



wwPDB X-ray Structure Validation Summary Report

Oct 30, 2014 – 05:03 PM EDT

PDB ID : 2XAV
Title : Ribonucleotide reductase Y731NO2Y and Y730F modified R1 subunit of E. coli
Authors : Yokoyama, K.; Uhlin, U.; Stubbe, J.
Deposited on : 2010-03-31
Resolution : 2.80 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

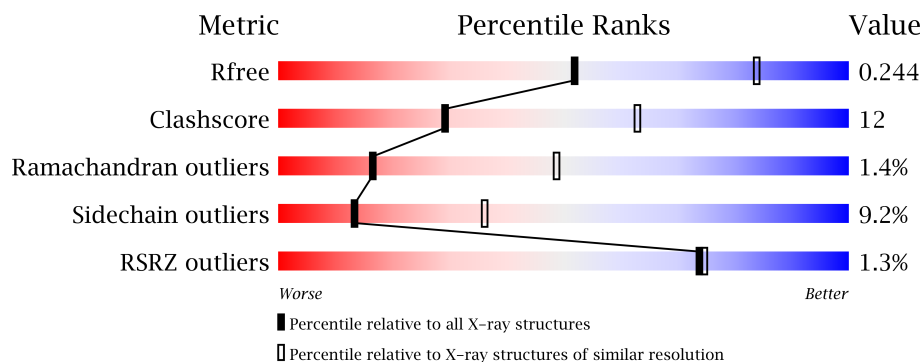
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable24103
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.1.3
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable24103

1 Overall quality at a glance

The reported resolution of this entry is 2.80 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}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	761	
1	B	761	
1	C	761	
2	D	20	
2	E	20	
2	F	20	
2	P	20	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18459 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called RIBONUCLEOSIDE-DIPHOSPHATEREDUCTASE 1 SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	0	0	0
			5806	3688	996	1098	24			
1	B	728	Total	C	N	O	S	0	0	0
			5806	3688	996	1098	24			
1	C	728	Total	C	N	O	S	0	0	0
			5806	3688	996	1098	24			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	730	PHE	TYR	ENGINEERED MUTATION	UNP P00452
B	730	PHE	TYR	ENGINEERED MUTATION	UNP P00452
C	730	PHE	TYR	ENGINEERED MUTATION	UNP P00452

- Molecule 2 is a protein called RIBONUCLEOSIDE-DIPHOSPHATEREDUCTASE 1 SUBUNIT BETA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	16	Total	C	N	O	0	0	0
			129	77	19	33			
2	E	16	Total	C	N	O	0	0	0
			129	77	19	33			
2	F	16	Total	C	N	O	0	0	0
			129	77	19	33			
2	P	3	Total	C	N	O	0	0	0
			27	20	3	4			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	176	Total	O	0	0
			176	176		

Continued on next page...

Continued from previous page...

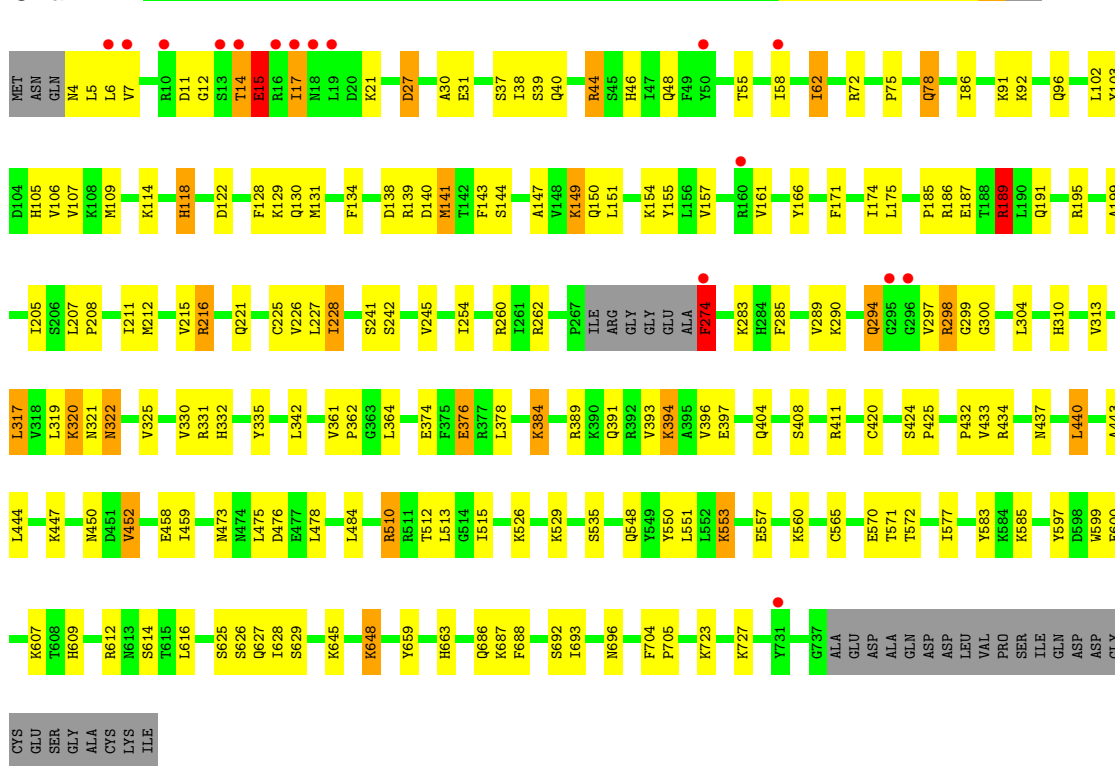
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	183	Total 183	O 183	0	0
3	C	259	Total 259	O 259	0	0
3	D	2	Total 2	O 2	0	0
3	F	3	Total 3	O 3	0	0
3	P	4	Total 4	O 4	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

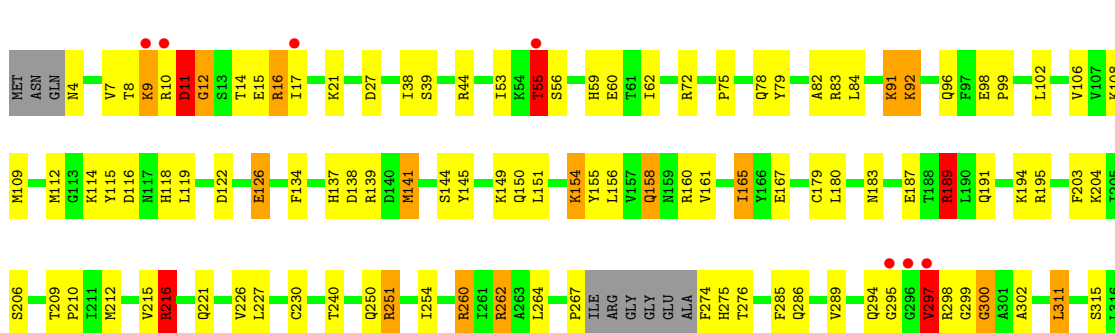
• Molecule 1: RIBONUCLEOSIDE-DIPHOSPHATEREDUCTASE 1 SUBUNIT ALPHA

Chain A:



• Molecule 1: RIBONUCLEOSIDE-DIPHOSPHATEREDUCTASE 1 SUBUNIT ALPHA

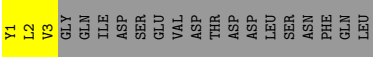
Chain B:





● Molecule 2: RIBONUCLEOSIDE-DIPHOSPHATEREDUCTASE 1 SUBUNIT BETA

Chain P: 



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	224.66Å 224.66Å 336.36Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	169.03 – 2.80 84.21 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.7 (169.03-2.80) 93.6 (84.21-2.80)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.169 , 0.247 0.169 , 0.244	Depositor DCC
R_{free} test set	3787 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	44.3	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 23.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	4 of 75021 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18459	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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: NIY

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	0.69	1/5916 (0.0%)	0.75	0/8010
1	B	0.69	1/5916 (0.0%)	0.78	5/8010 (0.1%)
1	C	0.82	3/5916 (0.1%)	0.83	1/8010 (0.0%)
2	D	0.58	0/129	0.66	0/173
2	E	0.66	0/129	0.79	0/173
2	F	0.61	0/129	0.73	0/173
2	P	0.85	0/27	0.98	0/36
All	All	0.73	5/18162 (0.0%)	0.78	6/24585 (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
1	A	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	278	CYS	CB-SG	-7.21	1.70	1.82
1	B	187	GLU	CG-CD	6.58	1.61	1.51
1	C	111	GLU	CG-CD	6.48	1.61	1.51
1	C	155	TYR	CE1-CZ	5.49	1.45	1.38
1	A	225	CYS	CB-SG	-5.16	1.73	1.81

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	505	ARG	NE-CZ-NH2	-6.30	117.15	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	616	LEU	CA-CB-CG	-5.61	102.41	115.30
1	B	264	LEU	CA-CB-CG	5.50	127.95	115.30
1	C	703	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	B	180	LEU	CA-CB-CG	5.11	127.04	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	274	PHE	Peptide

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5806	0	5725	138	0
1	B	5806	0	5726	149	0
1	C	5806	0	5725	142	0
2	D	129	0	111	4	0
2	E	129	0	111	2	0
2	F	129	0	111	2	0
2	P	27	0	31	3	0
3	A	176	0	0	42	0
3	B	183	0	0	52	1
3	C	259	0	0	50	1
3	D	2	0	0	1	0
3	F	3	0	0	0	0
3	P	4	0	0	2	0
All	All	18459	0	17540	436	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

The worst 5 of 436 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:299:GLY:HA3	3:A:2073:HOH:O	1.51	1.11
1:C:480:GLU:HB3	3:C:2070:HOH:O	1.59	1.03
1:A:294:GLN:HB2	1:A:298:ARG:HH11	1.23	1.02
1:B:204:LYS:HB3	3:B:2057:HOH:O	1.59	1.01
1:A:450:ASN:HB2	3:A:2120:HOH:O	1.60	1.00

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:B:2011:HOH:O	3:C:2016:HOH:O[15_554]	2.06	0.14

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	723/761 (95%)	669 (92%)	44 (6%)	10 (1%)	16	49
1	B	723/761 (95%)	673 (93%)	39 (5%)	11 (2%)	15	46
1	C	723/761 (95%)	680 (94%)	34 (5%)	9 (1%)	19	54
2	D	14/20 (70%)	12 (86%)	2 (14%)	0	100	100
2	E	14/20 (70%)	10 (71%)	4 (29%)	0	100	100
2	F	14/20 (70%)	11 (79%)	2 (14%)	1 (7%)	2	4
2	P	1/20 (5%)	1 (100%)	0	0	100	100
All	All	2212/2363 (94%)	2056 (93%)	125 (6%)	31 (1%)	16	49

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	294	GLN
1	B	294	GLN
1	B	300	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	294	GLN

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	625/650 (96%)	572 (92%)	53 (8%)	15	41
1	B	625/650 (96%)	560 (90%)	65 (10%)	10	28
1	C	625/650 (96%)	579 (93%)	46 (7%)	20	48
2	D	16/19 (84%)	11 (69%)	5 (31%)	0	1
2	E	16/19 (84%)	12 (75%)	4 (25%)	1	2
2	F	16/19 (84%)	13 (81%)	3 (19%)	2	7
2	P	3/19 (16%)	2 (67%)	1 (33%)	0	1
All	All	1926/2026 (95%)	1749 (91%)	177 (9%)	13	36

5 of 177 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	260	ARG
1	B	430	ILE
1	C	723	LYS
1	B	276	THR
1	B	330	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	130	GLN
1	B	328	ASN
1	C	661	HIS
1	B	150	GLN
1	B	183	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

3 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	NIY	A	731	1	15,15,16	4.79	2 (13%)	18,20,22	1.09	0
1	NIY	B	731	1	15,15,16	5.50	2 (13%)	18,20,22	1.87	3 (16%)
1	NIY	C	731	1	15,15,16	5.39	3 (20%)	18,20,22	1.51	3 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	NIY	A	731	1	-	0/8/10/12	0/1/1/1
1	NIY	B	731	1	-	0/8/10/12	0/1/1/1
1	NIY	C	731	1	-	0/8/10/12	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	731	NIY	O-C	20.72	1.25	1.11
1	C	731	NIY	O-C	20.20	1.25	1.11
1	A	731	NIY	O-C	18.14	1.23	1.11
1	B	731	NIY	CE1-NN	-4.48	1.39	1.46
1	C	731	NIY	CE1-NN	-3.91	1.40	1.46

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	731	NIY	CD1-CE1-NN	5.83	122.42	116.08
1	B	731	NIY	C-CA-N	3.95	117.77	113.83
1	C	731	NIY	CB-CG-CD1	-3.08	114.67	120.39
1	C	731	NIY	C-CA-N	2.43	116.26	113.83
1	C	731	NIY	CD1-CE1-NN	2.20	118.47	116.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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 ⓘ

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	A	728/761 (95%)	0.03	16 (2%) 59 60	27, 42, 68, 89	0
1	B	728/761 (95%)	-0.09	7 (0%) 79 79	25, 41, 66, 89	0
1	C	728/761 (95%)	-0.22	2 (0%) 91 93	17, 30, 55, 79	0
2	D	16/20 (80%)	0.75	2 (12%) 5 4	78, 90, 92, 94	0
2	E	16/20 (80%)	0.66	1 (6%) 19 18	69, 82, 93, 93	0
2	F	16/20 (80%)	0.54	0 100 100	64, 78, 84, 85	0
2	P	3/20 (15%)	0.15	0 100 100	33, 33, 36, 42	0
All	All	2235/2363 (94%)	-0.08	28 (1%) 74 75	17, 39, 69, 94	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	LEU	6.5
1	A	14	THR	5.0
2	E	372	ASN	4.3
1	A	274	PHE	3.7
1	B	10	ARG	3.5

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	NIY	A	731	15/16	0.21	1.60	36,41,51,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	NIY	B	731	15/16	0.17	-0.20	32,37,45,46	0
1	NIY	C	731	15/16	0.15	-1.09	22,27,39,42	0

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.