

# Full wwPDB X-ray Structure Validation Report (i)

#### Sep 17, 2023 – 02:04 PM EDT

PDB ID	:	4XT3
Title	:	Structure of a viral GPCR bound to human chemokine CX3CL1
Authors	:	Burg, J.S.; Jude, K.M.; Waghray, D.; Garcia, K.C.
Deposited on		
Resolution	:	3.80  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:

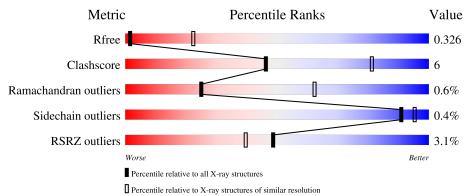
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

# 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 3.80 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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 c	hain	
1	А	362	% • 68%	11%	20%
2	В	91	62%	14%	24%
3	С	3	67%		33%



## 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 2774 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 G-protein coupled receptor homolog US28.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	А	288	Total 2243	C 1511	N 338	O 375	S 19	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	ASP	-	expression tag	UNP P69332
А	-6	TYR	-	expression tag	UNP P69332
А	-5	LYS	-	expression tag	UNP P69332
А	-4	ASP	-	expression tag	UNP P69332
А	-3	ASP	-	expression tag	UNP P69332
А	-2	ASP	-	expression tag	UNP P69332
А	-1	ASP	-	expression tag	UNP P69332
А	0	ALA	-	expression tag	UNP P69332

• Molecule 2 is a protein called Fractalkine.

Mol	Chain	Residues		Atc	$\mathbf{ms}$			ZeroOcc	AltConf	Trace
2	В	69	Total 475	C 294	N 83	O 93	${ m S}{ m 5}$	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Residue	Modelled	Actual	Comment	Reference
78	SER	-	expression tag	UNP P78423
79	GLY	-	expression tag	UNP P78423
80	SER	-	expression tag	UNP P78423
81	GLY	-	expression tag	UNP P78423
82	SER	-	expression tag	UNP P78423
83	ALA	-	expression tag	UNP P78423
84	ALA	-	expression tag	UNP P78423
85	ALA	-	expression tag	UNP P78423
	78 79 80 81 82 83 83 84	78         SER           79         GLY           80         SER           81         GLY           82         SER           83         ALA           84         ALA	78         SER         -           79         GLY         -           80         SER         -           81         GLY         -           82         SER         -           83         ALA         -           84         ALA         -	78SER-expression tag79GLY-expression tag80SER-expression tag81GLY-expression tag82SER-expression tag83ALA-expression tag84ALA-expression tag

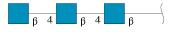
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Chain	Residue	Modelled	Actual	Comment	Reference
В	86	LEU	-	expression tag	UNP P78423
В	87	GLU	-	expression tag	UNP P78423
В	88	VAL	-	expression tag	UNP P78423
В	89	LEU	-	expression tag	UNP P78423
В	90	PHE	-	expression tag	UNP P78423
В	91	GLN	-	expression tag	UNP P78423

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• Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.

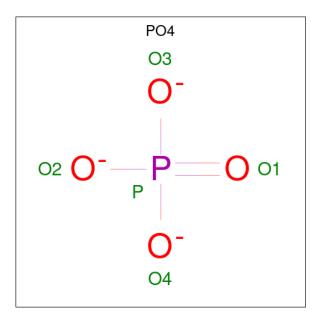


Mol	Chain	Residues	Aton	ns	ZeroOcc	AltConf	Trace
3	С	3	$\begin{array}{cc} \text{Total} & \text{C} \\ 42 & 24 \end{array}$	N O 3 15	0	0	0

• Molecule 4 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	Total C 9 9	0	0

• Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



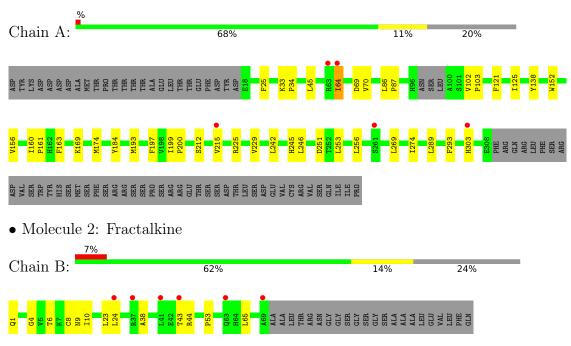


Mo	bl	Chain	Residues	Atoms			ZeroOcc	AltConf
5		А	1	Total 5	0 4	Р 1	0	0



# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.



• Molecule 1: G-protein coupled receptor homolog US28

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

Chain C:	67%	33%

NAG1 NAG2 NAG3



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	59.90Å 192.70Å 94.40Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	48.92 - 3.80	Depositor
Resolution (A)	48.92 - 3.62	EDS
% Data completeness	84.9 (48.92-3.80)	Depositor
(in resolution range)	$67.4 \ (48.92 - 3.62)$	EDS
R <sub>merge</sub>	0.28	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.57 (at 3.57 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1839)	Depositor
D D.	0.283 , $0.322$	Depositor
$R, R_{free}$	0.284 , $0.326$	DCC
$R_{free}$ test set	506 reflections $(10.02\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	77.0	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.29, $50.4$	EDS
L-test for twinning <sup>2</sup>	$< L >=0.47, < L^2>=0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	2774	wwPDB-VP
Average B, all atoms $(Å^2)$	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.43% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities 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: PO4, UNL, PCA, NAG

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).

Mol	Chain	Bond	lengths	Bond angles		
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.26	0/2306	0.42	0/3159	
2	В	0.22	0/476	0.41	0/656	
All	All	0.25	0/2782	0.42	0/3815	

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	2243	0	2212	25	0
2	В	475	0	395	10	0
3	С	42	0	37	2	0
4	А	9	0	0	0	0
5	А	5	0	0	0	0
All	All	2774	0	2644	34	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 6.

All (34) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	Interatomic distance (Å)	Clash
1:A:199:ILE:HG13	1:A:200:PRO:HD3	1.67	<b>overlap</b> (Å) 0.76
2:B:10:ILE:HD11			
-	3:C:1:NAG:H82	1.74	0.69
1:A:289:LEU:HA	1:A:293:PHE:HB3	1.77	0.65
1:A:161:PRO:O	1:A:184:TYR:OH	2.20	0.56
1:A:64:ILE:HG23	1:A:69:ASP:HB2	1.88	0.56
1:A:138:TYR:HE1	1:A:303:HIS:NE2	2.05	0.55
2:B:6:THR:HG22	2:B:8:CYS:H	1.71	0.55
1:A:102:VAL:HG12	1:A:103:PRO:HD2	1.88	0.55
2:B:23:LEU:O	2:B:44:ARG:N	2.41	0.53
1:A:251:ASP:HA	1:A:269:LEU:HD21	1.92	0.51
2:B:24:LEU:HA	2:B:43:THR:HA	1.93	0.50
1:A:197:PHE:HB2	1:A:245:HIS:CE1	2.46	0.49
1:A:64:ILE:HD13	1:A:70:VAL:HG22	1.93	0.49
1:A:274:ILE:HG23	2:B:4:GLY:HA2	1.95	0.48
2:B:9:ASN:OD1	2:B:9:ASN:N	2.45	0.48
2:B:38:ALA:HA	2:B:53:PRO:HD3	1.97	0.46
1:A:212:SER:HA	1:A:215:VAL:HG12	1.96	0.46
1:A:138:TYR:HE1	1:A:303:HIS:HE2	1.63	0.46
1:A:225:ARG:O	1:A:229:VAL:HG23	2.16	0.46
1:A:169:LYS:HB3	1:A:174:MET:HG2	1.99	0.45
2:B:24:LEU:HD23	2:B:43:THR:HG22	1.98	0.45
1:A:242:LEU:O	1:A:246:LEU:HB2	2.17	0.45
1:A:25:PHE:HB2	2:B:9:ASN:HA	1.99	0.44
1:A:193:MET:HA	1:A:245:HIS:HD2	1.82	0.43
3:C:2:NAG:H62	3:C:3:NAG:O7	2.19	0.43
1:A:152:TRP:O	1:A:156:VAL:HG23	2.19	0.42
1:A:121:PHE:O	1:A:125:ILE:HG13	2.19	0.42
1:A:256:LEU:HD12	1:A:256:LEU:HA	1.93	0.42
1:A:197:PHE:C	1:A:200:PRO:HD2	2.40	0.42
1:A:246:LEU:HD12	1:A:246:LEU:HA	1.92	0.41
1:A:160:ILE:HD13	1:A:163:PHE:CZ	2.56	0.41
2:B:24:LEU:HB2	2:B:65:LEU:HD21	2.03	0.41
1:A:33:LYS:HB3	1:A:34:PRO:HD3	2.02	0.41
1:A:86:LEU:N	1:A:87:PRO:HD2	2.36	0.41

There are no symmetry-related clashes.



 $4 \mathrm{XT3}$ 



## 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	Perce	entiles
1	А	284/362~(78%)	271 (95%)	11 (4%)	2(1%)	22	60
2	В	67/91~(74%)	64 (96%)	3~(4%)	0	100	100
All	All	351/453~(78%)	335~(95%)	14 (4%)	2(1%)	25	62

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	45	LEU
1	А	64	ILE

#### 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	237/334~(71%)	236 (100%)	1 (0%)	91 95
2	В	42/73~(58%)	42 (100%)	0	100 100
All	All	279/407~(69%)	278 (100%)	1 (0%)	91 95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	253	LEU

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



Mol	Chain	Res	Type
1	А	245	HIS

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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).

ſ	Mol	Type	e Chain Res	Dog	Link	B	ond leng	gths	В	ond ang	gles
	WIOI	туре		nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
	2	PCA	В	1	2	7,8,9	1.81	1 (14%)	9,10,12	2.24	<mark>5 (55%)</mark>

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	PCA	В	1	2	-	0/0/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
2	В	1	PCA	CD-N	4.69	1.47	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	В	1	PCA	CB-CA-C	-3.19	108.31	112.70
2	В	1	PCA	OE-CD-CG	-3.06	121.42	126.76
2	В	1	PCA	CA-N-CD	-2.91	103.61	113.58
2	В	1	PCA	CB-CA-N	2.63	110.85	103.30

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	1	PCA	CG-CD-N	2.44	114.71	108.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 5.5 Carbohydrates (i)

3 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	Turne	Chain	Res	Tiple	Bo	ond leng	ths	В	ond ang	les
MOI	Type	Chain	nes	Link	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
3	NAG	С	1	3,2	14,14,15	0.37	0	$17,\!19,\!21$	1.21	2 (11%)
3	NAG	С	2	3	14,14,15	0.58	0	17,19,21	0.71	0
3	NAG	С	3	3	14,14,15	0.64	0	17,19,21	0.61	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
3	NAG	С	1	3,2	-	1/6/23/26	0/1/1/1
3	NAG	С	2	3	-	2/6/23/26	0/1/1/1
3	NAG	С	3	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
3	С	1	NAG	C1-O5-C5	4.08	117.72	112.19
3	С	1	NAG	O4-C4-C5	2.09	114.49	109.30

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

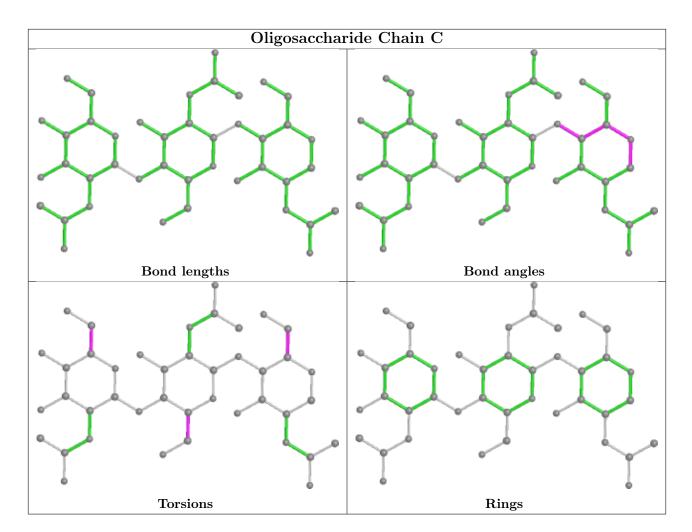
There are no ring outliers.

3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	С	3	NAG	1	0
3	С	2	NAG	1	0
3	С	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)

Of 2 ligands modelled in this entry, 1 is unknown - leaving 1 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	Aol Type Chain Res		Res Link		B	ond leng	$\operatorname{gths}$	Bond angles		
NIOI	туре	Ullalli	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
5	PO4	А	402	-	4,4,4	0.99	0	$6,\!6,\!6$	0.43	0

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	$\langle RSRZ \rangle$	# <b>RS</b>	#RSRZ>2		$OWAB(Å^2)$	Q < 0.9
1	А	288/362~(79%)	-0.16	5 (1%)	70	62	50, 83, 133, 154	0
2	В	68/91~(74%)	0.62	6 (8%)	10	8	70, 126, 147, 155	0
All	All	356/453~(78%)	-0.02	11 (3%)	49	40	50, 92, 139, 155	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	24	LEU	4.1
1	А	64	ILE	3.3
2	В	37	ARG	3.2
2	В	41	LEU	3.1
2	В	69	ALA	2.9
2	В	43	THR	2.2
1	А	63	ARG	2.2
1	А	261	SER	2.2
2	В	63	GLN	2.2
1	А	215	VAL	2.0
1	А	303	HIS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains (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
2	PCA	В	1	8/9	0.85	0.31	$95,\!105,\!109,\!128$	0

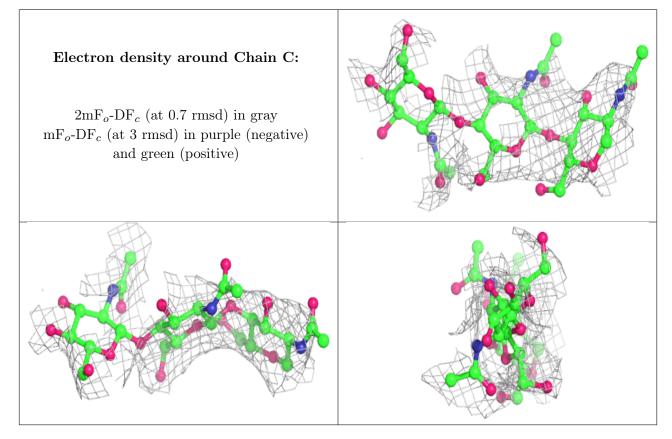


### 6.3 Carbohydrates (i)

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	NAG	С	3	14/15	0.54	0.27	$128,\!153,\!161,\!162$	0
3	NAG	С	2	14/15	0.73	0.34	118,155,161,164	0
3	NAG	С	1	14/15	0.85	0.45	101,127,146,158	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	$B-factors(Å^2)$	Q < 0.9
5	PO4	А	402	5/5	0.53	0.38	137,150,162,169	5
4	UNL	А	401	9/-	0.81	0.35	46,48,61,66	0

## 6.5 Other polymers (i)

There are no such residues in this entry.

