

Full wwPDB X-ray Structure Validation Report (i)

Oct 15, 2023 – 03:36 AM EDT

PDB ID	:	8E1P
Title	:	Crystal structure of BG505 SOSIP.v4.1-GT1.2 trimer in complex with gl-
		PGV20 and PGT124 Fabs
Authors	:	Sarkar, A.; Kumar, S.; Wilson, I.A.
Deposited on	:	2022-08-11
Resolution	:	3.82 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
buster-report	:	1.1.7(2018)
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 3.82 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.



Motric	Whole archive	Similar resolution
Wiethic	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R _{free}	130704	$1231 \ (4.04-3.60)$
Clashscore	141614	1031 (4.02-3.62)
Ramachandran outliers	138981	1261 (4.04-3.60)
Sidechain outliers	138945	1255 (4.04-3.60)
RSRZ outliers	127900	1139 (4.04-3.60)

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	Quality of chain									
1	F	225	8%	26%									
1	Н	225	81%	17%									
1	Ν	225	18%	20%									
2	Ι	210	9%	15%	•••								
3	L	210	^{2%} 77%	18%	••								



Mol	Chain	Length	Quality of chain								
2	0	910	14%								
3	0	210	80%	15% ••							
4	А	214	86%	12% •							
4	C	014	14%								
4	C	214	85%	13% ••							
4	J	214	81%	17% ·							
5	F	474	2%	100/							
0	Ľ	474	/4%	19% • 6%							
5	G	474	73%	20% • 5%							
5	М	474	73%	19% • 5%							
			8%	1370 . 370							
6	В	236	77%	18% •							
6	D	236	75%	20% •							
	τ.	224	6%								
6	K	236	77%	18% •							
7	Х	153	76%	8% 16%							
7	V	152	7404	100/ 100/							
	1	100	3%	10% 16%							
7	Z	153	71%	13% 16%							
8	Р	3	100%								
	-										
8	U	3	33% 67%								
8	с	3	67%	33%							
0	_	0									
8	e	3	100%								
9	Q	2	100%								
Q	S	2	50%	50%							
5	5	<u></u>	50%	50 %							
9	Т	2	50%	50%							
9	V	2	100%								
Q	W	9	100%								
3	v v		100%								
9	b	2	50%	50%							
9	d	2	100%								
9	f	2	100%								
L	1										



Mol	Chain	Length		Quality of chain
9	i	2		100%
10	R	7	14%	86%
11	a	9	22%	78%
12	g	6	33%	67%
13	h	3		100%

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
9	NAG	Т	2	-	-	-	Х



2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 34410 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Б	222	Total	С	Ν	0	\mathbf{S}	0	0	
		1690	1060	294	326	10	0	0	0	
1	п	222	Total	С	Ν	0	S	0	0	0
	ІН		1690	1060	294	326	10			
1	1 N	222	Total	С	Ν	0	S	0	0	0
			1690	1060	294	326	10	0	0	U

• Molecule 1 is a protein called germline PGV20 heavy chain.

• Molecule 2 is a protein called germline PGV20 light chain.

Mol	Chain	Residues		At	\mathbf{oms}			ZeroOcc	AltConf	Trace
2	Ι	205	Total 1526	C 954	N 250	0 316	S 6	0	0	0

• Molecule 3 is a protein called germline PGV20 light chain.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
3	L	204	Total	С	Ν	0	S	0	0	0
5 L	204	1521	952	249	314	6	0	0	0	
2	2 0	205	Total	С	Ν	0	S	0	0	0
3 0	0	205	1526	954	250	316	6	0	0	0

• Molecule 4 is a protein called PGT124 Fab Light Chain.

Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf	Trace
4	Λ	210	Total	С	Ν	0	S	0	0	
4 A	210	1595	1005	270	315	5	0	0	0	
4	C	210	Total	С	Ν	0	S	0	0	0
	U		1595	1005	270	315	5			0
4	4 I	910	Total	С	Ν	0	S	0	0	0
4 J	210	1595	1005	270	315	5	0	0		

• Molecule 5 is a protein called BG505-SOSIP.v4.1-GT1.2gp120.



Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
Б	Б	447	Total	С	Ν	0	\mathbf{S}	0	0	0
D E	447	3526	2219	622	658	27	0	0	0	
F	C	440	Total	С	Ν	0	S	0	0	0
5 G	449	3541	2227	625	662	27	0	0	U	
5	E M	440	Total	С	Ν	0	S	0	0	0
D M	449	3541	2227	625	662	27	0	0		

• Molecule 6 is a protein called PGT124 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
6 B	226	Total	С	Ν	0	S	0	0	0		
0	D	220	1720	1093	287	335	5	0	0	U	
6	П	226	Total	С	Ν	Ο	S	0	0	0	
0		220	1720	1093	287	335	5	0	0	0	
6	K	226	Total	С	Ν	0	S	0	0	0	
0	Γ	220	1720	1093	287	335	5	0	0	0	

• Molecule 7 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	7 V	120	Total	С	Ν	0	S	0	0	0
	I	129	1030	655	176	193	6	0	0	0
7	v	120	Total	С	Ν	0	S	0	0	0
	Λ	129	1030	655	176	193	6	0	0	0
7	7	120	Total	С	Ν	0	S	0	0	0
		129	1030	655	176	193	6	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	559	PRO	ILE	conflict	UNP Q2N0S6
Y	605	CYS	THR	conflict	UNP Q2N0S6
Х	559	PRO	ILE	conflict	UNP Q2N0S6
Х	605	CYS	THR	conflict	UNP Q2N0S6
Z	559	PRO	ILE	conflict	UNP Q2N0S6
Z	605	CYS	THR	conflict	UNP Q2N0S6

• 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.





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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
8	Р	3	Total C N O 39 22 2 15	0	0	0
8	U	3	Total C N O 39 22 2 15	0	0	0
8	С	3	Total C N O 39 22 2 15	0	0	0
8	е	3	Total C N O 39 22 2 15	0	0	0

• Molecule 9 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
9	Q	2	Total C N O 28 16 2 10	0	0	0
9	S	2	Total C N O 28 16 2 10	0	0	0
9	Т	2	Total C N O 28 16 2 10	0	0	0
9	V	2	Total C N O 28 16 2 10	0	0	0
9	W	2	Total C N O 28 16 2 10	0	0	0
9	b	2	Total C N O 28 16 2 10	0	0	0
9	d	2	Total C N O 28 16 2 10	0	0	0
9	f	2	Total C N O 28 16 2 10	0	0	0
9	i	2	Total C N O 28 16 2 10	0	0	0

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





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

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
11	a	9	Total C N O 108 60 3 45	0	0	0

• Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyra nose-(1-6)]alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

• Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyra nose-(1-2)-alpha-D-mannopyranose.





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
13	h	3	Total 33	C 18	O 15	0	0	0

• Molecule 14 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	A	ton	ns		ZeroOcc	AltConf
14	F	1	Total	С	Ν	0	0	0
14	Ľ	1	14	8	1	5	0	0
14	E	1	Total	С	Ν	Ο	0	Ο
14	Ľ	1	14	8	1	5	0	0
14	E	1	Total	С	Ν	Ο	0	0
17	Ц	I	14	8	1	5	0	0
14	E	1	Total	С	Ν	Ο	0	0
14	Ľ	1	14	8	1	5	0	0
14	E	1	Total	С	Ν	Ο	0	0
17	Ц	I	14	8	1	5	0	0
14	E	1	Total	С	Ν	Ο	0	0
		1	14	8	1	5	0	0
14	E	1	Total	С	Ν	Ο	0	0
		1	14	8	1	5	0	0
14	E	1	Total	С	Ν	Ο	0	0
		I.	14	8	1	5	Ŭ	0
14	G	1	Total	С	Ν	Ο	0	0
	<u> </u>	1	14	8	1	5		0
14	G	1	Total	С	Ν	Ο	0	0
		1	14	8	1	5		0



Continued from previous page...

Mol	Chain	Residues	A	ton	ns		ZeroOcc	AltConf
14	C	1	Total	С	Ν	0	0	0
14	G	1	14	8	1	5	0	0
14	C	1	Total	С	Ν	0	0	0
14	G	1	14	8	1	5	0	0
14	С	1	Total	С	Ν	0	0	0
14	G	1	14	8	1	5	0	0
14	С	1	Total	С	Ν	0	0	0
14	G	1	14	8	1	5	0	0
14	C	1	Total	С	Ν	0	0	0
14	u	I	14	8	1	5	0	0
14	М	1	Total	С	Ν	Ο	0	0
11	111	Ĩ	14	8	1	5	0	0
14	М	1	Total	С	Ν	Ο	0	0
		1	14	8	1	5	0	0
14	М	1	Total	С	Ν	Ο	0	0
		1	14	8	1	5	0	
14	М	1	Total	С	Ν	Ο	0	0
		-	14	8	1	5		Ŭ
14	М	1	Total	С	Ν	Ο	0	0
		-	14	8	1	5		
14	М	1	Total	С	Ν	0	0	0
		-	14	8	1	5		Ŭ
14	М	1	Total	С	Ν	0	0	0
		_	14	8	1	5	-	
14	М	1	Total	C	N	Õ	0	0
			14	8	1	5		
14	Y	1	Total	С	N	Õ	0	0
			14	8		5		
14	Y	1	Total	С	N	Õ	0	0
			14	8		5		
14	Y	1	Total	C	N	Õ	0	0
			14	8	1	5		
14	Х	1	Total	C	IN 1	U F	0	0
			14	8		5 0		
14	Х	1		U o	1N 1	U E	0	0
			14 Tet 1	8 ()		0		
14	Ζ	1	10tal	U o	1N 1	U E	0	0
			14 Tetal	ð C		$\frac{0}{0}$		
14	Ζ	1	10tal	U o	1N 1	U E	0	0
			14	ð	T	Э		



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: germline PGV20 heavy chain

• Molecule 1: germline PGV20 heavy chain



 \bullet Molecule 1: germline PGV20 heavy chain







• Molecule 2: germline PGV20 light chain





• Molecule 4: PGT124 Fab Light Chain





• Molecule 5: BG505-SOSIP.v4.1-GT1.2gp120



• Molecule 5: BG505-SOSIP.v4.1-GT1.2gp120







• Molecule 8: beta-D
-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:	100%
NAG1 NAG2 BMA3	

• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

$\alpha_1 \cdot \tau_1$		
Chain U:	33%	67%

NAG1 NAG2 BMA3



33%

67%

Chain c:

NAG 1 NAG 2 BMA 3

• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:	100%	
NAG1 NAG2 BMA3		
• Molecule 9: opyranose	2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamid	lo-2-deoxy-beta-D-gluc
Chain Q:	100%	•
NAG1 NAG2		
• Molecule 9: opyranose	2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamid	lo-2-deoxy-beta-D-gluc
Chain S:	50% 50%	

NAG1 NAG2

• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:	50%	50%	
NAG2 NAG2			

• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:

100%

NAG1 NAG2

• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:

100%



• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

50%

Chain b:

NAG1 NAG2

• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:

100%

50%

NAG1 NAG2

• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc opyranose

Chain f:	100%
NAG2 NAG2	
• Molecule 9: opyranose	eq:2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-a

Chain i:

100%

NAG1 NAG2

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

Chain R:	14%	86%	
NAG1 NAG2 BMA3 MAN4 MAN5 MAN5 MAN6 MAN7			

 $\label{eq:constraint} \bullet \mbox{Molecule 11: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4$

Chain a:	22%	78%	
NAG1 NAG2 MAN4 MAN5 MAN5 MAN6 MAN8 MAN8 MAN8			



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

Chain g: 33% 67%

NAG 1 NAG 2 BMA 3 MAN 4 MAN 5 MAN 5 MAN 6

 \bullet Molecule 13: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose

Chain h:

100%

MAN1 MAN2 MAN3 MAN3



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	146.06Å 157.67Å 158.56Å	Deperitor
a, b, c, α , β , γ	90.00° 102.97° 90.00°	Depositor
$\mathbf{P}_{\mathrm{exolution}}(\mathbf{\hat{A}})$	49.76 - 3.82	Depositor
Resolution (A)	49.76 - 3.82	EDS
% Data completeness	94.3 (49.76-3.82)	Depositor
(in resolution range)	94.3 (49.76-3.82)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.37 (at 3.88 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
D D	0.271 , 0.301	Depositor
n, n_{free}	0.270 , 0.300	DCC
R_{free} test set	3181 reflections $(4.97%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	104.9	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.27, 45.4	EDS
L-test for $twinning^2$	$ < L >=0.41, < L^2>=0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	34410	wwPDB-VP
Average B, all atoms $(Å^2)$	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.84% 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: NAG, MAN, BMA

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

Mal	Chain	Bond lengths		Bond angles	
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	F	0.27	0/1732	0.51	0/2354
1	Н	0.26	0/1732	0.49	0/2354
1	Ν	0.25	0/1732	0.50	0/2354
2	Ι	0.26	0/1564	0.46	0/2132
3	L	0.26	0/1558	0.47	0/2122
3	0	0.25	0/1563	0.46	0/2129
4	А	0.24	0/1638	0.47	0/2238
4	С	0.25	0/1638	0.46	0/2238
4	J	0.24	0/1638	0.46	0/2238
5	Е	0.25	0/3601	0.49	0/4889
5	G	0.26	0/3618	0.50	0/4916
5	М	0.25	0/3617	0.49	0/4913
6	В	0.25	0/1763	0.49	0/2407
6	D	0.25	0/1763	0.49	0/2407
6	Κ	0.25	0/1763	0.50	0/2407
7	Х	0.23	0/1048	0.42	0/1421
7	Y	0.24	0/1048	0.43	0/1421
7	Ζ	0.24	0/1048	0.43	0/1421
All	All	0.25	0/34064	0.48	0/46361

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1690	0	1645	38	0
1	Н	1690	0	1645	26	0
1	Ν	1690	0	1645	26	0
2	Ι	1526	0	1462	20	0
3	L	1521	0	1461	25	0
3	0	1526	0	1461	23	0
4	А	1595	0	1541	12	0
4	С	1595	0	1541	17	0
4	J	1595	0	1541	24	0
5	Е	3526	0	3463	65	0
5	G	3541	0	3478	68	0
5	М	3541	0	3477	70	0
6	В	1720	0	1686	24	0
6	D	1720	0	1686	27	0
6	Κ	1720	0	1686	27	0
7	Х	1030	0	1019	10	0
7	Y	1030	0	1018	16	0
7	Ζ	1030	0	1019	23	0
8	Р	39	0	34	0	0
8	U	39	0	34	1	0
8	с	39	0	34	0	0
8	е	39	0	34	0	0
9	Q	28	0	25	0	0
9	S	28	0	25	1	0
9	Т	28	0	25	2	0
9	V	28	0	25	0	0
9	W	28	0	25	0	0
9	b	28	0	25	0	0
9	d	28	0	25	0	0
9	f	28	0	25	0	0
9	i	28	0	25	0	0
10	R	83	0	70	0	0
11	a	108	0	91	0	0
12	g	72	0	61	0	0
13	h	33	0	28	0	0
14	Е	112	0	104	3	0
14	G	98	0	91	5	0
14	М	112	0	104	3	0
14	Х	28	0	26	0	0
14	Y	42	0	39	0	0
14	Z	$\overline{28}$	0	$\overline{26}$	0	0

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.



Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	34410	0	33475	495	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 7.

All (495) 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)
5:E:186(A):ASN:H	5:E:187:GLN:HA	1.41	0.86
1:N:121:SER:HA	1:N:122:SER:HB3	1.60	0.84
5:M:186(A):ASN:N	5:M:187:GLN:HA	1.94	0.82
4:A:148:TRP:HE1	4:A:176:SER:HG	1.25	0.81
5:E:186(A):ASN:N	5:E:187:GLN:HA	1.96	0.81
1:F:144:THR:HA	1:F:194:PRO:HA	1.61	0.80
5:G:186(A):ASN:N	5:G:187:GLN:HA	1.97	0.80
1:F:142:GLY:CA	1:F:144:THR:H	1.96	0.79
4:C:148:TRP:HE1	4:C:176:SER:HG	1.29	0.78
4:J:148:TRP:HE1	4:J:176:SER:HG	1.31	0.78
5:E:152:GLY:N	14:E:601:NAG:HO6	1.83	0.76
5:G:230:ASP:HB3	5:G:233:PHE:HB2	1.68	0.76
5:M:186(A):ASN:H	5:M:187:GLN:HA	1.50	0.75
7:Y:591:GLN:NE2	7:X:541:ALA:O	2.20	0.74
2:I:13:GLY:H	2:I:105:PHE:HE1	1.35	0.74
4:C:108:GLN:HG2	4:C:109:PRO:HD2	1.70	0.73
5:E:69:TRP:HB3	5:E:215:ILE:HD11	1.71	0.72
5:E:230:ASP:HB3	5:E:233:PHE:HB2	1.70	0.72
5:M:84:ILE:HD13	7:Z:522:PHE:H	1.53	0.72
5:G:186(A):ASN:H	5:G:187:GLN:HA	1.55	0.71
2:I:54:ARG:HD2	2:I:58:VAL:HG22	1.74	0.69
6:B:22:CYS:HB3	6:B:78:LEU:HB3	1.73	0.69
5:M:219:ALA:O	5:M:246:GLN:NE2	2.26	0.69
6:B:135:THR:HA	6:B:185:PRO:HA	1.75	0.69
5:G:220:PRO:HB3	7:Y:578:ALA:HB1	1.74	0.68
1:F:142:GLY:HA3	1:F:144:THR:H	1.59	0.68
5:M:230:ASP:HB3	5:M:233:PHE:HB2	1.76	0.67
5:G:219:ALA:O	5:G:246:GLN:NE2	2.27	0.67
5:M:37:THR:HG22	7:Z:605:CYS:HA	1.77	0.67
1:H:3:GLN:HB3	1:H:25:SER:HB2	1.77	0.66
5:M:363:ASN:O	5:M:469:ARG:NH1	2.26	0.66
6:D:123:PRO:HG3	6:D:209:LYS:HB3	1.76	0.66
1:H:144:THR:HA	1:H:195:SER:H	1.61	0.65



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
6:B:121:VAL:HG11	6:B:198:VAL:HG21	1.77	0.65
3:L:54:ARG:HD2	3:L:58:VAL:HG22	1.78	0.65
7:X:573:ILE:HD13	7:Z:568:LEU:HD21	1.79	0.65
7:Y:542:ARG:NH1	7:Z:647:GLU:OE2	2.30	0.65
2:I:152:ASP:OD2	2:I:190:LYS:HG3	1.97	0.65
5:G:308:ARG:NH1	5:M:197:ASN:O	2.30	0.65
5:M:276:ASP:HB3	5:M:279:ASP:HB2	1.78	0.65
4:C:34:GLN:HG3	4:C:49:TYR:HA	1.79	0.64
1:F:105:ARG:HG3	1:F:106:GLU:HB2	1.78	0.64
6:D:135:THR:HA	6:D:185:PRO:HA	1.78	0.64
5:E:156:ASN:ND2	14:E:602:NAG:O7	2.30	0.64
5:M:491:ILE:O	7:Z:585:ARG:NH2	2.31	0.64
1:F:103:GLN:NE2	1:F:108:ASP:OD2	2.29	0.63
5:E:201:ILE:HD11	5:E:435:TYR:HB2	1.80	0.63
5:E:164:GLU:HG3	5:E:165:LEU:HD12	1.80	0.63
1:F:10:GLU:HB2	1:F:118:VAL:HG12	1.79	0.63
7:Z:606:THR:HG21	7:Z:646:LEU:HD11	1.81	0.63
5:E:161:MET:HE3	5:E:162:THR:H	1.62	0.62
5:G:70:ALA:HB2	5:G:213:ILE:HD11	1.79	0.62
4:J:21:ILE:HB	4:J:73:LEU:HB3	1.81	0.62
1:H:6:GLN:H	1:H:114:GLN:HE22	1.47	0.62
1:H:7:SER:HB3	1:H:21:SER:HB3	1.81	0.62
5:E:36:VAL:HG12	7:X:610:TRP:HE3	1.64	0.62
14:G:601:NAG:H3	14:G:601:NAG:H83	1.82	0.62
7:X:606:THR:HG21	7:X:646:LEU:HD11	1.81	0.62
5:E:277:ILE:O	5:E:456:ARG:NH1	2.33	0.61
5:G:186(A):ASN:O	5:G:186(A):ASN:ND2	2.33	0.61
5:G:47:ASP:HA	5:G:489:VAL:HG12	1.82	0.61
5:M:36:VAL:HG12	7:Z:610:TRP:HE3	1.64	0.61
1:H:144:THR:HG22	1:H:194:PRO:HA	1.83	0.60
5:M:135:THR:O	5:M:137:ASN:N	2.34	0.60
5:E:69:TRP:HA	5:E:111:LEU:HD13	1.82	0.60
5:M:87:GLU:HB2	14:M:601:NAG:H82	1.83	0.60
4:A:134:CYS:HB3	4:A:176:SER:HB3	1.83	0.60
5:M:221:ALA:HB3	7:Z:582:ALA:HB1	1.84	0.60
4:A:25:ARG:NH2	4:A:88:CYS:O	2.34	0.60
14:G:604:NAG:H83	14:G:604:NAG:H3	1.83	0.60
6:B:11:LEU:HD11	6:B:112:SER:HB3	1.84	0.60
5:E:186(A):ASN:O	5:E:186(A):ASN:ND2	2.35	0.59
6:D:87:THR:HG23	6:D:110:THR:HA	1.84	0.59
5:M:94:ASN:HA	5:M:236:THR:HG22	1.84	0.59



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
5:M:201:ILE:HD11	5:M:435:TYR:HB2	1.84	0.59
5:G:55:ALA:HB3	5:G:216:HIS:HB2	1.84	0.59
6:K:123:PRO:HG3	6:K:209:LYS:HB3	1.85	0.59
2:I:107:LEU:HG	2:I:109:GLN:HA	1.84	0.59
5:M:34:LEU:HD21	7:Z:619:LEU:HD11	1.85	0.59
5:M:292:VAL:HB	5:M:449:ILE:HG23	1.83	0.59
4:J:25:ARG:NH2	4:J:88:CYS:O	2.35	0.59
1:H:168:LEU:HD21	1:H:191:VAL:HG21	1.83	0.59
5:G:122:LEU:HD13	5:G:125:LEU:HD22	1.85	0.59
6:K:65:SER:O	6:K:82(A):ARG:NH1	2.36	0.59
5:M:474:ASP:OD2	5:M:476:ARG:NH1	2.36	0.58
4:C:37:GLN:HB2	4:C:47:LEU:HD11	1.84	0.58
5:E:124:PRO:HA	5:M:166:ARG:HE	1.68	0.58
4:J:7:SER:HB3	4:J:102:THR:HA	1.84	0.58
1:F:144:THR:HG22	1:F:192:THR:HG22	1.86	0.58
5:E:292:VAL:HB	5:E:449:ILE:HG23	1.86	0.58
1:H:171:GLY:O	1:H:191:VAL:HA	2.04	0.58
5:E:308:ARG:NH1	5:G:197:ASN:O	2.37	0.58
1:F:142:GLY:CA	1:F:144:THR:N	2.66	0.58
5:G:299:PRO:HB2	5:G:327:ARG:HB2	1.84	0.58
5:G:321(A):ASP:HB3	14:G:602:NAG:H82	1.85	0.58
6:B:87:THR:HG23	6:B:110:THR:HA	1.84	0.58
3:O:54:ARG:HD2	3:O:58:VAL:HG22	1.84	0.58
5:E:474:ASP:OD1	5:E:475:MET:N	2.37	0.58
1:N:177:ALA:HB2	1:N:187:LEU:HD23	1.86	0.57
1:H:144:THR:HA	1:H:194:PRO:HA	1.84	0.57
1:F:99:ARG:HD2	1:F:105:ARG:HB2	1.87	0.57
3:L:116:VAL:O	3:L:205:LYS:NZ	2.31	0.57
4:C:134:CYS:HB3	4:C:176:SER:HB3	1.87	0.57
9:S:2:NAG:H83	9:S:2:NAG:H3	1.87	0.57
5:G:37:THR:HG22	7:Y:605:CYS:HA	1.87	0.57
1:H:177:ALA:HB2	1:H:187:LEU:HD23	1.87	0.57
4:C:21:ILE:HD12	4:C:73:LEU:HD23	1.87	0.56
5:G:94:ASN:HA	5:G:236:THR:HG22	1.87	0.56
5:G:201:ILE:HD11	5:G:435:TYR:HB2	1.87	0.56
1:F:6:GLN:NE2	1:F:116:THR:OG1	2.37	0.56
5:G:61:TYR:CD1	5:G:65:LYS:HB3	2.40	0.56
5:G:493:PRO:HG3	7:Y:544:LEU:HD21	1.88	0.56
1:H:67:ARG:NH2	1:H:90:ASP:OD2	2.38	0.56
1:N:144:THR:HA	1:N:194:PRO:HA	1.85	0.56
5:M:235:GLY:HA3	14:M:604:NAG:H82	1.86	0.56



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
5:E:297:THR:HG22	5:E:444:ARG:HG3	1.86	0.56
5:G:84:ILE:HD13	7:Y:521:GLY:HA3	1.88	0.56
6:D:138:LEU:O	6:D:182:VAL:N	2.38	0.56
1:N:14:PRO:HD3	1:N:121:SER:O	2.06	0.56
5:E:448:ASN:HD22	9:T:1:NAG:C7	2.19	0.56
5:E:273:ARG:NH1	5:E:287:GLN:OE1	2.35	0.55
6:K:40:SER:HB2	6:K:43:LYS:HD2	1.87	0.55
6:K:119:PRO:HB3	6:K:145:TYR:HB3	1.87	0.55
6:K:150:VAL:HB	6:K:178:LEU:HD21	1.86	0.55
2:I:116:VAL:O	2:I:205:LYS:NZ	2.30	0.55
6:K:51:ILE:HD13	6:K:71:ARG:HG3	1.88	0.55
1:N:3:GLN:HB3	1:N:25:SER:HB2	1.87	0.55
5:E:299:PRO:HB2	5:E:327:ARG:HB2	1.87	0.55
6:K:135:THR:HA	6:K:185:PRO:HA	1.88	0.55
1:F:177:ALA:HB2	1:F:187:LEU:HD23	1.89	0.55
5:G:173:HIS:CE1	5:G:305:LYS:HE3	2.42	0.55
3:O:109:GLN:NE2	3:0:141:TYR:0	2.40	0.55
3:L:107:LEU:HD11	3:L:110:PRO:HG3	1.89	0.54
3:O:133:LEU:HD12	3:O:179:LEU:HB3	1.89	0.54
5:M:55:ALA:HB3	5:M:216:HIS:HB2	1.90	0.54
5:G:36:VAL:HG12	7:Y:610:TRP:HE3	1.72	0.54
6:D:119:PRO:HB3	6:D:145:TYR:HB3	1.88	0.54
1:F:156:PRO:HD2	1:F:211:PRO:HB2	1.88	0.54
5:G:298:ARG:NH2	5:G:441:GLY:O	2.39	0.54
1:H:177:ALA:HA	1:H:187:LEU:HB3	1.90	0.54
1:N:147:LEU:HB2	1:N:220:VAL:HG11	1.89	0.54
5:E:101:VAL:HG13	5:E:479:TRP:HB2	1.90	0.54
1:F:171:GLY:O	1:F:191:VAL:HA	2.08	0.54
1:H:191:VAL:HG22	1:H:193:VAL:HG13	1.90	0.54
5:E:197:ASN:O	5:M:308:ARG:NH1	2.40	0.54
5:G:61:TYR:HD1	5:G:65:LYS:HB3	1.71	0.54
5:G:173:HIS:ND1	14:G:602:NAG:O7	2.41	0.53
1:F:147:LEU:HB2	1:F:220:VAL:HG11	1.90	0.53
3:L:31:ASN:N	3:L:66:LYS:HZ3	2.06	0.53
5:M:264:SER:O	5:M:287:GLN:NE2	2.34	0.53
6:D:126:PRO:HG2	6:D:213:PRO:HB3	1.90	0.53
5:E:84:ILE:HD13	7:X:521:GLY:HA3	1.90	0.53
5:E:490:LYS:HD2	7:X:585:ARG:HH12	1.73	0.53
6:D:11:LEU:HD11	6:D:112:SER:HB3	1.90	0.53
3:L:91:TYR:CE2	5:G:278:ARG:HB3	2.43	0.53
4:J:28:LEU:HB3	4:J:94:ARG:HD3	1.91	0.53



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:100:MET:HG2	1:F:110:GLN:HB2	1.91	0.53
6:D:144:ASP:HB3	6:D:175:LEU:HD23	1.91	0.53
5:G:67:ASN:HD21	5:G:70:ALA:H	1.56	0.53
5:M:164:GLU:HG3	5:M:165:LEU:HD12	1.91	0.53
6:K:22:CYS:HB3	6:K:78:LEU:HB3	1.90	0.53
1:N:36:TRP:CE2	1:N:81:MET:HB2	2.44	0.53
5:G:298:ARG:NH1	5:G:381:GLU:OE2	2.41	0.53
1:H:99:ARG:HD3	1:H:106:GLU:HG3	1.92	0.52
1:N:178:VAL:HG21	3:O:161:GLU:HB3	1.90	0.52
6:B:200:HIS:CD2	6:B:202:PRO:HD2	2.44	0.52
5:M:159:PHE:HA	14:M:603:NAG:H82	1.91	0.52
5:M:474:ASP:OD1	5:M:475:MET:N	2.41	0.52
3:L:83:ASP:OD1	3:L:83:ASP:N	2.43	0.52
3:O:109:GLN:HG2	3:O:142:PRO:HD3	1.91	0.52
5:E:263:GLY:O	9:T:1:NAG:H81	2.10	0.52
5:E:363:ASN:O	5:E:469:ARG:NH1	2.41	0.52
5:G:474:ASP:OD1	5:G:475:MET:N	2.43	0.52
5:M:257:THR:O	5:M:259:LEU:N	2.40	0.52
6:D:147:PRO:O	6:D:200:HIS:NE2	2.43	0.52
5:E:358:ILE:HB	5:E:465:THR:HA	1.92	0.52
5:G:297:THR:HG22	5:G:444:ARG:HG3	1.92	0.52
3:O:109:GLN:HB2	3:0:141:TYR:HD1	1.75	0.51
5:E:37:THR:HG22	7:X:605:CYS:HA	1.93	0.51
5:G:257:THR:HG22	5:G:258:GLN:HG3	1.93	0.51
5:M:476:ARG:HA	5:M:479:TRP:CD1	2.45	0.51
7:Y:587:LEU:HB3	7:X:545:LEU:HD21	1.92	0.51
5:E:67:ASN:ND2	5:E:70:ALA:H	2.08	0.51
5:M:493:PRO:HG3	7:Z:544:LEU:HD21	1.92	0.51
6:B:151:THR:HB	6:B:199:ASN:HB2	1.92	0.51
7:Z:650:GLN:O	7:Z:654:GLU:N	2.31	0.51
2:I:109:GLN:N	2:I:110:PRO:HD2	2.26	0.51
1:H:58:THR:H	5:G:366:GLY:HA3	1.76	0.51
1:H:147:LEU:HB2	1:H:220:VAL:HG11	1.93	0.51
3:L:79:GLN:H	3:L:82:GLU:HG3	1.74	0.51
3:L:184:GLU:O	3:L:188:SER:OG	2.24	0.51
5:E:370:GLU:HG2	5:E:384:TYR:HE2	1.76	0.51
4:J:89:HIS:CD2	4:J:91:TRP:HE1	2.28	0.51
5:M:134:VAL:HG12	5:M:156:ASN:HB2	1.93	0.51
4:A:59:PRO:HB2	4:A:61:ARG:HG3	1.92	0.51
5:G:96:TRP:HH2	5:G:285:LEU:HD23	1.76	0.51
6:D:150:VAL:HB	6:D:178:LEU:HD21	1.92	0.51



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
5:E:94:ASN:HA	5:E:236:THR:HG22	1.92	0.50
4:C:15:LEU:HB3	4:C:107:SER:HB3	1.93	0.50
6:K:39:GLN:HB2	6:K:45:LEU:HD23	1.93	0.50
5:E:67:ASN:HD21	5:E:70:ALA:H	1.60	0.50
6:K:144:ASP:HB3	6:K:175:LEU:HD23	1.94	0.50
2:I:184:GLU:O	2:I:188:SER:OG	2.29	0.50
5:G:317:PHE:CE2	5:G:319:ALA:HB2	2.47	0.50
5:E:70:ALA:HB2	5:E:213:ILE:HD11	1.92	0.50
4:J:83:GLU:OE1	4:J:166:LYS:NZ	2.32	0.50
4:J:134:CYS:HB3	4:J:176:SER:HB3	1.93	0.50
5:M:260:LEU:HD12	5:M:451:GLY:HA3	1.94	0.50
6:K:11:LEU:HD11	6:K:112:SER:HB3	1.94	0.50
4:J:37:GLN:HB2	4:J:47:LEU:HD11	1.94	0.50
6:K:28:SER:HB3	6:K:31:ASN:HB2	1.93	0.49
1:N:144:THR:HG22	1:N:192:THR:HG22	1.93	0.49
5:E:219:ALA:O	5:E:246:GLN:NE2	2.45	0.49
6:K:3:GLN:HB3	6:K:25:SER:HB2	1.94	0.49
3:0:116:VAL:O	3:O:205:LYS:NZ	2.32	0.49
5:M:131:CYS:HA	5:M:157:CYS:HA	1.93	0.49
5:G:175:LEU:HD11	14:G:602:NAG:H83	1.94	0.49
7:Y:606:THR:HG21	7:Y:646:LEU:HD11	1.94	0.49
1:N:122:SER:OG	1:N:123:ALA:N	2.45	0.49
5:M:161:MET:HE3	5:M:161:MET:HA	1.93	0.49
4:J:34:GLN:HB2	4:J:89:HIS:HB3	1.95	0.49
3:L:108:GLY:HA3	3:L:141:TYR:OH	2.13	0.49
6:B:121:VAL:HG12	6:B:142:VAL:HA	1.94	0.49
5:G:125:LEU:HA	5:G:161:MET:HE1	1.93	0.49
5:G:503:ARG:NE	7:Y:605:CYS:O	2.35	0.49
1:F:47:TRP:CZ2	1:F:49:GLY:HA2	2.48	0.49
3:L:23:CYS:N	3:L:71:ALA:O	2.44	0.49
1:N:143:GLY:N	1:N:195:SER:OG	2.46	0.49
5:M:54:CYS:HB2	7:Z:571:TRP:CE3	2.48	0.49
5:M:59:LYS:HD3	5:M:213:ILE:HD12	1.94	0.49
3:L:151:ALA:HB2	3:L:192:TYR:CE1	2.48	0.48
7:Y:603:ILE:HB	7:Z:655:LYS:HB3	1.94	0.48
3:L:19:ILE:HG22	3:L:75:ILE:HB	1.94	0.48
3:O:163:THR:HB	3:O:176:SER:H	1.79	0.48
4:J:93:SER:O	5:M:136:ASN:ND2	2.46	0.48
1:F:33:TYR:HB2	1:F:106:GLU:OE2	2.13	0.48
3:0:110:PRO:HD2	3:O:141:TYR:CE1	2.48	0.48
4:A:108:GLN:HB3	4:A:140:TYR:CE1	2.48	0.48



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
4:C:28:LEU:HB3	4:C:94:ARG:HD3	1.95	0.48
4:J:94:ARG:HA	5:M:136:ASN:ND2	2.27	0.48
5:M:203:GLN:HE22	5:M:317:PHE:HA	1.78	0.48
4:C:106:VAL:O	4:C:140:TYR:OH	2.27	0.48
5:G:456:ARG:HG2	5:G:468:PHE:HE1	1.78	0.48
1:F:168:LEU:HD21	1:F:191:VAL:HG21	1.94	0.48
6:B:40:SER:HB2	6:B:43:LYS:HD2	1.96	0.48
6:D:33:TYR:HB2	6:D:95:ALA:O	2.13	0.48
6:K:204:ASN:OD1	6:K:205:THR:N	2.47	0.48
1:F:35:HIS:NE2	1:F:106:GLU:OE2	2.39	0.48
2:I:50:GLU:O	2:I:52:SER:N	2.44	0.48
3:L:119:PHE:HB2	3:L:134:VAL:HB	1.95	0.48
5:G:69:TRP:HA	5:G:111:LEU:HD13	1.95	0.48
1:F:3:GLN:HB3	1:F:25:SER:HB2	1.95	0.48
3:O:61:ARG:CZ	3:O:79:GLN:HE22	2.25	0.48
5:E:111:LEU:HD11	7:X:571:TRP:HZ2	1.77	0.48
5:G:212:PRO:HG2	5:G:254:VAL:HG22	1.95	0.48
5:M:186(A):ASN:N	5:M:187:GLN:CA	2.74	0.48
5:E:448:ASN:O	5:E:450:THR:HG23	2.13	0.48
5:E:361:PHE:HB3	5:E:391:PHE:HB3	1.96	0.48
5:M:498:PRO:HB3	7:Z:610:TRP:CD2	2.49	0.48
6:B:119:PRO:HB3	6:B:145:TYR:HB3	1.95	0.48
5:G:257:THR:OG1	5:G:375:SER:OG	2.29	0.47
6:B:66:ARG:NH1	6:B:82(B):SER:O	2.47	0.47
6:K:123:PRO:HB3	6:K:211:VAL:HG22	1.95	0.47
6:B:35:THR:OG1	6:B:47:TRP:NE1	2.47	0.47
5:E:338:TRP:CZ2	5:E:390:LEU:HB3	2.48	0.47
5:M:257:THR:HG22	5:M:258:GLN:HG3	1.96	0.47
7:Y:601:LYS:HG2	7:Z:655:LYS:NZ	2.30	0.47
1:H:24:ALA:HB1	1:H:27:TYR:HE1	1.80	0.47
2:I:107:LEU:HD11	2:I:109:GLN:HG2	1.95	0.47
3:O:109:GLN:NE2	3:O:110:PRO:O	2.47	0.47
5:G:294:ILE:HB	5:G:333:VAL:HG22	1.96	0.47
6:D:39:GLN:HB2	6:D:45:LEU:HD23	1.95	0.47
1:H:12:LYS:HG3	1:H:18:VAL:HB	1.96	0.47
1:N:15:GLY:HA2	1:N:85:ARG:HA	1.97	0.47
5:M:218:CYS:HA	5:M:247:CYS:HA	1.96	0.47
3:L:19:ILE:HB	3:L:78:LEU:HD11	1.96	0.47
4:C:14:ALA:HA	4:C:106(A):LEU:HB2	1.96	0.47
5:E:231:LYS:HD2	5:E:267:GLU:HB3	1.95	0.47
5:G:67:ASN:ND2	5:G:70:ALA:H	2.12	0.47



Atom_1	Atom_2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
5:G:107:ASP:OD2	7:Y:574:LYS:NZ	2.48	0.47
5:G:270:VAL:HG23	5:G:348:GLN:HG3	1.95	0.47
5:G:294:ILE:HG23	5:G:447:SER:HB2	1.96	0.47
5:M:299:PRO:HB2	5:M:327:ARG:HB2	1.96	0.47
6:B:60:ASN:ND2	6:B:62:SER:OG	2.47	0.47
2:I:168:GLN:N	2:I:172:LYS:O	2.35	0.47
6:B:68:VAL:HG13	6:B:81:GLN:HB2	1.96	0.47
5:E:257:THR:HG22	5:E:258:GLN:HG3	1.97	0.47
5:M:36:VAL:HG12	7:Z:610:TRP:CE3	2.47	0.47
1:F:191:VAL:HG22	1:F:193:VAL:HG13	1.96	0.47
3:O:83:ASP:OD1	3:O:83:ASP:N	2.47	0.47
4:C:66(C):ASN:ND2	4:C:66(C):ASN:O	2.48	0.46
5:M:358:ILE:HB	5:M:465:THR:HA	1.97	0.46
1:F:207:VAL:HB	1:F:216:VAL:HG23	1.96	0.46
5:M:54:CYS:HB2	7:Z:571:TRP:CD2	2.51	0.46
1:N:88:SER:HA	1:N:120:VAL:HG11	1.97	0.46
1:N:153:ASP:HB3	1:N:184:LEU:HD13	1.97	0.46
1:N:7:SER:HB3	1:N:21:SER:HB3	1.98	0.46
1:N:177:ALA:HA	1:N:187:LEU:HB3	1.98	0.46
5:E:181:ILE:HG23	5:E:191:TYR:HB3	1.97	0.46
6:B:138:LEU:O	6:B:182:VAL:N	2.46	0.46
6:K:60:ASN:HB3	6:K:63:LEU:HD23	1.96	0.46
4:A:150:ALA:O	4:A:152:SER:N	2.49	0.46
5:G:74:CYS:SG	5:G:75:VAL:N	2.88	0.46
5:G:203:GLN:HG3	5:G:435:TYR:HD2	1.81	0.46
6:D:204:ASN:OD1	6:D:205:THR:N	2.48	0.46
7:X:650:GLN:HG3	7:X:651:ASN:H	1.81	0.46
5:M:65:LYS:HB2	5:M:66:HIS:H	1.67	0.46
1:F:39:GLN:HB2	1:F:45:LEU:HD23	1.97	0.46
1:H:141:SER:HA	1:H:144:THR:O	2.16	0.46
1:N:12:LYS:HG3	1:N:18:VAL:HB	1.97	0.46
6:B:146:PHE:HA	6:B:147:PRO:HA	1.78	0.46
5:G:69:TRP:HB3	5:G:215:ILE:HD11	1.97	0.46
4:J:94:ARG:O	5:M:136:ASN:HB2	2.15	0.45
5:M:180:ASP:OD2	5:M:422:GLN:N	2.43	0.45
5:M:297:THR:HG22	5:M:444:ARG:HG3	1.97	0.45
1:F:87:ARG:O	1:F:120:VAL:HG21	2.16	0.45
5:G:195:ASN:ND2	5:G:201:ILE:HB	2.32	0.45
5:G:343:GLY:O	5:G:347:LYS:HG2	2.16	0.45
5:M:203:GLN:HG3	5:M:435:TYR:HD2	1.81	0.45
5:G:350:ARG:HD3	5:G:355:ASN:O	2.16	0.45



Atom_1	Atom_2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
4:J:133:VAL:HG21	6:K:141:LEU:HD13	1.97	0.45
4:J:108:GLN:HB3	4:J:140:TYR:CE1	2.51	0.45
1:F:12:LYS:HG3	1:F:18:VAL:HB	1.98	0.45
2:I:140:PHE:HZ	2:I:165:PRO:HB3	1.82	0.45
1:N:30:THR:OG1	1:N:54:ASN:OD1	2.34	0.45
5:E:99:ASN:OD1	5:E:103:GLN:NE2	2.49	0.45
1:H:6:GLN:H	1:H:114:GLN:NE2	2.14	0.45
4:J:166:LYS:HA	4:J:172:TYR:HA	1.99	0.45
6:D:200:HIS:CE1	6:D:203:SER:HB2	2.51	0.45
1:F:157:GLU:OE2	1:F:177:ALA:HB3	2.17	0.45
1:N:170:SER:HA	1:N:171:GLY:HA2	1.63	0.45
1:F:141:SER:OG	1:F:142:GLY:N	2.48	0.45
3:O:75:ILE:HD13	3:O:82:GLU:OE2	2.17	0.45
5:E:369:LEU:HD22	5:E:370:GLU:HG3	1.98	0.45
6:D:123:PRO:HB3	6:D:211:VAL:HG22	1.98	0.45
4:C:13:VAL:HG13	4:C:17:GLU:HG3	1.98	0.45
5:E:186(A):ASN:N	5:E:187:GLN:CA	2.76	0.45
5:E:234:ASN:OD1	5:E:235:GLY:N	2.50	0.45
1:H:35:HIS:HD1	1:H:47:TRP:HE1	1.65	0.44
1:N:99:ARG:HD3	1:N:106:GLU:CD	2.38	0.44
4:A:85:ASP:HB3	4:A:101:ALA:HB1	2.00	0.44
5:G:360:ARG:HG2	5:G:467:THR:HG22	1.99	0.44
5:G:54:CYS:SG	5:G:55:ALA:N	2.90	0.44
5:G:292:VAL:HB	5:G:449:ILE:HG23	1.99	0.44
5:M:47:ASP:HA	5:M:489:VAL:HG12	1.99	0.44
6:D:60:ASN:HD22	6:D:61:PRO:HD2	1.82	0.44
1:F:60:TYR:HE1	1:F:70:MET:HB2	1.82	0.44
1:N:123:ALA:HB2	1:N:183:GLY:HA3	1.98	0.44
3:L:140:PHE:HE2	3:L:143:GLY:HA2	1.82	0.44
1:F:153:ASP:HB3	1:F:184:LEU:HD13	1.98	0.44
2:I:133:LEU:HD12	2:I:179:LEU:HB3	2.00	0.44
7:Z:635:ILE:O	7:Z:639:THR:HG23	2.17	0.44
1:H:144:THR:HA	1:H:195:SER:N	2.29	0.44
4:A:37:GLN:HB2	4:A:47:LEU:HD11	1.99	0.44
5:E:317:PHE:CE2	5:E:319:ALA:HB2	2.53	0.44
5:G:476:ARG:HA	5:G:479:TRP:CD1	2.53	0.44
6:D:72:ASP:OD1	6:D:74:SER:OG	2.24	0.44
6:K:68:VAL:HB	6:K:82(A):ARG:HH21	1.80	0.44
6:K:154:TRP:CZ2	6:K:196:CYS:HB3	2.52	0.44
4:A:94:ARG:HD2	5:G:324:GLY:O	2.18	0.44
5:E:69:TRP:HE1	5:E:108:ILE:HG23	1.82	0.44



A + 1	A t am 0	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
5:M:498:PRO:HB3	7:Z:610:TRP:CG	2.53	0.44
1:F:132:PRO:HD3	1:F:218:LYS:HE3	2.00	0.43
3:L:152:ASP:OD2	3:L:190:LYS:HG2	2.18	0.43
3:O:190:LYS:O	3:O:209:PRO:HD2	2.18	0.43
5:E:61:TYR:HD1	5:E:65:LYS:HB3	1.83	0.43
4:J:94:ARG:HD2	5:M:324:GLY:O	2.18	0.43
5:M:220:PRO:HB3	7:Z:578:ALA:HB1	1.98	0.43
2:I:106:VAL:HB	2:I:107:LEU:H	1.43	0.43
5:E:96:TRP:HH2	5:E:285:LEU:HD23	1.83	0.43
5:E:321(A):ASP:HB3	14:E:602:NAG:H82	2.00	0.43
5:E:359:ILE:HD13	5:E:466:GLU:HB3	2.00	0.43
4:J:21:ILE:HD12	4:J:73:LEU:HD23	1.99	0.43
6:B:159:LEU:HD13	6:B:182:VAL:HG11	2.00	0.43
3:L:140:PHE:CE2	3:L:143:GLY:HA2	2.53	0.43
4:A:21:ILE:HD12	4:A:73:LEU:HD23	2.01	0.43
4:C:32:ALA:N	4:C:91:TRP:O	2.51	0.43
6:D:154:TRP:CZ2	6:D:196:CYS:HB3	2.53	0.43
6:K:200:HIS:CE1	6:K:203:SER:HB2	2.53	0.43
2:I:129:ASN:HA	2:I:183:PRO:HG2	2.00	0.43
3:L:112:ALA:CB	3:L:141:TYR:HB3	2.48	0.43
1:N:133:LEU:HB3	3:O:119:PHE:CG	2.54	0.43
5:E:227:LYS:HG3	5:E:485:LYS:HD3	2.00	0.43
5:M:50:THR:O	5:M:103:GLN:NE2	2.32	0.43
1:N:60:TYR:HE1	1:N:70:MET:HB2	1.83	0.43
5:E:122:LEU:HB2	5:E:201:ILE:HG23	2.01	0.43
5:E:384:TYR:CE1	5:E:421:LYS:HD3	2.54	0.43
5:G:289:ASN:OD1	5:G:290:THR:N	2.51	0.43
1:H:36:TRP:CE2	1:H:81:MET:HB2	2.54	0.43
5:M:67:ASN:HD21	5:M:70:ALA:HB3	1.83	0.43
3:O:151:ALA:HA	3:O:152:ASP:HA	1.80	0.43
3:0:184:GLU:0	3:O:188:SER:OG	2.33	0.43
5:M:220:PRO:HG2	5:M:223:PHE:CD1	2.53	0.43
4:C:136:ILE:HG12	4:C:195:VAL:HG11	2.00	0.43
5:M:343:GLY:O	5:M:347:LYS:HG2	2.18	0.43
1:F:179:LEU:HD13	1:F:185:TYR:CE2	2.53	0.43
1:F:209:HIS:CD2	1:F:211:PRO:HD2	2.54	0.43
1:H:143:GLY:O	1:H:144:THR:OG1	2.25	0.43
4:C:13:VAL:O	4:C:106:VAL:HA	2.18	0.43
2:I:56:SER:HA	2:I:57:GLY:HA2	1.51	0.42
6:D:146:PHE:HA	6:D:147:PRO:HA	1.78	0.42
6:D:161:SER:HA	6:D:162:GLY:HA2	1.77	0.42



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:N:209:HIS:CD2	1:N:211:PRO:HD2	2.53	0.42
5:E:253:PRO:HA	5:E:479:TRP:HZ3	1.83	0.42
5:E:456:ARG:HG2	5:E:468:PHE:HE1	1.84	0.42
5:G:52:LEU:O	7:Y:574:LYS:HD3	2.19	0.42
5:G:370:GLU:HG2	5:G:384:TYR:HE2	1.84	0.42
4:A:145:THR:HB	4:A:196:THR:HB	2.01	0.42
5:E:257:THR:O	5:E:259:LEU:N	2.52	0.42
5:E:369:LEU:HB3	5:E:370:GLU:H	1.71	0.42
4:J:136:ILE:HG12	4:J:195:VAL:HG11	2.01	0.42
6:D:124:LEU:HD21	6:D:141:LEU:HB2	2.01	0.42
6:K:145:TYR:HB2	6:K:200:HIS:CE1	2.55	0.42
4:C:151:ASP:OD1	4:C:188:HIS:HB3	2.19	0.42
5:G:456:ARG:HG2	5:G:468:PHE:CE1	2.55	0.42
6:B:123:PRO:HB3	6:B:211:VAL:HG22	2.01	0.42
3:O:11:VAL:HG12	3:O:19:ILE:HD11	2.02	0.42
5:M:101:VAL:HG21	5:M:480:ARG:HG2	2.01	0.42
6:D:94:THR:O	6:D:100(P):MET:HA	2.19	0.42
4:C:21:ILE:HB	4:C:73:LEU:HB3	2.01	0.42
5:G:69:TRP:HE1	5:G:108:ILE:HG23	1.85	0.42
8:U:1:NAG:O6	8:U:2:NAG:N2	2.53	0.42
1:F:36:TRP:CE2	1:F:81:MET:HB2	2.54	0.42
3:L:50:GLU:O	3:L:52:SER:N	2.46	0.42
5:E:384:TYR:CZ	5:E:421:LYS:HD3	2.55	0.42
3:L:32:TYR:HB3	3:L:50:GLU:HA	2.02	0.42
3:L:152:ASP:OD1	3:L:189:HIS:HB3	2.20	0.42
4:A:34:GLN:HG2	6:B:100(O):TYR:HB3	2.00	0.42
5:E:61:TYR:CD1	5:E:65:LYS:HB3	2.55	0.42
5:E:260:LEU:HD12	5:E:451:GLY:HA3	2.01	0.42
6:D:34:TRP:HB3	6:D:78:LEU:HD22	2.02	0.42
6:K:11:LEU:HD12	6:K:110:THR:HB	2.00	0.42
1:F:128:PRO:HB3	1:F:154:TYR:HB3	2.01	0.42
2:I:55:PRO:O	2:I:58:VAL:HG13	2.20	0.42
6:K:151:THR:HB	6:K:199:ASN:HB2	2.01	0.42
4:J:35:TRP:CG	4:J:73:LEU:HD13	2.55	0.41
5:M:121:LYS:HA	5:M:202:THR:HA	2.02	0.41
6:B:33:TYR:HB2	6:B:95:ALA:O	2.20	0.41
6:D:18:LEU:HD11	6:D:109:VAL:HG11	2.01	0.41
6:D:18:LEU:HB3	6:D:82:LEU:HB3	2.02	0.41
3:0:152:ASP:OD1	3:O:152:ASP:N	2.54	0.41
5:G:125:LEU:HD12	5:G:161:MET:HE3	2.02	0.41
4:J:38:HIS:NE2	6:K:39:GLN:OE1	2.53	0.41



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
4:J:61:ARG:NH2	4:J:82:ASP:OD1	2.53	0.41
3:L:151:ALA:HA	3:L:152:ASP:HA	1.71	0.41
1:N:207:VAL:HB	1:N:216:VAL:HG23	2.03	0.41
5:M:369:LEU:HD22	5:M:370:GLU:HG2	2.03	0.41
7:Y:650:GLN:HG3	7:Y:651:ASN:H	1.85	0.41
7:Z:631:TRP:O	7:Z:635:ILE:HG12	2.20	0.41
1:F:177:ALA:HA	1:F:187:LEU:HB3	2.02	0.41
2:I:108:GLY:N	2:I:109:GLN:HA	2.36	0.41
3:L:151:ALA:HB2	3:L:192:TYR:CD1	2.55	0.41
2:I:151:ALA:HA	2:I:152:ASP:HA	1.86	0.41
5:G:181:ILE:HG23	5:G:191:TYR:HB3	2.02	0.41
5:G:494:LEU:HD23	5:G:494:LEU:HA	1.87	0.41
6:B:22:CYS:HB2	6:B:36:TRP:CH2	2.56	0.41
6:B:59:TYR:HE1	6:B:69:ILE:HG13	1.86	0.41
6:K:161:SER:HA	6:K:162:GLY:HA2	1.76	0.41
1:F:83:LEU:HD23	1:F:83:LEU:HA	1.94	0.41
1:H:98:ARG:HB2	1:H:98:ARG:HH11	1.86	0.41
2:I:36:TYR:O	2:I:86:TYR:HA	2.21	0.41
2:I:38:GLN:C	2:I:84:ALA:HB1	2.41	0.41
3:L:56:SER:HA	3:L:57:GLY:HA2	1.54	0.41
3:L:107:LEU:HD12	3:L:107:LEU:HA	1.87	0.41
5:G:273:ARG:NH1	5:G:287:GLN:OE1	2.51	0.41
4:J:15:LEU:HB2	4:J:107:SER:HB2	2.02	0.41
1:H:14:PRO:HG3	1:H:122:SER:HB2	2.03	0.41
1:N:156:PRO:HD2	1:N:211:PRO:HB2	2.02	0.41
5:G:437:PRO:HA	5:G:438:PRO:HD3	1.95	0.41
3:O:50:GLU:O	3:O:52:SER:N	2.51	0.41
3:O:129:ASN:HA	3:O:183:PRO:HG2	2.02	0.41
5:E:280:ASN:OD1	5:E:281:ALA:N	2.54	0.41
6:K:200:HIS:O	6:K:204:ASN:HA	2.21	0.41
4:J:137:SER:HA	4:J:173:ALA:HA	2.03	0.41
6:D:36:TRP:HD1	6:D:69:ILE:HD13	1.86	0.41
7:Y:540:GLN:O	7:Y:544:LEU:HB2	2.20	0.41
1:F:142:GLY:HA2	1:F:144:THR:N	2.36	0.40
1:F:170:SER:HA	1:F:171:GLY:HA2	1.60	0.40
5:E:54:CYS:SG	5:E:55:ALA:N	2.95	0.40
5:M:270:VAL:HG23	5:M:348:GLN:HG3	2.03	0.40
6:B:200:HIS:HD2	6:B:202:PRO:HD2	1.85	0.40
5:M:69:TRP:HB3	5:M:215:ILE:HD11	2.03	0.40
5:M:86:LEU:HD22	7:Z:523:LEU:O	2.21	0.40
5:M:181:ILE:HG23	5:M:191:TYR:HB3	2.03	0.40



Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
5:M:289:ASN:OD1	5:M:290:THR:N	2.55	0.40
1:H:24:ALA:HB1	1:H:27:TYR:CE1	2.57	0.40
3:O:19:ILE:HG22	3:O:75:ILE:HB	2.02	0.40
5:E:349:LEU:HD13	5:E:468:PHE:CE2	2.55	0.40
6:K:22:CYS:N	6:K:78:LEU:O	2.53	0.40
5:G:349:LEU:HD13	5:G:468:PHE:CE2	2.55	0.40
5:M:111:LEU:HD11	7:Z:571:TRP:CZ2	2.56	0.40
6:D:200:HIS:O	6:D:204:ASN:HA	2.22	0.40
3:O:6:GLN:HB3	3:O:102:THR:OG1	2.21	0.40
5:M:369:LEU:HB3	5:M:370:GLU:HG2	2.04	0.40
6:B:9:PRO:HD3	6:B:19:SER:O	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	Percentiles	
1	F	218/225~(97%)	203~(93%)	14 (6%)	1 (0%)	29	66
1	Η	218/225~(97%)	202 (93%)	15 (7%)	1 (0%)	29	66
1	Ν	218/225~(97%)	201 (92%)	17 (8%)	0	100	100
2	Ι	203/210~(97%)	187 (92%)	12 (6%)	4 (2%)	7	40
3	L	200/210~(95%)	183 (92%)	12 (6%)	5(2%)	5	36
3	Ο	201/210~(96%)	183 (91%)	17 (8%)	1 (0%)	29	66
4	А	208/214~(97%)	194 (93%)	12 (6%)	2(1%)	15	52
4	\mathbf{C}	208/214~(97%)	196 (94%)	11 (5%)	1 (0%)	29	66
4	J	208/214~(97%)	196 (94%)	11 (5%)	1 (0%)	29	66
5	Е	437/474~(92%)	405 (93%)	30 (7%)	2(0%)	29	66
5	G	$44\overline{3}/474~(94\%)$	403 (91%)	35 (8%)	5 (1%)	14	51



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
5	М	441/474~(93%)	406 (92%)	31 (7%)	4 (1%)	17 54
6	В	222/236~(94%)	214 (96%)	6 (3%)	2(1%)	17 54
6	D	222/236~(94%)	214 (96%)	8 (4%)	0	100 100
6	K	222/236~(94%)	211 (95%)	11 (5%)	0	100 100
7	Х	125/153~(82%)	119~(95%)	6~(5%)	0	100 100
7	Y	125/153~(82%)	121 (97%)	4 (3%)	0	100 100
7	Z	125/153~(82%)	120 (96%)	5 (4%)	0	100 100
All	All	4244/4536 (94%)	3958~(93%)	257 (6%)	29 (1%)	22 59

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All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	110	PRO
3	0	112	ALA
5	G	140	ASP
5	G	449	ILE
5	М	136	ASN
5	М	157	CYS
1	F	106	GLU
1	Н	144	THR
2	Ι	29	ASP
3	L	106	VAL
4	А	151	ASP
5	G	186	GLU
5	G	333	VAL
2	Ι	106	VAL
2	Ι	110	PRO
3	L	3	ALA
3	L	139	ASP
4	С	151	ASP
4	J	151	ASP
5	М	186	GLU
2	Ι	139	ASP
3	L	108	GLY
5	Е	186	GLU
5	М	258	GLN
6	В	82(B)	SER
6	В	144	ASP
4	А	60	GLU
5	Е	369	LEU



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Mol	Chain	Res	Type
5	G	369	LEU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	188/191~(98%)	182~(97%)	6 (3%)	39	65
1	Н	188/191~(98%)	182~(97%)	6 (3%)	39	65
1	Ν	188/191 (98%)	183~(97%)	5(3%)	44	68
2	Ι	173/176~(98%)	167 (96%)	6 (4%)	36	63
3	L	172/176~(98%)	166 (96%)	6 (4%)	36	63
3	Ο	173/176~(98%)	167 (96%)	6 (4%)	36	63
4	А	176/180~(98%)	173~(98%)	3(2%)	60	78
4	С	176/180~(98%)	174 (99%)	2(1%)	73	85
4	J	176/180~(98%)	172 (98%)	4 (2%)	50	71
5	Ε	399/422~(94%)	390~(98%)	9(2%)	50	71
5	G	401/422~(95%)	390~(97%)	11 (3%)	44	68
5	М	401/422~(95%)	386~(96%)	15~(4%)	34	61
6	В	194/204~(95%)	193 (100%)	1 (0%)	88	94
6	D	194/204~(95%)	192~(99%)	2(1%)	76	86
6	Κ	194/204~(95%)	191~(98%)	3~(2%)	65	80
7	Х	112/129~(87%)	112 (100%)	0	100	100
7	Y	112/129~(87%)	112 (100%)	0	100	100
7	Z	112/129~(87%)	112 (100%)	0	100	100
All	All	$372\overline{9/3906}\ (96\%)$	3644 (98%)	85 (2%)	50	71

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	72	ARG
	a r.	7	


Mol	Chain	Res	Type
1	F	83	LEU
1	F	104	ASP
1	F	117	LEU
1	F	217	ASP
1	F	225	CYS
1	Н	72	ARG
1	Н	83	LEU
1	Н	98	ARG
1	Н	105	ARG
1	Н	217	ASP
1	Н	225	CYS
2	Ι	58	VAL
2	Ι	83	GLU
2	Ι	105	PHE
2	Ι	106	VAL
2	Ι	184	GLU
2	Ι	192	TYR
3	L	58	VAL
3	L	96	GLU
3	L	103	LYS
3	L	109	GLN
3	L	184	GLU
3	L	192	TYR
1	N	54	ASN
1	N	72	ARG
1	N	83	LEU
1	N	217	ASP
1	N	225	CYS
3	0	58	VAL
3	0	96	GLU
3	0	109	GLN
3	0	152	ASP
3	0	184	GLU
3	0	192	TYR
4	А	72	THR
4	А	89	HIS
4	А	183	GLU
4	С	66(C)	ASN
4	С	183	GLU
5	Е	61	TYR
5	Е	65	LYS
5	Е	71	THR
	-		

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Mol	Chain	Res	Type
5	Е	186(A)	ASN
5	Е	189	THR
5	Е	342	LEU
5	Е	369	LEU
5	Е	449	ILE
5	Е	505	VAL
5	G	61	TYR
5	G	65	LYS
5	G	71	THR
5	G	74	CYS
5	G	87	GLU
5	G	186	GLU
5	G	186(A)	ASN
5	G	342	LEU
5	G	369	LEU
5	G	449	ILE
5	G	466	GLU
4	J	15	LEU
4	J	18	THR
4	J	54	ARG
4	J	183	GLU
5	М	65	LYS
5	М	71	THR
5	М	74	CYS
5	М	88	ASN
5	М	134	VAL
5	М	186	GLU
5	М	213	ILE
5	М	218	CYS
5	М	279	ASP
5	М	342	LEU
5	М	369	LEU
5	М	370	GLU
5	М	378	CYS
5	М	424	ILE
5	M	449	ILE
6	В	208	ASP
6	D	205	THR
6	D	206	LYS
6	K	76	ASN
6	K	81	GLN
6	K	205	THR

Continued from previous page.



Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
4	С	50	ASN
5	М	136	ASN
6	В	60	ASN
7	Ζ	651	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)

55 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	Turne	Chain	Dec	Tink	Bond lengths			Bond angles		
	туре	Unam	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	Р	1	5,8	14,14,15	0.18	0	17,19,21	0.55	0
8	NAG	Р	2	8	14,14,15	0.37	0	17,19,21	0.36	0
8	BMA	Р	3	8	11,11,12	0.77	0	$15,\!15,\!17$	0.75	0
9	NAG	Q	1	5,9	14,14,15	0.34	0	17,19,21	0.46	0
9	NAG	Q	2	9	14,14,15	0.31	0	17,19,21	0.37	0
10	NAG	R	1	5,10	14,14,15	0.39	0	17,19,21	0.45	0
10	NAG	R	2	10	14,14,15	0.46	0	17,19,21	0.82	1 (5%)
10	BMA	R	3	10	11,11,12	1.48	2 (18%)	$15,\!15,\!17$	1.52	3 (20%)
10	MAN	R	4	10	11,11,12	1.25	1 (9%)	$15,\!15,\!17$	2.47	3 (20%)
10	MAN	R	5	10	11,11,12	0.56	0	$15,\!15,\!17$	1.15	2 (13%)
10	MAN	R	6	10	11,11,12	0.73	0	$15,\!15,\!17$	0.98	1 (6%)
10	MAN	R	7	10	11,11,12	0.97	1 (9%)	$15,\!15,\!17$	1.50	2 (13%)



	T	Chain	Dag	T :1-	Bo	ond leng	ths	Bond angles		
IVIOI	Type	Chain	Res	Link	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
9	NAG	S	1	5,9	14,14,15	0.23	0	17,19,21	0.49	0
9	NAG	S	2	9	14,14,15	0.35	0	$17,\!19,\!21$	1.23	1 (5%)
9	NAG	Т	1	5,9	14,14,15	1.05	1 (7%)	17,19,21	1.12	3 (17%)
9	NAG	Т	2	9	14,14,15	0.35	0	17,19,21	0.66	0
8	NAG	U	1	5,8	14,14,15	0.35	0	$17,\!19,\!21$	0.42	0
8	NAG	U	2	8	14,14,15	0.39	0	17,19,21	0.67	0
8	BMA	U	3	8	11,11,12	0.64	0	$15,\!15,\!17$	0.72	0
9	NAG	V	1	5,9	14,14,15	0.28	0	17,19,21	0.38	0
9	NAG	V	2	9	14,14,15	0.22	0	17,19,21	0.38	0
9	NAG	W	1	5,9	14,14,15	0.39	0	17,19,21	0.43	0
9	NAG	W	2	9	14,14,15	0.31	0	17,19,21	0.48	0
	NAG	a		5,11	14,14,15	0.26	0	17,19,21	0.41	0
	NAG NAC	a	2	11	14,14,15 14.14.15	0.33	0	17,19,21	0.48	0
11	MAN	a	3	11	14,14,10	1.00	$\frac{1}{007}$	17,19,21	1.00	$\frac{1}{2}(3007)$
	MAN	a	4	11	11,11,12	1.28	1 (9%)	15,15,17	1.80	3(20%)
	MAN	a	5		11,11,12	0.75	0	15,15,17	1.07	2(13%)
11	MAN	a	6	11	11,11,12	0.71	0	15,15,17	1.37	2 (13%)
11	MAN	a	7	11	11,11,12	1.00	1 (9%)	15, 15, 17	0.95	1 (6%)
11	MAN	a	8	11	11,11,12	0.85	0	$15,\!15,\!17$	0.98	1 (6%)
11	MAN	a	9	11	11,11,12	0.95	1 (9%)	$15,\!15,\!17$	1.42	1 (6%)
9	NAG	b	1	5,9	14,14,15	0.28	0	$17,\!19,\!21$	0.36	0
9	NAG	b	2	9	14,14,15	0.57	0	$17,\!19,\!21$	1.30	2 (11%)
8	NAG	с	1	5,8	14,14,15	0.22	0	$17,\!19,\!21$	0.45	0
8	NAG	с	2	8	14,14,15	0.24	0	17,19,21	0.55	0
8	BMA	с	3	8	11,11,12	0.79	1 (9%)	$15,\!15,\!17$	0.77	0
9	NAG	d	1	5,9	14,14,15	0.14	0	17,19,21	0.56	0
9	NAG	d	2	9	14,14,15	0.26	0	17,19,21	0.57	0
8	NAG	е	1	5,8	14,14,15	0.21	0	$17,\!19,\!21$	0.75	0
8	NAG	е	2	8	14,14,15	0.52	0	17,19,21	0.52	0
8	BMA	е	3	8	11,11,12	0.78	0	$15,\!15,\!17$	0.76	0
9	NAG	f	1	5,9	14,14,15	0.33	0	17,19,21	0.42	0
9	NAG	f	2	9	14,14,15	0.27	0	17,19,21	0.37	0
12	NAG	g	1	5,12	14,14,15	0.37	0	17,19,21	0.40	0
12	NAG	g	$\frac{2}{2}$	12	14,14,15	0.29	0	17,19,21	0.55	
12	BMA	g	<u>う</u>	12	11,11,12	0.62	0	15,15,17	0.96	
12	MAN	g	4	12	11,11,12	0.83	0	15, 15, 17	1.35	2 (13%)
12	MAN	g	5	12	11,11,12	0.74	0	15, 15, 17	1.26	1 (6%)
12	MAN	g	6	12	11,11,12	0.81	1 (9%)	$15,\!15,\!17$	1.12	2 (13%)
13	MAN	h	1	13	11,11,12	1.00	1(9%)	$15,\!15,\!17$	1.28	1 (6%)



Mal	Mal Tuna Chain	Dec	Timle	Bo	Bond lengths			Bond angles		
IVIOI	Type	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	MAN	h	2	13	11,11,12	0.79	0	$15,\!15,\!17$	1.50	2 (13%)
13	MAN	h	3	13	11,11,12	0.68	0	15,15,17	0.94	1 (6%)
9	NAG	i	1	5,9	14,14,15	0.31	0	17,19,21	0.51	0
9	NAG	i	2	9	14,14,15	0.27	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. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	Р	1	5,8	-	2/6/23/26	0/1/1/1
8	NAG	Р	2	8	-	2/6/23/26	0/1/1/1
8	BMA	Р	3	8	-	1/2/19/22	0/1/1/1
9	NAG	Q	1	5,9	-	2/6/23/26	0/1/1/1
9	NAG	Q	2	9	-	0/6/23/26	0/1/1/1
10	NAG	R	1	5,10	-	1/6/23/26	0/1/1/1
10	NAG	R	2	10	-	3/6/23/26	0/1/1/1
10	BMA	R	3	10	-	1/2/19/22	0/1/1/1
10	MAN	R	4	10	-	0/2/19/22	0/1/1/1
10	MAN	R	5	10	-	2/2/19/22	0/1/1/1
10	MAN	R	6	10	-	0/2/19/22	0/1/1/1
10	MAN	R	7	10	-	0/2/19/22	0/1/1/1
9	NAG	S	1	5,9	-	3/6/23/26	0/1/1/1
9	NAG	S	2	9	-	3/6/23/26	0/1/1/1
9	NAG	Т	1	5,9	-	1/6/23/26	0/1/1/1
9	NAG	Т	2	9	-	2/6/23/26	0/1/1/1
8	NAG	U	1	5,8	-	2/6/23/26	0/1/1/1
8	NAG	U	2	8	-	3/6/23/26	0/1/1/1
8	BMA	U	3	8	-	1/2/19/22	0/1/1/1
9	NAG	V	1	5,9	-	3/6/23/26	0/1/1/1
9	NAG	V	2	9	-	1/6/23/26	0/1/1/1
9	NAG	W	1	5,9	-	3/6/23/26	0/1/1/1
9	NAG	W	2	9	-	2/6/23/26	0/1/1/1
11	NAG	a	1	5,11	-	1/6/23/26	0/1/1/1
11	NAG	a	2	11	-	4/6/23/26	0/1/1/1
11	NAG	a	3	11	-	2/6/23/26	0/1/1/1
11	MAN	a	4	11	-	2/2/19/22	0/1/1/1



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	MAN	a	5	11	-	2/2/19/22	0/1/1/1
11	MAN	a	6	11	-	2/2/19/22	0/1/1/1
11	MAN	a	7	11	-	2/2/19/22	0/1/1/1
11	MAN	a	8	11	-	0/2/19/22	0/1/1/1
11	MAN	a	9	11	-	0/2/19/22	0/1/1/1
9	NAG	b	1	5,9	-	2/6/23/26	0/1/1/1
9	NAG	b	2	9	-	5/6/23/26	0/1/1/1
8	NAG	с	1	5,8	-	3/6/23/26	0/1/1/1
8	NAG	с	2	8	-	2/6/23/26	0/1/1/1
8	BMA	с	3	8	-	1/2/19/22	0/1/1/1
9	NAG	d	1	5,9	-	0/6/23/26	0/1/1/1
9	NAG	d	2	9	-	2/6/23/26	0/1/1/1
8	NAG	е	1	5,8	-	2/6/23/26	0/1/1/1
8	NAG	е	2	8	-	2/6/23/26	0/1/1/1
8	BMA	е	3	8	-	2/2/19/22	0/1/1/1
9	NAG	f	1	5,9	-	2/6/23/26	0/1/1/1
9	NAG	f	2	9	-	2/6/23/26	0/1/1/1
12	NAG	g	1	5,12	-	1/6/23/26	0/1/1/1
12	NAG	g	2	12	-	1/6/23/26	0/1/1/1
12	BMA	g	3	12	-	0/2/19/22	0/1/1/1
12	MAN	g	4	12	-	0/2/19/22	1/1/1/1
12	MAN	g	5	12	-	0/2/19/22	0/1/1/1
12	MAN	g	6	12	-	0/2/19/22	0/1/1/1
13	MAN	h	1	13	-	0/2/19/22	0/1/1/1
13	MAN	h	2	13	-	1/2/19/22	0/1/1/1
13	MAN	h	3	13	-	2/2/19/22	0/1/1/1
9	NAG	i	1	5,9	-	2/6/23/26	0/1/1/1
9	NAG	i	2	9	-	2/6/23/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms		Observed(Å)	Ideal(Å)
9	Т	1	NAG	O5-C1	-3.88	1.37	1.43
11	а	4	MAN	C1-C2	3.35	1.59	1.52
10	R	3	BMA	O5-C1	-3.31	1.38	1.43
10	R	4	MAN	O5-C5	2.83	1.49	1.43
10	R	3	BMA	C4-C5	2.72	1.58	1.53
11	a	9	MAN	C1-C2	2.62	1.58	1.52
13	h	1	MAN	O5-C1	-2.53	1.39	1.43



• • • • • •												
Mol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(Å)					
11	a	7	MAN	O5-C1	-2.40	1.39	1.43					
10	R	7	MAN	O5-C5	2.24	1.48	1.43					
12	g	6	MAN	C1-C2	2.16	1.57	1.52					
8	с	3	BMA	C1-C2	2.05	1.56	1.52					

All (39) bond angle outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
10	R	4	MAN	C1-O5-C5	7.49	122.34	112.19
11	a	4	MAN	C1-O5-C5	5.48	119.62	112.19
10	R	7	MAN	C1-O5-C5	4.82	118.73	112.19
13	h	2	MAN	C1-O5-C5	4.41	118.17	112.19
9	S	2	NAG	C2-N2-C7	4.26	128.96	122.90
9	b	2	NAG	C2-N2-C7	4.21	128.90	122.90
10	R	4	MAN	O5-C1-C2	4.05	117.03	110.77
11	a	6	MAN	C1-O5-C5	4.01	117.62	112.19
12	g	5	MAN	C1-O5-C5	3.82	117.37	112.19
11	a	9	MAN	C1-O5-C5	3.73	117.25	112.19
12	g	4	MAN	C1-O5-C5	3.57	117.02	112.19
10	R	3	BMA	C3-C4-C5	3.23	116.00	110.24
10	R	4	MAN	C1-C2-C3	3.16	113.55	109.67
13	h	2	MAN	O2-C2-C3	-3.12	103.88	110.14
12	g	6	MAN	C1-O5-C5	3.04	116.31	112.19
13	h	1	MAN	O5-C1-C2	3.04	115.46	110.77
10	R	5	MAN	C1-O5-C5	2.94	116.18	112.19
11	a	5	MAN	C1-O5-C5	2.89	116.11	112.19
10	R	3	BMA	C1-O5-C5	2.89	116.11	112.19
10	R	5	MAN	O2-C2-C3	-2.65	104.83	110.14
11	a	4	MAN	O2-C2-C3	-2.53	105.07	110.14
12	g	4	MAN	O2-C2-C3	-2.42	105.29	110.14
11	a	3	NAG	C1-O5-C5	2.36	115.39	112.19
11	a	8	MAN	O2-C2-C3	-2.33	105.47	110.14
11	a	6	MAN	O2-C2-C3	-2.25	105.64	110.14
13	h	3	MAN	O2-C2-C3	-2.24	105.66	110.14
11	a	4	MAN	C1-C2-C3	2.22	112.40	109.67
10	R	2	NAG	O4-C4-C5	-2.21	103.81	109.30
10	R	3	BMA	O2-C2-C3	-2.21	105.72	110.14
12	g	6	MAN	O2-C2-C3	-2.21	105.72	110.14
9	Т	1	NAG	O4-C4-C3	-2.18	105.30	110.35
9	Т	1	NAG	C3-C4-C5	2.10	113.98	110.24
10	R	7	MAN	O2-C2-C3	-2.09	105.95	110.14
11	a	7	MAN	O2-C2-C3	-2.08	105.97	110.14



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
9	Т	1	NAG	O4-C4-C5	-2.07	104.17	109.30
10	R	6	MAN	O2-C2-C3	-2.06	106.00	110.14
11	a	5	MAN	O2-C2-C3	-2.04	106.05	110.14
9	b	2	NAG	C1-O5-C5	2.01	114.92	112.19
12	g	3	BMA	O2-C2-C3	-2.00	106.13	110.14

There are no chirality outliers.

(e) torsion outliers are insteal selow.	All	(87)	torsion	outliers	are	listed	below:	
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Mol	Chain	\mathbf{Res}	Type	Atoms
9	Т	2	NAG	C4-C5-C6-O6
9	W	1	NAG	C4-C5-C6-O6
9	b	2	NAG	C4-C5-C6-O6
11	a	3	NAG	C4-C5-C6-O6
11	a	4	MAN	C4-C5-C6-O6
11	a	7	MAN	O5-C5-C6-O6
9	i	2	NAG	C4-C5-C6-O6
10	R	5	MAN	O5-C5-C6-O6
9	Т	2	NAG	O5-C5-C6-O6
11	a	2	NAG	O5-C5-C6-O6
10	R	2	NAG	C4-C5-C6-O6
11	a	7	MAN	C4-C5-C6-O6
8	с	1	NAG	O5-C5-C6-O6
10	R	2	NAG	O5-C5-C6-O6
11	a	3	NAG	O5-C5-C6-O6
9	b	2	NAG	O5-C5-C6-O6
11	a	4	MAN	O5-C5-C6-O6
8	е	3	BMA	C4-C5-C6-O6
9	S	2	NAG	C8-C7-N2-C2
9	S	2	NAG	O7-C7-N2-C2
9	b	2	NAG	C8-C7-N2-C2
9	b	2	NAG	O7-C7-N2-C2
11	a	2	NAG	C8-C7-N2-C2
11	a	2	NAG	O7-C7-N2-C2
11	a	2	NAG	C4-C5-C6-O6
9	W	1	NAG	O5-C5-C6-O6
9	b	1	NAG	O5-C5-C6-O6
9	f	2	NAG	O5-C5-C6-O6
9	i	2	NAG	O5-C5-C6-O6
8	Р	3	BMA	O5-C5-C6-O6
9	V	1	NAG	O5-C5-C6-O6
10	R	5	MAN	C4-C5-C6-O6



Mol	Chain	Res	Type	Atoms
8	е	3	BMA	O5-C5-C6-O6
8	Р	1	NAG	O5-C5-C6-O6
8	U	2	NAG	O5-C5-C6-O6
13	h	3	MAN	O5-C5-C6-O6
8	U	3	BMA	O5-C5-C6-O6
8	е	2	NAG	C1-C2-N2-C7
8	с	2	NAG	O5-C5-C6-O6
8	с	3	BMA	O5-C5-C6-O6
9	V	2	NAG	O5-C5-C6-O6
8	с	1	NAG	C4-C5-C6-O6
9	i	1	NAG	O5-C5-C6-O6
9	Т	1	NAG	O5-C5-C6-O6
9	Q	1	NAG	C1-C2-N2-C7
8	Р	2	NAG	O5-C5-C6-O6
8	U	1	NAG	O5-C5-C6-O6
10	R	3	BMA	O5-C5-C6-O6
9	f	1	NAG	C1-C2-N2-C7
11	a	6	MAN	C4-C5-C6-O6
9	S	1	NAG	C4-C5-C6-O6
13	h	2	MAN	O5-C5-C6-O6
11	а	5	MAN	C4-C5-C6-O6
8	U	1	NAG	C1-C2-N2-C7
9	d	2	NAG	C1-C2-N2-C7
9	b	1	NAG	C4-C5-C6-O6
9	f	2	NAG	C4-C5-C6-O6
10	R	1	NAG	O5-C5-C6-O6
9	W	1	NAG	C1-C2-N2-C7
8	U	2	NAG	C3-C2-N2-C7
8	с	1	NAG	C3-C2-N2-C7
9	S	1	NAG	C3-C2-N2-C7
9	b	2	NAG	C3-C2-N2-C7
10	R	2	NAG	C3-C2-N2-C7
12	g	1	NAG	C3-C2-N2-C7
12	g	2	NAG	C3-C2-N2-C7
11	а	6	MAN	O5-C5-C6-O6
8	e	1	NAG	$C1-C2-N\overline{2-C7}$
9	S	1	NAG	O5-C5-C6-O6
11	a	1	NAG	O5-C5-C6-O6
9	V	1	NAG	C1-C2-N2-C7
9	V	1	NAG	C4-C5-C6-O6
11	a	5	MAN	O5-C5-C6-O6
9	i	1	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
13	h	3	MAN	C4-C5-C6-O6
8	U	2	NAG	C4-C5-C6-O6
9	W	2	NAG	C4-C5-C6-O6
8	Р	1	NAG	C4-C5-C6-O6
8	Р	2	NAG	C1-C2-N2-C7
8	с	2	NAG	C3-C2-N2-C7
8	е	1	NAG	C3-C2-N2-C7
8	е	2	NAG	C3-C2-N2-C7
9	Q	1	NAG	C3-C2-N2-C7
9	S	2	NAG	C3-C2-N2-C7
9	d	2	NAG	C3-C2-N2-C7
9	f	1	NAG	C3-C2-N2-C7
9	W	2	NAG	O5-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	g	4	MAN	C1-C2-C3-C4-C5-O5

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	S	2	NAG	1	0
9	Т	1	NAG	2	0
8	U	2	NAG	1	0
8	U	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.













Rings



Torsions





























































5.6 Ligand geometry (i)

30 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	Turne	Chain	Dec	Timle	Bo	ond leng	ths	В	ond ang	les
INIOI	туре	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
14	NAG	Е	607	5	14,14,15	0.37	0	17,19,21	0.48	0
14	NAG	Y	703	7	14,14,15	0.30	0	$17,\!19,\!21$	0.50	0
14	NAG	М	607	5	14,14,15	0.40	0	17,19,21	0.52	0
14	NAG	М	603	5	$14,\!14,\!15$	0.24	0	$17,\!19,\!21$	0.49	0
14	NAG	М	606	5	14,14,15	0.29	0	17,19,21	0.41	0
14	NAG	G	604	5	14,14,15	0.62	1 (7%)	17,19,21	1.29	2 (11%)
14	NAG	G	607	5	14,14,15	0.24	0	17,19,21	0.43	0
14	NAG	Х	701	7	14,14,15	0.29	0	17,19,21	0.38	0
14	NAG	Х	702	7	14,14,15	0.25	0	17,19,21	0.38	0
14	NAG	Е	602	5	14,14,15	0.55	0	17,19,21	0.62	0
14	NAG	G	601	5	14,14,15	0.49	0	17,19,21	1.22	1 (5%)



Mal	Tuno	Chain	Dog	Tink	Bond lengths		Bond angles			
	Type	Ullalli	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
14	NAG	E	604	5	$14,\!14,\!15$	0.30	0	17,19,21	0.43	0
14	NAG	М	605	5	14,14,15	0.29	0	17,19,21	0.42	0
14	NAG	Z	702	7	$14,\!14,\!15$	0.45	0	17,19,21	0.60	0
14	NAG	М	602	5	$14,\!14,\!15$	0.42	0	17,19,21	0.43	0
14	NAG	Y	702	7	14,14,15	0.19	0	17,19,21	0.47	0
14	NAG	E	601	5	$14,\!14,\!15$	0.40	0	17,19,21	0.41	0
14	NAG	E	606	5	$14,\!14,\!15$	0.24	0	17,19,21	0.35	0
14	NAG	G	603	5	$14,\!14,\!15$	0.32	0	17,19,21	0.50	0
14	NAG	Y	701	7	$14,\!14,\!15$	0.36	0	17,19,21	0.37	0
14	NAG	G	606	5	$14,\!14,\!15$	0.23	0	17,19,21	0.39	0
14	NAG	G	602	5	$14,\!14,\!15$	0.44	0	17,19,21	0.58	0
14	NAG	E	608	5	$14,\!14,\!15$	0.21	0	17,19,21	0.40	0
14	NAG	Е	605	5	$14,\!14,\!15$	0.22	0	17,19,21	0.41	0
14	NAG	G	605	5	$14,\!14,\!15$	0.23	0	17,19,21	0.41	0
14	NAG	Z	701	7	14,14,15	0.55	0	17,19,21	0.95	1 (5%)
14	NAG	М	608	5	14,14,15	0.28	0	17,19,21	0.56	0
14	NAG	E	603	5	14,14,15	0.20	0	17,19,21	0.38	0
14	NAG	М	604	5	14,14,15	0.20	0	17,19,21	0.47	0
14	NAG	М	601	5	14,14,15	0.35	0	17,19,21	0.48	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	Е	607	5	-	0/6/23/26	0/1/1/1
14	NAG	Y	703	7	-	0/6/23/26	0/1/1/1
14	NAG	М	607	5	-	0/6/23/26	0/1/1/1
14	NAG	М	603	5	-	0/6/23/26	0/1/1/1
14	NAG	М	606	5	-	0/6/23/26	0/1/1/1
14	NAG	G	604	5	-	5/6/23/26	0/1/1/1
14	NAG	G	607	5	-	2/6/23/26	0/1/1/1
14	NAG	Х	701	7	-	0/6/23/26	0/1/1/1
14	NAG	Х	702	7	-	1/6/23/26	0/1/1/1
14	NAG	Е	602	5	-	4/6/23/26	0/1/1/1
14	NAG	G	601	5	-	4/6/23/26	0/1/1/1
14	NAG	Е	604	5	-	1/6/23/26	0/1/1/1
14	NAG	М	605	5	-	1/6/23/26	0/1/1/1
14	NAG	Z	702	7	-	2/6/23/26	0/1/1/1
14	NAG	М	602	5	-	2/6/23/26	0/1/1/1



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WOI	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	NAG	Y	702	7	-	3/6/23/26	0/1/1/1
14	NAG	Е	601	5	-	4/6/23/26	0/1/1/1
14	NAG	Е	606	5	-	2/6/23/26	0/1/1/1
14	NAG	G	603	5	-	0/6/23/26	0/1/1/1
14	NAG	Y	701	7	-	0/6/23/26	0/1/1/1
14	NAG	G	606	5	-	1/6/23/26	0/1/1/1
14	NAG	G	602	5	-	3/6/23/26	0/1/1/1
14	NAG	Е	608	5	-	2/6/23/26	0/1/1/1
14	NAG	Е	605	5	-	0/6/23/26	0/1/1/1
14	NAG	G	605	5	-	2/6/23/26	0/1/1/1
14	NAG	Z	701	7	-	2/6/23/26	0/1/1/1
14	NAG	М	608	5	-	0/6/23/26	0/1/1/1
14	NAG	Е	603	5	-	0/6/23/26	0/1/1/1
14	NAG	М	604	5	-	2/6/23/26	0/1/1/1
14	NAG	М	601	5	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	604	NAG	C1-C2	2.06	1.55	1.52

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
14	G	604	NAG	C2-N2-C7	4.35	129.09	122.90
14	G	601	NAG	C2-N2-C7	4.22	128.91	122.90
14	Z	701	NAG	C1-O5-C5	3.51	116.95	112.19
14	G	604	NAG	C1-C2-N2	2.27	114.36	110.49

All (4) bond angle outliers are listed below:

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	Е	602	NAG	C3-C2-N2-C7
14	М	602	NAG	C4-C5-C6-O6
14	М	602	NAG	O5-C5-C6-O6
14	G	604	NAG	O5-C5-C6-O6
14	G	601	NAG	C8-C7-N2-C2
14	G	601	NAG	O7-C7-N2-C2



Mol	Chain	Res	Type	Atoms
14	G	604	NAG	C8-C7-N2-C2
14	G	604	NAG	O7-C7-N2-C2
14	Ζ	702	NAG	C8-C7-N2-C2
14	Ζ	702	NAG	O7-C7-N2-C2
14	G	605	NAG	O5-C5-C6-O6
14	М	604	NAG	C4-C5-C6-O6
14	G	605	NAG	C4-C5-C6-O6
14	М	604	NAG	O5-C5-C6-O6
14	Z	701	NAG	O5-C5-C6-O6
14	Е	606	NAG	C4-C5-C6-O6
14	Е	601	NAG	C1-C2-N2-C7
14	Е	604	NAG	O5-C5-C6-O6
14	Х	702	NAG	O5-C5-C6-O6
14	Е	606	NAG	O5-C5-C6-O6
14	G	604	NAG	C4-C5-C6-O6
14	G	601	NAG	O5-C5-C6-O6
14	М	605	NAG	O5-C5-C6-O6
14	G	602	NAG	O5-C5-C6-O6
14	G	606	NAG	O5-C5-C6-O6
14	Ζ	701	NAG	C4-C5-C6-O6
14	Y	702	NAG	C4-C5-C6-O6
14	Е	608	NAG	C4-C5-C6-O6
14	Y	702	NAG	O5-C5-C6-O6
14	Е	608	NAG	O5-C5-C6-O6
14	G	601	NAG	C3-C2-N2-C7
14	G	604	NAG	C3-C2-N2-C7
14	Y	702	NAG	C3-C2-N2-C7
14	G	607	NAG	C4-C5-C6-O6
14	Е	601	NAG	C4-C5-C6-O6
14	Е	601	NAG	05-C5-C6-O6
14	Е	602	NAG	O5-C5-C6-O6
14	Е	602	NAG	C4-C5-C6-O6
14	Е	602	NAG	C1-C2-N2-C7
14	G	607	NAG	O5-C5-C6-O6
14	Е	601	NAG	C3-C2-N2-C7
14	G	602	NAG	C3-C2-N2-C7
14	G	602	NAG	C1-C2-N2-C7

Continued from previous page...

There are no ring outliers.

8 monomers are involved in 11 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	М	603	NAG	1	0
14	G	604	NAG	1	0
14	Е	602	NAG	2	0
14	G	601	NAG	1	0
14	Е	601	NAG	1	0
14	G	602	NAG	3	0
14	М	604	NAG	1	0
14	М	601	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.


























































































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	F	222/225~(98%)	0.42	19 (8%) 10 8	79, 119, 185, 222	0
1	Н	222/225~(98%)	0.07	4 (1%) 68 61	71, 103, 145, 208	0
1	Ν	222/225~(98%)	0.95	41 (18%) 1 1	83, 123, 252, 272	0
2	Ι	205/210~(97%)	0.48	19 (9%) 8 7	81, 137, 179, 217	0
3	L	204/210~(97%)	0.13	4 (1%) 65 57	81, 112, 144, 186	0
3	Ο	205/210~(97%)	0.85	30 (14%) 2 2	87, 173, 239, 254	0
4	А	210/214~(98%)	0.53	24 (11%) 5 5	76, 158, 224, 235	0
4	С	210/214~(98%)	0.64	29 (13%) 2 3	77, 127, 224, 227	0
4	J	210/214~(98%)	0.89	34 (16%) 1 2	81, 156, 192, 206	0
5	Е	447/474 (94%)	0.12	9 (2%) 65 57	66, 95, 152, 181	0
5	G	449/474~(94%)	0.00	2 (0%) 92 88	53, 81, 140, 177	0
5	М	449/474~(94%)	0.09	13 (2%) 51 41	61, 92, 141, 195	0
6	В	226/236~(95%)	0.50	20 (8%) 10 8	70, 131, 203, 212	0
6	D	226/236~(95%)	0.69	38 (16%) 1 1	72, 122, 237, 252	0
6	Κ	226/236~(95%)	0.36	15 (6%) 18 14	78, 138, 195, 210	0
7	Х	129/153~(84%)	0.13	4 (3%) 49 39	68, 112, 169, 194	0
7	Y	129/153~(84%)	-0.00	0 100 100	62, 90, 136, 166	0
7	Z	129/153~(84%)	0.10	5 (3%) 39 32	70, 116, 164, 193	0
All	All	4320/4536~(95%)	0.35	310 (7%) 15 12	53, 109, 217, 272	0

All (310) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Ν	168	LEU	10.6
7	Х	518	VAL	9.7
6	В	126	PRO	8.8



Mol	Chain	Res	Type	RSRZ	
4	J	107	SER	8.4	
1	Ν	135	PRO	7.4	
1	F	225	CYS	7.3	
6	В	125	ALA	7.2	
4	С	201	THR	7.2	
1	Н	225	CYS	7.2	
6	D	150	VAL	7.1	
1	Ν	147	LEU	7.0	
1	N	203	TYR	6.8	
1	Ν	161	VAL	6.7	
7	Ζ	518	VAL	6.6	
1	N	146	ALA	6.3	
3	0	112	ALA	6.2	
4	J	133	VAL	6.2	
1	N	159	VAL	6.1	
5	М	186(A)	ASN	5.9	
3	0	156	VAL	5.6	
1	Ν	134	ALA	5.6	
3	0	147	VAL	5.6	
6	D	138	LEU	5.5	
1	Ν	199	GLY	5.4	
1	Ν	187	LEU	5.2	
3	0	111	LYS	5.2	
2	Ι	187	LYS	5.1	
4	J	202	VAL	5.0	
1	Ν	189	SER	5.0	
6	D	208	ASP	5.0	
6	D	137	ALA	5.0	
1	F	150	LEU	4.9	
4	J	201	THR	4.9	
3	0	157	LYS	4.9	
1	N	225	CYS	4.9	
4	J	116	THR	4.9	
4	A	206	VAL	4.8	
4	J	13	VAL	4.8	
6	D	141	LEU	4.7	
1	N	170	SER	4.7	
1	Н	224	SER	4.7	
5	Е	506	VAL	4.6	
3	0	148	ALA	4.6	
2	Ι	209	PRO	4.5	
4	J	200	SER	4.5	



Mol	Chain	Res	Type	RSRZ	
4	А	180	LEU	4.5	
4	С	196	THR	4.5	
4	А	15	LEU	4.5	
1	F	151	VAL	4.4	
1	F	224	SER	4.4	
1	Ν	188	SER	4.4	
4	J	15	LEU	4.4	
5	М	460	SER	4.4	
2	Ι	189	HIS	4.3	
4	А	190	SER	4.3	
1	N	169	THR	4.3	
6	В	168	ALA	4.3	
3	L	212	CYS	4.2	
4	J	195	VAL	4.2	
4	А	156	LYS	4.2	
4	С	119	PRO	4.2	
3	0	129	ASN	4.2	
4	А	191	TYR	4.2	
4	А	175	SER	4.1	
6	K	194	TYR	4.1	
7	Х	664	ASP	4.1	
6	K	207	VAL	4.1	
6	D	180	SER	4.1	
6	K	138	LEU	4.1	
4	J	203	GLU	4.1	
6	D	207	VAL	4.0	
2	Ι	13	GLY	4.0	
7	Х	519	PHE	4.0	
4	J	117	LEU	4.0	
4	J	155	VAL	4.0	
6	D	136	ALA	4.0	
4	A	185	TRP	3.9	
6	D	139	GLY	3.9	
1	N	193	VAL	3.9	
3	0	82	GLU	3.9	
3	Ō	153	SER	3.8	
4	J	146	VAL	3.8	
3	0	158	ALA	3.8	
3	0	117	THR	3.7	
6	D	133	GLY	3.7	
1	N	148	GLY	3.7	
1	Ν	24	ALA	3.7	



Mol	Chain	Res	Type	RSRZ	
6	D	167	PRO	3.7	
4	А	161	THR	3.7	
4	С	180	LEU	3.7	
1	N	151	VAL	3.7	
4	J	14	ALA	3.6	
5	G	72	HIS	3.6	
5	G	137	ASN	3.6	
1	Ν	215	LYS	3.5	
6	Κ	11	LEU	3.5	
1	F	203	TYR	3.5	
6	Κ	202	PRO	3.5	
4	J	207	ALA	3.5	
4	А	162	THR	3.5	
1	N	176	PRO	3.5	
6	Κ	8	GLY	3.5	
6	D	120	SER	3.5	
4	А	144	VAL	3.4	
2	Ι	14	SER	3.4	
4	J	80	VAL	3.4	
3	0	155	PRO	3.4	
2	Ι	186	TRP	3.4	
4	С	142	GLY	3.4	
6	В	116	THR	3.4	
6	D	184	VAL	3.4	
1	Ν	216	VAL	3.4	
4	С	200	SER	3.3	
1	F	219	LYS	3.3	
2	Ι	212	CYS	3.3	
5	М	152	GLY	3.3	
6	В	137	ALA	3.3	
6	В	163	VAL	3.3	
1	N	160	THR	3.2	
3	0	195	GLN	3.2	
4	A	155	VAL	3.2	
4	J	106(A)	LEU	3.2	
3	0	123	SER	3.2	
6	D	140	CYS	3.2	
4	J	109	PRO	3.1	
3	0	192	TYR	3.1	
1	F	135	PRO	3.1	
5	Е	72	HIS	3.1	
2	Ι	188	SER	3.1	



Mol	Chain	Res	Type	RSRZ	
4	J	191	TYR	3.1	
6	В	132	SER	3.1	
6	В	121	VAL	3.0	
1	F	220	VAL	3.0	
4	С	177	TYR	3.0	
1	N	129	SER	3.0	
1	F	129	SER	3.0	
6	K	9	PRO	3.0	
3	0	134	VAL	3.0	
4	J	78	VAL	3.0	
6	D	132	SER	3.0	
5	М	462	ASP	3.0	
1	F	188	SER	3.0	
6	В	213	PRO	3.0	
3	0	145	VAL	2.9	
1	N	163	TRP	2.9	
4	J	136	ILE	2.9	
2	Ι	190	LYS	2.9	
1	F	187	LEU	2.9	
6	D	210	LYS	2.9	
6	D	135	THR	2.9	
1	Ν	142	GLY	2.9	
3	0	2	SER	2.9	
5	М	185	ASN	2.9	
4	С	5	TYR	2.9	
4	С	133	VAL	2.9	
4	С	209	THR	2.9	
3	0	127	GLN	2.9	
6	D	159	LEU	2.9	
4	С	203	GLU	2.9	
6	D	179	SER	2.9	
6	D	163	VAL	2.8	
4	С	131	THR	2.8	
5	М	505	VAL	2.8	
4	A	120	PRO	2.8	
4	A	189	LYS	2.8	
2	I	132	THR	2.8	
4	J	208	PRO	2.8	
1	F	161	VAL	2.8	
6	D	178	LEU	2.8	
6	K	126	PRO	2.7	
1	N N	143	GLY	2.7	



Mol	Chain	Res	Type	RSRZ	
1	Ν	145	ALA	2.7	
4	J	115	VAL	2.7	
1	Ν	224	SER	2.7	
4	J	170	ASN	2.7	
2	Ι	2	SER	2.7	
4	А	116	THR	2.7	
3	L	27	SER	2.7	
4	J	209	THR	2.7	
3	0	21	ILE	2.7	
4	А	131	THR	2.7	
6	D	152	VAL	2.7	
7	Ζ	520	LEU	2.7	
6	K	198	VAL	2.7	
5	Е	473	GLY	2.7	
6	D	142	VAL	2.6	
6	D	185	PRO	2.6	
4	С	199	GLY	2.6	
6	Κ	27	GLY	2.6	
7	Ζ	567	LYS	2.6	
5	Е	189	THR	2.6	
2	Ι	86	TYR	2.6	
5	М	64	LYS	2.6	
1	Ν	217	ASP	2.6	
6	В	124	LEU	2.5	
2	Ι	210	THR	2.5	
1	Ν	186	SER	2.5	
4	С	132	LEU	2.5	
4	J	119	PRO	2.5	
6	D	191	THR	2.5	
4	J	144	VAL	2.5	
1	F	90	ASP	2.5	
4	А	174	ALA	2.5	
4	С	117	LEU	2.5	
4	С	120	PRO	2.5	
4	J	108	GLN	2.5	
5	Е	186	GLU	2.4	
6	D	126	PRO	2.4	
6	D	197	ASN	2.4	
1	Ν	214	THR	2.4	
4	J	206	VAL	2.4	
6	K	210	LYS	2.4	
6	В	90	TYR	2.4	



Mol	Chain	Res	Type	RSRZ	
3	0	132	THR	2.4	
2	Ι	117	THR	2.4	
3	0	162	THR	2.4	
6	D	206	LYS	2.4	
1	F	149	CYS	2.4	
6	D	149	PRO	2.4	
1	F	141	SER	2.4	
6	D	181	VAL	2.4	
1	Ν	167	ALA	2.4	
6	В	167	PRO	2.4	
4	С	186	LYS	2.4	
4	J	69	THR	2.4	
6	D	121	VAL	2.4	
5	М	72	HIS	2.4	
1	Ν	207	VAL	2.4	
6	D	124	LEU	2.4	
4	А	136	ILE	2.4	
4	А	119	PRO	2.4	
6	В	119	PRO	2.4	
4	С	115	VAL	2.4	
4	С	183	GLU	2.4	
3	L	62	PHE	2.4	
1	F	38	ARG	2.4	
7	Х	565	LEU	2.3	
5	М	186	GLU	2.3	
6	K	140	CYS	2.3	
2	Ι	211	GLU	2.3	
2	Ι	21	ILE	2.3	
5	М	341	THR	2.3	
6	D	160	THR	2.3	
1	F	118	VAL	2.3	
1	Ν	198	LEU	2.3	
6	В	212	GLU	2.3	
4	С	136	ILE	2.3	
4	C	146	VAL	2.3	
1	N	200	THR	2.3	
3	0	71	ALA	2.3	
6	K	208	ASP	2.3	
6	В	38	ARG	2.2	
5	М	395	TRP	2.2	
5	Е	186(A)	ASN	2.2	
6	В	11	LEU	2.2	



Mol	Chain	Res	Type	RSRZ	
4	J	190	SER	2.2	
3	Ο	184	GLU	2.2	
4	С	204	LYS	2.2	
1	F	223	LYS	2.2	
1	N	208	ASN	2.2	
4	А	67	PHE	2.2	
1	N	158	PRO	2.2	
4	С	191	TYR	2.2	
4	J	150	ALA	2.2	
6	D	211	VAL	2.2	
4	А	130	ALA	2.2	
6	В	100(N)	TYR	2.2	
4	С	202	VAL	2.2	
7	Ζ	565	LEU	2.2	
4	С	175	SER	2.2	
4	А	199	GLY	2.2	
4	А	157	ALA	2.2	
4	J	174	ALA	2.2	
2	Ι	142	PRO	2.1	
4	С	113	PRO	2.1	
5	М	506	VAL	2.1	
3	0	62	PHE	2.1	
5	М	73	ALA	2.1	
2	Ι	201	SER	2.1	
5	Е	195	ASN	2.1	
3	0	187	LYS	2.1	
5	Е	455	THR	2.1	
6	D	168	ALA	2.1	
1	Н	98	ARG	2.1	
6	В	28	SER	2.1	
4	J	68	GLY	2.1	
1	Н	200	THR	2.1	
6	D	182	VAL	2.1	
1	F	222	PRO	2.1	
6	K	118	GLY	2.1	
3	L	32	TYR	2.1	
3	0	204	GLU	2.1	
4	С	194	GLN	2.1	
1	Ν	174	THR	2.1	
6	В	146	PHE	2.1	
1	N	219	LYS	2.1	
3	0	133	LEU	2.1	



Mol	Chain	Res	Type	RSRZ	
2	Ι	12	SER	2.0	
3	0	122	SER	2.0	
3	0	196	VAL	2.0	
6	Κ	141	LEU	2.0	
6	D	164	HIS	2.0	
7	Ζ	615	SER	2.0	
4	С	20	ARG	2.0	
1	Ν	172	VAL	2.0	
6	D	190	GLY	2.0	
6	В	34	TRP	2.0	
5	Е	269	GLU	2.0	
4	А	207	ALA	2.0	
4	С	144	VAL 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
8	BMA	Р	3	11/12	0.69	0.24	129,129,129,129	0
10	MAN	R	7	11/12	0.70	0.31	111,111,111,111	0
8	BMA	е	3	11/12	0.75	0.27	116,116,116,116	0
8	BMA	U	3	11/12	0.75	0.26	113,113,113,113	0
9	NAG	b	2	14/15	0.76	0.29	110,110,110,110	0
9	NAG	Т	2	14/15	0.78	0.73	$157,\!157,\!157,\!157$	0
9	NAG	V	2	14/15	0.79	0.18	118,118,118,118	0
11	MAN	a	9	11/12	0.80	0.23	103,103,103,103	0
8	BMA	с	3	11/12	0.81	0.20	161,161,161,161	0
12	MAN	g	6	11/12	0.82	0.25	109,109,109,109	0
9	NAG	i	2	14/15	0.83	0.38	123,123,123,123	0
12	MAN	g	4	11/12	0.84	0.15	120,120,120,120	0
8	NAG	е	2	14/15	0.84	0.23	114,114,114,114	0
9	NAG	Q	2	14/15	0.85	0.21	134,134,134,134	0
8	NAG	с	2	14/15	0.86	0.18	144,144,144,144	0



8E1P

Mol		Chain	\mathbf{Res}	Atoms	RSCC	RSR	B -factors($Å^2$)	Q<0.9
9	NAG	Т	1	14/15	0.86	0.37	139.139.139.139	0
9	NAG	d	2	14/15	0.87	0.21	121,121,121,121	0
12	BMA	g	3	11/12	0.87	0.17	100,100,100,100	0
9	NAG	f	2	14/15	0.88	0.21	131,131,131,131	0
11	MAN	a	5	11/12	0.88	0.28	90,90,90,90	0
8	NAG	с	1	14/15	0.88	0.24	115,115,115,115	0
11	MAN	a	6	11/12	0.89	0.34	88,88,88,88	0
11	MAN	a	8	11/12	0.89	0.19	95,95,95,95	0
9	NAG	S	2	14/15	0.89	0.21	106,106,106,106	0
12	NAG	g	1	14/15	0.89	0.33	97,97,97,97	0
8	NAG	Р	2	14/15	0.89	0.17	127,127,127,127	0
11	NAG	a	3	14/15	0.89	0.25	88,88,88,88	0
9	NAG	W	1	14/15	0.89	0.27	104,104,104,104	0
9	NAG	i	1	14/15	0.90	0.25	111,111,111,111	0
9	NAG	d	1	14/15	0.90	0.27	111,111,111,111	0
9	NAG	W	2	14/15	0.90	0.29	114,114,114,114	0
12	MAN	g	5	11/12	0.90	0.13	123,123,123,123	0
8	NAG	е	1	14/15	0.90	0.27	103,103,103,103	0
11	MAN	a	4	11/12	0.91	0.17	86,86,86,86	0
13	MAN	h	1	11/12	0.91	0.18	96,96,96,96	0
9	NAG	f	1	14/15	0.92	0.20	112,112,112,112	0
8	NAG	U	2	14/15	0.92	0.15	116,116,116,116	0
10	NAG	R	2	14/15	0.92	0.20	94,94,94,94	0
10	BMA	R	3	11/12	0.92	0.20	94,94,94,94	0
12	NAG	g	2	14/15	0.92	0.21	95,95,95,95	0
10	NAG	R	1	14/15	0.93	0.23	95,95,95,95	0
9	NAG	b	1	14/15	0.93	0.18	91,91,91,91	0
9	NAG	S	1	14/15	0.93	0.17	100,100,100,100	0
10	MAN	R	4	11/12	0.93	0.27	90,90,90,90	0
9	NAG	Q	1	14/15	0.93	0.25	109,109,109,109	0
9	NAG	V	1	14/15	0.93	0.15	102,102,102,102	0
11	NAG	a	1	14/15	0.94	0.26	78,78,78,78	0
11	MAN	a	7	11/12	0.95	0.12	87,87,87,87	0
10	MAN	R	6	11/12	0.95	0.19	90,90,90,90	0
8	NAG	P	1	14/15	0.95	0.20	104,104,104,104	0
8	NAG	U	1	14/15	0.95	0.23	91,91,91,91	0
	NAG	a	2	14/15	0.95	0.17	00.00.00.00	0
13	MAN	h	2	$\frac{11}{12}$	0.95	0.20	99,99,99,99	0
13	MAN	h	3	11/12	0.95	0.29	107,107,107,107	0
10	MAN	\mid R	5	11/12	0.96	0.16	84,84,84,84	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	$B-factors(A^2)$	Q<0.9
14	NAG	М	606	14/15	0.64	0.33	147,147,147,147	0
14	NAG	Е	606	14/15	0.65	0.33	135,135,135,135	0
14	NAG	Z	702	14/15	0.66	0.31	198,198,198,198	0
14	NAG	Е	601	14/15	0.73	0.24	134,134,134,134	0
14	NAG	М	604	14/15	0.73	0.36	117,117,117,117	0
14	NAG	М	608	14/15	0.74	0.35	124,124,124,124	0
14	NAG	G	604	14/15	0.78	0.32	106,106,106,106	0
14	NAG	Y	703	14/15	0.78	0.32	140,140,140,140	0
14	NAG	G	606	14/15	0.78	0.25	138,138,138,138	0
14	NAG	Е	605	14/15	0.80	0.34	107,107,107,107	0
14	NAG	G	602	14/15	0.81	0.25	123,123,123,123	0
14	NAG	Х	701	14/15	0.81	0.34	$159,\!159,\!159,\!159,\!159$	0
14	NAG	Е	608	14/15	0.81	0.24	116,116,116,116	0
14	NAG	G	603	14/15	0.82	0.23	117,117,117,117	0
14	NAG	Х	702	14/15	0.82	0.51	152,152,152,152	0
14	NAG	М	601	14/15	0.82	0.39	131,131,131,131	0
14	NAG	Z	701	14/15	0.83	0.23	149,149,149,149	0
14	NAG	Y	701	14/15	0.84	0.24	139,139,139,139	0
14	NAG	G	605	14/15	0.84	0.23	126,126,126,126	0
14	NAG	E	603	14/15	0.84	0.30	$115,\!115,\!115,\!115$	0
14	NAG	М	607	14/15	0.85	0.26	109,109,109,109	0
14	NAG	М	602	14/15	0.85	0.24	126,126,126,126	0
14	NAG	E	602	14/15	0.86	0.25	$97,\!97,\!97,\!97$	0
14	NAG	E	607	14/15	0.87	0.43	$144,\!144,\!144,\!144$	0
14	NAG	G	607	14/15	0.87	0.28	102,102,102,102	0
14	NAG	G	601	14/15	0.88	0.30	99,99,99,99	0
14	NAG	М	605	14/15	0.89	0.20	102,102,102,102	0
14	NAG	E	604	14/15	0.89	0.21	114,114,114,114	0
14	NAG	Y	702	14/15	0.91	0.22	101,101,101,101	0
14	NAG	М	603	14/15	0.91	0.17	112,112,112,112	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.














































































6.5 Other polymers (i)

There are no such residues in this entry.

