



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 8, 2023 – 10:25 AM EDT

PDB ID : 6EBO  
Title : Crystal Structure of the Class Ie Ribonucleotide Reductase Beta Subunit from *Aerococcus urinae* in Unactivated Form  
Authors : Palowitch, G.M.; Alapati, R.B.; Boal, A.K.  
Deposited on : 2018-08-06  
Resolution : 1.58 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

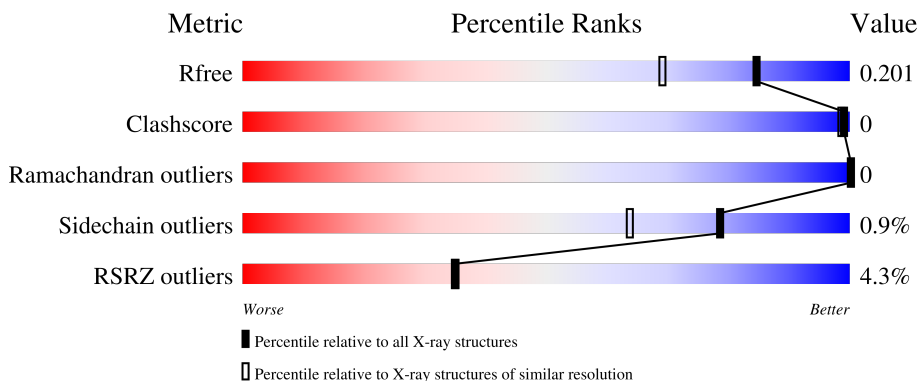
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.58 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))
$R_{free}$	130704	5534 (1.60-1.56)
Clashscore	141614	5861 (1.60-1.56)
Ramachandran outliers	138981	5708 (1.60-1.56)
Sidechain outliers	138945	5703 (1.60-1.56)
RSRZ outliers	127900	5431 (1.60-1.56)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	355	
1	B	355	
1	C	355	
1	D	355	

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 10774 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, beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	311	2537	1637	414	480	6	0	0	0
1	B	303	2467	1596	400	465	6	0	0	0
1	C	305	2483	1605	405	467	6	0	0	0
1	D	311	2537	1637	414	480	6	0	0	0

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	initiating methionine	UNP F2I8X9
A	-16	GLY	-	expression tag	UNP F2I8X9
A	-15	SER	-	expression tag	UNP F2I8X9
A	-14	SER	-	expression tag	UNP F2I8X9
A	-13	HIS	-	expression tag	UNP F2I8X9
A	-12	HIS	-	expression tag	UNP F2I8X9
A	-11	HIS	-	expression tag	UNP F2I8X9
A	-10	HIS	-	expression tag	UNP F2I8X9
A	-9	HIS	-	expression tag	UNP F2I8X9
A	-8	HIS	-	expression tag	UNP F2I8X9
A	-7	SER	-	expression tag	UNP F2I8X9
A	-6	SER	-	expression tag	UNP F2I8X9
A	-5	GLY	-	expression tag	UNP F2I8X9
A	-4	LEU	-	expression tag	UNP F2I8X9
A	-3	VAL	-	expression tag	UNP F2I8X9
A	-2	PRO	-	expression tag	UNP F2I8X9
A	-1	ARG	-	expression tag	UNP F2I8X9
A	0	GLY	-	expression tag	UNP F2I8X9
A	1	SER	-	expression tag	UNP F2I8X9
B	-17	MET	-	initiating methionine	UNP F2I8X9
B	-16	GLY	-	expression tag	UNP F2I8X9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	SER	-	expression tag	UNP F2I8X9
B	-14	SER	-	expression tag	UNP F2I8X9
B	-13	HIS	-	expression tag	UNP F2I8X9
B	-12	HIS	-	expression tag	UNP F2I8X9
B	-11	HIS	-	expression tag	UNP F2I8X9
B	-10	HIS	-	expression tag	UNP F2I8X9
B	-9	HIS	-	expression tag	UNP F2I8X9
B	-8	HIS	-	expression tag	UNP F2I8X9
B	-7	SER	-	expression tag	UNP F2I8X9
B	-6	SER	-	expression tag	UNP F2I8X9
B	-5	GLY	-	expression tag	UNP F2I8X9
B	-4	LEU	-	expression tag	UNP F2I8X9
B	-3	VAL	-	expression tag	UNP F2I8X9
B	-2	PRO	-	expression tag	UNP F2I8X9
B	-1	ARG	-	expression tag	UNP F2I8X9
B	0	GLY	-	expression tag	UNP F2I8X9
B	1	SER	-	expression tag	UNP F2I8X9
C	-17	MET	-	initiating methionine	UNP F2I8X9
C	-16	GLY	-	expression tag	UNP F2I8X9
C	-15	SER	-	expression tag	UNP F2I8X9
C	-14	SER	-	expression tag	UNP F2I8X9
C	-13	HIS	-	expression tag	UNP F2I8X9
C	-12	HIS	-	expression tag	UNP F2I8X9
C	-11	HIS	-	expression tag	UNP F2I8X9
C	-10	HIS	-	expression tag	UNP F2I8X9
C	-9	HIS	-	expression tag	UNP F2I8X9
C	-8	HIS	-	expression tag	UNP F2I8X9
C	-7	SER	-	expression tag	UNP F2I8X9
C	-6	SER	-	expression tag	UNP F2I8X9
C	-5	GLY	-	expression tag	UNP F2I8X9
C	-4	LEU	-	expression tag	UNP F2I8X9
C	-3	VAL	-	expression tag	UNP F2I8X9
C	-2	PRO	-	expression tag	UNP F2I8X9
C	-1	ARG	-	expression tag	UNP F2I8X9
C	0	GLY	-	expression tag	UNP F2I8X9
C	1	SER	-	expression tag	UNP F2I8X9
D	-17	MET	-	initiating methionine	UNP F2I8X9
D	-16	GLY	-	expression tag	UNP F2I8X9
D	-15	SER	-	expression tag	UNP F2I8X9
D	-14	SER	-	expression tag	UNP F2I8X9
D	-13	HIS	-	expression tag	UNP F2I8X9
D	-12	HIS	-	expression tag	UNP F2I8X9

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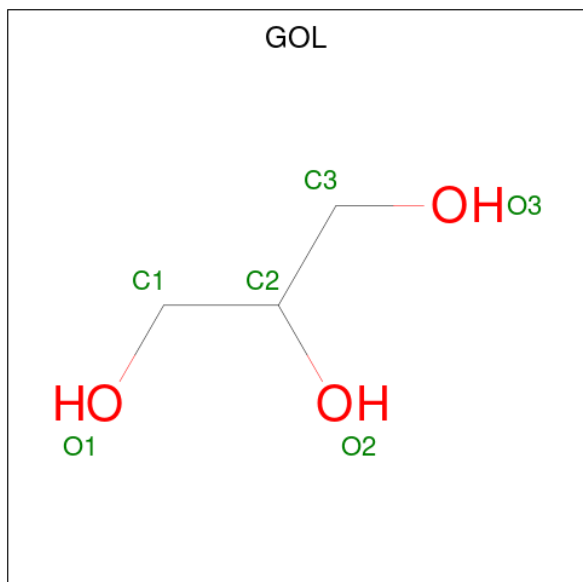
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-11	HIS	-	expression tag	UNP F2I8X9
D	-10	HIS	-	expression tag	UNP F2I8X9
D	-9	HIS	-	expression tag	UNP F2I8X9
D	-8	HIS	-	expression tag	UNP F2I8X9
D	-7	SER	-	expression tag	UNP F2I8X9
D	-6	SER	-	expression tag	UNP F2I8X9
D	-5	GLY	-	expression tag	UNP F2I8X9
D	-4	LEU	-	expression tag	UNP F2I8X9
D	-3	VAL	-	expression tag	UNP F2I8X9
D	-2	PRO	-	expression tag	UNP F2I8X9
D	-1	ARG	-	expression tag	UNP F2I8X9
D	0	GLY	-	expression tag	UNP F2I8X9
D	1	SER	-	expression tag	UNP F2I8X9

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	B	2	Total Ca 2 2	0	0
2	C	2	Total Ca 2 2	0	0
2	D	1	Total Ca 1 1	0	0

- Molecule 3 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
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	189	Total	O	0	0
			189	189		
4	B	201	Total	O	0	0
			201	201		
4	C	187	Total	O	0	0
			187	187		
4	D	143	Total	O	0	0
			143	143		



F314  
PHE  
SER  
GLY  
SER  
GLY  
SER  
SER  
TYR  
ILE  
ILE  
GLY  
THR  
SER  
GLU  
GLU  
THR  
LEU  
LEU  
ASP  
GLU  
ASP  
TRP  
ASP  
PHE



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.85Å 109.07Å 83.73Å 90.00° 90.04° 90.00°	Depositor
Resolution (Å)	39.67 – 1.58 39.67 – 1.58	Depositor EDS
% Data completeness (in resolution range)	96.5 (39.67-1.58) 97.2 (39.67-1.58)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.17 (at 1.58Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.162 , 0.172 0.189 , 0.201	Depositor DCC
$R_{free}$ test set	9453 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	12.8	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 41.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h 0.126 for h,-k,-l 0.002 for l,-k,h	Xtriage
Reported twinning fraction	0.604 for H, K, L 0.396 for h,-k,-l	Depositor
Outliers	0 of 189253 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10774	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.78% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.36	0/2602	0.57	0/3534
1	B	0.36	0/2530	0.57	0/3437
1	C	0.36	0/2546	0.55	0/3458
1	D	0.36	0/2602	0.54	0/3534
All	All	0.36	0/10280	0.56	0/13963

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	2537	0	2460	1	0
1	B	2467	0	2406	1	0
1	C	2483	0	2424	1	0
1	D	2537	0	2460	2	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	1	0	0	0	0
3	B	12	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	12	0	12	0	0
4	A	189	0	0	0	0
4	B	201	0	0	0	0
4	C	187	0	0	0	0
4	D	143	0	0	0	0
All	All	10774	0	9776	5	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 0.

All (5) 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:221:TYR:CZ	1:A:225:VAL:HG11	2.48	0.48
1:D:221:TYR:CZ	1:D:225:VAL:HG11	2.53	0.44
1:B:221:TYR:CZ	1:B:225:VAL:HG11	2.55	0.41
1:D:54:ILE:HD12	1:D:54:ILE:N	2.36	0.41
1:C:221:TYR:CZ	1:C:225:VAL:HG11	2.55	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	309/355 (87%)	307 (99%)	2 (1%)	0	100	100
1	B	301/355 (85%)	299 (99%)	2 (1%)	0	100	100
1	C	303/355 (85%)	301 (99%)	2 (1%)	0	100	100
1	D	309/355 (87%)	306 (99%)	3 (1%)	0	100	100
All	All	1222/1420 (86%)	1213 (99%)	9 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	273/311 (88%)	271 (99%)	2 (1%)	84	72
1	B	266/311 (86%)	263 (99%)	3 (1%)	73	55
1	C	267/311 (86%)	265 (99%)	2 (1%)	84	72
1	D	273/311 (88%)	270 (99%)	3 (1%)	73	55
All	All	1079/1244 (87%)	1069 (99%)	10 (1%)	78	64

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	179	LEU
1	A	307	ARG
1	B	121	ARG
1	B	179	LEU
1	B	232	LYS
1	C	121	ARG
1	C	283	LEU
1	D	31	LYS
1	D	121	ARG
1	D	179	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 6 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
3	GOL	C	403	2	5,5,5	0.37	0	5,5,5	0.25	0
3	GOL	B	404	2	5,5,5	0.28	0	5,5,5	0.24	0
3	GOL	C	404	2	5,5,5	0.30	0	5,5,5	0.14	0
3	GOL	B	403	2	5,5,5	0.29	0	5,5,5	0.23	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
3	GOL	C	403	2	-	2/4/4/4	-
3	GOL	B	404	2	-	1/4/4/4	-
3	GOL	C	404	2	-	0/4/4/4	-
3	GOL	B	403	2	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	403	GOL	C1-C2-C3-O3
3	B	403	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	C	403	GOL	O1-C1-C2-O2
3	C	403	GOL	O1-C1-C2-C3
3	B	404	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	311/355 (87%)	0.28	12 (3%) 39 40	6, 12, 21, 29	0
1	B	303/355 (85%)	0.29	12 (3%) 38 39	6, 11, 20, 26	0
1	C	305/355 (85%)	0.33	11 (3%) 42 44	8, 12, 22, 33	0
1	D	311/355 (87%)	0.47	18 (5%) 23 23	8, 15, 28, 38	0
All	All	1230/1420 (86%)	0.34	53 (4%) 35 35	6, 12, 23, 38	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	307	ARG	6.3
1	D	231	GLU	4.7
1	C	308	ALA	4.4
1	D	310	GLU	4.3
1	D	292	GLU	4.2
1	A	310	GLU	4.0
1	D	311	ASN	4.0
1	A	307	ARG	3.9
1	B	304	LEU	3.8
1	D	53	ASN	3.7
1	C	305	SER	3.6
1	A	55	PRO	3.5
1	D	291	LYS	3.2
1	C	97	ILE	3.2
1	C	231	GLU	3.2
1	B	305	SER	3.2
1	A	4	ASN	3.2
1	B	53	ASN	3.1
1	B	228	LEU	3.0
1	A	311	ASN	3.0
1	D	286	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	97	ILE	3.0
1	D	230	PRO	2.9
1	D	4	ASN	2.8
1	C	232	LYS	2.8
1	C	53	ASN	2.8
1	C	4	ASN	2.8
1	D	134	GLU	2.7
1	D	307	ARG	2.7
1	D	55	PRO	2.7
1	D	232	LYS	2.7
1	A	292	GLU	2.7
1	D	163	ASP	2.6
1	B	163	ASP	2.6
1	D	234	ALA	2.6
1	A	314	PHE	2.6
1	B	291	LYS	2.5
1	C	160	TYR	2.5
1	B	91	ILE	2.4
1	D	314	PHE	2.4
1	A	43	ARG	2.4
1	C	87	VAL	2.3
1	B	232	LYS	2.3
1	B	306	ALA	2.2
1	C	286	GLU	2.2
1	D	312	HIS	2.2
1	D	304	LEU	2.1
1	A	97	ILE	2.1
1	A	291	LYS	2.1
1	B	227	LYS	2.1
1	A	31	LYS	2.1
1	B	112	PHE	2.1
1	A	65	GLU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
3	GOL	B	403	6/6	0.78	0.17	25,26,26,27	0
3	GOL	C	404	6/6	0.84	0.14	23,23,23,23	0
3	GOL	B	404	6/6	0.89	0.18	19,19,20,20	0
3	GOL	C	403	6/6	0.90	0.16	20,21,21,22	0
2	CA	A	401	1/1	0.99	0.06	11,11,11,11	0
2	CA	B	402	1/1	0.99	0.06	17,17,17,17	0
2	CA	C	402	1/1	0.99	0.06	16,16,16,16	0
2	CA	D	401	1/1	0.99	0.04	12,12,12,12	0
2	CA	B	401	1/1	1.00	0.04	11,11,11,11	0
2	CA	C	401	1/1	1.00	0.04	11,11,11,11	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.