

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

### Apr 25, 2024 – 06:16 PM EDT

PDB ID	:	8VQR
Title	:	Crystal structure of chimeric SARS-CoV-2 RBD complexed with chimeric rac-
		coon dog ACE2
Authors	:	Hsueh, FC.; Shi, K.; Aihara, H.; Li, F.
Deposited on	:	2024-01-19
Resolution	:	2.56  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	:	2.36.2
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)	:	2.36.2

# 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 2.56 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive	Similar resolution		
	$(\# { m Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$		
$R_{free}$	130704	1279(2.58-2.54)		
Clashscore	141614	1327 (2.58-2.54)		
Ramachandran outliers	138981	1312(2.58-2.54)		
Sidechain outliers	138945	1312(2.58-2.54)		
RSRZ outliers	127900	1269 (2.58-2.54)		

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	Q	uality of chain	
1	А	602	6% 	/0	18% ••
1	В	602	2%	050/	120/
	D	002	9%	85%	13% ••
2	E	232	65%	17%	• 17%
2	F	232	65%	16%	• 16%
3	С	2	50%	509	6



Mol	Chain	Length	Quality of chain			
4	D	5	60%	40%		
5	G	2	50%	50%		
5	Ι	2	100%			
6	Н	4	75%	25%		
7	J	5	60%	40%		
8	К	3	67%	33%		



# 2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 13126 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 Angiotensin-converting enzyme,Processed angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	А	594	Total 4860	C 3108	N 804	O 920	S 28	0	0	0
1	В	595	Total 4866	C 3111	N 805	0 922	S 28	0	0	0

Chain	Residue	Modelled	Actual	Comment	Reference
А	616	HIS	-	expression tag	UNP Q9BYF1
А	617	HIS	-	expression tag	UNP Q9BYF1
А	618	HIS	-	expression tag	UNP Q9BYF1
А	619	HIS	-	expression tag	UNP Q9BYF1
А	620	HIS	-	expression tag	UNP Q9BYF1
А	621	HIS	-	expression tag	UNP Q9BYF1
В	616	HIS	-	expression tag	UNP Q9BYF1
В	617	HIS	-	expression tag	UNP Q9BYF1
В	618	HIS	-	expression tag	UNP Q9BYF1
В	619	HIS	-	expression tag	UNP Q9BYF1
В	620	HIS	-	expression tag	UNP Q9BYF1
В	621	HIS	-	expression tag	UNP Q9BYF1

There are 12 discrepancies between the modelled and reference sequences:

• Molecule 2 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	F	102	Total	С	Ν	0	S	0	0	0
		195	1524	982	246	287	9	0	0	0
9	Б	104	Total	С	Ν	0	S	0	0	0
	2 F	194	1531	984	248	290	9	0	0	0

There are 92 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
Е	321	VAL	GLN	engineered mutation	UNP P0DTC2
Е	323	SER	THR	engineered mutation	UNP P0DTC2
Е	324	GLY	GLU	engineered mutation	UNP P0DTC2
Е	325	ASP	SER	engineered mutation	UNP P0DTC2
Е	326	VAL	ILE	engineered mutation	UNP P0DTC2
Е	346	LYS	ARG	variant	UNP P0DTC2
Е	348	PRO	ALA	engineered mutation	UNP P0DTC2
Е	354	GLU	ASN	engineered mutation	UNP P0DTC2
E	357	LYS	ARG	engineered mutation	UNP P0DTC2
Е	372	THR	ALA	engineered mutation	UNP P0DTC2
E	373	PHE	SER	engineered mutation	UNP P0DTC2
E	384	ALA	PRO	engineered mutation	UNP P0DTC2
Ε	393	SER	THR	engineered mutation	UNP P0DTC2
E	402	VAL	ILE	engineered mutation	UNP P0DTC2
E	403	LYS	ARG	engineered mutation	UNP P0DTC2
E	406	ASP	GLU	engineered mutation	UNP P0DTC2
E	417	VAL	LYS	engineered mutation	UNP P0DTC2
E	430	MET	THR	engineered mutation	UNP P0DTC2
E	434	LEU	ILE	engineered mutation	UNP P0DTC2
E	438	THR	SER	engineered mutation	UNP P0DTC2
E	439	ARG	ASN	engineered mutation	UNP P0DTC2
E	441	ILE	LEU	engineered mutation	UNP P0DTC2
E	443	ALA	SER	engineered mutation	UNP P0DTC2
E	444	THR	LYS	variant	UNP P0DTC2
E	445	SER	VAL	engineered mutation	UNP P0DTC2
E	446	THR	GLY	engineered mutation	UNP P0DTC2
E	452	LYS	LEU	engineered mutation	UNP P0DTC2
E	519	ASN	HIS	engineered mutation	UNP P0DTC2
E	529	LEU	LYS	engineered mutation	UNP P0DTC2
E	532	ASP	ASN	engineered mutation	UNP P0DTC2
E	534	ILE	VAL	engineered mutation	UNP P0DTC2
E	536	SER	ASN	engineered mutation	UNP P0DTC2
E	537	GLY	-	expression tag	UNP P0DTC2
E	538	GLU	-	expression tag	UNP P0DTC2
E	539	ASN	-	expression tag	UNP P0DTC2
E	540	LEU	-	expression tag	UNP P0DTC2
E	541	TYR	-	expression tag	UNP P0DTC2
E	542	PHE	-	expression tag	UNP P0DTC2
E	543	GLN	-	expression tag	UNP P0DTC2
E	544	GLY	-	expression tag	UNP P0DTC2
E	545	HIS	-	expression tag	UNP P0DTC2
E	546	HIS	-	expression tag	UNP P0DTC2
E	547	HIS	-	expression tag	UNP P0DTC2



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Chain	Residue	Modelled	Actual	Comment	Reference
E	548	HIS	_	expression tag	UNP P0DTC2
E	549	HIS	_	expression tag	UNP P0DTC2
E	550	HIS	_	expression tag	UNP P0DTC2
F	321	VAL	GLN	engineered mutation	UNP P0DTC2
F	323	SER	THR	engineered mutation	UNP P0DTC2
F	324	GLY	GLU	engineered mutation	UNP P0DTC2
F	325	ASP	SER	engineered mutation	UNP P0DTC2
F	326	VAL	ILE	engineered mutation	UNP P0DTC2
F	346	LYS	ARG	variant	UNP P0DTC2
F	348	PRO	ALA	engineered mutation	UNP P0DTC2
F	354	GLU	ASN	engineered mutation	UNP P0DTC2
F	357	LYS	ARG	engineered mutation	UNP P0DTC2
F	372	THR	ALA	engineered mutation	UNP P0DTC2
F	373	PHE	SER	engineered mutation	UNP P0DTC2
F	384	ALA	PRO	engineered mutation	UNP P0DTC2
F	393	SER	THR	engineered mutation	UNP P0DTC2
F	402	VAL	ILE	engineered mutation	UNP P0DTC2
F	403	LYS	ARG	engineered mutation	UNP P0DTC2
F	406	ASP	GLU	engineered mutation	UNP P0DTC2
F	417	VAL	LYS	engineered mutation	UNP P0DTC2
F	430	MET	THR	engineered mutation	UNP P0DTC2
F	434	LEU	ILE	engineered mutation	UNP P0DTC2
F	438	THR	SER	engineered mutation	UNP P0DTC2
F	439	ARG	ASN	engineered mutation	UNP P0DTC2
F	441	ILE	LEU	engineered mutation	UNP P0DTC2
F	443	ALA	SER	engineered mutation	UNP P0DTC2
F	444	THR	LYS	variant	UNP P0DTC2
F	445	SER	VAL	engineered mutation	UNP P0DTC2
F	446	THR	GLY	engineered mutation	UNP P0DTC2
F	452	LYS	LEU	engineered mutation	UNP P0DTC2
F	519	ASN	HIS	engineered mutation	UNP P0DTC2
F	529	LEU	LYS	engineered mutation	UNP P0DTC2
F	532	ASP	ASN	engineered mutation	UNP P0DTC2
F	534	ILE	VAL	engineered mutation	UNP P0DTC2
F	536	SER	ASN	engineered mutation	UNP P0DTC2
F	537	GLY	-	expression tag	UNP PODTC2
F	538	GLU	-	expression tag	UNP P0DTC2
F	539	ASN	-	expression tag	UNP P0DTC2
F	540		-	expression tag	UNP PODTC2
F F	541	TYR	-	expression tag	UNP PODTC2
F'	542	PHE	-	expression tag	UNP P0DTC2
F	543	GLN	-	expression tag	UNP P0DTC2



Chain	Residue	Modelled	Actual	Comment	Reference
F	544	GLY	-	expression tag	UNP P0DTC2
F	545	HIS	-	expression tag	UNP P0DTC2
F	546	HIS	-	expression tag	UNP P0DTC2
F	547	HIS	-	expression tag	UNP P0DTC2
F	548	HIS	-	expression tag	UNP P0DTC2
F	549	HIS	-	expression tag	UNP P0DTC2
F	550	HIS	-	expression tag	UNP P0DTC2

• Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-bet a-D-glucopyranose.



Mol	Chain	Residues	A	Aton	ns		ZeroOcc	AltConf	Trace
3	С	2	Total 24	C 14	N 1	O 9	0	0	0

• Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-beta-D-mannopyranose -(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-aceta mido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	1	Aton	ns		ZeroOcc	AltConf	Trace
4	D	5	Total 60	С 34	N 2	O 24	0	0	0

• Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	I	Aton	ns		ZeroOcc	AltConf	Trace
5	G	2	Total 28	C 16	N 2	O 10	0	0	0



Continued from previous page...

Mol	Chain	Residues	ŀ	Aton	ns		ZeroOcc	AltConf	Trace
5	Ι	2	Total 28	C 16	N 2	O 10	0	0	0

• Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranos e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluco pyranose.



Mol	Chain	Residues	At	$\mathbf{toms}$		ZeroOcc	AltConf	Trace
6	Н	4	Total 50 2	C N 28 2	O 20	0	0	0

• Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranos e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acet amido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	I	Aton	ns		ZeroOcc	AltConf	Trace
7	J	5	Total 60	C 34	N 2	O 24	0	0	0

• Molecule 8 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	I	Aton	ns		ZeroOcc	AltConf	Trace
8	K	3	Total 39	C 22	N 2	O 15	0	0	0

• Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	А	1	Total Zn 1 1	0	0
9	В	1	Total Zn 1 1	0	0

• Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	А	1	Total Cl 1 1	0	0
10	В	1	Total Cl 1 1	0	0

• Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	A	ton	ns		ZeroOcc	AltConf
11	А	1	Total 14	C 8	N 1	O 5	0	0
11	В	1	Total 14	C 8	N 1	O 5	0	0

• Molecule 12 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
12	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0

• Molecule 13 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	А	8	Total O 8 8	0	0
13	В	6	Total O 6 6	0	0
13	Е	1	Total O 1 1	0	0
13	F	1	Total O 1 1	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: Angiotensin-converting enzyme, Processed angiotensin-converting enzyme 2





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• Molecule 2: Spike protein S1



9%				
Chain E:	65%	17% •	17%	
ARG VAL VAL PRO FRO GLY VAL ARG PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO	TILE THE ASN V350 V350 N350 N350 N350 N350 N350 N350 N350 N	V 389 F 373 F 377 F 377 K 378 C 379 C 370 C 370	F332 81334 11334 11336 11338 11358 11358 11358 11358 11358 11358 11358 11358 11358 11358 11358 11358 11358 11358 113588 113588 113588 113588 113588 113588 113588 113588 113588 1135	
0404 0405 0405 8408 0427 0427 0432 8439 8449 8449	Y451 Y451 Y453 Y453 Y453 R454 R454 R461 K462 R461 F462 E471 E471 E471 F473 E471	4932 4933 4944 7497 7499 7499 7499 7499 7499	L517 L518 N519 A520 P521 A522 V524 F527 LVS LEU	
SER THR ASP LEU LEU LEU LYS SER GLU GLU ASN ASN TYR PHE	HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS			
• Molecule 2: Spik	æ protein S1			
17% Cl. : D				
Chain F:	65%	16% ·	16%	
ARG VAL VAL VAL PRO SER SER GLY VAL VAL ARG PRO PRO PRO	T1332 11334 11335 11335 1335 1335 1335 1355 135	Badd Badd Y365 Y365 Y365 F373 F373 F373 F373 K378 Y379 Y380 Y380 Y380 Y388	C391 F392 N394 N395 V395 A395 A395 N401 R408	
P412 1418 1419 4419 4420 1420 1422 1422 1423 1429 1420 1430	451 8452 8453 8455 8455 8455 8455 8465 8465 8465 8465	A475 C476 C476 C476 C483 E484 E484 F490 F491 C492 C493 C493 C493 S494 F495 C495 C495 C495 C495 C495 C495 C495 C	L513 L514 E516 E516 E516 LEU LEU LEU A520 A520 A521 V524 V524	
C526 C526 C526 LYS LYS LEU SER ASP LEU LYS SER CLY	ASN TTYR TTYR TTYR CLN GLN HIS HIS HIS HIS HIS HIS			
• Molecule 3: alph	a-L-fucopyranose-(1-6)-2	2-acetamido-2-deoxy-be	ta-D-glucopyranose	
Chain C:	50%	50%		
NAG1 FUC2				
• Molecule 4: beta ta-D-glucopyranos e	a-D-mannopyranose-(1-4) se-(1-4)-[alpha-L-fucopyr	)-beta-D-mannopyranos ranose-(1-6)]2-acetamid	se-(1-4)-2-acetamido-2-deoxy- o-2-deoxy-beta-D-glucopyran	·be 10s
Chain D:	60%	40%		
NAG1 NAG2 BMA3 BMA4 FUC5				
• Molecule 5: 2-ac opyranose	etamido-2-deoxy-beta-D	-glucopyranose-(1-4)-2-	acetamido-2-deoxy-beta-D-gl	luc
Chain G:	50%	50%		

#### NAG1 NAG2

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



Chain I:

#### NAG 1 NAG 2

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

Chain H:	75%	25%
NAG1 NAG2 BMA3 MAN4		

100%

 • Molecule 7: alpha-D-mannopyranose-(1-3)-beta-D<br/>-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)] 2-acetamido-2-deoxy-beta-D-glucopyranose<br/> e

Chain J:	60%	40%
NAG1 NAG2 MAA3 FUG5 FUG5		

67%

Chain K:

33%

#### NAG1 NAG2 BMA3



# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	80.96Å 118.11Å 112.23Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $92.89^{\circ}$ $90.00^{\circ}$	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	58.41 - 2.56	Depositor
Resolution (A)	$112.09 \ - \ 2.56$	EDS
% Data completeness	62.8(58.41-2.56)	Depositor
(in resolution range)	59.5(112.09-2.56)	EDS
R <sub>merge</sub>	0.05	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.73 (at 2.58 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
D D	0.214 , $0.264$	Depositor
$\Pi, \Pi_{free}$	0.212 , $0.262$	DCC
$R_{free}$ test set	2203 reflections $(5.19%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	67.9	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent $k_{sol}(e/A^3)$ , $B_{sol}(A^2)$	0.28, $36.1$	EDS
L-test for twinning <sup>2</sup>	$< L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	13126	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 3.60% 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: FUC, NAG, MAN, BMA, ZN, CL, EDO

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	
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.24	0/4998	0.45	0/6790
1	В	0.24	0/5004	0.44	0/6798
2	Е	0.25	0/1568	0.48	0/2136
2	F	0.26	0/1574	0.48	0/2143
All	All	0.24	0/13144	0.45	0/17867

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	4860	0	4626	68	0
1	В	4866	0	4631	42	0
2	Е	1524	0	1437	21	0
2	F	1531	0	1440	27	0
3	С	24	0	22	1	0
4	D	60	0	52	0	0
5	G	28	0	25	1	0
5	Ι	28	0	25	0	0
6	H	50	0	43	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	J	60	0	52	0	0
8	К	39	0	34	1	0
9	А	1	0	0	0	0
9	В	1	0	0	0	0
10	А	1	0	0	0	0
10	В	1	0	0	1	0
11	А	14	0	13	0	0
11	В	14	0	13	0	0
12	В	8	0	12	0	0
13	А	8	0	0	0	0
13	В	6	0	0	0	0
13	Е	1	0	0	0	0
13	F	1	0	0	0	0
All	All	13126	0	12425	159	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 6.

All (159) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:98:GLN:HE22	1:A:210:ASN:HD21	1.25	0.81
1:B:338:ASP:N	1:B:338:ASP:OD1	2.22	0.73
1:A:416:LYS:NZ	1:A:541:LYS:O	2.21	0.72
2:F:363:ALA:HB2	2:F:525:CYS:HB3	1.72	0.71
1:A:520:LEU:HD22	1:A:579:MET:HE2	1.74	0.70
1:A:468:ILE:HD12	1:A:476:LYS:HG2	1.75	0.69
2:E:335:LEU:HB3	2:E:362:VAL:H	1.60	0.65
2:E:454:ARG:NH2	2:E:469:SER:O	2.30	0.65
1:A:293:VAL:HG12	1:A:296:ALA:HB3	1.79	0.64
1:B:177:ARG:NH1	1:B:181:GLU:OE2	2.31	0.63
1:A:482:ARG:HH22	1:A:611:SER:HB3	1.64	0.62
1:A:555:PHE:HA	1:A:558:LEU:HD22	1.81	0.61
2:F:378:LYS:HA	2:F:378:LYS:HE3	1.81	0.61
1:B:83:TYR:O	1:B:101:GLN:NE2	2.31	0.61
1:A:337:SER:OG	1:A:338:ASP:N	2.31	0.60
1:A:420:SER:HB2	5:G:1:NAG:H62	1.84	0.60
1:B:177:ARG:NH2	1:B:495:GLU:OE1	2.36	0.58
2:F:365:TYR:HB2	2:F:388:ASN:HD22	1.68	0.58
2:E:383:SER:HB2	2:E:386:LYS:HG2	1.86	0.58
2:E:448:ASN:HB3	2:E:497:PHE:HB2	1.85	0.57



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:70:SER:O	1:B:74:LYS:HG2	2.05	0.57
1:A:520:LEU:HD21	1:A:581:VAL:HG13	1.87	0.57
1:A:388:GLN:NE2	1:A:559:ARG:O	2.38	0.57
1:B:80:ALA:O	1:B:101:GLN:NE2	2.37	0.57
1:A:177:ARG:HD3	1:A:498:CYS:HB2	1.87	0.56
1:B:388:GLN:HG3	1:B:389:PRO:HD2	1.85	0.56
2:E:461:LEU:HD22	2:E:465:GLU:HB3	1.86	0.56
1:A:402:GLU:HB3	1:A:518:ARG:HH11	1.70	0.56
1:B:524:GLN:HG2	1:B:583:PRO:HG2	1.85	0.56
2:F:361:CYS:N	2:F:524:VAL:O	2.38	0.56
2:F:360:ASN:H	2:F:524:VAL:HA	1.70	0.56
2:F:333:THR:O	2:F:333:THR:OG1	2.22	0.56
1:A:524:GLN:HG2	1:A:583:PRO:HG2	1.88	0.55
1:B:99:ALA:O	1:B:103:ASN:HB2	2.06	0.55
2:E:335:LEU:HD23	2:E:361:CYS:HA	1.88	0.55
8:K:1:NAG:H83	8:K:1:NAG:H3	1.88	0.55
1:A:143:LEU:H	1:A:143:LEU:HD23	1.71	0.54
1:B:38:GLU:OE1	1:B:353:ARG:NH2	2.34	0.54
1:B:133:CYS:HA	1:B:141:CYS:HA	1.89	0.54
2:E:452:LYS:HG2	2:E:494:SER:HB3	1.89	0.54
1:B:245:ARG:NH2	1:B:605:GLY:O	2.41	0.54
2:F:461:LEU:HD22	2:F:465:GLU:HB3	1.89	0.54
1:A:331:SER:OG	1:A:358:ILE:O	2.25	0.54
1:A:294:THR:O	1:A:298:VAL:HG23	2.08	0.53
1:A:298:VAL:HG22	1:A:364:VAL:O	2.07	0.53
1:A:564:GLU:HB3	1:A:568:LEU:HD23	1.91	0.53
1:A:322:ASN:N	1:A:322:ASN:OD1	2.40	0.53
2:F:366:SER:OG	2:F:370:ASN:OD1	2.27	0.53
1:A:301:ALA:HA	1:A:364:VAL:HG11	1.91	0.52
1:A:435:GLU:HG3	1:A:540:HIS:CE1	2.43	0.52
1:A:51:ASN:HB3	1:A:359:LYS:HE2	1.90	0.52
1:B:88:ILE:HD11	1:B:97:LEU:HD23	1.91	0.52
1:B:337:SER:O	1:B:339:SER:N	2.42	0.52
1:A:417:HIS:O	1:A:421:ILE:HG12	2.09	0.52
2:F:412:PRO:HG3	2:F:429:PHE:HB3	1.92	0.51
1:A:314:PHE:O	1:A:318:VAL:HG23	2.11	0.51
1:A:133:CYS:HA	1:A:141:CYS:HA	1.91	0.51
1:A:305:GLN:O	1:A:309:LYS:HB2	2.11	0.51
1:B:468:ILE:HD12	1:B:476:LYS:HG2	1.93	0.51
2:E:452:LYS:HA	2:E:494:SER:HA	1.92	0.51
1:A:168:TRP:CD1	1:A:502:SER:HB2	2.46	0.51



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:F:454:ARG:NH1	2:F:467:ASP:O	2.44	0.50
2:E:498:GLN:H	2:E:501:ASN:HD21	1.59	0.50
1:B:455:MET:HE2	1:B:485:VAL:HG21	1.92	0.50
1:A:47:SER:HA	1:A:62:MET:HG3	1.93	0.50
1:B:143:LEU:HD23	1:B:143:LEU:H	1.77	0.50
1:A:343:VAL:HG23	1:A:359:LYS:NZ	2.27	0.50
2:E:439:ARG:HD2	2:E:499:PRO:HA	1.94	0.49
2:F:524:VAL:HG13	2:F:525:CYS:H	1.77	0.49
1:B:305:GLN:O	1:B:309:LYS:HB2	2.13	0.49
1:A:457:GLU:HG2	1:A:512:PHE:HB3	1.95	0.49
1:A:105:SER:OG	1:A:190:MET:SD	2.71	0.49
2:F:363:ALA:H	2:F:526:GLY:H	1.61	0.49
2:F:393:SER:HA	2:F:522:ALA:HA	1.95	0.48
2:E:350:VAL:HA	2:E:400:PHE:HB2	1.94	0.48
1:A:363:LYS:N	1:A:363:LYS:HD3	2.28	0.48
1:A:52:THR:HB	3:C:1:NAG:HN2	1.79	0.48
2:F:355:ARG:HD2	2:F:396:TYR:HD2	1.79	0.48
1:A:396:ALA:HB1	1:A:566:TRP:HA	1.94	0.47
2:E:462:LYS:HG2	2:E:465:GLU:OE1	2.14	0.47
1:A:55:THR:O	1:A:59:VAL:HG23	2.14	0.47
2:E:401:VAL:HG22	2:E:509:ARG:HG2	1.95	0.47
2:E:498:GLN:H	2:E:501:ASN:ND2	2.12	0.47
1:A:355:ASP:OD2	1:A:357:ARG:NH1	2.48	0.47
1:B:457:GLU:HG2	1:B:512:PHE:HB3	1.95	0.47
1:A:416:LYS:HE3	1:A:416:LYS:H	1.79	0.47
1:A:419:LYS:NZ	1:A:426:PRO:O	2.38	0.47
1:A:51:ASN:O	1:A:343:VAL:HG22	2.15	0.46
2:E:379:CYS:HA	2:E:432:CYS:HA	1.98	0.46
1:A:477:TRP:CE3	1:A:500:PRO:HG3	2.50	0.46
1:B:31:LYS:NZ	1:B:35:GLU:OE2	2.38	0.46
1:A:132:VAL:HG12	1:A:171:GLU:HG3	1.97	0.46
1:A:96:GLN:HB3	1:A:391:LEU:HD13	1.99	0.45
1:B:593:THR:HA	1:B:596:LYS:HE2	1.97	0.45
2:E:403:LYS:HE3	2:E:405:ASP:HB2	1.98	0.45
1:A:269:ASP:OD1	1:A:272:GLY:N	2.49	0.45
1:A:389:PRO:HG2	1:A:392:LEU:HD22	1.99	0.45
1:B:309:LYS:HD2	1:B:328:TRP:CH2	2.51	0.45
1:A:180:TYR:HA	1:A:183:TYR:HB3	1.99	0.45
1:A:239:HIS:CE1	1:A:604:VAL:HG11	2.52	0.45
1:B:365:THR:OG1	1:B:366:MET:N	2.50	0.45
2:F:524:VAL:HG13	2:F:525:CYS:N	2.32	0.44



	loue page	Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:B:177:ABG:HD3	1:B:498:CYS:HB2	2.00	0.44
1:B:365:THR:HG23	1:B:368:ASP:H	1.82	0.44
2:E:355:ABG:HD3	2:E:398:ASP:OD1	2.17	0.44
2:F:394:ASN:HA	2:F:524:VAL:HB	2.00	0.44
1:B:314:PHE:O	1:B:318:VAL:HG23	2.17	0.44
1:A:488:VAL:HG21	1:A:611:SEB:HA	2.00	0.44
1:A:81:LYS:HA	1:A:101:GLN:HE21	1.83	0.44
2:F:359:SEB:HA	2:F:524:VAL:HG23	2.00	0.44
2:F:401:VAL:HG22	2:F:509:ARG:HG2	1.99	0.44
1:A:359:LYS:HE3	1:A:359:LYS:HB3	1.85	0.43
1:A:113:SEB:O	1:A:117:ASN:ND2	2.51	0.43
1:A:310:GLU:OE2	1:A:421:ILE:HD12	2.19	0.43
1:B:268:GLY:O	1:B:277:ASN:ND2	2.39	0.43
2:F:421:TYR:HB3	2:F:454:ARG:HG2	1.99	0.43
1:A:213:ASP:OD1	1:A:213:ASP:N	2.51	0.43
1:A:229:THR:HG22	1:A:581:VAL:HG22	2.00	0.43
1:A:493:HIS:ND1	1:A:499:ASP:OD2	2.51	0.43
1:B:284:PRO:HG2	1:B:436:ILE:HG22	2.01	0.43
1:B:50:TYR:CE1	1:B:59:VAL:HG22	2.53	0.43
2:E:383:SER:OG	2:E:386:LYS:NZ	2.48	0.43
2:F:394:ASN:N	2:F:394:ASN:OD1	2.51	0.43
1:B:389:PRO:HG2	1:B:392:LEU:HD22	2.00	0.42
2:E:502:GLY:O	2:E:506:GLN:HG3	2.19	0.42
1:A:54:ILE:HB	1:A:341:LYS:HG2	2.01	0.42
1:A:245:ARG:HD3	1:A:258:PRO:HA	2.02	0.42
1:B:294:THR:HG23	1:B:365:THR:HA	2.02	0.42
2:F:373:PHE:HD1	2:F:373:PHE:HA	1.68	0.42
1:A:117:ASN:O	1:A:121:ASN:ND2	2.52	0.42
1:A:580:ASN:OD1	1:A:582:ARG:HG2	2.19	0.42
1:A:455:MET:HE2	1:A:480:MET:HB2	2.02	0.42
1:A:535:HIS:NE2	1:A:538:PRO:O	2.50	0.42
1:B:77:SER:O	1:B:81:LYS:HG3	2.20	0.41
1:B:345:HIS:O	1:B:359:LYS:NZ	2.52	0.41
1:A:83:TYR:HB2	1:A:97:LEU:HD21	2.02	0.41
1:B:169:ARG:HH22	1:B:271:TRP:HA	1.85	0.41
1:B:90:ASP:HB2	1:B:93:VAL:HB	2.02	0.41
1:B:269:ASP:OD1	1:B:272:GLY:N	2.47	0.41
2:F:419:ALA:O	2:F:424:LYS:HD3	2.20	0.41
2:F:452:LYS:HA	2:F:494:SER:HA	2.02	0.41
1:A:50:TYR:CD1	1:A:59:VAL:HG22	2.56	0.41
1:A:92:THR:O	1:A:96:GLN:HG3	2.20	0.41



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:520:LEU:HD21	1:B:581:VAL:HG13	2.01	0.41
2:E:355:ARG:HD2	2:E:396:TYR:HB3	2.03	0.41
2:F:368:LEU:HB3	2:F:377:PHE:CZ	2.56	0.41
2:E:471:GLU:O	2:E:491:PRO:HG3	2.21	0.41
1:B:423:LEU:HD23	1:B:423:LEU:HA	1.93	0.41
1:A:85:LEU:HD13	1:A:94:LYS:NZ	2.35	0.41
2:F:357:LYS:NZ	2:F:357:LYS:HB3	2.36	0.41
1:A:95:ARG:HD3	1:A:563:SER:O	2.20	0.41
2:F:418:ILE:HA	2:F:422:ASN:HD22	1.87	0.40
1:A:462:MET:HE3	1:A:468:ILE:HD11	2.02	0.40
1:B:45:LEU:HD23	1:B:45:LEU:HA	1.95	0.40
2:F:454:ARG:NH2	2:F:469:SER:O	2.53	0.40
1:A:365:THR:OG1	1:A:366:MET:N	2.53	0.40
1:B:389:PRO:O	1:B:393:ARG:HG3	2.22	0.40
1:B:499:ASP:HB3	10:B:702:CL:CL	2.59	0.40
1:B:351:LEU:HD12	1:B:355:ASP:OD2	2.21	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	$\mathbf{s}$
1	А	592/602~(98%)	567 (96%)	21 (4%)	4 (1%)	22	29	
1	В	593/602~(98%)	569~(96%)	20 (3%)	4 (1%)	22	29	
2	E	191/232~(82%)	171 (90%)	19 (10%)	1 (0%)	29	39	
2	F	190/232~(82%)	168 (88%)	19 (10%)	3(2%)	9	12	
All	All	1566/1668~(94%)	1475 (94%)	79~(5%)	12 (1%)	19	27	

All (12) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	В	338	ASP
1	В	147	GLY
1	В	340	TRP
1	А	212	VAL
1	А	337	SER
2	F	333	THR
1	А	301	ALA
1	А	334	THR
2	Ε	518	LEU
2	F	485	GLY
1	В	211	GLY
2	F	521	PRO

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	527/535~(98%)	496 (94%)	31~(6%)	19	25
1	В	528/535~(99%)	511 (97%)	17 (3%)	39	51
2	Ε	166/203~(82%)	156 (94%)	10 (6%)	19	24
2	F	167/203~(82%)	158 (95%)	9~(5%)	22	29
All	All	1388/1476~(94%)	$1321 \ (95\%)$	67~(5%)	25	34

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	55	THR
1	А	85	LEU
1	А	89	GLN
1	А	100	LEU
1	А	107	VAL
1	А	110	GLU
1	А	177	ARG
1	А	291	ILE
1	А	295	ASP
1	А	305	GLN



Mol	Chain	Res	Type
1	А	309	LYS
1	А	322	ASN
1	А	334	THR
1	А	335	GLU
1	А	338	ASP
1	А	357	ARG
1	А	358	ILE
1	А	363	LYS
1	А	381	TYR
1	А	388	GLN
1	А	394	ASN
1	А	416	LYS
1	А	427	ASP
1	А	455	MET
1	А	518	ARG
1	А	558	LEU
1	А	559	ARG
1	А	573	VAL
1	А	581	VAL
1	А	582	ARG
1	А	597	ASP
1	В	100	LEU
1	В	103	ASN
1	В	107	VAL
1	В	110	GLU
1	В	172	VAL
1	В	177	ARG
1	В	185	VAL
1	В	334	THR
1	В	338	ASP
1	В	381	TYR
1	В	388	GLN
1	В	427	ASP
1	В	455	MET
1	В	489	GLU
1	В	518	ARG
1	В	557	MET
1	В	581	VAL
2	Е	377	PHE
2	Е	386	LYS
2	Е	388	ASN
2	Е	408	ARG
	~	-	



$\overline{Mol}$	Chain	$\mathbf{Res}$	Type
2	Е	427	ASP
2	Е	450	ASN
2	Е	471	GLU
2	Е	478	THR
2	Е	493	GLN
2	Е	523	THR
2	F	336	CYS
2	F	357	LYS
2	F	373	PHE
2	F	377	PHE
2	F	378	LYS
2	F	408	ARG
2	F	458	LYS
2	F	462	LYS
2	F	525	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	117	ASN
1	А	121	ASN
1	А	194	ASN
1	А	210	ASN
1	А	388	GLN
1	А	472	GLN
1	В	117	ASN
1	В	121	ASN
1	В	194	ASN
1	В	388	GLN
2	Е	493	GLN
2	Е	501	ASN
2	F	334	ASN
2	F	388	ASN
2	F	474	GLN

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.



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

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

### 5.5 Carbohydrates (i)

#### 23 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Type	Chain	Bos	Link	Bo	Bond lengths		Bond angles		
WIOI	Type	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
3	NAG	С	1	1,3	14,14,15	0.27	0	17,19,21	0.77	1 (5%)
3	FUC	С	2	3	10,10,11	0.71	0	14,14,16	0.97	1 (7%)
4	NAG	D	1	1,4	14,14,15	0.36	0	17,19,21	0.54	0
4	NAG	D	2	4	14,14,15	0.52	0	17,19,21	0.66	0
4	BMA	D	3	4	11,11,12	1.46	2 (18%)	15,15,17	1.42	3 (20%)
4	BMA	D	4	4	11,11,12	0.97	0	$15,\!15,\!17$	1.06	1 (6%)
4	FUC	D	5	4	10,10,11	0.70	0	14,14,16	0.84	0
5	NAG	G	1	1,5	14,14,15	0.53	0	17,19,21	0.83	0
5	NAG	G	2	5	14,14,15	0.21	0	17,19,21	0.49	0
6	NAG	Н	1	1,6	14,14,15	0.38	0	17,19,21	0.44	0
6	NAG	Н	2	6	$14,\!14,\!15$	0.35	0	17,19,21	0.43	0
6	BMA	Н	3	6	$11,\!11,\!12$	0.70	0	$15,\!15,\!17$	0.87	0
6	MAN	Н	4	6	11,11,12	0.64	0	$15,\!15,\!17$	1.05	2 (13%)
5	NAG	Ι	1	1,5	$14,\!14,\!15$	0.30	0	17,19,21	0.58	0
5	NAG	Ι	2	5	14,14,15	0.38	0	17,19,21	0.49	0
7	NAG	J	1	1,7	14,14,15	0.31	0	17,19,21	0.54	0
7	NAG	J	2	7	14,14,15	0.19	0	17,19,21	0.47	0
7	BMA	J	3	7	11,11,12	1.46	2 (18%)	15,15,17	1.13	1 (6%)
7	MAN	J	4	7	11,11,12	0.79	1 (9%)	15,15,17	1.37	2 (13%)
7	FUC	J	5	7	10,10,11	0.74	0	14,14,16	0.83	0
8	NAG	К	1	2,8	14,14,15	0.42	0	17,19,21	1.27	2(11%)
8	NAG	K	2	8	14,14,15	0.31	0	17,19,21	0.43	0
8	BMA	K	3	8	11,11,12	0.60	0	15,15,17	0.86	0

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
3	NAG	С	1	1,3	-	3/6/23/26	0/1/1/1
3	FUC	С	2	3	-	-	0/1/1/1
4	NAG	D	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	BMA	D	3	4	-	1/2/19/22	0/1/1/1
4	BMA	D	4	4	-	2/2/19/22	0/1/1/1
4	FUC	D	5	4	-	-	0/1/1/1
5	NAG	G	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
6	NAG	Н	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	Н	2	6	-	2/6/23/26	0/1/1/1
6	BMA	Н	3	6	-	0/2/19/22	0/1/1/1
6	MAN	Н	4	6	-	0/2/19/22	0/1/1/1
5	NAG	Ι	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	Ι	2	5	-	2/6/23/26	0/1/1/1
7	NAG	J	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	J	2	7	-	2/6/23/26	0/1/1/1
7	BMA	J	3	7	-	2/2/19/22	0/1/1/1
7	MAN	J	4	7	-	0/2/19/22	1/1/1/1
7	FUC	J	5	7	-	-	0/1/1/1
8	NAG	Κ	1	2,8	-	3/6/23/26	0/1/1/1
8	NAG	Κ	2	8	-	0/6/23/26	0/1/1/1
8	BMA	K	3	8	-	$0/2/19/\overline{22}$	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.

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
7	J	3	BMA	C2-C3	3.48	1.57	1.52
4	D	3	BMA	C4-C3	2.86	1.59	1.52
4	D	3	BMA	C2-C3	2.55	1.56	1.52
7	J	3	BMA	O3-C3	2.49	1.48	1.43
7	J	4	MAN	C1-C2	2.08	1.56	1.52

All (13) bond angle outliers are listed below:



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v	QIU.

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
8	Κ	1	NAG	C2-N2-C7	4.33	129.06	122.90
7	J	4	MAN	C1-O5-C5	4.30	118.02	112.19
4	D	3	BMA	C2-C3-C4	3.16	116.36	110.89
6	Н	4	MAN	C1-O5-C5	2.72	115.88	112.19
3	С	1	NAG	C1-O5-C5	2.60	115.71	112.19
7	J	3	BMA	O3-C3-C2	2.55	114.88	109.99
7	J	4	MAN	O2-C2-C3	-2.27	105.60	110.14
6	Н	4	MAN	O2-C2-C3	-2.25	105.63	110.14
4	D	4	BMA	C2-C3-C4	2.22	114.73	110.89
4	D	3	BMA	C1-O5-C5	-2.20	109.21	112.19
3	С	2	FUC	C1-O5-C5	2.13	117.60	112.78
4	D	3	BMA	C3-C4-C5	2.01	113.83	110.24
8	Κ	1	NAG	C1-C2-N2	2.00	113.91	110.49

There are no chirality outliers.

All	(29)	) torsion	outliers	are	listed	below:
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Mol	Chain	Res	Type	Atoms
5	G	2	NAG	O5-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
4	D	4	BMA	O5-C5-C6-O6
5	Ι	1	NAG	O5-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	D	1	NAG	C8-C7-N2-C2
4	D	1	NAG	O7-C7-N2-C2
6	Н	1	NAG	C8-C7-N2-C2
6	Н	1	NAG	O7-C7-N2-C2
6	Н	2	NAG	C8-C7-N2-C2
6	Н	2	NAG	O7-C7-N2-C2
8	Κ	1	NAG	C8-C7-N2-C2
8	Κ	1	NAG	O7-C7-N2-C2
4	D	4	BMA	C4-C5-C6-O6
3	С	1	NAG	O5-C5-C6-O6
5	Ι	1	NAG	C4-C5-C6-O6
3	С	1	NAG	C4-C5-C6-O6
7	J	3	BMA	C4-C5-C6-O6
7	J	2	NAG	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	D	3	BMA	O5-C5-C6-O6
5	Ι	2	NAG	O5-C5-C6-O6
5	G	1	NAG	O5-C5-C6-O6
7	J	3	BMA	O5-C5-C6-O6
7	J	2	NAG	C4-C5-C6-O6



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Mol	Chain	$\mathbf{Res}$	Type	Atoms							
3	С	1	NAG	C3-C2-N2-C7							
5	G	1	NAG	C3-C2-N2-C7							
5	Ι	2	NAG	C3-C2-N2-C7							
8	Κ	1	NAG	C3-C2-N2-C7							

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All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	J	4	MAN	C1-C2-C3-C4-C5-O5

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	С	1	NAG	1	0
8	Κ	1	NAG	1	0
5	G	1	NAG	1	0

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





















### 5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal Tuna Chain		Dec	Tink	Bond lengths			Bond angles			
WIOI	туре	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
11	NAG	В	705	1	14,14,15	0.26	0	17,19,21	0.46	0
12	EDO	В	703	-	3,3,3	0.45	0	2,2,2	0.34	0
11	NAG	А	703	1	14,14,15	0.25	0	17,19,21	0.44	0
12	EDO	В	704	-	3,3,3	0.45	0	2,2,2	0.34	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
11	NAG	В	705	1	-	4/6/23/26	0/1/1/1
12	EDO	В	703	-	-	0/1/1/1	-
11	NAG	А	703	1	-	2/6/23/26	0/1/1/1
12	EDO	B	704	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	А	703	NAG	C8-C7-N2-C2
11	А	703	NAG	O7-C7-N2-C2
11	В	705	NAG	C8-C7-N2-C2
11	В	705	NAG	O7-C7-N2-C2
11	В	705	NAG	C4-C5-C6-O6
11	В	705	NAG	O5-C5-C6-O6
12	В	704	EDO	O1-C1-C2-O2



There are no ring outliers.

No monomer is involved in short contacts.

# 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



# 6 Fit of model and data (i)

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

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

Mol	Chain	Analysed	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	594/602~(98%)	0.37	39 (6%) 18 23	39, 83, 141, 203	0
1	В	595/602~(98%)	0.19	14 (2%) 59 67	37, 69, 134, 217	0
2	Е	193/232~(83%)	0.71	22 (11%) 5 7	45, 77, 167, 277	0
2	F	194/232~(83%)	1.17	39 (20%) 1 1	59, 112, 183, 248	0
All	All	1576/1668~(94%)	0.44	114 (7%) 15 20	37, 80, 155, 277	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Е	522	ALA	18.8
2	Е	521	PRO	18.7
2	F	331	ASN	14.4
2	F	332	ILE	8.4
2	F	522	ALA	8.3
2	Е	387	LEU	7.8
2	F	396	TYR	6.8
2	Е	517	LEU	6.6
2	Е	527	PRO	6.6
1	А	333	LEU	6.4
2	Е	392	PHE	6.1
2	F	483	VAL	6.1
2	Е	368	LEU	6.0
2	F	369	TYR	5.9
2	Е	515	PHE	5.6
2	F	338	PHE	5.4
2	Е	394	ASN	5.4
2	F	392	PHE	5.3
2	F	521	PRO	5.3
1	А	339	SER	5.2
2	F	523	THR	5.1



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Mol	Chain	Res	Type	RSRZ
1	В	97	LEU	5.1
1	А	362	THR	5.1
2	F	456	PHE	5.0
2	Е	520	ALA	4.9
2	F	357	LYS	4.4
1	В	106	SER	4.4
2	F	430	MET	4.4
2	Е	369	TYR	4.3
2	F	356	LYS	4.3
2	F	358	ILE	4.2
1	А	428	PHE	4.2
2	F	515	PHE	4.2
2	F	368	LEU	4.2
1	А	424	LEU	4.0
1	В	137	ASN	4.0
1	В	79	LEU	3.8
2	F	367	VAL	3.8
2	F	342	PHE	3.8
2	F	476	GLY	3.8
1	А	88	ILE	3.8
1	А	413	ALA	3.8
1	А	336	PRO	3.8
1	А	102	GLN	3.7
1	А	346	PRO	3.7
2	F	397	ALA	3.7
2	F	373	PHE	3.6
2	F	395	VAL	3.6
2	Е	384	ALA	3.5
1	А	298	VAL	3.5
2	F	335	LEU	3.4
1	А	360	MET	3.4
1	А	299	ASP	3.4
1	В	108	LEU	3.4
2	Е	395	VAL	3.3
2	F	391	CYS	3.3
2	F	355	ARG	3.3
1	В	136	ASP	3.3
1	А	85	LEU	3.2
2	F	492	LEU	3.2
1	А	429	GLN	3.2
1	А	409	SER	3.2
1	А	370	LEU	3.1



Mol	Chain	Res	Type	RSRZ
1	А	50 TYR		3.1
2	Е	359	SER	3.0
2	Е	518	LEU	3.0
2	Е	365	TYR	2.9
2	Е	390	LEU	2.9
2	Е	391	CYS	2.9
1	В	86	GLU	2.9
1	В	105	SER	2.9
1	В	85	LEU	2.9
1	А	46	ALA	2.8
1	А	343	VAL	2.8
2	F	431	GLY	2.8
2	F	380	TYR	2.8
2	F	490	PHE	2.8
2	F	362	VAL	2.7
2	F	455	LEU	2.7
2	F	513	LEU	2.7
1	В	217	TYR	2.6
1	А	421	ILE	2.6
1	А	292	ASP	2.6
1	А	369	PHE	2.5
2	F	336	CYS	2.5
2	Ε	524	VAL	2.4
1	А	416	LYS	2.4
1	А	334	THR	2.4
1	А	81	LYS	2.4
1	А	54	ILE	2.3
2	F	495	TYR	2.3
1	В	89	GLN	2.3
1	А	202	TYR	2.3
2	F	333	THR	2.3
1	A	390	PHE	2.3
1	А	305	GLN	2.3
2	F	524	VAL	2.3
1	А	340	TRP	2.3
1	В	179	LEU	2.2
1	В	202	TYR	2.2
1	А	106	SER	2.2
2	E	363	ALA	2.1
1	А	419	LYS	2.1
1	A	83	TYR	2.1
1	A	423	LEU	2.1



Mol	Chain	Res	Type	RSRZ
1	А	534	LYS	2.1
2	Е	360	ASN	2.1
2	F	516	GLU	2.1
1	А	176	LEU	2.0
1	А	363	LYS	2.0
2	F	475	ALA	2.0
1	В	342	VAL	2.0
1	А	525	PHE	2.0
2	Е	373	PHE	2.0

### 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
5	NAG	Ι	2	14/15	0.60	0.28	99,114,128,129	0
8	NAG	K	2	14/15	0.67	0.27	115,125,149,149	0
3	FUC	С	2	10/11	0.68	0.20	117,141,146,147	0
4	BMA	D	3	11/12	0.68	0.32	114,122,138,138	0
8	BMA	K	3	11/12	0.75	0.17	122,126,144,155	0
3	NAG	С	1	14/15	0.77	0.27	129,138,147,152	0
4	NAG	D	2	14/15	0.80	0.16	88,119,130,134	0
5	NAG	Ι	1	14/15	0.82	0.15	86,100,116,118	0
6	MAN	Н	4	11/12	0.82	0.30	71,100,112,118	0
7	NAG	J	1	14/15	0.83	0.24	101,116,124,129	0
4	BMA	D	4	11/12	0.84	0.21	78,109,117,122	0
5	NAG	G	2	14/15	0.86	0.15	84,118,138,150	0
7	NAG	J	2	14/15	0.86	0.21	80,102,111,115	0
4	NAG	D	1	14/15	0.87	0.19	120,128,136,138	0
4	FUC	D	5	10/11	0.87	0.39	90,102,118,121	0
7	BMA	J	3	11/12	0.88	0.20	84,98,112,114	0
7	FUC	J	5	10/11	0.89	0.23	90,101,114,115	0
5	NAG	G	1	14/15	0.89	0.21	99,116,123,128	0
6	BMA	Н	3	11/12	0.89	0.13	69,83,99,101	0



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9
7	MAN	J	4	11/12	0.90	0.13	57,79,93,96	0
8	NAG	Κ	1	14/15	0.90	0.13	$86,\!115,\!127,\!132$	0
6	NAG	Н	2	14/15	0.95	0.15	49,59,76,93	0
6	NAG	Н	1	14/15	0.98	0.13	35,54,73,82	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)

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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
11	NAG	А	703	14/15	0.74	0.16	98,133,141,147	0
11	NAG	В	705	14/15	0.83	0.26	76,93,105,116	0
12	EDO	В	704	4/4	0.88	0.21	44,52,55,58	0
10	CL	В	702	1/1	0.92	0.09	75,75,75,75	0
12	EDO	В	703	4/4	0.95	0.13	48,53,61,67	0
9	ZN	В	701	1/1	0.95	0.16	85,85,85,85	0
10	CL	А	702	1/1	0.97	0.11	64,64,64,64	0
9	ZN	А	701	1/1	0.97	0.16	85,85,85,85	0

### 6.5 Other polymers (i)

There are no such residues in this entry.

