

wwPDB X-ray Structure Validation Summary Report (i)

Oct 10, 2023 – 02:51 PM EDT

PDB ID	:	7K4Q
Title	:	Crystal structure of Kemp Eliminase HG3 in complex with the transition state
		analog 6-nitrobenzotriazole
Authors	:	Padua, R.A.P.; Otten, R.; Bunzel, A.; Nguyen, V.; Pitsawong, W.; Patterson,
		M.; Sui, S.; Perry, S.L.; Cohen, A.E.; Hilvert, D.; Kern, D.
Deposited on		
Resolution	:	1.28 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* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

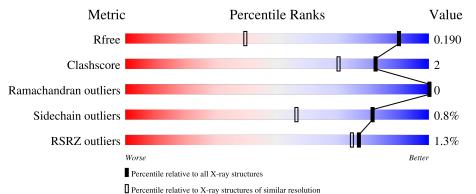
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.28 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	1850 (1.30-1.26)
Clashscore	141614	1926 (1.30-1.26)
Ramachandran outliers	138981	1860 (1.30-1.26)
Sidechain outliers	138945	1859 (1.30-1.26)
RSRZ outliers	127900	1807 (1.30-1.26)

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 >=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	А	308	% 91%	5% •
1	В	308	^{2%} 92%	5% • •



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10452 atoms, of which 4773 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 Endo-1,4-beta-xylanase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace		
1	А	297		C 1531	Н 2387	N 415	O 472	S 13	0	23	0
1	В	300	Total 4809	C 1534		N 416	O 469	S 12	0	20	0

$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	Chain	Residue	Modelled	Actual	Comment	Reference
A-2GLY-expression tagUNP P23360A-1MET-expression tagUNP P23360A0ALA-expression tagUNP P23360A1GLU-expression tagUNP P23360A42METGLNconflictUNP P23360A42METGLNconflictUNP P23360A44TRPTHRconflictUNP P23360A81GLYARGconflictUNP P23360A83GLYHISconflictUNP P23360A83GLYHISconflictUNP P23360A84METTHRconflictUNP P23360A130GLYASNconflictUNP P23360A130GLYASNconflictUNP P23360A234SERALAconflictUNP P23360A236LEUTHRconflictUNP P23360A236LEUTHRconflictUNP P23360A267PHETRPconflictUNP P23360B-3SER-expression tagUNP P23360B-1MET-expression tagUNP P23360B-1MET-expression tagUNP P23360B1GLU-expression tagUNP P23360B1MET-expression tagUNP P23360B1	А	-4	GLY	-	expression tag	UNP P23360
A-1MET-expression tagUNP P23360A0ALA-expression tagUNP P23360A1GLU-expression tagUNP P23360A42METGLNconflictUNP P23360A42METGLNconflictUNP P23360A44TRPTHRconflictUNP P23360A44TRPTHRconflictUNP P23360A81GLYARGconflictUNP P23360A83GLYHISconflictUNP P23360A84METTHRconflictUNP P23360A130GLYASNconflictUNP P23360A172METASNconflictUNP P23360A234SERALAconflictUNP P23360A236LEUTHRconflictUNP P23360A237METGLUconflictUNP P23360A267PHETRPconflictUNP P23360B-4GLY-expression tagUNP P23360B-3SER-expression tagUNP P23360B-1MET-expression tagUNP P23360B0ALA-expression tagUNP P23360B1GLU-expression tagUNP P23360B1GLU-expression tagUNP P23360B1<	А	-3	SER	-	expression tag	UNP P23360
A0ALA-expression tagUNP P23360A1GLU-expression tagUNP P23360A42METGLNconflictUNP P23360A44TRPTHRconflictUNP P23360A44TRPTHRconflictUNP P23360A44TRPTHRconflictUNP P23360A81GLYARGconflictUNP P23360A83GLYHISconflictUNP P23360A84METTHRconflictUNP P23360A130GLYASNconflictUNP P23360A130GLYASNconflictUNP P23360A234SERALAconflictUNP P23360A236LEUTHRconflictUNP P23360A236LEUTHRconflictUNP P23360A237METGLUconflictUNP P23360A267PHETRPconflictUNP P23360B-4GLY-expression tagUNP P23360B-3SER-expression tagUNP P23360B-1MET-expression tagUNP P23360B0ALA-expression tagUNP P23360B1GLU-expression tagUNP P23360B42METGLNconflictUNP P23360	А	-2	GLY	-	expression tag	UNP P23360
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	А	-1	MET	-	expression tag	UNP P23360
A42METGLNconflictUNP P23360A44TRPTHRconflictUNP P23360A81GLYARGconflictUNP P23360A83GLYHISconflictUNP P23360A83GLYHISconflictUNP P23360A84METTHRconflictUNP P23360A130GLYASNconflictUNP P23360A130GLYASNconflictUNP P23360A234SERALAconflictUNP P23360A236LEUTHRconflictUNP P23360A236LEUTHRconflictUNP P23360A237METGLUconflictUNP P23360B-4GLY-expression tagUNP P23360B-3SER-expression tagUNP P23360B-2GLY-expression tagUNP P23360B-1MET-expression tagUNP P23360B1GLU-expression tagUNP P23360B1GLU-expression tagUNP P23360B1GLU-expression tagUNP P23360B1GLU-expression tagUNP P23360B1GLU-expression tagUNP P23360B1GLU-expression tagUNP P23360B <td< td=""><td>А</td><td>0</td><td>ALA</td><td>-</td><td>expression tag</td><td>UNP P23360</td></td<>	А	0	ALA	-	expression tag	UNP P23360
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	А	1	GLU	-	expression tag	UNP P23360
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	А	42		GLN		UNP P23360
A83GLYHISconflictUNP P23360A84METTHRconflictUNP P23360A130GLYASNconflictUNP P23360A172METASNconflictUNP P23360A234SERALAconflictUNP P23360A236LEUTHRconflictUNP P23360A236LEUTHRconflictUNP P23360A237METGLUconflictUNP P23360A267PHETRPconflictUNP P23360B-4GLY-expression tagUNP P23360B-3SER-expression tagUNP P23360B-1MET-expression tagUNP P23360B0ALA-expression tagUNP P23360B1GLU-expression tagUNP P23360	A	44	TRP	THR	conflict	UNP P23360
A84METTHRconflictUNP P23360A130GLYASNconflictUNP P23360A172METASNconflictUNP P23360A234SERALAconflictUNP P23360A236LEUTHRconflictUNP P23360A236LEUTHRconflictUNP P23360A237METGLUconflictUNP P23360A267PHETRPconflictUNP P23360B-4GLY-expression tagUNP P23360B-3SER-expression tagUNP P23360B-2GLY-expression tagUNP P23360B0ALA-expression tagUNP P23360B0ALA-expression tagUNP P23360B1GLU-expression tagUNP P23360	А	81	GLY	ARG	conflict	UNP P23360
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	А	83	GLY	HIS	conflict	UNP P23360
A172METASNconflictUNP P23360A234SERALAconflictUNP P23360A236LEUTHRconflictUNP P23360A237METGLUconflictUNP P23360A267PHETRPconflictUNP P23360B-4GLY-expression tagUNP P23360B-3SER-expression tagUNP P23360B-2GLY-expression tagUNP P23360B-1MET-expression tagUNP P23360B0ALA-expression tagUNP P23360B1GLU-expression tagUNP P23360B1GLU-expression tagUNP P23360B1GLU-expression tagUNP P23360B1GLU-expression tagUNP P23360B1GLU-expression tagUNP P23360B1GLU-expression tagUNP P23360B42METGLNconflictUNP P23360	А	84	MET	THR	conflict	UNP P23360
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	А	130	GLY	ASN	conflict	UNP P23360
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	А	172	MET	ASN	conflict	UNP P23360
A237METGLUconflictUNP P23360A267PHETRPconflictUNP P23360B-4GLY-expression tagUNP P23360B-3SER-expression tagUNP P23360B-2GLY-expression tagUNP P23360B-1MET-expression tagUNP P23360B0ALA-expression tagUNP P23360B1GLU-expression tagUNP P23360B42METGLNconflictUNP P23360	А	234	SER	ALA	conflict	UNP P23360
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	A	236	LEU	THR	conflict	UNP P23360
B-4GLY-expression tagUNP P23360B-3SER-expression tagUNP P23360B-2GLY-expression tagUNP P23360B-1MET-expression tagUNP P23360B0ALA-expression tagUNP P23360B1GLU-expression tagUNP P23360B42METGLNconflictUNP P23360	А	237	MET	GLU	conflict	UNP P23360
B-3SER-expression tagUNP P23360B-2GLY-expression tagUNP P23360B-1MET-expression tagUNP P23360B0ALA-expression tagUNP P23360B1GLU-expression tagUNP P23360B42METGLNconflictUNP P23360	А	267	PHE	TRP	conflict	UNP P23360
B-2GLY-expression tagUNP P23360B-1MET-expression tagUNP P23360B0ALA-expression tagUNP P23360B1GLU-expression tagUNP P23360B42METGLNconflictUNP P23360	В	-4	GLY	-		UNP P23360
B-1MET-expression tagUNP P23360B0ALA-expression tagUNP P23360B1GLU-expression tagUNP P23360B42METGLNconflictUNP P23360	В	-3	SER	-	expression tag	UNP P23360
B0ALA-expression tagUNP P23360B1GLU-expression tagUNP P23360B42METGLNconflictUNP P23360	В	-2	GLY	-	expression tag	UNP P23360
B1GLU-expression tagUNP P23360B42METGLNconflictUNP P23360	В	-1	MET	-	expression tag	UNP P23360
B 42 MET GLN conflict UNP P23360	В		ALA	-	expression tag	UNP P23360
	В	1	GLU	-	expression tag	UNP P23360
B44TRPTHRconflictUNP P23360		42		GLN		
	В	44	TRP	THR	conflict	UNP P23360

There are 34 discrepancies between the modelled and reference sequences:



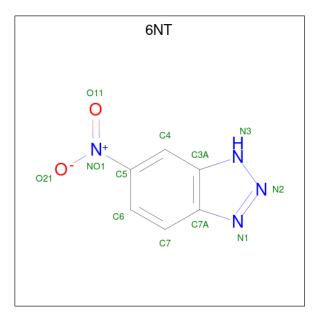
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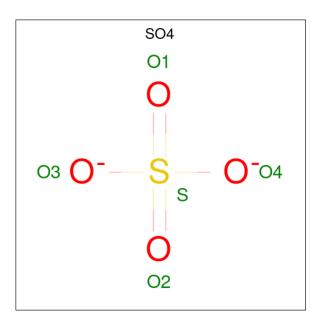
Commu	Continuea from previous page							
Chain	Residue	Modelled	Actual	Comment	Reference			
В	81	GLY	ARG	conflict	UNP P23360			
В	83	GLY	HIS	conflict	UNP P23360			
В	84	MET	THR	conflict	UNP P23360			
В	130	GLY	ASN	conflict	UNP P23360			
В	172	MET	ASN	conflict	UNP P23360			
В	234	SER	ALA	conflict	UNP P23360			
В	236	LEU	THR	conflict	UNP P23360			
В	237	MET	GLU	conflict	UNP P23360			
В	267	PHE	TRP	conflict	UNP P23360			

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M	ol	Chain	Residues		Ate	oms			ZeroOcc	AltConf
2		Δ	1	Total	С	Η	Ν	0	0	1
	Z A	1	16	6	4	4	2	0	1	
2		р	1	Total	С	Η	Ν	0	0	1
		D	1	16	6	4	4	2		





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

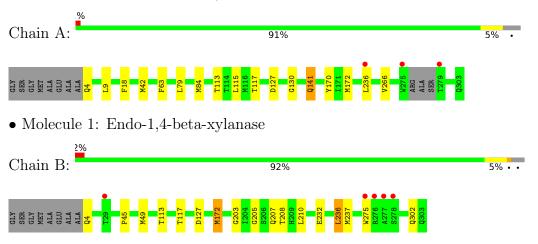
• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	386	Total O 388 388	0	4
4	В	395	Total O 395 395	0	5



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: Endo-1,4-beta-xylanase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	50.64Å 58.97 Å 88.76 Å	Depositor
a, b, c, α , β , γ	90.00° 104.94° 90.00°	Depositor
Resolution (Å)	48.59 - 1.28	Depositor
Resolution (A)	48.59 - 1.28	EDS
% Data completeness	96.2 (48.59-1.28)	Depositor
(in resolution range)	90.8 (48.59 - 1.28)	EDS
R _{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.84 (at 1.28 \text{\AA})$	Xtriage
Refinement program	PHENIX dev_3965	Depositor
R, R_{free}	0.168 , 0.190	Depositor
10, 10 free	0.168 , 0.190	DCC
R_{free} test set	1988 reflections (1.58%)	wwPDB-VP
Wilson B-factor $(Å^2)$	10.6	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.38 , 43.1	EDS
L-test for twinning ²	$< L > = 0.51, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	10452	wwPDB-VP
Average B, all atoms $(Å^2)$	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 50.56 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.3604e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

²Theoretical 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.



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: SO4, $6\mathrm{NT}$

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		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.31	0/2485	0.57	0/3385	
1	В	0.29	0/2485	0.57	0/3389	
All	All	0.30	0/4970	0.57	0/6774	

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	А	2431	2387	2371	12	0
1	В	2431	2378	2363	12	0
2	А	12	4	4	1	0
2	В	12	4	4	1	0
3	А	5	0	0	0	0
3	В	5	0	0	0	0
4	А	388	0	0	1	0
4	В	395	0	0	0	0
All	All	5679	4773	4742	24	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 2.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:GLN:HG2	1:A:9:LEU:HD11	1.63	0.80
1:A:117[B]:THR:HG22	4:A:549:HOH:O	1.88	0.73
1:A:172[B]:MET:HG2	1:A:236[B]:LEU:HD22	1.77	0.67
1:B:127[A]:ASP:OD2	2:B:401[A]:6NT:N3	2.23	0.66
1:A:127[A]:ASP:OD2	2:A:401[A]:6NT:N3	2.25	0.66

The worst 5 of 24 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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	А	317/308~(103%)	307~(97%)	10 (3%)	0	100	100
1	В	317/308~(103%)	307~(97%)	10 (3%)	0	100	100
All	All	634/616~(103%)	614 (97%)	20 (3%)	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	А	264/246~(107%)	262~(99%)	2(1%)	81 56	

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	В	261/246~(106%)	256~(98%)	5(2%)	57 19	
All	All	525/492~(107%)	518 (99%)	7 (1%)	81 34	

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

Mol	Chain	Res	Type
1	В	172[B]	MET
1	В	236[A]	LEU
1	В	275	TRP
1	В	236[B]	LEU
1	В	172[A]	MET

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

Mol	Chain	Res	Type
1	В	303	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)

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)

4 ligands 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



Mol	l Type Chain Res		Link	Bond lengths			Bond angles			
	Type	Ullaili	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	6NT	А	401[A]	-	8,13,13	1.39	1 (12%)	10,18,18	1.09	1 (10%)
2	6NT	В	401[A]	-	8,13,13	1.35	1 (12%)	10,18,18	1.05	1 (10%)
3	SO4	А	402	-	4,4,4	0.13	0	$6,\!6,\!6$	0.40	0
3	SO4	В	402	-	4,4,4	0.12	0	$6,\!6,\!6$	0.35	0

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).

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
2	6NT	А	401[A]	-	-	0/2/4/4	0/2/2/2
2	6NT	В	401[A]	-	-	0/2/4/4	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	А	401[A]	6NT	011-NO1	-3.17	1.17	1.22
2	В	401[A]	6NT	011-N01	-3.09	1.17	1.22

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
2	А	401[A]	6NT	N3-N2-N1	-2.47	108.04	111.25
2	В	401[A]	6NT	N3-N2-N1	-2.44	108.09	111.25

All (2) bond angle outliers are listed below:

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	401[A]	6NT	1	0
2	В	401[A]	6NT	1	0



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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	297/308~(96%)	-0.24	3 (1%) 82 80	8, 12, 24, 42	0
1	В	300/308~(97%)	-0.17	5 (1%) 70 67	8, 12, 25, 42	0
All	All	597/616~(96%)	-0.20	8 (1%) 77 74	8, 12, 24, 42	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	275	TRP	6.0
1	В	278	SER	5.6
1	В	277	ALA	4.6
1	А	275	TRP	3.3
1	В	276	ARG	2.6

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^{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	B-factors(Å ²)	Q < 0.9
2	6NT	А	401[A]	12/12	0.82	0.16	$16,\!22,\!31,\!37$	16
3	SO4	А	402	5/5	0.82	0.20	13,13,26,46	5
2	6NT	В	401[A]	12/12	0.88	0.11	13,21,31,37	16
3	SO4	В	402	5/5	0.94	0.10	11,12,30,35	5

6.5 Other polymers (i)

There are no such residues in this entry.

