

Full wwPDB X-ray Structure Validation Report (i)

Aug 8, 2020 - 05:20 AM BST

PDB ID	:	6NM6
Title	:	Crystal Structure of HIV-1 BG505 SOSIP.664 Prefusion Env Trimer Bound
		to N6 FR3-03 scFv in Complex with Crystallization Chaperones $3H109L$ Fab
		and 35O22 scFv at 3.2 Angstrom
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Deposited on	:	2019-01-10
Resolution	:	2.74 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 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	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
$\rm CCP4$:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.74 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}	130704	$1271 \ (2.76-2.72)$
Clashscore	141614	1322(2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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 on 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	п	159	2%		
	Б	193	69%	12% •	18%
			9%		
2	D	153	59%	22% •	16%
		100	6%		
3	E	130	65%	19%	15%
	a	10.1	2%		
4	G	481	68%	20%	• 11%
	тт	211	⁹ ∕₀		
5	H	244	72%	18%	• 7%
_	-		%		
6	L	217	75%	21	.% ••



Mol	Chain	Length	Quality	of chain
7	U	145	11% 72%	15% • 12%
8	V	122	66%	15% 19%
9	А	6	33% 17%	50%
10	С	2	100	0%
10	Ι	2	100	0%
10	K	2	100	0%
10	М	2	100	0%
10	Ν	2	100	2%
10	Р	2	100	0%
10	Q	2	50%	50%
11	F	5	60%	40%
12	J	4	50%	50%
13	0	10	10% 70%	20%

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
10	NAG	С	2	-	-	-	Х
10	NAG	Κ	2	-	-	-	Х



$6\mathrm{NM6}$

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 11893 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

• Molecule 1 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	В	126	Total 1001	$\begin{array}{c} \mathrm{C} \\ 635 \end{array}$	N 172	O 188	S 6	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	559	PRO	ILE	engineered mutation	UNP Q2N0S6
В	605	CYS	THR	engineered mutation	UNP Q2N0S6

• Molecule 2 is a protein called 35O22 scFv heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	128	Total 994	C 628	N 169	O 192	${ m S}{ m 5}$	0	0	0

• Molecule 3 is a protein called 35O22 scFv light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	110	Total 836	C 525	N 138	O 167	${ m S}{ m 6}$	0	0	0

• Molecule 4 is a protein called Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	429	Total 3383	C 2131	N 598	O 627	S 27	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	145	ALA	ASN	engineered mutation	UNP Q2N0S6
G	332	ASN	THR	engineered mutation	UNP Q2N0S6



Chain	Residue	Modelled	Actual	Comment	Reference
G	501	CYS	ALA	engineered mutation	UNP Q2N0S6
G	509	ARG	-	expression tag	UNP Q2N0S6
G	510	ARG	-	expression tag	UNP Q2N0S6
G	511	ARG	-	expression tag	UNP Q2N0S6
G	512	ARG	-	expression tag	UNP Q2N0S6
G	513	ARG	-	expression tag	UNP Q2N0S6

• Molecule 5 is a protein called 3H109L Fab heavy chain.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
5	н	226	Total	С	Ν	Ο	\mathbf{S}	0	0	0
0	11	220	1715	1093	278	338	6	0	0	0

• Molecule 6 is a protein called 3H109L Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	L	210	Total 1598	C 1006	N 275	O 310	S 7	0	0	0

• Molecule 7 is a protein called N6 FR3-03 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	U	128	Total	С	Ν	Ο	\mathbf{S}	0	0	0
•	Ŭ	120	1005	637	180	184	4	0	0	

• Molecule 8 is a protein called N6 FR3-03 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	V	99	Total 767	C 478	N 140	0 147	S 2	0	0	0

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





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	А	6	Total 72	C 40	N 2	O 30	0	0	0

• Molecule 10 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	С	2	Total C N O 28 16 2 10	0	0	0
10	Ι	2	Total C N O 28 16 2 10	0	0	0
10	K	2	Total C N O 28 16 2 10	0	0	0
10	М	2	Total C N O 28 16 2 10	0	0	0
10	Ν	2	Total C N O 28 16 2 10	0	0	0
10	Р	2	Total C N O 28 16 2 10	0	0	0
10	Q	2	Total C N O 28 16 2 10	0	0	0

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



Mol	Chain	Residues	A	Aton	ns		ZeroOcc	AltConf	Trace
11	F	5	Total 61	$\begin{array}{c} \mathrm{C} \\ \mathrm{34} \end{array}$	N 2	O 25	0	0	0

• Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyran ose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glu copyranose.





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

• Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyra nose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyr anose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyr anose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-g lucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	О	10	Total 116	C 64	N 2	O 50	0	0	0

• Molecule 14 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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



Continued from previous page...

Mol	Chain	Residues	A	ton	ns		ZeroOcc	AltConf
14	В	1	Total	С	Ν	Ο	0	0
14	D	T	14	8	1	5	0	0
14	В	1	Total	С	Ν	Ο	0	0
14	D	T	14	8	1	5	0	0
14	п	1	Total	С	Ν	Ο	0	0
14		T	14	8	1	5	0	0
14	C	1	Total	С	Ν	Ο	0	0
14	u	L	14	8	1	5	0	0
14	G	1	Total	С	Ν	Ο	0	0
14	u	L	14	8	1	5	0	0
14	G	1	Total	Ċ	N	Ō		0
1.4	G	L L	14	8	1	5		0

• Molecule 15 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	В	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: Envelope glycoprotein gp41





Hole Late 111 111 1000 111 1010 111 1010 111 1010 111 1115 111 1101 111 1115 111 1116 111 114 111 114 111 114 111 114 111 114 111 114 111 114

• Molecule 9: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A:	33%	17%	50%
NAG1 NAG2 BMA3 MAN4 MAN5 MAN6 MAN6			

100%

• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

NAG 1 NAG 2

• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

100%

NAG 1 NAG 2

• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

100%

NAG 1 NAG 2

• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:

100%

NAG 1 NAG 2

• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



Chain N:		100%		
NAG 1 NAG 2				
• Molecule 10: 2 copyranose	2-acetamido-2-deoxy-b	eta-D-glucopyrano	se-(1-4)-2-acetam	ido-2-deoxy-beta-D-glu
Chain P:		100%		•
NAG 1 NAG 2 NAG 2				
• Molecule 10: 2 copyranose	2-acetamido-2-deoxy-b	eta-D-glucopyrano	se-(1-4)-2-acetam	ido-2-deoxy-beta-D-glu
Chain Q:	50%		50%	•
NAG 1 NAG 2				
• Molecule 11: a ose-(1-4)-2-aceta nose	alpha-D-mannopyranos amido-2-deoxy-beta-D-	se-(1-3)-[alpha-D-m glucopyranose-(1-4	nannopyranose-(1- l)-2-acetamido-2-c	6)]beta-D-mannopyran leoxy-beta-D-glucopyra
Chain F:	60%		40%	•
NAG1 NAG2 BMA3 MAN4 MAN5				
• Molecule 12: a beta-D-glucopyr	alpha-D-mannopyrano ranose-(1-4)-2-acetamic	se-(1-6)-beta-D-ma lo-2-deoxy-beta-D-	nnopyranose-(1-4 glucopyranose)-2-acetamido-2-deoxy-
Chain J:	50%		50%	i -

NAG1 NAG2 BMA3 MAN4

• Molecule 13: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyra nose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranos e-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-g lucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants	128.24Å 128.24 Å 315.77 Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	37.02 - 2.74	Depositor
Resolution (A)	37.02 - 2.74	EDS
% Data completeness	45.1 (37.02-2.74)	Depositor
(in resolution range)	45.1 (37.02 - 2.74)	EDS
R _{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.57 (at 2.72 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
D D .	0.240 , 0.288	Depositor
Π, Π_{free}	0.240 , 0.287	DCC
R_{free} test set	1735 reflections $(5.00%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	33.8	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.24 , 20.7	EDS
L-test for twinning ²	$< L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	0.055 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	11893	wwPDB-VP
Average B, all atoms $(Å^2)$	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.26% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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		angles
		RMSZ	# Z > 5	RMSZ	# Z > 5
1	В	0.23	0/1019	0.39	0/1382
2	D	0.24	0/1021	0.47	0/1390
3	Е	0.25	0/860	0.42	0/1175
4	G	0.25	0/3452	0.45	0/4683
5	Н	0.25	0/1758	0.46	0/2397
6	L	0.24	0/1641	0.44	0/2239
7	U	0.24	0/1035	0.43	0/1408
8	V	0.25	0/787	0.45	0/1068
All	All	0.24	0/11573	0.44	0/15742

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	В	1001	0	982	15	0
2	D	994	0	952	21	0
3	Е	836	0	785	13	0
4	G	3383	0	3334	68	0
5	Н	1715	0	1685	31	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	L	1598	0	1548	28	0
7	U	1005	0	956	16	0
8	V	767	0	727	9	0
9	А	72	0	61	3	0
10	С	28	0	25	0	0
10	Ι	28	0	25	0	0
10	K	28	0	25	0	0
10	М	28	0	25	0	0
10	N	28	0	25	0	0
10	Р	28	0	25	0	0
10	Q	28	0	25	1	0
11	F	61	0	52	0	0
12	J	50	0	43	2	0
13	0	116	0	97	2	0
14	В	42	0	39	0	0
14	D	14	0	13	1	0
14	G	42	0	39	0	0
15	В	1	0	0	0	0
All	All	11893	0	11488	193	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 8.

All (193) 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)
4:G:230:ASP:HB3	4:G:233:PHE:HB2	1.54	0.89
4:G:201:ILE:HD11	4:G:435:TYR:HB2	1.70	0.74
5:H:59:TYR:HB2	5:H:64:LYS:HD2	1.68	0.74
4:G:227:LYS:HD3	4:G:229:LYS:HZ1	1.53	0.74
1:B:605:CYS:HA	4:G:37:THR:HG22	1.72	0.71
1:B:520:LEU:HB3	1:B:524:GLY:HA3	1.72	0.71
4:G:335:LYS:HB3	4:G:412:ASP:HB3	1.72	0.71
4:G:282:LYS:NZ	7:U:100:ASP:OD1	2.23	0.70
4:G:456:ARG:O	7:U:58:ASN:ND2	2.24	0.69
1:B:585:ARG:NH2	4:G:491:ILE:O	2.25	0.69
3:E:78:LEU:HD13	3:E:106:VAL:HG23	1.75	0.68
4:G:257:THR:HG22	4:G:258:GLN:HG3	1.76	0.68
4:G:299:PRO:HG2	4:G:327:ARG:HB2	1.76	0.68
7:U:39:GLN:HB2	7:U:45:LEU:HD23	1.75	0.67
4:G:69:TRP:HE1	4:G:108:ILE:HD12	1.60	0.67



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
4:G:259:LEU:HD23	4:G:449:ILE:HG21	1.76	0.67	
4:G:425:ASN:ND2	4:G:432:GLN:O	2.28	0.67	
4:G:271:MET:HB3	4:G:273:ARG:HE	1.59	0.66	
4:G:94:ASN:HB3	4:G:97:LYS:HG2	1.77	0.66	
1:B:574:LYS:NZ	4:G:107:ASP:OD1	2.29	0.65	
5:H:63:LEU:O	5:H:65:SER:N	2.29	0.64	
5:H:157:LEU:HD21	5:H:180:VAL:HG11	1.79	0.63	
6:L:54:ARG:NH2	6:L:62:PHE:O	2.30	0.63	
1:B:571:TRP:HA	1:B:574:LYS:HB2	1.81	0.63	
5:H:195:ASN:ND2	5:H:206:ASP:OD2	2.32	0.62	
6:L:39:ARG:NH1	6:L:81:GLY:O	2.30	0.62	
4:G:286:VAL:HG13	4:G:452:LEU:HB3	1.81	0.61	
7:U:35:PHE:HE1	7:U:95:ASP:HB2	1.64	0.61	
4:G:427:TRP:HZ3	4:G:475:MET:HG2	1.65	0.61	
5:H:39:GLN:HB2	5:H:45:LEU:HD23	1.82	0.61	
2:D:59:LEU:HD11	2:D:64:GLN:HA	1.82	0.61	
2:D:96:LEU:HG	2:D:97:LEU:HG	1.84	0.60	
6:L:50:ASN:O	6:L:52:GLN:N	2.35	0.60	
6:L:37:GLN:HB2	6:L:47:LEU:HD11	1.83	0.60	
5:H:92:CYS:O	5:H:102:GLY:N	2.36	0.59	
6:L:19:ALA:HB3	6:L:75:ILE:HB	1.84	0.59	
4:G:292:VAL:HG13	4:G:449:ILE:HG13	1.85	0.58	
9:A:2:NAG:H83	9:A:2:NAG:H3	1.86	0.57	
2:D:19:LYS:HE3	2:D:79:TYR:HB3	1.85	0.57	
4:G:475:MET:SD	4:G:478:ASN:ND2	2.78	0.57	
7:U:51:ILE:HD11	7:U:71:ARG:HD2	1.85	0.57	
7:U:72:GLN:HB3	7:U:77:ILE:HG23	1.86	0.57	
5:H:100:ARG:NH2	13:O:4:MAN:O6	2.37	0.57	
4:G:456:ARG:NH1	4:G:466:GLU:OE2	2.38	0.57	
4:G:360:ARG:HB3	4:G:467:THR:HG22	1.87	0.57	
4:G:279:ASN:OD1	7:U:100(C):TRP:NE1	2.37	0.56	
3:E:37:GLN:HB2	3:E:47:ILE:HD11	1.85	0.56	
5:H:136:LEU:HD13	5:H:209:VAL:HG21	1.87	0.56	
2:D:38:ARG:HD2	2:D:46:GLU:HB3	1.88	0.56	
4:G:258:GLN:NE2	4:G:371:VAL:O	2.34	0.56	
5:H:35:SER:HG	5:H:47:TRP:HE1	1.51	0.56	
5:H:35:SER:OG	5:H:47:TRP:NE1	2.39	0.56	
4:G:260:LEU:HD12	4:G:451:GLY:HA3	1.88	0.55	
5:H:150:VAL:HG22	5:H:196:VAL:HG22	1.89	0.55	
4:G:427:TRP:HD1	4:G:429:ARG:HD2	1.71	0.55	
1:B:650:GLN:NE2	1:B:654:GLU:OE2	2.40	0.54	



	Atom 2	Interatomic	Clash
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)
3:E:19:VAL:HG12	3:E:20:THR:H	1.71	0.54
3:E:47:ILE:HG22	3:E:48:ILE:HG13	1.89	0.54
2:D:35:ASN:ND2	2:D:100(D):TRP:O	2.40	0.54
6:L:8:VAL:HG11	6:L:103:ARG:HE	1.73	0.54
6:L:14:ALA:HB3	6:L:17:GLU:HG3	1.90	0.54
4:G:476:ARG:HA	4:G:479:TRP:CD1	2.43	0.54
5:H:117:PRO:HB3	5:H:143:TYR:HB3	1.89	0.53
6:L:59:PRO:HB2	6:L:61:ARG:HG2	1.89	0.53
6:L:83:GLU:OE1	6:L:167:LYS:NZ	2.41	0.53
8:V:39:LYS:HG2	8:V:84:ALA:HB2	1.91	0.53
8:V:37:GLN:HB2	8:V:47:LEU:HD11	1.89	0.53
6:L:124:GLU:OE1	6:L:124:GLU:N	2.40	0.53
2:D:68:ASN:HB2	2:D:81:GLU:HB2	1.90	0.53
4:G:256:SER:OG	4:G:257:THR:N	2.41	0.53
4:G:346:VAL:HA	4:G:349:LEU:HD12	1.90	0.53
4:G:42:VAL:HG23	4:G:44:VAL:HG12	1.90	0.53
5:H:142:ASP:OD1	5:H:142:ASP:N	2.41	0.53
8:V:21:ILE:HD13	8:V:102:SER:HB2	1.91	0.53
4:G:439:ILE:HB	4:G:443:ILE:HD11	1.89	0.53
4:G:256:SER:OG	4:G:259:LEU:O	2.24	0.52
5:H:18:LEU:HD11	5:H:107:VAL:HG11	1.92	0.52
4:G:69:TRP:NE1	4:G:108:ILE:HD12	2.24	0.52
1:B:519:PHE:HZ	1:B:542:ARG:HH22	1.57	0.52
4:G:374:HIS:HB3	4:G:385:CYS:HB2	1.92	0.52
5:H:18:LEU:HB2	5:H:82(C):VAL:HG11	1.93	0.51
1:B:629:LEU:HD23	4:G:44:VAL:HG23	1.93	0.50
6:L:83:GLU:HG3	6:L:106:VAL:HG23	1.93	0.50
3:E:24:THR:HB	3:E:70:SER:HB3	1.94	0.50
8:V:19:VAL:HG21	8:V:78:LEU:HD13	1.92	0.50
2:D:66:ARG:NH1	2:D:86:ASP:OD2	2.45	0.50
5:H:68:ILE:HG23	5:H:81:LYS:HB2	1.93	0.50
5:H:99:LYS:HE2	5:H:100(A):ILE:HD11	1.94	0.50
6:L:34:GLN:HB2	6:L:89:HIS:HB3	1.93	0.50
2:D:100(E):LEU:HD12	2:D:100(F):PRO:HD2	1.95	0.49
3:E:37:GLN:HG3	3:E:84:THR:HG21	1.93	0.49
6:L:52:GLN:N	6:L:52:GLN:OE1	2.46	0.49
2:D:109:LEU:HG	2:D:110:THR:H	1.76	0.49
1:B:569:THR:OG1	1:B:569:THR:O	2.28	0.49
4:G:104:MET:O	4:G:108:ILE:HG12	2.13	0.49
4:G:257:THR:HB	4:G:375:SER:H	1.77	0.49
4:G:360:ARG:HH11	4:G:467:THR:HG21	1.78	0.49



		Interatomic	Clash
Atom-1	Atom-2	$distance ({ m \AA})$	overlap (Å)
13:O:1:NAG:H83	13:O:1:NAG:H3	1.94	0.49
4:G:478:ASN:O	4:G:481:SER:OG	2.30	0.48
5:H:165:PRO:HG2	6:L:163:THR:HG21	1.96	0.48
5:H:24:VAL:HG12	5:H:76:ASN:HB3	1.96	0.48
5:H:4:LEU:HG	5:H:24:VAL:HG23	1.96	0.48
2:D:57:LYS:HE2	2:D:59:LEU:HD22	1.95	0.47
4:G:193:LEU:HB2	4:G:196:CYS:SG	2.54	0.47
6:L:52:GLN:NE2	6:L:53:ASP:OD1	2.47	0.47
14:D:201:NAG:O3	14:D:201:NAG:O7	2.31	0.47
4:G:219:ALA:O	4:G:246:GLN:NE2	2.47	0.47
1:B:609:PRO:HA	4:G:35:TRP:HA	1.96	0.47
1:B:606:THR:HG21	1:B:646:LEU:HD22	1.96	0.47
3:E:83:GLU:HG3	3:E:106:VAL:HG12	1.96	0.47
4:G:123:THR:N	4:G:124:PRO:HD2	2.30	0.47
6:L:34:GLN:HG3	6:L:49:TYR:HA	1.95	0.47
5:H:33:TYR:HB2	5:H:95:ALA:O	2.15	0.47
2:D:30:ASN:HA	2:D:52(A):PRO:HB2	1.96	0.46
1:B:526:ALA:HA	4:G:43:PRO:HB2	1.97	0.46
7:U:95:ASP:OD1	7:U:96:ARG:N	2.48	0.46
3:E:7:SER:HB2	3:E:22:SER:H	1.80	0.46
6:L:47:LEU:O	6:L:48:ILE:HG13	2.16	0.46
8:V:85:THR:HG22	8:V:103:ARG:HB2	1.96	0.46
5:H:103:LYS:HD2	5:H:103:LYS:N	2.31	0.46
6:L:109:GLN:HB2	6:L:141:TYR:CE1	2.51	0.46
4:G:231:LYS:HB3	4:G:268:GLU:HG3	1.97	0.46
4:G:299:PRO:HA	4:G:442:VAL:HG13	1.97	0.46
4:G:333:VAL:HG21	4:G:390:LEU:HD21	1.98	0.45
4:G:101:VAL:HG13	4:G:479:TRP:HB2	1.98	0.45
4:G:378:CYS:HB3	4:G:383:PHE:CE1	2.52	0.45
4:G:205:CYS:HB3	4:G:207:LYS:HD2	1.99	0.45
6:L:83:GLU:HG2	6:L:105:THR:HA	1.99	0.45
4:G:122:LEU:HD13	4:G:125:LEU:HD12	1.99	0.44
5:H:121:PRO:HG3	5:H:207:LYS:HG2	1.97	0.44
2:D:2:GLY:O	2:D:102:LEU:HD21	2.18	0.44
4:G:357:THR:HG1	4:G:465:THR:N	2.15	0.44
2:D:48:MET:HG2	2:D:63:PHE:CD2	2.53	0.44
9:A:4:MAN:H3	9:A:5:MAN:H2	1.63	0.44
4:G:291:PRO:HG3	10:Q:1:NAG:O6	2.18	0.44
4:G:96:TRP:CG	4:G:275:GLU:HG2	2.53	0.44
3:E:38:TRP:CE2	3:E:44:PRO:HG3	2.53	0.44
5:H:103:LYS:H	5:H:103:LYS:HD2	1.83	0.43



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
7:U:100(C):TRP:CZ3	8:V:96:GLN:HB3	2.53	0.43
7:U:29:PHE:CE2	7:U:52(A):PRO:HB3	2.53	0.43
4:G:261:LEU:HD13	12:J:1:NAG:H82	1.99	0.43
7:U:76(B):ASP:C	7:U:76(D):PRO:HD3	2.38	0.43
4:G:56:SER:O	4:G:77:THR:N	2.35	0.43
5:H:144:PHE:HA	5:H:145:PRO:HA	1.79	0.43
5:H:38:ARG:HG2	5:H:48:ILE:HD11	2.01	0.43
5:H:83:THR:O	5:H:109:VAL:HG21	2.19	0.43
6:L:111:LYS:HD2	6:L:199:GLU:HG3	2.00	0.43
7:U:29:PHE:CD2	7:U:76(G):GLY:HA3	2.54	0.43
2:D:13:LYS:HD2	2:D:13:LYS:HA	1.68	0.43
2:D:47:TRP:HZ2	2:D:50:TRP:CD1	2.37	0.42
7:U:87:THR:HG23	7:U:110:VAL:HA	2.00	0.42
2:D:6:GLN:H	2:D:105:GLN:NE2	2.17	0.42
7:U:67:VAL:HG22	7:U:82:ILE:HG12	2.02	0.42
1:B:544:LEU:HD12	4:G:222:GLY:HA2	2.01	0.42
6:L:121:PRO:HD3	6:L:133:LEU:HD13	2.02	0.42
6:L:143:GLY:HA3	6:L:173:TYR:CG	2.54	0.42
8:V:3:HIS:N	8:V:26:SER:HG	2.16	0.42
4:G:86:LEU:HB3	4:G:89:VAL:HG21	2.02	0.42
2:D:47:TRP:CZ2	2:D:49:GLY:HA2	2.54	0.42
4:G:104:MET:SD	4:G:479:TRP:HB3	2.60	0.42
2:D:6:GLN:H	2:D:105:GLN:HE22	1.67	0.42
4:G:272:ILE:HG12	4:G:286:VAL:HB	2.01	0.42
8:V:32:ASP:HA	8:V:50:HIS:HA	2.02	0.42
5:H:24:VAL:CG1	5:H:76:ASN:HB3	2.50	0.42
4:G:153:GLU:O	4:G:178:ARG:HB2	2.20	0.41
5:H:6:GLU:N	5:H:6:GLU:OE1	2.51	0.41
2:D:94:LYS:HG2	2:D:95:GLY:O	2.19	0.41
4:G:272:ILE:HD12	4:G:348:GLN:HB3	2.02	0.41
6:L:168:GLN:OE1	6:L:174:ALA:HB2	2.20	0.41
4:G:261:LEU:HD23	4:G:449:ILE:HG22	2.02	0.41
6:L:122:SER:OG	6:L:125:GLU:HG2	2.20	0.41
3:E:84:THR:OG1	3:E:85:THR:N	2.53	0.41
4:G:359:ILE:HD12	4:G:468:PHE:HE1	1.84	0.41
2:D:4:LEU:HG	2:D:24:THR:HG22	2.02	0.41
2:D:50:TRP:CH2	9:A:4:MAN:H62	2.55	0.41
3:E:27(C):CYS:HA	3:E:28:CYS:HA	1.62	0.41
4:G:396:ILE:HG22	4:G:397:SER:N	2.35	0.41
8:V:49:HIS:O	8:V:53:SER:HB2	2.20	0.41
1:B:656:ASN:O	1:B:660:LEU:HG	2.21	0.41



ge 20	Full wwf DD A-lay Stilu	cture vanuation ne	port
ontinued from previou	s page		
Atom-1	Atom-2	$\begin{array}{c c} \text{Interatomic} \\ \text{distance} (\text{\AA}) \end{array}$	$egin{array}{c} { m Clash} \ { m overlap} \ ({ m \AA}) \end{array}$
4:G:282:LYS:HA	4:G:282:LYS:HD3	1.73	0.41
7:U:35:PHE:CD2	7:U:50:TRP:HB3	2.55	0.41
5:H:115:LYS:HD2	5:H:115:LYS:HA	1.85	0.41
1:B:637:ASN:OD1	1:B:637:ASN:N	2.54	0.41
6:L:33:VAL:HG12	6:L:51:ASN:OD1	2.21	0.41
4:G:447:SER:HB3	12:J:1:NAG:HN2	1.85	0.40
3:E:19:VAL:HG12	3:E:20:THR:N	2.36	0.40
5:H:27:GLY:O	5:H:76:ASN:ND2	2.54	0.40
6:L:42:GLN:HG2	6:L:43:ALA:H	1.86	0.40
4:G:270:VAL:HG23	4:G:287:GLN:O	2.21	0.40
6:L:36:TYR:HD1	6:L:46:LEU:HA	1.85	0.40
6:L:61:ARG:NH2	6:L:82:ASP:OD2	2.47	0.40

2.02

1.77

0.40

0.40

7:U:78:ALA:HA

3:E:43:ALA:H

Continue

There are no symmetry-related clashes.

Torsion angles (i) 5.3

7:U:71:ARG:HA

3:E:42:ARG:HB3

5.3.1Protein 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	Perc	entiles
1	В	122/153~(80%)	113~(93%)	8 (7%)	1 (1%)	19	36
2	D	126/153~(82%)	113 (90%)	12 (10%)	1 (1%)	19	36
3	E	108/130~(83%)	88 (82%)	19 (18%)	1 (1%)	17	32
4	G	$417/481 \ (87\%)$	378 (91%)	38 (9%)	1 (0%)	47	69
5	Н	222/244~(91%)	198 (89%)	20 (9%)	4 (2%)	8	15
6	L	208/217~(96%)	189 (91%)	17 (8%)	2 (1%)	15	28
7	U	126/145~(87%)	119 (94%)	7 (6%)	0	100	100
8	V	97/122~(80%)	89 (92%)	7 (7%)	1 (1%)	15	28
All	All	1426/1645~(87%)	1287 (90%)	128 (9%)	11 (1%)	19	36





Mol	Chain	Res	Type
6	L	51	ASN
3	Е	8	ALA
5	Н	64	LYS
8	V	51	THR
5	Н	117	PRO
4	G	474	ASP
1	В	570	VAL
5	Н	124	PRO
6	L	95(A)	GLY
2	D	100(F)	PRO
5	Н	68	ILE

All (11) Ramachandran outliers are listed below:

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	Percentiles
1	В	108/129~(84%)	105~(97%)	3 (3%)	43 63
2	D	107/115~(93%)	103~(96%)	4 (4%)	34 54
3	Ε	96/113~(85%)	92~(96%)	4 (4%)	30 49
4	G	383/427~(90%)	372~(97%)	11 (3%)	42 62
5	Н	196/212~(92%)	192~(98%)	4 (2%)	55 72
6	L	174/181~(96%)	172~(99%)	2(1%)	73 84
7	U	102/115~(89%)	101~(99%)	1 (1%)	76 85
8	V	87/94~(93%)	87 (100%)	0	100 100
All	All	1253/1386~(90%)	1224 (98%)	29 (2%)	50 70

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	569	THR
1	В	570	VAL
1	В	571	TRP



Mol	Chain	Res	Type
2	D	38	ARG
2	D	68	ASN
2	D	91	PHE
2	D	100(C)	THR
3	Е	27(B)	VAL
3	Е	68	TYR
3	Е	89	CYS
3	Е	96	CYS
4	G	57	ASP
4	G	67	ASN
4	G	207	LYS
4	G	231	LYS
4	G	286	VAL
4	G	292	VAL
4	G	346	VAL
4	G	348	GLN
4	G	426	MET
4	G	429	ARG
4	G	444	ARG
5	Н	82(B)	SER
5	Н	100(P)	MET
5	Н	142	ASP
5	Н	207	LYS
6	L	25	ARG
6	L	54	ARG
7	U	71	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
4	G	425	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)

39 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	Tune	Chain	Dec	Tink	Bond lengths		Bond angles			
	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	А	1	9,4	14, 14, 15	0.30	0	$17,\!19,\!21$	0.45	0
9	NAG	А	2	9	14, 14, 15	0.44	0	$17,\!19,\!21$	1.27	1(5%)
9	BMA	А	3	9	11,11,12	0.69	0	$15,\!15,\!17$	0.92	0
9	MAN	А	4	9	11,11,12	0.97	1 (9%)	$15,\!15,\!17$	1.25	2 (13%)
9	MAN	А	5	9	11,11,12	1.53	1 (9%)	$15,\!15,\!17$	1.82	4 (26%)
9	MAN	А	6	9	11,11,12	0.60	0	$15,\!15,\!17$	1.06	2 (13%)
10	NAG	С	1	10,4	14,14,15	0.19	0	17,19,21	0.45	0
10	NAG	С	2	10	14,14,15	0.23	0	$17,\!19,\!21$	0.45	0
11	NAG	F	1	11,4	14, 14, 15	0.25	0	$17,\!19,\!21$	0.41	0
11	NAG	F	2	11	14, 14, 15	0.23	0	$17,\!19,\!21$	0.37	0
11	BMA	F	3	11	11,11,12	0.69	0	$15,\!15,\!17$	0.85	0
11	MAN	F	4	11	11,11,12	0.80	1(9%)	$15,\!15,\!17$	1.15	2 (13%)
11	MAN	F	5	11	11,11,12	0.73	0	$15,\!15,\!17$	1.07	2(13%)
10	NAG	Ι	1	10,4	14,14,15	0.28	0	17,19,21	0.48	0
10	NAG	Ι	2	10	14,14,15	0.26	0	17,19,21	0.36	0
12	NAG	J	1	12,4	14,14,15	0.28	0	17,19,21	0.54	0
12	NAG	J	2	12	14,14,15	0.24	0	17,19,21	0.45	0
12	BMA	J	3	12	11,11,12	0.64	0	$15,\!15,\!17$	0.78	0
12	MAN	J	4	12	11,11,12	0.66	0	$15,\!15,\!17$	1.14	2 (13%)
10	NAG	K	1	10,4	14,14,15	0.25	0	17,19,21	0.39	0
10	NAG	K	2	10	14,14,15	0.27	0	17,19,21	0.35	0
10	NAG	М	1	10,4	14,14,15	0.22	0	17,19,21	0.44	0
10	NAG	М	2	10	14,14,15	0.24	0	17,19,21	0.40	0
10	NAG	N	1	10,4	14, 14, 15	0.30	0	$17,\!19,\!21$	0.43	0
10	NAG	Ν	2	10	$14,\!14,\!15$	0.24	0	$17,\!19,\!21$	0.49	0
13	NAG	0	1	13,4	14, 14, 15	0.38	0	$17,\!19,\!21$	1.42	2 (11%)
13	MAN	Ο	10	13	11,11,12	1.10	2(18%)	$15,\!15,\!17$	1.60	4 (26%)
13	NAG	0	2	13	14,14,15	0.21	0	17, 19, 21	0.40	0
13	BMA	Ο	3	13	11, 11, 12	1.00	1 (9%)	$15,\!15,\!17$	0.96	0
13	MAN	O	4	13	11,11,12	0.77	1 (9%)	$15,\!1\overline{5},\!17$	1.39	2 (13%)



Mal	Tune	Chain	Dec	Ros Link	Bo	ond leng	\mathbf{ths}	В	ond ang	les
	туре	Chain	ries		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	MAN	Ο	5	13	11,11,12	0.67	0	$15,\!15,\!17$	0.97	1(6%)
13	MAN	Ο	6	13	11,11,12	0.72	0	$15,\!15,\!17$	0.86	1 (6%)
13	MAN	Ο	7	13	11,11,12	0.72	0	$15,\!15,\!17$	1.00	2 (13%)
13	MAN	Ο	8	13	11,11,12	0.69	0	$15,\!15,\!17$	1.06	1 (6%)
13	MAN	0	9	13	11,11,12	0.79	1(9%)	$15,\!15,\!17$	1.31	2(13%)
10	NAG	Р	1	10,4	14,14,15	0.29	0	17,19,21	0.48	0
10	NAG	Р	2	10	14,14,15	0.26	0	17,19,21	0.50	0
10	NAG	Q	1	10,4	14,14,15	0.99	1 (7%)	17,19,21	1.67	1 (5%)
10	NAG	Q	2	10	14,14,15	0.26	0	17,19,21	0.44	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
9	NAG	А	1	9,4	-	0/6/23/26	0/1/1/1
9	NAG	А	2	9	-	5/6/23/26	0/1/1/1
9	BMA	А	3	9	-	2/2/19/22	0/1/1/1
9	MAN	А	4	9	-	1/2/19/22	0/1/1/1
9	MAN	А	5	9	-	2/2/19/22	0/1/1/1
9	MAN	А	6	9	-	0/2/19/22	0/1/1/1
10	NAG	С	1	10,4	-	0/6/23/26	0/1/1/1
10	NAG	С	2	10	-	2/6/23/26	0/1/1/1
11	NAG	F	1	11,4	-	2/6/23/26	0/1/1/1
11	NAG	F	2	11	-	0/6/23/26	0/1/1/1
11	BMA	F	3	11	-	2/2/19/22	0/1/1/1
11	MAN	F	4	11	-	2/2/19/22	0/1/1/1
11	MAN	F	5	11	-	2/2/19/22	0/1/1/1
10	NAG	Ι	1	10,4	-	2/6/23/26	0/1/1/1
10	NAG	Ι	2	10	-	2/6/23/26	0/1/1/1
12	NAG	J	1	12,4	-	2/6/23/26	0/1/1/1
12	NAG	J	2	12	-	2/6/23/26	0/1/1/1
12	BMA	J	3	12	-	2/2/19/22	0/1/1/1
12	MAN	J	4	12	-	2/2/19/22	0/1/1/1
10	NAG	K	1	10,4	-	2/6/23/26	0/1/1/1
10	NAG	K	2	10	-	2/6/23/26	0/1/1/1



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	М	1	10,4	-	2/6/23/26	0/1/1/1
10	NAG	М	2	10	-	0/6/23/26	0/1/1/1
10	NAG	N	1	10,4	-	0/6/23/26	0/1/1/1
10	NAG	N	2	10	-	2/6/23/26	0/1/1/1
13	NAG	0	1	13,4	-	5/6/23/26	0/1/1/1
13	MAN	0	10	13	-	0/2/19/22	0/1/1/1
13	NAG	Ο	2	13	-	2/6/23/26	0/1/1/1
13	BMA	0	3	13	-	0/2/19/22	0/1/1/1
13	MAN	Ο	4	13	-	2/2/19/22	0/1/1/1
13	MAN	0	5	13	-	0/2/19/22	0/1/1/1
13	MAN	0	6	13	-	0/2/19/22	0/1/1/1
13	MAN	0	7	13	-	0/2/19/22	0/1/1/1
13	MAN	0	8	13	-	0/2/19/22	0/1/1/1
13	MAN	0	9	13	-	1/2/19/22	0/1/1/1
10	NAG	Р	1	10,4	-	2/6/23/26	0/1/1/1
10	NAG	Р	2	10	-	0/6/23/26	0/1/1/1
10	NAG	Q	1	10,4	-	2/6/23/26	0/1/1/1
10	NAG	Q	2	10	-	2/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	А	5	MAN	C1-C2	4.33	1.62	1.52
10	Q	1	NAG	O5-C1	3.55	1.49	1.43
13	0	9	MAN	C1-C2	2.36	1.57	1.52
13	0	10	MAN	C1-C2	2.36	1.57	1.52
13	0	4	MAN	C1-C2	2.27	1.57	1.52
13	0	10	MAN	C2-C3	2.25	1.55	1.52
11	F	4	MAN	C1-C2	2.22	1.57	1.52
13	0	3	BMA	O5-C1	-2.20	1.40	1.43
9	А	4	MAN	O5-C1	-2.12	1.40	1.43

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
10	Q	1	NAG	C1-O5-C5	6.44	120.91	112.19
13	0	1	NAG	C2-N2-C7	4.52	129.34	122.90
9	А	2	NAG	C2-N2-C7	4.28	129.00	122.90
9	А	5	MAN	C1-C2-C3	4.20	114.83	109.67
9	А	5	MAN	C1-O5-C5	4.00	117.62	112.19



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
13	0	4	MAN	C1-O5-C5	3.84	117.39	112.19
13	0	9	MAN	C1-O5-C5	3.62	117.10	112.19
13	0	10	MAN	C1-C2-C3	3.59	114.08	109.67
13	0	8	MAN	C1-O5-C5	3.03	116.30	112.19
12	J	4	MAN	C1-O5-C5	3.02	116.29	112.19
9	А	6	MAN	C1-O5-C5	2.83	116.03	112.19
11	F	5	MAN	C1-O5-C5	2.43	115.49	112.19
13	0	1	NAG	C1-C2-N2	2.43	114.64	110.49
11	F	4	MAN	C1-O5-C5	2.41	115.46	112.19
13	0	10	MAN	C1-O5-C5	2.41	115.46	112.19
9	А	4	MAN	C3-C4-C5	2.40	114.53	110.24
13	0	7	MAN	C1-O5-C5	2.38	115.42	112.19
9	А	4	MAN	O2-C2-C3	-2.33	105.48	110.14
13	0	4	MAN	O2-C2-C3	-2.31	105.50	110.14
13	0	10	MAN	O2-C2-C3	-2.27	105.59	110.14
9	А	6	MAN	O2-C2-C3	-2.26	105.61	110.14
13	0	9	MAN	O2-C2-C3	-2.24	105.65	110.14
13	0	10	MAN	O5-C1-C2	2.23	114.21	110.77
12	J	4	MAN	O2-C2-C3	-2.23	105.68	110.14
13	0	7	MAN	O2-C2-C3	-2.21	105.70	110.14
9	А	5	MAN	O2-C2-C3	-2.21	105.71	110.14
11	F	5	MAN	O2-C2-C3	-2.21	105.72	110.14
13	0	5	MAN	O2-C2-C3	-2.14	105.84	110.14
11	F	4	MAN	O2-C2-C3	-2.12	105.89	110.14
13	0	6	MAN	O2-C2-C3	-2.10	105.94	110.14
9	A	5	MAN	O5-C1-C2	2.09	114.00	110.77

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There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	Ι	2	NAG	O5-C5-C6-O6
9	А	2	NAG	O5-C5-C6-O6
10	М	1	NAG	O5-C5-C6-O6
12	J	1	NAG	O5-C5-C6-O6
9	А	5	MAN	O5-C5-C6-O6
10	Q	2	NAG	O5-C5-C6-O6
12	J	2	NAG	O5-C5-C6-O6
11	F	4	MAN	O5-C5-C6-O6
10	Ι	1	NAG	O5-C5-C6-O6
9	А	3	BMA	O5-C5-C6-O6
9	А	3	BMA	C4-C5-C6-O6



Mol	Chain	Res	Type	Atoms
12	J	4	MAN	O5-C5-C6-O6
10	Ι	2	NAG	C4-C5-C6-O6
11	F	3	BMA	C4-C5-C6-O6
12	J	2	NAG	C4-C5-C6-O6
13	0	1	NAG	O5-C5-C6-O6
13	0	1	NAG	C4-C5-C6-O6
9	A	2	NAG	C4-C5-C6-O6
10	М	1	NAG	C4-C5-C6-O6
12	J	1	NAG	C4-C5-C6-O6
10	Q	1	NAG	C8-C7-N2-C2
10	Q	1	NAG	O7-C7-N2-C2
9	A	2	NAG	C8-C7-N2-C2
9	А	2	NAG	O7-C7-N2-C2
13	Ο	1	NAG	C8-C7-N2-C2
13	0	1	NAG	O7-C7-N2-C2
11	F	4	MAN	C4-C5-C6-O6
13	0	4	MAN	O5-C5-C6-O6
11	F	5	MAN	C4-C5-C6-O6
10	Q	2	NAG	C4-C5-C6-O6
12	J	4	MAN	C4-C5-C6-O6
9	А	5	MAN	C4-C5-C6-O6
10	Р	1	NAG	O5-C5-C6-O6
13	0	4	MAN	C4-C5-C6-O6
11	F	3	BMA	O5-C5-C6-O6
12	J	3	BMA	O5-C5-C6-O6
10	K	1	NAG	O5-C5-C6-O6
11	F	1	NAG	C4-C5-C6-O6
11	F	5	MAN	O5-C5-C6-O6
10	K	1	NAG	C4-C5-C6-O6
10	Ι	1	NAG	C4-C5-C6-O6
11	F	1	NAG	O5-C5-C6-O6
13	0	2	NAG	C4-C5-C6-O6
10	С	2	NAG	C4-C5-C6-O6
10	K	2	NAG	C4-C5-C6-O6
10	N	2	NAG	C4-C5-C6-O6
13	0	2	NAG	O5-C5-C6-O6
10	Р	1	NAG	C4-C5-C6-O6
10	K	2	NAG	O5-C5-C6-O6
10	C	2	NAG	O5-C5-C6-O6
13	0	9	MAN	C4-C5-C6-O6
12	J	3	BMA	C4-C5-C6-O6
10	N	2	NAG	05-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	А	2	NAG	C3-C2-N2-C7
13	0	1	NAG	C3-C2-N2-C7
9	А	4	MAN	C4-C5-C6-O6

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	Q	1	NAG	1	0
13	0	4	MAN	1	0
9	А	5	MAN	1	0
9	А	2	NAG	1	0
9	А	4	MAN	2	0
13	0	1	NAG	1	0
12	J	1	NAG	2	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)

7 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	Dog	Tink	Bo	Bond lengths			Bond angles		
	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
14	NAG	G	638	4	14, 14, 15	0.20	0	17,19,21	0.43	0	
14	NAG	В	702	1	14, 14, 15	0.29	0	$17,\!19,\!21$	0.43	0	
14	NAG	В	701	1	14,14,15	0.34	0	17,19,21	0.58	0	
14	NAG	D	201	2	14,14,15	0.49	0	17,19,21	0.49	0	



Mol Ty	Type	Chain	Dog	Tink	Bond lengths				Bond angles		
	туре	Chain	I Ites		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
14	NAG	G	614	4	14, 14, 15	0.27	0	17,19,21	0.48	0	
14	NAG	G	617	4	14, 14, 15	0.23	0	17,19,21	0.45	0	
14	NAG	В	703	1	14,14,15	0.27	0	17,19,21	0.45	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
14	NAG	G	638	4	-	2/6/23/26	0/1/1/1
14	NAG	В	702	1	-	2/6/23/26	0/1/1/1
14	NAG	В	701	1	-	1/6/23/26	0/1/1/1
14	NAG	D	201	2	-	3/6/23/26	0/1/1/1
14	NAG	G	614	4	-	2/6/23/26	0/1/1/1
14	NAG	G	617	4	-	2/6/23/26	0/1/1/1
14	NAG	В	703	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	D	201	NAG	C1-C2-N2-C7
14	G	614	NAG	O5-C5-C6-O6
14	G	617	NAG	O5-C5-C6-O6
14	G	638	NAG	O5-C5-C6-O6
14	G	638	NAG	C4-C5-C6-O6
14	G	614	NAG	C4-C5-C6-O6
14	G	617	NAG	C4-C5-C6-O6
14	В	703	NAG	O5-C5-C6-O6
14	В	702	NAG	C4-C5-C6-O6
14	D	201	NAG	O5-C5-C6-O6
14	B	702	NAG	O5-C5-C6-O6
14	В	701	NAG	O5-C5-C6-O6
14	D	201	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	D	201	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	< RSRZ >	#RSRZ>2	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q<0.9
1	В	126/153~(82%)	-0.13	3 (2%) 59 66	13, 41, 76, 101	0
2	D	128/153~(83%)	0.46	14 (10%) 5 5	27, 75, 116, 127	0
3	E	110/130~(84%)	0.24	8 (7%) 15 17	31, 59, 103, 120	0
4	G	429/481~(89%)	-0.27	12 (2%) 53 60	10, 34, 85, 113	0
5	Н	226/244~(92%)	-0.18	3 (1%) 77 82	15,51,92,111	0
6	L	210/217~(96%)	-0.43	3 (1%) 75 80	16,39,66,91	0
7	U	128/145~(88%)	0.79	16 (12%) 3 4	37, 87, 123, 143	0
8	V	99/122~(81%)	1.65	33 (33%) 0 0	68, 108, 136, 152	0
All	All	1456/1645~(88%)	0.06	92 (6%) 20 22	10, 49, 112, 152	0

All (92) RSRZ outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	RSRZ
7	U	14	PRO	8.4
8	V	58	VAL	6.5
8	V	76	SER	6.3
8	V	12	SER	6.0
3	Е	107	GLY	5.8
4	G	72	HIS	5.8
7	U	15	GLY	5.6
1	В	660	LEU	5.4
2	D	109	LEU	4.8
8	V	57	GLY	4.8
2	D	41	ALA	4.8
4	G	188	ASN	4.7
8	V	80	ALA	4.6
8	V	86	TYR	4.5
2	D	10	THR	4.5
8	V	104	LEU	4.5



Mol	Chain	Res	Type	RSRZ
4	G	505	VAL	4.4
2	D	18	VAL	4.3
6	L	210	THR	4.3
8	V	48	ILE	4.2
7	U	8	GLY	4.2
3	Е	106	VAL	4.1
4	G	430	ILE	3.9
2	D	8	GLY	3.9
2	D	43	ARG	3.8
2	D	5	VAL	3.7
3	Е	106(A)	LEU	3.6
7	U	2	ALA	3.6
7	U	82(A)	ARG	3.6
8	V	89	GLN	3.6
7	U	3	HIS	3.5
8	V	13	VAL	3.5
3	Е	80	PRO	3.5
4	G	411	ASN	3.4
8	V	99	GLY	3.4
1	В	548	ILE	3.4
7	U	13	LYS	3.3
2	D	84	SER	3.3
4	G	135	THR	3.3
3	Е	68	TYR	3.1
2	D	19	LYS	3.1
8	V	19	VAL	3.1
3	Е	69	TRP	3.0
8	V	69	THR	3.0
7	U	17	SER	3.0
2	D	82(C)	LEU	3.0
5	Н	187	LEU	3.0
8	V	103	ARG	2.9
8	V	14	SER	2.9
4	G	504	ARG	2.8
3	Е	8	ALA	2.8
8	V	67	PHE	2.8
4	G	465	THR	2.8
8	V	74	THR	2.7
6	L	184	MET	2.7
6	L	7	TYR	2.7
7	U	18	VAL	2.6
1	В	662	ALA	2.5



Mol

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7

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V

V

Η

D

U

V

D

V

V

RSRZ

2.5

2.5

Type

GLN

ALA

V	11	LEU	2.5	
V	98	PHE	2.5	
D	107	THR	2.5	
V	63	SER	2.5	
U	109	VAL	2.4	
V	10	SER	2.4	
U	7	SER	2.4	
U	90	TYR	2.4	
U	82	ILE	2.4	
G	428	GLN	2.4	
V	105	HIS	2.3	
G	80	ASN	2.3	
Е	65	TYR	2.3	
G	151	ARG	2.3	
V	40	PRO	2.3	
D	108	LEU	2.3	
V	36	TYR	2.2	
V	45	LYS	2.2	
V	81	ASP	2.2	
G	412	ASP	2.2	
V	62	PHE	2.2	
U	65	ASP	2.2	
Η	28	SER	2.1	

VAL

ILE

PRO

THR

GLY

ASP

ARG

THR

ARG

2.1

2.1

2.1

2.1

2.1

2.1

2.0

2.0

2.0

54

21

183

83

82(B)

77

82(A)

20

100

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 \mathbf{Res}

27

10

Chain

V

U

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	\mathbf{Res}	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{A}^2)$	Q<0.9
10	NAG	С	2	14/15	0.61	0.43	$114,\!146,\!158,\!165$	0
11	BMA	F	3	11/12	0.62	0.34	123,127,141,142	0
10	NAG	K	2	14/15	0.74	0.52	$100,\!137,\!149,\!149$	0
10	NAG	Q	2	14/15	0.78	0.29	84,114,126,146	0
10	NAG	Р	2	14/15	0.78	0.21	48,88,101,106	0
11	MAN	F	4	11/12	0.79	0.27	$94,\!119,\!128,\!131$	0
10	NAG	Ι	2	14/15	0.80	0.26	$72,\!103,\!117,\!121$	0
12	BMA	J	3	11/12	0.80	0.24	$86,\!107,\!130,\!134$	0
10	NAG	М	2	14/15	0.80	0.35	$77,\!92,\!117,\!120$	0
10	NAG	K	1	14/15	0.83	0.26	$67,\!98,\!117,\!128$	0
9	MAN	А	4	11/12	0.83	0.22	$79,\!88,\!107,\!114$	0
10	NAG	N	2	14/15	0.83	0.33	$77,\!87,\!116,\!135$	0
10	NAG	С	1	14/15	0.84	0.24	$87,\!108,\!130,\!143$	0
12	MAN	J	4	11/12	0.85	0.39	115,128,149,153	0
9	MAN	A	5	11/12	0.87	0.30	$85,\!95,\!100,\!105$	0
13	NAG	0	1	14/15	0.87	0.18	$33,\!58,\!71,\!77$	0
13	MAN	0	8	11/12	0.89	0.14	42,59,71,72	0
13	MAN	0	9	11/12	0.89	0.24	$79,\!86,\!103,\!103$	0
11	NAG	F	2	14/15	0.89	0.19	$63,\!80,\!113,\!120$	0
11	MAN	F	5	11/12	0.89	0.41	$54,\!111,\!124,\!128$	0
13	NAG	0	2	14/15	0.89	0.16	$32,\!57,\!74,\!82$	0
10	NAG	Ι	1	14/15	0.90	0.16	$75,\!96,\!103,\!114$	0
12	NAG	J	2	14/15	0.92	0.15	$41,\!61,\!102,\!104$	0
10	NAG	Р	1	14/15	0.93	0.12	$46,\!58,\!70,\!94$	0
13	MAN	0	10	11/12	0.94	0.20	$37,\!51,\!77,\!85$	0
11	NAG	F	1	14/15	0.94	0.16	$24,\!56,\!69,\!73$	0
13	MAN	0	6	11/12	0.94	0.14	$30,\!37,\!43,\!47$	0
9	BMA	А	3	11/12	0.94	0.12	$38,\!43,\!51,\!85$	0
10	NAG	Q	1	14/15	0.94	0.12	$54,\!68,\!94,\!108$	0
9	NAG	А	1	14/15	0.95	0.14	$17,\!24,\!30,\!35$	0
10	NAG	М	1	14/15	0.95	0.15	$36,\!52,\!76,\!81$	0
10	NAG	N	1	14/15	0.95	0.19	28,43,64,65	0
9	NAG	A	2	14/15	0.95	0.11	$24,\!33,\!51,\!63$	0
9	MAN	А	6	11/12	0.96	0.10	$31,\!42,\!50,\!58$	0
13	BMA	0	3	11/12	0.96	0.07	$20,\!39,\!45,\!50$	0
13	MAN	Ο	7	11/12	0.96	0.13	$37,\!49,\!66,\!80$	0
12	NAG	J	1	14/15	0.97	0.13	12,26,49,51	0



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
13	MAN	0	4	11/12	0.97	0.10	25,29,39,44	0
13	MAN	Ο	5	11/12	0.97	0.13	22,32,41,44	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	${f B} ext{-factors}({ m \AA}^2)$	Q<0.9
14	NAG	В	702	14/15	0.80	0.26	$58,\!96,\!101,\!102$	0
14	NAG	В	701	14/15	0.85	0.41	85,111,128,139	0
14	NAG	D	201	14/15	0.85	0.29	$64,\!106,\!122,\!128$	0
14	NAG	G	617	14/15	0.85	0.26	$68,\!91,\!99,\!99$	0
14	NAG	В	703	14/15	0.88	0.33	$67,\!103,\!116,\!120$	0
14	NAG	G	614	14/15	0.91	0.16	47,70,96,99	0
14	NAG	G	638	14/15	0.93	0.15	$48,\!57,\!67,\!74$	0

6.5 Other polymers (i)

There are no such residues in this entry.

