

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

Jan 14, 2024 - 12:25 am GMT

PDB ID	:	6S9J
Title	:	Crystal structure of TfR1 mimicry in complex with GP1 from MACV
Authors	:	Diskin, R.; Cohen-Dvashi, H.
Deposited on	:	2019-07-15
Resolution	:	2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY\;DIFFRACTION$ 

The reported resolution of this entry is 2.70 Å.

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



Metric	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R <sub>free</sub>	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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					
			5%					
1	В	168	71%	20% • 8%				
			7%					
1	D	168	71%	18% • 10%				
			40%					
1	F	168	54%	34% • 11%				
			29%					
1	Н	168	63%	29% 8%				
			5%					
2	А	178	65%	20% • 15%				



Mol	Chain	Length	Quality of chain					
2	С	178	6% 67%	17%		16%		
2	Е	178	8%	20%	•	16%		
2	G	178	60%	23%	•	16%		
3	Ι	5	40%	60%				
4	J	2	50%	50%				

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
3	MAN	Ι	4	-	-	-	Х



# 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9715 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	155	Total	С	Ν	0	$\mathbf{S}$	0	0	0
	D	100	1247	785	216	232	14	0	0	0
1	П	159	Total	С	Ν	0	S	0	0	0
	D	152	1218	766	211	227	14	0		0
1	Б	140	Total	С	Ν	0	S	0	0	0
	Г	149	1192	750	207	221	14	0	0	0
1	ц	154	Total	С	Ν	0	S	0	0	0
		104	1238	780	215	229	14	0	0	0

• Molecule 1 is a protein called Pre-glycoprotein polyprotein GP complex.

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	245	GLY	-	expression tag	UNP Q8AZ57
В	246	SER	-	expression tag	UNP Q8AZ57
В	247	HIS	-	expression tag	UNP Q8AZ57
В	248	HIS	-	expression tag	UNP Q8AZ57
В	249	HIS	-	expression tag	UNP Q8AZ57
В	250	HIS	-	expression tag	UNP Q8AZ57
В	251	HIS	-	expression tag	UNP Q8AZ57
В	252	HIS	-	expression tag	UNP Q8AZ57
D	245	GLY	-	expression tag	UNP Q8AZ57
D	246	SER	-	expression tag	UNP Q8AZ57
D	247	HIS	-	expression tag	UNP Q8AZ57
D	248	HIS	-	expression tag	UNP Q8AZ57
D	249	HIS	-	expression tag	UNP Q8AZ57
D	250	HIS	-	expression tag	UNP Q8AZ57
D	251	HIS	-	expression tag	UNP Q8AZ57
D	252	HIS	-	expression tag	UNP Q8AZ57
F	245	GLY	-	expression tag	UNP Q8AZ57
F	246	SER	-	expression tag	UNP Q8AZ57
F	247	HIS	-	expression tag	UNP Q8AZ57
F	248	HIS	-	expression tag	UNP Q8AZ57
F	249	HIS	-	expression tag	UNP Q8AZ57



Chain	Residue	Modelled	Actual	Comment	Reference
F	250	HIS	-	expression tag	UNP Q8AZ57
F	251	HIS	-	expression tag	UNP Q8AZ57
F	252	HIS	-	expression tag	UNP Q8AZ57
Н	245	GLY	-	expression tag	UNP Q8AZ57
Н	246	SER	-	expression tag	UNP Q8AZ57
Н	247	HIS	-	expression tag	UNP Q8AZ57
Н	248	HIS	-	expression tag	UNP Q8AZ57
Н	249	HIS	-	expression tag	UNP Q8AZ57
Н	250	HIS	-	expression tag	UNP Q8AZ57
Н	251	HIS	-	expression tag	UNP Q8AZ57
Н	252	HIS	-	expression tag	UNP Q8AZ57

• Molecule 2 is a protein called Transferrin receptor 1, Transferrin receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
0	Δ	151	Total	С	Ν	0	S	0	0	0
	A	101	1170	737	201	229	3	0	0	0
0	C	140	Total	С	Ν	0	S	0	0	0
	U	149	1159	731	199	226	3	0		0
0	Б	140	Total	С	Ν	0	S	0	0	0
	E	149	1159	731	199	226	3	0	0	0
0	C	140	Total	С	Ν	0	S	0	0	0
	G	149	1159	731	199	226	3	0	0	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	194	CYS	GLY	conflict	UNP A0A060BIS8
А	?	-	VAL	deletion	UNP A0A060BIS8
А	283	LYS	MET	conflict	UNP A0A060BIS8
А	288	TYR	PHE	conflict	UNP A0A060BIS8
А	291	SER	VAL	conflict	UNP A0A060BIS8
А	295	GLU	ILE	conflict	UNP A0A060BIS8
А	324	GLN	PHE	conflict	UNP A0A060BIS8
А	380	CYS	ALA	conflict	UNP A0A060BIS8
А	384	GLY	-	expression tag	UNP A0A060BIS8
A	385	THR	-	expression tag	UNP A0A060BIS8
А	386	SER	-	expression tag	UNP A0A060BIS8
A	387	GLY	-	expression tag	UNP A0A060BIS8
A	388	HIS	-	expression tag	UNP A0A060BIS8
А	389	HIS	-	expression tag	UNP A0A060BIS8
А	390	HIS	-	expression tag	UNP A0A060BIS8



Chain	Residue	Modelled	Actual	Comment	Reference
А	391	HIS	-	expression tag	UNP A0A060BIS8
А	392	HIS	-	expression tag	UNP A0A060BIS8
А	393	HIS	-	expression tag	UNP A0A060BIS8
С	194	CYS	GLY	conflict	UNP A0A060BIS8
С	?	-	VAL	deletion	UNP A0A060BIS8
С	283	LYS	MET	conflict	UNP A0A060BIS8
С	288	TYR	PHE	conflict	UNP A0A060BIS8
С	291	SER	VAL	conflict	UNP A0A060BIS8
С	295	GLU	ILE	conflict	UNP A0A060BIS8
С	324	GLN	PHE	conflict	UNP A0A060BIS8
С	380	CYS	ALA	conflict	UNP A0A060BIS8
С	384	GLY	-	expression tag	UNP A0A060BIS8
С	385	THR	-	expression tag	UNP A0A060BIS8
С	386	SER	-	expression tag	UNP A0A060BIS8
С	387	GLY	-	expression tag	UNP A0A060BIS8
С	388	HIS	-	expression tag	UNP A0A060BIS8
С	389	HIS	-	expression tag	UNP A0A060BIS8
С	390	HIS	-	expression tag	UNP A0A060BIS8
С	391	HIS	-	expression tag	UNP A0A060BIS8
С	392	HIS	-	expression tag	UNP A0A060BIS8
С	393	HIS	-	expression tag	UNP A0A060BIS8
Е	194	CYS	GLY	conflict	UNP A0A060BIS8
Е	?	-	VAL	deletion	UNP A0A060BIS8
Е	283	LYS	MET	conflict	UNP A0A060BIS8
Е	288	TYR	PHE	conflict	UNP A0A060BIS8
Е	291	SER	VAL	conflict	UNP A0A060BIS8
Е	295	GLU	ILE	conflict	UNP A0A060BIS8
Е	324	GLN	PHE	conflict	UNP A0A060BIS8
Е	380	CYS	ALA	conflict	UNP A0A060BIS8
Е	384	GLY	-	expression tag	UNP A0A060BIS8
Е	385	THR	-	expression tag	UNP A0A060BIS8
Е	386	SER	-	expression tag	UNP A0A060BIS8
Е	387	GLY	-	expression tag	UNP A0A060BIS8
Е	388	HIS	-	expression tag	UNP A0A060BIS8
Е	389	HIS	-	expression tag	UNP A0A060BIS8
Е	390	HIS	-	expression tag	UNP A0A060BIS8
E	391	HIS	-	expression tag	UNP A0A060BIS8
Е	392	HIS	-	expression tag	UNP A0A060BIS8
Е	393	HIS	-	expression tag	UNP A0A060BIS8
G	194	CYS	GLY	conflict	UNP A0A060BIS8
G	?	-	VAL	deletion	UNP A0A060BIS8
G	283	LYS	MET	conflict	UNP A0A060BIS8



Chain	Residue	Modelled	Actual	Comment	Reference
G	288	TYR	PHE	conflict	UNP A0A060BIS8
G	291	SER	VAL	conflict	UNP A0A060BIS8
G	295	GLU	ILE	conflict	UNP A0A060BIS8
G	324	GLN	PHE	conflict	UNP A0A060BIS8
G	380	CYS	ALA	conflict	UNP A0A060BIS8
G	384	GLY	-	expression tag	UNP A0A060BIS8
G	385	THR	-	expression tag	UNP A0A060BIS8
G	386	SER	-	expression tag	UNP A0A060BIS8
G	387	GLY	-	expression tag	UNP A0A060BIS8
G	388	HIS	-	expression tag	UNP A0A060BIS8
G	389	HIS	-	expression tag	UNP A0A060BIS8
G	390	HIS	-	expression tag	UNP A0A060BIS8
G	391	HIS	-	expression tag	UNP A0A060BIS8
G	392	HIS	-	expression tag	UNP A0A060BIS8
G	393	HIS	-	expression tag	UNP A0A060BIS8

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



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace		
3	Ι	5	Total 61	C 34	N 2	O 25	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	J	2	Total 28	C 16	N 2	O 10	0	0	0

• Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).





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

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	В	8	Total O 8 8	0	0
6	А	8	Total O 8 8	0	0
6	D	2	Total O 2 2	0	0
6	С	9	Total O 9 9	0	0
6	F	5	Total O 5 5	0	0
6	Е	6	Total O 6 6	0	0
6	Н	2	Total O 2 2	0	0
6	G	2	Total O 2 2	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: Pre-glycoprotein polyprotein GP complex



• Molecule 1: Pre-glycoprotein polyprotein GP complex



• Molecule 1: Pre-glycoprotein polyprotein GP complex







NAG1 NAG2

# KZ67 LY8 V268 LY8 V268 LY8 V268 LY8 V266 LY8 T281 CY8 T286 ALA T286 ALA T286 ALA T286 ALA T286 ALA T286 ALA T289 P187 T296 T202 CLW N198 RCL T202 CLW T202 CLW T202 CLW T202 CLW T202 CLW T202 CLW T202 T204 T202 T205 T204 T204 T202 T205 T204 T306 T202 T307 T202 T304 T202 T305 T204 T306 T202 T307 T202 T308 T202<

 $\bullet$  Molecule 3: 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 nose

Chain I:	40%	60%	
NAG1 NAG2 BMA3 MAN4 MAN5			
• Molecule 4:	2-acetamido-2-de	eoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deox	y-beta-D

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

Unain J:	50%	50%



# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants	104.63Å 104.63Å 281.36Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Bosolution(A)	49.56 - 2.70	Depositor
Resolution (A)	49.56 - 2.70	EDS
% Data completeness	83.1 (49.56-2.70)	Depositor
(in resolution range)	83.1 (49.56-2.70)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.07 (at 2.69 \text{\AA})$	Xtriage
Refinement program	PHENIX (dev_2871: ???)	Depositor
P. P.	0.241 , $0.267$	Depositor
$n, n_{free}$	0.244 , $0.272$	DCC
$R_{free}$ test set	1999 reflections $(5.46\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	43.4	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.29, $50.6$	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	9715	wwPDB-VP
Average B, all atoms $(Å^2)$	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 13.82% 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: BMA, NAG, MAN

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	Bond lengths		ond angles
WIOI	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	В	0.40	0/1279	0.58	0/1724
1	D	0.36	0/1248	0.54	0/1682
1	F	0.32	0/1222	0.58	1/1646~(0.1%)
1	Н	0.32	0/1270	0.56	1/1712~(0.1%)
2	А	0.43	0/1189	0.62	0/1611
2	С	0.36	0/1178	0.59	0/1595
2	Е	0.36	0/1178	0.58	0/1595
2	G	0.33	0/1178	0.57	0/1595
All	All	0.36	0/9742	0.58	2/13160~(0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
1	F	193	ARG	NE-CZ-NH1	-6.31	117.15	120.30
1	Н	184	ASP	CB-CG-OD2	-5.27	113.55	118.30

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	В	1247	0	1176	26	0



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	Choin	Non H	<b>H</b> (model)	H(addad)	Claches	Symm Clashes
IVIOI	Chain		n(model)	n(audeu)	Clashes	Symm-Clasnes
1	D	1218	0	1158	27	0
1	$\mathbf{F}$	1192	0	1135	47	0
1	Н	1238	0	1171	55	0
2	А	1170	0	1172	22	0
2	С	1159	0	1164	20	0
2	Е	1159	0	1164	34	0
2	G	1159	0	1164	48	0
3	Ι	61	0	52	1	0
4	J	28	0	25	0	0
5	А	14	0	13	0	0
5	В	28	0	26	0	0
6	А	8	0	0	0	0
6	В	8	0	0	0	0
6	С	9	0	0	1	0
6	D	2	0	0	0	0
6	Е	6	0	0	1	0
6	F	5	0	0	2	0
6	G	2	0	0	0	0
6	Н	2	0	0	1	0
All	All	9715	0	9420	261	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 14.

All (261) 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 (Å)	overlap (Å)
1:F:155:ASP:OD2	2:G:221:ALA:HB2	1.36	1.25
1:H:181:LYS:HE3	1:H:193:ARG:NH1	1.51	1.22
2:G:220:VAL:HG11	2:G:335:GLN:NE2	1.61	1.13
1:H:181:LYS:NZ	1:H:207:CYS:O	1.82	1.11
1:F:181:LYS:HE2	1:F:193:ARG:HH12	1.01	1.11
1:F:155:ASP:OD2	2:G:221:ALA:CB	2.03	1.06
1:H:181:LYS:NZ	1:H:207:CYS:C	2.11	1.02
1:H:181:LYS:CE	1:H:193:ARG:NH1	2.24	1.00
2:G:220:VAL:CG1	2:G:335:GLN:NE2	2.28	0.96
2:G:220:VAL:HG11	2:G:335:GLN:CD	1.88	0.93
1:F:181:LYS:HE2	1:F:193:ARG:NH1	1.84	0.92
1:H:181:LYS:HE3	1:H:193:ARG:HH11	1.26	0.92
2:G:220:VAL:CG1	2:G:335:GLN:HE22	1.82	0.91
1:F:155:ASP:CG	2:G:221:ALA:HB2	1.90	0.91



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:H:181:LYS:O	1:H:186:ARG:NH2	2.02	0.90
1:H:181:LYS:CE	1:H:193:ARG:HH12	1.87	0.87
2:E:217:GLU:N	2:E:217:GLU:OE1	2.07	0.85
1:F:94:LEU:HD21	1:F:236:LYS:HE3	1.60	0.83
1:D:129:PRO:HB3	1:D:146:HIS:HD2	1.44	0.81
2:G:297:LEU:O	2:G:297:LEU:HD12	1.80	0.81
1:H:181:LYS:CD	1:H:193:ARG:HH12	1.94	0.79
2:C:203:THR:HG22	2:C:209:LEU:HG	1.66	0.77
2:E:262:ILE:HB	2:E:266:GLU:OE1	1.86	0.76
2:E:198:ASN:ND2	2:E:220:VAL:HG21	2.00	0.75
1:H:181:LYS:HZ2	1:H:207:CYS:C	1.89	0.75
2:G:198:ASN:ND2	2:G:220:VAL:CG2	2.51	0.73
1:B:129:PRO:HB3	1:B:146:HIS:CD2	2.24	0.73
2:G:220:VAL:HG11	2:G:335:GLN:HE22	1.42	0.73
1:H:181:LYS:NZ	1:H:207:CYS:HB2	2.04	0.72
2:E:203:THR:HG22	2:E:209:LEU:HG	1.71	0.72
1:H:118:LEU:H	1:H:176:GLN:HE22	1.36	0.72
2:G:204:ASN:HA	2:G:371:ARG:HG2	1.71	0.72
2:G:203:THR:HG22	2:G:209:LEU:HG	1.72	0.71
2:E:199:SER:HG	2:E:376:THR:HG1	1.30	0.71
1:D:129:PRO:HB3	1:D:146:HIS:CD2	2.26	0.70
2:C:233:VAL:HG13	2:C:248:TYR:CE2	2.27	0.70
2:G:220:VAL:HG13	2:G:335:GLN:HE22	1.56	0.69
2:C:272:GLN:NE2	2:C:331:SER:OG	2.25	0.69
2:A:233:VAL:HG13	2:A:248:TYR:CE2	2.28	0.69
1:H:181:LYS:HZ1	1:H:207:CYS:C	1.91	0.68
2:G:281:ILE:HB	2:G:336:THR:HG22	1.75	0.68
1:H:180:SER:OG	1:H:212:VAL:HA	1.92	0.68
1:B:136:LEU:O	1:B:167:LYS:NZ	2.24	0.68
1:H:181:LYS:NZ	1:H:207:CYS:CB	2.57	0.67
2:A:203:THR:HG22	2:A:209:LEU:HG	1.76	0.67
1:H:98:PHE:HD1	1:H:109:LEU:HD11	1.59	0.66
1:H:181:LYS:HZ1	1:H:207:CYS:HB2	1.59	0.66
1:B:129:PRO:HB3	1:B:146:HIS:HD2	1.61	0.65
2:G:295:GLU:HB3	2:G:296:PRO:HD2	1.79	0.65
2:C:201:THR:HG22	2:C:212:LEU:HA	1.78	0.65
2:E:198:ASN:HD21	2:E:220:VAL:HG21	1.61	0.65
1:F:177:PHE:HB2	1:F:215:LEU:HB3	1.79	0.65
1:F:98:PHE:HD1	1:F:109:LEU:HD11	1.61	0.64
1:H:180:SER:OG	1:H:213:CYS:N	2.29	0.64
1:F:118:LEU:HB2	1:F:176:GLN:OE1	1.97	0.64



	to do pagom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:H:113:SER:HG	2:G:211:TYR:HH	1.46	0.64
2:A:258:ARG:NH1	2:A:284:ASP:OD2	2.28	0.63
1:D:116:SER:CB	1:D:176:GLN:HE22	2.11	0.62
2:A:199:SER:HG	2:A:376:THR:HG1	1.47	0.62
2:G:201:THR:HG22	2:G:212:LEU:HA	1.82	0.62
1:D:181:LYS:HE2	1:D:193:ARG:NH1	2.14	0.62
1:B:186:ARG:NH2	1:B:209:GLU:OE2	2.33	0.61
2:G:202:ILE:HD11	2:G:345:LEU:HD23	1.82	0.61
1:H:118:LEU:HB2	1:H:176:GLN:OE1	1.99	0.61
1:H:181:LYS:HE3	1:H:193:ARG:HH12	1.44	0.61
1:D:116:SER:HB2	1:D:176:GLN:HE22	1.66	0.60
2:E:202:ILE:HD11	2:E:345:LEU:HD23	1.82	0.60
2:G:217:GLU:N	2:G:217:GLU:OE1	2.34	0.60
2:E:201:THR:HG22	2:E:212:LEU:HA	1.84	0.60
2:A:202:ILE:HD11	2:A:345:LEU:HD23	1.84	0.60
2:E:268:VAL:HG11	2:E:334:VAL:HG21	1.84	0.59
2:G:233:VAL:HG13	2:G:248:TYR:CE2	2.37	0.59
2:A:201:THR:HG22	2:A:212:LEU:HA	1.83	0.59
1:D:98:PHE:C	1:D:99:TYR:HD1	2.06	0.59
2:G:232:LEU:HD22	2:G:373:VAL:HG21	1.84	0.59
1:H:111:ARG:NH2	1:H:218:ASN:OD1	2.33	0.59
2:E:261:LYS:N	6:E:401:HOH:O	2.33	0.59
2:C:283:LYS:HD3	2:C:287:LYS:HE3	1.85	0.58
1:B:181:LYS:HE2	1:B:193:ARG:HH12	1.68	0.58
2:G:295:GLU:OE1	2:G:296:PRO:HD2	2.03	0.57
2:G:220:VAL:HG11	2:G:335:GLN:OE1	2.04	0.57
2:C:243:PHE:HB3	2:C:274:PHE:CE2	2.39	0.57
1:H:123:ASP:OD2	2:G:344:LYS:NZ	2.38	0.57
1:F:98:PHE:CE1	1:F:111:ARG:HD3	2.40	0.57
1:F:155:ASP:OD2	2:G:221:ALA:HB3	2.00	0.57
2:A:243:PHE:HB3	2:A:274:PHE:CE2	2.41	0.56
2:A:285:ARG:HH21	2:A:339:ARG:HH12	1.53	0.56
1:H:174:ASN:OD1	1:H:216:THR:HG23	2.06	0.56
1:H:181:LYS:CE	1:H:193:ARG:HH11	2.05	0.56
1:H:118:LEU:N	1:H:176:GLN:HE22	2.02	0.56
1:F:117:VAL:H	1:F:176:GLN:NE2	2.03	0.55
1:H:130:GLU:O	1:H:130:GLU:HG3	2.06	0.55
1:D:164:CYS:HA	1:D:174:ASN:O	2.05	0.55
1:H:181:LYS:CG	1:H:193:ARG:HH12	2.19	0.55
2:G:340:GLU:HG2	2:G:344:LYS:HE2	1.89	0.55
1:B:181:LYS:CE	1:B:193:ARG:HH12	2.20	0.55



	ti a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:A:243:PHE:HB3	2:A:274:PHE:CD2	2.43	0.54
1:F:134:ASN:HA	1:F:167:LYS:NZ	2.22	0.54
2:E:232:LEU:HD22	2:E:373:VAL:HG21	1.89	0.54
2:C:227:GLU:OE2	2:C:374:LYS:HE3	2.08	0.54
2:G:197:PRO:HG2	2:G:215:TYR:CE1	2.42	0.54
2:G:198:ASN:ND2	2:G:220:VAL:HG22	2.22	0.54
2:E:227:GLU:OE2	2:E:374:LYS:HE3	2.07	0.54
2:C:202:ILE:HD11	2:C:345:LEU:HD23	1.91	0.53
2:E:222:TYR:CD2	2:E:222:TYR:O	2.61	0.53
1:H:129:PRO:HB3	1:H:146:HIS:CD2	2.43	0.53
1:B:107:THR:C	1:B:108:PHE:HD1	2.12	0.53
1:H:116:SER:HB3	1:H:214:TYR:CE2	2.44	0.53
1:F:118:LEU:N	1:F:176:GLN:HE22	2.07	0.53
1:F:140:ASP:OD1	1:F:141:SER:N	2.42	0.52
2:E:233:VAL:HG13	2:E:248:TYR:CE2	2.44	0.52
1:B:140:ASP:OD1	1:B:141:SER:N	2.42	0.52
1:B:164:CYS:HA	1:B:174:ASN:O	2.09	0.52
1:D:107:THR:C	1:D:108:PHE:HD1	2.12	0.52
2:E:222:TYR:O	2:E:222:TYR:HD2	1.93	0.52
2:G:295:GLU:CB	2:G:296:PRO:HD2	2.39	0.52
2:E:237:PHE:O	2:E:267:LYS:NZ	2.39	0.52
1:H:117:VAL:H	1:H:176:GLN:NE2	2.08	0.52
1:H:181:LYS:HZ1	1:H:207:CYS:CB	2.21	0.52
1:H:181:LYS:HG2	1:H:193:ARG:HH12	1.74	0.52
1:B:189:GLY:C	1:B:193:ARG:HE	2.14	0.51
1:F:132:LEU:HD13	1:F:145:ILE:HG22	1.92	0.51
1:B:98:PHE:C	1:B:99:TYR:HD1	2.14	0.51
1:F:143:TRP:O	1:F:146:HIS:HB2	2.10	0.51
1:D:116:SER:HB3	1:D:214:TYR:CE2	2.46	0.51
2:E:215:TYR:O	2:E:217:GLU:OE1	2.28	0.51
2:E:220:VAL:HG11	2:E:335:GLN:OE1	2.09	0.51
2:E:199:SER:HB3	2:E:215:TYR:HE1	1.75	0.51
1:H:140:ASP:OD1	1:H:141:SER:N	2.44	0.51
1:D:98:PHE:HD1	1:D:109:LEU:HD11	1.76	0.50
1:D:106:ASN:HB3	1:D:108:PHE:HE1	1.77	0.50
2:A:263:THR:HG23	2:A:266:GLU:H	1.76	0.50
1:F:164:CYS:HA	1:F:174:ASN:O	2.12	0.50
2:E:199:SER:HB3	2:E:215:TYR:CE1	2.46	0.50
1:H:135:CYS:HB2	1:H:136:LEU:HD12	1.93	0.50
2:G:201:THR:OG1	2:G:374:LYS:HB3	2.11	0.50
2:A:272:GLN:NE2	2:A:331:SER:OG	2.45	0.50



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:106:ASN:HB3	1:B:108:PHE:HE1	1.77	0.49	
2:A:209:LEU:C	2:A:211:TYR:HD1	2.15	0.49	
1:D:140:ASP:OD1	1:D:141:SER:N	2.45	0.49	
1:B:135:CYS:HB2	1:B:136:LEU:HD12	1.94	0.49	
2:E:340:GLU:HG2	2:E:344:LYS:HE2	1.93	0.49	
1:H:118:LEU:HD11	1:H:174:ASN:O	2.12	0.49	
1:B:183:ASP:OD2	3:I:2:NAG:H3	2.12	0.49	
1:H:181:LYS:HG2	1:H:193:ARG:NH1	2.28	0.49	
1:F:140:ASP:O	1:F:143:TRP:HD1	1.95	0.49	
2:C:352:ASP:OD1	2:C:364:LYS:NZ	2.46	0.49	
1:H:120:LYS:HG2	1:H:163:LEU:HD21	1.95	0.49	
1:H:181:LYS:HZ2	1:H:207:CYS:CB	2.25	0.48	
2:C:209:LEU:C	2:C:211:TYR:HD1	2.17	0.48	
1:F:126:ILE:HG22	1:F:156:TRP:HZ3	1.77	0.48	
1:D:134:ASN:HA	1:D:167:LYS:HE3	1.95	0.48	
1:H:115:ILE:HD13	2:G:202:ILE:HG22	1.96	0.48	
2:C:263:THR:HG23	2:C:266:GLU:H	1.79	0.48	
1:D:118:LEU:HD12	1:D:176:GLN:HB2	1.96	0.47	
2:C:367:LEU:HD22	2:C:373:VAL:HG23	1.96	0.47	
1:D:99:TYR:HD1	1:D:99:TYR:N	2.13	0.47	
2:A:339:ARG:NH1	2:A:343:GLU:OE2	2.46	0.47	
1:B:116:SER:HB3	1:B:214:TYR:CE2	2.49	0.47	
1:F:186:ARG:NH2	1:F:209:GLU:OE2	2.47	0.47	
1:H:117:VAL:O	2:G:344:LYS:HD3	2.15	0.47	
1:F:155:ASP:O	1:F:159:ASP:HB2	2.15	0.47	
1:F:118:LEU:H	1:F:176:GLN:HE22	1.61	0.47	
1:D:135:CYS:HB2	1:D:136:LEU:HD12	1.97	0.47	
2:C:240:LYS:O	2:C:244:GLU:HG3	2.15	0.47	
2:A:227:GLU:OE2	2:A:374:LYS:HE3	2.15	0.47	
1:D:204:HIS:O	1:D:206:PRO:HD3	2.15	0.47	
1:F:126:ILE:HG23	1:F:131:ASP:HB2	1.97	0.46	
2:E:344:LYS:O	2:E:347:GLN:HG2	2.15	0.46	
2:G:235:ALA:HB3	2:G:257:VAL:HG12	1.97	0.46	
1:D:181:LYS:HE3	1:D:207:CYS:HB2	1.97	0.46	
1:B:99:TYR:HE2	1:B:203:PHE:HD1	1.61	0.46	
2:A:340:GLU:HG2	2:A:344:LYS:HE2	1.96	0.46	
1:D:99:TYR:N	1:D:99:TYR:CD1	2.83	0.46	
1:F:116:SER:HB3	1:F:214:TYR:CE2	2.50	0.46	
1:H:226:PHE:HE2	2:G:209:LEU:HB3	1.81	0.46	
1:F:181:LYS:HB2	1:F:208:GLU:O	2.16	0.46	
1:B:212:VAL:HG12	1:B:214:TYR:CE2	2.51	0.46	



	h h	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:194:ASN:ND2	6:F:302:HOH:O	2.35	0.46
1:F:226:PHE:CE2	2:E:209:LEU:HB3	2.51	0.46
1:H:164:CYS:HA	1:H:174:ASN:O	2.16	0.46
1:F:134:ASN:HA	1:F:167:LYS:HZ1	1.79	0.45
1:H:107:THR:C	1:H:108:PHE:HD1	2.20	0.45
1:D:118:LEU:HA	2:C:344:LYS:HZ2	1.81	0.45
1:H:116:SER:HB3	1:H:214:TYR:CZ	2.51	0.45
1:F:115:ILE:HD13	2:E:202:ILE:HG22	1.98	0.45
1:F:113:SER:OG	2:E:211:TYR:OH	2.26	0.45
2:E:262:ILE:HD12	2:E:266:GLU:HB3	1.97	0.45
1:F:99:TYR:HE2	1:F:203:PHE:HD1	1.65	0.45
1:H:126:ILE:HB	1:H:162:MET:SD	2.57	0.45
1:B:174:ASN:OD1	1:B:216:THR:HG23	2.17	0.45
1:H:169:LYS:O	6:H:301:HOH:O	2.21	0.45
1:B:231:VAL:O	1:B:235:SER:CB	2.65	0.45
1:F:107:THR:C	1:F:108:PHE:HD1	2.20	0.45
1:H:226:PHE:CE2	2:G:209:LEU:HB3	2.52	0.45
2:G:217:GLU:H	2:G:217:GLU:CD	2.21	0.45
2:G:222:TYR:O	2:G:222:TYR:CD2	2.70	0.45
2:E:225:ALA:HA	2:E:377:VAL:O	2.17	0.45
1:H:89:PRO:HA	1:H:102:ARG:O	2.17	0.44
1:H:204:HIS:O	1:H:206:PRO:HD3	2.17	0.44
2:G:223:SER:OG	2:G:330:PRO:O	2.22	0.44
2:A:350:GLU:O	2:A:351:ARG:HB2	2.17	0.44
2:G:240:LYS:O	2:G:244:GLU:HG3	2.18	0.44
1:H:140:ASP:O	1:H:143:TRP:HD1	2.01	0.43
2:G:198:ASN:ND2	2:G:220:VAL:HG21	2.31	0.43
2:E:263:THR:O	2:E:266:GLU:HB2	2.18	0.43
1:D:89:PRO:HA	1:D:102:ARG:O	2.19	0.43
1:D:118:LEU:HB2	1:D:176:GLN:OE1	2.18	0.43
2:E:216:PRO:HA	2:E:217:GLU:OE1	2.19	0.43
1:F:229:CYS:O	6:F:301:HOH:O	2.21	0.43
2:E:198:ASN:O	2:E:216:PRO:HD2	2.19	0.43
1:D:226:PHE:CE2	2:C:209:LEU:HB3	2.53	0.43
1:F:126:ILE:O	1:F:161:PRO:HB3	2.18	0.43
2:E:209:LEU:C	2:E:211:TYR:HD1	2.21	0.43
1:H:181:LYS:CE	1:H:207:CYS:HB2	2.48	0.43
1:B:148:PHE:CE2	1:B:152:LEU:HD11	2.54	0.43
1:D:226:PHE:HE2	2:C:209:LEU:HB3	1.84	0.43
1:F:180:SER:HA	1:F:213:CYS:HB3	2.01	0.43
2:E:203:THR:CG2	2:E:209:LEU:HG	2.45	0.43



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
2:C:344:LYS:O	2:C:347:GLN:HG2	2.19	0.43
1:F:162:MET:HB2	1:F:176:GLN:O	2.19	0.43
1:H:186:ARG:NH2	1:H:209:GLU:HG2	2.34	0.43
1:H:229:CYS:HA	1:H:234:LEU:HD13	2.01	0.43
1:F:91:LEU:HB3	1:F:200:PHE:CE1	2.55	0.42
2:G:233:VAL:O	2:G:255:VAL:HA	2.19	0.42
2:G:263:THR:HG23	2:G:266:GLU:H	1.84	0.42
2:A:198:ASN:ND2	2:A:220:VAL:HG11	2.34	0.42
1:B:99:TYR:HE2	1:B:203:PHE:CD1	2.36	0.42
1:B:108:PHE:HE2	1:B:145:ILE:HG12	1.83	0.42
1:D:174:ASN:OD1	1:D:216:THR:HG23	2.19	0.42
2:C:243:PHE:HB3	2:C:274:PHE:CD2	2.55	0.42
1:F:91:LEU:HD13	1:F:199:LEU:HB3	2.01	0.42
1:B:133:GLY:O	1:B:167:LYS:HE2	2.20	0.42
1:B:226:PHE:N	1:B:226:PHE:CD1	2.87	0.42
1:F:99:TYR:HE2	1:F:203:PHE:CD1	2.38	0.41
1:F:184:ASP:OD1	2:G:297:LEU:HA	2.20	0.41
1:B:231:VAL:O	1:B:235:SER:HB3	2.20	0.41
2:A:234:HIS:O	2:A:248:TYR:OH	2.34	0.41
2:C:339:ARG:NH1	6:C:403:HOH:O	2.53	0.41
1:F:102:ARG:HH22	1:F:234:LEU:HD23	1.84	0.41
2:A:203:THR:CG2	2:A:209:LEU:HG	2.47	0.41
1:D:226:PHE:N	1:D:226:PHE:CD1	2.88	0.41
2:A:367:LEU:HD22	2:A:373:VAL:HG23	2.03	0.41
2:G:268:VAL:HG11	2:G:334:VAL:HG21	2.02	0.41
1:F:181:LYS:HG3	1:F:207:CYS:HB3	2.03	0.41
2:G:209:LEU:C	2:G:211:TYR:HD1	2.24	0.41
1:B:116:SER:HB2	1:B:176:GLN:HE22	1.86	0.41
2:A:233:VAL:O	2:A:255:VAL:HA	2.21	0.41
1:D:148:PHE:CE2	1:D:152:LEU:HD11	2.56	0.41
1:H:118:LEU:HA	2:G:344:LYS:NZ	2.36	0.41
1:H:165:ARG:HG3	1:H:169:LYS:HD3	2.02	0.41
2:E:367:LEU:HD22	2:E:373:VAL:HG23	2.03	0.41
2:A:259:ALA:HA	2:A:267:LYS:HE3	2.03	0.40
2:C:242:ASP:O	2:C:246:LEU:HG	2.21	0.40
1:F:160:PRO:HA	1:F:161:PRO:HD3	1.99	0.40
1:F:175:ILE:HB	1:F:217:ILE:HB	2.03	0.40
1:F:204:HIS:O	1:F:206:PRO:HD3	2.22	0.40
1:F:226:PHE:N	1:F:226:PHE:CD1	2.90	0.40
2:G:203:THR:CG2	2:G:209:LEU:HG	2.48	0.40
2:G:280:LEU:HA	2:G:335:GLN:O	2.21	0.40



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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:264:ILE:HG23 2:E:281:ILE:CD1		2.51	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	153/168~(91%)	146 (95%)	7(5%)	0	100	100
1	D	150/168~(89%)	145 (97%)	5(3%)	0	100	100
1	F	147/168~(88%)	140 (95%)	7(5%)	0	100	100
1	Н	152/168~(90%)	148 (97%)	4(3%)	0	100	100
2	А	147/178~(83%)	141 (96%)	5(3%)	1 (1%)	22	46
2	С	145/178~(82%)	137 (94%)	8 (6%)	0	100	100
2	Е	145/178~(82%)	136 (94%)	9~(6%)	0	100	100
2	G	145/178~(82%)	138 (95%)	6 (4%)	1 (1%)	22	46
All	All	1184/1384 (86%)	1131 (96%)	51 (4%)	2 (0%)	47	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	351	ARG
2	А	351	ARG

#### 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.



Mol	Chain	Analysed	Rotameric	Outliers	Percentile	es
1	В	140/152~(92%)	136~(97%)	4 (3%)	42 71	
1	D	137/152~(90%)	135~(98%)	2(2%)	65 86	
1	F	134/152~(88%)	133 (99%)	1 (1%)	84 94	
1	Н	139/152~(91%)	138 (99%)	1 (1%)	84 94	
2	А	129/152~(85%)	129 (100%)	0	100 100	)
2	С	128/152~(84%)	128 (100%)	0	100 100	)
2	Е	128/152~(84%)	125~(98%)	3(2%)	50 78	
2	G	128/152~(84%)	127 (99%)	1 (1%)	81 93	
All	All	1063/1216~(87%)	1051 (99%)	12 (1%)	73 90	

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

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	В	99	TYR
1	В	162	MET
1	В	177	PHE
1	В	193	ARG
1	D	99	TYR
1	D	177	PHE
1	F	237	CYS
2	Е	217	GLU
2	Е	220	VAL
2	Е	222	TYR
1	Н	179	ILE
2	G	217	GLU

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

Mol	Chain	Res	Type
1	В	146	HIS
1	В	150	ASN
1	В	176	GLN
2	А	272	GLN
1	D	146	HIS
1	D	176	GLN
2	С	272	GLN



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Mol	Chain	Res	Type
1	F	150	ASN
1	F	176	GLN
2	Е	347	GLN
1	Н	146	HIS
1	Н	150	ASN
1	Н	176	GLN
2	G	335	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)

7 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	l Type Chain F		Dec	Tink	Bo	Bond lengths			Bond angles		
	туре	Unain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2	
3	NAG	Ι	1	3,1	14,14,15	0.38	0	17,19,21	0.53	0	
3	NAG	Ι	2	3	14,14,15	0.48	0	17,19,21	0.82	0	
3	BMA	Ι	3	3	11,11,12	1.02	0	$15,\!15,\!17$	0.96	1 (6%)	
3	MAN	Ι	4	3	11,11,12	1.46	1 (9%)	$15,\!15,\!17$	1.75	5 (33%)	
3	MAN	Ι	5	3	11,11,12	0.79	0	15,15,17	0.84	0	
4	NAG	J	1	4,1	14,14,15	0.49	0	17,19,21	0.61	1 (5%)	
4	NAG	J	2	4	14,14,15	0.32	0	17,19,21	0.42	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.



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	Ι	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	Ι	2	3	-	0/6/23/26	0/1/1/1
3	BMA	Ι	3	3	-	2/2/19/22	0/1/1/1
3	MAN	Ι	4	3	-	0/2/19/22	0/1/1/1
3	MAN	Ι	5	3	-	2/2/19/22	0/1/1/1
4	NAG	J	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1

'-' means no outliers of that kind were identified.

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
3	Ι	4	MAN	C1-C2	4.36	1.62	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	Ι	4	MAN	C1-C2-C3	3.50	113.97	109.67
3	Ι	4	MAN	C1-O5-C5	3.01	116.28	112.19
3	Ι	4	MAN	O2-C2-C3	-2.33	105.47	110.14
3	Ι	4	MAN	O5-C1-C2	2.27	114.28	110.77
3	Ι	4	MAN	C3-C4-C5	-2.20	106.31	110.24
3	Ι	3	BMA	C3-C4-C5	2.04	113.89	110.24
4	J	1	NAG	C1-O5-C5	2.02	114.93	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	Ι	5	MAN	O5-C5-C6-O6
3	Ι	5	MAN	C4-C5-C6-O6
3	Ι	3	BMA	C4-C5-C6-O6
3	Ι	3	BMA	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Ι	2	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,





bond angles, torsion angles, and ring geometry for oligosaccharide.





## 5.6 Ligand geometry (i)

3 ligands are modelled in this entry.

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

Mal	Type Chain Bes	Tink	Bo	ond leng	$_{\rm sths}$	Bond angles				
MIOI	туре	Unain	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	В	306	1	14,14,15	0.46	0	17,19,21	0.65	1 (5%)
5	NAG	В	307	1	14,14,15	0.47	0	17,19,21	0.69	1 (5%)
5	NAG	А	401	2	14,14,15	0.52	0	17,19,21	0.64	1 (5%)



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
5	NAG	В	306	1	-	2/6/23/26	0/1/1/1
5	NAG	В	307	1	-	2/6/23/26	0/1/1/1
5	NAG	А	401	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	В	307	NAG	C1-O5-C5	2.52	115.61	112.19
5	В	306	NAG	C1-O5-C5	2.31	115.32	112.19
5	А	401	NAG	C1-O5-C5	2.22	115.20	112.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	В	306	NAG	O5-C5-C6-O6
5	А	401	NAG	O5-C5-C6-O6
5	В	306	NAG	C4-C5-C6-O6
5	В	307	NAG	O5-C5-C6-O6
5	А	401	NAG	C4-C5-C6-O6
5	В	307	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

#### 5.7 Other polymers (i)

There are no such residues in this entry.

#### 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



# 6 Fit of model and data (i)

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

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	< <b>RSRZ</b> >	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	В	155/168~(92%)	0.34	9 (5%) 23 22	19, 47, 98, 149	0
1	D	152/168~(90%)	0.40	12 (7%) 12 10	22, 57, 127, 214	0
1	F	149/168~(88%)	2.11	68~(45%) 0 0	55, 136, 174, 202	0
1	Н	154/168~(91%)	1.74	49 (31%) 0 0	67, 129, 174, 223	0
2	А	151/178~(84%)	0.21	9 (5%) 21 20	13, 34, 114, 153	0
2	С	149/178~(83%)	0.23	11 (7%) 14 12	19, 44, 139, 182	0
2	Ε	149/178~(83%)	0.64	14 (9%) 8 6	22, 61, 159, 201	0
2	G	149/178~(83%)	0.98	27 (18%) 1 1	46, 84, 153, 184	0
All	All	1208/1384 (87%)	0.83	199 (16%) 1 1	13, 68, 165, 223	0

All (199) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Е	219	TYR	10.4
1	F	154	HIS	8.1
1	F	201	ARG	7.6
1	Н	240	ASP	7.3
1	F	197	ARG	6.9
1	D	232	ASN	6.8
1	F	234	LEU	6.7
1	Н	148	PHE	6.2
1	F	147	TRP	6.0
1	F	158	MET	6.0
2	G	217	GLU	6.0
2	Е	296	PRO	6.0
2	С	224	LYS	6.0
2	Е	294	ASP	5.9
1	Н	105	VAL	5.8
1	Н	144	ALA	5.6



6S9J

Mol	Chain	Res	Type	RSRZ
1	F	235	SER	5.4
2	Е	331	SER	5.4
1	Н	154	HIS	5.4
1	Н	241	HIS	5.4
1	F	97	SER	5.2
1	Н	234	LEU	5.1
1	F	157	LEU	5.1
1	F	148	PHE	5.1
1	Н	229	CYS	5.1
1	Н	192	ILE	5.0
2	С	296	PRO	5.0
2	G	206	SER	5.0
2	G	223	SER	5.0
1	F	89	PRO	4.9
1	F	94	LEU	4.9
1	Н	136	LEU	4.9
1	F	202	GLY	4.8
1	Н	232	ASN	4.8
2	Е	222	TYR	4.8
1	F	92	CYS	4.7
2	G	221	ALA	4.7
1	Н	92	CYS	4.7
1	Н	230	GLY	4.7
1	Н	98	PHE	4.7
1	Н	238	GLN	4.7
1	Н	145	ILE	4.7
1	F	98	PHE	4.6
1	Н	231	VAL	4.6
1	F	152	LEU	4.5
2	Е	223	SER	4.5
2	G	222	TYR	4.4
1	F	203	PHE	4.4
2	G	333	PRO	4.3
1	F	135	CYS	4.3
1	F	105	VAL	4.3
2	G	219	TYR	4.2
1	Н	94	LEU	4.2
1	В	241	HIS	4.2
2	G	230	GLY	4.1
2	С	222	TYR	4.1
2	С	223	SER	4.1
1	Н	239	PHE	4.1



6S9J	

Mol	Chain	Res	Type	RSRZ
1	F	156	TRP	4.1
2	А	293	ALA	4.1
1	D	204	HIS	4.1
1	F	192	ILE	4.1
1	F	149	SER	4.0
1	F	199	LEU	4.0
2	А	222	TYR	4.0
1	F	233	HIS	3.9
1	F	185	ALA	3.9
1	F	177	PHE	3.8
2	G	334	VAL	3.8
1	F	236	LYS	3.8
1	F	91	LEU	3.8
1	Н	107	THR	3.7
1	Н	200	PHE	3.7
1	F	145	ILE	3.7
1	Н	97	SER	3.7
1	F	231	VAL	3.6
2	G	330	PRO	3.6
1	F	131	ASP	3.6
1	F	96	ASN	3.6
1	F	132	LEU	3.6
2	Е	221	ALA	3.5
1	В	236	LYS	3.5
1	F	101	MET	3.5
1	D	235	SER	3.5
1	F	232	ASN	3.5
1	В	239	PHE	3.4
1	Н	233	HIS	3.4
2	С	297	LEU	3.4
1	F	200	PHE	3.4
2	А	223	SER	3.4
2	Е	330	PRO	3.4
1	Н	201	ARG	3.4
1	F	102	ARG	3.2
2	Е	295	GLU	3.2
1	F	143	TRP	3.2
1	F	188	TYR	3.1
1	Н	102	ARG	3.1
2	G	296	PRO	3.1
1	F	128	GLU	3.1
1	Н	193	ARG	3.1



Mol	Chain	Res	Type	RSRZ
1	F	196	MET	3.1
2	G	373	VAL	3.0
1	Н	139	SER	3.0
1	Н	199	LEU	3.0
1	Н	215	LEU	3.0
1	F	198	HIS	3.0
1	F	229	CYS	3.0
1	F	108	PHE	3.0
1	F	226	PHE	3.0
1	Н	220	CYS	2.9
1	Н	237	CYS	2.9
2	G	202	ILE	2.9
1	Н	109	LEU	2.9
1	В	87	GLU	2.9
1	Н	141	SER	2.9
2	А	330	PRO	2.9
1	F	134	ASN	2.9
1	F	155	ASP	2.9
2	А	294	ASP	2.9
1	Н	235	SER	2.9
1	F	162	MET	2.9
2	С	220	VAL	2.9
1	F	141	SER	2.9
1	Н	100	TYR	2.9
2	С	221	ALA	2.8
1	Н	147	TRP	2.8
1	F	107	THR	2.8
1	В	103	GLY	2.8
1	F	230	GLY	2.8
1	Н	151	ALA	2.8
1	Н	189	GLY	2.8
2	С	217	GLU	2.8
1	Н	226	PHE	2.8
1	F	153	GLY	2.8
1	F	100	TYR	2.7
1	F	212	VAL	2.7
1	D	238	GLN	2.7
2	A	206	SER	2.7
2	Е	226	THR	2.7
1	D	198	HIS	2.6
1	Н	89	PRO	2.5
2	G	294	ASP	2.5



Mol

1

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2

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22

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1

1

285	ARG	2.5	
91	LEU	2.4	
197	ARG	2.4	
375	LEU	2.4	
237	CYS	2.4	
297	LEU	2.4	
203	PHE	2.4	
170	LYS	2.4	
294	ASP	2.4	
196	ALA	2.4	
230	GLY	2.4	
151	ALA	2.3	
377	VAL	2.3	
97	SER	2.3	
297	LEU	2.3	
193	ARG	2.3	
205	ALA	2.3	
177	PHE	2.3	
206	SER	2.3	
227	GLU	2.3	

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Η

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D

F

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Е

F

G

Η Η

G

F

Е Н

F

С

А D

F

G D

А F

G

Η

 $\overline{\mathbf{C}}$ G

Е

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G

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G

В

F

Η

С

Η

G

D

В

 $\mathbf{Res}$ 

135

179

136

104

95

285

140

Type

CYS

ILE

LEU

GLY

ASN

ARG

ASP

RSRZ

2.5

2.5

2.5

2.5

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2.5

2.5

LEU Continued on next page...

GLY

LEU

VAL

VAL

GLY

GLY

VAL

LEU

LEU

GLY

GLU

ILE LYS

ASN

207

209

220

228

207

260

213

234

136

104

295

179

224

96

88



Mol	Chain	Res	Type	RSRZ
1	В	233	HIS	2.1
1	В	232	ASN	2.1
2	А	224	LYS	2.1
1	F	138	LYS	2.1
1	D	94	LEU	2.1
1	F	106	ASN	2.1
1	F	139	SER	2.1
1	Н	146	HIS	2.1
1	F	99	TYR	2.1
1	Н	174	ASN	2.1
1	D	199	LEU	2.0
2	G	286	THR	2.0
2	Е	248	TYR	2.0
1	F	113	SER	2.0
1	D	138	LYS	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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q < 0.9
3	MAN	Ι	4	11/12	0.65	0.50	93,98,102,106	0
3	BMA	Ι	3	11/12	0.72	0.31	86,93,97,98	0
3	MAN	Ι	5	11/12	0.75	0.23	92,103,106,107	0
3	NAG	Ι	2	14/15	0.81	0.25	66,86,92,95	0
3	NAG	Ι	1	14/15	0.83	0.29	42,60,74,80	0
4	NAG	J	2	14/15	0.86	0.19	73,79,87,88	0
4	NAG	J	1	14/15	0.95	0.11	$23,\!47,\!55,\!62$	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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
5	NAG	В	306	14/15	0.84	0.19	$58,\!68,\!81,\!89$	0
5	NAG	В	307	14/15	0.84	0.17	63,68,84,85	0
5	NAG	А	401	14/15	0.84	0.21	56,63,80,86	0

## 6.5 Other polymers (i)

There are no such residues in this entry.

