

wwPDB X-ray Structure Validation Summary Report (i)

Aug 8, 2020 - 09:56 AM BST

PDB ID	:	3VQQ
Title	:	HIV-1 integrase core domain in complex with 2,1,3-benzothiadiazol-4-amine
Authors	:	Wielens, J.; Chalmers, D.K.; Parker, M.W.; Scanlon, M.J.
Deposited on	:	2012-03-29
Resolution	:	2.00 Å(reported)

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

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

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

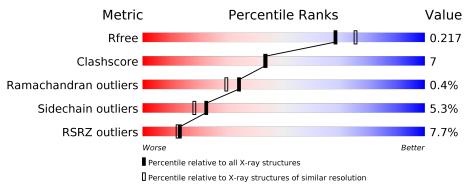
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
$\rm CCP4$:	$7.0.044 (\mathrm{Gargrove})$
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.00 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain	
1	А	158	8%	13% <mark>•</mark> 9%
1	В	158	6% 70%	16% • 11%
2	С	2	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
4	SO4	В	303	-	-	Х	-



$\mathbf{2}$ Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 2330 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	Ī
1	Δ	144	Total	С	Ν	Ο	S	0	0	Ī
1	А	144	1106	703	193	206	4	0	0	
1	D	140	Total	С	Ν	Ο	S	0	0	Γ
1	D	140	1079	670	190	200	4	0		

679

• Molecule 1 is a protein called POL polyprotein.

1072

There are 8 discrepancies between the modelled and reference sequences:

189

200 - 4

Chain	Residue	Modelled	Actual	Comment	Reference
A	56	SER	CYS	engineered mutation	UNP Q72498
A	131	ASP	TRP	engineered mutation	UNP Q72498
А	139	ASP	PHE	engineered mutation	UNP Q72498
А	185	HIS	PHE	engineered mutation	UNP Q72498
В	56	SER	CYS	engineered mutation	UNP Q72498
В	131	ASP	TRP	engineered mutation	UNP Q72498
В	139	ASP	PHE	engineered mutation	UNP Q72498
В	185	HIS	PHE	engineered mutation	UNP Q72498

• Molecule 2 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.



Mol	Chain	Residues	At	\mathbf{oms}		ZeroOcc	AltConf	Trace
2	С	2	Total 23	C 12	0 11	0	0	0

• Molecule 3 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Ator	ns	ZeroOcc	AltConf
3	В	2	Total 2	$\begin{array}{c} \mathrm{Cd} \\ 2 \end{array}$	0	0
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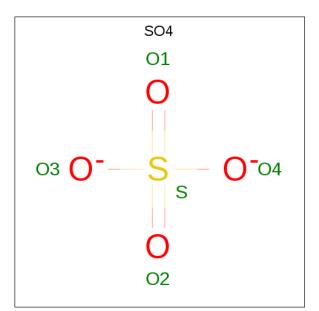
Trace

0

0

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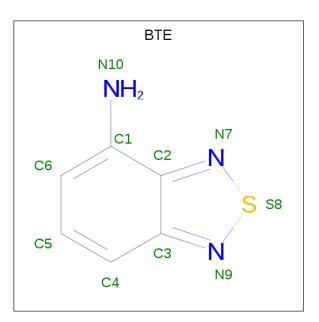
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	2	Total Cd 2 2	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 5 is 2,1,3-benzothiadiazol-4-amine (three-letter code: BTE) (formula: $C_6H_5N_3S$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	$\begin{array}{cccc} \mathrm{Total} & \mathrm{C} & \mathrm{N} & \mathrm{S} \\ 10 & 6 & 3 & 1 \end{array}$	0	0
5	А	1	$\begin{array}{cccc} \text{Total} & \text{C} & \text{N} & \text{S} \\ 10 & 6 & 3 & 1 \end{array}$	0	0

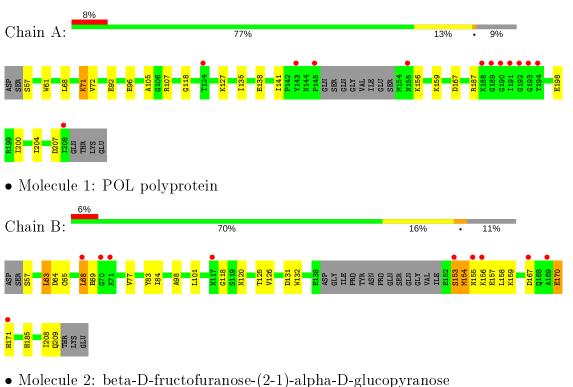
• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	60	Total O 60 60	0	0
6	В	35	$\begin{array}{cc} {\rm Total} & {\rm O} \\ 35 & 35 \end{array}$	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: POL polyprotein

Chain C:

100%

GLC1 FRU2



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	60.40Å 61.68 Å 81.89 Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.18 - 2.00	Depositor
Resolution (A)	38.18 - 2.00	EDS
% Data completeness	99.6 (38.18-2.00)	Depositor
(in resolution range)	99.6 (38.18 - 2.00)	EDS
R _{merge}	0.10	Depositor
R _{sym}	0.10	Depositor
$< I/\sigma(I) > 1$	$3.53 (at 2.00 \text{\AA})$	Xtriage
Refinement program	REFMAC $5.6.0117$	Depositor
R, R_{free}	0.180 , 0.220	Depositor
Λ, Λ_{free}	0.180 , 0.217	DCC
R_{free} test set	1090 reflections (5.14%)	wwPDB-VP
Wilson B-factor $(Å^2)$	24.7	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.39 , 51.9	EDS
L-test for twinning ²	$< L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	0.027 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2330	wwPDB-VP
Average B, all atoms $(Å^2)$	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.11% 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: BTE, GLC, SO4, FRU, CD

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	Bo	nd lengths	Bond angles	
Mol	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	1.12	2/1128~(0.2%)	0.99	4/1528~(0.3%)
1	В	1.16	2/1091~(0.2%)	1.01	2/1475~(0.1%)
All	All	1.14	4/2219~(0.2%)	1.00	6/3003~(0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
1	А	61	TRP	CD2-CE2	6.46	1.49	1.41
1	А	96	GLU	CD-OE2	-5.99	1.19	1.25
1	В	83	TYR	CG-CD2	5.15	1.45	1.39
1	В	132	TRP	CD2-CE2	5.10	1.47	1.41

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$\mathbf{Ideal}(^{o})$
1	В	131	ASP	CB-CG-OD2	6.65	124.29	118.30
1	А	167	ASP	CB-CG-OD1	6.25	123.92	118.30
1	А	187	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	А	207	ASP	CB-CG-OD1	5.34	123.10	118.30
1	В	101	LEU	CB-CG-CD2	-5.33	101.95	111.00

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	1106	0	1107	11	0
1	В	1072	0	1075	21	0
2	С	23	0	21	0	0
3	А	2	0	0	0	0
3	В	2	0	0	0	0
4	А	5	0	0	0	0
4	В	5	0	0	2	0
5	А	20	0	10	1	0
6	А	60	0	0	3	0
6	В	35	0	0	2	0
All	All	2330	0	2213	30	0

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

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.

The worst 5 of 30 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:GLU:HG2	1:B:171:HIS:CD2	2.19	0.77
1:B:65:CYS:SG	6:B:425:HOH:O	2.53	0.67
1:B:154:MET:HA	1:B:157:GLU:HB3	1.79	0.65
1:A:68:LEU:HD13	1:A:159:LYS:HE2	1.79	0.64
1:B:84:ILE:HD13	1:B:158:LEU:HD13	1.79	0.63

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	140/158~(89%)	138~(99%)	2(1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	В	136/158~(86%)	134~(98%)	1 (1%)	1 (1%)	22 16
All	All	276/316 (87%)	272 (99%)	3 (1%)	1 (0%)	34 30

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	69	GLU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	116/129~(90%)	112~(97%)	4(3%)	37 36
1	В	112/129~(87%)	104~(93%)	8 (7%)	14 10
All	All	228/258~(88%)	216~(95%)	12~(5%)	22 18

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	63	LEU
1	В	68	LEU
1	В	167	ASP
1	В	57	SER
1	В	154	MET

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

Mol	Chain	Res	Type
1	В	209	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)

2 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).

Γ	Mal	True	Chain	Res	Link	Bond lengths			B	ond ang	les
	IVIOI	Type	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
	2	GLC	С	1	2	11, 11, 12	1.40	2 (18%)	$15,\!15,\!17$	1.12	1 (6%)
	2	FRU	С	2	2	11,12,12	1.27	1 (9%)	$10,\!18,\!18$	2.39	3 (30%)

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	GLC	С	1	2	-	0/2/19/22	0/1/1/1
2	FRU	С	2	2	-	3/5/24/24	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
2	С	2	FRU	O5-C2	-2.85	1.38	1.43
2	С	1	GLC	O5-C5	-2.72	1.38	1.43
2	С	1	GLC	O5-C1	-2.71	1.39	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	С	2	FRU	O2-C2-O5	-4.49	100.83	109.50
2	С	2	FRU	C6-C5-C4	-3.73	106.09	115.09
2	С	2	FRU	O1-C1-C2	3.67	119.67	111.86

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	С	1	GLC	C1-O5-C5	2.89	116.11	112.19

There are no chirality outliers.

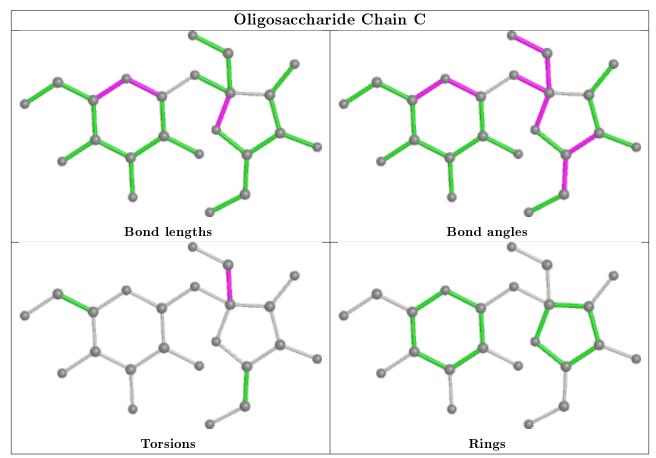
All (3) torsion outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms
2	С	2	FRU	O1-C1-C2-C3
2	С	2	FRU	O1-C1-C2-O5
2	С	2	FRU	O1-C1-C2-O2

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)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.



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	Type	Chain	Res	Link	Bo	Bond lengths			Bond angles		
	туре	Cham	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2	
5	BTE	А	305	-	11,11,11	1.50	1 (9%)	8,15,15	2.42	4 (50%)	
5	BTE	А	306	-	11,11,11	1.72	4 (36%)	8,15,15	<mark>5.38</mark>	<mark>6 (75%)</mark>	
4	SO4	А	303	-	4,4,4	1.06	0	$6,\!6,\!6$	1.23	0	
4	SO4	В	303	-	4,4,4	0.39	0	$6,\!6,\!6$	0.50	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
5	BTE	А	305	-	-	-	0/2/2/2
5	BTE	А	306	-	-	-	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
5	А	305	BTE	C2-C3	3.11	1.53	1.42
5	А	306	BTE	C1-C2	-3.09	1.37	1.42
5	А	306	BTE	S8-N9	2.51	1.73	1.65
5	А	306	BTE	C2-C3	2.31	1.50	1.42
5	А	306	BTE	C5-C6	2.20	1.43	1.38

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
5	А	306	BTE	C6-C1-N10	9.43	139.21	120.36
5	А	306	BTE	C2-N7-S8	-6.67	98.97	104.97
5	А	306	BTE	C2-C1-N10	-6.66	105.36	118.07
5	А	306	BTE	C5-C6-C1	4.84	130.51	121.19
5	А	306	BTE	C4-C5-C6	-4.55	113.73	120.99

There are no chirality outliers.

There are no torsion outliers.



There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	А	305	BTE	1	0
4	В	303	SO4	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ $>$	#RSRZ >2		$\mathbf{OWAB}(\mathrm{\AA}^2)$	$\mathbf{Q}{<}0.9$
1	А	144/158~(91%)	0.14	12 (8%) 11	10	14, 22, 49, 65	1 (0%)
1	В	140/158~(88%)	0.22	10 (7%) 16	15	13, 22, 53, 78	0
All	All	284/316~(89%)	0.18	22 (7%) 13	12	13, 22, 50, 78	1 (0%)

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	189	GLY	7.3
1	А	190	GLY	4.3
1	А	143	TYR	3.9
1	В	117	ASN	3.4
1	А	191	ILE	3.2

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

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

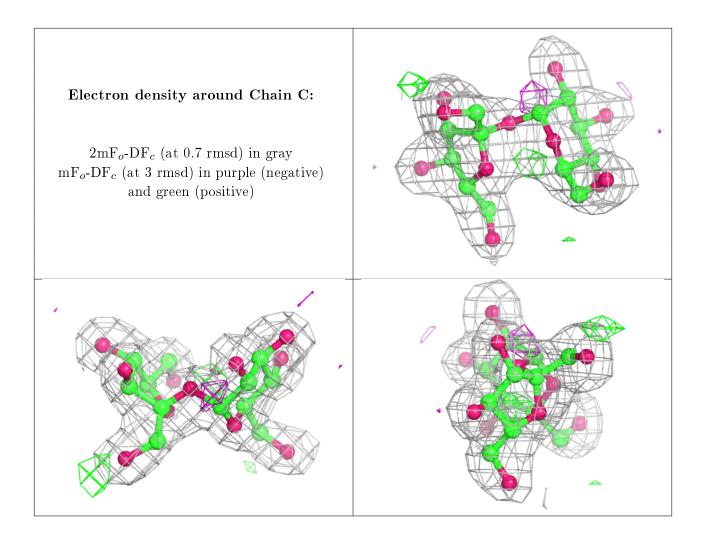
6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
2	GLC	С	1	11/12	0.92	0.13	$22,\!27,\!29,\!32$	0
2	FRU	С	2	12/12	0.93	0.10	$21,\!27,\!33,\!34$	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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	$Q{<}0.9$
4	SO4	А	303	5/5	0.83	0.22	$30,\!38,\!39,\!42$	0
4	SO4	В	303	5/5	0.86	0.28	$71,\!78,\!80,\!87$	0
5	BTE	А	306	10/10	0.87	0.17	$19,\!26,\!35,\!42$	0
5	BTE	А	305	10/10	0.95	0.13	$25,\!27,\!29,\!32$	0
3	CD	В	302	1/1	0.99	0.03	$43,\!43,\!43,\!43$	0
3	CD	А	302	1/1	0.99	0.06	27,27,27,27	0
3	CD	В	301	1/1	1.00	0.03	$38,\!38,\!38,\!38$	0
3	CD	А	301	1/1	1.00	0.07	$19,\!19,\!19,\!19$	1



6.5 Other polymers (i)

There are no such residues in this entry.

