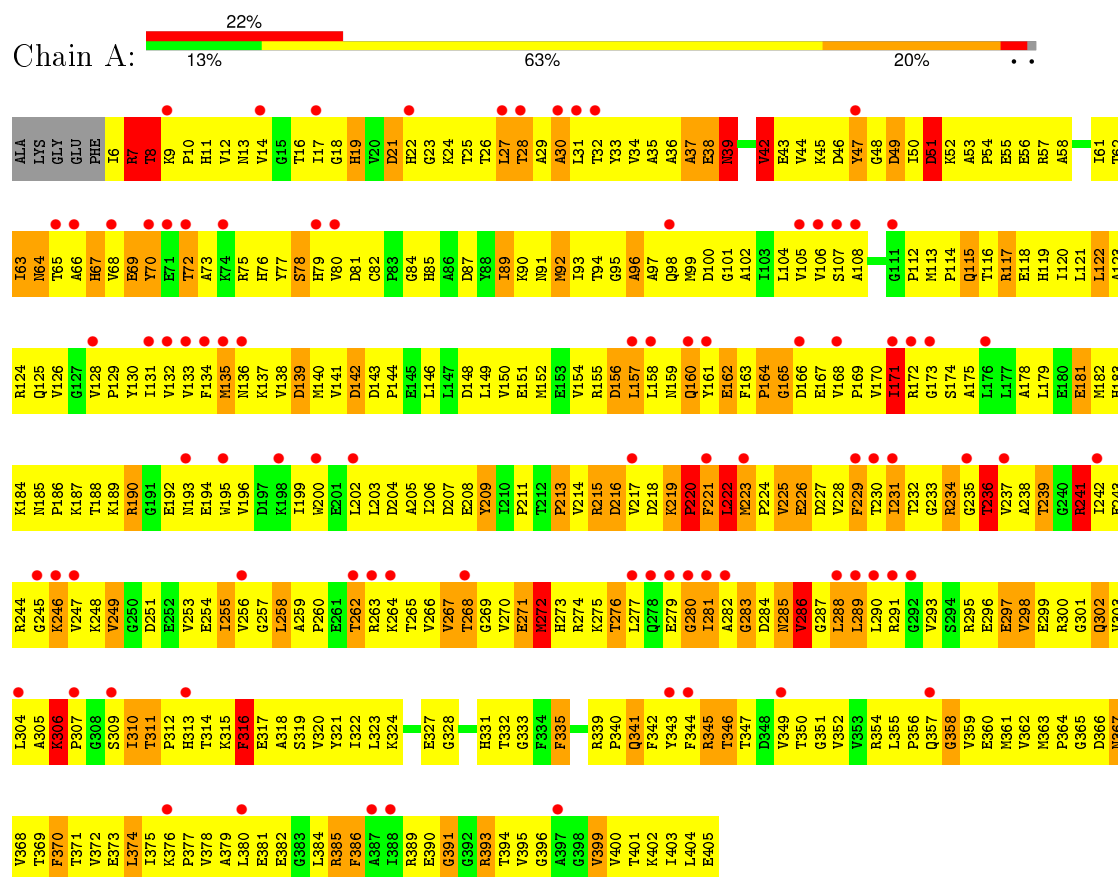


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Cl	N	O	0	0
			47	33	2	1	11		
5	C	1	Total	C	Cl	N	O	0	0
			47	33	2	1	11		
5	E	1	Total	C	Cl	N	O	0	0
			47	33	2	1	11		

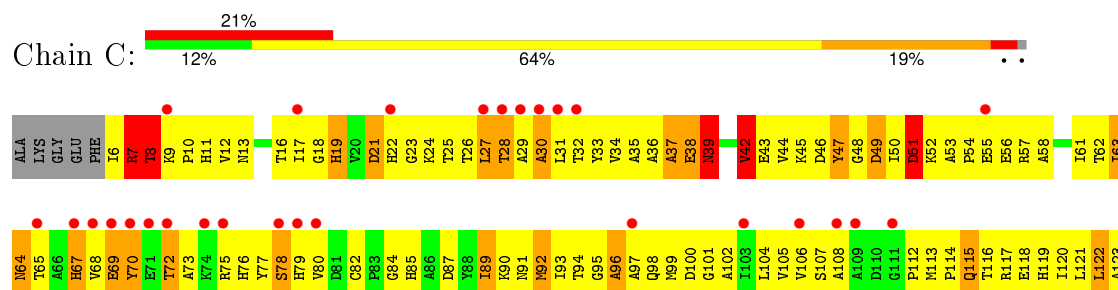
### 3 Residue-property plots [i](#)

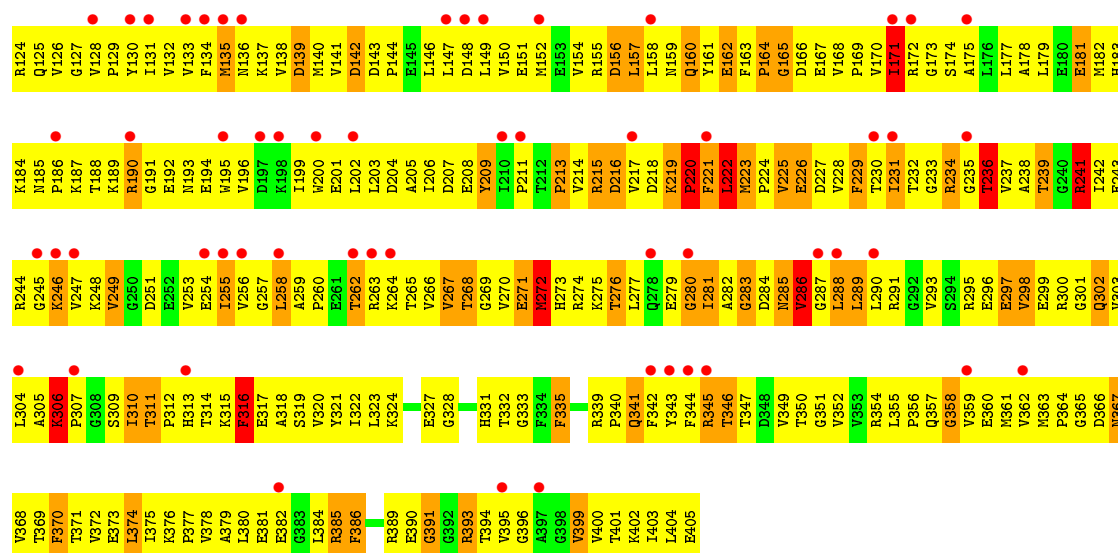
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: ELONGATION FACTOR TU

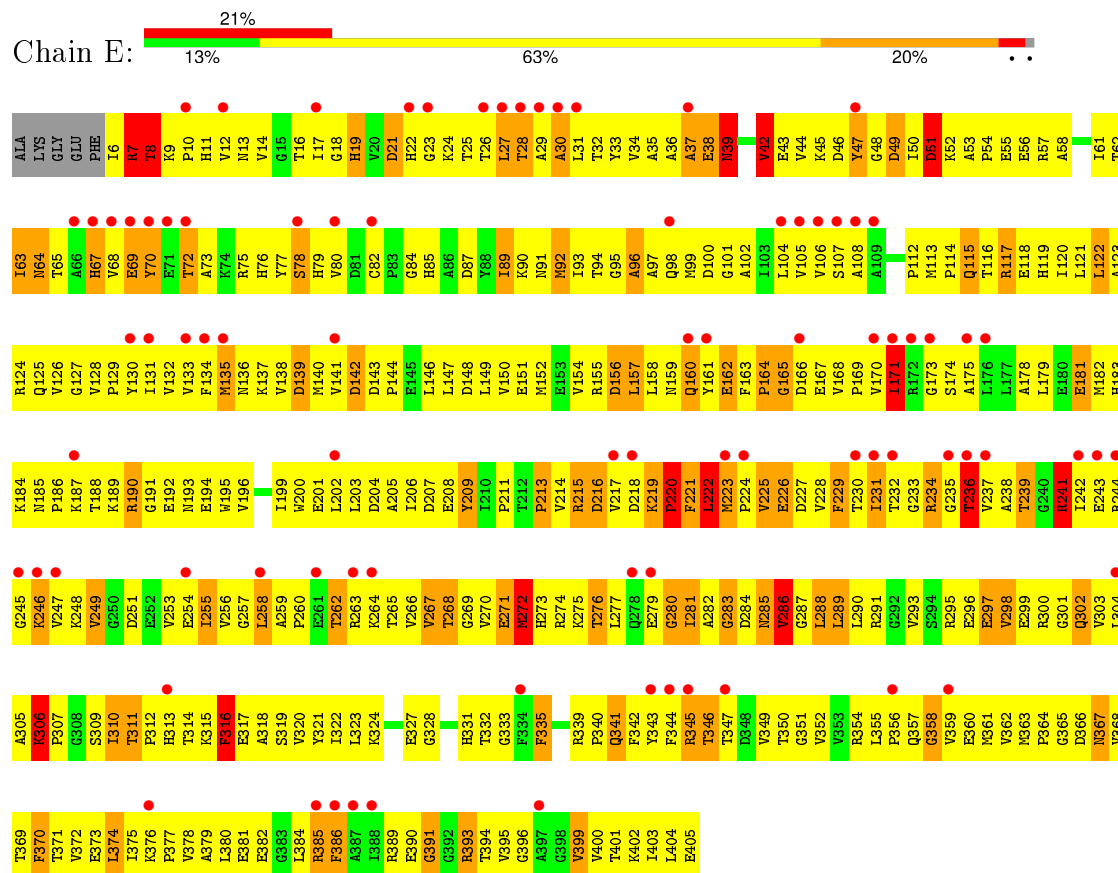


#### • Molecule 1: ELONGATION FACTOR TU

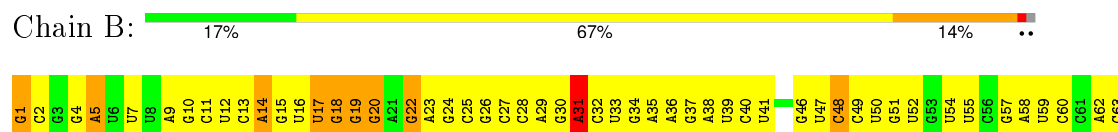




### • Molecule 1: ELONGATION FACTOR TU



### • Molecule 2: TRANSFER-RNA, PHE







● Molecule 2: TRANSFER-RNA, PHE



● Molecule 2: TRANSFER-RNA, PHE



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	212.57Å 122.33Å 135.68Å 90.00° 121.30° 90.00°	Depositor
Resolution (Å)	29.54 – 3.10 29.54 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.54-3.10) 96.6 (29.54-3.00)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.81 (at 3.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.280 , 0.294 0.277 , 0.296	Depositor DCC
$R_{free}$ test set	1584 reflections (3.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	63.7	Xtriage
Anisotropy	0.826	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 62.4	EDS
Estimated twinning fraction	0.448 for $1/2^*h-3/2^*k,-1/2^*h-1/2^*k,-1/2^*h+1/2^*k-l$ 0.449 for $1/2^*h+3/2^*k,1/2^*h-1/2^*k,-1/2^*h-1/2^*k-l$	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	1 of 57601 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	14547	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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, 0.375 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: OMC, 5MU, GNP, OMG, H2U, PHA, MG, YG, 1MA, 2MG, 5MC, ENX, M2G, 7MG, PSU

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	0.55	0/3165	0.86	1/4294 (0.0%)
1	C	0.55	0/3165	0.86	1/4294 (0.0%)
1	E	0.55	0/3165	0.86	1/4294 (0.0%)
2	B	0.81	1/1485 (0.1%)	0.87	2/2307 (0.1%)
2	D	0.81	1/1485 (0.1%)	0.87	2/2307 (0.1%)
2	F	0.81	1/1485 (0.1%)	0.87	2/2307 (0.1%)
All	All	0.65	3/13950 (0.0%)	0.86	9/19803 (0.0%)

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
2	B	0	4
2	D	0	4
2	F	0	4
All	All	0	12

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	G	OP3-P	-6.99	1.52	1.61
2	B	1	G	OP3-P	-6.99	1.52	1.61
2	F	1	G	OP3-P	-6.96	1.52	1.61

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	48	C	O5'-P-OP2	-5.99	100.31	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	48	C	O5'-P-OP2	-5.97	100.33	105.70
2	F	48	C	O5'-P-OP2	-5.96	100.33	105.70
1	C	222	LEU	CA-CB-CG	5.51	127.97	115.30
1	E	222	LEU	CA-CB-CG	5.51	127.96	115.30

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	31	A	Sidechain
2	B	38	A	Sidechain
2	B	51	G	Sidechain
2	B	52	U	Sidechain
2	D	31	A	Sidechain

## 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	3106	0	3122	747	2
1	C	3106	0	3122	734	2
1	E	3106	0	3122	743	2
2	B	1663	0	869	133	0
2	D	1663	0	869	137	0
2	F	1663	0	869	140	0
3	A	32	0	13	7	0
3	C	32	0	13	7	0
3	E	32	0	13	8	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
5	A	47	0	45	5	0
5	C	47	0	45	5	0
5	E	47	0	45	5	0
All	All	14547	0	12147	2502	3

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 94.

The worst 5 of 2502 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:368:VAL:HG22	1:A:369:THR:H	1.03	1.19
1:A:221:PHE:HB3	1:A:306:LYS:H	1.08	1.19
1:A:234:ARG:HH11	1:A:234:ARG:HB2	1.04	1.16
1:C:75:ARG:HH21	1:C:207:ASP:HA	1.04	1.15
1:C:234:ARG:HB2	1:C:234:ARG:HH11	1.04	1.14

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:TYR:OH	1:C:148:ASP:OD1[3_545]	1.71	0.49
1:C:130:TYR:OH	1:E:148:ASP:OD1[1_565]	1.76	0.44
1:A:148:ASP:OD1	1:E:130:TYR:OH[3_555]	1.82	0.38

## 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	
1	A	398/405 (98%)	250 (63%)	90 (23%)	58 (15%)	0	1
1	C	398/405 (98%)	250 (63%)	90 (23%)	58 (15%)	0	1
1	E	398/405 (98%)	250 (63%)	90 (23%)	58 (15%)	0	1
All	All	1194/1215 (98%)	750 (63%)	270 (23%)	174 (15%)	0	1

5 of 174 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	8	THR

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Mol	Chain	Res	Type
1	A	19	HIS
1	A	27	LEU
1	A	39	ASN

### 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	
1	A	335/338 (99%)	275 (82%)	60 (18%)	2	10
1	C	335/338 (99%)	275 (82%)	60 (18%)	2	10
1	E	335/338 (99%)	275 (82%)	60 (18%)	2	10
All	All	1005/1014 (99%)	825 (82%)	180 (18%)	2	10

5 of 180 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	156	ASP
1	C	262	THR
1	E	297	GLU
1	C	171	ILE
1	C	223	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	76	HIS
1	C	273	HIS
1	E	278	GLN
1	C	79	HIS
1	C	91	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	73/78 (93%)	9 (12%)	2 (2%)
2	D	73/78 (93%)	9 (12%)	2 (2%)
2	F	73/78 (93%)	9 (12%)	2 (2%)
All	All	219/234 (93%)	27 (12%)	6 (2%)

5 of 27 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	5	A
2	B	14	A
2	B	17	H2U
2	B	18	G
2	B	19	G

5 of 6 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	D	17	H2U
2	F	19	G
2	D	19	G
2	B	19	G
2	F	17	H2U

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

45 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	2MG	B	10	2	17,26,27	1.20	1 (5%)	21,38,41	2.60	3 (14%)
2	H2U	B	16	2	17,21,22	0.75	0	23,30,33	0.99	2 (8%)
2	H2U	B	17	2	17,21,22	0.81	0	23,30,33	1.29	3 (13%)
2	M2G	B	26	2	17,27,28	1.26	2 (11%)	22,40,43	2.14	2 (9%)
2	OMC	B	32	2	13,22,23	0.74	0	20,31,34	1.03	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	OMG	B	34	2	17,26,27	1.19	1 (5%)	21,38,41	2.63	3 (14%)
2	YG	B	37	2	27,42,43	1.84	6 (22%)	29,62,65	2.53	12 (41%)
2	PSU	B	39	2	13,21,22	1.85	3 (23%)	18,30,33	6.15	5 (27%)
2	5MC	B	40	2	13,22,23	1.12	2 (15%)	15,32,35	0.50	0
2	7MG	B	46	2	19,26,27	1.64	3 (15%)	24,39,42	2.26	4 (16%)
2	5MC	B	49	2	13,22,23	0.93	1 (7%)	15,32,35	0.76	0
2	5MU	B	54	2	12,22,23	1.27	2 (16%)	14,32,35	4.35	2 (14%)
2	PSU	B	55	2	13,21,22	1.37	2 (15%)	18,30,33	5.92	4 (22%)
2	1MA	B	58	2	14,25,26	1.04	2 (14%)	15,37,40	1.55	3 (20%)
2	PHA	B	77	2	10,11,11	0.66	0	10,13,13	0.35	0
2	2MG	D	10	2	17,26,27	1.21	1 (5%)	21,38,41	2.59	3 (14%)
2	H2U	D	16	2	17,21,22	0.74	0	23,30,33	0.99	2 (8%)
2	H2U	D	17	2	17,21,22	0.81	0	23,30,33	1.29	3 (13%)
2	M2G	D	26	2	17,27,28	1.27	2 (11%)	22,40,43	2.14	2 (9%)
2	OMC	D	32	2	13,22,23	0.73	0	20,31,34	1.02	1 (5%)
2	OMG	D	34	2	17,26,27	1.19	1 (5%)	21,38,41	2.63	3 (14%)
2	YG	D	37	2	27,42,43	1.85	6 (22%)	29,62,65	2.53	12 (41%)
2	PSU	D	39	2	13,21,22	1.84	3 (23%)	18,30,33	6.14	5 (27%)
2	5MC	D	40	2	13,22,23	1.13	2 (15%)	15,32,35	0.50	0
2	7MG	D	46	2	19,26,27	1.64	3 (15%)	24,39,42	2.27	4 (16%)
2	5MC	D	49	2	13,22,23	0.93	1 (7%)	15,32,35	0.75	0
2	5MU	D	54	2	12,22,23	1.27	2 (16%)	14,32,35	4.38	2 (14%)
2	PSU	D	55	2	13,21,22	1.38	2 (15%)	18,30,33	5.93	4 (22%)
2	1MA	D	58	2	14,25,26	1.04	2 (14%)	15,37,40	1.54	3 (20%)
2	PHA	D	77	2	10,11,11	0.66	0	10,13,13	0.35	0
2	2MG	F	10	2	17,26,27	1.20	1 (5%)	21,38,41	2.60	3 (14%)
2	H2U	F	16	2	17,21,22	0.75	0	23,30,33	0.99	2 (8%)
2	H2U	F	17	2	17,21,22	0.81	0	23,30,33	1.29	3 (13%)
2	M2G	F	26	2	17,27,28	1.25	2 (11%)	22,40,43	2.14	2 (9%)
2	OMC	F	32	2	13,22,23	0.74	0	20,31,34	1.03	1 (5%)
2	OMG	F	34	2	17,26,27	1.20	1 (5%)	21,38,41	2.62	3 (14%)
2	YG	F	37	2	27,42,43	1.85	6 (22%)	29,62,65	2.53	13 (44%)
2	PSU	F	39	2	13,21,22	1.85	3 (23%)	18,30,33	6.16	5 (27%)
2	5MC	F	40	2	13,22,23	1.12	2 (15%)	15,32,35	0.49	0
2	7MG	F	46	2	19,26,27	1.65	3 (15%)	24,39,42	2.27	4 (16%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	5MC	F	49	2	13,22,23	0.92	1 (7%)	15,32,35	0.76	0
2	5MU	F	54	2	12,22,23	1.27	2 (16%)	14,32,35	4.35	2 (14%)
2	PSU	F	55	2	13,21,22	1.38	2 (15%)	18,30,33	5.92	4 (22%)
2	1MA	F	58	2	14,25,26	1.04	2 (14%)	15,37,40	1.56	3 (20%)
2	PHA	F	77	2	10,11,11	0.66	0	10,13,13	0.34	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
2	2MG	B	10	2	-	0/5/27/28	0/3/3/3
2	H2U	B	16	2	-	0/7/38/39	0/2/2/2
2	H2U	B	17	2	-	0/7/38/39	0/2/2/2
2	M2G	B	26	2	-	0/7/29/30	0/3/3/3
2	OMC	B	32	2	-	0/5/27/28	0/2/2/2
2	OMG	B	34	2	-	0/5/27/28	0/3/3/3
2	YG	B	37	2	-	2/20/42/43	0/4/4/4
2	PSU	B	39	2	-	0/7/25/26	0/2/2/2
2	5MC	B	40	2	-	0/3/25/26	0/2/2/2
2	7MG	B	46	2	-	0/7/37/38	0/3/3/3
2	5MC	B	49	2	-	0/3/25/26	0/2/2/2
2	5MU	B	54	2	-	0/3/25/26	0/2/2/2
2	PSU	B	55	2	-	0/7/25/26	0/2/2/2
2	1MA	B	58	2	-	0/3/25/26	0/3/3/3
2	PHA	B	77	2	-	0/4/6/6	0/1/1/1
2	2MG	D	10	2	-	0/5/27/28	0/3/3/3
2	H2U	D	16	2	-	0/7/38/39	0/2/2/2
2	H2U	D	17	2	-	0/7/38/39	0/2/2/2
2	M2G	D	26	2	-	0/7/29/30	0/3/3/3
2	OMC	D	32	2	-	0/5/27/28	0/2/2/2
2	OMG	D	34	2	-	0/5/27/28	0/3/3/3
2	YG	D	37	2	-	2/20/42/43	0/4/4/4
2	PSU	D	39	2	-	0/7/25/26	0/2/2/2
2	5MC	D	40	2	-	0/3/25/26	0/2/2/2
2	7MG	D	46	2	-	0/7/37/38	0/3/3/3
2	5MC	D	49	2	-	0/3/25/26	0/2/2/2
2	5MU	D	54	2	-	0/3/25/26	0/2/2/2
2	PSU	D	55	2	-	0/7/25/26	0/2/2/2
2	1MA	D	58	2	-	0/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PHA	D	77	2	-	0/4/6/6	0/1/1/1
2	2MG	F	10	2	-	0/5/27/28	0/3/3/3
2	H2U	F	16	2	-	0/7/38/39	0/2/2/2
2	H2U	F	17	2	-	0/7/38/39	0/2/2/2
2	M2G	F	26	2	-	0/7/29/30	0/3/3/3
2	OMC	F	32	2	-	0/5/27/28	0/2/2/2
2	OMG	F	34	2	-	0/5/27/28	0/3/3/3
2	YG	F	37	2	-	2/20/42/43	0/4/4/4
2	PSU	F	39	2	-	0/7/25/26	0/2/2/2
2	5MC	F	40	2	-	0/3/25/26	0/2/2/2
2	7MG	F	46	2	-	0/7/37/38	0/3/3/3
2	5MC	F	49	2	-	0/3/25/26	0/2/2/2
2	5MU	F	54	2	-	0/3/25/26	0/2/2/2
2	PSU	F	55	2	-	0/7/25/26	0/2/2/2
2	1MA	F	58	2	-	0/3/25/26	0/3/3/3
2	PHA	F	77	2	-	0/4/6/6	0/1/1/1

The worst 5 of 75 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	46	7MG	C8-N9	-5.41	1.37	1.45
2	D	46	7MG	C8-N9	-5.39	1.37	1.45
2	B	46	7MG	C8-N9	-5.38	1.37	1.45
2	F	37	YG	O23-C21	-3.97	1.28	1.34
2	B	39	PSU	C6-C5	-3.93	1.32	1.38

The worst 5 of 133 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	39	PSU	N1-C2-N3	-21.33	114.72	128.33
2	B	39	PSU	N1-C2-N3	-21.28	114.76	128.33
2	D	39	PSU	N1-C2-N3	-21.23	114.79	128.33
2	D	55	PSU	N1-C2-N3	-20.65	115.16	128.33
2	F	55	PSU	N1-C2-N3	-20.61	115.19	128.33

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	37	YG	C24-O23-C21-N20
2	B	37	YG	C24-O23-C21-N20

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Mol	Chain	Res	Type	Atoms
2	F	37	YG	C24-O23-C21-N20
2	B	37	YG	C24-O23-C21-O22
2	D	37	YG	C24-O23-C21-O22

There are no ring outliers.

45 monomers are involved in 152 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	10	2MG	4	0
2	B	16	H2U	2	0
2	B	17	H2U	1	0
2	B	26	M2G	8	0
2	B	32	OMC	4	0
2	B	34	OMG	3	0
2	B	37	YG	9	0
2	B	39	PSU	3	0
2	B	40	5MC	4	0
2	B	46	7MG	3	0
2	B	49	5MC	2	0
2	B	54	5MU	1	0
2	B	55	PSU	1	0
2	B	58	1MA	2	0
2	B	77	PHA	7	0
2	D	10	2MG	5	0
2	D	16	H2U	3	0
2	D	17	H2U	1	0
2	D	26	M2G	9	0
2	D	32	OMC	4	0
2	D	34	OMG	5	0
2	D	37	YG	10	0
2	D	39	PSU	3	0
2	D	40	5MC	4	0
2	D	46	7MG	3	0
2	D	49	5MC	2	0
2	D	54	5MU	1	0
2	D	55	PSU	1	0
2	D	58	1MA	2	0
2	D	77	PHA	7	0
2	F	10	2MG	5	0
2	F	16	H2U	2	0
2	F	17	H2U	1	0
2	F	26	M2G	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	32	OMC	4	0
2	F	34	OMG	5	0
2	F	37	YG	10	0
2	F	39	PSU	3	0
2	F	40	5MC	4	0
2	F	46	7MG	3	0
2	F	49	5MC	2	0
2	F	54	5MU	1	0
2	F	55	PSU	1	0
2	F	58	1MA	2	0
2	F	77	PHA	7	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 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	$\# Z  > 2$
3	GNP	A	1406	4	28,34,34	1.93	7 (25%)	33,54,54	2.51	9 (27%)
5	ENX	A	1408	-	42,47,47	1.36	6 (14%)	41,62,62	1.17	3 (7%)
3	GNP	C	1406	4	28,34,34	1.93	7 (25%)	33,54,54	2.51	9 (27%)
5	ENX	C	1408	-	42,47,47	1.36	6 (14%)	41,62,62	1.17	3 (7%)
3	GNP	E	1406	4	28,34,34	1.93	7 (25%)	33,54,54	2.50	9 (27%)
5	ENX	E	1408	-	42,47,47	1.37	6 (14%)	41,62,62	1.17	3 (7%)

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	GNP	A	1406	4	-	0/12/38/38	0/3/3/3
5	ENX	A	1408	-	-	2/49/71/71	0/1/1/1
3	GNP	C	1406	4	-	0/12/38/38	0/3/3/3
5	ENX	C	1408	-	-	2/49/71/71	0/1/1/1
3	GNP	E	1406	4	-	0/12/38/38	0/3/3/3
5	ENX	E	1408	-	-	2/49/71/71	0/1/1/1

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1406	GNP	PG-O2G	-3.48	1.47	1.56
3	E	1406	GNP	PG-O2G	-3.46	1.47	1.56
3	A	1406	GNP	PG-O2G	-3.46	1.47	1.56
5	E	1408	ENX	C8-C7	-2.10	1.50	1.53
5	A	1408	ENX	C8-C7	-2.08	1.50	1.53

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1406	GNP	C5-C6-N1	-7.72	113.04	123.59
3	A	1406	GNP	C5-C6-N1	-7.68	113.08	123.59
3	E	1406	GNP	C5-C6-N1	-7.67	113.10	123.59
3	E	1406	GNP	O1G-PG-N3B	-4.99	104.24	111.90
3	A	1406	GNP	O1G-PG-N3B	-4.99	104.25	111.90

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	1408	ENX	C5-O29-C42-O44
5	A	1408	ENX	C5-O29-C42-O44
5	C	1408	ENX	C5-O29-C42-O44
5	A	1408	ENX	C5-O29-C42-N43
5	C	1408	ENX	C5-O29-C42-N43

There are no ring outliers.

6 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1406	GNP	7	0
5	A	1408	ENX	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1406	GNP	7	0
5	C	1408	ENX	5	0
3	E	1406	GNP	8	0
5	E	1408	ENX	5	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 [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, 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	A	400/405 (98%)	1.08	88 (22%) <b>1</b> <b>0</b>	24, 83, 127, 155	0
1	C	400/405 (98%)	0.95	84 (21%) <b>1</b> <b>0</b>	24, 83, 127, 155	0
1	E	400/405 (98%)	0.97	85 (21%) <b>1</b> <b>0</b>	24, 83, 127, 155	0
2	B	62/78 (79%)	0.06	0 <b>100</b> <b>100</b>	22, 62, 102, 111	0
2	D	62/78 (79%)	-0.15	0 <b>100</b> <b>100</b>	22, 62, 102, 111	0
2	F	62/78 (79%)	-0.02	0 <b>100</b> <b>100</b>	22, 62, 102, 111	0
All	All	1386/1449 (95%)	0.86	257 (18%) <b>2</b> <b>1</b>	22, 80, 126, 155	0

The worst 5 of 257 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	235	GLY	13.7
1	E	235	GLY	10.8
1	A	247	VAL	9.6
1	A	278	GLN	8.1
1	E	245	GLY	6.8

### 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
2	OMG	B	34	24/25	0.89	0.20	-	2,29,39,50	0
2	YG	F	37	39/40	0.92	0.19	-	13,44,86,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	OMC	F	32	21/22	0.88	0.21	-	44,63,73,89	0
2	YG	B	37	39/40	0.91	0.20	-	13,44,86,93	0
2	H2U	D	16	20/21	0.87	0.15	-	50,92,109,111	0
2	2MG	D	10	24/25	0.86	0.13	-	76,85,97,103	0
2	5MC	D	40	21/22	0.92	0.16	-	23,42,56,65	0
2	5MC	D	49	21/22	0.91	0.20	-	19,28,35,50	0
2	1MA	B	58	23/24	0.91	0.21	-	6,25,34,37	0
2	PSU	F	39	20/21	0.90	0.18	-	16,36,50,54	0
2	1MA	F	58	23/24	0.92	0.25	-	6,25,34,37	0
2	5MU	D	54	21/22	0.89	0.22	-	3,28,45,54	0
2	PHA	D	77	11/11	0.81	0.52	-	98,114,124,126	0
2	7MG	D	46	24/25	0.91	0.18	-	25,53,93,99	0
2	OMC	D	32	21/22	0.89	0.21	-	44,63,73,89	0
2	5MU	B	54	21/22	0.84	0.24	-	3,28,45,54	0
2	7MG	F	46	24/25	0.91	0.17	-	25,53,93,99	0
2	5MC	F	49	21/22	0.93	0.17	-	19,28,35,50	0
2	M2G	D	26	25/26	0.87	0.12	-	67,87,114,121	0
2	OMG	F	34	24/25	0.91	0.19	-	2,29,39,50	0
2	PSU	D	39	20/21	0.93	0.16	-	16,36,50,54	0
2	5MC	F	40	21/22	0.93	0.15	-	23,42,56,65	0
2	M2G	F	26	25/26	0.90	0.16	-	67,87,114,121	0
2	PHA	F	77	11/11	0.71	0.94	-	98,114,124,126	0
2	2MG	B	10	24/25	0.83	0.17	-	76,85,97,103	0
2	7MG	B	46	24/25	0.91	0.17	-	25,53,93,99	0
2	OMG	D	34	24/25	0.87	0.21	-	2,29,39,50	0
2	5MU	F	54	21/22	0.93	0.17	-	3,28,45,54	0
2	H2U	D	17	20/21	0.85	0.18	-	91,123,146,146	0
2	1MA	D	58	23/24	0.92	0.20	-	6,25,34,37	0
2	H2U	B	16	20/21	0.87	0.15	-	50,92,109,111	0
2	H2U	F	16	20/21	0.87	0.18	-	50,92,109,111	0
2	PSU	B	55	20/21	0.86	0.21	-	18,38,54,57	0
2	PSU	D	55	20/21	0.90	0.18	-	18,38,54,57	0
2	PHA	B	77	11/11	0.72	0.52	-	98,114,124,126	0
2	PSU	F	55	20/21	0.89	0.20	-	18,38,54,57	0
2	YG	D	37	39/40	0.88	0.20	-	13,44,86,93	0
2	2MG	F	10	24/25	0.82	0.17	-	76,85,97,103	0
2	H2U	F	17	20/21	0.85	0.17	-	91,123,146,146	0
2	OMC	B	32	21/22	0.88	0.22	-	44,63,73,89	0
2	5MC	B	40	21/22	0.91	0.15	-	23,42,56,65	0
2	M2G	B	26	25/26	0.88	0.20	-	67,87,114,121	0
2	H2U	B	17	20/21	0.87	0.17	-	91,123,146,146	0
2	5MC	B	49	21/22	0.91	0.18	-	19,28,35,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PSU	B	39	20/21	0.88	0.19	-	16,36,50,54	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( $\text{\AA}^2$ )	Q<0.9
4	MG	C	1407	1/1	0.95	0.26	1.22	57,57,57,57	0
5	ENX	A	1408	47/47	0.63	0.53	1.19	45,74,86,109	0
5	ENX	E	1408	47/47	0.63	0.52	0.82	45,74,86,109	0
5	ENX	C	1408	47/47	0.71	0.43	0.48	45,74,86,109	0
4	MG	A	1407	1/1	0.98	0.23	0.34	57,57,57,57	0
4	MG	E	1407	1/1	0.88	0.20	-0.53	57,57,57,57	0
3	GNP	C	1406	32/32	0.93	0.18	-0.83	47,70,85,90	0
3	GNP	A	1406	32/32	0.90	0.18	-0.84	47,70,85,90	0
3	GNP	E	1406	32/32	0.91	0.18	-0.92	47,70,85,90	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.