



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 6, 2025 – 04:18 PM JST

PDB ID : 8YDT
Title : Crystal structure of the receptor binding domain of SARS-CoV-2 Alpha variant spike protein in complex with Ce41
Authors : Nakamura, S.; Numoto, N.; Fujiyoshi, Y.
Deposited on : 2024-02-21
Resolution : 2.50 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

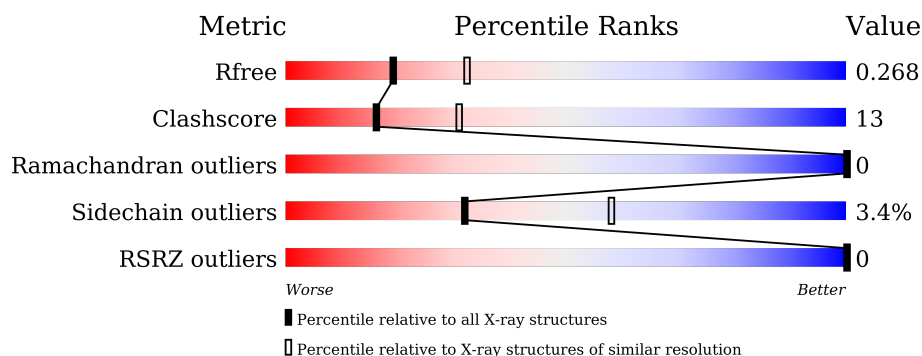
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
R_{free}	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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 $\leq 5\%$. 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	39	<div> <div>59%</div> <div>38%</div> <div>.</div> </div>
1	C	39	<div> <div>59%</div> <div>36%</div> <div>5%</div> </div>
2	B	230	<div> <div>66%</div> <div>18%</div> <div>.</div> <div>15%</div> </div>
2	D	230	<div> <div>57%</div> <div>27%</div> <div>.</div> <div>15%</div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3806 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 SARS-CoV-2 inhibiting peptide Ce41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	39	Total	C	N	O	S	0	0	0
			336	213	56	65	2			
1	C	39	Total	C	N	O	S	0	0	0
			336	213	56	65	2			

- Molecule 2 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	196	Total	C	N	O	S	0	0	0
			1553	995	258	292	8			
2	D	196	Total	C	N	O	S	0	0	0
			1553	995	258	292	8			

There are 74 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	501	TYR	ASN	variant	UNP P0DTC2
B	527	SER	-	expression tag	UNP P0DTC2
B	528	ASN	-	expression tag	UNP P0DTC2
B	529	SER	-	expression tag	UNP P0DTC2
B	530	GLU	-	expression tag	UNP P0DTC2
B	531	ASN	-	expression tag	UNP P0DTC2
B	532	LEU	-	expression tag	UNP P0DTC2
B	533	TYR	-	expression tag	UNP P0DTC2
B	534	PHE	-	expression tag	UNP P0DTC2
B	535	GLN	-	expression tag	UNP P0DTC2
B	536	GLY	-	expression tag	UNP P0DTC2
B	537	SER	-	expression tag	UNP P0DTC2
B	538	HIS	-	expression tag	UNP P0DTC2
B	539	HIS	-	expression tag	UNP P0DTC2
B	540	HIS	-	expression tag	UNP P0DTC2
B	541	HIS	-	expression tag	UNP P0DTC2

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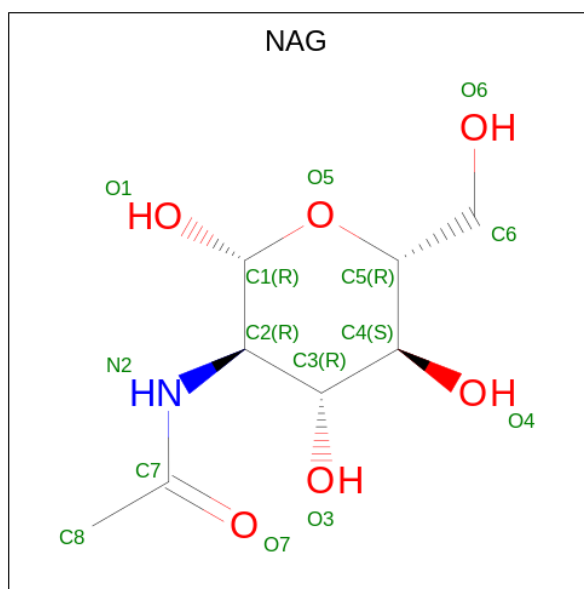
Chain	Residue	Modelled	Actual	Comment	Reference
B	542	HIS	-	expression tag	UNP P0DTC2
B	543	HIS	-	expression tag	UNP P0DTC2
B	544	HIS	-	expression tag	UNP P0DTC2
B	545	HIS	-	expression tag	UNP P0DTC2
B	546	HIS	-	expression tag	UNP P0DTC2
B	547	HIS	-	expression tag	UNP P0DTC2
B	548	GLY	-	expression tag	UNP P0DTC2
B	549	LEU	-	expression tag	UNP P0DTC2
B	550	ASN	-	expression tag	UNP P0DTC2
B	551	ASP	-	expression tag	UNP P0DTC2
B	552	ILE	-	expression tag	UNP P0DTC2
B	553	PHE	-	expression tag	UNP P0DTC2
B	554	GLU	-	expression tag	UNP P0DTC2
B	555	ALA	-	expression tag	UNP P0DTC2
B	556	GLN	-	expression tag	UNP P0DTC2
B	557	LYS	-	expression tag	UNP P0DTC2
B	558	ILE	-	expression tag	UNP P0DTC2
B	559	GLU	-	expression tag	UNP P0DTC2
B	560	TRP	-	expression tag	UNP P0DTC2
B	561	HIS	-	expression tag	UNP P0DTC2
B	562	GLU	-	expression tag	UNP P0DTC2
D	501	TYR	ASN	variant	UNP P0DTC2
D	527	SER	-	expression tag	UNP P0DTC2
D	528	ASN	-	expression tag	UNP P0DTC2
D	529	SER	-	expression tag	UNP P0DTC2
D	530	GLU	-	expression tag	UNP P0DTC2
D	531	ASN	-	expression tag	UNP P0DTC2
D	532	LEU	-	expression tag	UNP P0DTC2
D	533	TYR	-	expression tag	UNP P0DTC2
D	534	PHE	-	expression tag	UNP P0DTC2
D	535	GLN	-	expression tag	UNP P0DTC2
D	536	GLY	-	expression tag	UNP P0DTC2
D	537	SER	-	expression tag	UNP P0DTC2
D	538	HIS	-	expression tag	UNP P0DTC2
D	539	HIS	-	expression tag	UNP P0DTC2
D	540	HIS	-	expression tag	UNP P0DTC2
D	541	HIS	-	expression tag	UNP P0DTC2
D	542	HIS	-	expression tag	UNP P0DTC2
D	543	HIS	-	expression tag	UNP P0DTC2
D	544	HIS	-	expression tag	UNP P0DTC2
D	545	HIS	-	expression tag	UNP P0DTC2
D	546	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	547	HIS	-	expression tag	UNP P0DTC2
D	548	GLY	-	expression tag	UNP P0DTC2
D	549	LEU	-	expression tag	UNP P0DTC2
D	550	ASN	-	expression tag	UNP P0DTC2
D	551	ASP	-	expression tag	UNP P0DTC2
D	552	ILE	-	expression tag	UNP P0DTC2
D	553	PHE	-	expression tag	UNP P0DTC2
D	554	GLU	-	expression tag	UNP P0DTC2
D	555	ALA	-	expression tag	UNP P0DTC2
D	556	GLN	-	expression tag	UNP P0DTC2
D	557	LYS	-	expression tag	UNP P0DTC2
D	558	ILE	-	expression tag	UNP P0DTC2
D	559	GLU	-	expression tag	UNP P0DTC2
D	560	TRP	-	expression tag	UNP P0DTC2
D	561	HIS	-	expression tag	UNP P0DTC2
D	562	GLU	-	expression tag	UNP P0DTC2

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



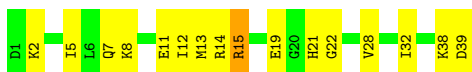
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

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: SARS-CoV-2 inhibiting peptide Ce41

Chain A: 



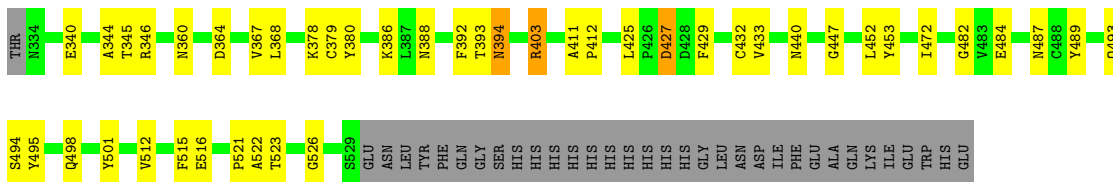
- Molecule 1: SARS-CoV-2 inhibiting peptide Ce41

Chain C: 



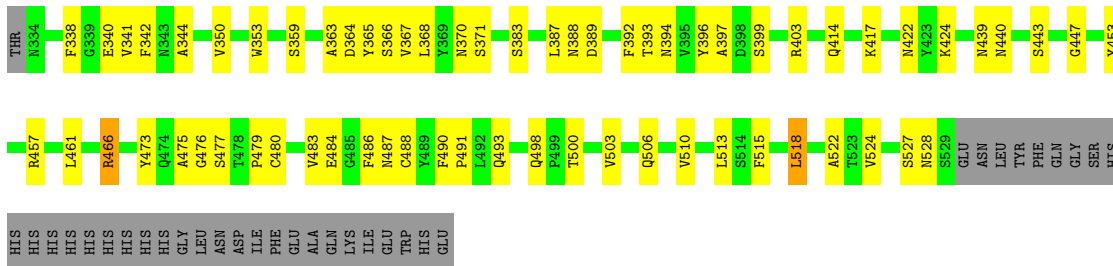
- Molecule 2: Spike protein S1

Chain B: 



- Molecule 2: Spike protein S1

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	73.31Å 73.31Å 99.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.23 – 2.50 39.23 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (39.23-2.50) 99.6 (39.23-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.229 , 0.268 0.229 , 0.268	Depositor DCC
R_{free} test set	1040 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	80.8	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 75.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.037 for -h,-k,l 0.145 for h,-h-k,-l 0.054 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3806	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.52	0/341	0.54	0/452
1	C	0.41	0/341	0.56	0/452
2	B	0.49	0/1597	0.64	0/2173
2	D	0.45	0/1597	0.58	0/2173
All	All	0.47	0/3876	0.60	0/5250

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	A	336	0	333	13	0
1	C	336	0	333	15	0
2	B	1553	0	1464	30	0
2	D	1553	0	1464	44	0
3	B	14	0	13	1	0
3	D	14	0	13	1	0
All	All	3806	0	3620	96	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 13.

The worst 5 of 96 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)
2:D:393:THR:HA	2:D:522:ALA:HA	1.69	0.73
2:B:393:THR:HA	2:B:522:ALA:HA	1.77	0.66
1:C:6:LEU:O	1:C:9:ILE:HG12	1.96	0.65
2:D:341:VAL:HG11	2:D:397:ALA:HB1	1.81	0.62
1:A:5:ILE:H	1:A:5:ILE:HD12	1.64	0.62

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	37/39 (95%)	34 (92%)	3 (8%)	0	100	100
1	C	37/39 (95%)	33 (89%)	4 (11%)	0	100	100
2	B	194/230 (84%)	175 (90%)	19 (10%)	0	100	100
2	D	194/230 (84%)	174 (90%)	20 (10%)	0	100	100
All	All	462/538 (86%)	416 (90%)	46 (10%)	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	Outliers	Percentiles	
1	A	36/36 (100%)	34 (94%)	2 (6%)	17	36
1	C	36/36 (100%)	33 (92%)	3 (8%)	9	19
2	B	169/200 (84%)	164 (97%)	5 (3%)	36	63
2	D	169/200 (84%)	165 (98%)	4 (2%)	44	70
All	All	410/472 (87%)	396 (97%)	14 (3%)	32	58

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	2	LYS
1	C	17	ASP
2	D	518	LEU
2	D	466	ARG
2	D	484	GLU

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	$\# Z > 2$
3	NAG	D	601	2	14,14,15	0.84	1 (7%)	17,19,21	0.83	1 (5%)
3	NAG	B	601	2	14,14,15	0.53	0	17,19,21	0.51	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	D	601	2	-	2/6/23/26	0/1/1/1
3	NAG	B	601	2	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	601	NAG	O5-C1	2.76	1.48	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	601	NAG	C1-O5-C5	2.69	115.84	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	601	NAG	O5-C5-C6-O6
3	B	601	NAG	C4-C5-C6-O6
3	D	601	NAG	O5-C5-C6-O6
3	D	601	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	601	NAG	1	0
3	B	601	NAG	1	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	OWAB(Å ²)	Q<0.9
1	A	39/39 (100%)	-1.07	0 100 100	69, 82, 107, 131	0
1	C	39/39 (100%)	-0.98	0 100 100	75, 94, 115, 131	0
2	B	196/230 (85%)	-1.09	0 100 100	64, 82, 103, 113	0
2	D	196/230 (85%)	-1.02	0 100 100	69, 89, 111, 121	0
All	All	470/538 (87%)	-1.05	0 100 100	64, 86, 110, 131	0

There are no RSRZ outliers to report.

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, 95th 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	B	601	14/15	0.97	0.07	105,115,118,120	0
3	NAG	D	601	14/15	0.97	0.04	100,107,114,115	0

6.5 Other polymers [i](#)

There are no such residues in this entry.