

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	2AAI
Title	:	Crystallographic refinement of ricin to 2.5 Angstroms
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Deposited on	:	1993-09-07
Resolution	:	2.50 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
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 2.50 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	Similar resolution
WIEUIIC	$(\# \mathbf{Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
Clashscore	141614	$5346\ (2.50-2.50)$
Ramachandran outliers	138981	5231(2.50-2.50)
Sidechain outliers	138945	5233(2.50-2.50)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of	chain	
1	А	267	51%	30%	14% 5%
2	В	262	53%	31%	14% •
3	С	2	100%		
3	D	2	100%		
4	Е	5	80%		20%
4	F	5	100%		

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	Ε	1	X	-	-	-
4	NAG	F	1	Х	-	-	-



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4440 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 RICIN (A CHAIN).

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	А	267	Total 2114	C 1342	N 372	O 395	S 5	0	0	0

• Molecule 2 is a protein called RICIN (B CHAIN).

Mol	Chain	Residues		At	\mathbf{oms}			ZeroOcc	AltConf	Trace
2	В	262	Total 2035	C 1273	N 357	O 393	S 12	0	0	0

• Molecule 3 is an oligosaccharide called beta-D-galactopyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	С	2	Total C O 23 12 11	0	0	0
3	D	2	Total C O 23 12 11	0	0	0

• Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyran ose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	Е	5	Total C N O 61 34 2 25	0	0	0
4	F	5	Total C N O 61 34 2 25	0	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	61	Total O 61 61	0	0
5	В	62	$\begin{array}{cc} \text{Total} & \text{O} \\ 62 & 62 \end{array}$	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. 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. 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.

30%

14%

5%

Note EDS was not executed.

• Molecule 1: RICIN (A CHAIN)

Chain A: 51%



• Molecule 2: RICIN (B CHAIN)



• Molecule 3: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain C:

100%



• Molecule 3: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

80%

Chain D:

BGC1 GAL2

 $\label{eq:mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]} beta-D-mannopyranose-(1-6)] beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2$

20%

Chain E:

100%

NAG 1 NAG 2 BMA 3 MAN 4 MAN 5 MAN 5

 $\label{eq:mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]} beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gl$

Chain F:

100%

NAG1 NAG2 BMA3 MAN4 MAN5



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	72.74Å 78.49 Å 114.34 Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) - 2.50	Depositor
% Data completeness	(Not available) ((Not available)-2.50)	Depositor
(in resolution range)	(Not available) ((Not available)-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.212 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4440	wwPDB-VP
Average B, all atoms $(Å^2)$	26.0	wwPDB-VP



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: MAN, GAL, BGC, BMA, NAG

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).

Mal	Chain	Bo	nd lengths	Bond angles		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	1.04	0/2162	2.00	89/2941~(3.0%)	
2	В	1.04	2/2080~(0.1%)	2.12	86/2842~(3.0%)	
All	All	1.04	2/4242~(0.0%)	2.06	175/5783~(3.0%)	

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	А	0	3
2	В	0	3
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
2	В	131	TRP	CD1-NE1	-5.74	1.28	1.38
2	В	195	SER	CA-CB	5.14	1.60	1.52

All (175) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	В	200	THR	CA-C-N	-13.18	88.21	117.20
1	А	234	ARG	NE-CZ-NH2	-13.11	113.74	120.30
1	А	234	ARG	NE-CZ-NH1	11.23	125.91	120.30
2	В	37	TRP	CD1-CG-CD2	10.77	114.92	106.30
1	А	258	ARG	NE-CZ-NH1	10.62	125.61	120.30
2	В	170	GLU	CA-C-N	-10.60	93.88	117.20
2	В	258	TRP	CD1-CG-CD2	10.53	114.72	106.30



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	216	TRP	CD1-CG-CD2	10.32	114.56	106.30
2	В	258	TRP	CG-CD2-CE3	10.12	143.01	133.90
1	А	236	ASN	CA-C-N	10.08	136.35	116.20
1	А	125	ARG	NE-CZ-NH1	9.92	125.26	120.30
1	А	258	ARG	NE-CZ-NH2	-9.90	115.35	120.30
2	В	212	SER	CA-C-N	9.67	135.54	116.20
2	В	258	TRP	CB-CG-CD1	-9.46	114.70	127.00
2	В	131	TRP	CD1-CG-CD2	9.46	113.86	106.30
2	В	187	ARG	NE-CZ-NH1	9.29	124.94	120.30
2	В	198	ARG	CA-CB-CG	9.13	133.48	113.40
2	В	131	TRP	CE2-CD2-CG	-8.96	100.13	107.30
2	В	160	TRP	CD1-CG-CD2	8.88	113.41	106.30
2	В	90	TRP	CG-CD2-CE3	8.72	141.75	133.90
2	В	258	TRP	CE2-CD2-CG	-8.52	100.48	107.30
1	А	114	ARG	NE-CZ-NH1	8.46	124.53	120.30
2	В	200	THR	O-C-N	8.44	136.21	122.70
1	А	235	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	А	125	ARG	NE-CZ-NH2	-8.37	116.11	120.30
2	В	37	TRP	CE2-CD2-CG	-8.25	100.70	107.30
1	А	196	ARG	NE-CZ-NH2	-8.16	116.22	120.30
1	А	65	HIS	N-CA-CB	8.16	125.29	110.60
1	А	226	PHE	CB-CG-CD2	-7.95	115.23	120.80
2	В	212	SER	O-C-N	-7.93	109.72	123.20
1	А	29	ARG	NE-CZ-NH1	7.92	124.26	120.30
2	В	27	ARG	NE-CZ-NH2	-7.91	116.35	120.30
1	А	240	PHE	N-CA-C	7.89	132.30	111.00
2	В	90	TRP	CD1-CG-CD2	7.84	112.57	106.30
1	А	65	HIS	CA-C-N	-7.82	99.99	117.20
1	А	197	ARG	NE-CZ-NH1	7.80	124.20	120.30
1	А	17	THR	N-CA-CB	-7.77	95.54	110.30
2	В	216	TRP	CE2-CD2-CG	-7.77	101.08	107.30
1	A	6	TYR	CB-CG-CD2	-7.70	116.38	121.00
2	В	43	THR	CA-CB-CG2	7.69	123.17	112.40
1	А	159	THR	CA-CB-CG2	7.69	123.17	112.40
2	В	173	TRP	CD1-CG-CD2	7.57	112.35	106.30
2	В	24	ARG	NE-CZ-NH1	7.50	124.05	120.30
2	В	16	ARG	NE-CZ-NH1	7.49	124.04	120.30
1	А	133	LEU	CA-CB-CG	7.48	132.51	115.30
2	В	248	TYR	CB-CG-CD1	-7.44	116.54	121.00
2	В	202	VAL	CG1-CB-CG2	-7.39	99.07	110.90
2	В	216	TRP	CG-CD1-NE1	-7.38	102.72	110.10
1	А	211	TRP	CD1-CG-CD2	7.36	112.19	106.30



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	90	TRP	CE2-CD2-CG	-7.34	101.43	107.30
1	А	226	PHE	N-CA-C	7.33	130.80	111.00
1	А	245	VAL	CA-C-N	7.30	133.25	117.20
2	В	258	TRP	CG-CD1-NE1	-7.27	102.83	110.10
2	В	104	SER	O-C-N	7.25	134.31	122.70
2	В	53	ARG	NE-CZ-NH1	7.17	123.88	120.30
2	В	43	THR	N-CA-CB	-7.15	96.71	110.30
1	А	174	MET	CG-SD-CE	7.13	111.62	100.20
1	А	192	ILE	CG1-CB-CG2	-7.09	95.79	111.40
1	А	242	VAL	CG1-CB-CG2	-7.07	99.58	110.90
2	В	198	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	А	114	ARG	NE-CZ-NH2	-7.03	116.78	120.30
2	В	173	TRP	CE2-CD2-CG	-7.01	101.69	107.30
2	В	236	ARG	NE-CZ-NH1	7.01	123.80	120.30
1	А	28	VAL	CG1-CB-CG2	-6.99	99.72	110.90
2	В	160	TRP	CE2-CD2-CG	-6.93	101.75	107.30
2	В	37	TRP	CG-CD1-NE1	-6.90	103.20	110.10
1	А	266	GLN	N-CA-C	6.84	129.48	111.00
2	В	74	TYR	CB-CG-CD2	-6.79	116.92	121.00
1	А	64	ASN	CA-C-N	6.74	132.03	117.20
2	В	102	ARG	NE-CZ-NH2	-6.69	116.96	120.30
1	А	251	ILE	CG1-CB-CG2	-6.68	96.71	111.40
1	А	65	HIS	O-C-N	6.65	133.34	122.70
2	В	93	TRP	CE2-CD2-CG	-6.62	102.00	107.30
1	А	223	GLN	N-CA-C	-6.61	93.16	111.00
1	А	226	PHE	CB-CA-C	-6.54	97.31	110.40
2	В	49	TRP	CE2-CD2-CG	-6.53	102.08	107.30
2	В	49	TRP	CD1-CG-CD2	6.52	111.51	106.30
1	А	226	PHE	CA-C-N	-6.50	102.89	117.20
1	A	180	ARG	NE-CZ-NH2	-6.49	117.05	120.30
2	В	58	ARG	NE-CZ-NH2	-6.47	117.07	120.30
1	A	60	VAL	CG1-CB-CG2	-6.44	100.60	110.90
1	A	232	LEU	CA-CB-CG	6.43	130.09	115.30
1	A	211	TRP	CE2-CD2-CG	-6.38	102.19	107.30
2	В	225	LEU	CA-CB-CG	6.36	129.92	115.30
2	В	90	TRP	CB-CG-CD1	-6.34	118.76	127.00
2	В	24	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	A	71	THR	CA-CB-CG2	6.30	121.23	112.40
1	A	226	PHE	CA-CB-CG	6.30	129.03	113.90
1	A	62	LEU	CA-CB-CG	6.29	129.76	115.30
1	А	222	ASN	OD1-CG-ND2	-6.26	107.51	121.90
2	В	237	ALA	CB-CA-C	-6.25	100.72	110.10



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	85	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	А	113	ASN	CA-C-N	-6.21	103.53	117.20
1	А	197	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	А	64	ASN	CB-CG-ND2	6.13	131.42	116.70
1	А	245	VAL	O-C-N	-6.12	112.91	122.70
2	В	131	TRP	CG-CD1-NE1	-6.10	104.00	110.10
2	В	43	THR	CA-CB-OG1	-6.05	96.29	109.00
1	А	238	SER	CA-C-N	-6.04	103.90	117.20
2	В	137	THR	N-CA-CB	-6.04	98.83	110.30
1	А	236	ASN	O-C-N	-6.02	112.96	123.20
2	В	131	TRP	CG-CD2-CE3	6.02	139.32	133.90
1	А	14	ALA	CA-C-N	6.01	128.22	116.20
2	В	22	ASP	O-C-N	-6.00	113.10	122.70
1	А	44	VAL	CG1-CB-CG2	-5.95	101.37	110.90
1	А	238	SER	C-N-CA	5.94	136.55	121.70
1	А	67	GLU	N-CA-C	5.91	126.97	111.00
1	А	91	TYR	CB-CG-CD2	-5.89	117.47	121.00
2	В	160	TRP	CG-CD1-NE1	-5.87	104.23	110.10
2	В	90	TRP	CG-CD1-NE1	-5.85	104.25	110.10
1	А	53	ILE	CB-CA-C	-5.81	99.99	111.60
2	В	145	VAL	CG1-CB-CG2	-5.80	101.62	110.90
2	В	173	TRP	CG-CD2-CE3	5.79	139.11	133.90
1	А	56	ARG	N-CA-C	5.76	126.56	111.00
2	В	102	ARG	CA-C-N	-5.76	104.53	117.20
2	В	93	TRP	CD1-CG-CD2	5.75	110.90	106.30
1	А	56	ARG	NE-CZ-NH1	5.75	123.18	120.30
2	В	67	TYR	CB-CG-CD1	-5.72	117.57	121.00
2	В	198	ARG	CA-C-N	-5.70	104.67	117.20
2	В	250	LEU	CA-CB-CG	5.70	128.40	115.30
2	В	48	LEU	CA-CB-CG	5.66	128.33	115.30
2	В	106	VAL	N-CA-CB	-5.66	99.05	111.50
1	А	84	TYR	CB-CG-CD2	-5.64	117.62	121.00
2	В	200	THR	CA-C-O	5.61	131.87	120.10
2	В	165	SER	N-CA-C	-5.59	95.91	111.00
1	А	238	SER	O-C-N	5.59	131.64	122.70
1	A	197	ARG	N-CA-C	-5.55	96.01	111.00
1	A	239	LYS	N-CA-C	5.54	125.95	111.00
2	В	169	ALA	N-CA-C	-5.54	96.05	111.00
1	A	113	ASN	O-C-N	5.52	131.54	122.70
1	A	180	ARG	NE-CZ-NH1	5.50	123.05	120.30
2	В	155	ASN	CA-C-N	-5.50	$1\overline{05.10}$	117.20
1	A	64	ASN	O-C-N	-5.49	113.92	122.70



Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	65	HIS	CB-CA-C	-5.47	99.46	110.40
1	А	71	THR	CA-CB-OG1	-5.47	97.52	109.00
1	А	127	GLU	CA-CB-CG	5.45	125.38	113.40
2	В	22	ASP	N-CA-CB	-5.44	100.80	110.60
1	А	159	THR	OG1-CB-CG2	-5.42	97.54	110.00
1	А	123	TYR	CB-CG-CD2	-5.41	117.76	121.00
1	А	235	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	А	29	ARG	NE-CZ-NH2	-5.37	117.62	120.30
2	В	184	GLN	CA-CB-CG	-5.37	101.59	113.40
1	А	134	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	А	37	ASP	CB-CG-OD1	5.34	123.10	118.30
2	В	173	TRP	CB-CG-CD1	-5.33	120.07	127.00
1	А	26	ARG	CD-NE-CZ	-5.33	116.14	123.60
2	В	239	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	А	76	VAL	N-CA-CB	-5.33	99.78	111.50
1	А	2	PHE	N-CA-CB	-5.26	101.13	110.60
1	А	190	THR	CA-CB-CG2	5.25	119.75	112.40
1	А	192	ILE	CA-CB-CG1	5.23	120.94	111.00
2	В	131	TRP	CB-CG-CD1	-5.22	120.21	127.00
2	В	216	TRP	CG-CD2-CE3	5.22	138.60	133.90
2	В	22	ASP	CA-C-N	5.21	128.66	117.20
2	В	205	LEU	CA-CB-CG	5.19	127.23	115.30
1	А	221	SER	CA-CB-OG	5.18	125.18	111.20
2	В	176	TYR	CB-CG-CD2	-5.18	117.89	121.00
2	В	104	SER	CA-C-N	-5.17	105.82	117.20
1	А	89	SER	N-CA-CB	-5.16	102.76	110.50
2	В	161	ILE	CA-CB-CG1	-5.16	101.20	111.00
1	А	230	ILE	CG1-CB-CG2	-5.14	100.10	111.40
2	В	102	ARG	NE-CZ-NH1	5.11	122.85	120.30
2	В	109	ALA	CA-C-N	5.09	128.40	117.20
2	В	184	GLN	N-CA-C	5.09	124.75	111.00
1	А	113	ASN	CA-CB-CG	-5.09	102.21	113.40
1	А	240	PHE	CB-CG-CD2	-5.08	117.25	120.80
2	В	41	SER	CA-C-N	-5.06	106.06	117.20
1	А	211	TRP	CG-CD1-NE1	-5.06	105.04	110.10
1	A	238	SER	N-CA-C	5.05	124.65	111.00
1	А	104	ILE	N-CA-CB	-5.04	99.21	110.80
1	A	109	THR	CA-CB-CG2	5.04	119.45	112.40
2	В	231	LEU	CA-CB-CG	5.03	126.88	115.30
2	В	68	GLY	O-C-N	-5.03	114.65	122.70
2	В	201	VAL	N-CA-C	-5.03	97.41	111.00
1	A	211	TRP	CG-CD2-CE3	5.03	138.43	133.90

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There are no chirality outliers.

Mol	Chain	\mathbf{Res}	\mathbf{Type}	Group
1	А	158	GLY	Mainchain
1	А	262	PRO	Peptide
1	А	56	ARG	Sidechain
2	В	170	GLU	Mainchain
2	В	199	GLU	Mainchain
2	В	74	TYR	Sidechain

All (6) planarity outliers are listed below:

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	2114	0	2083	63	0
2	В	2035	0	1974	51	0
3	С	23	0	21	0	0
3	D	23	0	21	0	0
4	Е	61	0	52	1	0
4	F	61	0	52	0	0
5	А	61	0	0	2	0
5	В	62	0	0	4	0
All	All	4440	0	4203	112	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 13.

All (112) 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:1:ILE:HG23	1:A:2:PHE:H	1.51	0.76
1:A:236:ASN:HD21	1:A:238:SER:HB2	1.53	0.73
1:A:225:ALA:HB1	1:A:226:PHE:CD1	2.29	0.67
2:B:193:SER:HA	2:B:201:VAL:O	1.94	0.67
2:B:198:ARG:HB3	2:B:199:GLU:OE1	1.94	0.67
1:A:224:GLY:HA2	5:A:625:HOH:O	1.94	0.67
1:A:1:ILE:HG12	1:A:53:ILE:HD11	1.76	0.66



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:B:102:ARG:HB2	5:B:671:HOH:O	1.95	0.66	
1:A:1:ILE:HG23	1:A:2:PHE:N	2.13	0.62	
1:A:225:ALA:HB3	1:A:244:ASP:HA	1.81	0.62	
2:B:165:SER:HB3	2:B:168:LYS:HB2	1.82	0.62	
2:B:201:VAL:HG12	2:B:203:LYS:NZ	2.15	0.61	
1:A:266:GLN:HG3	1:A:267:PHE:N	2.15	0.61	
1:A:260:ALA:O	2:B:4:CYS:SG	2.58	0.61	
2:B:12:ARG:HD3	2:B:20:CYS:SG	2.42	0.60	
1:A:229:PRO:HB3	1:A:243:TYR:CE2	2.37	0.59	
1:A:53:ILE:HG21	1:A:106:HIS:CD2	2.37	0.58	
2:B:16:ARG:HH11	2:B:128:SER:HB3	1.67	0.58	
1:A:91:TYR:OH	1:A:155:SER:HA	2.04	0.58	
1:A:154:TYR:CE1	1:A:159:THR:HG23	2.39	0.57	
2:B:78:TYR:HD2	2:B:83:ALA:HB2	1.69	0.57	
1:A:236:ASN:ND2	1:A:238:SER:HB2	2.18	0.56	
1:A:119:PHE:HB2	1:A:125:ARG:HG2	1.86	0.56	
2:B:182:ARG:NE	2:B:207:CYS:SG	2.78	0.56	
2:B:236:ARG:HD3	2:B:242:LEU:HD13	1.87	0.55	
1:A:40:HIS:H	1:A:267:PHE:HB3	1.72	0.55	
2:B:67:TYR:HB3	2:B:73:VAL:HB	1.89	0.55	
1:A:9:ILE:HD11	1:A:31:ARG:HG2	1.87	0.54	
2:B:145:VAL:HG21	2:B:261:LEU:HD12	1.90	0.54	
1:A:66:ALA:O	1:A:67:GLU:HB2	2.07	0.54	
2:B:141:VAL:HA	2:B:173:TRP:O	2.07	0.53	
2:B:153:GLN:HG2	5:B:651:HOH:O	2.08	0.53	
1:A:221:SER:O	1:A:222:ASN:HB2	2.08	0.53	
1:A:39:ARG:HA	1:A:267:PHE:HB2	1.90	0.53	
1:A:88:ASN:HB2	1:A:112:GLN:OE1	2.09	0.52	
1:A:206:THR:HG22	1:A:232:LEU:HD12	1.90	0.52	
1:A:266:GLN:HG3	1:A:267:PHE:CG	2.45	0.52	
1:A:102:GLU:O	1:A:105:THR:HB	2.10	0.52	
1:A:53:ILE:HG21	1:A:106:HIS:HD2	1.75	0.52	
2:B:99:ILE:HD11	2:B:104:SER:HA	1.92	0.52	
2:B:90:TRP:CZ3	2:B:100:ASN:HB2	2.45	0.51	
1:A:60:VAL:HG12	1:A:62:LEU:HD13	1.93	0.51	
2:B:27:ARG:O	2:B:32:ASN:ND2	2.43	0.51	
1:A:29:ARG:HD2	1:A:179:ALA:O	2.10	0.51	
1:A:39:ARG:HA	1:A:267:PHE:CB	2.42	0.49	
1:A:23:ASN:HA	1:A:26:ARG:HD3	1.93	0.49	
2:B:90:TRP:CE3	2:B:100:ASN:HB2	2.47	0.49	
1:A:64:ASN:HB3	1:A:66:ALA:HB3	1.95	0.48	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:B:78:TYR:CD2	2:B:83:ALA:HB2	2.48	0.48	
2:B:201:VAL:HG12	2:B:203:LYS:HZ2	1.78	0.47	
2:B:238:SER:O	2:B:240:PRO:HD3	2.14	0.47	
1:A:229:PRO:HA	1:A:242:VAL:O	2.14	0.47	
2:B:161:ILE:HD12	2:B:258:TRP:CZ3	2.50	0.47	
2:B:34:ILE:HD12	2:B:49:TRP:HH2	1.79	0.47	
2:B:12:ARG:HH11	2:B:12:ARG:CG	2.28	0.47	
2:B:8:GLU:HA	2:B:51:LEU:O	2.15	0.47	
2:B:93:TRP:CZ2	4:E:2:NAG:H83	2.49	0.47	
1:A:224:GLY:O	1:A:225:ALA:HB2	2.15	0.47	
2:B:186:ASN:OD1	2:B:189:ASN:ND2	2.48	0.47	
1:A:222:ASN:HB3	1:A:223:GLN:O	2.15	0.46	
1:A:40:HIS:O	1:A:41:GLU:HB2	2.15	0.46	
2:B:191:LEU:HD23	2:B:216:TRP:CE2	2.50	0.46	
1:A:70:VAL:HG11	1:A:151:LEU:HD23	1.97	0.46	
2:B:161:ILE:HD12	2:B:258:TRP:HZ3	1.80	0.45	
2:B:124:ILE:O	2:B:212:SER:HB3	2.16	0.45	
1:A:154:TYR:CD1	1:A:159:THR:HA	2.52	0.45	
2:B:201:VAL:HA	2:B:203:LYS:HZ2	1.81	0.45	
2:B:175:LEU:HD22	2:B:181:ILE:HG12	1.99	0.45	
2:B:213:GLY:HA2	2:B:226:ASN:HD21	1.82	0.45	
1:A:134:ARG:HH22	1:A:209:ASN:HD21	1.63	0.45	
1:A:191:ARG:NH2	1:A:198:SER:HB3	2.31	0.45	
2:B:233:LEU:HD22	2:B:245:ILE:HG21	1.99	0.45	
2:B:160:TRP:CD2	2:B:243:LYS:HD3	2.52	0.45	
1:A:18:VAL:HB	1:A:189:ARG:HG3	1.98	0.45	
2:B:223:THR:HG21	2:B:250:LEU:HD23	1.99	0.44	
1:A:11:PHE:HB2	1:A:24:PHE:CD1	2.53	0.44	
1:A:251:ILE:HD13	2:B:260:PRO:HG2	2.00	0.44	
1:A:43:PRO:HD2	1:A:253:ALA:O	2.18	0.43	
2:B:228:TYR:N	5:B:675:HOH:O	2.45	0.43	
2:B:199:GLU:HA	2:B:246:ILE:HB	2.00	0.43	
2:B:183:PRO:O	2:B:185:GLN:N	2.51	0.43	
1:A:191:ARG:HH21	1:A:198:SER:HB3	1.83	0.43	
1:A:4:LYS:NZ	1:A:55:GLN:HE22	2.17	0.43	
1:A:211:TRP:CH2	1:A:256:VAL:HB	2.53	0.43	
2:B:96:GLY:O	2:B:130:GLY:HA2	2.19	0.43	
2:B:19:LEU:HB2	2:B:36:LEU:HG	2.01	0.43	
1:A:190:THR:HG23	1:A:196:ARG:HH12	1.84	0.42	
1:A:122:ASN:HD22	1:A:124:ASP:HB2	1.84	0.42	
2:B:100:ASN:ND2	5:B:671:HOH:O	2.52	0.42	



Atom 1		Interatomic	Clash
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)
1:A:4:LYS:O	1:A:5:GLN:HG2	2.19	0.42
2:B:64:LEU:HD23	2:B:90:TRP:NE1	2.34	0.42
2:B:233:LEU:HD22	2:B:245:ILE:CG2	2.49	0.42
1:A:236:ASN:O	1:A:236:ASN:ND2	2.52	0.42
1:A:154:TYR:HD1	1:A:159:THR:HA	1.84	0.41
2:B:213:GLY:CA	2:B:226:ASN:HD21	2.32	0.41
1:A:161:LEU:HB3	1:A:162:PRO:HD3	2.02	0.41
1:A:39:ARG:HG2	1:A:267:PHE:HD2	1.84	0.41
1:A:10:ASN:HB3	1:A:61:GLU:HB3	2.03	0.41
1:A:8:ILE:HA	1:A:59:LEU:O	2.21	0.41
1:A:166:ARG:O	1:A:170:ILE:HG13	2.21	0.41
1:A:1:ILE:CG2	1:A:2:PHE:H	2.27	0.41
2:B:140:PHE:CD2	2:B:142:THR:HG23	2.56	0.41
1:A:238:SER:OG	1:A:239:LYS:HD3	2.20	0.41
1:A:267:PHE:HE2	5:A:310:HOH:O	2.02	0.41
1:A:108:PHE:O	1:A:111:VAL:HG22	2.21	0.41
2:B:195:SER:O	2:B:197:ILE:N	2.53	0.41
1:A:107:LEU:HA	1:A:107:LEU:HD13	1.91	0.41
1:A:68:LEU:HD12	1:A:149:SER:HA	2.02	0.41
1:A:17:THR:HG22	1:A:20:SER:H	1.85	0.41
1:A:119:PHE:HA	1:A:125:ARG:NH1	2.36	0.41
2:B:33:ALA:HB1	2:B:117:THR:HG23	2.03	0.41
2:B:2:ASP:HB3	2:B:5:MET:SD	2.62	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	А	$265/267 \ (99\%)$	231 (87%)	17~(6%)	17~(6%)	1 1
2	В	260/262 (99%)	222 (85%)	20 (8%)	18 (7%)	1 1



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	525/529~(99%)	453 (86%)	37 (7%)	35(7%)	1 1	

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	3	PRO
1	А	14	ALA
1	А	66	ALA
1	А	67	GLU
1	А	222	ASN
1	А	226	PHE
1	А	239	LYS
1	А	240	PHE
1	А	263	PRO
2	В	42	ASN
2	В	166	SER
2	В	184	GLN
2	В	195	SER
2	В	199	GLU
2	В	228	TYR
1	А	105	THR
1	А	134	ARG
1	А	237	GLY
1	А	264	SER
2	В	5	MET
2	В	25	ASP
2	В	196	ASN
2	В	201	VAL
2	В	206	SER
1	А	5	GLN
1	А	112	GLN
1	А	157	GLY
2	В	197	ILE
2	В	237	ALA
1	A	156	THR
2	В	7	PRO
2	В	84	ALA
2	В	85	THR
2	В	38	PRO
2	В	101	PRO



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	Pe	erce	enti	les
1	А	226/226~(100%)	184 (81%)	42 (19%)		1	2	
2	В	227/227~(100%)	$197 \ (87\%)$	30 (13%)		4	7	
All	All	453/453~(100%)	381 (84%)	72 (16%)		2	4	

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	3	PRO
1	А	17	THR
1	А	19	GLN
1	А	34	THR
1	А	46	PRO
1	А	48	ARG
1	А	53	ILE
1	А	62	LEU
1	А	65	HIS
1	А	67	GLU
1	А	70	VAL
1	А	85	ARG
1	А	102	GLU
1	А	104	ILE
1	А	107	LEU
1	А	109	THR
1	А	110	ASP
1	А	113	ASN
1	А	114	ARG
1	А	126	LEU
1	A	133	LEU
1	A	135	GLU
1	А	151	LEU
1	A	160	GLN
1	А	164	LEU
1	А	190	THR
1	A	192	ILE



Mol	Chain	Res	Type
1	A	198	SER
1	A	203	SER
1	A	222	ASN
1	A	226	PHE
1	A	230	ILE
1	А	232	LEU
1	А	235	ARG
1	А	236	ASN
1	А	238	SER
1	А	239	LYS
1	А	240	PHE
1	А	247	ILE
1	А	251	ILE
1	А	263	PRO
1	А	264	SER
2	В	5	MET
2	В	6	ASP
2	В	8	GLU
2	В	12	ARG
2	В	24	ARG
2	В	38	PRO
2	В	47	GLN
2	В	48	LEU
2	В	51	LEU
2	В	64	LEU
2	В	78	TYR
2	В	122	THR
2	В	136	ASN
$2^{$	B	156	SER
2	В	158	GLN
2	В	166	SER
2	В	167	GLU
2	В	184	GLN
2	В	188	ASP
2	В	194	ASP
2	В	196	ASN
2	В	199	GLU
2	В	201	VAL
2	В	205	LEU
2	В	225	LEU
2	В	231	LEU
2	В	236	ARG



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Mol	Chain	Res	Type
2	В	241	SER
2	В	251	HIS
2	В	261	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	19	GLN
1	А	98	GLN
1	А	128	GLN
1	А	132	ASN
1	А	173	GLN
1	А	209	ASN
1	А	233	GLN
1	А	236	ASN
2	В	55	ASN
2	В	186	ASN
2	В	189	ASN
2	В	196	ASN
2	В	220	ASN
2	В	226	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)

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

5.5 Carbohydrates (i)

14 monosaccharides 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	Tuno	Chain	Dog	Tink	Bo	Bond lengths		B	ond ang	gles
	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BGC	С	1	3	12,12,12	1.28	1 (8%)	17,17,17	1.71	3(17%)
3	GAL	С	2	3	11,11,12	1.00	1 (9%)	15,15,17	1.41	2(13%)
3	BGC	D	1	3	12,12,12	1.18	1 (8%)	17,17,17	2.06	3 (17%)
3	GAL	D	2	3	11,11,12	1.12	1 (9%)	$15,\!15,\!17$	2.01	7 (46%)
4	NAG	Е	1	2,4	14,14,15	1.26	1 (7%)	17,19,21	1.79	5 (29%)
4	NAG	Е	2	4	14,14,15	1.76	6 (42%)	17,19,21	3.64	7 (41%)
4	BMA	Е	3	4	11,11,12	1.61	2 (18%)	15,15,17	4.15	<mark>9 (60%)</mark>
4	MAN	Е	4	4	11,11,12	1.42	2 (18%)	15,15,17	1.08	0
4	MAN	Е	5	4	11,11,12	2.20	5(45%)	15,15,17	2.38	8 (53%)
4	NAG	F	1	2,4	14,14,15	0.86	0	17,19,21	1.46	4 (23%)
4	NAG	F	2	4	14,14,15	1.08	1 (7%)	17,19,21	2.83	8 (47%)
4	BMA	F	3	4	11,11,12	1.86	2 (18%)	15,15,17	2.04	7 (46%)
4	MAN	F	4	4	11,11,12	1.25	1 (9%)	15,15,17	3.09	11 (73%)
4	MAN	F	5	4	11,11,12	1.42	0	15,15,17	<mark>3.95</mark>	9 (60%)

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
3	BGC	С	1	3	-	0/2/22/22	0/1/1/1
3	GAL	С	2	3	-	0/2/19/22	0/1/1/1
3	BGC	D	1	3	-	2/2/22/22	0/1/1/1
3	GAL	D	2	3	-	0/2/19/22	0/1/1/1
4	NAG	Е	1	2,4	1/1/5/7	1/6/23/26	0/1/1/1
4	NAG	Е	2	4	-	2/6/23/26	0/1/1/1
4	BMA	Е	3	4	-	2/2/19/22	0/1/1/1
4	MAN	Е	4	4	-	2/2/19/22	0/1/1/1
4	MAN	Е	5	4	-	2/2/19/22	0/1/1/1
4	NAG	F	1	2,4	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	4/6/23/26	0/1/1/1
4	BMA	F	3	4	-	1/2/19/22	0/1/1/1
4	MAN	F	4	4	-	0/2/19/22	1/1/1/1
4	MAN	F	5	4	-	1/2/19/22	1/1/1/1



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Ε	5	MAN	C2-C3	3.94	1.58	1.52
4	Е	4	MAN	C2-C3	-3.93	1.46	1.52
4	F	3	BMA	O5-C5	3.90	1.51	1.43
4	Ε	3	BMA	O2-C2	3.32	1.50	1.43
4	F	3	BMA	C2-C3	3.18	1.57	1.52
4	Ε	2	NAG	C3-C2	3.07	1.59	1.52
4	Е	2	NAG	C1-C2	2.98	1.56	1.52
4	Е	5	MAN	C1-C2	2.90	1.58	1.52
4	Ε	2	NAG	O5-C5	2.72	1.49	1.43
4	Е	5	MAN	C6-C5	2.61	1.60	1.51
4	Е	1	NAG	O5-C1	-2.53	1.39	1.43
3	С	2	GAL	C2-C3	-2.50	1.48	1.52
4	Е	5	MAN	O3-C3	2.45	1.48	1.43
4	F	2	NAG	O5-C1	-2.41	1.39	1.43
3	С	1	BGC	O1-C1	2.35	1.47	1.39
3	D	2	GAL	O4-C4	2.30	1.48	1.43
4	Е	2	NAG	C4-C3	2.20	1.57	1.52
4	Ε	2	NAG	O3-C3	2.19	1.48	1.43
4	Е	3	BMA	O3-C3	2.16	1.48	1.43
4	Е	2	NAG	O4-C4	2.15	1.48	1.43
4	F	4	MAN	C2-C3	2.13	1.55	1.52
3	D	1	BGC	C6-C5	2.10	1.58	1.51
4	Е	5	MAN	O5-C5	2.07	1.47	1.43
4	Е	4	MAN	04-C4	2.02	1.47	1.43

All (24) bond length outliers are listed below:

All (83) bond angle outliers are listed belo	w:
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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	F	5	MAN	O5-C1-C2	-11.35	93.25	110.77
4	Ε	3	BMA	C1-C2-C3	-10.34	96.96	109.67
4	Е	2	NAG	C1-O5-C5	-7.93	101.44	112.19
4	Е	2	NAG	O5-C1-C2	-7.86	98.88	111.29
4	F	2	NAG	C2-N2-C7	-7.01	112.92	122.90
4	Е	3	BMA	O5-C5-C6	6.83	117.91	107.20
3	D	1	BGC	C3-C4-C5	-6.61	98.45	110.24
4	Е	2	NAG	C3-C4-C5	-6.38	98.86	110.24
4	Ε	2	NAG	C4-C3-C2	-6.21	101.92	111.02
4	F	4	MAN	O5-C1-C2	-5.79	101.83	110.77
4	Е	3	BMA	C6-C5-C4	-5.26	100.69	113.00
4	Е	3	BMA	C3-C4-C5	5.01	119.18	110.24
4	F	2	NAG	O5-C1-C2	-4.64	103.97	111.29
4	Е	3	BMA	C1-O5-C5	-4.63	105.92	112.19

PROT

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	F	2	NAG	C1-C2-N2	-4.61	102.61	110.49
3	С	1	BGC	C6-C5-C4	-4.27	103.00	113.00
4	F	5	MAN	C1-O5-C5	4.08	117.72	112.19
4	F	5	MAN	O4-C4-C5	4.04	119.32	109.30
4	F	4	MAN	C1-C2-C3	-3.91	104.87	109.67
4	F	4	MAN	O2-C2-C1	3.88	117.09	109.15
4	F	5	MAN	C3-C4-C5	-3.86	103.35	110.24
4	F	5	MAN	O4-C4-C3	-3.85	101.44	110.35
4	F	1	NAG	O5-C1-C2	3.82	117.33	111.29
4	Е	5	MAN	C1-C2-C3	3.77	114.30	109.67
4	F	3	BMA	O6-C6-C5	3.73	124.10	111.29
4	F	4	MAN	O2-C2-C3	-3.73	102.66	110.14
3	D	2	GAL	O2-C2-C3	-3.69	102.74	110.14
4	F	4	MAN	C2-C3-C4	-3.68	104.53	110.89
4	Е	1	NAG	C8-C7-N2	3.61	122.22	116.10
3	D	1	BGC	O5-C1-C2	3.46	116.47	110.28
4	F	5	MAN	O3-C3-C4	-3.40	102.49	110.35
3	С	1	BGC	O5-C5-C6	3.38	114.85	106.44
4	Е	5	MAN	O3-C3-C2	3.28	116.27	109.99
4	Е	5	MAN	C2-C3-C4	-3.16	105.43	110.89
4	F	2	NAG	O7-C7-N2	-3.14	116.19	121.95
3	С	1	BGC	O5-C5-C4	3.10	115.33	109.69
4	F	3	BMA	O2-C2-C1	-3.08	102.85	109.15
4	F	4	MAN	O5-C5-C6	3.07	112.02	107.20
4	Е	5	MAN	O5-C5-C6	3.03	111.96	107.20
3	С	2	GAL	C1-C2-C3	2.99	113.34	109.67
4	F	5	MAN	O3-C3-C2	2.94	115.63	109.99
4	F	2	NAG	C1-O5-C5	-2.92	108.23	112.19
4	Е	5	MAN	O4-C4-C3	-2.91	103.61	110.35
4	Е	1	NAG	O5-C1-C2	2.90	115.87	111.29
3	С	2	GAL	O5-C1-C2	-2.89	106.31	110.77
4	F	4	MAN	C6-C5-C4	-2.85	106.32	113.00
4	Е	5	MAN	O5-C1-C2	2.83	115.14	110.77
4	Е	5	MAN	C6-C5-C4	-2.78	106.49	113.00
4	F	2	NAG	O7-C7-C8	2.78	127.22	122.06
4	F	3	BMA	C1-O5-C5	-2.75	108.47	112.19
4	F	4	MAN	O3-C3-C4	-2.73	104.03	110.35
3	D	2	GAL	C1-C2-C3	2.71	113.00	109.67
4	Е	1	NAG	C1-C2-N2	-2.69	105.89	110.49
4	F	3	BMA	O5-C5-C6	2.68	111.41	107.20
4	E	3	BMA	O5-C1-C2	-2.66	106.66	110.77
4	F	4	MAN	O3-C3-C2	2.65	115.07	109.99

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Mol	Chain	Res	Type	Atoms Z		$Observed(^{o})$	$Ideal(^{o})$
4	F	3	BMA	C6-C5-C4	-2.59	106.94	113.00
4	F	4	MAN	C3-C4-C5	-2.59	105.62	110.24
4	Е	2	NAG	O6-C6-C5	-2.59	102.42	111.29
3	D	2	GAL	O2-C2-C1	2.58	114.43	109.15
4	F	2	NAG	O5-C5-C4	-2.57	104.58	110.83
4	Е	3	BMA	O5-C5-C4	2.53	116.99	110.83
3	D	2	GAL	O5-C5-C6	2.50	111.12	107.20
4	F	1	NAG	C1-O5-C5	2.50	115.58	112.19
4	Е	3	BMA	O2-C2-C1	2.50	114.26	109.15
3	D	1	BGC	O4-C4-C5	2.42	115.30	109.30
4	F	3	BMA	C3-C4-C5	2.37	114.46	110.24
3	D	2	GAL	C1-O5-C5	2.36	115.39	112.19
3	D	2	GAL	C6-C5-C4	-2.36	107.48	113.00
4	Е	1	NAG	C4-C3-C2	-2.33	107.60	111.02
4	Е	2	NAG	C1-C2-N2	2.33	114.46	110.49
4	F	5	MAN	O2-C2-C1	-2.31	104.42	109.15
4	F	1	NAG	C3-C4-C5	-2.31	106.12	110.24
3	D	2	GAL	O3-C3-C4	-2.27	105.10	110.35
4	F	4	MAN	O6-C6-C5	-2.22	103.68	111.29
4	F	5	MAN	C2-C3-C4	-2.20	107.09	110.89
4	Е	2	NAG	O4-C4-C5	2.19	114.73	109.30
4	Е	3	BMA	O4-C4-C5	-2.17	103.92	109.30
4	F	3	BMA	O2-C2-C3	2.14	114.42	110.14
4	Е	5	MAN	O3-C3-C4	-2.12	105.44	110.35
4	F	1	NAG	C1-C2-N2	-2.11	106.88	110.49
4	F	2	NAG	C4-C3-C2	-2.01	108.07	111.02
4	E	1	NAG	O4-C4-C5	2.00	114.27	109.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	Е	1	NAG	C1
4	F	1	NAG	C1

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	2	NAG	C8-C7-N2-C2
4	F	2	NAG	O7-C7-N2-C2
4	Е	3	BMA	O5-C5-C6-O6
4	Е	4	MAN	C4-C5-C6-O6
4	Е	3	BMA	C4-C5-C6-O6



Mol	Chain	\mathbf{Res}	Type	Atoms
4	Е	5	MAN	O5-C5-C6-O6
4	Е	4	MAN	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
3	D	1	BGC	C4-C5-C6-O6
4	Е	5	MAN	C4-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
4	Е	2	NAG	C1-C2-N2-C7
3	D	1	BGC	O5-C5-C6-O6
4	Е	1	NAG	O5-C5-C6-O6
4	F	3	BMA	O5-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
4	F	5	MAN	O5-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6

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All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	5	MAN	C1-C2-C3-C4-C5-O5
4	F	4	MAN	C1-C2-C3-C4-C5-O5

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Ε	2	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.













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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

