



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 24, 2024 – 10:25 PM EDT

PDB ID : 6EBZ  
Title : Crystal Structure of the Class Ie Ribonucleotide Reductase Beta Subunit from *Aerococcus urinae* in Activated Form with Thiocyanate Bound  
Authors : Palowitch, G.M.; Boal, A.K.  
Deposited on : 2018-08-07  
Resolution : 1.66 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

<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>.

---

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	:	2.37.1
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)	:	2.37.1

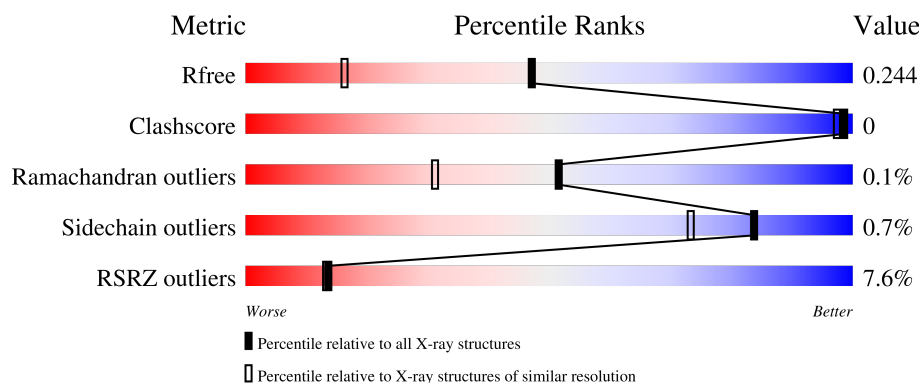
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.66 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	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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

There are 5 unique types of molecules in this entry. The entry contains 10753 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
1	A	312	Total	C	N	O	S	0	3	0
			2567	1657	417	487	6			
1	B	302	Total	C	N	O	S	0	1	0
			2469	1597	400	466	6			
1	C	303	Total	C	N	O	S	0	1	0
			2474	1599	401	468	6			
1	D	313	Total	C	N	O	S	0	1	0
			2564	1655	418	485	6			

There are 80 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
A	123	DAH	TYR	see remark 999	UNP F2I8X9
B	-17	MET	-	initiating methionine	UNP F2I8X9

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	GLY	-	expression tag	UNP F2I8X9
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
B	123	DAH	TYR	see remark 999	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
C	123	DAH	TYR	see remark 999	UNP F2I8X9
D	-17	MET	-	initiating methionine	UNP F2I8X9
D	-16	GLY	-	expression tag	UNP F2I8X9
D	-15	SER	-	expression tag	UNP F2I8X9

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	-14	SER	-	expression tag	UNP F2I8X9
D	-13	HIS	-	expression tag	UNP F2I8X9
D	-12	HIS	-	expression tag	UNP F2I8X9
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
D	123	DAH	TYR	see remark 999	UNP F2I8X9

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

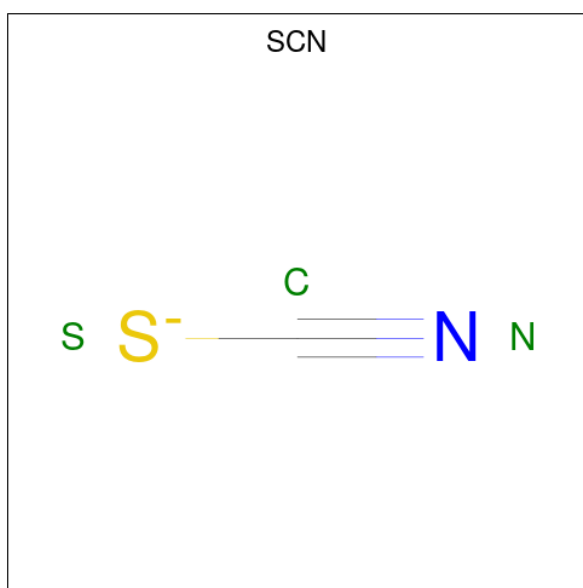
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	B	2	Total Ca 2 2	0	0
2	C	2	Total Ca 2 2	0	0
2	D	1	Total Ca 1 1	0	0

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

- Molecule 4 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	S	0	0
			3	1	1	1		
4	B	1	Total	C	N	S	0	0
			3	1	1	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total 3	C 1	N 1	S 1	0	0
4	C	1	Total 3	C 1	N 1	S 1	0	0
4	C	1	Total 3	C 1	N 1	S 1	0	0


- Molecule 5 is water.

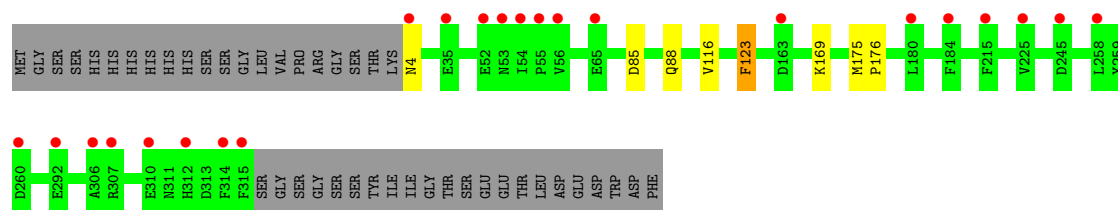
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	167	Total 167	O 167	0	0
5	B	177	Total 177	O 177	0	0
5	C	167	Total 167	O 167	0	0
5	D	135	Total 135	O 135	0	0

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


These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

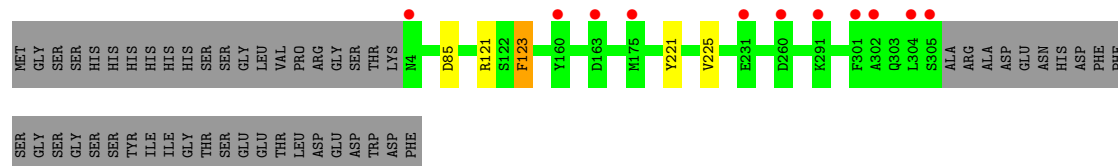
- Molecule 1: Ribonucleoside-diphosphate reductase, beta subunit

Chain A: 




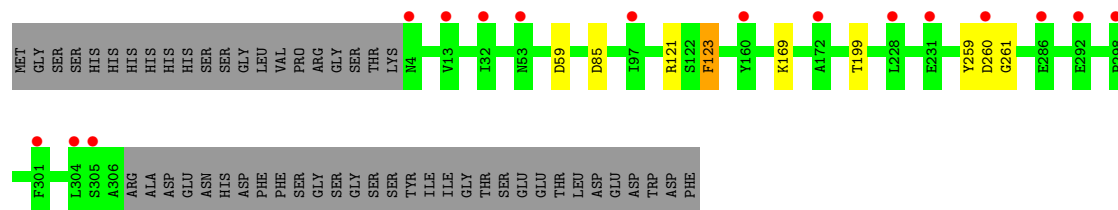
- Molecule 1: Ribonucleoside-diphosphate reductase, beta subunit

Chain B: 




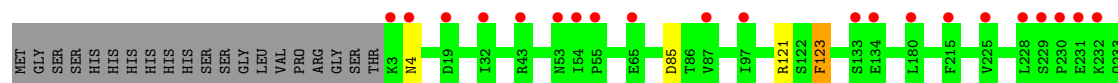
- Molecule 1: Ribonucleoside-diphosphate reductase, beta subunit

Chain C: 

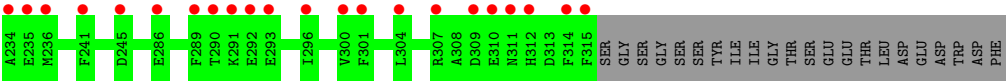


- Molecule 1: Ribonucleoside-diphosphate reductase, beta subunit

Chain D: 







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.04Å 108.97Å 84.03Å 90.00° 90.14° 90.00°	Depositor
Resolution (Å)	45.04 – 1.66 45.04 – 1.66	Depositor EDS
% Data completeness (in resolution range)	86.4 (45.04-1.66) 91.2 (45.04-1.66)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.08 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.196 , 0.215 0.224 , 0.244	Depositor DCC
$R_{free}$ test set	7941 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.3	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 37.0	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 0.117 for h,-k,-l 0.003 for l,-k,h	Xtriage
Reported twinning fraction	0.733 for H, K, L 0.267 for -h,-k,l	Depositor
Outliers	0 of 156066 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10753	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% 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: DAH, SCN, GOL, CA

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	0.38	0/2621	0.56	0/3557
1	B	0.38	0/2520	0.55	0/3421
1	C	0.38	0/2521	0.54	0/3421
1	D	0.38	0/2615	0.54	0/3548
All	All	0.38	0/10277	0.55	0/13947

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	2567	0	2479	3	0
1	B	2469	0	2406	2	0
1	C	2474	0	2408	3	0
1	D	2564	0	2483	1	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	A	6	0	8	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	6	0	8	0	0
4	B	9	0	0	0	0
4	C	6	0	0	0	0
5	A	167	0	0	0	0
5	B	177	0	0	0	0
5	C	167	0	0	0	0
5	D	135	0	0	0	0
All	All	10753	0	9792	9	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.

The worst 5 of 9 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:B:85:ASP:OD2	1:B:123:DAH:OE2	2.21	0.58
1:C:259:TYR:O	1:C:261:GLY:N	2.42	0.53
1:C:85:ASP:OD2	1:C:123:DAH:OE2	2.29	0.50
1:A:85:ASP:OD2	1:A:123:DAH:OE2	2.33	0.46
1:D:85:ASP:OD2	1:D:123:DAH:OE2	2.35	0.45

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	312/355 (88%)	307 (98%)	5 (2%)	0	100	100
1	B	300/355 (84%)	297 (99%)	3 (1%)	0	100	100
1	C	301/355 (85%)	296 (98%)	4 (1%)	1 (0%)	41	22
1	D	311/355 (88%)	307 (99%)	4 (1%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1224/1420 (86%)	1207 (99%)	16 (1%)	1 (0%)	51 31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	260	ASP

### 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	275/310 (89%)	273 (99%)	2 (1%)	84 73
1	B	266/310 (86%)	265 (100%)	1 (0%)	91 85
1	C	266/310 (86%)	264 (99%)	2 (1%)	81 70
1	D	275/310 (89%)	273 (99%)	2 (1%)	84 73
All	All	1082/1240 (87%)	1075 (99%)	7 (1%)	84 76

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	121	ARG
1	C	169	LYS
1	D	121	ARG
1	D	4	ASN
1	B	121	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	DAH	A	123	1	12,13,14	1.56	1 (8%)	14,17,19	0.93	0
1	DAH	C	123	1	12,13,14	1.73	1 (8%)	14,17,19	1.01	0
1	DAH	B	123	1	12,13,14	1.67	1 (8%)	14,17,19	0.88	0
1	DAH	D	123	1	12,13,14	1.63	1 (8%)	14,17,19	0.84	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
1	DAH	A	123	1	-	0/5/6/8	0/1/1/1
1	DAH	C	123	1	-	0/5/6/8	0/1/1/1
1	DAH	B	123	1	-	0/5/6/8	0/1/1/1
1	DAH	D	123	1	-	0/5/6/8	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	123	DAH	CZ-CE2	5.81	1.49	1.40
1	B	123	DAH	CZ-CE2	5.58	1.49	1.40
1	D	123	DAH	CZ-CE2	5.41	1.48	1.40
1	A	123	DAH	CZ-CE2	5.18	1.48	1.40

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	123	DAH	1	0
1	C	123	DAH	1	0
1	B	123	DAH	1	0
1	D	123	DAH	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 6 are monoatomic - leaving 7 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	SCN	B	403	-	1,2,2	0.33	0	0,1,1	-	-
4	SCN	B	401	-	1,2,2	0.33	0	0,1,1	-	-
4	SCN	B	402	-	1,2,2	0.19	0	0,1,1	-	-
4	SCN	C	401	-	1,2,2	0.34	0	0,1,1	-	-
4	SCN	C	402	-	1,2,2	0.29	0	0,1,1	-	-
3	GOL	B	406	-	5,5,5	0.33	0	5,5,5	0.21	0
3	GOL	A	402	-	5,5,5	0.26	0	5,5,5	0.29	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	B	406	-	-	2/4/4/4	-
3	GOL	A	402	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	406	GOL	O1-C1-C2-O2
3	B	406	GOL	O1-C1-C2-C3
3	A	402	GOL	O2-C2-C3-O3

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 [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	311/355 (87%)	0.65	23 (7%) 14 14	6, 14, 29, 38	0
1	B	301/355 (84%)	0.52	11 (3%) 41 41	6, 12, 22, 31	0
1	C	302/355 (85%)	0.59	16 (5%) 26 25	8, 14, 24, 35	0
1	D	312/355 (87%)	0.93	43 (13%) 2 2	9, 18, 34, 41	0
All	All	1226/1420 (86%)	0.67	93 (7%) 13 13	6, 14, 27, 41	0

The worst 5 of 93 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	305	SER	7.4
1	D	231	GLU	6.1
1	A	315	PHE	5.3
1	A	53	ASN	5.3
1	A	307	ARG	5.1

### 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. 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
1	DAH	D	123	13/14	0.89	0.13	15,16,17,17	1
1	DAH	C	123	13/14	0.90	0.12	10,12,14,15	1
1	DAH	B	123	13/14	0.90	0.13	10,12,13,14	1
1	DAH	A	123	13/14	0.92	0.12	11,13,14,14	1

### 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	406	6/6	0.53	0.27	33,33,34,34	0
3	GOL	A	402	6/6	0.66	0.34	26,27,27,27	0
4	SCN	B	402	3/3	0.84	0.17	33,33,33,35	0
4	SCN	C	402	3/3	0.87	0.13	29,29,29,30	0
4	SCN	C	401	3/3	0.93	0.17	26,26,26,26	0
4	SCN	B	401	3/3	0.95	0.20	28,28,29,30	0
4	SCN	B	403	3/3	0.95	0.22	26,26,26,26	0
2	CA	D	401	1/1	0.96	0.06	17,17,17,17	0
2	CA	B	405	1/1	0.98	0.04	14,14,14,14	0
2	CA	B	404	1/1	0.99	0.06	16,16,16,16	0
2	CA	A	401	1/1	0.99	0.04	14,14,14,14	0
2	CA	C	403	1/1	0.99	0.05	16,16,16,16	0
2	CA	C	404	1/1	0.99	0.05	15,15,15,15	0

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

There are no such residues in this entry.