

Full wwPDB X-ray Structure Validation Report (i)

Nov 14, 2023 – 11:54 PM JST

PDB ID	:	6IK8
Title	:	Crystal structure of tomato beta-galactosidase (TBG) 4 in complex with beta
		-1,6-galactobiose
Authors	:	Matsuyama, K.; Nakae, S.; Igarashi, K.; Tada, T.; Ishimaru, M.
Deposited on	:	2018-10-15
Resolution	:	2.80 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:

:	4.02b-467
:	1.8.5 (274361), CSD as541be (2020)
:	1.13
:	2.36
:	20191225.v01 (using entries in the PDB archive December 25th 2019)
:	5.8.0158
:	7.0.044 (Gargrove)
:	Engh & Huber (2001)
:	Parkinson et al. (1996)
:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569(2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain					
1	А	718	77%		20%			
1	В	718	^{2%} 75%		22%			
2	С	2	100	%				
2	Е	2	50%	50%				
3	D	2	50%	50%				
3	F	2	50%	50%				



The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	В	803	-	-	Х	-



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 11450 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 Beta-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	В	705	$\begin{array}{c} \text{Total} \\ 5527 \end{array}$	C 3533	N 944	O 1023	S 27	0	0	0
1	А	705	Total 5527	C 3533	N 944	O 1023	S 27	0	0	0

Chain	Residue	Modelled	Actual	Comment	Reference
В	18	GLU	-	expression tag	UNP 081100
В	19	ALA	-	expression tag	UNP 081100
В	20	GLU	-	expression tag	UNP 081100
В	21	ALA	-	expression tag	UNP 081100
В	22	GLU	-	expression tag	UNP 081100
В	23	PHE	-	expression tag	UNP 081100
В	181	ALA	GLU	engineered mutation	UNP 081100
В	725	SER	-	expression tag	UNP 081100
В	726	ALA	-	expression tag	UNP 081100
В	727	ALA	-	expression tag	UNP 081100
В	728	ALA	-	expression tag	UNP 081100
В	729	ALA	-	expression tag	UNP 081100
В	730	SER	-	expression tag	UNP 081100
В	731	PHE	-	expression tag	UNP 081100
В	732	LEU	-	expression tag	UNP 081100
В	733	GLU	-	expression tag	UNP 081100
В	734	GLN	-	expression tag	UNP 081100
В	735	LYS	-	expression tag	UNP 081100
A	18	GLU	-	expression tag	UNP 081100
A	19	ALA	-	expression tag	UNP 081100
A	20	GLU	-	expression tag	UNP 081100
А	21	ALA	-	expression tag	UNP 081100
A	22	GLU	-	expression tag	UNP 081100
A	23	PHE	-	expression tag	UNP 081100
A	181	ALA	GLU	engineered mutation	UNP 081100

There are 36 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
А	725	SER	-	expression tag	UNP 081100
А	726	ALA	-	expression tag	UNP 081100
А	727	ALA	-	expression tag	UNP 081100
А	728	ALA	-	expression tag	UNP 081100
А	729	ALA	-	expression tag	UNP 081100
А	730	SER	-	expression tag	UNP 081100
А	731	PHE	-	expression tag	UNP 081100
А	732	LEU	-	expression tag	UNP 081100
А	733	GLU	-	expression tag	UNP 081100
A	734	GLN	-	expression tag	UNP 081100
А	735	LYS	-	expression tag	UNP 081100

• Molecule 2 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
2	С	2	Total C N O 28 16 2 10	0	0	0
2	Е	2	Total C N O 28 16 2 10	0	0	0

• Molecule 3 is an oligosaccharide called beta-D-galactopyranose-(1-6)-beta-D-galactopyranos e.



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
3	D	2	Total 0 23 1	C O 12 11	0	0	0
3	F	2	Total (23 1	C O 12 11	0	0	0

• Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).





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

• Molecule 5 is beta-D-galactopyranose (three-letter code: GAL) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	Total C O 12 6 6	0	0

• Molecule 6 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	В	106	Total O 106 106	0	0
6	А	148	Total O 148 148	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: Beta-galactosidase

• Molecule 1: Beta-galactosidase





N455 E456 S465 N465 N469 V470	N4 1 N4 1 N4 75 N4 75 N4 75 E480 E481 F483 K484 K487 K487 K487 K487 K487 K487 K487	Y613 C514 C514 C514 C514 C514 C521 V541 V541 V563 S566 C567 C567 C567 C567 C567 C573 R573 R573 R573 R573 K577	
S597 S598 S599 S600 S601 S601	1622 642 1645 1645 1646 1646 1654 1658 1659 1659 1703 1702 1707	E7 08 E7 08 ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	
• Molecule opyranose	2: 2-acetamido-2-deoxy-beta-I	D-glucopyranose-(1-4)-2-acetamide	o-2-deoxy-beta-D-gluc
Chain C:	10	00%	
NAG1 NAG2			
• Molecule opyranose	2: 2-acetamido-2-deoxy-beta-I	D-glucopyranose-(1-4)-2-acetamid	o-2-deoxy-beta-D-gluc
Chain E:	50%	50%	
NAG1 NAG2			
• Molecule	3: beta-D-galactopyranose-(1-6	6)-beta-D-galactopyranose	
Chain D:	50%	50%	
GAL1 GAL2			
• Molecule	3: beta-D-galactopyranose-(1-6	6)-beta-D-galactopyranose	
Chain F:	50%	50%	
GAL1 GAL2			



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	92.94Å 95.95 Å 158.96 Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
$\mathbf{P}_{\text{accolution}}\left(\overset{}{\boldsymbol{\lambda}}\right)$	48.02 - 2.80	Depositor
Resolution (A)	47.98 - 2.80	EDS
% Data completeness	99.7 (48.02-2.80)	Depositor
(in resolution range)	99.7(47.98-2.80)	EDS
R _{merge}	0.15	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$3.02 (at 2.81 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
D D.	0.182 , 0.248	Depositor
n, n_{free}	0.182 , 0.248	DCC
R_{free} test set	1777 reflections (4.98%)	wwPDB-VP
Wilson B-factor $(Å^2)$	50.0	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.28 , 46.0	EDS
L-test for twinning ²	$< L >=0.47, < L^2>=0.30$	Xtriage
Estimated twinning fraction	0.023 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11450	wwPDB-VP
Average B, all atoms $(Å^2)$	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.35% 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, GAL

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	Bo	ond angles
1VIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.37	0/5690	0.70	0/7734
1	В	0.37	0/5690	0.72	1/7734~(0.0%)
All	All	0.37	0/11380	0.71	1/15468~(0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	В	682	CYS	CA-CB-SG	-5.90	103.38	114.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	5527	0	5349	184	1
1	В	5527	0	5348	190	1
2	С	28	0	25	0	0
2	Е	28	0	25	1	0
3	D	23	0	21	5	0
3	F	23	0	21	3	0
4	А	14	0	13	5	0
4	В	14	0	13	10	0



Jerre Jerre Frederick						
Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	А	12	0	11	0	0
6	А	148	0	0	8	0
6	В	106	0	0	12	0
All	All	11450	0	10826	373	1

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 17.

All (373) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:108:TYR:CB	1:A:174:ILE:HD11	1.58	1.34
1:B:494:MET:SD	1:B:522:THR:CG2	2.18	1.32
1:B:494:MET:SD	1:B:522:THR:HG22	1.72	1.29
1:A:269:GLU:HG3	1:A:669:TYR:CB	1.63	1.27
1:A:108:TYR:HB3	1:A:174:ILE:CD1	1.66	1.24
1:A:370:CYS:O	1:A:405:CYS:SG	2.01	1.18
1:A:108:TYR:CG	1:A:174:ILE:HD11	1.78	1.17
1:A:269:GLU:HG3	1:A:669:TYR:CG	1.80	1.16
1:A:485:ASN:HB2	1:A:487:LYS:NZ	1.59	1.16
1:A:485:ASN:ND2	1:A:487:LYS:HZ1	1.51	1.09
1:A:269:GLU:CG	1:A:669:TYR:CB	2.31	1.09
1:A:108:TYR:CB	1:A:174:ILE:CD1	2.29	1.08
1:B:456:GLU:OE1	1:B:458:LYS:HG2	1.54	1.07
1:B:472:THR:HG23	1:B:580:TRP:CE3	1.89	1.06
1:B:456:GLU:H	4:B:803:NAG:H81	1.10	1.05
1:B:494:MET:SD	1:B:522:THR:HG21	1.98	1.00
1:B:402:LEU:HD23	1:B:408:ALA:HA	1.42	1.00
1:B:630:ASP:N	1:B:694:ARG:NH2	2.11	0.98
1:A:485:ASN:CG	1:A:487:LYS:HZ1	1.65	0.98
1:B:607:GLY:O	1:B:610:MET:HG2	1.60	0.98
1:B:630:ASP:N	1:B:694:ARG:HH22	1.43	0.98
1:B:74:TYR:CG	1:B:117:VAL:HG13	1.98	0.97
1:B:577:LYS:HE2	1:B:577:LYS:HA	1.46	0.96
1:A:485:ASN:CB	1:A:487:LYS:NZ	2.28	0.96
1:A:402:LEU:HD23	1:A:408:ALA:HA	1.46	0.95
1:A:269:GLU:HG3	1:A:669:TYR:HB2	1.47	0.94
1:B:472:THR:HG23	1:B:580:TRP:CD2	2.00	0.94
1:B:530:ARG:NH1	1:B:531:ALA:HB3	1.83	0.94
1:A:485:ASN:ND2	1:A:487:LYS:NZ	2.16	0.94
1:A:269:GLU:CG	1:A:669:TYR:HB2	1.95	0.93



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:B:308:THR:HG21	1:B:653:ARG:O	1.70	0.91
1:B:132:TYR:OH	1:B:458:LYS:HG3	1.71	0.90
1:B:472:THR:CG2	1:B:580:TRP:CD2	2.54	0.90
1:A:445:ASP:HA	1:A:448:THR:OG1	1.72	0.90
1:B:402:LEU:HD23	1:B:408:ALA:CA	2.00	0.90
1:A:77:TRP:HB3	1:A:152:PHE:CZ	2.07	0.90
1:B:308:THR:CG2	1:B:653:ARG:O	2.21	0.88
1:B:494:MET:CE	1:B:522:THR:HG22	2.04	0.88
1:A:402:LEU:HD23	1:A:408:ALA:CA	2.03	0.87
1:A:485:ASN:HB2	1:A:487:LYS:HZ3	1.35	0.87
1:B:530:ARG:NH1	1:B:531:ALA:CB	2.40	0.84
1:A:269:GLU:OE2	1:A:669:TYR:HB3	1.77	0.84
1:B:577:LYS:HA	1:B:577:LYS:CE	2.04	0.84
1:A:402:LEU:CD2	1:A:408:ALA:N	2.42	0.83
1:B:456:GLU:N	4:B:803:NAG:H81	1.92	0.83
1:A:269:GLU:CG	1:A:669:TYR:HB3	2.06	0.82
1:A:370:CYS:C	1:A:405:CYS:SG	2.58	0.82
1:B:402:LEU:CD2	1:B:408:ALA:N	2.43	0.82
1:A:108:TYR:HB3	1:A:174:ILE:HD12	1.60	0.82
1:B:431:LEU:CD2	1:B:623:PHE:HB3	2.09	0.82
1:B:443:ALA:HB2	1:B:471:MET:HB3	1.61	0.81
1:A:354:LEU:HD13	1:A:385:VAL:HG11	1.63	0.81
1:A:45:SER:HB2	1:A:290:MET:HE2	1.61	0.80
1:B:605:VAL:HG12	1:B:609:LEU:O	1.80	0.80
1:B:74:TYR:CD1	1:B:117:VAL:HG13	2.16	0.79
1:B:494:MET:CE	1:B:522:THR:CG2	2.60	0.79
1:B:120:GLU:OE2	3:D:2:GAL:H3	1.82	0.78
1:A:108:TYR:CD2	1:A:174:ILE:HD11	2.18	0.78
1:A:456:GLU:H	4:A:803:NAG:H81	1.48	0.78
1:B:629:ASN:C	1:B:694:ARG:HH12	1.88	0.77
1:A:513:TYR:C	1:A:521:LEU:HD11	2.06	0.76
1:B:237:PHE:O	1:B:246:LYS:HE3	1.83	0.76
1:A:312:TYR:HH	3:F:2:GAL:HO3	0.88	0.76
1:B:38:ARG:HB2	1:B:345:VAL:CG1	2.15	0.76
1:B:431:LEU:HD21	1:B:623:PHE:HB3	1.66	0.76
1:A:269:GLU:HG3	1:A:669:TYR:HB3	1.65	0.76
1:A:45:SER:CB	1:A:290:MET:HE2	2.16	0.75
1:A:485:ASN:CG	1:A:487:LYS:NZ	2.37	0.75
1:A:570:GLU:OE2	1:A:573:ARG:NH2	2.20	0.75
1:A:402:LEU:CD2	1:A:408:ALA:CA	2.65	0.75
1:B:184:PRO:HG2	3:D:1:GAL:O3	1.86	0.74



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:361:HIS:HD2	6:B:911:HOH:O	1.70	0.74
1:B:602:VAL:HG12	1:B:603:GLU:H	1.53	0.74
1:B:402:LEU:CD2	1:B:408:ALA:CA	2.65	0.74
1:B:455:TRP:HA	4:B:803:NAG:H82	1.71	0.73
1:B:38:ARG:HB2	1:B:345:VAL:HG13	1.70	0.73
1:A:485:ASN:HD22	1:A:487:LYS:NZ	1.86	0.73
1:A:92:ARG:NH1	1:A:297:PHE:HB2	2.03	0.72
1:A:354:LEU:HD13	1:A:385:VAL:CG1	2.19	0.72
1:B:605:VAL:CG1	1:B:609:LEU:O	2.38	0.72
1:A:269:GLU:HG2	1:A:669:TYR:HB2	1.70	0.72
1:B:472:THR:HG21	1:B:580:TRP:CE2	2.24	0.72
1:A:237:PHE:O	1:A:246:LYS:HE3	1.89	0.72
1:A:485:ASN:HB2	1:A:487:LYS:HZ2	1.54	0.71
1:A:455:TRP:CD1	4:A:803:NAG:H82	2.25	0.71
1:A:367:SER:OG	1:A:368:GLY:N	2.19	0.70
1:B:74:TYR:CG	1:B:117:VAL:CG1	2.74	0.69
1:B:179:GLU:HG3	1:B:180:ASN:H	1.57	0.69
1:A:115:PRO:HD2	6:A:1008:HOH:O	1.92	0.69
1:B:530:ARG:HH12	1:B:531:ALA:HB3	1.52	0.68
1:B:666:LYS:CD	6:B:901:HOH:O	2.40	0.68
1:A:179:GLU:HG3	1:A:180:ASN:H	1.57	0.68
1:A:402:LEU:HD23	1:A:408:ALA:N	2.08	0.68
1:A:402:LEU:CD2	1:A:407:THR:C	2.62	0.68
6:A:996:HOH:O	2:E:1:NAG:H4	1.95	0.67
1:B:455:TRP:CD1	4:B:803:NAG:H82	2.29	0.67
1:A:269:GLU:CD	1:A:669:TYR:HB3	2.16	0.67
1:B:629:ASN:HA	1:B:694:ARG:NH1	2.10	0.66
1:B:530:ARG:HH11	1:B:531:ALA:H	1.44	0.66
1:B:402:LEU:CD2	1:B:407:THR:C	2.64	0.66
1:A:54:GLN:HG3	1:A:695:SER:CB	2.26	0.65
1:B:456:GLU:H	4:B:803:NAG:C8	1.99	0.65
1:B:38:ARG:CB	1:B:345:VAL:HG13	2.26	0.65
1:B:431:LEU:HD23	1:B:623:PHE:HB3	1.78	0.65
1:A:440:THR:HG23	6:A:1036:HOH:O	1.97	0.65
1:B:402:LEU:HD23	1:B:408:ALA:N	2.09	0.65
1:A:485:ASN:OD1	1:A:485:ASN:N	2.30	0.65
1:B:472:THR:HG21	1:B:580:TRP:CD2	2.31	0.64
1:B:602:VAL:HG12	1:B:603:GLU:N	2.12	0.64
1:B:248:TRP:CE2	1:B:251:VAL:HG22	2.33	0.64
1:B:530:ARG:HH12	1:B:531:ALA:CB	2.08	0.64
1:B:354:LEU:HB3	1:B:385:VAL:CG2	2.27	0.64



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:248:TRP:CE2	1:A:251:VAL:HG22	2.34	0.63
1:A:367:SER:O	1:A:368:GLY:O	2.16	0.63
1:B:436:TYR:CE2	1:B:602:VAL:HG11	2.34	0.63
1:A:514:GLY:N	1:A:521:LEU:HD11	2.13	0.63
1:B:629:ASN:C	1:B:694:ARG:NH1	2.51	0.63
1:B:634:LEU:HD23	1:B:636:MET:CE	2.28	0.63
1:A:370:CYS:O	1:A:371:ALA:C	2.38	0.63
1:B:472:THR:HG22	1:B:579:LYS:O	1.99	0.62
1:A:289:TYR:CG	1:A:290:MET:HE3	2.34	0.62
1:B:475:ASN:OD1	1:B:533:ILE:HG12	1.99	0.62
1:B:629:ASN:C	1:B:694:ARG:HH22	2.02	0.62
1:A:445:ASP:HA	1:A:448:THR:HG1	1.65	0.62
1:B:312:TYR:OH	3:D:2:GAL:O3	2.18	0.61
1:B:424:MET:HB3	1:B:720:VAL:HG21	1.81	0.61
1:A:358:GLN:HG2	1:A:383:VAL:HG21	1.83	0.61
1:B:115:PRO:O	1:B:117:VAL:HG23	2.01	0.60
1:A:77:TRP:HB3	1:A:152:PHE:CE2	2.36	0.60
1:B:610:MET:O	1:B:612:GLN:HG2	2.01	0.60
1:B:308:THR:HG23	1:B:653:ARG:O	2.02	0.60
1:A:108:TYR:HB2	1:A:174:ILE:HD11	1.73	0.59
1:A:591:LEU:O	1:A:599:SER:O	2.20	0.59
1:A:54:GLN:HG3	1:A:695:SER:HB3	1.84	0.59
1:B:472:THR:CG2	1:B:580:TRP:CE3	2.75	0.59
1:A:513:TYR:CA	1:A:521:LEU:HD11	2.33	0.58
1:B:354:LEU:HB3	1:B:385:VAL:HG21	1.84	0.58
1:B:627:GLY:O	1:B:721:ARG:NH2	2.36	0.58
1:A:290:MET:HE2	1:A:290:MET:HA	1.84	0.58
1:A:501:HIS:HE1	1:A:709:GLU:OE2	1.87	0.58
1:B:167:GLU:HA	1:B:171:GLY:O	2.03	0.58
1:A:402:LEU:HD23	1:A:407:THR:C	2.23	0.57
1:B:70:VAL:HG22	1:B:108:TYR:HB2	1.86	0.57
1:A:108:TYR:HB3	1:A:174:ILE:CG1	2.31	0.57
1:A:455:TRP:HA	4:A:803:NAG:C8	2.35	0.57
1:A:570:GLU:OE1	1:A:573:ARG:HG3	2.04	0.57
1:A:167:GLU:HA	1:A:171:GLY:O	2.04	0.57
1:B:455:TRP:HA	4:B:803:NAG:C8	2.34	0.57
1:B:308:THR:OG1	1:B:687:GLN:NE2	2.38	0.56
1:B:710:TRP:HB3	6:B:915:HOH:O	2.04	0.56
1:A:87:TYR:CD2	1:A:155:LYS:HE2	2.41	0.56
1:B:402:LEU:HD21	1:B:408:ALA:HB2	1.88	0.56
1:A:646:ILE:HD11	1:A:704:LEU:HD13	1.88	0.55



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:402:LEU:HD22	1:B:407:THR:C	2.27	0.55
1:B:63:ALA:HB1	1:B:68:LEU:HD12	1.89	0.55
1:A:440:THR:CG2	6:A:1036:HOH:O	2.54	0.55
1:B:238:ARG:HD3	6:B:972:HOH:O	2.07	0.55
1:B:494:MET:SD	1:B:522:THR:CB	2.93	0.55
1:A:654:HIS:HA	1:A:690:TYR:CE2	2.42	0.55
1:B:646:ILE:HD11	1:B:704:LEU:HD13	1.89	0.54
1:B:642:GLY:HA3	1:B:707:PHE:O	2.07	0.54
1:A:622:THR:HA	1:A:702:ASN:O	2.07	0.54
1:A:54:GLN:CG	1:A:695:SER:CB	2.84	0.54
1:A:289:TYR:CD1	1:A:290:MET:HE3	2.42	0.54
1:A:402:LEU:CD2	1:A:408:ALA:HA	2.25	0.54
1:B:308:THR:OG1	1:B:687:GLN:CD	2.45	0.54
1:B:622:THR:HA	1:B:702:ASN:O	2.07	0.54
1:B:654:HIS:HA	1:B:690:TYR:CE2	2.42	0.54
1:B:262:PRO:HB3	1:B:682:CYS:SG	2.47	0.54
1:A:402:LEU:HD21	1:A:408:ALA:HB2	1.89	0.54
1:A:442:THR:O	1:A:443:ALA:C	2.45	0.54
1:B:402:LEU:CD2	1:B:408:ALA:HA	2.25	0.54
1:B:577:LYS:HE2	1:B:577:LYS:CA	2.30	0.54
1:A:718:SER:HB2	6:A:985:HOH:O	2.07	0.54
1:B:299:ARG:HD3	6:B:954:HOH:O	2.08	0.54
1:B:308:THR:OG1	1:B:687:GLN:OE1	2.23	0.53
1:B:331:ARG:NH1	1:B:332:ASP:OD1	2.41	0.53
1:A:115:PRO:O	1:A:117:VAL:HG13	2.09	0.53
1:B:266:ARG:O	1:B:326:LYS:NZ	2.41	0.53
1:B:324:GLU:HB2	1:B:420:SER:HB3	1.90	0.53
1:B:459:ASN:HD22	4:B:803:NAG:H83	1.73	0.53
1:B:404:ASP:O	1:B:405:CYS:HB2	2.08	0.53
1:A:111:LEU:O	1:A:176:ALA:HA	2.09	0.53
1:B:139:ARG:NH1	1:B:179:GLU:OE2	2.36	0.53
1:B:474:VAL:HG13	1:B:573:ARG:HH21	1.74	0.53
1:A:642:GLY:HA3	1:A:707:PHE:O	2.09	0.53
1:B:188:GLU:CD	1:B:550:VAL:HG21	2.28	0.52
1:B:629:ASN:CA	1:B:694:ARG:NH1	2.72	0.52
1:B:87:TYR:CG	1:B:155:LYS:HE2	2.44	0.52
1:A:485:ASN:HD22	1:A:487:LYS:HZ2	1.58	0.52
1:A:494:MET:HG3	1:A:562:PRO:HD2	1.91	0.52
1:B:565:LEU:HG	1:B:568:LEU:HD11	1.92	0.52
1:A:594:HIS:HB2	1:A:645:TRP:CG	2.45	0.52
1:B:402:LEU:HD23	1:B:407:THR:C	2.29	0.51



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:594:HIS:HB2	1:B:645:TRP:CG	2.45	0.51	
1:A:513:TYR:HA	1:A:521:LEU:HD11	1.91	0.51	
1:B:602:VAL:CG1	1:B:603:GLU:H	2.21	0.51	
1:A:290:MET:HA	1:A:290:MET:CE	2.41	0.51	
1:B:605:VAL:HG11	1:B:609:LEU:HG	1.92	0.51	
1:B:111:LEU:O	1:B:176:ALA:HA	2.11	0.51	
1:A:113:ILE:O	1:A:115:PRO:HA	2.11	0.51	
1:B:312:TYR:HH	3:D:2:GAL:HO3	1.55	0.51	
1:B:238:ARG:CD	6:B:972:HOH:O	2.59	0.50	
1:A:116:TYR:HB2	1:A:126:PHE:CZ	2.47	0.50	
1:A:179:GLU:HG3	1:A:180:ASN:N	2.25	0.50	
1:B:634:LEU:HD23	1:B:636:MET:HE3	1.92	0.50	
1:B:629:ASN:C	1:B:694:ARG:NH2	2.62	0.50	
1:B:48:TYR:CG	1:B:49:PRO:HD3	2.47	0.50	
1:A:269:GLU:HG3	1:A:669:TYR:CD2	2.42	0.50	
1:A:402:LEU:HD22	1:A:407:THR:C	2.32	0.50	
1:A:448:THR:HB	1:A:581:SER:HB3	1.94	0.50	
1:A:501:HIS:CE1	1:A:709:GLU:OE2	2.65	0.50	
1:A:289:TYR:CE2	1:A:290:MET:HE1	2.47	0.50	
1:A:438:GLU:HB3	1:A:616:LEU:HB3	1.94	0.50	
1:A:599:SER:O	1:A:600:SER:HB3	2.12	0.50	
1:B:238:ARG:HB2	6:B:972:HOH:O	2.12	0.49	
1:A:48:TYR:CG	1:A:49:PRO:HD3	2.47	0.49	
1:B:530:ARG:NH1	1:B:531:ALA:HB2	2.25	0.49	
1:A:480:GLU:HG3	6:A:961:HOH:O	2.12	0.49	
1:A:563:VAL:HG12	1:A:575:LEU:HD13	1.95	0.49	
1:B:22:GLU:N	6:B:907:HOH:O	2.45	0.49	
1:A:137:GLU:HB2	1:A:142:ASN:ND2	2.28	0.49	
1:B:179:GLU:HG3	1:B:180:ASN:N	2.25	0.49	
1:B:530:ARG:HH11	1:B:531:ALA:CB	2.23	0.49	
1:A:354:LEU:HD11	1:A:374:LEU:HD22	1.94	0.49	
1:B:94:ASP:OD2	1:B:97:ARG:HB2	2.12	0.48	
1:B:308:THR:HG1	1:B:687:GLN:CD	2.15	0.48	
1:B:366:LYS:HA	1:B:366:LYS:HD3	1.56	0.48	
1:B:469:TRP:CE2	1:B:539:LEU:HD13	2.48	0.48	
1:A:77:TRP:HA	1:A:80:HIS:HB2	1.95	0.48	
1:A:289:TYR:CD2	1:A:290:MET:CE	2.97	0.48	
1:B:42:ILE:HG22	1:B:68:LEU:HD23	1.95	0.48	
1:B:116:TYR:HB2	1:B:126:PHE:CZ	2.48	0.48	
1:B:205:VAL:HG21	1:B:224:PRO:HD2	1.96	0.48	
1:A:56:TRP:HB2	1:A:57:PRO:HD3	1.95	0.48	



		Interatomic	Clash	
Atom-1	Atom-2	distance $(Å)$	overlap (Å)	
1:A:455:TRP:HD1	4:A:803:NAG:H82	1.75	0.48	
1:B:666:LYS:CE	6:B:901:HOH:O	2.49	0.48	
1:A:513:TYR:HA	1:A:521:LEU:CD1	2.44	0.48	
1:B:526:ASN:HD21	1:A:597:SER:HB2	1.77	0.48	
1:A:455:TRP:HA	4:A:803:NAG:H81	1.96	0.48	
1:A:480:GLU:OE2	1:A:568:LEU:HB3	2.14	0.48	
1:B:165:LEU:O	1:B:172:PRO:HD2	2.14	0.48	
1:B:443:ALA:HB2	1:B:471:MET:CB	2.40	0.48	
1:A:94:ASP:CG	1:A:97:ARG:HB2	2.34	0.48	
1:B:247:MET:N	6:B:904:HOH:O	2.43	0.47	
1:B:139:ARG:HD2	1:B:179:GLU:OE2	2.14	0.47	
1:A:248:TRP:CD2	1:A:251:VAL:HG22	2.49	0.47	
1:A:448:THR:HG22	1:A:471:MET:HE1	1.96	0.47	
1:A:430:GLY:O	1:A:431:LEU:HB2	2.14	0.47	
1:B:456:GLU:CD	1:B:458:LYS:HG2	2.32	0.47	
1:A:179:GLU:HG2	1:A:182:TYR:HB2	1.95	0.47	
1:A:469:TRP:CE2	1:A:539:LEU:HD13	2.50	0.47	
1:A:87:TYR:CG	1:A:155:LYS:HE2	2.50	0.47	
1:B:184:PRO:HA	1:B:187:TRP:CE3	2.50	0.47	
1:A:179:GLU:CG	1:A:182:TYR:HB2	2.45	0.47	
1:A:375:SER:HB3	1:A:399:ILE:HG12	1.97	0.47	
1:B:42:ILE:HG12	1:B:286:PHE:CZ	2.50	0.47	
1:B:74:TYR:HA	1:B:112:ARG:O	2.14	0.47	
1:A:78:ASN:HD21	1:A:121:TRP:HE1	1.62	0.47	
1:A:493:VAL:HG13	1:A:563:VAL:HG22	1.97	0.47	
1:B:431:LEU:H	1:B:431:LEU:HD12	1.80	0.46	
1:B:441:PRO:HD2	1:B:469:TRP:CZ2	2.50	0.46	
1:A:112:ARG:HA	1:A:177:GLN:HB3	1.97	0.46	
1:B:459:ASN:HD22	4:B:803:NAG:C7	2.28	0.46	
1:A:445:ASP:CA	1:A:448:THR:OG1	2.55	0.46	
1:B:112:ARG:HA	1:B:177:GLN:HB3	1.98	0.46	
1:B:248:TRP:CD2	1:B:251:VAL:HG22	2.50	0.46	
1:B:87:TYR:CD1	1:B:155:LYS:HE2	2.50	0.46	
1:B:113:ILE:O	1:B:115:PRO:HA	2.15	0.46	
1:A:448:THR:HG21	1:A:471:MET:HE3	1.97	0.46	
1:B:375:SER:HB3	1:B:399:ILE:HG12	1.98	0.46	
1:B:269:GLU:HB2	1:B:669:TYR:HB2	1.98	0.45	
1:A:45:SER:HB3	1:A:290:MET:HE2	1.97	0.45	
1:A:54:GLN:CG	1:A:695:SER:HB3	2.47	0.45	
1:A:237:PHE:O	1:A:246:LYS:CE	2.62	0.45	
1:A:384:LYS:HE2	1:A:384:LYS:HB3	1.85	0.45	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:666:LYS:HD2	6:B:901:HOH:O	2.09	0.45	
1:B:543:VAL:HG13	1:B:543:VAL:O	2.17	0.45	
1:B:490:TYR:HB3	1:B:566:SER:OG	2.16	0.45	
1:A:351:VAL:HG22	1:A:361:HIS:CE1	2.51	0.45	
1:A:448:THR:CG2	1:A:471:MET:HE3	2.47	0.45	
1:A:74:TYR:HA	1:A:112:ARG:O	2.16	0.45	
1:A:77:TRP:NE1	1:A:115:PRO:HB2	2.32	0.45	
1:B:361:HIS:CD2	6:B:911:HOH:O	2.53	0.44	
1:A:231:GLY:HA2	1:A:252:TRP:CZ3	2.52	0.44	
1:A:474:VAL:HG22	1:A:575:LEU:HD23	1.98	0.44	
1:B:612:GLN:O	1:B:614:GLN:HG3	2.18	0.44	
1:A:577:LYS:HA	1:A:577:LYS:HD3	1.79	0.44	
1:B:231:GLY:HA2	1:B:252:TRP:CZ3	2.52	0.44	
1:B:494:MET:HE3	1:B:522:THR:HG22	1.95	0.44	
1:A:120:GLU:OE1	3:F:2:GAL:H3	2.18	0.44	
1:A:493:VAL:HA	1:A:563:VAL:HG22	1.99	0.44	
1:B:56:TRP:HB2	1:B:57:PRO:HD3	1.98	0.44	
1:A:42:ILE:HG12	1:A:286:PHE:CZ	2.52	0.44	
1:A:165:LEU:O	1:A:172:PRO:HD2	2.18	0.44	
1:B:94:ASP:CG	1:B:97:ARG:HB2	2.38	0.44	
1:B:434:GLN:HG2	1:B:606:ARG:HG3	2.00	0.44	
1:A:402:LEU:HD21	1:A:408:ALA:CA	2.46	0.44	
1:B:530:ARG:HG3	1:B:531:ALA:N	2.32	0.44	
1:A:45:SER:CB	1:A:290:MET:CE	2.92	0.44	
1:A:406:LYS:HA	1:A:406:LYS:HD2	1.74	0.44	
1:B:602:VAL:CG1	1:B:603:GLU:N	2.80	0.43	
1:A:296:ASN:HB3	1:A:301:SER:OG	2.18	0.43	
1:B:112:ARG:NH2	1:B:250:GLU:OE1	2.47	0.43	
1:A:108:TYR:CB	1:A:174:ILE:HD12	2.29	0.43	
1:A:247:MET:N	6:A:905:HOH:O	2.40	0.43	
1:B:611:ALA:HB3	1:B:617:THR:HG21	2.00	0.43	
1:B:146:LYS:O	1:B:150:GLN:HB2	2.18	0.43	
1:A:77:TRP:HD1	1:A:77:TRP:H	1.66	0.43	
1:B:420:SER:HA	1:B:725:SER:O	2.19	0.43	
1:A:358:GLN:CG	1:A:383:VAL:HG21	2.46	0.43	
1:A:591:LEU:HD22	1:A:600:SER:OG	2.19	0.43	
1:B:632:LEU:CD2	1:B:721:ARG:HG2	2.48	0.43	
1:A:180:ASN:OD1	1:A:216:CYS:SG	2.76	0.43	
1:A:465:SER:HB2	6:A:1017:HOH:O	2.19	0.43	
1:A:203:MET:HB2	1:A:203:MET:HE3	1.86	0.43	
1:A:354:LEU:CD1	1:A:385:VAL:HG11	2.43	0.43	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:68:LEU:HD11	1:B:291:TYR:CD1	2.53	0.42
1:A:94:ASP:OD2	1:A:97:ARG:HB2	2.19	0.42
1:A:363:TYR:O	1:A:370:CYS:HA	2.18	0.42
1:A:312:TYR:OH	3:F:2:GAL:O3	1.88	0.42
1:A:448:THR:CG2	1:A:471:MET:CE	2.97	0.42
1:A:289:TYR:CD2	1:A:290:MET:HE3	2.54	0.42
1:B:74:TYR:CD2	1:B:117:VAL:CG1	3.02	0.42
1:B:568:LEU:HD12	1:B:568:LEU:N	2.34	0.42
1:B:494:MET:HE1	1:B:522:THR:CG2	2.48	0.42
1:B:455:TRP:HD1	4:B:803:NAG:H82	1.80	0.42
1:A:92:ARG:HH12	1:A:297:PHE:HB2	1.80	0.42
1:A:191:ALA:N	1:A:192:PRO:CD	2.83	0.42
1:B:191:ALA:N	1:B:192:PRO:CD	2.83	0.42
1:A:448:THR:HG22	1:A:471:MET:CE	2.49	0.42
1:B:49:PRO:O	1:B:92:ARG:HD2	2.20	0.42
1:B:74:TYR:CD2	1:B:117:VAL:HG13	2.52	0.42
1:B:431:LEU:HD12	1:B:431:LEU:N	2.35	0.42
1:A:78:ASN:ND2	1:A:121:TRP:HE1	2.17	0.41
1:B:201:ALA:HB1	1:B:225:VAL:HG21	2.02	0.41
1:A:513:TYR:CA	1:A:521:LEU:CD1	2.98	0.41
1:A:205:VAL:HG21	1:A:224:PRO:HD2	2.01	0.41
1:B:436:TYR:HB3	1:B:618:TRP:HB2	2.02	0.41
1:A:475:ASN:O	1:A:573:ARG:NH1	2.53	0.41
1:A:591:LEU:O	1:A:600:SER:HB3	2.20	0.41
1:B:43:SER:HA	1:B:70:VAL:O	2.20	0.41
1:A:499:VAL:HB	1:A:541:VAL:HB	2.01	0.41
1:B:71:ILE:O	1:B:109:VAL:HA	2.20	0.41
1:B:179:GLU:CG	1:B:182:TYR:HB2	2.50	0.41
1:B:434:GLN:CA	1:B:610:MET:HE1	2.51	0.41
1:A:77:TRP:O	1:A:81:GLU:N	2.50	0.41
1:B:112:ARG:HG2	1:B:177:GLN:HB2	2.03	0.41
1:B:472:THR:CG2	1:B:580:TRP:CE2	2.92	0.41
1:A:43:SER:HA	1:A:70:VAL:O	2.20	0.41
1:A:97:ARG:O	1:A:101:MET:HG3	2.21	0.41
1:B:38:ARG:HB3	1:B:345:VAL:HG13	2.02	0.41
1:B:60:ILE:O	1:B:63:ALA:HB3	2.21	0.41
1:B:184:PRO:HG2	3:D:1:GAL:C3	2.51	0.41
1:A:312:TYR:O	1:A:313:ASP:C	2.58	0.41
1:A:402:LEU:HD21	1:A:408:ALA:N	2.29	0.41
1:A:480:GLU:HG2	1:A:482:PHE:CE2	2.56	0.41
1:B:487:LYS:NZ	1:A:601:SER:HB3	$2.\overline{35}$	0.41



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:142:ASN:OD1	1:A:144:PRO:HD2	2.20	0.41
1:A:255:TRP:HB3	1:A:264:PRO:HG2	2.03	0.41
1:A:266:ARG:HA	1:A:267:PRO:HD3	1.91	0.41
1:A:490:TYR:HB3	1:A:566:SER:OG	2.21	0.41
1:B:112:ARG:HG2	1:B:177:GLN:CB	2.51	0.40
1:B:434:GLN:HA	1:B:610:MET:HE1	2.02	0.40
1:B:591:LEU:HD13	1:B:602:VAL:HG21	2.03	0.40
1:B:634:LEU:HD13	1:B:692:VAL:HG21	2.02	0.40
1:A:83:SER:OG	1:A:86:LYS:HD3	2.20	0.40
1:A:108:TYR:HB2	1:A:174:ILE:CD1	2.34	0.40
1:A:112:ARG:NH2	1:A:250:GLU:OE2	2.36	0.40
1:B:459:ASN:HD22	4:B:803:NAG:C8	2.34	0.40
1:A:83:SER:HA	1:A:129:TRP:CD1	2.57	0.40
1:B:130:LEU:O	1:B:136:MET:HG2	2.22	0.40
1:B:470:TYR:HB2	1:B:538:LEU:HB2	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)	
1:B:530:ARG:NH2	1:A:484:LYS:O[4_545]	2.18	0.02	

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	А	703/718~(98%)	657~(94%)	44 (6%)	2~(0%)	41 72
1	В	703/718~(98%)	663~(94%)	40 (6%)	0	100 100
All	All	1406/1436~(98%)	1320 (94%)	84 (6%)	2(0%)	51 81

All (2) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	А	368	GLY
1	А	443	ALA

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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	590/598~(99%)	582~(99%)	8 (1%)	67	90
1	В	590/598~(99%)	579~(98%)	11 (2%)	57	85
All	All	1180/1196~(99%)	1161 (98%)	19 (2%)	62	88

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	123	PHE
1	В	167	GLU
1	В	312	TYR
1	В	366	LYS
1	В	374	LEU
1	В	458	LYS
1	В	507	LYS
1	В	518	ASN
1	В	577	LYS
1	В	658	TYR
1	В	694	ARG
1	А	77	TRP
1	А	123	PHE
1	А	203	MET
1	А	312	TYR
1	А	406	LYS
1	А	485	ASN
1	А	658	TYR
1	A	718	SER

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



Mol	Chain	Res	Type
1	В	103	GLN
1	В	265	GLN
1	В	361	HIS
1	В	526	ASN
1	В	551	HIS
1	А	103	GLN
1	А	141	ASN
1	А	158	ASN
1	А	292	HIS
1	А	388	GLN
1	А	393	ASN
1	А	416	ASN
1	А	485	ASN
1	А	501	HIS
1	А	612	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

8 monosaccharides are modelled in this entry.

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

Mol Tuno Chain B		Dec	Tink	Bond lengths			Bond angles			
WIOI	туре	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
2	NAG	С	1	2,1	$14,\!14,\!15$	0.59	0	17,19,21	1.99	2 (11%)
2	NAG	С	2	2	14,14,15	0.98	1 (7%)	17,19,21	1.99	7 (41%)
3	GAL	D	1	3	12,12,12	0.47	0	17,17,17	1.03	0
3	GAL	D	2	3	11,11,12	0.81	1 (9%)	15,15,17	1.03	1 (6%)



Mal	Turne	Chain	Dec	Tink	Bo	ond leng	\mathbf{ths}	Bond angles		
INIOI	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	NAG	Е	1	2,1	14,14,15	0.76	1 (7%)	17,19,21	1.82	3 (17%)
2	NAG	Е	2	2	14,14,15	0.70	1 (7%)	17,19,21	1.45	2 (11%)
3	GAL	F	1	3	12,12,12	0.40	0	17,17,17	0.83	1 (5%)
3	GAL	F	2	3	11,11,12	0.74	0	15,15,17	0.97	2 (13%)

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
2	NAG	С	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	С	2	2	-	2/6/23/26	0/1/1/1
3	GAL	D	1	3	-	2/2/22/22	0/1/1/1
3	GAL	D	2	3	-	2/2/19/22	0/1/1/1
2	NAG	Е	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	Е	2	2	-	2/6/23/26	0/1/1/1
3	GAL	F	1	3	-	0/2/22/22	0/1/1/1
3	GAL	F	2	3	-	2/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	С	2	NAG	C1-C2	2.59	1.56	1.52
2	Е	1	NAG	C1-C2	2.18	1.55	1.52
2	Е	2	NAG	C1-C2	2.16	1.55	1.52
3	D	2	GAL	O5-C5	2.04	1.47	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	С	1	NAG	C1-O5-C5	7.07	121.78	112.19
2	Е	1	NAG	C1-O5-C5	4.34	118.07	112.19
2	С	2	NAG	O5-C5-C6	4.21	113.80	107.20
2	Е	2	NAG	C1-C2-N2	3.73	116.87	110.49
2	С	2	NAG	C2-N2-C7	3.58	128.00	122.90
2	Е	1	NAG	C1-C2-N2	3.51	116.48	110.49
2	Е	2	NAG	C2-N2-C7	3.50	127.89	122.90
2	Е	1	NAG	C2-N2-C7	-3.25	118.27	122.90



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	D	2	GAL	O2-C2-C3	2.64	115.43	110.14
2	С	2	NAG	C4-C3-C2	2.46	114.62	111.02
2	С	2	NAG	C1-C2-N2	2.42	114.62	110.49
3	F	1	GAL	O1-C1-C2	2.36	115.69	109.03
2	С	2	NAG	C3-C4-C5	-2.36	106.02	110.24
2	С	2	NAG	O5-C1-C2	2.25	114.83	111.29
2	С	1	NAG	O4-C4-C3	-2.16	105.35	110.35
3	F	2	GAL	O5-C1-C2	-2.12	107.50	110.77
2	С	2	NAG	O5-C5-C4	-2.08	105.77	110.83
3	F	2	GAL	O2-C2-C3	2.07	114.29	110.14

There are no chirality outliers.

Mol	Chain	Res	Type	Atoms
3	D	2	GAL	O5-C5-C6-O6
3	F	2	GAL	O5-C5-C6-O6
2	Е	2	NAG	O5-C5-C6-O6
2	Е	1	NAG	C4-C5-C6-O6
3	F	2	GAL	C4-C5-C6-O6
2	Е	1	NAG	O5-C5-C6-O6
3	D	2	GAL	C4-C5-C6-O6
2	С	1	NAG	O5-C5-C6-O6
2	Е	2	NAG	C4-C5-C6-O6
3	D	1	GAL	O5-C5-C6-O6
2	С	2	NAG	C4-C5-C6-O6
2	С	1	NAG	C4-C5-C6-O6
2	С	2	NAG	O5-C5-C6-O6
3	D	1	GAL	C4-C5-C6-O6

All (14) torsion outliers are listed below:

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1	GAL	2	0
3	D	2	GAL	3	0
3	F	2	GAL	3	0
2	Е	1	NAG	1	0

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

















5.6 Ligand geometry (i)

3 ligands are modelled in this entry.

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

Mal	Turne	Chain	Dog	Bog Link Bond lengths			Bond angles			
	туре	Unain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	В	803	1	14,14,15	0.89	0	17,19,21	1.96	5 (29%)
5	GAL	А	806	-	12,12,12	0.65	0	17,17,17	0.92	1 (5%)
4	NAG	А	803	1	14,14,15	0.73	0	17,19,21	1.43	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	В	803	1	-	2/6/23/26	0/1/1/1
5	GAL	А	806	-	-	0/2/22/22	0/1/1/1
4	NAG	А	803	1	-	3/6/23/26	0/1/1/1

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	В	803	NAG	C2-N2-C7	4.53	129.36	122.90
4	В	803	NAG	C1-O5-C5	4.22	117.91	112.19
4	В	803	NAG	O5-C5-C4	2.64	117.25	110.83
5	А	806	GAL	O5-C5-C6	2.49	112.62	106.44
4	А	803	NAG	O7-C7-C8	-2.19	117.98	122.06
4	В	803	NAG	C8-C7-N2	2.13	119.71	116.10
4	В	803	NAG	O7-C7-C8	-2.02	118.30	122.06

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	В	803	NAG	C8-C7-N2-C2
4	В	803	NAG	O7-C7-N2-C2
4	А	803	NAG	C8-C7-N2-C2
4	А	803	NAG	O7-C7-N2-C2
4	А	803	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	В	803	NAG	10	0
4	А	803	NAG	5	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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	705/718~(98%)	-0.46	3 (0%) 92 91	32, 49, 80, 151	0
1	В	705/718~(98%)	-0.40	11 (1%) 72 66	28, 48, 87, 158	0
All	All	1410/1436~(98%)	-0.43	14 (0%) 82 77	28, 48, 84, 158	0

All (14) RSRZ outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	RSRZ
1	В	565	LEU	3.5
1	В	572	SER	3.1
1	В	573	ARG	3.1
1	В	448	THR	3.0
1	В	447	ASP	2.8
1	А	439	GLU	2.6
1	В	609	LEU	2.3
1	А	392	TYR	2.3
1	В	476	ILE	2.1
1	В	429	GLY	2.1
1	В	608	SER	2.1
1	В	428	GLY	2.1
1	В	610	MET	2.0
1	А	601	SER	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,



6IK8

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q < 0.9
2	NAG	Ε	2	14/15	0.77	0.21	83,118,132,134	0
3	GAL	F	1	12/12	0.77	0.39	77,109,121,137	0
3	GAL	D	1	12/12	0.84	0.35	83,101,117,123	0
2	NAG	С	2	14/15	0.85	0.24	80,110,126,133	0
3	GAL	D	2	11/12	0.87	0.32	$59,\!78,\!95,\!122$	0
3	GAL	F	2	11/12	0.91	0.41	70,82,102,109	0
2	NAG	Е	1	14/15	0.94	0.11	54,62,76,99	0
2	NAG	С	1	14/15	0.95	0.12	44,55,57,75	0

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.

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.















6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
4	NAG	В	803	14/15	0.85	0.20	47,77,86,87	0
4	NAG	А	803	14/15	0.85	0.16	70,85,90,91	0
5	GAL	А	806	12/12	0.86	0.24	70,114,127,130	0

6.5 Other polymers (i)

There are no such residues in this entry.

