W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 06:31 AM GMT

|		
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)

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 2.80 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.
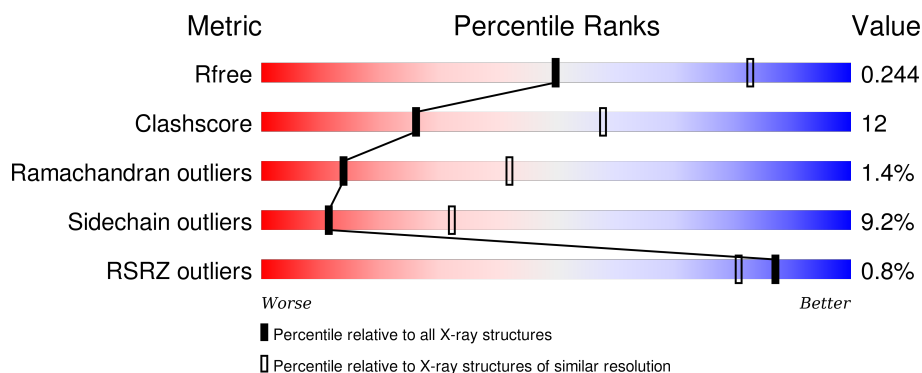
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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. 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 <=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	761	
1	B	761	
1	C	761	
2	D	20	
2	E	20	

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Mol	Chain	Length	Quality of chain
2	F	20	50% 　　　 30% 　　　 20%
2	P	20	15% 　　　 85%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 18459 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 RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT ALPHA.

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

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-DIPHOSPHATE REDUCTASE 1 SUBUNIT BETA.

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

- Molecule 3 is water.

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

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WORLDWIDE
wwPDB
PROTEIN DATA BANK

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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-DIPHOSPHATE REDUCTASE 1 SUBUNIT ALPHA
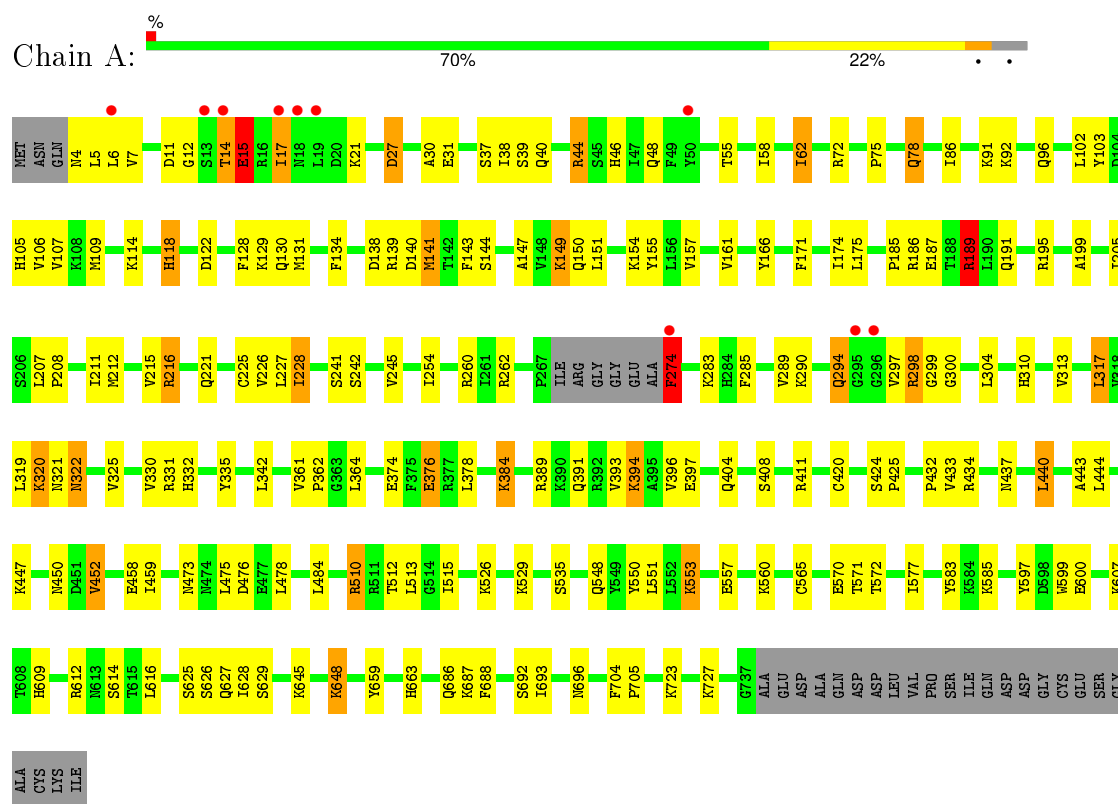
- Molecule 1: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT ALPHA

• Molecule 1: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT ALPHA

Chain C:

• Molecule 2: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT BETA

Chain D:

• Molecule 2: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT BETA

Chain E:

• Molecule 2: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT BETA

Chain F:

50%   30%   20%

TYR LEU VAL GLY Q360 I361 E364 T367 F373 Q374 L375

● Molecule 2: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT BETA

Chain P:

15%   85%

Y1 L2 V3 GLY GLN ILE ASP SER GLU VAL ASP THR ASP ASP LEU SER ASN PHE GLN LEU
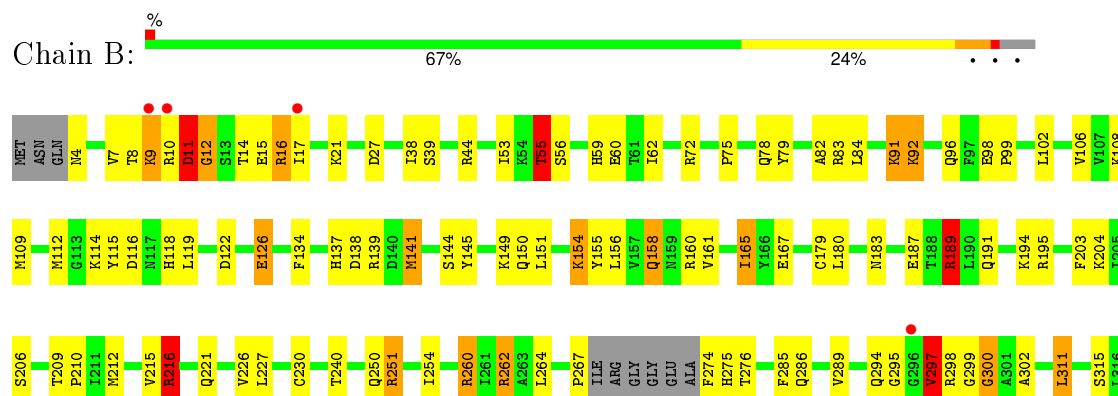
4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 , 55.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.29$	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.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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(^{o})	Ideal(^{o})
1	B	505	ARG	NE-CZ-NH2	-6.30	117.15	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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 Too-close contacts (i)

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	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

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 12.

The worst 5 of 436 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: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	Interatomic distance (Å)	Clash overlap (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%)	14	42
1	B	723/761 (95%)	673 (93%)	39 (5%)	11 (2%)	13	40
1	C	723/761 (95%)	680 (94%)	34 (5%)	9 (1%)	16	47
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%)	1	3
2	P	1/20 (5%)	1 (100%)	0	0	100	100
All	All	2212/2363 (94%)	2056 (93%)	125 (6%)	31 (1%)	14	42

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	294	GLN

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Mol	Chain	Res	Type
1	B	294	GLN
1	B	300	GLY
1	C	294	GLN

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	625/650 (96%)	572 (92%)	53 (8%)	13	36
1	B	625/650 (96%)	560 (90%)	65 (10%)	9	25
1	C	625/650 (96%)	579 (93%)	46 (7%)	17	43
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	6
2	P	3/19 (16%)	2 (67%)	1 (33%)	0	1
All	All	1926/2026 (95%)	1749 (91%)	177 (9%)	11	32

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

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Mol	Chain	Res	Type
1	B	183	ASN

5.3.3   RNA (i)

There are no RNA molecules in this entry.

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

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	11,15,16	0.78	0	10,20,22	1.08	1 (10%)
1	NIY	B	731	1	11,15,16	0.64	0	10,20,22	0.92	0
1	NIY	C	731	1	11,15,16	0.79	0	10,20,22	1.48	1 (10%)

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	-	0/7/10/12	0/1/1/1
1	NIY	B	731	1	-	0/7/10/12	0/1/1/1
1	NIY	C	731	1	-	0/7/10/12	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	731	NIY	CB-CG-CD1	-2.95	114.67	120.36
1	A	731	NIY	O-C-CA	-2.00	120.27	125.49

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	C	731	NIY	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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, 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(Å²)	Q<0.9
1	A	727/761 (95%)	-0.04	10 (1%)	78	69	27, 42, 68, 89	0
1	B	727/761 (95%)	-0.14	4 (0%)	90	86	25, 41, 66, 89	0
1	C	727/761 (95%)	-0.26	2 (0%)	94	92	17, 30, 55, 79	0
2	D	16/20 (80%)	0.78	1 (6%)	23	14	78, 90, 92, 94	0
2	E	16/20 (80%)	0.70	1 (6%)	23	14	69, 82, 93, 93	0
2	F	16/20 (80%)	0.36	0	100	100	64, 78, 84, 85	0
2	P	3/20 (15%)	0.11	0	100	100	33, 33, 36, 42	0
All	All	2232/2363 (94%)	-0.13	18 (0%)	87	81	17, 39, 69, 94	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	LEU	6.1
1	A	14	THR	4.5
2	E	372	ASN	4.3
2	D	372	ASN	3.5
1	A	274	PHE	3.1

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, 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(Å²)	Q<0.9
1	NIY	A	731	15/16	0.93	0.20	-	36,41,51,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	NIY	B	731	15/16	0.94	0.17	-	32,37,45,46	0
1	NIY	C	731	15/16	0.96	0.15	-	22,27,39,42	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.