

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

#### Aug 26, 2024 – 02:26 PM JST

PDB ID	:	8ZER
Title	:	Crystal structure of the complex of Wuhan SARS-CoV-2 RBD (319-541) with
		P2C5 nanobody
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Deposited on	:	2024-05-06
Resolution	:	3.10 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
$\mathrm{EDS}$	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

# 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 3.10 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.



Metric	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	164625	1351 (3.10-3.10)
Clashscore	180529	1454 (3.10-3.10)
Ramachandran outliers	177936	1391 (3.10-3.10)
Sidechain outliers	177891	1391 (3.10-3.10)
RSRZ outliers	164620	1351 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain								
1	В	235	3% 57%	21%	•• 17%						
1	С	235	5%	20% 5%	• 18%						
1	Е	235	4% 53%	23% 6	% • 17%						
1	G	235	9%	18% 8%	• 18%						
1	Ι	235	6%	17%	• 18%						
2	А	146	% 63%	15%	•• 18%						



Contr	nueu jron	i previous	paye			
$\mathbf{Mol}$	Chain	Length	Quality of chain			
2	D	146	65%	14%	••	18%
2	F	146	2% 67%	12%	•	18%
2	Н	146	2% 65%	15%	••	16%
2	J	146	6% 70%	9%	·	18%
3	К	3	100%			
3	Ν	3	100%			
4	L	2	100%			
4	М	2	100%			
5	О	7	100%			



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# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12475 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		At	oms			ZeroOcc	AltConf	Trace
1	р	105	Total	С	Ν	0	S	0	1	0
	D	195	1542	988	259	287	8	0	1	0
1	С	102	Total	С	Ν	Ο	S	0	0	0
1		192	1514	972	252	282	8	0	0	0
1	F	104	Total	С	Ν	0	S	0	0	0
1	Ľ	194	1525	977	254	286	8	0	0	0
1	C	102	Total	С	Ν	0	S	0	0	0
1	G	192	1520	976	253	283	8	0	0	0
1	т	103	Total	С	Ν	0	S	0	0	0
	1	195	1521	975	253	285	8		U	0

• Molecule 1 is a protein called Spike protein S1.

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	542	GLY	-	expression tag	UNP P0DTC2
В	543	SER	-	expression tag	UNP P0DTC2
В	544	HIS	-	expression tag	UNP P0DTC2
В	545	HIS	-	expression tag	UNP P0DTC2
В	546	HIS	-	expression tag	UNP P0DTC2
В	547	HIS	-	expression tag	UNP P0DTC2
В	548	HIS	-	expression tag	UNP P0DTC2
В	549	HIS	-	expression tag	UNP P0DTC2
В	550	HIS	-	expression tag	UNP P0DTC2
В	551	HIS	-	expression tag	UNP P0DTC2
В	552	HIS	-	expression tag	UNP P0DTC2
В	553	HIS	-	expression tag	UNP P0DTC2
С	542	GLY	-	expression tag	UNP P0DTC2
С	543	SER	-	expression tag	UNP P0DTC2
С	544	HIS	-	expression tag	UNP P0DTC2
С	545	HIS	-	expression tag	UNP P0DTC2
C	546	HIS	-	expression tag	UNP P0DTC2
С	547	HIS	-	expression tag	UNP P0DTC2
С	548	HIS	-	expression tag	UNP P0DTC2



Chain	Residue	Modelled	Actual	Comment	Reference
C	549	HIS	_	expression tag	UNP P0DTC2
C	550	HIS	_	expression tag	UNP P0DTC2
C	551	HIS	-	expression tag	UNP P0DTC2
С	552	HIS	-	expression tag	UNP P0DTC2
С	553	HIS	_	expression tag	UNP P0DTC2
Е	542	GLY	_	expression tag	UNP P0DTC2
Е	543	SER	_	expression tag	UNP P0DTC2
Е	544	HIS	-	expression tag	UNP P0DTC2
Е	545	HIS	-	expression tag	UNP P0DTC2
Е	546	HIS	-	expression tag	UNP P0DTC2
Е	547	HIS	-	expression tag	UNP P0DTC2
Е	548	HIS	-	expression tag	UNP P0DTC2
Е	549	HIS	-	expression tag	UNP P0DTC2
Е	550	HIS	-	expression tag	UNP P0DTC2
Е	551	HIS	-	expression tag	UNP P0DTC2
Е	552	HIS	-	expression tag	UNP P0DTC2
Е	553	HIS	-	expression tag	UNP P0DTC2
G	542	GLY	-	expression tag	UNP P0DTC2
G	543	SER	-	expression tag	UNP P0DTC2
G	544	HIS	-	expression tag	UNP P0DTC2
G	545	HIS	-	expression tag	UNP P0DTC2
G	546	HIS	-	expression tag	UNP P0DTC2
G	547	HIS	-	expression tag	UNP P0DTC2
G	548	HIS	-	expression tag	UNP P0DTC2
G	549	HIS	-	expression tag	UNP P0DTC2
G	550	HIS	-	expression tag	UNP P0DTC2
G	551	HIS	-	expression tag	UNP P0DTC2
G	552	HIS	-	expression tag	UNP P0DTC2
G	553	HIS	-	expression tag	UNP P0DTC2
I	542	GLY	-	expression tag	UNP P0DTC2
Ι	543	SER	-	expression tag	UNP P0DTC2
I	544	HIS	-	expression tag	UNP P0DTC2
I	545	HIS	-	expression tag	UNP P0DTC2
I	546	HIS	-	expression tag	UNP P0DTC2
I	547	HIS	-	expression tag	UNP P0DTC2
I	548	HIS	-	expression tag	UNP P0DTC2
I	549	HIS	-	expression tag	UNP P0DTC2
I	550	HIS	-	expression tag	UNP P0DTC2
I	551	HIS	-	expression tag	UNP P0DTC2
Ī	552	HIS	-	expression tag	UNP P0DTC2
Ι	553	HIS	-	expression tag	UNP P0DTC2

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• Molecule 2 is a protein called Nanobody P2C5.



Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
0	0 A	120	Total	С	Ν	0	S	0	0	0
	A		922	572	157	186	$\overline{7}$	0	0	0
0	Л	120	Total	С	Ν	0	S	0	1	0
	2 D	120	929	575	160	187	7	0	1	0
0	Б	120	Total	С	Ν	0	S	0	0	0
	Г	120	914	567	155	185	$\overline{7}$	0	0	0
0	ц	192	Total	С	Ν	0	S	0	0	0
		125	945	585	161	192	$\overline{7}$	0	0	0
0	т	120	Total	С	Ν	0	S	0	1	0
	J	120	923	572	157	187	$\overline{7}$		1	U

• Molecule 3 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
3	Κ	3	Total 39	C 22	N 2	O 15	0	0	0
3	Ν	3	Total 39	C 22	N 2	O 15	0	0	0

• Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	L	2	Total 28	C 16	N 2	O 10	0	0	0
4	М	2	Total 28	C 16	N 2	O 10	0	0	0

• Molecule 5 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-b eta-D-glucopyranose-(1-4)-beta-D-mannopyranose-(1-4)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-de oxy-beta-D-glucopyranose.





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	Ο	7	Total 86	C 48	N 3	O 35	0	0	0



# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.



• Molecule 1: Spike protein S1





• Molecule 3: beta-D<br/>-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:	100%
NAG1 NAG2 BMA3	

• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:

100%

#### NAG1 NAG2 BMA3

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

Chain L:

100%



#### NAG1 NAG2

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

Chain M:

100%

#### NAG1 NAG2

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

Chain O:

100%

NAG1 NAG2 BMA3 BMA4 BMA4 NAG5 GAL6 GAL6 BMA7



# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	72.48Å 177.46Å 209.86Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Bosolution (Å)	45.17 - 3.10	Depositor
Itesolution (A)	45.17 - 3.10	EDS
% Data completeness	98.7 (45.17-3.10)	Depositor
(in resolution range)	98.7 (45.17 - 3.10)	EDS
$R_{merge}$	0.18	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.75 (at 3.12 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
B B.	0.222 , $0.283$	Depositor
$\Pi, \Pi_{free}$	0.224 , $0.284$	DCC
$R_{free}$ test set	2386 reflections $(4.83%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	76.1	Xtriage
Anisotropy	0.683	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.29, 46.3	EDS
L-test for $twinning^2$	$ < L >=0.46, < L^2>=0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	12475	wwPDB-VP
Average B, all atoms $(Å^2)$	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.50% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities 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: NAG, GAL, 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).

Mal	Chain	Bond lengths		Bond angles		
WIOI	Unain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	В	0.83	1/1591~(0.1%)	1.56	22/2167~(1.0%)	
1	С	0.87	1/1557~(0.1%)	1.59	25/2120~(1.2%)	
1	Ε	0.88	2/1568~(0.1%)	1.62	31/2137~(1.5%)	
1	G	0.86	4/1563~(0.3%)	1.66	37/2128~(1.7%)	
1	Ι	0.80	0/1564	1.53	21/2132~(1.0%)	
2	А	0.76	1/941~(0.1%)	1.53	14/1272~(1.1%)	
2	D	0.81	2/952~(0.2%)	1.73	27/1287~(2.1%)	
2	F	0.79	1/933~(0.1%)	1.62	17/1263~(1.3%)	
2	Н	0.77	0/964	1.57	15/1303~(1.2%)	
2	J	0.82	1/946~(0.1%)	1.53	8/1280~(0.6%)	
All	All	0.83	13/12579~(0.1%)	1.60	217/17089~(1.3%)	

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	В	0	8
1	С	0	6
1	Ε	0	7
1	G	0	10
1	Ι	0	6
2	А	0	5
2	D	0	5
2	F	0	3
2	Н	0	4
2	J	0	4
All	All	0	58

All (13) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Е	417	LYS	CB-CG	7.90	1.73	1.52
2	J	35	SER	CA-CB	-6.74	1.42	1.52
1	G	346	ARG	NE-CZ	6.30	1.41	1.33
1	В	468	ILE	CB-CG1	-5.94	1.37	1.54
2	D	46	GLU	CG-CD	5.79	1.60	1.51
1	Е	383	SER	CA-CB	5.69	1.61	1.52
1	G	525	CYS	C-O	5.62	1.34	1.23
1	С	484	GLU	CD-OE2	5.52	1.31	1.25
1	G	399	SER	CA-CB	5.52	1.61	1.52
2	А	35	SER	CA-CB	-5.46	1.44	1.52
2	F	35	SER	CA-CB	-5.16	1.45	1.52
2	D	104	GLU	CD-OE2	5.11	1.31	1.25
1	G	484	GLU	CD-OE1	5.04	1.31	1.25

All (217) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	G	346	ARG	NE-CZ-NH1	15.11	127.85	120.30
1	В	466	ARG	NE-CZ-NH1	12.49	126.54	120.30
1	В	466	ARG	NE-CZ-NH2	-11.75	114.42	120.30
2	F	92	MET	CG-SD-CE	11.70	118.92	100.20
1	Е	417	LYS	CB-CG-CD	11.11	140.49	111.60
1	Ι	355	ARG	NE-CZ-NH1	11.09	125.84	120.30
1	Е	355	ARG	NE-CZ-NH1	10.81	125.71	120.30
1	G	346	ARG	CD-NE-CZ	10.57	138.40	123.60
1	С	408	ARG	NE-CZ-NH1	10.56	125.58	120.30
1	Е	355	ARG	NE-CZ-NH2	-10.21	115.19	120.30
2	F	29	TYR	CB-CG-CD1	9.97	126.98	121.00
2	Н	52	ARG	NE-CZ-NH1	9.88	125.24	120.30
2	D	38	ARG	NE-CZ-NH2	-9.72	115.44	120.30
2	D	46	GLU	CG-CD-OE2	9.50	137.30	118.30
2	F	104	GLU	CB-CA-C	9.30	129.00	110.40
2	F	71	ARG	NE-CZ-NH1	-9.22	115.69	120.30
1	G	471	GLU	N-CA-CB	9.19	127.15	110.60
1	С	355	ARG	NE-CZ-NH1	9.13	124.86	120.30
2	А	38	ARG	NE-CZ-NH1	9.09	124.84	120.30
1	Ι	355	ARG	NE-CZ-NH2	-8.81	115.89	120.30
2	А	27	TYR	CB-CA-C	8.78	127.95	110.40
2	D	46	GLU	OE1-CD-OE2	-8.76	112.79	123.30
2	F	29	TYR	CB-CG-CD2	-8.59	115.84	121.00
1	В	471	GLU	N-CA-CB	8.59	126.06	110.60
1	С	517	LEU	CB-CG-CD2	8.58	125.58	111.00
1	Е	471	GLU	N-CA-CB	8.55	125.99	110.60



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	Н	45	ARG	NE-CZ-NH1	8.55	124.58	120.30
1	С	417	LYS	CD-CE-NZ	8.30	130.79	111.70
2	Н	52	ARG	NE-CZ-NH2	-8.20	116.20	120.30
1	G	458	LYS	CA-CB-CG	7.95	130.88	113.40
2	F	27	TYR	CA-CB-CG	7.93	128.46	113.40
2	D	27	TYR	CB-CA-C	7.91	126.21	110.40
2	А	66	ARG	NE-CZ-NH1	7.78	124.19	120.30
2	F	27	TYR	CB-CA-C	7.71	125.81	110.40
2	J	27	TYR	CB-CA-C	7.67	125.73	110.40
1	В	420	ASP	CB-CA-C	7.66	125.71	110.40
2	D	19	ARG	CG-CD-NE	7.63	127.83	111.80
1	G	517	LEU	CB-CG-CD2	7.61	123.94	111.00
1	С	415	THR	CA-CB-CG2	7.61	123.05	112.40
1	С	509	ARG	NE-CZ-NH1	7.49	124.04	120.30
2	D	104	GLU	CB-CA-C	7.40	125.20	110.40
2	Н	27	TYR	CB-CA-C	7.34	125.08	110.40
1	G	354	ASN	CB-CA-C	-7.29	95.83	110.40
2	D	71[A]	ARG	N-CA-CB	-7.28	97.50	110.60
2	D	71[B]	ARG	N-CA-CB	-7.28	97.50	110.60
2	D	46	GLU	CB-CG-CD	7.26	133.80	114.20
2	D	28	THR	OG1-CB-CG2	7.23	126.63	110.00
1	G	355	ARG	NE-CZ-NH1	7.20	123.90	120.30
2	А	18	LEU	CB-CG-CD1	7.17	123.19	111.00
2	Н	59	TYR	CB-CG-CD2	7.17	125.30	121.00
2	D	52	ARG	NE-CZ-NH2	-7.14	116.73	120.30
2	А	34	MET	CG-SD-CE	7.08	111.53	100.20
2	D	29	TYR	CB-CG-CD1	7.03	125.22	121.00
2	D	71[A]	ARG	CG-CD-NE	6.98	126.45	111.80
2	D	71[B]	ARG	CG-CD-NE	6.98	126.45	111.80
1	Ε	398	ASP	CB-CG-OD1	-6.94	112.05	118.30
2	Н	104	GLU	CB-CA-C	6.92	124.23	110.40
1	С	417	LYS	CA-CB-CG	6.91	128.60	113.40
1	Ε	405	ASP	CB-CA-C	6.91	124.21	110.40
1	Ι	337	PRO	N-CA-CB	-6.87	95.04	102.60
2	F	45	ARG	NE-CZ-NH1	6.87	123.73	120.30
2	D	13	GLN	CB-CA-C	6.86	124.12	110.40
1	Е	427	ASP	CB-CA-C	6.85	124.10	110.40
1	С	351	TYR	N-CA-CB	6.84	122.90	110.60
1	С	506	GLN	CB-CA-C	6.83	124.06	110.40
1	Е	363	ALA	N-CA-CB	6.79	119.60	110.10
2	F	104	GLU	CB-CG-CD	6.75	132.42	114.20
1	Ι	509	ARG	NE-CZ-NH1	6.74	123.67	120.30



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Conti	Continued from previous page							
Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$	
1	Е	466	ARG	NE-CZ-NH1	6.73	123.67	120.30	
1	Е	403	ARG	NE-CZ-NH2	-6.72	116.94	120.30	
2	D	13	GLN	N-CA-CB	-6.71	98.51	110.60	
2	А	38	ARG	NE-CZ-NH2	-6.70	116.95	120.30	
1	G	346	ARG	CA-CB-CG	6.69	128.12	113.40	
1	G	346	ARG	CG-CD-NE	6.68	125.83	111.80	
1	Ι	491	PRO	N-CA-CB	-6.64	95.29	102.60	
2	J	52	ARG	NE-CZ-NH2	-6.62	116.99	120.30	
1	В	506	GLN	CB-CA-C	6.59	123.58	110.40	
1	G	398	ASP	CB-CG-OD1	-6.59	112.37	118.30	
1	В	466	ARG	CD-NE-CZ	6.58	132.81	123.60	
1	В	415	THR	CA-CB-OG1	-6.56	95.23	109.00	
1	Ι	351	TYR	N-CA-CB	6.56	122.40	110.60	
1	В	398	ASP	CB-CG-OD1	-6.53	112.42	118.30	
1	G	491	PRO	N-CA-CB	-6.50	95.45	102.60	
2	J	38	ARG	NE-CZ-NH1	6.45	123.53	120.30	
1	Ι	398	ASP	CB-CG-OD1	-6.44	112.50	118.30	
2	Н	108	GLN	CB-CA-C	6.44	123.28	110.40	
1	Е	506	GLN	CB-CA-C	6.41	123.21	110.40	
2	F	66	ARG	NE-CZ-NH1	6.41	123.50	120.30	
2	А	71	ARG	CB-CA-C	6.40	123.20	110.40	
1	В	355	ARG	CD-NE-CZ	6.39	132.55	123.60	
1	С	403	ARG	CG-CD-NE	6.39	125.23	111.80	
1	G	405	ASP	CB-CA-C	6.39	123.18	110.40	
1	Е	355	ARG	CD-NE-CZ	6.39	132.54	123.60	
1	Е	523	THR	N-CA-CB	6.38	122.42	110.30	
1	С	471	GLU	N-CA-CB	6.35	122.04	110.60	
2	А	92	MET	CG-SD-CE	6.35	110.35	100.20	
2	Н	20	LEU	CB-CG-CD2	6.33	121.76	111.00	
1	G	471	GLU	CB-CA-C	-6.33	97.75	110.40	
2	D	38	ARG	NE-CZ-NH1	6.30	123.45	120.30	
1	Е	403	ARG	CB-CA-C	-6.30	97.81	110.40	
2	Н	92	MET	CG-SD-CE	6.29	110.26	100.20	
1	G	506	GLN	CB-CA-C	6.28	122.96	110.40	
1	Ι	471	GLU	N-CA-CB	6.26	121.88	110.60	
1	Ι	466	ARG	NE-CZ-NH1	6.25	123.42	120.30	
1	С	398	ASP	CB-CG-OD1	-6.17	112.75	118.30	
1	G	379	CYS	CB-CA-C	6.15	122.71	110.40	
1	С	374	PHE	N-CA-CB	6.15	121.67	110.60	
1	С	335	LEU	CB-CG-CD1	6.15	121.46	111.00	
1	В	405	ASP	CB-CA-C	6.12	122.63	110.40	
1	Е	346	ARG	CD-NE-CZ	6.08	132.12	123.60	



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Ι	506	GLN	CB-CA-C	6.08	122.56	110.40
1	G	337	PRO	N-CA-CB	-6.08	95.91	102.60
1	G	427	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	G	357	ARG	NE-CZ-NH2	5.92	123.26	120.30
1	С	451	TYR	CB-CG-CD1	-5.91	117.45	121.00
1	Ι	405	ASP	CB-CA-C	5.90	122.20	110.40
1	В	525	CYS	CB-CA-C	5.85	122.11	110.40
2	J	60	THR	CA-CB-OG1	-5.85	96.72	109.00
1	G	462	LYS	CB-CG-CD	5.83	126.75	111.60
1	Е	387	LEU	N-CA-CB	5.82	122.03	110.40
1	В	415	THR	OG1-CB-CG2	5.81	123.37	110.00
1	G	523	THR	N-CA-CB	5.81	121.33	110.30
1	Ι	523	THR	N-CA-CB	5.80	121.31	110.30
1	G	427	ASP	CB-CA-C	5.79	121.98	110.40
1	Ι	470	THR	OG1-CB-CG2	5.79	123.32	110.00
1	G	386	LYS	CA-CB-CG	5.78	126.11	113.40
1	G	466	ARG	NE-CZ-NH1	5.77	123.19	120.30
2	А	27	TYR	CA-CB-CG	5.75	124.33	113.40
1	В	357	ARG	NE-CZ-NH1	-5.74	117.43	120.30
1	С	355	ARG	CD-NE-CZ	5.74	131.63	123.60
2	J	37	TYR	CB-CG-CD1	5.74	124.44	121.00
1	С	454	ARG	NE-CZ-NH1	-5.73	117.44	120.30
1	G	362	VAL	N-CA-CB	5.72	124.08	111.50
1	G	408	ARG	NE-CZ-NH1	5.72	123.16	120.30
2	D	52	ARG	NE-CZ-NH1	5.71	123.16	120.30
2	D	53	ARG	N-CA-CB	5.71	120.88	110.60
1	В	403	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	Ι	424	LYS	N-CA-CB	5.68	120.82	110.60
1	В	457	ARG	NE-CZ-NH1	-5.67	117.47	120.30
2	D	60	THR	CA-CB-OG1	-5.65	97.14	109.00
2	J	27	TYR	CA-CB-CG	5.64	124.11	113.40
1	Е	466	ARG	NE-CZ-NH2	-5.63	117.49	120.30
2	F	71	ARG	CB-CA-C	5.62	121.63	110.40
1	В	387	LEU	N-CA-CB	5.60	121.61	110.40
1	G	483	VAL	CA-CB-CG2	5.59	119.29	110.90
1	G	357	ARG	NE-CZ-NH1	-5.58	117.51	120.30
2	Н	108	GLN	N-CA-CB	-5.55	100.60	110.60
2	F	104	GLU	CG-CD-OE1	5.55	129.40	118.30
2	Н	45	ARG	N-CA-CB	5.54	120.58	110.60
1	В	523	THR	N-CA-CB	5.54	120.83	110.30
2	J	45	ARG	NE-CZ-NH1	5.53	123.06	120.30
2	А	53	ARG	N-CA-CB	5.52	120.54	110.60



Continued from previous page... Mol Chain Res Type Atoms

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Ε	424	LYS	N-CA-CB	5.51	120.51	110.60
1	G	377	PHE	CB-CG-CD2	-5.50	116.95	120.80
2	Н	66	ARG	NE-CZ-NH1	5.49	123.05	120.30
2	А	2	VAL	N-CA-CB	5.49	123.58	111.50
1	Е	525	CYS	CB-CA-C	5.49	121.37	110.40
2	F	66	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	С	523	THR	N-CA-CB	5.48	120.71	110.30
1	G	335	LEU	N-CA-CB	5.47	121.34	110.40
1	Ι	390	LEU	CB-CG-CD2	5.42	120.21	111.00
2	D	28	THR	CA-CB-OG1	-5.39	97.68	109.00
1	Е	351	TYR	CB-CG-CD2	5.38	124.23	121.00
2	А	53	ARG	CG-CD-NE	5.38	123.09	111.80
1	G	470	THR	CA-CB-OG1	-5.37	97.73	109.00
1	С	483	VAL	N-CA-CB	5.36	123.28	111.50
2	А	105	TYR	CA-CB-CG	5.36	123.58	113.40
1	С	525	CYS	CB-CA-C	5.35	121.09	110.40
1	С	457	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	С	337	PRO	N-CA-CB	-5.33	96.74	102.60
1	G	403	ARG	NE-CZ-NH2	-5.32	117.64	120.30
2	D	45	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	Е	513	LEU	CB-CG-CD2	5.31	120.03	111.00
1	Ε	379	CYS	CB-CA-C	5.30	121.01	110.40
1	В	427	ASP	CB-CA-C	5.29	120.99	110.40
1	Ι	363	ALA	N-CA-CB	5.29	117.50	110.10
1	G	365	TYR	CB-CG-CD2	5.27	124.16	121.00
1	Е	340	GLU	CG-CD-OE1	5.26	128.83	118.30
2	Н	46	GLU	CB-CA-C	5.26	120.92	110.40
2	D	29	TYR	CB-CG-CD2	-5.25	117.85	121.00
1	С	491	PRO	N-CA-CB	-5.24	96.84	102.60
1	С	466	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	Ι	417	LYS	CB-CG-CD	5.22	125.17	111.60
1	В	424	LYS	CD-CE-NZ	5.21	123.67	111.70
2	D	71[A]	ARG	CA-CB-CG	5.20	124.84	113.40
2	D	71[B]	ARG	CA-CB-CG	5.20	124.84	113.40
1	Е	369	TYR	CA-CB-CG	5.20	123.28	113.40
2	J	27	TYR	N-CA-CB	-5.20	101.24	110.60
1	В	483	VAL	N-CA-CB	5.20	122.93	111.50
1	Ι	355	ARG	CD-NE-CZ	5.20	130.87	123.60
1	Ι	445	VAL	CA-CB-CG2	5.18	118.68	110.90
1	Е	517	LEU	CB-CG-CD2	5.18	119.81	111.00
2	D	53	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	Е	351	TYR	CB-CG-CD1	-5.18	117.89	121.00



Mol	Chain	$\operatorname{Res}$	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	F	45	ARG	N-CA-CB	5.17	119.91	110.60
1	Е	491	PRO	N-CA-CB	-5.17	96.92	102.60
2	F	46	GLU	CB-CA-C	5.16	120.72	110.40
1	G	387	LEU	N-CA-CB	5.14	120.69	110.40
2	А	53	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	G	500	THR	OG1-CB-CG2	5.13	121.79	110.00
2	Н	29	TYR	N-CA-CB	-5.12	101.38	110.60
1	Е	385	THR	CA-CB-CG2	5.12	119.56	112.40
1	Ι	387	LEU	CB-CG-CD1	5.11	119.69	111.00
1	С	385	THR	CA-CB-CG2	5.11	119.55	112.40
1	В	484	GLU	OE1-CD-OE2	5.10	129.42	123.30
1	G	407	VAL	CA-CB-CG2	5.09	118.53	110.90
1	В	408	ARG	NE-CZ-NH2	-5.08	117.76	120.30
2	F	71	ARG	CD-NE-CZ	5.08	130.71	123.60
2	F	108	GLN	CB-CA-C	5.08	120.55	110.40
2	Н	106	LEU	CB-CG-CD2	-5.07	102.37	111.00
1	G	509	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	G	467	ASP	CB-CG-OD1	5.05	122.85	118.30
1	Е	403	ARG	NE-CZ-NH1	5.03	122.82	120.30
2	D	105	TYR	CB-CG-CD1	-5.03	117.98	121.00
1	Е	387	LEU	CB-CG-CD1	5.03	119.54	111.00
1	Ι	470	THR	CA-CB-OG1	-5.01	98.47	109.00
1	Е	340	GLU	CG-CD-OE2	-5.01	108.28	118.30

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There are no chirality outliers.

$\mathbf{Mol}$	Chain	Res	Type	Group
2	А	101	SER	Peptide
2	А	2	VAL	Mainchain
2	А	45	ARG	Sidechain
2	А	52	ARG	Sidechain
2	А	9	GLY	Peptide
1	В	333	THR	Peptide
1	В	357	ARG	Sidechain
1	В	371	SER	Peptide
1	В	381	GLY	Peptide
1	В	408	ARG	Sidechain
1	В	466	ARG	Sidechain
1	В	476	GLY	Peptide
1	В	526	GLY	Peptide
1	С	346	ARG	Sidechain



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Mol	Chain	Res	Type	Group
1	С	357	ARG	Sidechain
1	С	371	SER	Peptide
1	С	381	GLY	Peptide
1	С	476	GLY	Peptide
1	С	519	HIS	Peptide
2	D	101	SER	Peptide
2	D	19	ARG	Sidechain
2	D	52	ARG	Sidechain
2	D	71[A]	ARG	Sidechain
2	D	71[B]	ARG	Sidechain
1	Е	357	ARG	Sidechain
1	Е	371	SER	Peptide
1	Е	379	CYS	Mainchain
1	Е	381	GLY	Peptide
1	Е	408	ARG	Sidechain
1	Е	466	ARG	Sidechain
1	Е	476	GLY	Peptide
2	F	101	SER	Peptide
2	F	52	ARG	Sidechain
2	F	71	ARG	Sidechain
1	G	346	ARG	Sidechain
1	G	357	ARG	Sidechain
1	G	371	SER	Peptide
1	G	379	CYS	Mainchain
1	G	381	GLY	Peptide
1	G	408	ARG	Sidechain
1	G	466	ARG	Sidechain
1	G	476	GLY	Peptide
1	G	483	VAL	Peptide
1	G	519	HIS	Peptide
2	Н	101	SER	Peptide
2	Н	122	ALA	Peptide
2	Н	52	ARG	Sidechain
2	Н	53	ARG	Sidechain
1	Ι	357	ARG	Sidechain
1	Ι	371	SER	Peptide
1	Ι	381	GLY	Peptide
1	Ι	408	ARG	Sidechain
1	Ι	466	ARG	Sidechain
1	Ι	476	GLY	Peptide
2	J	101	SER	Peptide
2	J	52	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	J	53	ARG	Sidechain
2	J	66	ARG	Sidechain

### 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	В	1542	0	1455	12	0
1	С	1514	0	1426	10	0
1	Е	1525	0	1428	10	0
1	G	1520	0	1435	13	0
1	Ι	1521	0	1425	7	0
2	А	922	0	860	9	0
2	D	929	0	864	8	0
2	F	914	0	843	4	0
2	Н	945	0	885	7	0
2	J	923	0	853	3	0
3	K	39	0	34	0	0
3	N	39	0	34	0	0
4	L	28	0	25	0	0
4	М	28	0	25	0	0
5	0	86	0	73	0	0
All	All	12475	0	11665	74	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 3.

All (74) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:466:ARG:HH21	2:J:106:LEU:HD22	1.59	0.68
2:A:53:ARG:HH11	2:A:53:ARG:HB3	1.59	0.67
1:I:425:LEU:HD21	1:I:512:VAL:HG11	1.85	0.58
2:D:19:ARG:HH11	2:D:19:ARG:HG3	1.68	0.58
1:B:406:GLU:OE2	1:B:495:TYR:OH	2.22	0.56
2:A:53:ARG:HH11	2:A:53:ARG:CB	2.19	0.56



A 4 1	A 4 D	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:470:THR:HG21	2:A:50:ILE:HD11	1.88	0.54
1:C:406:GLU:OE2	1:C:495:TYR:OH	2.22	0.53
1:G:425:LEU:HD21	1:G:512:VAL:HG11	1.91	0.53
2:H:53:ARG:HB3	2:H:53:ARG:HH11	1.74	0.52
1:B:425:LEU:HD21	1:B:512:VAL:HG11	1.91	0.52
1:I:480:CYS:O	1:I:483:VAL:HG22	2.10	0.52
1:C:466:ARG:HH21	2:D:106:LEU:HD13	1.75	0.51
1:C:425:LEU:HD21	1:C:512:VAL:HG11	1.91	0.51
2:H:49:SER:HB3	2:H:59:TYR:HD1	1.75	0.51
2:F:82:MET:HB3	2:F:85:LEU:HD21	1.94	0.50
1:G:466:ARG:HH21	2:H:106:LEU:HD22	1.77	0.50
2:H:28:THR:HG21	2:H:32:TYR:HE2	1.77	0.49
2:J:70:SER:OG	2:J:79:TYR:HB2	2.13	0.49
1:I:522:ALA:O	1:I:523:THR:HG23	2.12	0.49
1:B:341:VAL:HG11	1:B:397:ALA:HB1	1.95	0.47
1:G:375:SER:HB3	1:G:436:TRP:HA	1.96	0.47
1:E:522:ALA:O	1:E:523:THR:HG23	2.15	0.47
2:H:53:ARG:HH11	2:H:53:ARG:CB	2.28	0.47
1:C:470:THR:O	1:C:471:GLU:HB2	2.16	0.46
1:G:380:TYR:CE2	1:G:412:PRO:HD2	2.50	0.46
1:G:384:PRO:HA	1:G:387:LEU:HG	1.96	0.46
1:G:410:ILE:O	1:G:433:VAL:HG21	2.16	0.46
2:A:82:MET:HB3	2:A:85:LEU:HD21	1.97	0.46
2:D:82:MET:HB3	2:D:85:LEU:HD21	1.98	0.46
1:C:522:ALA:O	1:C:523:THR:HG23	2.16	0.46
1:B:468:ILE:HD12	2:A:99:ALA:HB3	1.98	0.46
2:F:53:ARG:HH11	2:F:53:ARG:HB3	1.81	0.46
1:G:362:VAL:HG12	1:G:525:CYS:C	2.36	0.46
1:G:474:GLN:HE22	1:G:479:PRO:HA	1.81	0.46
1:E:410:ILE:HD11	1:E:418:ILE:HG21	1.97	0.45
2:F:53:ARG:HH11	2:F:53:ARG:CB	2.29	0.45
1:B:522:ALA:O	1:B:523:THR:HG23	2.16	0.45
1:I:341:VAL:HG11	1:I:397:ALA:HB1	1.99	0.45
1:G:426:PRO:HD3	1:G:464:PHE:CE2	2.51	0.45
1:I:470:THR:O	1:I:471:GLU:CB	2.65	0.45
1:B:468:ILE:HD12	2:A:99:ALA:CB	2.47	0.44
1:C:466:ARG:NH2	2:D:106:LEU:HD22	2.32	0.44
2:H:82:MET:HB3	2:H:85:LEU:HD21	1.98	0.44
1:E:380:TYR:CE2	1:E:412:PRO:HD2	2.53	0.44
1:B:380:TYR:CE2	1:B:412:PRO:HD2	2.53	0.43
1:B:468:ILE:HD11	2:A:100:CYS:HA	1.99	0.43



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:E:470:THR:O	1:E:471:GLU:HB2	2.17	0.43	
1:B:492:LEU:HD13	2:A:98:TRP:CZ3	2.53	0.43	
1:E:382:VAL:HG12	1:E:386:LYS:NZ	2.33	0.43	
1:G:470:THR:O	1:G:471:GLU:CB	2.67	0.43	
2:H:9:GLY:H	2:H:18:LEU:HD11	1.84	0.43	
1:G:522:ALA:O	1:G:523:THR:HG23	2.19	0.43	
1:I:354:ASN:O	1:I:398:ASP:HA	2.20	0.42	
2:D:4:LEU:HB3	2:D:95:CYS:SG	2.59	0.42	
1:E:425:LEU:HD21	1:E:512:VAL:HG11	2.01	0.42	
1:E:457:ARG:CZ	1:E:461:LEU:HD23	2.50	0.42	
1:C:354:ASN:O	1:C:398:ASP:HA	2.19	0.42	
1:C:453:TYR:CZ	1:C:493:GLN:HB2	2.55	0.42	
1:C:470:THR:O	1:C:471:GLU:CB	2.67	0.42	
2:D:71[A]:ARG:HH11	2:D:71[A]:ARG:HD2	1.67	0.41	
2:D:71[B]:ARG:HH11	2:D:71[B]:ARG:HG2	1.85	0.41	
2:F:29:TYR:CD1	2:F:29:TYR:N	2.87	0.41	
1:G:457:ARG:CZ	1:G:461:LEU:HD23	2.50	0.41	
1:B:384:PRO:HA	1:B:387:LEU:HG	2.02	0.41	
1:E:354:ASN:O	1:E:398:ASP:HA	2.20	0.41	
2:A:34:MET:HB3	2:A:78:LEU:HD22	2.02	0.41	
1:E:358:ILE:HB	1:E:395:VAL:HB	2.02	0.41	
1:C:380:TYR:HE1	1:C:433:VAL:HG23	1.85	0.41	
1:E:364:ASP:OD2	1:E:367:VAL:HG23	2.21	0.41	
1:G:354:ASN:O	1:G:398:ASP:HA	2.21	0.41	
1:B:470:THR:O	1:B:471:GLU:HB2	2.21	0.40	
2:D:90:THR:HG23	2:D:118:THR:HA	2.04	0.40	
2:J:73:ASN:OD1	2:J:73:ASN:N	2.52	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	entiles
1	В	194/235~(83%)	161 (83%)	21 (11%)	12~(6%)	1	7
1	С	190/235~(81%)	157 (83%)	22 (12%)	11 (6%)	1	8
1	Ε	192/235~(82%)	158 (82%)	21 (11%)	13 (7%)	1	6
1	G	190/235~(81%)	158 (83%)	21 (11%)	11 (6%)	1	8
1	Ι	191/235~(81%)	162 (85%)	19 (10%)	10~(5%)	1	10
2	А	118/146~(81%)	111 (94%)	7 (6%)	0	100	100
2	D	119/146~(82%)	113~(95%)	6 (5%)	0	100	100
2	F	118/146~(81%)	110 (93%)	8 (7%)	0	100	100
2	Н	121/146~(83%)	112 (93%)	8 (7%)	1 (1%)	16	48
2	J	119/146~(82%)	110 (92%)	9 (8%)	0	100	100
All	All	1552/1905~(82%)	1352 (87%)	142 (9%)	58 (4%)	2	16

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	363	ALA
1	В	372	ALA
1	С	363	ALA
1	С	372	ALA
1	С	417	LYS
1	С	519	HIS
1	Е	363	ALA
1	Ε	372	ALA
1	Ε	519	HIS
1	G	372	ALA
1	G	471	GLU
1	G	519	HIS
1	Ι	335	LEU
1	Ι	363	ALA
1	Ι	372	ALA
1	В	471	GLU
1	В	519	HIS
1	В	523	THR
1	С	471	GLU
1	С	523	THR
1	Е	471	GLU
1	Е	523	THR
1	G	335	LEU
1	G	472	ILE



Mol	Chain	Res	Type
1	G	523	THR
1	Ι	471	GLU
1	Ι	519	HIS
1	Ι	523	THR
1	В	339	GLY
1	В	362	VAL
1	Е	417	LYS
1	В	478	THR
1	С	339	GLY
1	С	478	THR
1	Е	339	GLY
1	Е	478	THR
1	G	339	GLY
1	G	377	PHE
1	G	478	THR
1	Ι	339	GLY
1	Ι	478	THR
1	Е	470	THR
1	G	521	PRO
2	Н	64	LYS
1	В	335	LEU
1	В	417	LYS
1	В	470	THR
1	С	362	VAL
1	C	520	ALA
1	Е	360	ASN
1	Е	521	PRO
1	Ι	362	VAL
1	I	520	ALA
1	В	520	ALA
1	E	520	ALA
1	С	521	PRO
1	G	520	ALA
1	E	362	VAL

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#### 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 sidechain conformation was analysed, and the total number of residues.



Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
1	В	167/207~(81%)	147 (88%)	20~(12%)	4	16
1	С	163/207~(79%)	136~(83%)	27~(17%)	2	8
1	Ε	164/207~(79%)	140~(85%)	24~(15%)	2	11
1	G	164/207~(79%)	144 (88%)	20~(12%)	4	16
1	Ι	164/207~(79%)	143 (87%)	21~(13%)	3	15
2	А	97/117~(83%)	87~(90%)	10 (10%)	6	22
2	D	98/117~(84%)	91~(93%)	7~(7%)	12	39
2	F	95/117~(81%)	86 (90%)	9~(10%)	7	26
2	Н	99/117~(85%)	91~(92%)	8 (8%)	9	33
2	J	97/117~(83%)	88 (91%)	9  (9%)	7	27
All	All	1308/1620~(81%)	1153 (88%)	155 (12%)	4	17

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	$\operatorname{Res}$	Type
1	В	334	ASN
1	В	335	LEU
1	В	337	PRO
1	В	347	PHE
1	В	356	LYS
1	В	368	LEU
1	В	383	SER
1	В	385	THR
1	В	386	LYS
1	В	387	LEU
1	В	407	VAL
1	В	417	LYS
1	В	424	LYS
1	В	430	THR
1	В	441	LEU
1	В	491	PRO
1	В	501	ASN
1	В	506	GLN
1	В	514	SER
1	В	518	LEU
2	А	13	GLN
2	А	18	LEU
2	А	19	ARG
2	A	27	TYR



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Mol	Chain	Res	Type
2	A	43	LYS
2	A	53	ARG
2	A	56	SER
2	A	70	SER
2	A	101	SER
2	А	121	SER
1	С	337	PRO
1	С	341	VAL
1	С	347	PHE
1	С	351	TYR
1	С	356	LYS
1	С	373	SER
1	С	383	SER
1	С	385	THR
1	С	388	ASN
1	C	399	SER
1	С	403	ARG
1	С	407	VAL
1	С	415	THR
1	С	417	LYS
1	С	424	LYS
1	С	430	THR
1	С	441	LEU
1	С	466	ARG
1	С	468	ILE
1	С	483	VAL
1	С	484	GLU
1	С	491	PRO
1	С	493	GLN
1	С	501	ASN
1	С	506	GLN
1	С	514	SER
1	С	518	LEU
2	D	19	ARG
2	D	22	CYS
2	D	27	TYR
2	D	56	SER
2	D	70	SER
2	D	71[A]	ARG
2	D	71[B]	ARG
1	Е	333	THR
1	Е	334	ASN
			·



Mol	Chain	Res	Type
1	Е	337	PRO
1	Е	341	VAL
1	Е	347	PHE
1	Е	356	LYS
1	Е	373	SER
1	Е	383	SER
1	Е	385	THR
1	Е	386	LYS
1	Е	387	LEU
1	Е	388	ASN
1	Е	407	VAL
1	Е	415	THR
1	Е	417	LYS
1	Е	424	LYS
1	Е	430	THR
1	Е	441	LEU
1	Е	491	PRO
1	Е	501	ASN
1	Е	506	GLN
1	Е	514	SER
1	Е	518	LEU
1	Е	519	HIS
2	F	3	GLN
2	F	19	ARG
2	F	21	SER
2	F	53	ARG
2	F	56	SER
2	F	70	SER
2	F	101	SER
2	F	118	THR
2	F	121	SER
1	G	337	PRO
1	G	341	VAL
1	G	347	PHE
1	G	354	ASN
1	G	356	LYS
1	G	362	VAL
1	G	383	SER
1	G	386	LYS
1	G	387	LEU
1	G	399	SER
1	G	403	ARG



Mol	Chain	Res	Type
1	G	407	VAL
1	G	417	LYS
1	G	430	THR
1	G	462	LYS
1	G	471	GLU
1	G	491	PRO
1	G	506	GLN
1	G	514	SER
1	G	518	LEU
2	Н	18	LEU
2	Н	44	GLU
2	Н	46	GLU
2	Н	53	ARG
2	Н	71	ARG
2	Н	76	ASN
2	Н	113	GLN
2	Н	120	SER
1	Ι	334	ASN
1	Ι	337	PRO
1	Ι	347	PHE
1	Ι	373	SER
1	Ι	383	SER
1	Ι	387	LEU
1	Ι	388	ASN
1	Ι	390	LEU
1	Ι	403	ARG
1	Ι	407	VAL
1	Ι	415	THR
1	Ι	417	LYS
1	Ι	430	THR
1	Ι	441	LEU
1	Ι	445	VAL
1	Ι	484	GLU
1	Ι	491	PRO
1	Ι	501	ASN
1	Ι	514	SER
1	Ι	517	LEU
1	Ι	518	LEU
2	J	3[A]	GLN
2	J	3[B]	GLN
2	J	27	TYR
ი	.I	53	ARG



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Mol	Chain	Res	Type
2	J	56	SER
2	J	71	ARG
2	J	73	ASN
2	J	101	SER
2	J	113	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	В	334	ASN
2	А	73	ASN
1	С	501	ASN
1	Е	409	GLN
1	G	354	ASN
1	G	450	ASN
1	G	474	GLN
2	Н	73	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)

17 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).

Mol	Type	ype Chain Res	Dog	Link	Bo	ond leng	$_{\rm ths}$	E	Bond ang	gles
WIOI	туре		Res Link	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2	
3	NAG	K	1	3,1	14,14,15	1.41	3 (21%)	17,19,21	2.81	8 (47%)



Mal	Type	Chain	Dog	Link	Bo	ond leng	$_{\rm ths}$	Bond angles		
	туре	Ullalli	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
3	NAG	K	2	3	14,14,15	0.84	1 (7%)	17,19,21	1.45	3 (17%)
3	BMA	К	3	3	11,11,12	0.74	0	15,15,17	2.68	3 (20%)
4	NAG	L	1	1,4	14,14,15	0.66	0	17,19,21	2.78	9 (52%)
4	NAG	L	2	4	14,14,15	1.27	2 (14%)	17,19,21	3.46	10 (58%)
4	NAG	М	1	1,4	14,14,15	1.04	1 (7%)	17,19,21	2.62	5 (29%)
4	NAG	М	2	4	14,14,15	0.71	0	17,19,21	2.53	7 (41%)
3	NAG	Ν	1	3,1	14,14,15	0.56	0	17,19,21	2.09	6 (35%)
3	NAG	Ν	2	3	14,14,15	0.81	1 (7%)	17,19,21	1.92	4 (23%)
3	BMA	Ν	3	3	11,11,12	1.92	3 (27%)	15,15,17	2.72	6 (40%)
5	NAG	Ο	1	1,5	14,14,15	0.86	0	17,19,21	<mark>3.58</mark>	4 (23%)
5	NAG	Ο	2	5	14,14,15	0.76	0	17,19,21	3.26	7 (41%)
5	BMA	Ο	3	5	11,11,12	1.87	2 (18%)	$15,\!15,\!17$	2.47	7 (46%)
5	BMA	Ο	4	5	11,11,12	1.95	2 (18%)	$15,\!15,\!17$	2.64	5 (33%)
5	NAG	0	5	5	14,14,15	0.94	1 (7%)	17,19,21	1.54	3 (17%)
5	GAL	Ο	6	5	11,11,12	0.94	0	15,15,17	1.51	1 (6%)
5	BMA	0	7	5	11,11,12	1.19	2 (18%)	15, 15, 17	1.52	3 (20%)

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	Κ	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	Κ	2	3	-	4/6/23/26	0/1/1/1
3	BMA	К	3	3	-	2/2/19/22	0/1/1/1
4	NAG	L	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	L	2	4	-	4/6/23/26	0/1/1/1
4	NAG	М	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	М	2	4	-	3/6/23/26	0/1/1/1
3	NAG	Ν	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	Ν	2	3	-	3/6/23/26	0/1/1/1
3	BMA	N	3	3	-	1/2/19/22	0/1/1/1
5	NAG	Ο	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	Ο	2	5	-	3/6/23/26	0/1/1/1
5	BMA	Ο	3	5	-	2/2/19/22	0/1/1/1



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BMA	Ο	4	5	-	2/2/19/22	0/1/1/1
5	NAG	О	5	5	-	2/6/23/26	0/1/1/1
5	GAL	Ο	6	5	-	2/2/19/22	0/1/1/1
5	BMA	Ο	7	5	-	2/2/19/22	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	3	BMA	C2-C3	4.89	1.59	1.52
5	0	4	BMA	C2-C3	4.40	1.59	1.52
5	0	3	BMA	O5-C5	3.97	1.51	1.43
5	0	4	BMA	O5-C5	3.44	1.50	1.43
5	0	3	BMA	C2-C3	3.44	1.57	1.52
3	Κ	1	NAG	O6-C6	2.99	1.55	1.42
5	0	7	BMA	C2-C3	2.90	1.56	1.52
3	Κ	1	NAG	O4-C4	2.62	1.49	1.43
5	0	5	NAG	C1-C2	2.62	1.56	1.52
3	Κ	1	NAG	C6-C5	2.59	1.60	1.51
4	L	2	NAG	C2-N2	2.48	1.50	1.46
4	L	2	NAG	C3-C2	2.45	1.57	1.52
3	N	3	BMA	C1-C2	2.39	1.57	1.52
3	N	2	NAG	O4-C4	2.19	1.48	1.43
3	N	3	BMA	O5-C5	2.16	1.47	1.43
5	0	7	BMA	O5-C5	2.11	1.47	1.43
4	М	1	NAG	O4-C4	2.06	1.47	1.43
3	Κ	2	NAG	O4-C4	2.02	1.47	1.43

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
5	0	1	NAG	C1-O5-C5	10.48	126.39	112.19
4	L	2	NAG	C2-N2-C7	9.67	136.67	122.90
5	0	2	NAG	C2-N2-C7	9.06	135.80	122.90
5	0	1	NAG	C1-C2-N2	7.45	123.22	110.49
3	Κ	3	BMA	C1-O5-C5	7.30	122.08	112.19
4	М	1	NAG	C1-O5-C5	6.87	121.50	112.19
5	0	3	BMA	C1-O5-C5	6.60	121.14	112.19
5	0	4	BMA	C1-O5-C5	6.38	120.84	112.19
3	Ν	3	BMA	C1-O5-C5	6.35	120.79	112.19
3	Ν	3	BMA	C1-C2-C3	5.93	116.95	109.67
3	K	3	BMA	C1-C2-C3	5.85	116.85	109.67



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	$Ideal(^{o})$
4	М	1	NAG	C2-N2-C7	5.78	131.13	122.90
5	0	1	NAG	C2-N2-C7	5.73	131.06	122.90
3	К	1	NAG	C1-O5-C5	5.69	119.90	112.19
5	0	2	NAG	C1-C2-N2	5.66	120.15	110.49
3	N	1	NAG	C2-N2-C7	5.31	130.46	122.90
4	М	2	NAG	C1-O5-C5	5.18	119.22	112.19
4	L	1	NAG	C2-N2-C7	5.13	130.21	122.90
4	L	1	NAG	O5-C1-C2	5.01	119.20	111.29
3	K	1	NAG	C2-N2-C7	4.99	130.01	122.90
5	0	6	GAL	C1-O5-C5	4.87	118.79	112.19
4	L	2	NAG	O5-C1-C2	4.83	118.92	111.29
4	L	2	NAG	C4-C3-C2	4.69	117.89	111.02
4	М	2	NAG	C2-N2-C7	4.63	129.50	122.90
4	L	1	NAG	C1-O5-C5	4.58	118.39	112.19
5	0	2	NAG	O5-C5-C6	4.49	114.24	107.20
4	М	2	NAG	O3-C3-C2	4.44	118.65	109.47
3	K	1	NAG	O6-C6-C5	4.44	126.51	111.29
5	0	4	BMA	C1-C2-C3	4.40	115.07	109.67
3	N	2	NAG	C1-C2-N2	4.38	117.97	110.49
4	М	2	NAG	C1-C2-N2	4.26	117.77	110.49
5	0	5	NAG	C2-N2-C7	4.06	128.69	122.90
3	K	1	NAG	O3-C3-C2	-3.90	101.40	109.47
4	L	1	NAG	O5-C5-C4	-3.89	101.36	110.83
5	0	2	NAG	C1-O5-C5	3.83	117.38	112.19
3	N	2	NAG	C4-C3-C2	3.64	116.35	111.02
4	L	2	NAG	O5-C5-C4	-3.63	102.00	110.83
4	L	2	NAG	O4-C4-C3	3.55	118.55	110.35
5	0	3	BMA	C1-C2-C3	3.47	113.93	109.67
3	K	2	NAG	C2-N2-C7	3.43	127.79	122.90
4	L	1	NAG	C4-C3-C2	-3.30	106.19	111.02
5	0	5	NAG	C1-C2-N2	3.24	116.03	110.49
3	Ν	1	NAG	C1-C2-N2	3.16	115.88	110.49
5	Ο	4	BMA	O4-C4-C3	3.11	117.54	110.35
3	K	1	NAG	C6-C5-C4	3.10	120.27	113.00
3	Κ	1	NAG	C4-C3-C2	3.07	115.52	111.02
4	L	2	NAG	C1-C2-N2	3.06	115.71	110.49
5	Ο	4	BMA	C3-C4-C5	-3.03	104.84	110.24
4	М	1	NAG	C6-C5-C4	3.01	120.06	113.00
3	N	1	NAG	C4-C3-C2	3.00	115.41	111.02
3	N	3	BMA	O5-C1-C2	2.99	115.39	110.77
3	K	1	NAG	C1-C2-N2	-2.92	105.50	110.49
5	Ο	4	BMA	O4-C4-C5	2.89	116.48	109.30

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	0	7	BMA	C1-O5-C5	2.86	116.07	112.19
5	0	7	BMA	C2-C3-C4	2.79	115.73	110.89
3	Κ	3	BMA	O5-C1-C2	2.78	115.06	110.77
5	0	2	NAG	O3-C3-C2	2.77	115.20	109.47
3	Ν	3	BMA	O2-C2-C1	2.77	114.81	109.15
5	0	2	NAG	O4-C4-C3	-2.77	103.95	110.35
4	М	1	NAG	C3-C4-C5	-2.68	105.46	110.24
5	0	3	BMA	C3-C4-C5	-2.66	105.49	110.24
5	0	3	BMA	O4-C4-C5	2.64	115.86	109.30
4	L	2	NAG	O3-C3-C2	-2.62	104.04	109.47
4	L	1	NAG	O3-C3-C2	2.61	114.88	109.47
3	Ν	3	BMA	C3-C4-C5	-2.52	105.74	110.24
5	0	3	BMA	O2-C2-C3	2.47	115.09	110.14
4	М	1	NAG	O6-C6-C5	2.42	119.58	111.29
4	L	2	NAG	C1-O5-C5	2.38	115.41	112.19
4	L	1	NAG	C6-C5-C4	2.37	118.56	113.00
5	0	1	NAG	O6-C6-C5	2.37	119.44	111.29
3	Ν	2	NAG	C1-O5-C5	2.35	115.38	112.19
4	L	2	NAG	O4-C4-C5	-2.33	103.51	109.30
4	L	1	NAG	O6-C6-C5	2.32	119.25	111.29
4	L	1	NAG	C8-C7-N2	2.32	120.02	116.10
5	0	2	NAG	O4-C4-C5	2.31	115.03	109.30
3	Κ	2	NAG	07-C7-N2	-2.30	117.73	121.95
3	Ν	1	NAG	O4-C4-C5	2.27	114.94	109.30
5	0	7	BMA	O2-C2-C3	2.25	114.64	110.14
3	Κ	2	NAG	C4-C3-C2	2.20	114.24	111.02
4	L	2	NAG	C6-C5-C4	2.17	118.08	113.00
4	М	2	NAG	O5-C1-C2	-2.16	107.88	111.29
3	Κ	1	NAG	O3-C3-C4	2.14	115.30	110.35
4	М	2	NAG	C4-C3-C2	-2.12	107.91	111.02
3	Ν	3	BMA	O4-C4-C5	2.12	114.55	109.30
5	0	5	NAG	O4-C4-C5	2.11	114.54	109.30
5	0	3	BMA	O6-C6-C5	2.11	118.53	111.29
4	М	2	NAG	O7-C7-N2	-2.10	118.09	121.95
3	Ν	2	NAG	O3-C3-C2	-2.08	105.15	109.47
5	0	3	BMA	O5-C5-C6	2.07	110.45	107.20
3	Ν	1	NAG	O5-C5-C4	-2.04	105.87	110.83
3	Ν	1	NAG	C6-C5-C4	2.01	117.70	113.00

There are no chirality outliers.

All (41) torsion outliers are listed below:



8ZER
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Mol	Chain	Res	Type	Atoms
3	Κ	2	NAG	C8-C7-N2-C2
3	Κ	2	NAG	O7-C7-N2-C2
3	N	1	NAG	C8-C7-N2-C2
3	N	1	NAG	O7-C7-N2-C2
3	Ν	2	NAG	C8-C7-N2-C2
3	Ν	2	NAG	O7-C7-N2-C2
4	L	2	NAG	C3-C2-N2-C7
4	L	2	NAG	C8-C7-N2-C2
4	L	2	NAG	O7-C7-N2-C2
4	М	1	NAG	C8-C7-N2-C2
4	М	1	NAG	O7-C7-N2-C2
4	М	2	NAG	C8-C7-N2-C2
4	М	2	NAG	O7-C7-N2-C2
5	0	1	NAG	C1-C2-N2-C7
5	0	2	NAG	C8-C7-N2-C2
5	0	2	NAG	O7-C7-N2-C2
3	Κ	2	NAG	O5-C5-C6-O6
3	Κ	3	BMA	O5-C5-C6-O6
5	0	3	BMA	O5-C5-C6-O6
3	Κ	3	BMA	C4-C5-C6-O6
3	Ν	1	NAG	C1-C2-N2-C7
4	L	1	NAG	C1-C2-N2-C7
5	0	4	BMA	O5-C5-C6-O6
5	0	3	BMA	C4-C5-C6-O6
5	0	7	BMA	C4-C5-C6-O6
4	L	2	NAG	C1-C2-N2-C7
5	0	4	BMA	C4-C5-C6-O6
5	0	6	GAL	O5-C5-C6-O6
4	М	1	NAG	C4-C5-C6-O6
3	Κ	2	NAG	C4-C5-C6-O6
4	М	1	NAG	O5-C5-C6-O6
5	0	2	NAG	C1-C2-N2-C7
5	0	7	BMA	O5-C5-C6-O6
5	0	1	NAG	O5-C5-C6-O6
3	N	3	BMA	O5-C5-C6-O6
5	Ο	5	NAG	O5-C5-C6-O6
4	L	1	NAG	C3-C2-N2-C7
3	Ν	2	NAG	C3-C2-N2-C7
5	Ο	5	NAG	O7-C7-N2-C2
4	Μ	2	NAG	C3-C2-N2-C7
5	0	6	GAL	C4-C5-C6-O6

There are no ring outliers.



No monomer is involved in short contacts.

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



















### 5.6 Ligand geometry (i)

There are no ligands in this entry.

### 5.7 Other polymers (i)

There are no such residues in this entry.

### 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



# 6 Fit of model and data (i)

### 6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median,  $95^{th}$  percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	В	195/235~(82%)	0.45	7 (3%) 46 27	47, 83, 143, 190	1 (0%)
1	С	192/235~(81%)	0.54	11 (5%) 30 18	46, 76, 136, 203	0
1	Ε	194/235~(82%)	0.39	10 (5%) 34 20	50, 80, 128, 189	0
1	G	192/235~(81%)	0.67	20 (10%) 13 8	50, 85, 134, 161	0
1	Ι	193/235~(82%)	0.79	15 (7%) 20 11	54, 91, 144, 172	0
2	А	120/146~(82%)	0.19	2 (1%) 69 50	45, 74, 113, 145	0
2	D	120/146~(82%)	0.52	10 (8%) 19 10	43, 86, 112, 127	1 (0%)
2	$\mathbf{F}$	120/146~(82%)	0.27	3 (2%) 58 39	52, 86, 117, 130	0
2	Н	123/146~(84%)	0.39	3 (2%) 59 41	56, 78, 104, 133	0
2	J	$12\overline{0/146}\ (82\%)$	0.60	9 (7%) 22 12	53, 86, 111, 122	1 (0%)
All	All	1569/1905~(82%)	0.50	90 (5%) 30 18	43, 83, 132, 203	3(0%)

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	432	CYS	6.0
2	D	24	ALA	5.7
1	Ι	363	ALA	5.5
1	G	382	VAL	4.2
1	Ι	442	ASP	4.2
1	Ι	383	SER	4.2
2	D	23	VAL	4.0
1	G	433	VAL	3.8
2	J	104	GLU	3.8
2	D	22	CYS	3.5
1	G	386	LYS	3.4
1	С	392	PHE	3.4
2	Н	27	TYR	3.4



Mol	Chain	Res	Type	RSRZ
2	J	3[A]	GLN	3.3
1	Ι	341	VAL	3.3
1	Е	417	LYS	3.2
2	D	65	GLY	3.2
1	G	383	SER	3.1
2	J	7	SER	3.1
1	В	346[A]	ARG	3.1
1	Ι	432	CYS	3.0
1	С	383	SER	3.0
1	С	448	ASN	2.9
1	Е	424	LYS	2.9
1	Е	420	ASP	2.9
1	G	378	LYS	2.9
1	G	369	TYR	2.8
1	G	363	ALA	2.7
1	Е	480	CYS	2.7
1	Ι	367	VAL	2.7
1	Ι	400	PHE	2.6
1	В	436	TRP	2.6
1	G	480	CYS	2.6
2	J	76	ASN	2.6
1	Ι	434	ILE	2.5
1	Е	521	PRO	2.5
1	С	526	GLY	2.5
1	С	521	PRO	2.5
1	G	362	VAL	2.5
1	G	435	ALA	2.5
1	Ε	483	VAL	2.5
1	G	511	VAL	2.4
1	С	443	SER	2.4
1	Ι	334	ASN	2.4
2	J	64	LYS	2.4
1	С	459	SER	2.4
1	E	402	ILE	2.4
2	F	121	SER	2.4
1	I	337	PRO	2.3
1	G	438	SER	2.3
1	E	419	ALA	2.3
1	G	434	ILE	2.3
2	Н	95	CYS	2.2
1	В	424	LYS	2.2
1	Ι	446	GLY	2.2



Mol	Chain	Res	Type	RSRZ	
1	В	489	TYR	2.2	
1	G	512	VAL	2.2	
2	D	48	VAL	2.2	
1	Ι	340	GLU	2.2	
1	В	494	SER	2.2	
1	С	391	CYS	2.2	
1	С	480	CYS	2.2	
1	G	351	TYR	2.2	
2	А	74	ALA	2.2	
2	А	49	SER	2.2	
1	С	376	THR	2.2	
1	Ι	399	SER	2.2	
2	D	121	SER	2.2	
1	G	406	GLU	2.1	
1	Ι	521	PRO	2.1	
1	G	510	VAL	2.1	
1	Ι	362	VAL	2.1	
2	D	76	ASN	2.1	
1	Е	418	ILE	2.1	
2	D	93	TYR	2.1	
1	G	377	PHE	2.1	
2	F	53	ARG	2.1	
2	Н	108	GLN	2.1	
1	Е	356	LYS	2.1	
1	G	431	GLY	2.1	
2	J	115	THR	2.1	
1	В	377	PHE	2.1	
1	C	442	ASP	2.1	
2	D	27	TYR	2.0	
2	D	25	SER	2.0	
2	J	70	SER	2.0	
1	В	392	PHE	2.0	
2	F	46	GLU	2.0	
2	J	40	ALA	2.0	
2	J	99	ALA	2.0	

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

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



### 6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9
3	NAG	K	2	14/15	0.31	0.17	131,161,185,186	0
3	BMA	K	3	11/12	0.33	0.13	143,161,167,179	0
5	BMA	0	7	11/12	0.47	0.11	$138,\!152,\!190,\!227$	0
4	NAG	L	2	14/15	0.54	0.14	$102,\!128,\!155,\!155$	0
5	GAL	0	6	11/12	0.61	0.10	$163,\!175,\!189,\!199$	0
5	NAG	0	2	14/15	0.64	0.13	$115,\!158,\!190,\!205$	0
5	NAG	0	5	14/15	0.64	0.11	156,203,221,233	0
4	NAG	М	2	14/15	0.65	0.14	$97,\!146,\!175,\!191$	0
3	BMA	N	3	11/12	0.67	0.11	104,137,168,173	0
5	BMA	0	3	11/12	0.68	0.10	177,189,208,248	0
5	BMA	0	4	11/12	0.69	0.11	144,206,244,258	0
3	NAG	K	1	14/15	0.78	0.12	$77,\!91,\!110,\!126$	0
3	NAG	Ν	2	14/15	0.79	0.09	$82,\!130,\!160,\!164$	0
4	NAG	L	1	14/15	0.86	0.10	77,100,111,125	0
5	NAG	0	1	14/15	0.87	0.11	82,111,127,146	0
4	NAG	М	1	14/15	0.88	0.10	96,106,112,131	0
3	NAG	N	1	14/15	0.90	0.13	$90,\!116,\!\overline{137},\!140$	0

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)

There are no ligands in this entry.

## 6.5 Other polymers (i)

There are no such residues in this entry.

