

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

#### Jan 17, 2024 – 06:04 AM EST

PDB ID	:	8U1G
Title	:	Prefusion-stabilized SARS-CoV-2 S2 subunit
Authors	:	Hsieh, CL.; McLellan, J.S.
Deposited on	:	2023-08-31
Resolution	:	3.20  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 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
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 3.20 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	1133 (3.20-3.20)	
Clashscore	141614	1253 (3.20-3.20)	
Ramachandran outliers	138981	1234 (3.20-3.20)	
Sidechain outliers	138945	1233 (3.20-3.20)	
RSRZ outliers	127900	1095 (3.20-3.20)	

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	530	15%	69%	7%	23%	
1	В	530	12%	72%	•	24%	

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
2	NAG	В	1301	-	-	-	Х



## 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6244 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 Spike protein S2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	А	406	Total 3124	C 1988	N 525	O 594	S 17	0	0	0
1	В	403	Total 3106	C 1973	N 521	O 595	S 17	0	0	0

Chain	Residue	Modelled	Actual Comment		Reference
А	671	MET	-	initiating methionine	UNP P0DTC2
А	672	ARG	-	expression tag	UNP P0DTC2
А	673	PRO	-	expression tag	UNP P0DTC2
А	674	THR	-	expression tag	UNP P0DTC2
А	675	TRP	-	expression tag	UNP P0DTC2
А	676	ALA	-	expression tag	UNP P0DTC2
А	677	TRP	-	expression tag	UNP P0DTC2
A	678	TRP	-	expression tag	UNP P0DTC2
А	679	LEU	-	expression tag	UNP P0DTC2
А	680	PHE	-	expression tag	UNP P0DTC2
А	681	LEU	-	expression tag	UNP P0DTC2
A	682	VAL	-	expression tag	UNP P0DTC2
А	683	LEU	-	expression tag	UNP P0DTC2
А	684	LEU	-	expression tag	UNP P0DTC2
A	685	LEU	-	expression tag	UNP P0DTC2
А	686	ALA	-	expression tag	UNP P0DTC2
А	687	LEU	-	expression tag	UNP P0DTC2
А	688	TRP	-	expression tag	UNP P0DTC2
А	689	ALA	-	expression tag	UNP P0DTC2
А	690	PRO	-	expression tag	UNP P0DTC2
А	691	ALA	-	expression tag	UNP P0DTC2
А	692	ARG	-	expression tag	UNP P0DTC2
А	693	GLY	-	expression tag	UNP P0DTC2
А	694	ALA	-	expression tag	UNP P0DTC2
А	695	SER	-	expression tag	UNP P0DTC2

There are 188 discrepancies between the modelled and reference sequences:



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0	U	Т	G

Chain	Residue	Modelled	Actual	Comment	Reference
А	696	GLN	-	expression tag	UNP P0DTC2
А	704	CYS	SER	engineered mutation	UNP P0DTC2
А	790	CYS	LYS	engineered mutation	UNP P0DTC2
А	817	PRO	PHE	engineered mutation	UNP P0DTC2
А	892	PRO	ALA	engineered mutation	UNP P0DTC2
А	899	PRO	ALA	engineered mutation	UNP P0DTC2
А	942	PRO	ALA	engineered mutation	UNP P0DTC2
А	957	GLU	GLN	engineered mutation	UNP P0DTC2
А	986	PRO	LYS	engineered mutation	UNP P0DTC2
А	987	PRO	VAL	engineered mutation	UNP P0DTC2
А	1142	GLY	-	expression tag	UNP P0DTC2
А	1143	SER	-	expression tag	UNP P0DTC2
А	1144	GLY	-	expression tag	UNP P0DTC2
А	1145	TYR	-	expression tag	UNP P0DTC2
А	1146	ILE	-	expression tag	UNP P0DTC2
А	1147	PRO	-	expression tag	UNP P0DTC2
A	1148	GLU	-	expression tag	UNP P0DTC2
A	1149	ALA	-	expression tag	UNP P0DTC2
A	1150	PRO	-	expression tag	UNP P0DTC2
A	1151	ARG	-	expression tag	UNP P0DTC2
A	1152	ASP	-	expression tag	UNP P0DTC2
A	1153	GLY	-	expression tag	UNP P0DTC2
A	1154	GLN	-	expression tag	UNP P0DTC2
A	1155	ALA	-	expression tag	UNP P0DTC2
A	1156	TYR	-	expression tag	UNP P0DTC2
A	1157	VAL	-	expression tag	UNP P0DTC2
A	1158	ARG	-	expression tag	UNP P0DTC2
A	1159	LYS	-	expression tag	UNP P0DTC2
A	1160	ASP	-	expression tag	UNP P0DTC2
A	1161	GLY	-	expression tag	UNP P0DTC2
A	1162	GLU	-	expression tag	UNP P0DTC2
A	1163	TRP	-	expression tag	UNP P0DTC2
A	1164	VAL	-	expression tag	UNP P0DTC2
A	1165	LEU	-	expression tag	UNP P0DTC2
A	1166	LEU	-	expression tag	UNP P0DTC2
A	1167	SER	-	expression tag	UNP P0DTC2
A	1168	THR	-	expression tag	UNP P0DTC2
A	1169	PHE	-	expression tag	UNP P0DTC2
A	1170	LEU	-	expression tag	UNP P0DTC2
A	1171	GLY	-	expression tag	UNP P0DTC2
A	1172	ARG	-	expression tag	UNP P0DTC2
A	1173	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1174	LEU	-	expression tag	UNP P0DTC2
A	1175	GLU	_	expression tag	UNP P0DTC2
A	1176	VAL	_	expression tag	UNP P0DTC2
A	1177	LEU	-	expression tag	UNP P0DTC2
A	1178	PHE	-	expression tag	UNP P0DTC2
A	1179	GLN	-	expression tag	UNP P0DTC2
A	1180	GLY	-	expression tag	UNP P0DTC2
A	1181	PRO	_	expression tag	UNP P0DTC2
A	1182	GLY	_	expression tag	UNP P0DTC2
A	1183	HIS	-	expression tag	UNP P0DTC2
A	1184	HIS	-	expression tag	UNP P0DTC2
A	1185	HIS	-	expression tag	UNP P0DTC2
A	1186	HIS	-	expression tag	UNP P0DTC2
A	1187	HIS	-	expression tag	UNP P0DTC2
А	1188	HIS	-	expression tag	UNP P0DTC2
А	1189	HIS	-	expression tag	UNP P0DTC2
А	1190	HIS	-	expression tag	UNP P0DTC2
А	1191	SER	-	expression tag	UNP P0DTC2
А	1192	ALA	-	expression tag	UNP P0DTC2
А	1193	TRP	-	expression tag	UNP P0DTC2
А	1194	SER	-	expression tag	UNP P0DTC2
А	1195	HIS	-	expression tag	UNP P0DTC2
А	1196	PRO	-	expression tag	UNP P0DTC2
А	1197	GLN	-	expression tag	UNP P0DTC2
А	1198	PHE	-	expression tag	UNP P0DTC2
А	1199	GLU	-	expression tag	UNP P0DTC2
А	1200	LYS	-	expression tag	UNP P0DTC2
В	671	MET	-	initiating methionine	UNP P0DTC2
В	672	ARG	-	expression tag	UNP P0DTC2
В	673	PRO	-	expression tag	UNP P0DTC2
В	674	THR	-	expression tag	UNP P0DTC2
В	675	TRP	-	expression tag	UNP P0DTC2
В	676	ALA	-	expression tag	UNP P0DTC2
В	677	TRP	-	expression tag	UNP P0DTC2
В	678	TRP	-	expression tag	UNP P0DTC2
B	679	LEU	-	expression tag	UNP P0DTC2
В	680	PHE	-	expression tag	UNP P0DTC2
В	681	LEU	-	expression tag	UNP P0DTC2
В	682	VAL	-	expression tag	UNP P0DTC2
В	683	LEU	-	expression tag	UNP P0DTC2
В	684	LEU	-	expression tag	UNP P0DTC2
В	685	LEU	-	expression tag	UNP P0DTC2

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O	ТΤ	1	$\mathbf{\alpha}$
0	U	Τ	G.

Chain	Residue	Modelled	Actual	Comment	Reference
В	686	ALA	_	expression tag	UNP P0DTC2
В	687	LEU	-	expression tag	UNP P0DTC2
В	688	TRP	-	expression tag	UNP P0DTC2
В	689	ALA	_	expression tag	UNP P0DTC2
В	690	PRO	-	expression tag	UNP P0DTC2
В	691	ALA	_	expression tag	UNP P0DTC2
В	692	ARG	_	expression tag	UNP P0DTC2
В	693	GLY	-	expression tag	UNP P0DTC2
В	694	ALA	-	expression tag	UNP P0DTC2
В	695	SER	-	expression tag	UNP P0DTC2
В	696	GLN	-	expression tag	UNP P0DTC2
В	704	CYS	SER	engineered mutation	UNP P0DTC2
В	790	CYS	LYS	engineered mutation	UNP P0DTC2
В	817	PRO	PHE	engineered mutation	UNP P0DTC2
В	892	PRO	ALA	engineered mutation	UNP P0DTC2
В	899	PRO	ALA	engineered mutation	UNP P0DTC2
В	942	PRO	ALA	engineered mutation	UNP P0DTC2
В	957	GLU	GLN	engineered mutation	UNP P0DTC2
В	986	PRO	LYS	engineered mutation	UNP P0DTC2
В	987	PRO	VAL	engineered mutation	UNP P0DTC2
В	1142	GLY	-	expression tag	UNP P0DTC2
В	1143	SER	-	expression tag	UNP P0DTC2
В	1144	GLY	-	expression tag	UNP P0DTC2
В	1145	TYR	-	expression tag	UNP P0DTC2
В	1146	ILE	-	expression tag	UNP P0DTC2
В	1147	PRO	-	expression tag	UNP P0DTC2
В	1148	GLU	-	expression tag	UNP P0DTC2
В	1149	ALA	-	expression tag	UNP P0DTC2
В	1150	PRO	-	expression tag	UNP P0DTC2
В	1151	ARG	-	expression tag	UNP P0DTC2
В	1152	ASP	-	expression tag	UNP P0DTC2
В	1153	GLY	-	expression tag	UNP P0DTC2
В	1154	GLN	-	expression tag	UNP P0DTC2
В	1155	ALA	-	expression tag	UNP P0DTC2
В	1156	TYR	-	expression tag	UNP P0DTC2
В	1157	VAL	-	expression tag	UNP P0DTC2
В	1158	ARG	-	expression tag	UNP P0DTC2
B	1159	LYS	-	expression tag	UNP P0DTC2
В	1160	ASP	-	expression tag	UNP P0DTC2
B	1161	GLY	-	expression tag	UNP P0DTC2
В	1162	GLU	-	expression tag	UNP P0DTC2
В	1163	TRP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
В	1164	VAL	-	expression tag	UNP P0DTC2
В	1165	LEU	-	expression tag	UNP P0DTC2
В	1166	LEU	-	expression tag	UNP P0DTC2
В	1167	SER	-	expression tag	UNP P0DTC2
В	1168	THR	-	expression tag	UNP P0DTC2
В	1169	PHE	-	expression tag	UNP P0DTC2
В	1170	LEU	-	expression tag	UNP P0DTC2
В	1171	GLY	-	expression tag	UNP P0DTC2
В	1172	ARG	-	expression tag	UNP P0DTC2
В	1173	SER	-	expression tag	UNP P0DTC2
В	1174	LEU	-	expression tag	UNP P0DTC2
В	1175	GLU	-	expression tag	UNP P0DTC2
В	1176	VAL	-	expression tag	UNP P0DTC2
В	1177	LEU	-	expression tag	UNP P0DTC2
В	1178	PHE	-	expression tag	UNP P0DTC2
В	1179	GLN	-	expression tag	UNP P0DTC2
В	1180	GLY	-	expression tag	UNP P0DTC2
В	1181	PRO	-	expression tag	UNP P0DTC2
В	1182	GLY	-	expression tag	UNP P0DTC2
В	1183	HIS	-	expression tag	UNP P0DTC2
В	1184	HIS	-	expression tag	UNP P0DTC2
В	1185	HIS	-	expression tag	UNP P0DTC2
В	1186	HIS	-	expression tag	UNP P0DTC2
В	1187	HIS	-	expression tag	UNP P0DTC2
В	1188	HIS	-	expression tag	UNP P0DTC2
В	1189	HIS	-	expression tag	UNP P0DTC2
В	1190	HIS	-	expression tag	UNP P0DTC2
В	1191	SER	-	expression tag	UNP P0DTC2
В	1192	ALA	-	expression tag	UNP P0DTC2
В	1193	TRP	-	expression tag	UNP P0DTC2
В	1194	SER	-	expression tag	UNP P0DTC2
В	1195	HIS	-	expression tag	UNP P0DTC2
В	1196	PRO	-	expression tag	UNP P0DTC2
В	1197	GLN	-	expression tag	UNP P0DTC2
В	1198	PHE	-	expression tag	UNP P0DTC2
В	1199	GLU	-	expression tag	UNP P0DTC2
В	1200	LYS	-	expression tag	UNP P0DTC2

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





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	В	1	Total	С	Ν	Ο	0	0
	D	I	14	8	1	5	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: Spike protein S2



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	Н 3	Depositor
Cell constants	78.99Å 78.99Å 479.53Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	67.72 - 3.20	Depositor
Resolution (A)	67.72 - 3.20	EDS
% Data completeness	99.6 (67.72-3.20)	Depositor
(in resolution range)	99.6 (67.72-3.20)	EDS
R <sub>merge</sub>	(Not available)	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1913.28 (at 3.19 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
D D.	0.226 , $0.262$	Depositor
$n, n_{free}$	0.229 , $0.275$	DCC
$R_{free}$ test set	958 reflections $(5.21\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	52.8	Xtriage
Anisotropy	0.656	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.30 , $16.3$	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.37, < L^2 > = 0.19$	Xtriage
Estimated twinning fraction	0.329 for -h-k,k,-l	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	6244	wwPDB-VP
Average B, all atoms $(Å^2)$	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.15% 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: 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).

Mal	Chain	Bond	lengths	Bond angles		
Moi Chain		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.25	0/3185	0.48	0/4330	
1	В	0.25	0/3167	0.46	0/4308	
All	All	0.25	0/6352	0.47	0/8638	

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	3124	0	3103	20	1
1	В	3106	0	3077	14	2
2	В	14	0	13	0	0
All	All	6244	0	6193	34	3

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 3.

The worst 5 of 34 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:808:ASP:OD2	1:A:810:SER:OG	1.99	0.81
1:B:777:ASN:OD1	1:B:1019:ARG:NH1	2.21	0.74
1:A:795:LYS:HG2	1:A:806:LEU:HD12	1.76	0.68
1:B:903:ALA:HA	1:B:916:LEU:HD13	1.81	0.63
1:A:887:THR:H	1:A:893:ALA:HB2	1.65	0.62

All (3) 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:A:704:CYS:CB	1:A:790:CYS:SG[2_545]	1.60	0.60
1:B:704:CYS:SG	1:B:790:CYS:CB[3_655]	1.78	0.42
1:B:704:CYS:CB	1:B:790:CYS:SG[3_655]	1.98	0.22

### 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	396/530~(75%)	379~(96%)	16 (4%)	1 (0%)	41 74
1	В	393/530~(74%)	376~(96%)	17 (4%)	0	100 100
All	All	789/1060~(74%)	755~(96%)	33~(4%)	1 (0%)	51 83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	856	ASN

#### 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.



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	348/450~(77%)	346~(99%)	2(1%)	86 94
1	В	349/450~(78%)	346~(99%)	3 (1%)	78 91
All	All	697/900~(77%)	692~(99%)	5 (1%)	84 94

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

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	А	786	LYS
1	А	787	GLN
1	В	851	CYS
1	В	966	LEU
1	В	1004	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

#### 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)

There are no monosaccharides in this entry.

#### 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).

Mol	Type	Chain	Res	Tink	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	В	1301	1	14,14,15	0.23	0	17,19,21	0.33	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
2	NAG	В	1301	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	В	1301	NAG	C4-C5-C6-O6
2	В	1301	NAG	O5-C5-C6-O6

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		$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q < 0.9	
1	А	406/530~(76%)	1.26	79 (19%)	1	1	34, 51, 101, 155	0
1	В	403/530~(76%)	1.14	64 (15%)	1	1	29, 50, 90, 149	0
All	All	809/1060 (76%)	1.20	143 (17%)	1	1	29, 50, 93, 155	0

The worst 5 of 143 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	761	THR	8.1
1	В	829	ALA	7.4
1	А	831	ALA	6.8
1	А	844	ILE	6.2
1	В	1140	PRO	6.1

### 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 monosaccharides 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. 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
2	NAG	В	1301	14/15	0.46	0.55	47,60,70,70	0

## 6.5 Other polymers (i)

There are no such residues in this entry.

