

Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2024 - 12:42 am GMT

:	8CR5
:	Murine Interleukin-12 receptor beta 1 domain 1 in complex with murine
	Interleukin-12 beta.
:	Merceron, R.; Bloch, Y.; Felix, J.; Savvides, S.N.
:	2023-03-07
:	2.15 Å(reported)
	::

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

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

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

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

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	344	22%		69%	15%	•	15%	
2	В	265	6%	39%		57%			
3	С	4			75%		25	%	



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3363 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 Interleukin-12 subunit beta.

Mol	Chain	Residues		Atoms					AltConf	Trace
1	А	292	Total 2267	C 1432	N 371	0 447	S 17	0	2	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	197	SER	CYS	engineered mutation	UNP P43432
А	336	GLY	-	expression tag	UNP P43432
А	337	THR	-	expression tag	UNP P43432
А	338	LYS	-	expression tag	UNP P43432
А	339	HIS	-	expression tag	UNP P43432
А	340	HIS	-	expression tag	UNP P43432
А	341	HIS	-	expression tag	UNP P43432
А	342	HIS	-	expression tag	UNP P43432
А	343	HIS	-	expression tag	UNP P43432
А	344	HIS	-	expression tag	UNP P43432

• Molecule 2 is a protein called Interleukin-12 receptor subunit beta-1.

Mol	Chain	Residues		Atoms					AltConf	Trace
2	В	114	Total 919	$\begin{array}{c} \mathrm{C} \\ 583 \end{array}$	N 161	O 169	S 6	0	0	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	3	MET	-	initiating methionine	UNP Q60837
В	4	GLY	-	expression tag	UNP Q60837
В	5	VAL	-	expression tag	UNP Q60837
В	6	LYS	-	expression tag	UNP Q60837
В	7	VAL	-	expression tag	UNP Q60837
В	8	LEU	-	expression tag	UNP Q60837



Chain	Residue	Modelled	Actual	Comment	Reference
В	9	PHE	-	expression tag	UNP Q60837
В	10	ALA	-	expression tag	UNP Q60837
В	11	LEU	-	expression tag	UNP Q60837
В	12	ILE	-	expression tag	UNP Q60837
В	13	CYS	-	expression tag	UNP Q60837
В	14	ILE	-	expression tag	UNP Q60837
В	15	ALA	-	expression tag	UNP Q60837
В	16	VAL	-	expression tag	UNP Q60837
В	17	ALA	-	expression tag	UNP Q60837
В	18	GLU	-	expression tag	UNP Q60837
В	19	ALA	-	expression tag	UNP Q60837
В	259	GLY	-	expression tag	UNP Q60837
В	260	THR	-	expression tag	UNP Q60837
В	261	LYS	-	expression tag	UNP Q60837
В	262	HIS	-	expression tag	UNP Q60837
В	263	HIS	-	expression tag	UNP Q60837
В	264	HIS	-	expression tag	UNP Q60837
В	265	HIS	-	expression tag	UNP Q60837
В	266	HIS	-	expression tag	UNP Q60837
В	267	HIS	-	expression tag	UNP Q60837

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



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace		
3	С	4	Total 50	C 28	N 2	O 20	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	Atoms				ZeroOcc	AltConf
4	В	1	Total 14	C 8	N 1	O 5	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	73	Total O 73 73	0	0
5	В	40	Total O 40 40	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: Interleukin-12 subunit beta

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

Chain C: 75% 25%





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	29.22Å 165.09 Å 51.87 Å	Deperitor
a, b, c, α , β , γ	90.00° 90.44° 90.00°	Depositor
$\mathbf{P}_{\text{oscolution}}(\hat{\mathbf{A}})$	49.48 - 2.15	Depositor
Resolution (A)	49.48 - 2.15	EDS
% Data completeness	99.3 (49.48-2.15)	Depositor
(in resolution range)	99.4 (49.48-2.15)	EDS
R_{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.42 (at 2.16 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
D D.	0.241 , 0.282	Depositor
n, n_{free}	0.241 , 0.282	DCC
R_{free} test set	1325 reflections $(5.00%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	38.0	Xtriage
Anisotropy	0.755	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.33, 54.9	EDS
L-test for twinning ²	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.063 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3363	wwPDB-VP
Average B, all atoms $(Å^2)$	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.75% of the height of the origin peak. No significant pseudotranslation is detected.

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



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, MAN

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

Mal	Chain	Bond	lengths	Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.27	0/2319	0.51	0/3156	
2	В	0.27	0/949	0.51	0/1294	
All	All	0.27	0/3268	0.51	0/4450	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	2267	0	2084	35	0
2	В	919	0	853	9	0
3	С	50	0	43	0	0
4	В	14	0	13	0	0
5	А	73	0	0	6	0
5	В	40	0	0	1	0
All	All	3363	0	2993	42	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 (42) 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 (\AA)	overlap (Å)	
1:A:215:GLN:OE1	5:A:401:HOH:O	2.11	0.69	
1:A:165:VAL:HG12	1:A:193:GLU:HA	1.78	0.65	
1:A:108:GLU:OE1	5:A:402:HOH:O	2.14	0.65	
1:A:269:LYS:HE2	1:A:317:ARG:HA	1.80	0.62	
1:A:238:ASN:ND2	1:A:254:GLU:OE2	2.32	0.62	
2:B:94:ARG:HH21	2:B:96:ARG:HH21	1.51	0.58	
1:A:136:ARG:HG3	1:A:192:GLN:HE22	1.69	0.58	
1:A:249:VAL:N	1:A:303:VAL:O	2.35	0.57	
2:B:55:ARG:O	5:B:401:HOH:O	2.18	0.57	
2:B:151:PRO:HB2	2:B:152:LEU:HD22	1.89	0.54	
1:A:40:ASP:O	5:A:403:HOH:O	2.19	0.53	
1:A:27:GLU:OE2	1:A:213[B]:ARG:NH2	2.42	0.51	
2:B:94:ARG:HE	2:B:96:ARG:NH2	2.09	0.51	
1:A:232:LYS:HG3	1:A:323:CYS:O	2.12	0.50	
1:A:238:ASN:HB3	1:A:240:GLN:HE22	1.76	0.49	
1:A:238:ASN:O	1:A:253:TRP:HA	2.13	0.49	
1:A:273:ARG:O	1:A:311:CYS:N	2.33	0.49	
1:A:115:GLU:O	5:A:405:HOH:O	2.20	0.48	
1:A:64:GLN:NE2	1:A:85:ALA:O	2.45	0.48	
1:A:144:GLN:NE2	5:A:417:HOH:O	2.34	0.48	
1:A:165:VAL:HG21	1:A:208:LEU:HD21	1.96	0.47	
1:A:136:ARG:HG3	1:A:192:GLN:NE2	2.29	0.47	
1:A:269:LYS:CE	1:A:317:ARG:HA	2.44	0.46	
1:A:227:ILE:O	1:A:231:ILE:HG12	2.16	0.46	
1:A:270:PHE:C	1:A:271:PHE:HD1	2.19	0.46	
1:A:39:PRO:HD3	2:B:143:TYR:CZ	2.52	0.44	
1:A:106:LYS:HE2	1:A:217:LYS:HE3	1.99	0.44	
1:A:155:SER:HB3	1:A:165:VAL:HG22	1.98	0.44	
2:B:94:ARG:HE	2:B:96:ARG:HH22	1.64	0.44	
1:A:244:LEU:N	1:A:248:GLN:O	2.51	0.43	
1:A:122:ASN:ND2	1:A:124:THR:OG1	2.51	0.43	
2:B:55:ARG:HG2	2:B:57:SER:O	2.19	0.43	
1:A:115:GLU:OE2	2:B:58:LYS:HB3	2.19	0.43	
1:A:225:PHE:CE2	1:A:230:ILE:HD13	2.53	0.43	
1:A:143:VAL:HG22	1:A:187:TYR:HE1	1.83	0.42	
1:A:296:VAL:HG11	1:A:301:THR:OG1	2.20	0.42	
1:A:208:LEU:HD12	1:A:225:PHE:HE1	1.84	0.42	
1:A:41:ALA:O	1:A:80:LYS:NZ	2.51	0.41	
1:A:253:TRP:CE2	1:A:299:THR:HA	2.56	0.41	
2:B:82:PHE:CE1	2:B:84:PRO:HG3	2.55	0.41	
1:A:274:ILE:HA	1:A:310:VAL:HA	2.02	0.40	



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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:GLN:OE1	5:A:406:HOH:O	2.22	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	А	286/344~(83%)	273~(96%)	13~(4%)	0	100 100
2	В	112/265~(42%)	110 (98%)	2(2%)	0	100 100
All	All	398/609~(65%)	383~(96%)	15 (4%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Rotameric Outliers	
1	А	244/315~(78%)	236~(97%)	8 (3%)	38 37
2	В	102/230~(44%)	101~(99%)	1 (1%)	76 81
All	All	346/545~(64%)	337~(97%)	9(3%)	46 47

All (9) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	А	40	ASP
1	А	99	HIS
1	А	122	ASN
1	А	224	SER
1	А	257	ASP
1	А	265	TYR
1	А	297	GLU
1	А	319	TYR
2	В	109	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	122	ASN
1	А	192	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)

4 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	Tinle	Bo	ond leng	$_{\rm ths}$	B	ond ang	les
MOI	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	C	1	1,3	14,14,15	0.53	0	17,19,21	0.45	0
3	NAG	С	2	3	14,14,15	0.21	0	17,19,21	0.40	0
3	BMA	С	3	3	11,11,12	0.45	0	15,15,17	0.76	0
3	MAN	С	4	3	11,11,12	0.76	0	$15,\!15,\!17$	0.94	1 (6%)



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
3	NAG	С	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	С	2	3	-	2/6/23/26	0/1/1/1
3	BMA	С	3	3	-	2/2/19/22	0/1/1/1
3	MAN	С	4	3	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	C	4	MAN	O2-C2-C3	-2.21	105.70	110.14

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	С	4	MAN	O5-C5-C6-O6
3	С	2	NAG	C4-C5-C6-O6
3	С	2	NAG	O5-C5-C6-O6
3	С	4	MAN	C4-C5-C6-O6
3	С	3	BMA	C4-C5-C6-O6
3	С	3	BMA	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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)

1 ligand is 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	Mol Type Chain Res		Link	Bond lengths			Bond angles			
	Type	Ullalli	nes	LIUK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	В	301	2	14,14,15	0.31	0	17,19,21	0.47	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
4	NAG	В	301	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.



There are no bond angle outliers. There are no chirality outliers. There are no torsion outliers. There are no ring outliers. No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ $>$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	292/344~(84%)	1.78	75~(25%) 0 0	30, 63, 151, 220	0
2	В	114/265~(43%)	1.11	15 (13%) 3 4	28, 43, 111, 134	0
All	All	406/609~(66%)	1.59	90 (22%) 0 0	28, 57, 139, 220	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	306	LYS	16.8
1	А	310	VAL	12.3
1	А	241	MET	11.1
1	А	242	LYS	9.0
1	А	305	CYS	8.1
1	А	303	VAL	7.9
1	А	329	VAL	7.8
1	А	161	ASP	7.7
1	А	244	LEU	7.7
1	А	311	CYS	7.5
1	А	251	VAL	7.0
1	А	301	THR	6.3
1	А	289	ASN	6.0
1	А	274	ILE	6.0
1	А	239	LEU	5.9
1	А	249	VAL	5.9
1	А	272	VAL	5.8
1	А	304	GLN	5.8
1	А	288	CYS	5.6
1	A	294	PHE	5.4
1	A	300	SER	5.4
2	В	91	GLY	5.2
1	A	250	GLU	5.1
2	В	89	HIS	5.1



Mol	Chain	Res	Type	RSRZ
2	В	88	THR	5.0
1	А	307	GLY	4.8
1	А	308	GLY	4.8
1	А	238	ASN	4.7
1	А	330	PRO	4.7
1	А	299	THR	4.6
2	В	87	HIS	4.6
1	А	328	CYS	4.6
1	А	295	LEU	4.5
1	А	297	GLU	4.4
1	А	164	ALA	4.4
1	А	195	VAL	4.4
1	А	287	GLY	4.3
1	А	331	CYS	4.3
2	В	70	PRO	4.2
1	А	327	ALA	4.1
1	А	296	VAL	3.9
1	А	253	TRP	3.8
1	А	240	GLN	3.8
1	А	248	GLN	3.7
1	А	309	ASN	3.7
1	A	326	TRP	3.6
1	A	203	THR	3.6
1	А	275	GLN	3.5
1	A	48	LEU	3.5
1	A	318	TYR	3.5
1	A	252	SER	3.4
1	A	292	GLY	3.4
1	A	257	ASP	3.3
2	В	86	ASN	3.3
1	A	236	PRO	3.1
1	A	194	ASP	3.0
1	A	204	LEU	3.0
1	A	270	PHE	2.9
1	A	245	LYS	2.9
1	A	293	ALA	2.9
1	A	199	THR	2.9
1	A	179	LEU	2.9
1	A	271	PHE	2.8
1	A	291	LYS	2.8
2	В	71	GLU	2.8
1	A	243	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
2	В	90	THR	2.8
1	А	273	ARG	2.8
2	В	92	GLN	2.7
2	В	73	ASN	2.7
1	А	198	PRO	2.6
1	А	197	SER	2.5
1	А	255	TYR	2.5
1	А	165	VAL	2.5
1	А	180	ASP	2.4
1	А	184	TYR	2.4
2	В	128	LEU	2.4
2	В	159	GLN	2.4
1	А	139	CYS	2.3
1	А	143	VAL	2.3
2	В	63	CYS	2.3
2	В	132	THR	2.2
1	А	99	HIS	2.2
1	А	312	VAL	2.2
1	А	68	VAL	2.2
1	А	210	LEU	2.2
1	А	189	VAL	2.1
1	А	147[A]	MET	2.1
1	А	208	LEU	2.1
2	В	116	VAL	2.1

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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
3	MAN	С	4	11/12	0.52	0.25	64,93,100,103	0
3	BMA	С	3	11/12	0.82	0.18	56,74,86,90	0
3	NAG	С	1	14/15	0.90	0.17	36,42,57,60	0
3	NAG	С	2	14/15	0.95	0.13	39,49,58,63	0



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



6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
4	NAG	В	301	14/15	0.94	0.17	29,35,42,44	0

6.5 Other polymers (i)

There are no such residues in this entry.

