



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 27, 2017 – 05:42 AM EDT

PDB ID : 1FQ7  
Title : X-RAY STRUCTURE OF INHIBITOR CP-72,647 BOUND TO SACCHAROPEPSIN  
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Deposited on : unknown  
Resolution : 2.80 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

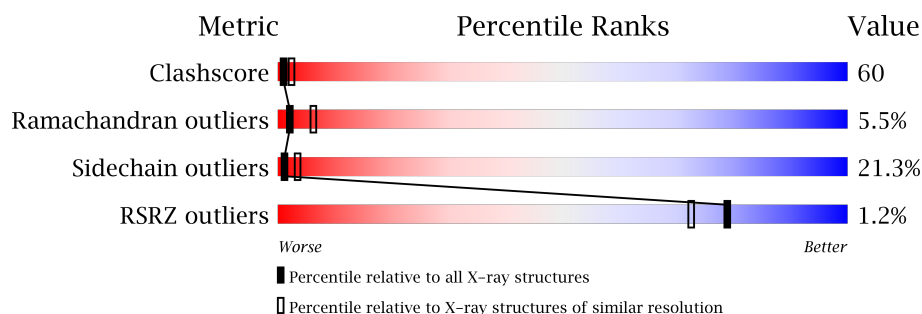
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . 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	A	329	

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 2717 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.

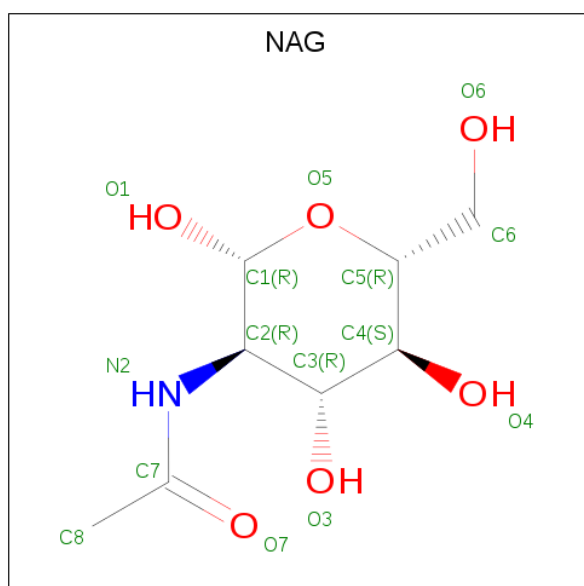
- Molecule 1 is a protein called SACCHAROPEPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	0	0
			2528	1618	396	508	6			

There is a discrepancy between the modelled and reference sequences:

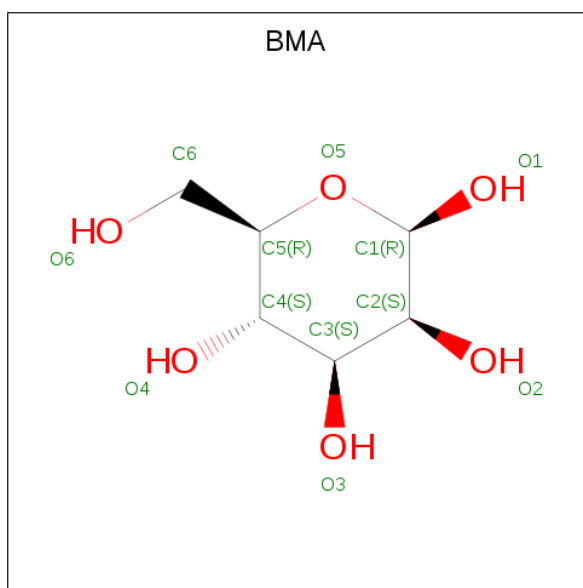
Chain	Residue	Modelled	Actual	Comment	Reference
A	315	ILE	LEU	CONFLICT	UNP P07267

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



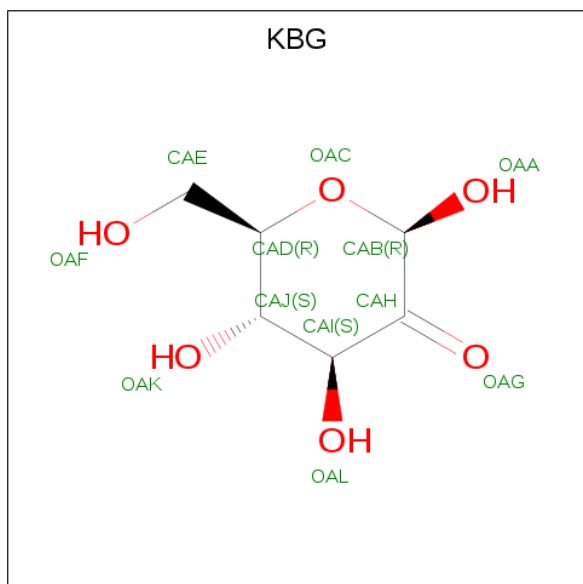
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is BETA-D-MANNOSE (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).



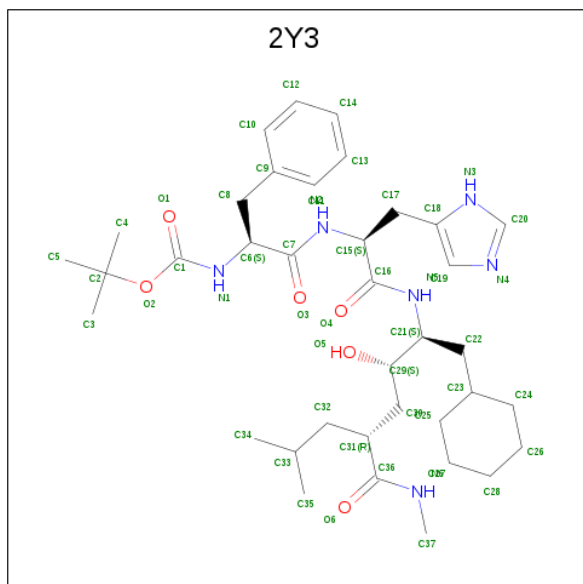
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is 2-KETO-BETA-D-GLUCOSE (three-letter code: KBG) (formula:  $C_6H_{10}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is N-(tert-butoxycarbonyl)-L-phenylalanyl-N-[(2S,3S,5R)-1-cyclohexyl-3-hydroxy-7-methyl-5-(methylcarbamoyl)octan-2-yl]-L-histidinamide (three-letter code: 2Y3) (formula: C<sub>37</sub>H<sub>58</sub>N<sub>6</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			49	37	6	6		

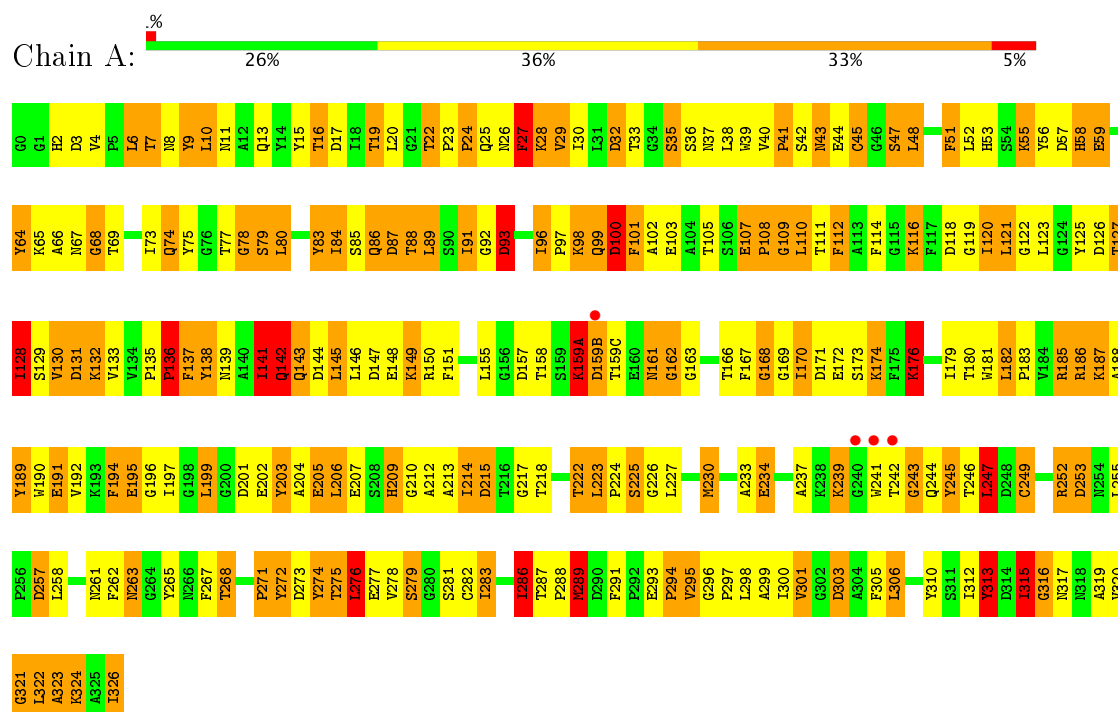
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	65	Total	O	0	0
			65	65		

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 ( $\text{RSRZ} > 2$ ). 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: SACCHAROPEPSIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.43Å 86.43Å 109.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.30 – 2.80 27.40 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (28.30-2.80) 94.5 (27.40-2.80)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.84 (at 2.80Å)	Xtriage
Refinement program	RESTRAIN	Depositor
R, $R_{free}$	0.190 , 0.270 0.187 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	53.4	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 100.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	2717	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.66% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<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.

## 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: KBG, BMA, 2Y3, 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	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.06	1/2592 (0.0%)	2.44	178/3526 (5.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	3	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	289	MET	SD-CE	5.07	2.06	1.77

The worst 5 of 178 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	ARG	NE-CZ-NH1	-18.10	111.25	120.30
1	A	101	PHE	CB-CG-CD1	-13.58	111.29	120.80
1	A	133	VAL	CA-CB-CG2	13.52	131.18	110.90
1	A	185	ARG	NE-CZ-NH2	13.15	126.87	120.30
1	A	201	ASP	CB-CG-OD2	-13.01	106.60	118.30

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	88	THR	CA
1	A	161	ASN	CA
1	A	315	ILE	CB



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	A	2528	0	2401	301	0
2	A	42	0	37	1	0
3	A	22	0	18	2	0
4	A	11	0	7	0	0
5	A	49	0	58	17	0
6	A	65	0	0	10	0
All	All	2717	0	2521	309	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 60.

The worst 5 of 309 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:A:289:MET:SD	1:A:289:MET:CE	2.06	1.42
1:A:242:THR:HG22	1:A:242:THR:O	1.41	1.15
1:A:287:THR:HG23	1:A:288:PRO:HD2	1.24	1.14
1:A:84:ILE:HG22	1:A:85:SER:H	1.09	1.12
1:A:84:ILE:CG2	1:A:85:SER:H	1.62	1.10

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	A	327/329 (99%)	278 (85%)	31 (10%)	18 (6%)	<b>2</b> <b>6</b>

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	ASP
1	A	188	ALA
1	A	24	PRO
1	A	44	GLU
1	A	59	GLU

### 5.3.2 Protein sidechains ⓘ

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	A	268/268 (100%)	211 (79%)	57 (21%)	<b>1</b> <b>3</b>

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	LYS
1	A	170	ILE
1	A	313	TYR
1	A	141	ILE
1	A	148	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	GLN
1	A	317	ASN
1	A	209	HIS
1	A	25	GLN
1	A	161	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

7 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	NAG	A	332	1,2	14,14,15	1.70	4 (28%)	15,19,21	3.17	4 (26%)
2	NAG	A	333	3,2	14,14,15	1.33	3 (21%)	15,19,21	2.30	6 (40%)
3	BMA	A	334	3,2	11,11,12	1.21	1 (9%)	13,15,17	3.96	4 (30%)
3	BMA	A	335	3,4	11,11,12	2.06	3 (27%)	13,15,17	2.78	6 (46%)
4	KBG	A	336	3	11,11,12	4.14	5 (45%)	11,15,17	1.89	3 (27%)
2	NAG	A	337	1	14,14,15	1.34	2 (14%)	15,19,21	3.32	5 (33%)
5	2Y3	A	400	-	47,51,51	1.16	3 (6%)	60,69,69	1.99	17 (28%)

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	A	332	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	333	3,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	A	334	3,2	-	0/2/19/22	0/1/1/1
3	BMA	A	335	3,4	-	0/2/19/22	0/1/1/1
4	KBG	A	336	3	-	0/2/19/22	0/1/1/1
2	NAG	A	337	1	-	0/6/23/26	0/1/1/1
5	2Y3	A	400	-	-	0/55/63/63	0/3/3/3

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	336	KBG	CAI-CAH	-4.87	1.44	1.52
4	A	336	KBG	CAB-CAH	-3.58	1.47	1.51
2	A	332	NAG	C1-C2	-3.37	1.47	1.52
5	A	400	2Y3	C17-C15	-2.77	1.47	1.54
5	A	400	2Y3	O2-C2	-2.00	1.44	1.48

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	332	NAG	C2-N2-C7	-10.05	108.28	122.94
2	A	337	NAG	O5-C1-C2	-9.32	98.51	111.47
3	A	335	BMA	O5-C1-C2	-5.79	101.72	110.79
2	A	337	NAG	C8-C7-N2	-5.73	105.76	116.11
3	A	335	BMA	C1-O5-C5	-5.40	104.72	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	332	NAG	1	0
3	A	334	BMA	1	0
3	A	335	BMA	2	0
5	A	400	2Y3	17	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	329/329 (100%)	-0.63	4 (1%) 79 72	6, 28, 56, 102	4 (1%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	242	THR	4.8
1	A	240	GLY	4.6
1	A	241	TRP	3.4
1	A	159(B)	ASP	2.8

### 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](#)

There are no carbohydrates in this entry.

### 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	A	332	14/15	0.93	0.17	1.88	20,43,71,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	2Y3	A	400	49/49	0.93	0.16	0.08	4,24,49,77	0
3	BMA	A	335	11/12	0.97	0.18	-	7,25,58,101	0
2	NAG	A	337	14/15	0.93	0.08	-	15,38,146,156	0
4	KBG	A	336	11/12	0.80	0.16	-	34,51,156,156	0
3	BMA	A	334	11/12	0.93	0.12	-	15,30,67,83	0
2	NAG	A	333	14/15	0.96	0.12	-	3,33,62,87	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.