

Full wwPDB X-ray Structure Validation Report (i)

Aug 21, 2020 - 06:43 AM BST

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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at 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 (i) symbol.

The following versions of software and data (see references (1)) 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 : 2.13.1

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)

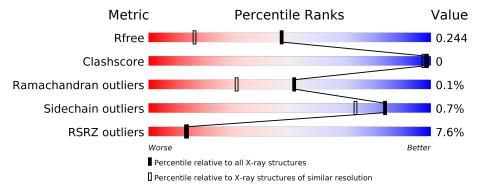
Validation Pipeline (wwPDB-VP) : 2.13.1

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 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
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 on the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	86%	·	12%
1	В	355	84%		15%
1	С	355	83%	·	15%
1	D	355	12% 87%		12%



2 Entry composition (i)

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	${f Atoms}$			ZeroOcc	AltConf	Trace		
1	Λ	312	Total	С	N	О	S	0	3	0
1	A	312	2567	1657	417	487	6	0	J	
1	В	302	Total	С	N	О	S	0	1	0
1	Б	302	2469	1597	400	466	6	0	1	0
1	С	303	Total	С	N	О	S	0	1	0
1		303	2474	1599	401	468	6	0	1	
1	1 D	313	Total	С	N	О	S	0	1	0
1		919	2564	1655	418	485	6		1	U

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
В	-17	MET	_	initiating methionine	UNP F2I8X9



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Chain	Residue	$oxed{egin{array}{c} \textit{wious page} \\ \mathbf{Modelled} \end{array}}$	Actual	Comment	Reference
В	-16	GLY	-	expression tag	UNP F2I8X9
В	-15	SER	-	expression tag	UNP F2I8X9
В	-14	SER	-	expression tag	UNP F2I8X9
В	-13	HIS	-	expression tag	UNP F2I8X9
В	-12	HIS	_	expression tag	UNP F2I8X9
В	-11	HIS	_	expression tag	UNP F2I8X9
В	-10	HIS	_	expression tag	UNP F2I8X9
В	-9	HIS	-	expression tag	UNP F2I8X9
В	-8	HIS	-	expression tag	UNP F2I8X9
В	-7	SER	-	expression tag	UNP F2I8X9
В	-6	SER	-	expression tag	UNP F2I8X9
В	-5	GLY	-	expression tag	UNP F2I8X9
В	-4	LEU	-	expression tag	UNP F2I8X9
В	-3	VAL	-	expression tag	UNP F2I8X9
В	-2	PRO	-	expression tag	UNP F2I8X9
В	-1	ARG	-	expression tag	UNP F2I8X9
В	0	GLY	-	expression tag	UNP F2I8X9
В	1	SER	_	expression tag	UNP F2I8X9
В	123	DAH	TYR	see remark 999	UNP F2I8X9
С	-17	MET	-	initiating methionine	UNP F2I8X9
С	-16	GLY	-	expression tag	UNP F2I8X9
С	-15	SER	_	expression tag	UNP F2I8X9
С	-14	SER	_	expression tag	UNP F2I8X9
С	-13	HIS	-	expression tag	UNP F2I8X9
С	-12	HIS	_	expression tag	UNP F2I8X9
С	-11	HIS	_	expression tag	UNP F2I8X9
С	-10	HIS	-	expression tag	UNP F2I8X9
С	-9	HIS	-	expression tag	UNP F2I8X9
С	-8	HIS	-	expression tag	UNP F2I8X9
С	-7	SER	-	expression tag	UNP F2I8X9
С	-6	SER	-	expression tag	UNP F2I8X9
С	-5	GLY	-	expression tag	UNP F2I8X9
С	-4	LEU	-	expression tag	UNP F2I8X9
С	-3	VAL	-	expression tag	UNP F2I8X9
С	-2	PRO	-	expression tag	UNP F2I8X9
С	-1	ARG	-	expression tag	UNP F2I8X9
С	0	GLY	-	expression tag	UNP F2I8X9
С	1	SER	-	expression tag	UNP F2I8X9
С	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



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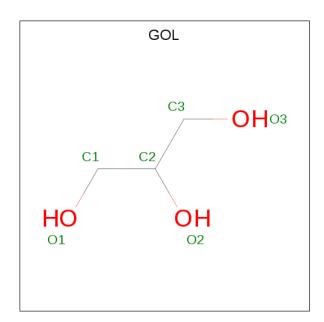
Chain	Residue	Modelled	Actual	Comment	Reference
D	-14	SER	-	expression tag	UNP F2I8X9
D	-13	HIS	-	expression tag	UNP F2I8X9
D	-12	HIS	_	expression tag	UNP F2I8X9
D	-11	HIS	-	expression tag	UNP F2I8X9
D	-10	HIS	_	expression tag	UNP F2I8X9
D	-9	HIS	-	expression tag	UNP F2I8X9
D	-8	HIS	-	expression tag	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	В	2	Total Ca 2 2	0	0
2	A	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0
2	C	2	Total Ca 2 2	0	0

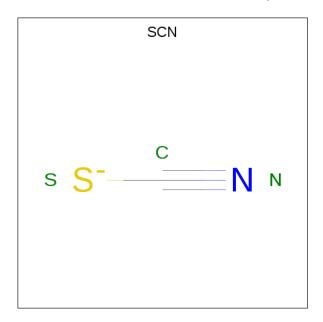
• Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	В	1	Total C O 6 3 3	0	0

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



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



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

• Molecule 5 is water.

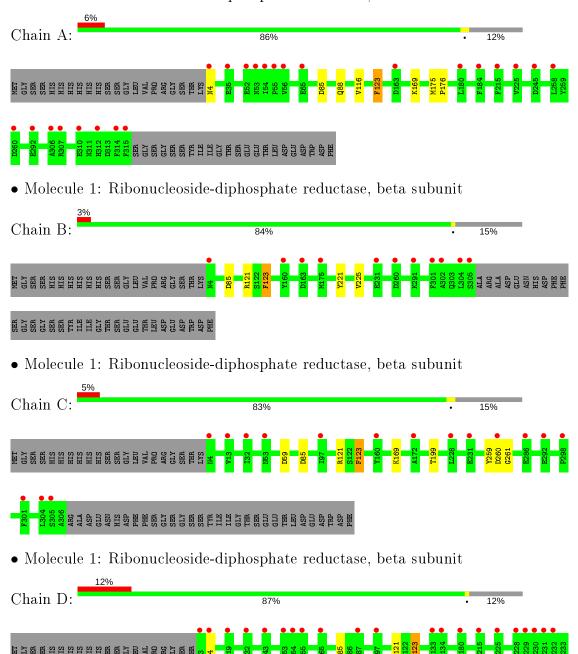
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	167	Total O 167 167	0	0
5	В	177	Total O 177 177	0	0
5	С	167	Total O 167 167	0	0
5	D	135	Total O 135 135	0	0



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







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	80.04Å 108.97Å 84.03Å	Depositor
a, b, c, α , β , γ	90.00° 90.14° 90.00°	Depositor
Resolution (Å)	45.04 - 1.66	Depositor
Resolution (A)	45.04 - 1.66	EDS
% Data completeness	86.4 (45.04-1.66)	Depositor
(in resolution range)	91.2 (45.04-1.66)	EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$0.08~({\rm at}~1.65{\rm \AA})$	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
P. P.	0.196 , 0.215	Depositor
R, R_{free}	0.224 , 0.244	DCC
R_{free} test set	7941 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	17.3	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.40 , 37.0	EDS
L-test for twinning ²	$< L > = 0.52, < L^2> = 0.36$	Xtriage
	0.000 for l,k,-h	
Estimated twinning fraction	0.117 for h,-k,-l	Xtriage
	0.003 for l,-k,h	
Reported twinning fraction	0.733 for H, K, L	Depositor
	0.267 for -h,-k,l	_
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 $(Å^2)$	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.

²Theoretical values of <|L|>, $< L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



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: GOL, CA, SCN, DAH

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		
IVIOI		RMSZ	# Z >5	RMSZ	# Z > 5	
1	A	0.38	0/2621	0.56	0/3557	
1	В	0.38	0/2520	0.55	0/3421	
1	С	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	$\mathbf{H}(\mathbf{model})$	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
1	A	2567	0	2479	3	0
1	В	2469	0	2406	2	0
1	С	2474	0	2408	3	0
1	D	2564	0	2483	1	0
2	A	1	0	0	0	0
2	В	2	0	0	0	0
2	С	2	0	0	0	0
2	D	1	0	0	0	0
3	A	6	0	8	0	0



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-	110111	picolous	payc

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	В	6	0	8	0	0
4	В	9	0	0	0	0
4	С	6	0	0	0	0
5	A	167	0	0	0	0
5	В	177	0	0	0	0
5	С	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.

All (9) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} ({\rm \AA}) \end{array}$	$egin{array}{c} ext{Clash} \ ext{overlap } (ext{Å}) \end{array}$
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
1:B:221:TYR:CZ	1:B:225:VAL:HG11	2.54	0.42
1:C:59:ASP:OD2	1:C:199:THR:HG23	2.20	0.41
1:A:88:GLN:HB3	1:A:116:VAL:HG11	2.03	0.41
1:A:175:MET:HB3	1:A:176:PRO:HD3	2.02	0.40

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



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	$_{ m ntiles}$
1	В	300/355~(84%)	297 (99%)	3 (1%)	0	100	100
1	С	301/355~(85%)	296 (98%)	4 (1%)	1 (0%)	41	22
1	D	311/355 (88%)	307 (99%)	4 (1%)	0	100	100
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	С	260	ASP

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	275/310 (89%)	273 (99%)	2 (1%)		84	73
1	В	$266/310 \ (86\%)$	265 (100%)	1 (0%)		91	85
1	С	$266/310 \ (86\%)$	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

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	169	LYS
1	В	121	ARG
1	С	121	ARG
1	С	169	LYS
1	D	4	ASN
1	D	121	ARG

Some 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 (i)

There are no RNA molecules in this entry.

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

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	Tuno	Chain	in Res	Link	Bo	ond leng	$ ag{ths}$	В	ond ang	les
MIOI	Type	Chain	nes	Lilik	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	В	123	1	12,13,14	1.67	1 (8%)	14,17,19	0.88	0
1	DAH	С	123	1	12,13,14	1.73	1 (8%)	14,17,19	1.01	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	В	123	1	-	0/5/6/8	0/1/1/1
1	DAH	С	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	\mathbf{Z}	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(ext{\AA})$
1	С	123	DAH	CZ-CE2	5.81	1.49	1.40
1	В	123	DAH	CZ-CE2	5.58	1.49	1.40
1	D	123	DAH	CZ-CE2	5.41	1.48	1.40



Mol	Chain	Res	Type	Atoms	Z	${ m Observed}({ m \AA})$	$Ideal(\AA)$	
1	Α	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	В	123	DAH	1	0
1	С	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	Trees	Chain	Res	Link	В	ond leng	$_{ m gths}$	Bond angles		
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SCN	С	402	-	1,2,2	0.29	0	0,1,1	0.00	_
3	GOL	В	406	-	5,5,5	0.33	0	5,5,5	0.21	0
4	SCN	С	401	-	1,2,2	0.34	0	0,1,1	0.00	_
4	SCN	В	401	-	1,2,2	0.33	0	0,1,1	0.00	_
4	SCN	В	402	-	1,2,2	0.19	0	0,1,1	0.00	_
3	GOL	A	402	-	5,5,5	0.26	0	5,5,5	0.29	0
4	SCN	В	403	-	1,2,2	0.33	0	0,1,1	0.00	-



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	В	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	В	406	GOL	O1-C1-C2-O2
3	В	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^{th} 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 $>$	$\#\mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q < 0.9
1	A	311/355~(87%)	0.65	23 (7%) 14 14	6, 14, 29, 38	0
1	В	301/355~(84%)	0.52	11 (3%) 41 41	6, 12, 22, 31	0
1	С	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

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	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
1	D	315	PHE	5.0
1	В	304	LEU	4.7
1	С	260	ASP	4.6
1	D	3	LYS	4.3
1	С	231	GLU	4.1
1	A	4	ASN	4.1
1	D	292	GLU	3.9
1	D	291	LYS	3.9
1	D	215	PHE	3.8
1	A	55	PRO	3.8
1	D	229	SER	3.7
1	D	310	GLU	3.7
1	D	228	LEU	3.7
1	A	260	ASP	3.6
1	D	311	ASN	3.6
1	D	54	ILE	3.4



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Mol	Chain	Res	Type	RSRZ
1	A	312	HIS	3.4
1	С	4	ASN	3.4
1	D	230	PRO	3.3
1	С	301	PHE	3.2
1	D	225	VAL	3.2
1	D	180	LEU	3.2
1	В	301	PHE	3.1
1	D	53	ASN	3.1
1	A	306	ALA	3.0
1	D	301	PHE	3.0
1	D	296	ILE	2.9
1	A	163	ASP	2.9
1	D	290	THR	2.8
1	С	304	LEU	2.8
1	С	53	ASN	2.8
1	D	314	PHE	2.7
1	D	286	GLU	2.7
1	В	163	ASP	2.7
1	В	305	SER	2.7
1	A	314	PHE	2.7
1	A	56	VAL	2.6
1	D	304	LEU	2.6
1	С	292	GLU	2.6
1	В	175	MET	2.6
1	A	310	GLU	2.6
1	D	234	ALA	2.6
1	D	55	PRO	2.6
1	D	307	ARG	2.5
1	A	292	GLU	2.5
1	D	309	ASP	2.5
1	D	289	PHE	2.5
1	D	87	VAL	2.5
1	D	232	LYS	2.5
1	D	300	VAL	2.5
1	D	241	PHE	2.5
1	A	180	LEU	2.5
1	В	291	LYS	2.5
1	В	4	ASN	2.4
1	D	4	ASN	2.4
1	С	228	LEU	2.4
1	D	293	GLU	2.4
1	A	52	GLU	2.4



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Mol	Chain	Res	Type	RSRZ
1	В	260	ASP	2.4
1	D	312	HIS	2.4
1	В	302	ALA	2.4
1	С	286	GLU	2.4
1	D	65	GLU	2.3
1	A	225	VAL	2.3
1	D	43	ARG	2.3
1	D	245	ASP	2.2
1	С	160	TYR	2.2
1	D	133	SER	2.2
1	D	235	GLU	2.2
1	В	231	GLU	2.2
1	A	65	GLU	2.2
1	С	172	ALA	2.2
1	A	215	PHE	2.1
1	С	97	ILE	2.1
1	D	97	ILE	2.1
1	A	184	PHE	2.1
1	С	298	PRO	2.1
1	В	160	TYR	2.1
1	С	13	VAL	2.1
1	D	32	ILE	2.1
1	A	245	ASP	2.1
1	D	236	MET	2.1
1	A	258	LEU	2.1
1	A	35	GLU	2.1
1	D	134	GLU	2.1
1	D	19	ASP	2.1
1	A	54	ILE	2.1
1	С	32	ILE	2.1

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^{th} 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	${f B-factors}({f \AA}^2)$	Q<0.9
1	DAH	D	123	13/14	0.89	0.13	15,16,17,17	1
1	DAH	С	123	13/14	0.90	0.12	10,12,14,15	1
1	DAH	В	123	13/14	0.90	0.13	10,12,13,14	1



Mol	Type	Chain	Res	Atoms	RSCC	RSR	${f B-factors}({f \AA}^2)$	Q < 0.9
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^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
3	GOL	В	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	В	402	3/3	0.84	0.17	33,33,33,35	0
4	SCN	С	402	3/3	0.87	0.13	29,29,29,30	0
4	SCN	С	401	3/3	0.93	0.17	26,26,26,26	0
4	SCN	В	401	3/3	0.95	0.20	28,28,29,30	0
4	SCN	В	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	В	405	1/1	0.98	0.04	14,14,14,14	0
2	CA	A	401	1/1	0.99	0.04	14,14,14,14	0
2	CA	С	404	1/1	0.99	0.05	15,15,15,15	0
2	CA	С	403	1/1	0.99	0.05	16,16,16,16	0
2	CA	В	404	1/1	0.99	0.06	16,16,16,16	0

6.5 Other polymers (i)

There are no such residues in this entry.

