

# Full wwPDB X-ray Structure Validation Report (i)

#### Mar 23, 2024 – 09:32 PM EDT

PDB ID	:	10VW
Title	:	ENDOGLUCANASE I COMPLEXED WITH NON-HYDROLYSABLE SUB-
		STRATE ANALOGUE
Authors	:	Sulzenbacher, G.; Davies, G.J.; Schulein, M.
Deposited on	:	1996-10-17
Resolution	:	2.70 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 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)	:	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)	:	2.36.1

## 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 2.70 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain		
1	А	398	69%	25%	5%•
1	В	398	65%	27%	8% •
1	С	398	70%	23%	6% •
1	D	398	70%	25%	5%•
2	Е	3	100%		
2	F	3	100%		
2	G	3	33% 67%		
2	Н	3	33% 67%		



#### 10VW

## 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13412 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Δ	208	Total	С	Ν	0	$\mathbf{S}$	0	0	0
	A	398	3023	1870	534	590	29	0	0	U
1	В	308	Total	С	Ν	0	S	0	0	0
	I D	390	3023	1870	534	590	29	0	0	U
1	C	C 398	Total	С	Ν	0	S	0	0	0
			3023	1870	534	590	29			
1 D	208	Total	С	Ν	0	S	0	0	0	
		398	3023	1870	534	590	29	0		U

• Molecule 1 is a protein called ENDOGLUCANASE I.

• Molecule 2 is an oligosaccharide called 4-thio-beta-D-glucopyranose-(1-4)-4-thio-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace		
2	E	3	Total	С	Ο	$\mathbf{S}$	0	0	Ο
2	Ľ	5	34	18	12	4	0	0	0
2	F	2	Total	С	Ο	$\mathbf{S}$	0	0	0
	Ľ	5	34	18	12	4	0	0	0
0	С	2	Total	С	Ο	S	0	0	0
	G	ა	34	18	12	4	0		
0	ц	2	Total	С	Ο	S	0	0	0
	11	ა	34	18	12	4	0	0	0

• Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total         C         N         O           14         8         1         5	0	0
3	А	1	Total         C         N         O           14         8         1         5	0	0
3	В	1	Total         C         N         O           14         8         1         5	0	0
3	В	1	Total C N O 14 8 1 5	0	0
3	С	1	Total C N O 14 8 1 5	0	0
3	С	1	Total         C         N         O           14         8         1         5	0	0
3	D	1	Total         C         N         O           14         8         1         5	0	0
3	D	1	Total         C         N         O           14         8         1         5	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	275	Total O 275 275	0	0
4	В	267	Total O 267 267	0	0
4	С	248	Total O 248 248	0	0
4	D	282	Total         O           282         282	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.

Note EDS was not executed.



• Molecule 1: ENDOGLUCANASE I



• Molecule 1: ENDOGLUCANASE I

Chain D:		70%	25%	5%•
Q1 P3 D4 B8 B8 C9 C9	R17 C18 T19 R20 R20 R21 C23 C23 C23 C23 C23 C23 C23 C23 C23 C23	453 K64 P55 P55 P61 P61 D62 S85 S85 S85 S85 S85 S85 S85 S87 S77 S77 S77	K81 186 K91 L92 R93 R93 R96	Q101 L102 V103 S104 P105 R105 V107 V107
K114 K116 K116 L120 E126 E126	L136 L136 L136 C138 G139 G139 A141 C136 A144 C144 C144 C144 C144 C144 C144 C144	E148 E148 Q151 Q152 Q153 C154 C155 S156 S156 S156 S156 S156 S156 S156 S	CL/0 1182 1182 1188 1189 1189 C193 C194 C195	E197 L198 D199 M201 E202 A203 R203
A207 1208 1210 1210 2212 1213 1213 1213	C233 R245 R245 R266 R266 R266	1267 1267 1271 1272 1277 1278 1278 1288 1288 128	N1291 N1291 1294 1294 P304 F322 F322 R325	V346 W347 W347 W348 S349 E350 E350 D358
E369 G370 D371 D371 R373 K373 N374 I375 V376 V376	v378 q379 5384 v384 r390 f394 1394 s398 r394 s398			

• Molecule 2: 4-thio-beta-D-glucopyranose-(1-4)-4-thio-beta-D-glucopyranose-(1-4)-1,4-dithio-bet a-D-glucopyranose

Chai	ain E: 100%	
SSG1 SGC2 SGC3		
• Mo a-D-	Molecule 2: 4-thio-beta-D-glucopyranose-(1-4)-4-thio-beta-D-glucopyranose-(1-2)-glucopyranose	-4)-1,4-dithio-bet

Chain F:

100%



• Molecule 2: 4-thio-beta-D-glucopyranose-(1-4)-4-thio-beta-D-glucopyranose-(1-4)-1,4-dithio-bet a-D-glucopyranose

67%

$\alpha$ · $\alpha$		
Chain G:	33%	



#### SSG1 SGC2 SGC3

• Molecule 2: 4-thio-beta-D-glucopyranose-(1-4)-4-thio-beta-D-glucopyranose-(1-4)-1,4-dithio-beta-D-glucopyranose

Chain H: 33% 67%

SSG1 SGC2 SGC3



## 4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	68.16Å 78.28Å 142.46Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $96.89^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	15.00 - 2.70	Depositor
% Data completeness	89.5 (15.00-2.70)	Depositor
(in resolution range)	00.0 (10.00 2.10)	Depositor
$R_{merge}$	0.12	Depositor
R <sub>sym</sub>	(Not available)	Depositor
Refinement program	REFMAC	Depositor
$R, R_{free}$	0.197 , $0.284$	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13412	wwPDB-VP
Average B, all atoms $(Å^2)$	23.0	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: SGC, NAG, PCA, SSG

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	Bond lengths		Bond angles		
IVIOI	Unain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.64	0/3077	1.54	31/4155~(0.7%)	
1	В	0.67	0/3077	1.62	45/4155~(1.1%)	
1	С	0.66	0/3077	1.61	49/4155~(1.2%)	
1	D	0.67	0/3077	1.57	38/4155~(0.9%)	
All	All	0.66	0/12308	1.58	163/16620~(1.0%)	

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	1
1	В	0	1
All	All	0	2

There are no bond length outliers.

All (163) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	390	ARG	NE-CZ-NH1	21.63	131.11	120.30
1	D	390	ARG	NE-CZ-NH1	18.99	129.80	120.30
1	С	325	ARG	NE-CZ-NH1	17.52	129.06	120.30
1	С	390	ARG	NE-CZ-NH1	16.93	128.77	120.30
1	А	325	ARG	CD-NE-CZ	14.97	144.56	123.60
1	С	93	ARG	NE-CZ-NH2	-14.90	112.85	120.30
1	А	390	ARG	NE-CZ-NH1	14.01	127.30	120.30
1	А	226	ASP	CB-CG-OD2	-13.14	106.48	118.30
1	В	93	ARG	NE-CZ-NH2	-12.16	114.22	120.30
1	B	264	ARG	NE-CZ-NH2	-11.79	114.40	120.30



1	$\cap$	17	117	
Т	U	v	vv	

Mol	Chain	Res	Type	Atoms	Z	Observed( <sup>o</sup> )	Ideal(°)
1	С	325	ARG	NE-CZ-NH2	-11.02	114.79	120.30
1	В	325	ARG	NE-CZ-NH1	10.79	125.70	120.30
1	А	338	ARG	NE-CZ-NH2	-10.79	114.91	120.30
1	С	152	ASP	CB-CG-OD1	10.29	127.56	118.30
1	С	352	ASP	CB-CG-OD1	10.24	127.51	118.30
1	А	334	ASP	CB-CG-OD2	-9.82	109.46	118.30
1	В	325	ARG	NE-CZ-NH2	-9.82	115.39	120.30
1	В	106	ARG	NE-CZ-NH2	9.78	125.19	120.30
1	В	358	ASP	CB-CG-OD2	9.50	126.85	118.30
1	А	325	ARG	NE-CZ-NH2	-9.11	115.75	120.30
1	D	325	ARG	NE-CZ-NH2	-8.89	115.86	120.30
1	С	62	ASP	CB-CG-OD2	-8.83	110.35	118.30
1	В	325	ARG	CD-NE-CZ	8.83	135.96	123.60
1	В	17	ARG	NE-CZ-NH2	-8.80	115.90	120.30
1	D	285	ARG	NE-CZ-NH1	8.76	124.68	120.30
1	D	325	ARG	CD-NE-CZ	8.66	135.73	123.60
1	D	325	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	D	264	ARG	NE-CZ-NH2	-8.61	115.99	120.30
1	С	250	ASP	CB-CG-OD1	8.59 126.03		118.30
1	А	325	ARG	NE-CZ-NH1	8.39	124.50	120.30
1	D	285	ARG	NE-CZ-NH2	-8.30	116.15	120.30
1	D	390	ARG	NH1-CZ-NH2	-8.26	110.31	119.40
1	А	390	ARG	CD-NE-CZ	8.24	135.14	123.60
1	С	159	ARG	NE-CZ-NH2	-8.23	116.19	120.30
1	С	17	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	D	93	ARG	NE-CZ-NH2	-7.83	116.38	120.30
1	А	250	ASP	CB-CG-OD1	7.68	125.21	118.30
1	С	390	ARG	CA-CB-CG	7.59	130.09	113.40
1	В	390	ARG	NH1-CZ-NH2	-7.55	111.10	119.40
1	С	390	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	D	152	ASP	CB-CG-OD1	7.44	125.00	118.30
1	В	346	VAL	CB-CA-C	-7.42	97.30	111.40
1	А	390	ARG	NH1-CZ-NH2	-7.39	111.27	119.40
1	D	261	ASP	CB-CG-OD1	7.33	124.90	118.30
1	В	117	TYR	CB-CG-CD2	7.25	125.35	121.00
1	D	358	ASP	$CB-CG-\overline{OD1}$	7.23	124.81	118.30
1	D	261	ASP	CB-CG-OD2	-7.23	111.80	118.30
1	С	325	ARG	CD-NE-CZ	7.20	133.68	123.60
1	D	34	ASP	$CB-CG-\overline{OD2}$	7.09	124.68	118.30
1	D	203	ALA	N-CA-CB	-7.05	100.23	110.10
1	D	390	ARG	CD-NE-CZ	6.94	133.32	123.60
1	A	312	ASP	CB-CG-OD1	6.90	124.51	118.30



1	$\cap$	17	111	
Т	U	v	vv	

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	390	ARG	CA-CB-CG	6.79	128.33	113.40
1	C	17	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	A	203	ALA	CB-CA-C	-6.66	100.11	110.10
1	С	371	ASP	CB-CG-OD1	6.66	124.29	118.30
1	D	346	VAL	CB-CA-C	-6.64	98.78	111.40
1	В	254	ARG	NE-CZ-NH2	6.61	123.61	120.30
1	С	245	ARG	NE-CZ-NH2	6.53	123.56	120.30
1	В	245	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	В	159	ARG	NE-CZ-NH2	-6.49	117.05	120.30
1	С	106	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	С	173	ASP	CB-CG-OD2	-6.44	112.50	118.30
1	D	76	ASP	CB-CG-OD1	6.42	124.08	118.30
1	D	62	ASP	CB-CG-OD1	6.41	124.07	118.30
1	С	338	ARG	NE-CZ-NH1	-6.40	117.10	120.30
1	В	254	ARG	NE-CZ-NH1	-6.33	117.13	120.30
1	D	104	SER	N-CA-CB	-6.33	101.00	110.50
1	С	226	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	D	159	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	В	171	TYR	CB-CG-CD2	-6.31 117.22		121.00
1	В	390	ARG	CA-CB-CG	6.29	127.25	113.40
1	В	56	ASN	CB-CG-OD1	-6.28	109.04	121.60
1	В	261	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	D	254	ARG	NE-CZ-NH2	6.17	123.39	120.30
1	В	203	ALA	N-CA-CB	-6.15	101.49	110.10
1	D	390	ARG	CA-CB-CG	6.14	126.92	113.40
1	С	203	ALA	N-CA-CB	-6.09	101.57	110.10
1	С	338	ARG	CD-NE-CZ	6.05	132.08	123.60
1	D	245	ARG	NE-CZ-NH1	-5.95	117.32	120.30
1	А	264	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	А	346	VAL	N-CA-CB	5.91	124.50	111.50
1	В	346	VAL	N-CA-CB	5.89	124.47	111.50
1	В	390	ARG	CD-NE-CZ	5.88	131.83	123.60
1	A	62	ASP	CB-CG-OD1	5.87	123.58	118.30
1	В	71	ILE	CB-CA-C	-5.85	99.91	111.60
1	A	221	TYR	CB-CG-CD1	5.84	124.51	121.00
1	С	132	GLU	OE1-CD-OE2	-5.84	116.29	123.30
1	D	106	ARG	CD-NE-CZ	5.83	131.76	123.60
1	A	346	VAL	CB-CA-C	-5.83	100.33	111.40
1	D	254	ARG	NE-CZ-NH1	-5.81	117.39	120.30
1	С	346	VAL	CA-CB-CG2	5.80	119.60	110.90
1	В	152	ASP	CB-CG-OD1	5.80	123.52	118.30
1	В	62	ASP	CB-CG-OD1	5.78	123.50	118.30



$1 \cap$	17	TX7
IU	v	vv

Continued from previous page								
Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$	
1	С	334	ASP	CB-CG-OD2	-5.75	113.12	118.30	
1	А	30	TYR	CB-CG-CD1	-5.75	117.55	121.00	
1	В	80	TYR	CB-CG-CD1	-5.71	117.58	121.00	
1	D	182	ILE	CB-CA-C	-5.69	100.21	111.60	
1	С	346	VAL	CB-CA-C	-5.69	100.59	111.40	
1	С	306	LYS	CA-CB-CG	5.68	125.89	113.40	
1	С	152	ASP	OD1-CG-OD2	-5.63	112.60	123.30	
1	D	17	ARG	NE-CZ-NH2	-5.61	117.50	120.30	
1	С	208	THR	N-CA-CB	5.60	120.94	110.30	
1	А	254	ARG	NE-CZ-NH1	-5.59	117.50	120.30	
1	С	56	ASN	CB-CG-OD1	-5.58	110.44	121.60	
1	D	369	GLU	OE1-CD-OE2	-5.56	116.62	123.30	
1	А	154	GLY	CA-C-O	-5.52	110.66	120.60	
1	D	202	GLU	N-CA-CB	5.51	120.52	110.60	
1	D	141	ASN	CA-CB-CG	5.49	125.47	113.40	
1	С	206	ARG	NE-CZ-NH1	5.48	123.04	120.30	
1	В	285	ARG	NE-CZ-NH2	-5.47	117.56	120.30	
1	В	10	HIS	CA-CB-CG	5.47	122.89	113.60	
1	В	312	ASP	CB-CG-OD1	B-CG-OD1 5.47 123.22		118.30	
1	С	93	ARG	NH1-CZ-NH2	5.46	125.41	119.40	
1	С	171	TYR	CB-CG-CD2	-5.46	117.73	121.00	
1	С	245	ARG	NE-CZ-NH1	-5.45	117.58	120.30	
1	В	76	ASP	CB-CG-OD1	5.43	123.19	118.30	
1	В	104	SER	N-CA-CB	-5.42	102.37	110.50	
1	С	137	PRO	N-CA-CB	5.41	109.79	103.30	
1	С	142	GLY	N-CA-C	-5.40	99.60	113.10	
1	В	215	CYS	CA-CB-SG	5.40	123.71	114.00	
1	С	334	ASP	CB-CG-OD1	5.40	123.16	118.30	
1	С	62	ASP	CB-CG-OD1	5.39	123.15	118.30	
1	D	8	GLU	OE1-CD-OE2	-5.38	116.85	123.30	
1	В	182	ILE	CB-CA-C	-5.38	100.85	111.60	
1	С	3	PRO	N-CA-CB	5.37	109.74	103.30	
1	В	306	LYS	CA-CB-CG	5.37	125.20	113.40	
1	A	106	ARG	NE-CZ-NH2	5.36	122.98	120.30	
1	С	199	ASP	CB-CG-OD2	-5.36	113.48	118.30	
1	D	279	ASP	CB-CG-OD1	-5.35	113.48	118.30	
1	В	245	ARG	NH1-CZ-NH2	5.34	125.28	119.40	
1	С	346	VAL	N-CA-CB	5.32	123.19	111.50	
1	A	34	ASP	CB-CG-OD1	-5.30	113.53	118.30	
1	В	36	GLY	O-C-N	-5.29	114.24	122.70	
1	А	203	ALA	N-CA-CB	-5.28	102.71	110.10	
1	A	137	PRO	N-CA-CB	N-CA-CB 5.28		103.30	



Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	140	MET	CA-CB-CG	5.27	122.26	113.30
1	В	245	ARG	NE-CZ-NH1	NE-CZ-NH1 -5.26		120.30
1	D	17	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	С	14	GLU	CG-CD-OE2	5.25	128.80	118.30
1	С	182	ILE	CB-CA-C	-5.24	101.13	111.60
1	В	250	ASP	CB-CG-OD1	5.23	123.00	118.30
1	В	50	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	С	208	THR	CA-CB-CG2	-5.20	105.12	112.40
1	А	285	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	С	138	CYS	CA-CB-SG	5.19	123.35	114.00
1	В	276	LYS	CA-CB-CG	5.19	124.81	113.40
1	D	93	ARG	NH1-CZ-NH2	5.18	125.10	119.40
1	D	142	GLY	N-CA-C	-5.17	100.16	113.10
1	С	203	ALA	CB-CA-C	-5.16	102.36	110.10
1	А	30	TYR	CA-CB-CG	-5.16	103.61	113.40
1	D	3	PRO	N-CA-CB	5.15	109.48	103.30
1	А	208	THR	CA-CB-CG2	-5.12	105.24	112.40
1	В	166	TYR	CB-CG-CD2	-5.08	117.95	121.00
1	В	338	ARG	CD-NE-CZ	5.08	130.71	123.60
1	D	148	GLU	CG-CD-OE1	5.07	128.44	118.30
1	С	348	TRP	CA-CB-CG	5.06	123.32	113.70
1	А	171	TYR	CB-CG-CD2	-5.05	117.97	121.00
1	С	104	SER	N-CA-CB	-5.04	102.94	110.50
1	С	212	PRO	N-CA-CB	5.04	109.34	103.30
1	В	390	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	В	27	GLN	CB-CA-C	-5.03	100.35	110.40
1	А	305	PRO	N-CA-CB	5.01	109.31	103.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	15	THR	Mainchain
1	В	15	THR	Mainchain

#### 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	3023	0	2905	79	0
1	В	3023	0	2905	82	0
1	С	3023	0	2905	65	0
1	D	3023	0	2905	65	0
2	Е	34	0	30	6	0
2	F	34	0	30	6	0
2	G	34	0	30	4	0
2	Н	34	0	29	6	0
3	А	28	0	26	0	0
3	В	28	0	26	0	0
3	С	28	0	26	0	0
3	D	28	0	26	0	0
4	А	275	0	0	13	0
4	В	267	0	0	13	0
4	С	248	0	0	12	0
4	D	282	0	0	9	0
All	All	13412	0	11843	302	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 12.

All (302) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	$distance ( { m \AA} )$	overlap (Å)
1:D:182:ILE:HG21	4:D:940:HOH:O	1.64	0.95
1:A:203:ALA:HB2	1:A:208:THR:HG23	1.50	0.93
1:D:78:ASN:HB3	4:D:858:HOH:O	1.67	0.93
1:B:203:ALA:HB2	1:B:208:THR:HG23	1.52	0.88
1:D:203:ALA:HB2	1:D:208:THR:HG23	1.55	0.88
1:B:41:ARG:HD3	4:B:584:HOH:O	1.75	0.86
1:C:203:ALA:HB2	1:C:208:THR:HG23	1.56	0.86
1:A:226:ASP:HB2	4:A:632:HOH:O	1.78	0.84
2:H:1:SSG:S4	2:H:2:SGC:H4	2.22	0.79
2:G:1:SSG:S4	2:G:2:SGC:H4	2.22	0.79
1:B:374:ASN:HA	1:B:377:LYS:HD2	1.62	0.79
1:A:19:THR:HA	1:A:393:GLU:HG3	1.64	0.78
2:E:1:SSG:S4	2:E:2:SGC:H4	2.24	0.78
1:A:374:ASN:HA	1:A:377:LYS:HD2	1.65	0.78
1:B:303:GLY:HA3	4:B:627:HOH:O	1.84	0.77
1:A:54:LYS:HB2	1:A:55:PRO:HD2	1.67	0.77
2:F:1:SSG:S4	2:F:2:SGC:H4	2.25	0.76
1:A:182:ILE:HD11	1:A:187:ASN:HA	1.68	0.76



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:54:LYS:HB2	1:B:55:PRO:HD2	1.68	0.75
1:D:374:ASN:HA	1:D:377:LYS:HD2	1.69	0.75
1:C:374:ASN:HA	1:C:377:LYS:HD2	1.69	0.73
1:A:259:LYS:NZ	4:A:653:HOH:O	2.18	0.72
1:C:5:LYS:HD3	1:C:5:LYS:H	1.54	0.71
1:D:182:ILE:HD11	1:D:187:ASN:HA	1.72	0.70
1:D:54:LYS:HB2	1:D:55:PRO:HD2	1.73	0.70
1:D:19:THR:HA	1:D:393:GLU:HG3	1.74	0.70
1:C:14:GLU:HG2	4:C:566:HOH:O	1.90	0.70
1:D:201:TRP:CZ3	1:D:208:THR:HG21	2.27	0.69
1:C:182:ILE:HG23	1:C:193:VAL:HG22	1.75	0.69
1:A:5:LYS:HD3	1:A:5:LYS:H	1.58	0.68
1:B:201:TRP:CZ3	1:B:208:THR:HG21	2.29	0.68
1:B:113:ASN:O	1:B:114:LYS:HB2	1.92	0.68
1:D:5:LYS:H	1:D:5:LYS:HD3	1.59	0.67
1:D:116:LYS:HB3	1:D:151:GLN:HG2	1.77	0.67
1:B:19:THR:HA	1:B:393:GLU:HG3	1.74	0.67
1:B:5:LYS:H	1:B:5:LYS:HD3	1.59	0.67
1:D:261:ASP:OD2	1:D:264:ARG:HD3	1.94	0.66
1:B:276:LYS:HB2	4:B:657:HOH:O	1.96	0.66
1:A:116:LYS:HB3	1:A:151:GLN:HG2	1.77	0.66
1:C:182:ILE:HD11	1:C:187:ASN:HA	1.78	0.66
1:C:19:THR:HA	1:C:393:GLU:HG3	1.80	0.64
2:H:1:SSG:S4	2:H:2:SGC:C4	2.86	0.64
1:C:116:LYS:HB3	1:C:151:GLN:HG2	1.80	0.63
2:E:1:SSG:S4	2:E:2:SGC:C4	2.86	0.63
2:G:1:SSG:S4	2:G:2:SGC:C4	2.86	0.63
1:B:116:LYS:HB3	1:B:151:GLN:HG2	1.79	0.63
1:B:261:ASP:OD2	1:B:264:ARG:HD3	1.99	0.62
1:C:201:TRP:CZ3	1:C:208:THR:HG21	2.34	0.62
1:C:113:ASN:O	1:C:114:LYS:HB2	1.99	0.62
1:C:120:LEU:HD12	1:C:146:LEU:HD21	1.81	0.62
1:C:54:LYS:HB2	1:C:55:PRO:HD2	1.82	0.62
1:C:299:VAL:HG11	1:C:304:PRO:HB2	1.80	0.62
1:B:182:ILE:HD11	1:B:187:ASN:HA	1.83	0.61
1:B:182:ILE:HG23	1:B:193:VAL:HG22	1.83	0.61
1:B:96:GLN:HA	1:B:96:GLN:HE21	1.65	0.61
1:C:195:CYS:HA	4:C:576:HOH:O	2.01	0.61
1:B:151:GLN:HB3	4:B:647:HOH:O	2.00	0.60
1:A:261:ASP:OD2	1:A:264:ARG:HD3	2.00	0.60
2:F:1:SSG:S4	2:F:2:SGC:C4	2.88	0.60



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:D:182:ILE:HG13	1:D:187:ASN:HB2	1.83	0.60	
1:A:290:ASP:O	1:A:291:ASN:HB2	2.00	0.60	
1:A:194:CYS:O	1:A:195:CYS:HB3	2.02	0.59	
1:C:182:ILE:HG13	1:C:187:ASN:HB2	1.83	0.59	
1:B:54:LYS:HB2	1:B:55:PRO:CD	2.32	0.59	
1:A:54:LYS:HB2	1:A:55:PRO:CD	2.32	0.59	
1:A:201:TRP:CZ3	1:A:208:THR:HG21	2.37	0.59	
1:C:231:SER:HB3	4:C:487:HOH:O	2.02	0.58	
1:C:96:GLN:HA	1:C:96:GLN:HE21	1.69	0.58	
1:D:5:LYS:H	1:D:5:LYS:CD	2.15	0.57	
1:C:5:LYS:H	1:C:5:LYS:CD	2.15	0.57	
1:B:376:VAL:HA	1:B:379:GLN:O	2.05	0.57	
1:B:137:PRO:HB2	4:B:524:HOH:O	2.04	0.57	
1:A:5:LYS:H	1:A:5:LYS:CD	2.14	0.57	
1:D:96:GLN:HA	1:D:96:GLN:HE21	1.70	0.57	
1:C:208:THR:HG22	1:C:209:HIS:H	1.69	0.56	
1:A:182:ILE:HG13	1:A:187:ASN:HB2	1.87	0.56	
1:C:14:GLU:OE1	1:C:26:LYS:HD2	2.06	0.56	
1:C:290:ASP:O	1:C:291:ASN:HB2	2.05	0.56	
1:D:376:VAL:HA	1:D:379:GLN:O	2.05	0.56	
1:A:151:GLN:HB3	4:A:611:HOH:O	2.06	0.55	
1:D:120:LEU:HD12	1:D:146:LEU:HD21	1.87	0.55	
1:C:271:GLN:HB2	1:C:284:HIS:HB2	1.89	0.55	
1:A:113:ASN:O	1:A:114:LYS:HB2	2.06	0.55	
1:D:54:LYS:HB2	1:D:55:PRO:CD	2.36	0.55	
1:D:113:ASN:O	1:D:114:LYS:HB2	2.06	0.55	
1:B:213:HIS:HE1	2:F:1:SSG:H2	1.70	0.55	
1:D:182:ILE:HG23	1:D:193:VAL:HG22	1.88	0.54	
1:B:299:VAL:HG11	1:B:304:PRO:HB2	1.89	0.54	
1:C:20:LYS:N	1:C:393:GLU:OE2	2.35	0.54	
1:D:194:CYS:O	1:D:195:CYS:HB3	2.07	0.54	
1:D:256:LYS:HD3	4:D:796:HOH:O	2.06	0.54	
1:B:290:ASP:O	1:B:291:ASN:HB2	2.06	0.54	
1:A:212:PRO:HD2	1:A:239:CYS:O	2.08	0.54	
1:A:137:PRO:HG3	1:A:379:GLN:HB3	1.90	0.53	
1:B:288:ILE:CD1	1:B:398:SER:HB2	2.39	0.53	
1:B:371:ASP:OD1	1:B:373:LYS:HB3	2.08	0.53	
1:D:9:GLN:OE1	1:D:76:ASP:HB2	2.09	0.53	
1:A:299:VAL:HG11	1:A:304:PRO:HB2	1.89	0.53	
1:A:208:THR:HG22	1:A:209:HIS:H	1.73	0.53	
1:B:179:THR:HB	4:B:592:HOH:O	2.09	0.53	



	ti a	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:C:159:ARG:NH2	4:C:616:HOH:O	2.35	0.53	
1:D:208:THR:HG22	1:D:209:HIS:H	1.74	0.53	
1:A:271:GLN:HB2	1:A:284:HIS:HB2	1.90	0.53	
1:B:120:LEU:HD12	1:B:146:LEU:HD21	1.91	0.53	
1:A:96:GLN:HE21	1:A:96:GLN:HA	1.73	0.52	
1:C:388:ASN:OD1	1:C:390:ARG:NH1	2.39	0.52	
1:A:388:ASN:OD1	1:A:390:ARG:NH1	2.32	0.52	
1:B:388:ASN:OD1	1:B:390:ARG:NH1	2.41	0.52	
1:D:137:PRO:HG2	1:D:375:ILE:HG23	1.92	0.52	
1:B:159:ARG:HB3	4:B:621:HOH:O	2.09	0.52	
1:D:212:PRO:HD2	1:D:239:CYS:O	2.10	0.52	
1:C:115:LYS:HE3	4:C:613:HOH:O	2.09	0.52	
1:A:14:GLU:OE1	1:A:26:LYS:HD2	2.10	0.52	
1:D:137:PRO:HB2	4:D:600:HOH:O	2.10	0.52	
1:D:299:VAL:HG11	1:D:304:PRO:HB2	1.92	0.52	
1:A:14:GLU:HG2	4:A:569:HOH:O	2.10	0.51	
1:B:194:CYS:O	1:B:195:CYS:HB3	2.10	0.51	
1:C:194:CYS:O	1:C:195:CYS:HB3	2.10	0.51	
1:C:193:VAL:HG13	1:C:220:LEU:HD21	1.93	0.51	
1:A:182:ILE:HG23	1:A:193:VAL:HG22	1.93	0.51	
1:C:53:GLN:NE2	1:C:54:LYS:O	2.44	0.51	
1:A:136:LEU:HD11	1:A:384:VAL:HB	1.92	0.50	
1:B:208:THR:HG22	1:B:209:HIS:H	1.74	0.50	
1:C:35:ALA:O	1:C:38:HIS:HB2	2.11	0.50	
1:D:371:ASP:OD1	1:D:373:LYS:HB3	2.11	0.50	
1:A:53:GLN:NE2	1:A:54:LYS:O	2.44	0.50	
1:A:371:ASP:O	1:A:375:ILE:HG13	2.11	0.50	
1:B:5:LYS:H	1:B:5:LYS:CD	2.19	0.50	
1:B:115:LYS:HD2	4:B:614:HOH:O	2.12	0.50	
1:A:9:GLN:OE1	1:A:76:ASP:HB2	2.11	0.50	
1:A:41:ARG:HD3	4:A:585:HOH:O	2.11	0.50	
1:D:290:ASP:O	1:D:291:ASN:HB2	2.11	0.50	
1:C:212:PRO:HD2	1:C:239:CYS:O	2.12	0.49	
1:C:223:CYS:HB2	1:C:227:GLU:HB2	1.95	0.49	
1:D:213:HIS:HE1	2:H:1:SSG:H2	1.76	0.49	
1:B:259:LYS:HE3	4:B:634:HOH:O	2.11	0.49	
1:B:35:ALA:O	1:B:38:HIS:HB2	2.13	0.49	
1:A:16:TYR:CE2	1:A:26:LYS:HG3	2.48	0.49	
1:A:380:PRO:HG2	4:A:672:HOH:O	2.12	0.49	
1:C:137:PRO:HB2	4:C:524:HOH:O	2.12	0.49	
1:A:202:GLU:OE2	2:E:1:SSG:S4	2.71	0.49	



	lo us pagem	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:32:VAL:HB	1:B:110:LEU:HD11	1.94	0.48	
1:B:195:CYS:HA	4:B:572:HOH:O	2.12	0.48	
1:A:292:LYS:O	1:A:294:ILE:HD12	2.14	0.48	
1:B:182:ILE:HG13	1:B:187:ASN:HB2	1.95	0.48	
1:C:144:LEU:C	1:C:144:LEU:HD23	2.34	0.48	
1:D:91:LYS:HE2	4:D:587:HOH:O	2.14	0.48	
1:D:254:ARG:HG3	4:D:500:HOH:O	2.14	0.48	
1:C:376:VAL:HA	1:C:379:GLN:O	2.14	0.48	
1:A:159:ARG:NH2	4:A:637:HOH:O	2.47	0.48	
1:A:203:ALA:CB	1:A:208:THR:HG23	2.35	0.48	
1:B:137:PRO:HG3	1:B:379:GLN:HB3	1.96	0.48	
1:C:257:GLN:HB3	4:C:610:HOH:O	2.13	0.48	
1:B:14:GLU:OE2	1:B:26:LYS:HB2	2.14	0.47	
1:D:54:LYS:HG2	4:D:860:HOH:O	2.14	0.47	
1:D:100:ASN:ND2	4:D:805:HOH:O	2.47	0.47	
1:A:199:ASP:OD2	2:E:1:SSG:O3	2.33	0.47	
1:A:31:ILE:HG23	1:A:107:VAL:HB	1.97	0.47	
1:B:213:HIS:CE1	2:F:1:SSG:H2	2.49	0.47	
1:D:210:ILE:HD11	1:D:285:ARG:NH1	2.30	0.47	
1:B:16:TYR:HB2	1:B:390:ARG:HB3	1.95	0.47	
1:B:54:LYS:CB	1:B:55:PRO:CD	2.92	0.47	
1:B:280:LEU:HD23	1:B:329:THR:CG2	2.45	0.47	
1:A:288:ILE:CD1	1:A:398:SER:HB2	2.44	0.47	
1:A:347:TRP:CE3	2:E:3:SGC:H5	2.50	0.47	
1:D:144:LEU:HD23	1:D:144:LEU:C	2.35	0.47	
1:C:303:GLY:HA3	4:C:611:HOH:O	2.14	0.47	
1:A:50:ASP:O	1:A:51:TRP:C	2.54	0.47	
1:A:322:GLU:HG3	1:A:325:ARG:HH11	1.80	0.46	
1:C:261:ASP:OD2	1:C:264:ARG:HD3	2.15	0.46	
1:A:277:GLN:NE2	4:A:606:HOH:O	2.46	0.46	
1:B:175:GLN:O	1:B:176:CYS:HB2	2.15	0.46	
1:B:247:ASN:HB3	1:B:300:ASN:HB3	1.97	0.46	
1:B:288:ILE:HD11	1:B:398:SER:HB2	1.98	0.46	
1:A:77:SER:O	1:A:81:LYS:HD2	2.16	0.46	
1:A:54:LYS:CB	1:A:55:PRO:CD	2.92	0.46	
1:B:9:GLN:OE1	1:B:76:ASP:HB2	2.16	0.46	
1:C:313:LYS:HD3	4:C:522:HOH:O	2.15	0.46	
1:B:18:CYS:HA	1:B:23:GLY:O	2.15	0.46	
1:D:136:LEU:HD11	1:D:384:VAL:HB	1.98	0.46	
1:D:175:GLN:O	1:D:176:CYS:HB2	2.16	0.46	
1:A:20:LYS:N	1:A:393:GLU:OE2	2.46	0.45	



	louo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:371:ASP:O	1:C:375:ILE:HG13	2.16	0.45
1:D:126:GLU:HB2	1:D:394:ILE:HA	1.99	0.45
2:F:1:SSG:O3	2:F:2:SGC:C1	2.64	0.45
1:A:272:PHE:HB3	1:A:280:LEU:HD11	1.97	0.45
1:D:197:GLU:OE1	2:H:2:SGC:O2	2.32	0.45
1:A:54:LYS:CB	1:A:55:PRO:HD2	2.42	0.45
1:A:137:PRO:HG2	1:A:375:ILE:HG23	1.99	0.45
1:A:371:ASP:OD1	1:A:373:LYS:HB3	2.16	0.45
1:B:280:LEU:HD23	1:B:329:THR:HG22	1.98	0.45
2:H:1:SSG:O3	2:H:2:SGC:C1	2.65	0.45
1:A:322:GLU:HG3	1:A:325:ARG:NH1	2.32	0.45
1:A:120:LEU:HD12	1:A:146:LEU:HD21	1.99	0.45
1:D:206:ARG:HG3	1:D:206:ARG:HH11	1.82	0.45
1:A:91:LYS:HE2	4:A:511:HOH:O	2.17	0.45
1:A:116:LYS:HB3	1:A:151:GLN:CG	2.46	0.45
1:B:31:ILE:HG23	1:B:107:VAL:HB	1.98	0.45
1:D:31:ILE:HG23	1:D:107:VAL:HB	1.99	0.45
1:B:81:LYS:HE2	1:B:85:ILE:O	2.17	0.45
1:C:54:LYS:CB	1:C:55:PRO:HD2	2.46	0.45
1:D:53:GLN:NE2	1:D:54:LYS:O	2.50	0.45
1:C:9:GLN:OE1	1:C:76:ASP:HB2	2.17	0.44
1:B:20:LYS:N	1:B:393:GLU:OE2	2.44	0.44
1:B:325:ARG:NH2	1:B:326:LEU:HD21	2.32	0.44
1:C:172:CYS:HB3	1:C:193:VAL:HG12	2.00	0.44
1:C:213:HIS:HE1	2:G:1:SSG:H2	1.82	0.44
1:D:208:THR:HG22	1:D:209:HIS:N	2.32	0.44
1:A:246:ILE:H	1:A:246:ILE:HG13	1.70	0.44
1:B:63:GLU:HG2	1:B:160:ASN:HD22	1.83	0.44
1:C:158:SER:OG	1:C:159:ARG:N	2.51	0.44
1:C:371:ASP:OD1	1:C:373:LYS:HB3	2.18	0.44
1:B:257:GLN:HG3	4:B:596:HOH:O	2.16	0.44
1:C:137:PRO:HG3	1:C:379:GLN:HB3	2.00	0.44
1:C:306:LYS:HE2	1:C:306:LYS:N	2.33	0.44
1:D:18:CYS:HA	1:D:23:GLY:O	2.16	0.44
1:D:203:ALA:CB	1:D:208:THR:HG23	2.37	0.44
1:A:16:TYR:HB3	1:A:24:CYS:HB3	1.99	0.44
1:B:193:VAL:HG13	1:B:220:LEU:HD21	1.99	0.44
1:B:208:THR:HG22	1:B:209:HIS:N	2.32	0.44
1:C:81:LYS:HD3	4:C:638:HOH:O	2.18	0.44
1:A:19:THR:HA	1:A:393:GLU:CG	2.41	0.44
1:A:126:GLU:HB2	1:A:394:ILE:HA	1.99	0.44



	, and page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:50:ASP:H	1:B:53:GLN:NE2	2.15	0.44
1:D:271:GLN:HB2	1:D:284:HIS:HB2	2.00	0.44
1:D:383:GLU:HG3	4:D:770:HOH:O	2.17	0.44
1:A:20:LYS:H	1:A:393:GLU:CD	2.21	0.43
1:A:96:GLN:HE21	1:A:96:GLN:CA	2.29	0.43
1:A:210:ILE:HG13	4:A:413:HOH:O	2.17	0.43
1:A:376:VAL:HA	1:A:379:GLN:O	2.18	0.43
1:C:19:THR:HA	1:C:393:GLU:CG	2.46	0.43
1:B:366:ASP:CG	1:B:369:GLU:HG2	2.39	0.43
1:C:137:PRO:HG2	1:C:375:ILE:HG23	2.01	0.43
1:D:61:PRO:HD2	1:D:65:SER:HB2	2.00	0.43
1:A:280:LEU:HD23	1:A:329:THR:HG22	2.01	0.43
1:B:203:ALA:CB	1:B:208:THR:HG23	2.38	0.43
1:D:54:LYS:CB	1:D:55:PRO:CD	2.97	0.43
1:D:267:THR:HB	1:D:288:ILE:HB	2.00	0.43
1:D:322:GLU:HG3	1:D:325:ARG:NH1	2.34	0.43
1:B:144:LEU:C	1:B:144:LEU:HD23	2.38	0.43
1:A:35:ALA:O	1:A:38:HIS:HB2	2.19	0.43
1:A:144:LEU:C	1:A:144:LEU:HD23	2.40	0.43
1:A:356:TRP:CZ2	2:E:1:SSG:H5	2.54	0.43
1:D:139:GLY:HA3	1:D:375:ILE:HD11	2.01	0.42
1:A:4:ASP:HB2	1:A:5:LYS:HD3	2.02	0.42
1:B:54:LYS:CB	1:B:55:PRO:HD2	2.42	0.42
1:B:50:ASP:H	1:B:53:GLN:HE21	1.67	0.42
1:C:208:THR:HG22	1:C:209:HIS:N	2.32	0.42
1:C:366:ASP:CG	1:C:369:GLU:HG2	2.40	0.42
1:D:272:PHE:HB3	1:D:280:LEU:HD11	2.02	0.42
2:G:1:SSG:O3	2:G:2:SGC:C1	2.67	0.42
1:A:120:LEU:O	1:A:339:GLY:HA2	2.19	0.42
1:A:192:GLY:HA3	1:A:223:CYS:SG	2.59	0.42
1:B:347:TRP:CE3	2:F:3:SGC:H5	2.54	0.42
1:C:20:LYS:H	1:C:393:GLU:CD	2.22	0.42
1:B:162:LYS:NZ	4:B:532:HOH:O	2.52	0.42
1:B:348:TRP:CE2	1:B:372:PRO:HB3	2.54	0.42
1:C:31:ILE:HG23	1:C:107:VAL:HB	2.01	0.42
1:C:325:ARG:NH2	1:C:326:LEU:HD21	2.33	0.42
1:C:77:SER:HB3	4:C:638:HOH:O	2.19	0.42
1:D:4:ASP:HB3	1:D:71:ILE:CG2	2.49	0.42
1:B:56:ASN:HB3	1:B:59:ALA:HB3	2.00	0.42
1:C:16:TYR:HB2	1:C:390:ARG:HB3	2.01	0.42
1:C:54:LYS:HB2	1:C:55:PRO:CD	2.48	0.42



	lo ao pagom	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:C:203:ALA:CB	1:C:208:THR:HG23	2.40	0.42	
1:D:172:CYS:HB3	1:D:193:VAL:HG12	2.01	0.42	
1:D:292:LYS:O	1:D:294:ILE:HD12	2.19	0.42	
1:A:116:LYS:HB3	1:A:116:LYS:HE3	1.88	0.41	
1:B:292:LYS:O	1:B:294:ILE:HD12	2.20	0.41	
1:B:53:GLN:HE21	1:B:53:GLN:HB3	1.75	0.41	
1:D:199:ASP:OD2	2:H:1:SSG:O3	2.38	0.41	
1:A:194:CYS:HB3	1:A:234:CYS:SG	2.61	0.41	
1:B:12:LYS:HE2	4:B:564:HOH:O	2.20	0.41	
1:B:20:LYS:H	1:B:393:GLU:CD	2.24	0.41	
1:C:264:ARG:NH2	1:C:290:ASP:OD1	2.53	0.41	
1:A:275:ASN:HB2	4:A:665:HOH:O	2.19	0.41	
1:B:210:ILE:HD11	1:B:285:ARG:NH1	2.36	0.41	
1:B:322:GLU:HG3	1:B:325:ARG:HH11	1.86	0.41	
1:D:155:LYS:HA	1:D:161:SER:OG	2.20	0.41	
1:B:16:TYR:HB3	1:B:24:CYS:HB3	2.02	0.41	
1:B:53:GLN:NE2	1:B:54:LYS:O	2.54	0.41	
1:B:210:ILE:O	1:B:240:GLY:HA2	2.21	0.41	
1:B:271:GLN:HB2	1:B:284:HIS:HB2	2.01	0.41	
1:A:371:ASP:HA	1:A:372:PRO:HD3	1.82	0.41	
1:B:267:THR:HB	1:B:288:ILE:HB	2.02	0.41	
1:D:371:ASP:O	1:D:375:ILE:HG13	2.20	0.41	
1:D:374:ASN:O	1:D:375:ILE:C	2.59	0.41	
1:C:136:LEU:HD11	1:C:384:VAL:HB	2.03	0.41	
1:B:188:ILE:H	1:B:188:ILE:HG12	1.70	0.41	
1:D:20:LYS:N	1:D:393:GLU:OE2	2.51	0.41	
1:B:288:ILE:HD12	1:B:398:SER:HB2	2.01	0.40	
1:D:154:GLY:O	1:D:157:THR:HG23	2.21	0.40	
1:D:288:ILE:CD1	1:D:398:SER:HB2	2.51	0.40	
1:B:8:GLU:HG2	1:B:10:HIS:CE1	2.56	0.40	
1:C:330:LYS:HB2	4:C:591:HOH:O	2.21	0.40	
1:D:54:LYS:CB	1:D:55:PRO:HD2	2.48	0.40	
1:A:113:ASN:HB3	4:A:577:HOH:O	2.21	0.40	
1:B:272:PHE:HB3	1:B:280:LEU:HD11	2.04	0.40	
1:A:41:ARG:HD3	1:A:41:ARG:HH11	1.75	0.40	
1:C:97:LEU:HA	1:C:101:GLN:O	2.21	0.40	
1:A:162:LYS:NZ	4:A:532:HOH:O	2.54	0.40	
1:C:139:GLY:HA3	1:C:375:ILE:HD11	2.04	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	Perce	ntiles
1	А	396/398~(100%)	377~(95%)	18 (4%)	1 (0%)	41	66
1	В	396/398~(100%)	379~(96%)	16 (4%)	1 (0%)	41	66
1	С	396/398~(100%)	378~(96%)	17~(4%)	1 (0%)	41	66
1	D	396/398~(100%)	381~(96%)	14 (4%)	1 (0%)	41	66
All	All	1584/1592~(100%)	1515 (96%)	65 (4%)	4 (0%)	41	66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	195	CYS
1	А	195	CYS
1	В	195	CYS
1	С	195	CYS

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perc	$\mathbf{entiles}$
1	А	323/323~(100%)	291~(90%)	32 (10%)	8	18
1	В	323/323~(100%)	285~(88%)	38 (12%)	5	12
1	С	323/323~(100%)	289~(90%)	34 (10%)	7	16
1	D	323/323~(100%)	292~(90%)	31 (10%)	8	19
All	All	1292/1292~(100%)	1157 (90%)	135 (10%)	7	16



Mol	Chain	Res	Type
1	А	5	LYS
1	А	20	LYS
1	А	22	SER
1	А	26	LYS
1	А	41	ARG
1	А	53	GLN
1	А	54	LYS
1	А	58	THR
1	А	81	LYS
1	А	96	GLN
1	А	102	LEU
1	А	116	LYS
1	А	132	GLU
1	А	137	PRO
1	А	155	LYS
1	А	156	SER
1	А	182	ILE
1	А	189	LYS
1	А	208	THR
1	А	231	SER
1	А	236	LYS
1	А	254	ARG
1	А	276	LYS
1	А	277	GLN
1	А	286	HIS
1	А	292	LYS
1	А	322	GLU
1	А	346	VAL
1	А	348	TRP
1	А	350	GLU
1	А	390	ARG
1	А	393	GLU
1	В	5	LYS
1	В	20	LYS
1	В	22	SER
1	В	26	LYS
1	В	41	ARG
1	В	43	LYS
1	В	53	GLN
1	В	54	LYS
1	В	58	THR
1	В	81	LYS

All (135) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	В	96	GLN
1	В	97	LEU
1	В	102	LEU
1	В	116	LYS
1	В	132	GLU
1	В	137	PRO
1	В	147	SER
1	В	155	LYS
1	В	156	SER
1	В	182	ILE
1	В	189	LYS
1	В	208	THR
1	В	231	SER
1	В	236	LYS
1	В	254	ARG
1	В	276	LYS
1	В	277	GLN
1	В	286	HIS
1	В	292	LYS
1	В	322	GLU
1	В	331	GLN
1	В	346	VAL
1	В	348	TRP
1	В	350	GLU
1	В	373	LYS
1	В	390	ARG
1	В	393	GLU
1	В	398	SER
1	С	5	LYS
1	С	19	THR
1	С	20	LYS
1	C	22	SER
1	С	41	ARG
1	C	43	LYS
1	С	53	GLN
1	C	$5\overline{4}$	LYS
1	C	58	THR
1	С	81	LYS
1	C	96	GLN
1	С	97	LEU
1	С	102	LEU
1	С	116	LYS



Mol	Chain	Res	Type
1	С	132	GLU
1	С	147	SER
1	С	155	LYS
1	С	180	PRO
1	С	182	ILE
1	С	189	LYS
1	С	208	THR
1	С	231	SER
1	С	236	LYS
1	С	276	LYS
1	С	277	GLN
1	С	292	LYS
1	С	305	PRO
1	С	322	GLU
1	С	346	VAL
1	C	348	TRP
1	С	350	GLU
1	С	390	ARG
1	С	393	GLU
1	С	398	SER
1	D	5	LYS
1	D	20	LYS
1	D	22	SER
1	D	41	ARG
1	D	53	GLN
1	D	54	LYS
1	D	58	THR
1	D	81	LYS
1	D	86	THR
1	D	96	GLN
1	D	102	LEU
1	D	116	LYS
1	D	132	GLU
1	D	147	SER
1	D	155	LYS
1	D	156	SER
1	D	182	ILE
1	D	189	LYS
1	D	208	THR
1	D	231	SER
1	D	254	ARG
1	D	276	LYS



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Mol	Chain	$\operatorname{Res}$	Type								
1	D	277	GLN								
1	D	292	LYS								
1	D	322	GLU								
1	D	346	VAL								
1	D	348	TRP								
1	D	350	GLU								
1	D	390	ARG								
1	D	393	GLU								
1	D	398	SER								

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	53	GLN
1	А	96	GLN
1	А	286	HIS
1	А	331	GLN
1	В	53	GLN
1	В	95	GLN
1	В	96	GLN
1	С	53	GLN
1	С	96	GLN
1	С	286	HIS
1	D	53	GLN
1	D	96	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).



Mal Tuna		Chain	Dec	Tiple	Bond lengths			Bond angles		
WIOI	туре	Unain	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
1	PCA	В	1	1	7,8,9	1.29	0	9,10,12	1.87	2 (22%)
1	PCA	D	1	1	7,8,9	1.18	0	9,10,12	1.80	3 (33%)
1	PCA	А	1	1	7,8,9	1.23	0	9,10,12	1.77	3 (33%)
1	PCA	С	1	1	7,8,9	1.41	0	9,10,12	2.28	2 (22%)

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	PCA	В	1	1	-	0/0/11/13	0/1/1/1
1	PCA	D	1	1	-	0/0/11/13	0/1/1/1
1	PCA	А	1	1	-	0/0/11/13	0/1/1/1
1	PCA	С	1	1	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	С	1	PCA	OE-CD-CG	-4.61	118.73	126.76
1	В	1	PCA	OE-CD-CG	-4.17	119.48	126.76
1	А	1	PCA	OE-CD-CG	-3.64	120.40	126.76
1	С	1	PCA	O-C-CA	-3.32	116.08	124.78
1	D	1	PCA	OE-CD-CG	-2.99	121.54	126.76
1	D	1	PCA	OE-CD-N	-2.67	118.65	124.86
1	В	1	PCA	OE-CD-N	-2.48	119.08	124.86
1	D	1	PCA	CB-CA-C	-2.42	109.38	112.70
1	А	1	PCA	CA-N-CD	-2.08	106.45	113.58
1	А	1	PCA	O-C-CA	-2.03	119.46	124.78

All (10) bond angle outliers are listed below:

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

#### 5.5 Carbohydrates (i)

12 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 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).

Mal	Type	Chain	Dog	Link	Bo	ond leng	ths	Bond angles		
WIOI	туре	Ullalli	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SSG	Е	1	2	$10,\!12,\!12$	1.91	3 (30%)	11,17,17	2.69	7 (63%)
2	SGC	Е	2	2	$10,\!11,\!12$	1.95	2 (20%)	12,15,17	2.69	4 (33%)
2	SGC	Е	3	2	$10,\!11,\!12$	0.90	0	12,15,17	1.61	3 (25%)
2	SSG	F	1	2	$10,\!12,\!12$	1.89	2 (20%)	11,17,17	2.19	5(45%)
2	SGC	F	2	2	$10,\!11,\!12$	1.11	0	12,15,17	2.66	3 (25%)
2	SGC	F	3	2	$10,\!11,\!12$	0.86	0	12,15,17	1.37	2(16%)
2	SSG	G	1	2	$10,\!12,\!12$	1.97	3 (30%)	11,17,17	2.65	5(45%)
2	SGC	G	2	2	$10,\!11,\!12$	1.44	2 (20%)	12,15,17	2.61	3 (25%)
2	SGC	G	3	2	$10,\!11,\!12$	1.12	1 (10%)	12,15,17	1.52	2 (16%)
2	SSG	Н	1	2	$10,\!12,\!12$	1.84	2 (20%)	11,17,17	2.50	5 (45%)
2	SGC	Н	2	2	10,11,12	1.63	2 (20%)	12,15,17	2.74	3 (25%)
2	SGC	Н	3	2	10,11,12	1.36	1 (10%)	12,15,17	1.44	2 (16%)

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	SSG	Е	1	2	-	0/2/22/22	0/1/1/1
2	SGC	Е	2	2	-	0/2/19/22	0/1/1/1
2	SGC	Е	3	2	-	0/2/19/22	0/1/1/1
2	SSG	F	1	2	-	0/2/22/22	0/1/1/1
2	SGC	F	2	2	-	0/2/19/22	0/1/1/1
2	SGC	F	3	2	-	1/2/19/22	0/1/1/1
2	SSG	G	1	2	-	0/2/22/22	0/1/1/1
2	SGC	G	2	2	-	0/2/19/22	0/1/1/1
2	SGC	G	3	2	-	0/2/19/22	0/1/1/1
2	SSG	Н	1	2	-	0/2/22/22	0/1/1/1
2	SGC	Н	2	2	-	0/2/19/22	0/1/1/1
2	SGC	Н	3	2	-	0/2/19/22	0/1/1/1



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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Ε	2	SGC	C3-C4	4.38	1.57	1.53
2	Н	1	SSG	C1-C2	-4.17	1.46	1.53
2	Е	1	SSG	C5-C4	-3.55	1.50	1.53
2	G	1	SSG	C5-C4	-3.47	1.50	1.53
2	F	1	SSG	C5-C4	-3.41	1.50	1.53
2	G	1	SSG	C1-C2	-3.39	1.47	1.53
2	F	1	SSG	C1-C2	-3.35	1.47	1.53
2	Н	3	SGC	C5-C4	-3.22	1.50	1.53
2	Е	1	SSG	C1-C2	-3.19	1.47	1.53
2	Н	2	SGC	C5-C4	-3.11	1.50	1.53
2	G	2	SGC	C5-C4	-3.03	1.50	1.53
2	G	1	SSG	C3-C4	-2.90	1.51	1.53
2	Н	2	SGC	O5-C1	-2.88	1.39	1.43
2	Ε	2	SGC	C5-C4	-2.83	1.50	1.53
2	G	3	SGC	C5-C4	-2.81	1.50	1.53
2	G	2	SGC	O3-C3	-2.33	1.37	1.43
2	Е	1	SSG	C3-C4	-2.16	1.51	1.53
2	Н	1	SSG	C5-C4	-2.10	1.51	1.53

All (18) bond length outliers are listed below:

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	F	2	SGC	O5-C1-C2	6.61	120.98	110.77
2	Н	2	SGC	O5-C1-C2	6.22	120.37	110.77
2	Е	2	SGC	O5-C1-C2	6.15	120.26	110.77
2	G	2	SGC	O5-C1-C2	5.94	119.95	110.77
2	Ε	2	SGC	C1-O5-C5	5.20	119.24	112.19
2	Е	1	SSG	O3-C3-C4	5.14	119.67	109.12
2	Н	2	SGC	C1-O5-C5	5.08	119.07	112.19
2	G	1	SSG	O3-C3-C4	4.97	119.33	109.12
2	G	2	SGC	C1-O5-C5	4.83	118.74	112.19
2	G	1	SSG	O5-C1-C2	4.57	116.06	110.31
2	Н	1	SSG	O3-C3-C4	4.44	118.25	109.12
2	Н	1	SSG	O5-C1-C2	4.26	115.67	110.31
2	F	2	SGC	C1-O5-C5	4.07	117.71	112.19
2	Ε	1	SSG	O5-C1-C2	4.06	115.42	110.31
2	Ε	3	SGC	O3-C3-C4	4.03	117.39	109.12
2	G	3	SGC	O3-C3-C4	3.78	116.89	109.12
2	F	1	SSG	O3-C3-C4	3.77	116.86	109.12
2	Н	3	SGC	O3-C3-C4	3.70	116.72	109.12
2	F	2	SGC	C5-C4-S4	-3.58	101.45	110.16
2	Е	2	SGC	$\overline{C}$ 5-C4-S4	-3.53	101.58	110.16



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	Н	2	SGC	C5-C4-S4	-3.46	101.75	110.16
2	G	2	SGC	C5-C4-S4	-3.41	101.87	110.16
2	Н	1	SSG	C1-O5-C5	-3.16	106.75	112.57
2	F	3	SGC	O3-C3-C4	3.07	115.42	109.12
2	Е	1	SSG	C1-O5-C5	-3.03	107.00	112.57
2	F	1	SSG	C1-O5-C5	-2.93	107.18	112.57
2	Е	1	SSG	C6-C5-C4	2.92	119.10	112.69
2	G	1	SSG	C6-C5-C4	2.87	119.00	112.69
2	F	1	SSG	O5-C1-C2	2.87	113.92	110.31
2	G	1	SSG	C1-O5-C5	-2.71	107.58	112.57
2	G	3	SGC	O3-C3-C2	-2.53	105.16	109.99
2	Н	3	SGC	C1-O5-C5	2.48	115.55	112.19
2	Е	1	SSG	O3-C3-C2	-2.39	104.82	110.35
2	F	1	SSG	C6-C5-C4	2.38	117.92	112.69
2	Е	1	SSG	O6-C6-C5	2.34	119.31	111.29
2	G	1	SSG	C1-C2-C3	-2.30	106.04	110.59
2	Н	1	SSG	O6-C6-C5	2.26	119.04	111.29
2	F	3	SGC	C1-O5-C5	2.25	115.24	112.19
2	F	1	SSG	C1-C2-C3	-2.16	106.32	110.59
2	Е	3	SGC	C1-O5-C5	2.13	115.07	112.19
2	Н	1	SSG	C6-C5-C4	2.13	117.36	112.69
2	Е	1	SSG	C1-C2-C3	-2.10	106.45	110.59
2	Е	3	SGC	O3-C3-C2	-2.04	106.09	109.99
2	Е	2	SGC	O2-C2-C1	2.00	113.25	109.15

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	3	SGC	C4-C5-C6-O6

There are no ring outliers.

10 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Н	2	SGC	4	0
2	Е	2	SGC	2	0
2	G	1	SSG	4	0
2	F	3	SGC	1	0
2	F	1	SSG	5	0
2	G	2	SGC	3	0



Continued from previous page									
Mol	Chain	Res	Type	Clashes	Symm-Clashes				
2	Н	1	SSG	5	0				
2	Е	1	SSG	5	0				
2	F	2	SGC	3	0				
2	Е	3	SGC	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)

8 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 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).

Mal	Turne	Chain	Res Link		Bo	ond leng	ths	Bond angles		
INIOI	туре	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
3	NAG	В	400	1	14,14,15	1.20	1 (7%)	17,19,21	1.54	4 (23%)
3	NAG	С	400	1	14,14,15	1.26	1 (7%)	17,19,21	1.51	3 (17%)
3	NAG	А	399	1	14,14,15	1.33	2 (14%)	17,19,21	1.18	1 (5%)
3	NAG	D	399	1	14,14,15	1.34	2 (14%)	17,19,21	2.20	5 (29%)
3	NAG	В	399	1	14,14,15	1.34	2 (14%)	17,19,21	1.75	3 (17%)
3	NAG	D	400	1	14,14,15	1.15	1 (7%)	17,19,21	1.31	2 (11%)
3	NAG	А	400	1	14,14,15	1.23	1 (7%)	17,19,21	1.50	3 (17%)



Mal	Mol Tuno Chain		Bos	Link	Bond lengths			Bond angles		
WIOI	Moi Type Chain	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2	
3	NAG	С	399	1	14,14,15	1.21	1 (7%)	17,19,21	2.10	5 (29%)

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	NAG	В	400	1	-	2/6/23/26	0/1/1/1
3	NAG	С	400	1	-	2/6/23/26	0/1/1/1
3	NAG	А	399	1	-	0/6/23/26	0/1/1/1
3	NAG	D	399	1	-	0/6/23/26	0/1/1/1
3	NAG	В	399	1	-	0/6/23/26	0/1/1/1
3	NAG	D	400	1	-	2/6/23/26	0/1/1/1
3	NAG	А	400	1	-	2/6/23/26	0/1/1/1
3	NAG	С	399	1	-	0/6/23/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
3	С	400	NAG	O7-C7	-3.69	1.14	1.23
3	В	399	NAG	O7-C7	-3.68	1.14	1.23
3	А	400	NAG	O7-C7	-3.66	1.15	1.23
3	А	399	NAG	O7-C7	-3.66	1.15	1.23
3	С	399	NAG	O7-C7	-3.51	1.15	1.23
3	В	400	NAG	O7-C7	-3.39	1.15	1.23
3	D	399	NAG	O7-C7	-3.36	1.15	1.23
3	D	400	NAG	O7-C7	-3.25	1.15	1.23
3	D	399	NAG	O5-C1	2.22	1.47	1.43
3	В	399	NAG	O5-C1	2.20	1.47	1.43
3	А	399	NAG	O5-C1	2.11	1.47	1.43

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
3	С	399	NAG	O5-C1-C2	-5.29	102.94	111.29
3	D	399	NAG	C1-O5-C5	-5.01	105.41	112.19
3	В	399	NAG	C1-C2-N2	4.53	118.23	110.49
3	D	399	NAG	O5-C1-C2	-3.89	105.14	111.29
3	С	399	NAG	C1-O5-C5	-3.86	106.96	112.19
3	В	399	NAG	C1-O5-C5	-3.45	107.52	112.19



Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
3	В	400	NAG	O5-C1-C2	-3.40	105.92	111.29
3	D	399	NAG	C2-N2-C7	-3.39	118.07	122.90
3	В	399	NAG	O5-C1-C2	-3.35	105.99	111.29
3	D	399	NAG	C8-C7-N2	-3.34	110.45	116.10
3	С	399	NAG	C8-C7-N2	-3.14	110.79	116.10
3	А	400	NAG	O5-C1-C2	-3.06	106.46	111.29
3	С	400	NAG	C4-C3-C2	-3.01	106.60	111.02
3	С	400	NAG	O5-C1-C2	-2.99	106.57	111.29
3	D	400	NAG	O5-C5-C6	2.92	111.78	107.20
3	С	400	NAG	O6-C6-C5	2.78	120.81	111.29
3	А	400	NAG	O6-C6-C5	2.77	120.78	111.29
3	D	399	NAG	O7-C7-C8	2.58	126.84	122.06
3	В	400	NAG	C4-C3-C2	-2.55	107.29	111.02
3	С	399	NAG	C1-C2-N2	2.49	114.75	110.49
3	А	400	NAG	C4-C3-C2	-2.36	107.56	111.02
3	В	400	NAG	C1-O5-C5	-2.23	109.17	112.19
3	С	399	NAG	O7-C7-C8	2.21	126.16	122.06
3	D	400	NAG	O5-C1-C2	-2.18	107.84	111.29
3	А	399	NAG	C1-O5-C5	-2.09	109.35	112.19
3	В	400	NAG	O4-C4-C5	-2.00	104.32	109.30

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	400	NAG	O5-C5-C6-O6
3	А	400	NAG	O5-C5-C6-O6
3	В	400	NAG	O5-C5-C6-O6
3	С	400	NAG	O5-C5-C6-O6
3	D	400	NAG	C4-C5-C6-O6
3	В	400	NAG	C4-C5-C6-O6
3	С	400	NAG	C4-C5-C6-O6
3	А	400	NAG	C4-C5-C6-O6

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)

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.

