

Full wwPDB X-ray Structure Validation Report (i)

Sep 27, 2023 – 12:47 AM EDT

PDB ID	:	6CH8
Title	:	Crystal structure of a natively-glycosylated BG505 SOSIP.664 HIV-1 Envelope
		Trimer in complex with the broadly-neutralizing antibodies BG18 and 35O22
Authors	:	Barnes, C.O.; Bjorkman, P.J.
Deposited on	:	2018-02-22
Resolution	:	4.10 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)	:	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 4.10 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.



Motria	Whole archive	Similar resolution
wietric	$(\# {\rm Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R _{free}	130704	1193 (4.50-3.70)
Clashscore	141614	$1003 \ (4.44-3.76)$
Ramachandran outliers	138981	1005 (4.48-3.72)
Sidechain outliers	138945	1199 (4.50-3.70)

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%

Mol	Chain	Length	Quality of chain		
1	В	153	63%	25%	• 9%
2	D	243	69%	25%	••
3	Е	216	74%	239	% •
4	G	479	58%	33%	• 6%
5	Q	241	65%	25%	• 5%
6	R	215	60%	33%	5% •
7	А	3	33% 6	7%	



Mol	Chain	Length		Quality of chain	
7	0	3	33%	33%	33%
8	С	5	40%	20%	40%
8	J	5	20%	60%	20%
9	F	7	43%		57%
10	Н	5	40%	40%	20%
10	U	5	40%	(50%
11	Ι	7	43%		57%
12	Κ	4	50%		50%
12	Т	4		75%	25%
13	L	4	25%	75%	
14	М	7	14%	57%	29%
15	Ν	8	50%		50%
16	Р	6	33%	67%)
17	S	8	38%	25%	38%
18	V	9	679	%	33%

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
17	NAG	S	1	-	-	Х	-



$6\mathrm{CH8}$

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 12325 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 Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	В	139	Total 1109	C 700	N 195	O 208	S 6	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	605	CYS	THR	engineered mutation	UNP Q2N0S7

• Molecule 2 is a protein called 35O22 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	235	Total 1753	C 1110	N 295	O 340	S 8	0	0	0

• Molecule 3 is a protein called 35O22 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Е	210	Total 1592	C 998	N 264	O 322	S 8	0	0	0

• Molecule 4 is a protein called Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	451	Total 3537	C 2220	N 625	O 665	S 27	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	332	ASN	THR	conflict	UNP Q2N0S6
G	501	CYS	ALA	engineered mutation	UNP Q2N0S6



• Molecule 5 is a protein called BG18 Heavy Chain.

Mol	Chain	Residues		Ate	oms		ZeroOcc	AltConf	Trace	
5	0	228	Total	С	Ν	0	\mathbf{S}	0	0	0
5	Q	220	1678	1055	286	329	8	0	0	0

• Molecule 6 is a protein called BG18 Light Chain.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
6	R	211	Total 1514	C 947	N 253	O 308	S 6	0	0	0

• Molecule 7 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b eta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	А	3	Total 39	C 22	N 2	O 15	0	0	0
7	О	3	Total 39	C 22	N 2	O 15	0	0	0

• Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-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
8	С	5	Total C N O 61 34 2 25	0	0	0
8	J	5	Total C N O 61 34 2 25	0	0	0

• Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyran ose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyran ose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.





Mol	Chain	Residues	I	Aton	ns		ZeroOcc	AltConf	Trace
9	F	7	Total 83	C 46	N 2	O 35	0	0	0

• Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyra nose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	Н	5	Total C N O 61 34 2 25	0	0	0
10	U	5	Total C N O 61 34 2 25	0	0	0

• Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyra nose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-beta-D-mannopyra nose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	I	Aton	ns		ZeroOcc	AltConf	Trace
11	Ι	7	Total 83	C 46	N 2	O 35	0	0	0

• Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyran ose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glu copyranose.





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
12	K	4	Total C N O 50 28 2 20	0	0	0
12	Т	4	Total C N O 50 28 2 20	0	0	0

• Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyran ose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glu copyranose.



Mol	Chain	Residues	I	Aton	ns		ZeroOcc	AltConf	Trace
13	L	4	Total 50	C 28	N 2	O 20	0	0	0

• Molecule 14 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyra nose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyra nose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	М	7	Total 83	C 46	N 2	O 35	0	0	0

• Molecule 15 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyra nose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopy ranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	I	Aton	ns		ZeroOcc	AltConf	Trace
15	N	8	Total 94	C 52	N 2	O 40	0	0	0



• Molecule 16 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyra nose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	I	Aton	ns		ZeroOcc	AltConf	Trace
16	Р	6	Total 72	C 40	N 2	O 30	0	0	0

• Molecule 17 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyra nose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopy ranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
17	S	8	Total C 94 52	N O 2 40	0	0	0

• Molecule 18 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyra nose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deo xy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace		
18	V	9	Total 105	C 58	N 2	O 45	0	0	0

• Molecule 19 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	В	1	Total C N O 14 8 1 5	0	0
19	G	1	Total C N O 14 8 1 5	0	0
19	G	1	Total C N O 14 8 1 5	0	0
19	G	1	Total C N O 14 8 1 5	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.



• Molecule 1: Envelope glycoprotein gp41





Chain A: 33% 67%

• Molecule 7: beta-D
-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



α · α			
Chain O:	33%	33%	33%

NAG1 NAG2 BMA3

 \bullet Molecule 8: alpha-D-mannopyranose-(1-6)-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-glucopyranose

Chain C:	40%	20%	40%	
NAG1 NAG2 BMA3 MAN4 MAN5 MAN5				

• Molecule 8: alpha-D-mannopyranose-(1-6)-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-glucopyranose

Chain J:	20%	60%	20%
NAC1 NAC2 BMA3 MAN4 MAN5			

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

Chain F:	43%	57%
NAG1 NAG2 BMA3 MAN4 MAN5 MAN5 MAN7		

 \bullet Molecule 10: alpha-D-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-glucopyranose

Chain H:	40%	40%	20%
NAG1 BMA2 BMA3 MAN5 MAN5			

 \bullet Molecule 10: alpha-D-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-glucopyranose

$\alpha_1 \cdot \mathbf{T}$		
Chain L	40%	60%
Unam U.	40 /8	0078

NAG1 NAG2 BMA3 MAN4 MAN5

 $\bullet \ Molecule \ 11: \ alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)] \\ alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-deoxy-b$



D-glucopyranose	-(1-4)-2-acetamide	o-2-deoxy-beta-D-glu	copyranose	
Chain I:	43%	-	57%	
NAG1 NAG2 BMA3 MAN4 MAN5 MAN6 MAN7				
• Molecule 12: a beta-D-glucopyra	lpha-D-mannopyr anose-(1-4)-2-acet	ranose-(1-3)-beta-D-r amido-2-deoxy-beta-	nannopyranose-(1-4 D-glucopyranose	l)-2-acetamido-2-deoxy-
Chain K:	50%		50%	-
NAG1 NAG2 BMA3 MAN4 MAN4				
• Molecule 12: a beta-D-glucopyra	lpha-D-mannopyr anose-(1-4)-2-acet	amido-2-deoxy-beta-	nannopyranose-(1-4 D-glucopyranose	l)-2-acetamido-2-deoxy-
Chain T:	75	5%	25%	-
NAG1 NAG2 BMA3 MAN4				
• Molecule 13: a beta-D-glucopyra	lpha-D-mannopyr anose-(1-4)-2-acet	anose-(1-6)-beta-D-r amido-2-deoxy-beta-	nannopyranose-(1-4 D-glucopyranose	l)-2-acetamido-2-deoxy-

Chain L:	25%	75%	
NAG1 NAG2 BMA3 MAN4			
			<i>.</i>

 $\label{eq:constraint} \bullet \mbox{Molecule 14: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose (1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose (1-4)-2-acetamido-2-deoxy-beta-D-$

Chain M:	14%	57%	29%
NAG1 NAG2 BMA3 MAN4 MAN5 MAN5 MAN7			

 \bullet Molecule 15: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D

Chain N: 50% 50%

NAG1 NAG2 BMA3 MAN4 MAN5 MAN5 MAN7 MAN7 MAN8

 $\bullet \ Molecule \ 16: \ alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)] \\ beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-g$



67%

mido-2-deoxy-beta-D-glucopyranose

Chain P: 33%

NAG1 NAG2 BMA3 MAN4 MAN5 MAN6

 \bullet Molecule 17: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranoy-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetami

Chain S:	38%	25%	38%
NAG1 NAG2 BMA3 MAN4 MAN6 MAN6 MAN7 MAN7 MAN7			

 $\label{eq:solution} \bullet \mbox{Molecule 18: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-$

Chain V:	67%	33%
161 162 143 144 146 146 147 147 148 149 149		



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants	239.22Å 239.22Å 355.27Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Bosolution(A)	39.51 - 4.10	Depositor
Resolution (A)	39.51 - 4.10	EDS
% Data completeness	99.8 (39.51-4.10)	Depositor
(in resolution range)	99.8 (39.51-4.10)	EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.36 (at 4.13 \text{\AA})$	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
B B.	0.229 , 0.274	Depositor
n, n_{free}	0.259 , 0.306	DCC
R_{free} test set	1551 reflections (5.04%)	wwPDB-VP
Wilson B-factor $(Å^2)$	163.4	Xtriage
Anisotropy	0.427	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.23, 152.4	EDS
L-test for $twinning^2$	$ < L >=0.45, < L^2>=0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	12325	wwPDB-VP
Average B, all atoms $(Å^2)$	226.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.11% of the height of the origin peak. No significant pseudotranslation is detected.

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: MAN, NAG, BMA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol Chain		Bond lengths		Bond angles	
IVIOI	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	В	0.28	0/1127	0.60	2/1527~(0.1%)
2	D	0.27	0/1798	0.52	1/2450~(0.0%)
3	Е	0.25	0/1635	0.48	0/2235
4	G	0.28	0/3610	0.54	3/4901~(0.1%)
5	Q	0.27	0/1721	0.51	0/2353
6	R	0.27	0/1552	0.59	2/2129~(0.1%)
All	All	0.27	0/11443	0.54	8/15595~(0.1%)

There are no bond length outliers.

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
1	В	627	THR	N-CA-C	6.58	128.77	111.00
4	G	464	THR	N-CA-C	6.11	127.51	111.00
4	G	279	ASN	N-CA-C	-5.83	95.27	111.00
1	В	556	LEU	CA-CB-CG	5.75	128.53	115.30
6	R	137	VAL	N-CA-C	-5.70	95.60	111.00
6	R	182	LEU	CA-CB-CG	5.44	127.81	115.30
4	G	188	ASN	N-CA-C	-5.23	96.88	111.00
2	D	203	SER	N-CA-C	5.11	124.79	111.00

All (8) bond angle outliers are listed below:

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	В	1109	0	1103	47	1
2	D	1753	0	1713	66	0
3	Е	1592	0	1530	35	0
4	G	3537	0	3469	158	0
5	Q	1678	0	1590	55	0
6	R	1514	0	1411	81	0
7	А	39	0	34	2	0
7	0	39	0	34	2	0
8	С	61	0	52	1	0
8	J	61	0	52	1	0
9	F	83	0	70	4	0
10	Н	61	0	52	2	0
10	U	61	0	52	3	0
11	Ι	83	0	70	5	0
12	Κ	50	0	43	2	0
12	Т	50	0	43	0	0
13	L	50	0	43	0	0
14	М	83	0	69	3	0
15	Ν	94	0	79	3	0
16	Р	72	0	61	0	0
17	S	94	0	79	15	0
18	V	105	0	87	4	0
19	В	14	0	13	0	0
19	G	42	0	39	1	0
All	All	12325	0	11788	432	1

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.

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 18.

All (432) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
	1100111 =	distance (A)	overlap (Å)
4:G:386:ASN:HD21	17:S:1:NAG:C2	1.24	1.48
4:G:386:ASN:ND2	17:S:1:NAG:C1	1.75	1.45
1:B:626:MET:O	1:B:627:THR:CG2	1.79	1.30
1:B:624:ASP:O	2:D:98:ARG:HG3	1.35	1.22
4:G:386:ASN:ND2	17:S:1:NAG:N2	1.86	1.21
2:D:201:LYS:HB2	2:D:202:PRO:CD	1.71	1.20
4:G:386:ASN:HD21	17:S:1:NAG:C1	1.38	1.16



Atom 1	Atom 1 Atom 2		Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
4:G:386:ASN:HD22	17:S:1:NAG:H83	1.04	1.12
6:R:163:VAL:HG11	6:R:182:LEU:HA	1.17	1.12
1:B:626:MET:O	1:B:627:THR:HG22	0.97	1.11
4:G:386:ASN:HD22	17:S:1:NAG:C8	1.63	1.10
1:B:547:GLY:O	1:B:550:GLN:HG3	1.54	1.08
2:D:201:LYS:CB	2:D:202:PRO:HD3	1.84	1.07
6:R:163:VAL:CG1	6:R:182:LEU:HA	1.85	1.06
6:R:163:VAL:HG11	6:R:182:LEU:CA	1.85	1.04
4:G:364:SER:O	4:G:365:SER:OG	1.76	1.03
6:R:163:VAL:HG21	6:R:182:LEU:HD12	1.41	1.02
2:D:201:LYS:CB	2:D:202:PRO:CD	2.35	0.99
4:G:386:ASN:CG	17:S:1:NAG:C1	2.29	0.99
2:D:201:LYS:HB2	2:D:202:PRO:HD3	0.96	0.96
1:B:624:ASP:O	2:D:98:ARG:CG	2.13	0.96
4:G:365:SER:HB3	4:G:469:ARG:HD2	1.46	0.96
1:B:625:ASN:OD1	2:D:32:TYR:OH	1.81	0.96
6:R:163:VAL:HG21	6:R:183:SER:H	1.34	0.93
6:R:139:LEU:HD12	6:R:140:ILE:N	1.86	0.91
2:D:201:LYS:H	2:D:201:LYS:HD3	1.34	0.91
2:D:98:ARG:HD3	9:F:1:NAG:H81	1.50	0.91
2:D:201:LYS:CG	2:D:202:PRO:HD2	2.02	0.90
4:G:386:ASN:ND2	17:S:1:NAG:C8	2.34	0.90
1:B:626:MET:C	1:B:627:THR:HG22	1.92	0.90
6:R:163:VAL:CG2	6:R:182:LEU:HD12	2.02	0.89
4:G:358:ILE:O	4:G:465:THR:OG1	1.92	0.88
2:D:119:PRO:HG3	2:D:201:LYS:NZ	1.89	0.88
2:D:201:LYS:HG2	2:D:202:PRO:HD2	1.55	0.87
2:D:16:ALA:O	2:D:17:SER:OG	1.91	0.87
4:G:220:PRO:HG2	4:G:223:PHE:CD2	2.12	0.85
6:R:134:ALA:H	6:R:186:PRO:HG3	1.41	0.85
4:G:386:ASN:ND2	17:S:1:NAG:H83	1.90	0.85
1:B:530:MET:HG2	1:B:628:TRP:CD1	2.11	0.84
4:G:386:ASN:ND2	17:S:1:NAG:C7	2.41	0.83
6:R:152:TRP:HE1	6:R:161:ALA:HB3	1.42	0.83
4:G:466:GLU:HG2	4:G:468:PHE:CE1	2.15	0.82
6:R:36:TRP:HB2	6:R:48:ILE:HG21	1.61	0.81
2:D:201:LYS:CG	2:D:202:PRO:CD	2.58	0.81
2:D:119:PRO:HG3	2:D:201:LYS:HZ1	1.43	0.79
4:G:49:GLU:HG2	4:G:99:ASN:HB3	1.62	0.79
4:G:295:ASN:HB3	4:G:446:VAL:HG12	1.65	0.79
4:G:219:ALA:HB1	4:G:220:PRO:HD2	1.64	0.79



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
6:R:49:ILE:HD11	6:R:58:GLY:HA2	1.66	0.77
5:Q:17:THR:HG22	5:Q:84:THR:HA	1.66	0.76
4:G:462:ASN:O	4:G:463:SER:OG	2.04	0.75
4:G:295:ASN:OD1	4:G:295:ASN:N	2.17	0.75
5:Q:167:VAL:HA	5:Q:218:LYS:HE2	1.68	0.75
5:Q:167:VAL:HG21	5:Q:195:LEU:HD13	1.69	0.75
1:B:555:LEU:O	1:B:555:LEU:HD23	1.87	0.74
6:R:22:ILE:HD12	6:R:105:THR:HG21	1.69	0.74
2:D:201:LYS:HD3	2:D:201:LYS:N	2.02	0.74
4:G:95:MET:H	4:G:236:THR:HG21	1.51	0.74
6:R:163:VAL:HG11	6:R:182:LEU:C	2.08	0.73
4:G:219:ALA:CB	4:G:220:PRO:HD2	2.18	0.73
1:B:530:MET:HA	1:B:628:TRP:CD1	2.24	0.73
4:G:279:ASN:O	4:G:281:ALA:N	2.21	0.73
4:G:83:GLU:C	4:G:84:ILE:HD12	2.08	0.73
4:G:277:ILE:C	4:G:278:THR:HG23	2.09	0.73
5:Q:28:SER:HB2	18:V:6:MAN:H2	1.70	0.73
4:G:277:ILE:HD11	4:G:352:HIS:O	1.89	0.73
5:Q:186:VAL:HG13	5:Q:188:GLN:H	1.55	0.72
4:G:125:LEU:HA	4:G:161:MET:HE1	1.70	0.72
4:G:294:ILE:CD1	4:G:296:CYS:SG	2.78	0.72
4:G:356:ASN:O	4:G:357:THR:HG23	1.90	0.71
4:G:358:ILE:HB	4:G:465:THR:OG1	1.91	0.71
4:G:233:PHE:HB3	4:G:273:ARG:HH21	1.56	0.70
4:G:364:SER:O	4:G:365:SER:CB	2.39	0.70
1:B:548:ILE:HG21	4:G:78:ASP:OD2	1.92	0.70
5:Q:33:HIS:HA	5:Q:101:ILE:HG22	1.74	0.70
5:Q:117:MET:SD	5:Q:117:MET:N	2.65	0.70
3:E:136:LEU:H	3:E:182:LEU:HB3	1.56	0.70
4:G:84:ILE:HD12	4:G:84:ILE:N	2.06	0.69
1:B:554:ASN:OD1	1:B:567:LYS:NZ	2.19	0.69
6:R:152:TRP:HE1	6:R:161:ALA:CB	2.06	0.69
2:D:47:TRP:HZ2	2:D:50:TRP:HD1	1.41	0.69
6:R:63:PHE:O	6:R:64:SER:HB3	1.92	0.69
3:E:132:ASN:HB3	3:E:186:PRO:HG3	1.74	0.68
4:G:294:ILE:HD11	4:G:296:CYS:SG	2.33	0.68
6:R:40:LYS:HE2	6:R:41:PRO:HD2	1.76	0.68
2:D:96:LEU:HA	2:D:101:TYR:HB2	1.75	0.68
4:G:313:PRO:O	4:G:315:GLN:N	2.25	0.68
5:Q:50:GLY:HA2	5:Q:60:TYR:HA	1.76	0.67
3:E:121:LEU:HD12	3:E:197:CYS:HB2	1.75	0.67



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
6:R:129:LEU:H	6:R:129:LEU:HD12	1.57	0.67
4:G:277:ILE:O	4:G:278:THR:HG23	1.95	0.67
4:G:328:GLN:HB3	5:Q:109:LEU:HD21	1.76	0.67
2:D:67:VAL:HG22	2:D:82:ILE:HG22	1.74	0.67
4:G:466:GLU:HG2	4:G:468:PHE:HE1	1.59	0.66
6:R:152:TRP:NE1	6:R:161:ALA:HB3	2.10	0.66
4:G:50:THR:HG21	4:G:220:PRO:HG3	1.77	0.66
6:R:63:PHE:HD1	6:R:76:ILE:HG13	1.60	0.66
4:G:130:GLN:OE1	4:G:188:ASN:ND2	2.29	0.66
5:Q:88:ALA:HA	5:Q:128:VAL:HG11	1.78	0.66
4:G:386:ASN:ND2	17:S:1:NAG:C2	2.09	0.66
10:U:3:BMA:H61	10:U:5:MAN:H5	1.78	0.66
10:U:3:BMA:H3	10:U:4:MAN:H5	1.76	0.66
6:R:201:HIS:H	6:R:205:THR:HG21	1.61	0.65
11:I:4:MAN:H4	11:I:5:MAN:H5	1.78	0.65
4:G:327:ARG:HH22	18:V:2:NAG:H61	1.61	0.65
4:G:360:ARG:HB3	4:G:467:THR:OG1	1.95	0.65
5:Q:91:THR:HB	5:Q:127:THR:HA	1.76	0.65
3:E:63:ARG:HD3	3:E:81:ARG:CZ	2.29	0.63
5:Q:188:GLN:NE2	6:R:164:GLU:OE2	2.28	0.63
1:B:627:THR:O	1:B:628:TRP:HB2	1.98	0.63
3:E:26:ASN:HA	3:E:29:CYS:HB2	1.79	0.63
6:R:139:LEU:HD12	6:R:140:ILE:CA	2.28	0.63
5:Q:34:SER:OG	5:Q:99:ASN:ND2	2.31	0.63
2:D:159:LEU:HD21	2:D:184:VAL:HG11	1.81	0.62
10:H:3:BMA:H3	10:H:4:MAN:H5	1.81	0.62
4:G:279:ASN:ND2	4:G:282:LYS:HG2	2.14	0.62
6:R:119:VAL:O	6:R:140:ILE:HD12	1.99	0.62
4:G:279:ASN:O	4:G:280:ASN:C	2.37	0.62
4:G:325:ASP:OD2	6:R:54:GLN:NE2	2.31	0.62
4:G:356:ASN:O	4:G:357:THR:CG2	2.48	0.62
4:G:388:SER:HB3	17:S:1:NAG:HN2	1.65	0.61
2:D:1:GLU:N	2:D:1:GLU:OE1	2.33	0.61
1:B:616:ASN:O	7:A:1:NAG:N2	2.34	0.61
5:Q:162:TYR:HE2	5:Q:195:LEU:H	1.47	0.61
17:S:2:NAG:H5	17:S:3:BMA:H2	1.82	0.61
4:G:331:CYS:HB2	4:G:416:LEU:HB2	1.82	0.61
6:R:63:PHE:HA	6:R:76:ILE:HA	1.81	0.60
6:R:133:LYS:HA	6:R:186:PRO:HD3	1.83	0.60
1:B:627:THR:CG2	1:B:630:GLN:HG3	2.32	0.60
6:R:6:LEU:HG	6:R:102:GLY:HA3	1.83	0.60



Atom 1	A + a	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
6:R:164:GLU:O	6:R:181:TYR:O	2.20	0.59
4:G:358:ILE:HA	4:G:396:ILE:HG21	1.82	0.59
17:S:1:NAG:O3	17:S:2:NAG:N2	2.36	0.59
4:G:60:ALA:HB1	4:G:65:LYS:HA	1.84	0.59
10:U:3:BMA:H5	10:U:5:MAN:H3	1.84	0.59
1:B:625:ASN:HA	2:D:98:ARG:CD	2.33	0.59
1:B:589:ASP:HA	1:B:592:LEU:HD12	1.85	0.59
4:G:286:VAL:HB	4:G:452:LEU:HB2	1.85	0.59
4:G:197:ASN:OD1	12:K:1:NAG:H82	2.03	0.59
4:G:212:PRO:HG3	14:M:1:NAG:H82	1.85	0.59
4:G:275:GLU:OE1	4:G:282:LYS:HE3	2.03	0.59
6:R:37:TYR:H	6:R:48:ILE:HG22	1.67	0.58
6:R:128:GLU:OE2	6:R:135:THR:OG1	2.21	0.58
1:B:628:TRP:CZ3	4:G:42:VAL:HG21	2.37	0.58
6:R:163:VAL:HG11	6:R:183:SER:N	2.17	0.58
4:G:83:GLU:HA	4:G:245:VAL:HG12	1.83	0.58
1:B:658:GLN:HB3	1:B:662:ALA:HB2	1.86	0.58
2:D:28:ARG:NH2	2:D:72(B):GLU:OE1	2.37	0.58
4:G:70:ALA:HB2	4:G:213:ILE:HD11	1.86	0.58
4:G:476:ARG:HA	4:G:479:TRP:CE3	2.39	0.58
3:E:114:LYS:HG2	3:E:145:PRO:HD3	1.85	0.58
4:G:294:ILE:O	4:G:294:ILE:HG13	2.04	0.58
6:R:139:LEU:HD12	6:R:139:LEU:C	2.24	0.58
4:G:291:PRO:HB2	4:G:448:ASN:HB3	1.86	0.57
1:B:596:TRP:HE1	1:B:647:GLU:HG3	1.68	0.57
3:E:41:PRO:HB2	3:E:44:ARG:HB2	1.87	0.57
4:G:386:ASN:OD1	17:S:1:NAG:C1	2.52	0.57
6:R:134:ALA:N	6:R:186:PRO:HG3	2.17	0.57
4:G:265:LEU:HD21	4:G:450:THR:HB	1.85	0.57
4:G:138:ILE:HD13	6:R:30:THR:HG22	1.87	0.57
4:G:294:ILE:C	4:G:294:ILE:HD12	2.25	0.57
1:B:627:THR:HG21	1:B:630:GLN:HG3	1.86	0.57
2:D:166:PHE:HE2	3:E:139:LEU:HB3	1.70	0.57
6:R:196:SER:HA	6:R:210:VAL:HG23	1.87	0.57
2:D:119:PRO:CG	2:D:201:LYS:NZ	2.66	0.56
4:G:270:VAL:HG12	4:G:288:PHE:HA	1.87	0.56
4:G:273:ARG:NH1	4:G:287:GLN:OE1	2.39	0.56
6:R:93:ASP:OD1	6:R:94:THR:N	2.38	0.56
2:D:59:LEU:HD21	2:D:63:PHE:HB2	1.88	0.56
6:R:182:LEU:HD12	6:R:183:SER:H	1.71	0.55
1:B:625:ASN:HA	2:D:98:ARG:HD2	1.88	0.55



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
4:G:258:GLN:HG2	4:G:472:GLY:H	1.70	0.55
6:R:63:PHE:O	6:R:64:SER:CB	2.53	0.55
4:G:95:MET:N	4:G:236:THR:HG21	2.19	0.55
4:G:331:CYS:O	4:G:415:THR:HA	2.05	0.55
6:R:136:LEU:HB2	6:R:182:LEU:HG	1.89	0.55
6:R:163:VAL:HG21	6:R:183:SER:N	2.13	0.55
4:G:80:ASN:OD1	4:G:80:ASN:N	2.40	0.55
4:G:466:GLU:CG	4:G:468:PHE:CE1	2.88	0.55
4:G:119:CYS:SG	4:G:120:VAL:N	2.80	0.55
4:G:311:ILE:HD11	4:G:317:PHE:HB2	1.87	0.55
4:G:425:ASN:HB3	4:G:433:ALA:HA	1.88	0.55
6:R:155:ASP:OD1	6:R:156:SER:N	2.38	0.54
3:E:82:PRO:HB2	3:E:174:ASN:HD22	1.72	0.54
4:G:280:ASN:OD1	4:G:280:ASN:N	2.40	0.54
6:R:129:LEU:HD23	6:R:189:TRP:NE1	2.22	0.54
4:G:281:ALA:HA	4:G:456:ARG:HD3	1.89	0.54
1:B:530:MET:HA	1:B:628:TRP:NE1	2.23	0.54
3:E:124:PRO:HG3	3:E:189:TRP:HZ2	1.73	0.54
4:G:125:LEU:HD23	4:G:193:LEU:HD11	1.90	0.54
4:G:260:LEU:HD12	4:G:451:GLY:HA3	1.89	0.53
6:R:197:CYS:O	6:R:207:GLU:HG3	2.08	0.53
4:G:358:ILE:HG23	4:G:396:ILE:HD13	1.90	0.53
4:G:105:HIS:HD1	4:G:479:TRP:HZ3	1.57	0.53
4:G:90:THR:HG22	4:G:240:PRO:HA	1.91	0.53
3:E:50:ILE:HD13	3:E:56:ARG:HA	1.91	0.53
4:G:94:ASN:O	4:G:98:ASN:HB2	2.09	0.53
5:Q:38:VAL:HG23	5:Q:95:TYR:HB2	1.90	0.53
2:D:100:GLY:HA3	9:F:3:BMA:H61	1.91	0.52
5:Q:164:PRO:HG2	5:Q:218:LYS:HG3	1.91	0.52
4:G:163:THR:OG1	4:G:164:GLU:N	2.42	0.52
1:B:569:THR:HG21	4:G:71:THR:HG21	1.91	0.52
2:D:10:GLU:HG2	2:D:18:VAL:HG11	1.92	0.52
4:G:84:ILE:N	4:G:84:ILE:CD1	2.73	0.51
4:G:274:SER:OG	4:G:276:ASN:C	2.49	0.51
3:E:4:LEU:HD22	3:E:102:GLY:HA2	1.93	0.51
10:H:2:NAG:H61	10:H:3:BMA:H2	1.93	0.51
4:G:50:THR:CG2	4:G:220:PRO:HG3	2.40	0.51
4:G:291:PRO:HB3	4:G:450:THR:HG22	1.92	0.51
2:D:10:GLU:OE2	2:D:18:VAL:HG12	2.11	0.51
4:G:209:SER:HB3	4:G:211:GLU:HG2	1.93	0.51
4:G:276:ASN:C	4:G:276:ASN:OD1	2.49	0.51



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:D:119:PRO:CG	2:D:201:LYS:HZ2	2.23	0.51
1:B:548:ILE:O	1:B:551:GLN:OE1	2.29	0.50
2:D:131:THR:HB	2:D:136:ALA:HB2	1.92	0.50
4:G:474:ASP:OD1	4:G:475:MET:N	2.44	0.50
5:Q:10:GLY:HA2	5:Q:126:VAL:HG12	1.93	0.50
2:D:150:VAL:HG11	2:D:200:HIS:HA	1.94	0.50
5:Q:38:VAL:HG21	5:Q:120:TRP:HZ3	1.76	0.50
14:M:4:MAN:O6	14:M:4:MAN:O4	2.26	0.50
4:G:251:ILE:HG23	4:G:482:GLU:HG2	1.94	0.50
5:Q:52:ILE:HD13	5:Q:58:THR:HG22	1.94	0.50
5:Q:115:TYR:CE1	6:R:50:SER:HB2	2.46	0.50
5:Q:167:VAL:HG11	5:Q:195:LEU:HD22	1.94	0.50
6:R:37:TYR:H	6:R:48:ILE:CG2	2.24	0.50
4:G:232:LYS:HE2	4:G:234:ASN:HB3	1.93	0.50
6:R:95:SER:C	6:R:97:SER:H	2.14	0.50
5:Q:64:LEU:O	5:Q:68:VAL:HG22	2.11	0.50
3:E:124:PRO:HG3	3:E:189:TRP:CZ2	2.47	0.50
4:G:360:ARG:HG3	4:G:394:THR:OG1	2.11	0.50
6:R:53:SER:HB3	18:V:9:MAN:O3	2.12	0.49
4:G:189:LYS:HD3	4:G:191:TYR:OH	2.12	0.49
1:B:601:LYS:HB2	1:B:604:CYS:SG	2.52	0.49
6:R:140:ILE:HG22	6:R:141:SER:N	2.27	0.49
6:R:140:ILE:CG2	6:R:141:SER:N	2.76	0.49
2:D:119:PRO:HG3	2:D:201:LYS:HZ2	1.71	0.49
4:G:160:ASN:OD1	4:G:171:LYS:HG2	2.13	0.49
4:G:311:ILE:HD11	4:G:317:PHE:CB	2.43	0.49
4:G:391:PHE:CD2	4:G:470:PRO:HG3	2.47	0.49
4:G:281:ALA:HB2	4:G:456:ARG:HH21	1.77	0.49
5:Q:38:VAL:HG21	5:Q:120:TRP:CZ3	2.47	0.49
1:B:555:LEU:HD23	1:B:555:LEU:C	2.33	0.49
6:R:163:VAL:HG12	6:R:164:GLU:N	2.27	0.49
2:D:100(E):LEU:HD23	2:D:100(E):LEU:H	1.77	0.48
2:D:167:PRO:HG3	3:E:169:SER:HB3	1.95	0.48
4:G:163:THR:O	4:G:312:GLY:N	2.43	0.48
5:Q:186:VAL:HG22	5:Q:187:LEU:HD23	1.95	0.48
6:R:12:VAL:O	6:R:107:LEU:HD12	2.12	0.48
2:D:198:VAL:HB	2:D:200:HIS:NE2	2.28	0.48
5:Q:163:PHE:H	5:Q:164:PRO:HD2	1.78	0.48
6:R:163:VAL:CG2	6:R:182:LEU:CD1	2.86	0.48
3:E:82:PRO:HB2	3:E:174:ASN:ND2	2.28	0.48
6:R:119:VAL:O	6:R:140:ILE:CD1	2.61	0.48



Atom 1	Atom 2	Interatomic	Clash
Atom-1	m-1 Atom-2		overlap (Å)
9:F:2:NAG:O3	9:F:3:BMA:O2	2.20	0.48
4:G:55:ALA:HB3	4:G:216:HIS:HB2	1.95	0.48
4:G:277:ILE:O	4:G:278:THR:CB	2.62	0.48
6:R:87:TYR:O	6:R:104:GLY:HA3	2.13	0.48
6:R:165:THR:CG2	6:R:166:THR:N	2.76	0.48
1:B:605:CYS:HB2	4:G:503:ARG:HG3	1.96	0.48
1:B:628:TRP:CZ3	4:G:42:VAL:CG2	2.97	0.48
6:R:189:TRP:NE1	6:R:190:LYS:HD3	2.29	0.48
6:R:35:TYR:HB2	6:R:90:GLN:HB3	1.96	0.47
1:B:601:LYS:HE2	1:B:604:CYS:SG	2.54	0.47
2:D:201:LYS:HG2	2:D:202:PRO:CD	2.30	0.47
4:G:277:ILE:O	4:G:278:THR:CG2	2.62	0.47
5:Q:18:LEU:HD13	5:Q:20:LEU:HD13	1.95	0.47
5:Q:218:LYS:HB3	5:Q:218:LYS:HE3	1.66	0.47
1:B:650:GLN:O	1:B:654:GLU:HB3	2.14	0.47
3:E:121:LEU:HD22	3:E:210:VAL:HG23	1.95	0.47
4:G:365:SER:CB	4:G:469:ARG:HD2	2.32	0.47
5:Q:32:ASP:O	5:Q:53:HIS:NE2	2.44	0.47
6:R:163:VAL:CG1	6:R:164:GLU:N	2.77	0.47
1:B:544:LEU:HD21	4:G:493:PRO:HG3	1.97	0.47
4:G:277:ILE:C	4:G:278:THR:CG2	2.80	0.47
1:B:530:MET:HG2	1:B:628:TRP:CG	2.49	0.47
6:R:122:PHE:O	6:R:137:VAL:O	2.32	0.47
15:N:3:BMA:H61	15:N:6:MAN:H62	1.97	0.47
12:K:1:NAG:H61	12:K:2:NAG:HN2	1.80	0.47
2:D:36:TRP:CZ3	2:D:92:CYS:HB3	2.50	0.47
2:D:150:VAL:HG21	2:D:200:HIS:ND1	2.30	0.47
4:G:55:ALA:HA	4:G:75:VAL:O	2.15	0.47
5:Q:130:SER:OG	5:Q:131:ALA:N	2.47	0.47
6:R:189:TRP:CD1	6:R:190:LYS:HG2	2.50	0.47
4:G:122:LEU:HD23	4:G:125:LEU:HD22	1.97	0.46
4:G:317:PHE:CE1	4:G:319:ALA:HB2	2.50	0.46
4:G:60:ALA:HB1	4:G:64:GLU:O	2.15	0.46
4:G:277:ILE:HG23	4:G:278:THR:HG23	1.96	0.46
6:R:129:LEU:HD23	6:R:189:TRP:HE1	1.80	0.46
6:R:190:LYS:HD2	6:R:190:LYS:HA	1.69	0.46
2:D:59:LEU:HD23	2:D:60:ALA:N	2.31	0.46
3:E:78:SER:O	3:E:81:ARG:NH2	2.45	0.46
4:G:69:TRP:HA	4:G:111:LEU:HD21	1.96	0.46
11:I:4:MAN:HO2	11:I:5:MAN:C1	2.28	0.46
2:D:4:LEU:O	2:D:104:GLY:HA2	2.14	0.46



Atom 1 Atom 2		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
5:Q:133:THR:HG21	5:Q:219:PRO:HG2	1.96	0.46
5:Q:117:MET:N	6:R:37:TYR:OH	2.46	0.46
7:A:2:NAG:H4	7:A:3:BMA:H2	1.63	0.46
6:R:38:ARG:HB3	6:R:87:TYR:CE1	2.51	0.46
2:D:210:ARG:HG2	2:D:211:VAL:H	1.81	0.46
1:B:627:THR:HG23	1:B:630:GLN:H	1.81	0.46
4:G:206:PRO:HG2	4:G:207:LYS:HE3	1.97	0.46
4:G:305:LYS:HA	4:G:305:LYS:HD3	1.77	0.46
4:G:368:ASP:OD1	4:G:369:LEU:N	2.49	0.45
6:R:165:THR:HG22	6:R:166:THR:N	2.31	0.45
2:D:163:VAL:HG12	2:D:182:VAL:HG23	1.98	0.45
3:E:14:LEU:HD12	3:E:80:LEU:O	2.15	0.45
1:B:653:GLN:O	1:B:657:GLU:HG2	2.16	0.45
4:G:356:ASN:C	4:G:357:THR:HG23	2.36	0.45
19:G:671:NAG:HO3	19:G:671:NAG:C7	2.29	0.45
5:Q:113:PHE:CE2	6:R:53:SER:HA	2.51	0.45
6:R:163:VAL:HB	6:R:182:LEU:CD1	2.47	0.45
1:B:610:TRP:CE3	4:G:498:PRO:HB3	2.52	0.45
3:E:119:VAL:HG11	3:E:199:VAL:HG21	1.98	0.45
1:B:555:LEU:C	1:B:555:LEU:CD2	2.85	0.45
1:B:625:ASN:HA	2:D:98:ARG:CG	2.47	0.45
4:G:280:ASN:O	4:G:456:ARG:HG2	2.16	0.45
6:R:95:SER:O	6:R:97:SER:N	2.49	0.45
4:G:96:TRP:CZ2	4:G:274:SER:C	2.90	0.45
4:G:335:LYS:HD3	4:G:414:ILE:HD11	1.98	0.45
5:Q:172:ASN:HB2	5:Q:211:TYR:HD1	1.81	0.45
6:R:168:PRO:HB3	6:R:176:TYR:HB3	1.99	0.45
8:C:2:NAG:H4	8:C:3:BMA:H2	1.69	0.45
2:D:53:TYR:O	2:D:55:GLY:N	2.47	0.45
4:G:294:ILE:CD1	4:G:294:ILE:C	2.85	0.45
5:Q:68:VAL:HA	5:Q:82:LYS:O	2.17	0.45
2:D:201:LYS:N	2:D:201:LYS:CD	2.73	0.45
5:Q:76:ILE:HG13	5:Q:77:PRO:HD2	1.99	0.45
3:E:149:THR:OG1	3:E:200:THR:HB	2.17	0.44
15:N:1:NAG:H62	15:N:2:NAG:HN2	1.80	0.44
1:B:658:GLN:O	1:B:662:ALA:N	2.22	0.44
3:E:56:ARG:H	3:E:56:ARG:HG2	1.63	0.44
4:G:175:LEU:O	4:G:320:THR:OG1	2.31	0.44
5:Q:187:LEU:HD23	5:Q:187:LEU:H	1.83	0.44
5:Q:217:HIS:CB	5:Q:222:THR:H	2.29	0.44
2:D:102:LEU:HA	2:D:102:LEU:HD23	1.77	0.44



A + amo 1	At	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
4:G:50:THR:HG21	4:G:220:PRO:CG	2.45	0.44
4:G:276:ASN:OD1	4:G:277:ILE:O	2.35	0.44
5:Q:22:CYS:HB2	5:Q:37:TRP:CH2	2.53	0.44
3:E:39:GLN:HG3	3:E:88:TYR:HE2	1.83	0.44
2:D:47:TRP:HZ2	2:D:50:TRP:CD1	2.29	0.44
2:D:166:PHE:CD2	3:E:139:LEU:HD22	2.52	0.44
4:G:129:LEU:HB3	4:G:157:CYS:SG	2.58	0.44
3:E:115:ALA:O	3:E:143:PHE:HA	2.18	0.44
3:E:119:VAL:HG22	3:E:140:ILE:HG22	2.00	0.44
2:D:16:ALA:O	2:D:17:SER:CB	2.66	0.43
4:G:220:PRO:HG2	4:G:223:PHE:CG	2.52	0.43
5:Q:91:THR:OG1	5:Q:128:VAL:HG12	2.18	0.43
6:R:138:CYS:O	6:R:180:SER:O	2.35	0.43
4:G:219:ALA:HA	4:G:220:PRO:HD3	1.71	0.43
6:R:163:VAL:HB	6:R:182:LEU:HD13	1.99	0.43
6:R:163:VAL:CB	6:R:182:LEU:HD12	2.46	0.43
1:B:536:THR:O	1:B:537:LEU:HB3	2.18	0.43
2:D:135:THR:HB	2:D:185:PRO:HA	2.01	0.43
2:D:181:VAL:HG21	3:E:139:LEU:CD1	2.48	0.43
4:G:112:TRP:CG	4:G:427:TRP:HH2	2.36	0.43
4:G:299:PRO:HB2	4:G:327:ARG:HB2	2.00	0.43
11:I:4:MAN:H61	11:I:7:MAN:H2	1.46	0.43
18:V:1:NAG:H83	18:V:1:NAG:H2	1.79	0.43
4:G:33:ASN:N	4:G:33:ASN:OD1	2.51	0.43
4:G:257:THR:HG22	4:G:258:GLN:HG3	2.01	0.43
4:G:343:GLY:O	4:G:346:VAL:HG12	2.19	0.43
1:B:537:LEU:HD22	1:B:603:ILE:HD11	2.00	0.43
3:E:196:SER:HA	3:E:209:THR:HG23	2.00	0.43
4:G:277:ILE:O	4:G:278:THR:OG1	2.33	0.43
4:G:453:ILE:HG21	4:G:472:GLY:HA2	2.01	0.43
3:E:37:TRP:HB2	3:E:50:ILE:HB	2.01	0.43
3:E:95:HIS:CD2	9:F:6:MAN:H3	2.54	0.43
4:G:171:LYS:NZ	8:J:2:NAG:O6	2.51	0.43
4:G:355:ASN:HB3	4:G:356:ASN:H	1.52	0.43
2:D:33:HIS:O	2:D:95:GLY:N	2.39	0.43
5:Q:99:ASN:HD21	5:Q:114:HIS:CD2	2.37	0.43
11:I:4:MAN:O2	11:I:5:MAN:O5	2.29	0.43
2:D:11:LEU:HD11	2:D:147:PRO:HG2	2.01	0.42
5:Q:101:ILE:HG23	5:Q:101:ILE:O	2.19	0.42
6:R:126:SER:O	6:R:128:GLU:N	2.45	0.42
11:I:1:NAG:HO6	11:I:2:NAG:HN2	1.65	0.42



A + amo 1	A + 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:628:TRP:CE3	4:G:42:VAL:CG1	3.02	0.42
2:D:2:GLY:HA3	2:D:26:GLY:HA3	2.01	0.42
4:G:332:ASN:HB3	7:O:1:NAG:H82	2.00	0.42
6:R:76:ILE:HG12	6:R:77:ARG:H	1.83	0.42
6:R:129:LEU:H	6:R:129:LEU:CD1	2.27	0.42
5:Q:39:ARG:NH2	5:Q:47:GLU:OE1	2.51	0.42
6:R:198:GLN:HA	6:R:207:GLU:HG3	2.01	0.42
2:D:166:PHE:CE2	3:E:139:LEU:HB3	2.52	0.42
4:G:129:LEU:O	4:G:191:TYR:N	2.35	0.42
4:G:447:SER:HB3	14:M:1:NAG:H3	2.02	0.42
5:Q:155:LEU:O	5:Q:198:VAL:HG23	2.18	0.42
5:Q:33:HIS:HA	5:Q:101:ILE:CG2	2.47	0.42
5:Q:162:TYR:OH	5:Q:195:LEU:HB2	2.18	0.42
5:Q:162:TYR:CZ	5:Q:193:TYR:HB2	2.54	0.42
6:R:33:PHE:CG	6:R:34:THR:N	2.87	0.42
1:B:614:TRP:O	1:B:638:TYR:OH	2.31	0.42
4:G:279:ASN:C	4:G:281:ALA:N	2.72	0.42
4:G:494:LEU:HA	4:G:494:LEU:HD23	1.75	0.42
3:E:65:SER:HB2	3:E:76:THR:HB	2.02	0.42
4:G:275:GLU:OE1	4:G:282:LYS:CE	2.68	0.42
2:D:190:GLY:H	2:D:194:TYR:HE2	1.68	0.41
4:G:135:THR:HG21	6:R:54:GLN:HG3	2.01	0.41
4:G:154:LEU:HG	4:G:177:TYR:HA	2.01	0.41
5:Q:93:MET:HA	5:Q:125:ALA:HA	2.02	0.41
2:D:128:SER:HB3	2:D:217:ASP:OD1	2.20	0.41
2:D:165:THR:HA	2:D:180:SER:HA	2.02	0.41
4:G:96:TRP:HH2	4:G:235:GLY:HA2	1.85	0.41
5:Q:172:ASN:HA	5:Q:212:ILE:HG22	2.02	0.41
15:N:2:NAG:H61	15:N:3:BMA:H2	2.01	0.41
2:D:200:HIS:HB3	2:D:201:LYS:HD3	2.02	0.41
4:G:444:ARG:NH1	7:O:1:NAG:O6	2.45	0.41
3:E:25:PRO:HD2	3:E:28:VAL:HG12	2.02	0.41
4:G:281:ALA:CA	4:G:456:ARG:HD3	2.50	0.41
4:G:387:THR:HB	4:G:391:PHE:HE2	1.86	0.41
5:Q:188:GLN:O	5:Q:190:SER:N	2.51	0.41
5:Q:186:VAL:HG22	5:Q:187:LEU:H	1.86	0.41
2:D:97:LEU:HD23	2:D:97:LEU:HA	1.72	0.41
5:Q:113:PHE:HD2	6:R:51:ARG:CZ	2.34	0.41
2:D:47:TRP:CZ2	2:D:50:TRP:HD1	2.28	0.41
3:E:86:THR:OG1	3:E:87:THR:N	2.53	0.41
3:E:91:CYS:HB2	3:E:99:CYS:HB3	2.02	0.41



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
4:G:359:ILE:O	4:G:394:THR:HG23	2.21	0.41
1:B:625:ASN:HB2	2:D:97:LEU:HD22	2.03	0.41
4:G:117:LYS:HB3	4:G:118:PRO:HD3	2.03	0.41
5:Q:139:PHE:HE1	6:R:128:GLU:N	2.19	0.41
1:B:627:THR:O	1:B:628:TRP:CB	2.69	0.40
1:B:628:TRP:CE3	4:G:42:VAL:HG11	2.56	0.40
2:D:143:LYS:HD2	2:D:177:SER:OG	2.21	0.40
3:E:121:LEU:HD23	3:E:122:PHE:N	2.35	0.40
4:G:178:ARG:HG2	4:G:179:LEU:N	2.36	0.40
4:G:192:ARG:CZ	4:G:197:ASN:HB2	2.51	0.40
5:Q:31:SER:O	5:Q:54:TYR:HB2	2.20	0.40
2:D:35:ASN:OD1	2:D:50:TRP:HB3	2.21	0.40
5:Q:165:GLU:N	5:Q:166:PRO:HD2	2.37	0.40
1:B:548:ILE:O	1:B:551:GLN:HB2	2.21	0.40
5:Q:113:PHE:HZ	6:R:52:SER:O	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-1 Atom-2		Clash overlap (Å)
1:B:535:MET:O	$1:B:652:GLN:NE2[2_545]$	2.11	0.09

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	Percenti	iles
1	В	135/153~(88%)	124 (92%)	10 (7%)	1 (1%)	22 60	0
2	D	233/243~(96%)	205 (88%)	25 (11%)	3 (1%)	12 4'	7
3	Ε	208/216~(96%)	185 (89%)	23 (11%)	0	100 10	00
4	G	443/479~(92%)	386 (87%)	54 (12%)	3 (1%)	22 60	0



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Pe	erc	entile	\mathbf{s}
5	Q	226/241~(94%)	184 (81%)	35 (16%)	7 (3%)		4	31	
6	R	209/215~(97%)	143 (68%)	57 (27%)	9 (4%)		2	24	
All	All	1454/1547~(94%)	1227 (84%)	204 (14%)	23~(2%)		9	43	

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	554	ASN
2	D	201	LYS
5	Q	50	GLY
6	R	62	ARG
6	R	212	PRO
4	G	280	ASN
4	G	314	GLY
6	R	64	SER
6	R	98	TYR
4	G	365	SER
5	Q	143	PRO
5	Q	162	TYR
5	Q	218	LYS
6	R	53	SER
6	R	135	THR
2	D	82(B)	ASN
2	D	17	SER
5	Q	84	THR
5	Q	140	PRO
6	R	96	ASP
6	R	195	TYR
5	Q	219	PRO
6	R	210	VAL

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	Perce	entiles
1	В	121/129~(94%)	115~(95%)	6~(5%)	24	52
2	D	194/206~(94%)	183 (94%)	11 (6%)	20	49
3	Ε	183/189~(97%)	182 (100%)	1 (0%)	88	93
4	G	400/426~(94%)	376~(94%)	24~(6%)	19	47
5	Q	181/208~(87%)	171 (94%)	10 (6%)	21	50
6	R	161/182~(88%)	152 (94%)	9~(6%)	21	49
All	All	1240/1340~(92%)	1179 (95%)	61 (5%)	25	52

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	549	VAL
1	В	556	LEU
1	В	565	LEU
1	В	583	VAL
1	В	606	THR
1	В	624	ASP
2	D	18	VAL
2	D	28	ARG
2	D	72(B)	GLU
2	D	82(C)	LEU
2	D	100(E)	LEU
2	D	128	SER
2	D	150	VAL
2	D	170	LEU
2	D	196	CYS
2	D	199	ASN
2	D	201	LYS
3	Е	81	ARG
4	G	33	ASN
4	G	72	HIS
4	G	74	CYS
4	G	80	ASN
4	G	82	GLN
4	G	207	LYS
4	G	234	ASN
4	G	268	GLU
4	G	271	MET
4	G	274	SER
4	G	275	GLU
4	G	294	ILE



Mol	Chain	Res	Type		
4	G	295	ASN		
4	G	297	THR		
4	G	321(A)	ASP		
4	G	322	ILE		
4	G	325	ASP		
4	G	350	ARG		
4	G	355	ASN		
4	G	363	ASN		
4	G	364	SER		
4	G	444	ARG		
4	G	445	CYS		
4	G	455	THR		
5	Q	54	TYR		
5	Q	60	TYR		
5	Q	112	TRP		
5	Q	113	PHE		
5	Q	117	MET		
5	Q	155	LEU		
5	Q	157	CYS		
5	Q	187	LEU		
5	Q	218	LYS		
5	Q	228	VAL		
6	R	6	LEU		
6	R	48	ILE		
6	R	54	GLN		
6	R	60	SER		
6	R	82	ASP		
6	R	129	LEU		
6	R	139	LEU		
6	R	150	VAL		
6	R	171	GLN		

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such side chains are listed below:

Mol	Chain	Res	Type
3	Ε	96	ASN
3	Е	174	ASN
4	G	386	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)

90 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	ol Type Chain B		Dog	Tink	Bo	ond leng	ths	Bond angles		
	туре	Ullalli	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
7	NAG	А	1	7,1	14,14,15	0.27	0	17,19,21	1.36	1 (5%)
7	NAG	А	2	7	14,14,15	0.34	0	17,19,21	0.66	0
7	BMA	А	3	7	11,11,12	0.24	0	$15,\!15,\!17$	0.97	1 (6%)
8	NAG	С	1	1,8	14,14,15	0.29	0	17,19,21	0.85	0
8	NAG	С	2	8	14,14,15	0.32	0	17,19,21	1.17	3 (17%)
8	BMA	С	3	8	11,11,12	0.45	0	$15,\!15,\!17$	1.17	2 (13%)
8	MAN	С	4	8	11,11,12	0.36	0	15,15,17	1.15	1 (6%)
8	MAN	С	5	8	11,11,12	0.22	0	15,15,17	0.77	0
9	NAG	F	1	9,4	14,14,15	0.29	0	17,19,21	1.87	6 (35%)
9	NAG	F	2	9	14,14,15	0.27	0	17,19,21	1.58	2 (11%)
9	BMA	F	3	9	11,11,12	0.38	0	15,15,17	1.33	2 (13%)
9	MAN	F	4	9	11,11,12	0.32	0	15,15,17	1.15	1 (6%)
9	MAN	F	5	9	11,11,12	0.26	0	15,15,17	0.90	1 (6%)
9	MAN	F	6	9	11,11,12	0.47	0	15,15,17	1.07	1 (6%)
9	MAN	F	7	9	11,11,12	0.26	0	15,15,17	0.94	1 (6%)
10	NAG	Н	1	10,4	14,14,15	0.28	0	17,19,21	0.87	0
10	NAG	Н	2	10	14,14,15	0.30	0	17,19,21	0.58	0
10	BMA	Н	3	10	11,11,12	0.32	0	15,15,17	0.92	0
10	MAN	Н	4	10	11,11,12	0.98	1 (9%)	$15,\!15,\!17$	2.08	3 (20%)



Mal	Turne	Chain	Dec	Tinle	Bo	Bond lengths		Bond angles		
NIOI	туре	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
10	MAN	Н	5	10	11,11,12	0.26	0	$15,\!15,\!17$	0.76	0
11	NAG	I	1	11,4	14,14,15	0.28	0	17,19,21	0.89	1 (5%)
11	NAG	Ι	2	11	14,14,15	0.29	0	17,19,21	0.72	0
11	BMA	Ι	3	11	11,11,12	0.32	0	15,15,17	0.91	1 (6%)
11	MAN	Ι	4	11	11,11,12	0.81	0	$15,\!15,\!17$	2.28	<mark>5 (33%)</mark>
11	MAN	Ι	5	11	11,11,12	0.50	0	$15,\!15,\!17$	1.35	2 (13%)
11	MAN	Ι	6	11	11,11,12	0.31	0	$15,\!15,\!17$	0.95	1 (6%)
11	MAN	Ι	7	11	11,11,12	0.44	0	$15,\!15,\!17$	1.19	2 (13%)
8	NAG	J	1	8,4	14,14,15	0.67	0	17,19,21	0.87	1 (5%)
8	NAG	J	2	8	14,14,15	0.41	0	17,19,21	1.06	1 (5%)
8	BMA	J	3	8	11,11,12	0.30	0	15, 15, 17	1.03	2 (13%)
8	MAN	J	4	8	11,11,12	0.25	0	$15,\!15,\!17$	0.74	0
8	MAN	J	5	8	11,11,12	0.26	0	$15,\!15,\!17$	0.84	1 (6%)
12	NAG	К	1	12,4	14,14,15	0.47	0	17,19,21	2.21	<mark>6 (35%)</mark>
12	NAG	K	2	12	14,14,15	0.36	0	17,19,21	0.92	1 (5%)
12	BMA	K	3	12	11,11,12	0.31	0	$15,\!15,\!17$	1.18	1 (6%)
12	MAN	К	4	12	11,11,12	0.27	0	15,15,17	0.92	1 (6%)
13	NAG	L	1	4,13	14,14,15	0.27	0	17,19,21	0.96	0
13	NAG	L	2	13	14,14,15	0.39	0	$17,\!19,\!21$	1.05	1 (5%)
13	BMA	L	3	13	11,11,12	0.31	0	$15,\!15,\!17$	0.82	1 (6%)
13	MAN	L	4	13	11,11,12	0.26	0	$15,\!15,\!17$	0.72	1 (6%)
14	NAG	М	1	14,4	14,14,15	0.31	0	17,19,21	0.91	1 (5%)
14	NAG	М	2	14	14,14,15	0.42	0	17,19,21	0.85	1 (5%)
14	BMA	М	3	14	11,11,12	0.75	0	$15,\!15,\!17$	1.49	4 (26%)
14	MAN	М	4	14	11,11,12	0.37	0	15,15,17	2.01	4 (26%)
14	MAN	М	5	14	11,11,12	0.47	0	15,15,17	1.41	2 (13%)
14	MAN	М	6	14	11,11,12	0.27	0	15,15,17	0.77	0
14	MAN	М	7	14,4	11,11,12	0.58	0	$15,\!15,\!17$	1.29	3 (20%)
15	NAG	Ν	1	15	14,14,15	0.95	1 (7%)	17,19,21	<mark>3.11</mark>	<mark>6 (35%)</mark>
15	NAG	N	2	15	14,14,15	0.28	0	17,19,21	0.80	1 (5%)
15	BMA	N	3	15	11,11,12	0.32	0	$15,\!15,\!17$	1.51	1 (6%)
15	MAN	N	4	15	11,11,12	0.28	0	15,15,17	0.86	1 (6%)
15	MAN	N	5	15	11,11,12	0.26	0	15,15,17	0.97	1 (6%)
15	MAN	N	6	15	11,11,12	0.24	0	15,15,17	0.89	1 (6%)
15	MAN	N	7	15	11,11,12	0.25	0	15,15,17	0.79	1 (6%)
15	MAN	N	8	15	11,11,12	0.57	0	15,15,17	1.45	2 (13%)



Mal	Turne	Chain	Dec	Tink	Bo	ond leng	ths	Bond angles		
WIOI	туре	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
7	NAG	Ο	1	7,4	14,14,15	0.31	0	$17,\!19,\!21$	2.27	4 (23%)
7	NAG	0	2	7	14,14,15	0.29	0	17,19,21	0.94	1 (5%)
7	BMA	0	3	7	11,11,12	0.22	0	$15,\!15,\!17$	0.80	0
16	NAG	Р	1	16,4	14,14,15	0.26	0	$17,\!19,\!21$	1.14	1 (5%)
16	NAG	Р	2	16	14,14,15	0.44	0	17,19,21	1.41	2 (11%)
16	BMA	Р	3	16	11,11,12	0.52	0	$15,\!15,\!17$	1.26	1 (6%)
16	MAN	Р	4	16	11,11,12	0.31	0	$15,\!15,\!17$	0.77	0
16	MAN	Р	5	16	11,11,12	0.28	0	$15,\!15,\!17$	0.90	1 (6%)
16	MAN	Р	6	16	11,11,12	0.27	0	$15,\!15,\!17$	0.88	0
17	NAG	S	1	17	14,14,15	0.27	0	17,19,21	1.52	3 (17%)
17	NAG	S	2	17	14,14,15	0.50	0	17,19,21	1.25	1 (5%)
17	BMA	S	3	17	11,11,12	0.53	0	$15,\!15,\!17$	1.46	1 (6%)
17	MAN	S	4	17	11,11,12	0.34	0	$15,\!15,\!17$	0.81	0
17	MAN	S	5	17	11,11,12	0.25	0	$15,\!15,\!17$	0.75	0
17	MAN	S	6	17	11,11,12	0.31	0	$15,\!15,\!17$	0.85	1 (6%)
17	MAN	S	7	17	11,11,12	0.27	0	$15,\!15,\!17$	0.82	0
17	MAN	S	8	17	11,11,12	0.24	0	$15,\!15,\!17$	0.81	1 (6%)
12	NAG	Т	1	12,4	14,14,15	0.32	0	17,19,21	0.71	0
12	NAG	Т	2	12	14,14,15	0.33	0	17,19,21	0.93	0
12	BMA	Т	3	12	11,11,12	0.25	0	$15,\!15,\!17$	0.90	0
12	MAN	Т	4	12	11,11,12	0.33	0	$15,\!15,\!17$	1.01	1 (6%)
10	NAG	U	1	10,4	14,14,15	0.27	0	17,19,21	1.05	2 (11%)
10	NAG	U	2	10	14,14,15	0.40	0	17,19,21	1.92	4 (23%)
10	BMA	U	3	10	11,11,12	0.47	0	$15,\!15,\!17$	2.03	<mark>5 (33%)</mark>
10	MAN	U	4	10	11,11,12	1.08	1 (9%)	$15,\!15,\!17$	1.99	3 (20%)
10	MAN	U	5	10	11,11,12	0.94	1 (9%)	$15,\!15,\!17$	2.15	3 (20%)
18	NAG	V	1	18,4	14,14,15	0.29	0	17,19,21	0.95	1 (5%)
18	NAG	V	2	18	14,14,15	0.30	0	17,19,21	0.66	0
18	BMA	V	3	18	11,11,12	0.30	0	15,15,17	1.21	1 (6%)
18	MAN	V	4	18	11,11,12	0.25	0	$15,\!15,\!17$	1.04	1 (6%)
18	MAN	V	5	18	11,11,12	0.23	0	15,15,17	1.07	1 (6%)
18	MAN	V	6	18,5	11,11,12	0.23	0	15,15,17	1.04	1 (6%)
18	MAN	V	7	18	11,11,12	0.54	0	$15,\!15,\!17$	1.30	1 (6%)
18	MAN	V	8	18	11,11,12	0.51	0	15,15,17	1.18	2 (13%)
18	MAN	V	9	18	11,11,12	0.59	0	15,15,17	1.32	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	А	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	А	2	7	-	3/6/23/26	0/1/1/1
7	BMA	A	3	7	_	1/2/19/22	0/1/1/1
8	NAG	С	1	1,8	_	$\frac{2}{6}/\frac{23}{26}$	0/1/1/1
8	NAG	С	2	8	-	$\frac{4}{6}/\frac{23}{26}$	0/1/1/1
8	BMA	С	3	8	-	0/2/19/22	0/1/1/1
8	MAN	С	4	8	-	$\frac{2}{2}/\frac{2}{19}/22$	0/1/1/1
8	MAN	С	5	8	-	1/2/19/22	0/1/1/1
9	NAG	F	1	9,4	_	3/6/23/26	0/1/1/1
9	NAG	F	2	9	_	$\frac{5}{6}/\frac{23}{26}$	0/1/1/1
9	BMA	F	3	9	_	$\frac{1/2}{19/22}$	0/1/1/1
9	MAN	F	4	9	_	$\frac{2/2}{19/22}$	0/1/1/1
9	MAN	F	5	9	_	0/2/19/22	0/1/1/1
9	MAN	F	6	9	-	1/2/19/22	0/1/1/1
9	MAN	F	7	9	-	0/2/19/22	0/1/1/1
10	NAG	Н	1	10,4	-	0/6/23/26	0/1/1/1
10	NAG	Н	2	10	-	5/6/23/26	0/1/1/1
10	BMA	Н	3	10	-	0/2/19/22	0/1/1/1
10	MAN	Н	4	10	-	0/2/19/22	0/1/1/1
10	MAN	Н	5	10	-	0/2/19/22	0/1/1/1
11	NAG	Ι	1	11,4	-	5/6/23/26	0/1/1/1
11	NAG	Ι	2	11	-	4/6/23/26	0/1/1/1
11	BMA	Ι	3	11	-	0/2/19/22	0/1/1/1
11	MAN	Ι	4	11	-	2/2/19/22	0/1/1/1
11	MAN	Ι	5	11	-	1/2/19/22	0/1/1/1
11	MAN	Ι	6	11	-	0/2/19/22	0/1/1/1
11	MAN	Ι	7	11	-	1/2/19/22	0/1/1/1
8	NAG	J	1	8,4	-	3/6/23/26	0/1/1/1
8	NAG	J	2	8	-	3/6/23/26	0/1/1/1
8	BMA	J	3	8	_	2/2/19/22	0/1/1/1
8	MAN	J	4	8	-	0/2/19/22	0/1/1/1
8	MAN	J	5	8	-	1/2/19/22	0/1/1/1
12	NAG	К	1	12,4	-	2/6/23/26	0/1/1/1
12	NAG	K	2	12	_	3/6/23/26	0/1/1/1
12	BMA	K	3	12	-	0/2/19/22	0/1/1/1
12	MAN	К	4	12	-	1/2/19/22	0/1/1/1

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.



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	NAG	L	1	4,13	-	2/6/23/26	0/1/1/1
13	NAG	L	2	13	-	3/6/23/26	0/1/1/1
13	BMA	L	3	13	_	2/2/19/22	0/1/1/1
13	MAN	L	4	13	_	0/2/19/22	0/1/1/1
14	NAG	М	1	14,4	-	4/6/23/26	0/1/1/1
14	NAG	М	2	14	_	3/6/23/26	0/1/1/1
14	BMA	М	3	14	-	0/2/19/22	0/1/1/1
14	MAN	М	4	14	-	1/2/19/22	0/1/1/1
14	MAN	М	5	14	-	0/2/19/22	0/1/1/1
14	MAN	М	6	14	-	0/2/19/22	0/1/1/1
14	MAN	М	7	14,4	-	2/2/19/22	0/1/1/1
15	NAG	N	1	15	-	5/6/23/26	0/1/1/1
15	NAG	Ν	2	15	-	3/6/23/26	0/1/1/1
15	BMA	Ν	3	15	-	2/2/19/22	0/1/1/1
15	MAN	N	4	15	-	2/2/19/22	0/1/1/1
15	MAN	N	5	15	-	2/2/19/22	0/1/1/1
15	MAN	Ν	6	15	-	0/2/19/22	0/1/1/1
15	MAN	Ν	7	15	-	2/2/19/22	0/1/1/1
15	MAN	Ν	8	15	-	0/2/19/22	0/1/1/1
7	NAG	0	1	7,4	-	3/6/23/26	0/1/1/1
7	NAG	0	2	7	-	3/6/23/26	0/1/1/1
7	BMA	0	3	7	-	0/2/19/22	0/1/1/1
16	NAG	Р	1	16,4	-	2/6/23/26	0/1/1/1
16	NAG	Р	2	16	-	1/6/23/26	0/1/1/1
16	BMA	Р	3	16	-	1/2/19/22	0/1/1/1
16	MAN	Р	4	16	-	2/2/19/22	0/1/1/1
16	MAN	Р	5	16	-	0/2/19/22	0/1/1/1
16	MAN	Р	6	16	-	0/2/19/22	0/1/1/1
17	NAG	S	1	17	-	5/6/23/26	0/1/1/1
17	NAG	S	2	17	-	4/6/23/26	0/1/1/1
17	BMA	S	3	17	-	2/2/19/22	0/1/1/1
17	MAN	S	4	17	-	1/2/19/22	0/1/1/1
17	MAN	S	5	17	-	1/2/19/22	0/1/1/1
17	MAN	S	6	17	-	2/2/19/22	0/1/1/1
17	MAN	S	7	17	-	1/2/19/22	0/1/1/1
17	MAN	S	8	17	-	1/2/19/22	0/1/1/1
12	NAG	Т	1	12,4	-	2/6/23/26	0/1/1/1



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	Т	2	12	-	2/6/23/26	0/1/1/1
12	BMA	Т	3	12	_	0/2/19/22	0/1/1/1
12	MAN	Т	4	12	-	0/2/19/22	0/1/1/1
10	NAG	U	1	10,4	-	2/6/23/26	0/1/1/1
10	NAG	U	2	10	-	4/6/23/26	0/1/1/1
10	BMA	U	3	10	-	2/2/19/22	0/1/1/1
10	MAN	U	4	10	-	2/2/19/22	0/1/1/1
10	MAN	U	5	10	-	0/2/19/22	0/1/1/1
18	NAG	V	1	18,4	-	4/6/23/26	0/1/1/1
18	NAG	V	2	18	-	0/6/23/26	0/1/1/1
18	BMA	V	3	18	-	0/2/19/22	0/1/1/1
18	MAN	V	4	18	-	2/2/19/22	0/1/1/1
18	MAN	V	5	18	-	0/2/19/22	0/1/1/1
18	MAN	V	6	18,5	-	0/2/19/22	0/1/1/1
18	MAN	V	7	18	-	0/2/19/22	0/1/1/1
18	MAN	V	8	18	-	2/2/19/22	0/1/1/1
18	MAN	V	9	18	-	2/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
15	Ν	1	NAG	O5-C1	-3.03	1.38	1.43
10	U	4	MAN	O5-C1	2.86	1.48	1.43
10	Н	4	MAN	O5-C1	2.46	1.47	1.43
10	U	5	MAN	O5-C1	2.25	1.47	1.43

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
15	Ν	1	NAG	C1-O5-C5	-9.59	99.20	112.19
7	0	1	NAG	C1-O5-C5	-6.18	103.82	112.19
10	U	2	NAG	O4-C4-C5	-5.67	95.22	109.30
12	Κ	1	NAG	C1-O5-C5	-5.44	104.83	112.19
10	U	5	MAN	C1-O5-C5	5.18	119.21	112.19
11	Ι	4	MAN	O3-C3-C2	4.95	119.47	109.99
10	U	4	MAN	C1-O5-C5	4.94	118.88	112.19
10	Н	4	MAN	C1-O5-C5	4.77	118.65	112.19
17	S	3	BMA	O5-C1-C2	-4.65	103.59	110.77
15	Ν	1	NAG	O5-C1-C2	4.64	118.61	111.29
14	М	4	MAN	O3-C3-C4	4.59	120.97	110.35



Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Z} = \mathbf{Observed}(^{o})$	
7	А	1	NAG	C1-O5-C5	-4.56	106.01	112.19
18	V	7	MAN	O2-C2-C1	4.55	118.46	109.15
10	U	3	BMA	O5-C5-C6	4.47	114.21	107.20
10	U	5	MAN	O5-C1-C2	-4.47	103.87	110.77
10	Н	4	MAN	O5-C1-C2	-4.47	103.88	110.77
9	F	2	NAG	C2-N2-C7	4.43	129.22	122.90
9	F	1	NAG	C2-N2-C7	4.41	129.18	122.90
15	Ν	1	NAG	O4-C4-C5	-4.36	98.47	109.30
7	0	1	NAG	O4-C4-C5	-4.29	98.65	109.30
10	U	4	MAN	O5-C1-C2	-4.28	104.16	110.77
12	K	1	NAG	O4-C4-C3	-4.14	100.78	110.35
15	Ν	3	BMA	O3-C3-C2	-4.11	102.12	109.99
10	Н	4	MAN	C1-C2-C3	4.07	114.67	109.67
10	U	5	MAN	C1-C2-C3	3.97	114.55	109.67
15	Ν	1	NAG	C1-C2-N2	3.95	117.23	110.49
10	U	3	BMA	C1-O5-C5	-3.89	106.92	112.19
14	М	5	MAN	O5-C1-C2	-3.68	105.09	110.77
11	Ι	5	MAN	O5-C1-C2	-3.60	105.22	110.77
14	М	4	MAN	O5-C1-C2	-3.56	105.27	110.77
11	Ι	4	MAN	O2-C2-C3	3.53	117.21	110.14
17	S	2	NAG	O4-C4-C5	3.48	117.94	109.30
7	0	1	NAG	O4-C4-C3	-3.43	102.41	110.35
15	Ν	8	MAN	O5-C1-C2	-3.43	105.47	110.77
10	U	4	MAN	C1-C2-C3	3.39	113.84	109.67
9	F	4	MAN	O5-C5-C6	3.32	112.41	107.20
15	Ν	8	MAN	C1-O5-C5	3.27	116.62	112.19
17	S	1	NAG	O4-C4-C3	-3.25	102.83	110.35
7	0	1	NAG	C1-C2-N2	3.23	116.00	110.49
16	Р	3	BMA	O5-C1-C2	-3.22	105.80	110.77
16	Р	2	NAG	O4-C4-C3	3.20	117.74	110.35
11	Ι	4	MAN	O3-C3-C4	-3.16	103.05	110.35
9	F	2	NAG	C1-C2-N2	-3.14	105.13	110.49
14	М	5	MAN	C1-O5-C5	3.12	116.42	112.19
14	М	4	MAN	O3-C3-C2	-3.11	104.05	109.99
11	Ι	4	MAN	O2-C2-C1	-3.10	102.81	109.15
18	V	6	MAN	O5-C1-C2	-3.09	106.01	110.77
13	L	2	NAG	O4-C4-C5	3.07	116.93	109.30
18	V	5	MAN	O5-C1-C2	-3.06	106.05	110.77
17	S	1	NAG	C1-O5-C5	-3.03	108.09	112.19
18	V	3	BMA	O3-C3-C4	3.02	117.33	110.35
16	Р	2	NAG	C2-N2-C7	2.97	127.13	122.90
11	Ι	7	MAN	O5-C1-C2	-2.95	106.22	110.77



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	K	1	NAG	C3-C4-C5	2.89	115.39	110.24
14	М	3	BMA	O3-C3-C4	2.87	116.98	110.35
9	F	1	NAG	C8-C7-N2	-2.84	111.28	116.10
8	С	4	MAN	O5-C1-C2	-2.83	106.41	110.77
8	J	2	NAG	O5-C1-C2	-2.78	106.90	111.29
12	Κ	1	NAG	C1-C2-N2	2.76	115.20	110.49
14	М	3	BMA	O5-C5-C6	2.73	111.48	107.20
9	F	3	BMA	O5-C1-C2	-2.73	106.56	110.77
12	К	1	NAG	C2-N2-C7	-2.73	119.02	122.90
8	С	2	NAG	C2-N2-C7	2.72	126.77	122.90
8	С	3	BMA	O5-C1-C2	-2.70	106.61	110.77
9	F	1	NAG	C1-O5-C5	-2.67	108.58	112.19
9	F	6	MAN	O5-C1-C2	-2.66	106.66	110.77
14	М	3	BMA	O5-C1-C2	-2.66	106.67	110.77
10	U	2	NAG	O4-C4-C3	-2.64	104.25	110.35
14	М	7	MAN	O5-C1-C2	-2.60	106.77	110.77
18	V	9	MAN	C1-C2-C3	2.58	112.84	109.67
7	А	3	BMA	O5-C1-C2	-2.58	106.78	110.77
10	U	2	NAG	C1-O5-C5	-2.56	108.72	112.19
10	U	1	NAG	C4-C3-C2	-2.54	107.29	111.02
17	S	1	NAG	C1-C2-N2	2.53	114.82	110.49
9	F	1	NAG	C1-C2-N2	-2.51	106.19	110.49
12	K	2	NAG	C4-C3-C2	-2.47	107.39	111.02
11	I	5	MAN	C1-O5-C5	2.45	115.50	112.19
15	N	6	MAN	O5-C1-C2	-2.42	107.04	110.77
15	N	5	MAN	O5-C5-C6	2.40	110.97	107.20
8	J	1	NAG	O4-C4-C3	2.39	115.89	110.35
18	V	8	MAN	C1-C2-C3	-2.39	106.73	109.67
8	С	3	BMA	O5-C5-C6	2.37	110.92	107.20
14	М	7	MAN	C1-C2-C3	2.37	112.58	109.67
12	K	1	NAG	O4-C4-C5	-2.36	103.43	109.30
15	N	2	NAG	O4-C4-C3	-2.36	104.90	110.35
15	N	1	NAG	O5-C5-C6	2.33	110.86	107.20
8	С	2	NAG	C1-C2-N2	-2.33	106.51	110.49
16	P	1	NAG	C2-N2-C7	-2.32	119.60	122.90
12	Т	4	MAN	O5-C1-C2	-2.31	107.20	110.77
11	l	4	MAN	O5-C1-C2	-2.31	107.21	110.77
14	M	7	MAN	<u>O3-C3-C4</u>	-2.30	105.02	110.35
8	C	2	NAG	05-C5-C6	2.29	110.79	107.20
9	F,	7	MAN	05-C1-C2	-2.28	107.25	110.77
12	K	4	MAN	C1-O5-C5	-2.28	109.11	112.19
8	J	3	BMA	O5-C5-C6	2.26	110.75	107.20



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
8	J	3	BMA	O5-C1-C2	-2.25	107.30	110.77
14	М	3	BMA	O3-C3-C2	2.23	114.27	109.99
11	Ι	7	MAN	C1-C2-C3	2.20	112.37	109.67
11	Ι	1	NAG	C1-C2-N2	-2.20	106.73	110.49
14	М	4	MAN	C2-C3-C4	-2.19	107.10	110.89
9	F	5	MAN	O5-C1-C2	-2.19	107.40	110.77
10	U	3	BMA	O3-C3-C2	-2.18	105.81	109.99
15	Ν	4	MAN	O5-C1-C2	-2.18	107.41	110.77
7	0	2	NAG	O5-C1-C2	-2.17	107.86	111.29
14	М	2	NAG	O5-C1-C2	-2.17	107.86	111.29
9	F	1	NAG	O4-C4-C3	-2.17	105.33	110.35
10	U	1	NAG	C2-N2-C7	-2.16	119.82	122.90
10	U	3	BMA	C2-C3-C4	-2.16	107.16	110.89
18	V	1	NAG	O4-C4-C5	-2.13	104.00	109.30
18	V	8	MAN	C1-O5-C5	-2.13	109.31	112.19
15	Ν	1	NAG	C2-N2-C7	2.10	125.90	122.90
11	Ι	3	BMA	C1-O5-C5	-2.07	109.39	112.19
15	Ν	7	MAN	O5-C1-C2	-2.06	107.59	110.77
18	V	4	MAN	O5-C1-C2	-2.05	107.60	110.77
8	J	5	MAN	O5-C1-C2	-2.05	107.61	110.77
14	М	1	NAG	C2-N2-C7	2.05	125.82	122.90
11	Ι	6	MAN	O5-C1-C2	-2.04	107.62	110.77
17	S	6	MAN	O5-C1-C2	-2.04	107.62	110.77
12	Κ	3	BMA	O2-C2-C1	-2.04	104.99	109.15
16	Р	5	MAN	O5-C5-C6	2.04	110.39	107.20
10	U	3	BMA	C1-C2-C3	2.03	112.17	109.67
9	F	1	NAG	O4-C4-C5	-2.02	104.28	109.30
9	F	3	BMA	O2-C2-C3	-2.02	106.09	110.14
13	L	4	MAN	O5-C1-C2	-2.01	107.66	110.77
17	S	8	MAN	O5-C1-C2	-2.01	107.67	110.77
13	L	3	BMA	O5-C1-C2	-2.00	107.68	110.77
10	U	2	NAG	C4-C3-C2	2.00	113.95	111.02

There are no chirality outliers.

All (146) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	А	1	NAG	C8-C7-N2-C2
7	А	1	NAG	O7-C7-N2-C2
7	А	2	NAG	C8-C7-N2-C2
7	А	2	NAG	O7-C7-N2-C2
8	С	2	NAG	C3-C2-N2-C7



Mol	Chain	Res	Type	Atoms
8	J	1	NAG	C3-C2-N2-C7
8	J	1	NAG	C8-C7-N2-C2
8	J	1	NAG	O7-C7-N2-C2
8	J	2	NAG	O7-C7-N2-C2
9	F	1	NAG	C3-C2-N2-C7
10	Н	2	NAG	C3-C2-N2-C7
10	Н	2	NAG	C8-C7-N2-C2
10	Н	2	NAG	O7-C7-N2-C2
11	Ι	1	NAG	C8-C7-N2-C2
11	Ι	1	NAG	O7-C7-N2-C2
11	Ι	2	NAG	C8-C7-N2-C2
11	Ι	2	NAG	O7-C7-N2-C2
12	K	1	NAG	C8-C7-N2-C2
12	K	1	NAG	O7-C7-N2-C2
12	K	2	NAG	C8-C7-N2-C2
12	K	2	NAG	O7-C7-N2-C2
13	L	2	NAG	C8-C7-N2-C2
13	L	2	NAG	O7-C7-N2-C2
14	М	1	NAG	C8-C7-N2-C2
14	М	1	NAG	O7-C7-N2-C2
14	М	2	NAG	C3-C2-N2-C7
14	М	2	NAG	C8-C7-N2-C2
14	М	2	NAG	O7-C7-N2-C2
15	N	1	NAG	C1-C2-N2-C7
15	N	1	NAG	C8-C7-N2-C2
15	N	1	NAG	O7-C7-N2-C2
15	N	2	NAG	C3-C2-N2-C7
15	N	2	NAG	C8-C7-N2-C2
15	N	2	NAG	O7-C7-N2-C2
16	Р	1	NAG	O7-C7-N2-C2
17	S	1	NAG	C3-C2-N2-C7
17	S	1	NAG	C8-C7-N2-C2
17	S	1	NAG	O7-C7-N2-C2
17	S	2	NAG	C3-C2-N2-C7
17	S	2	NAG	C8-C7-N2-C2
17	S	2	NAG	07-C7-N2-C2
18	V	1	NAG	C8-C7-N2-C2
18	V	1	NAG	07-C7-N2-C2
18	V	4	MAN	C4-C5-C6-O6
7	0	1	NAG	C8-C7-N2-C2
8	J	2	NAG	C8-C7-N2-C2
16	Р	1	NAG	C8-C7-N2-C2

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Mol

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MAN

Atoms

O5-C5-C6-O6

O5-C5-C6-O6 O5-C5-C6-O6

V	9	MAN	C4-C5-C6-O6	
V	4	MAN	O5-C5-C6-O6	
U	4	MAN	C4-C5-C6-O6	
S	3	BMA	C4-C5-C6-O6	
0	1	NAG	O7-C7-N2-C2	
0	2	NAG	C8-C7-N2-C2	
U	1	NAG	C8-C7-N2-C2	
С	4	MAN	O5-C5-C6-O6	
J	3	BMA	C4-C5-C6-O6	
М	7	MAN	C4-C5-C6-O6	
Р	4	MAN	O5-C5-C6-O6	
V	1	NAG	O5-C5-C6-O6	
М	7	MAN	O5-C5-C6-O6	
V	9	MAN	O5-C5-C6-O6	
U	2	NAG	C4-C5-C6-O6	
С	2	NAG	C8-C7-N2-C2	
F	1	NAG	C8-C7-N2-C2	
F	2	NAG	C8-C7-N2-C2	
U	4	MAN	O5-C5-C6-O6	
N	3	BMA	C4-C5-C6-O6	
М	1	NAG	C1-C2-N2-C7	
Ν	5	MAN	O5-C5-C6-O6	
F	4	MAN	O5-C5-C6-O6	
N	1	NAG	O5-C5-C6-O6	
0	2	NAG	O7-C7-N2-C2	
С	1	NAG	C8-C7-N2-C2	
С	2	NAG	O7-C7-N2-C2	
F	1	NAG	O7-C7-N2-C2	
	V V U S O O U C J M P V M V U C F F F U N N N F N O C F F	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	V 9 MAN V 4 MAN U 4 MAN S 3 BMA O 1 NAG O 2 NAG U 1 NAG O 2 NAG U 1 NAG C 4 MAN J 3 BMA M 7 MAN P 4 MAN V 1 NAG M 7 MAN V 9 MAN V 9 MAN U 2 NAG C 2 NAG F 1 NAG F 2 NAG M 1 NAG N 3 BMA M 1 NAG N 3 BMA M 1 NAG	V 9 MAN C4-C5-C6-O6 V 4 MAN O5-C5-C6-O6 U 4 MAN C4-C5-C6-O6 S 3 BMA C4-C5-C6-O6 O 1 NAG O7-C7-N2-C2 O 2 NAG C8-C7-N2-C2 U 1 NAG C8-C7-N2-C2 U 1 NAG C8-C7-N2-C2 C 4 MAN O5-C5-C6-O6 J 3 BMA C4-C5-C6-O6 M 7 MAN O5-C5-C6-O6 P 4 MAN O5-C5-C6-O6 V 1 NAG O5-C5-C6-O6 V 9 MAN O5-C5-C6-O6 V 9 MAN O5-C5-C6-O6 U 2 NAG C8-C7-N2-C2 F 1 NAG C8-C7-N2-C2 V 9 MAN O5-C5-C6-O6 N 3 BMA C4-C5-C6-O6

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3

3

2

Type

BMA

BMA

NAG

Chain Res

Ν

J

U

Continued on next page...

O7-C7-N2-C2 O7-C7-N2-C2

C4-C5-C6-O6

O5-C5-C6-O6

O5-C5-C6-O6

C4-C5-C6-O6

C4-C5-C6-O6

C1-C2-N2-C7

O7-C7-N2-C2

O5-C5-C6-O6

O5-C5-C6-O6



Mol	Chain	Res	Type	Atoms
17	S	2	NAG	O5-C5-C6-O6
14	М	4	MAN	O5-C5-C6-O6
9	F	2	NAG	C1-C2-N2-C7
18	V	8	MAN	C4-C5-C6-O6
18	V	8	MAN	O5-C5-C6-O6
11	Ι	4	MAN	O5-C5-C6-O6
9	F	2	NAG	O5-C5-C6-O6
11	Ι	1	NAG	C1-C2-N2-C7
11	Ι	2	NAG	O5-C5-C6-O6
13	L	3	BMA	C4-C5-C6-O6
8	С	5	MAN	O5-C5-C6-O6
7	А	2	NAG	O5-C5-C6-O6
17	S	7	MAN	O5-C5-C6-O6
12	K	4	MAN	O5-C5-C6-O6
7	А	3	BMA	O5-C5-C6-O6
17	S	5	MAN	O5-C5-C6-O6
15	Ν	5	MAN	C4-C5-C6-O6
11	Ι	2	NAG	C1-C2-N2-C7
8	J	5	MAN	O5-C5-C6-O6
17	S	8	MAN	O5-C5-C6-O6
7	0	2	NAG	O5-C5-C6-O6
11	Ι	4	MAN	C4-C5-C6-O6
11	Ι	5	MAN	O5-C5-C6-O6
12	Κ	2	NAG	O5-C5-C6-O6
17	S	4	MAN	O5-C5-C6-O6
9	F	3	BMA	O5-C5-C6-O6
11	Ι	1	NAG	O5-C5-C6-O6
15	N	4	MAN	C4-C5-C6-O6
10	U	3	BMA	C4-C5-C6-O6
9	F	2	NAG	C3-C2-N2-C7
11	Ι	1	NAG	C3-C2-N2-C7
17	S	6	MAN	C4-C5-C6-O6
17	S	1	NAG	C4-C5-C6-O6
17	S	1	NAG	O5-C5-C6-O6
9	F	4	MAN	C4-C5-C6-O6
10	Н	2	NAG	C4-C5-C6-O6
7	0	1	NAG	C1-C2-N2-C7
17	S	6	MAN	O5-C5-C6-O6
10	Н	2	NAG	O5-C5-C6-O6
10	U	2	NAG	C1-C2-N2-C7
8	J	2	NAG	C3-C2-N2-C7
13	L	1	NAG	C3-C2-N2-C7

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6CH8

Mol	Chain	Res	Type	Atoms
8	С	2	NAG	C4-C5-C6-O6
15	Ν	7	MAN	C4-C5-C6-O6
15	Ν	7	MAN	O5-C5-C6-O6
9	F	6	MAN	O5-C5-C6-O6
13	L	1	NAG	C1-C2-N2-C7
12	Т	1	NAG	C8-C7-N2-C2
16	Р	3	BMA	C4-C5-C6-O6
13	L	2	NAG	O5-C5-C6-O6
13	L	3	BMA	O5-C5-C6-O6
10	U	2	NAG	C3-C2-N2-C7
12	Т	2	NAG	C3-C2-N2-C7
14	М	1	NAG	C3-C2-N2-C7
12	Т	1	NAG	O7-C7-N2-C2
15	Ν	1	NAG	C4-C5-C6-O6
12	Т	2	NAG	C1-C2-N2-C7

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There are no ring outliers.

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	А	3	BMA	1	0
7	А	2	NAG	1	0
18	V	1	NAG	1	0
18	V	2	NAG	1	0
7	А	1	NAG	1	0
8	С	3	BMA	1	0
11	Ι	5	MAN	3	0
10	U	4	MAN	1	0
14	М	4	MAN	1	0
11	Ι	4	MAN	4	0
18	V	9	MAN	1	0
11	Ι	2	NAG	1	0
10	Н	2	NAG	1	0
15	N	1	NAG	1	0
7	0	1	NAG	2	0
11	Ι	7	MAN	1	0
9	F	2	NAG	1	0
12	Κ	1	NAG	2	0
17	S	3	BMA	1	0
15	N	6	MAN	1	0
10	U	5	MAN	2	0
9	F	3	BMA	2	0



Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	N	3	BMA	2	0
18	V	6	MAN	1	0
8	С	2	NAG	1	0
17	S	1	NAG	14	0
9	F	1	NAG	1	0
10	Н	3	BMA	2	0
12	Κ	2	NAG	1	0
8	J	2	NAG	1	0
10	U	3	BMA	3	0
10	Н	4	MAN	1	0
17	S	2	NAG	2	0
15	N	2	NAG	2	0
14	М	1	NAG	2	0
11	Ι	1	NAG	1	0
9	F	6	MAN	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)

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 expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	NAG	В	701	1	14,14,15	0.29	0	17,19,21	0.63	0
19	NAG	G	658	4	14,14,15	0.34	0	17,19,21	0.93	0
19	NAG	G	671	4	14,14,15	0.31	0	17,19,21	0.84	0
19	NAG	G	657	4	14,14,15	0.29	0	17,19,21	0.77	0



In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	NAG	В	701	1	-	2/6/23/26	0/1/1/1
19	NAG	G	658	4	-	3/6/23/26	0/1/1/1
19	NAG	G	671	4	-	3/6/23/26	0/1/1/1
19	NAG	G	657	4	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	В	701	NAG	C8-C7-N2-C2
19	В	701	NAG	O7-C7-N2-C2
19	G	671	NAG	C3-C2-N2-C7
19	G	671	NAG	C8-C7-N2-C2
19	G	671	NAG	O7-C7-N2-C2
19	G	658	NAG	C8-C7-N2-C2
19	G	657	NAG	C8-C7-N2-C2
19	G	658	NAG	O7-C7-N2-C2
19	G	657	NAG	O7-C7-N2-C2
19	G	658	NAG	C1-C2-N2-C7
19	G	657	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	G	671	NAG	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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.











































6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

