



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 8IAN / pdb_00008ian
Title : Crystal structure of CtPL-H210S/F214I mutant
Authors : Li, X.; Shi, B.L.; Zeng, Z.Y.; Huang, J.-W.; Chen, C.-C.; Guo, R.-T.
Deposited on : 2023-02-08
Resolution : 2.08 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 ⓘ 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

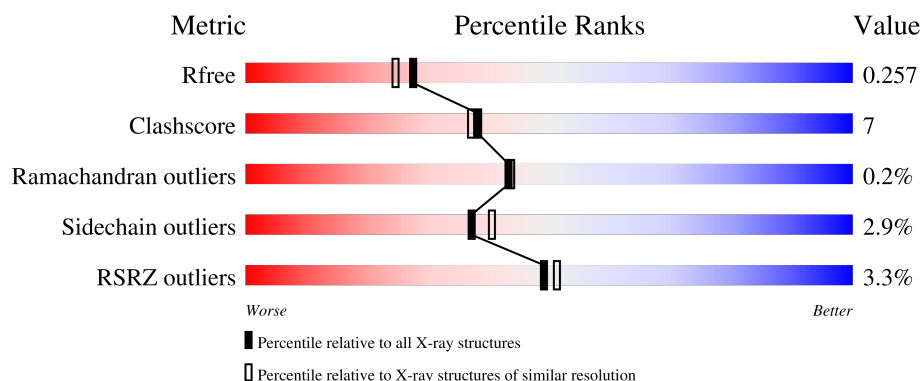
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 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}	180053	8172 (2.10-2.06)
Clashscore	190562	8714 (2.10-2.06)
Ramachandran outliers	187476	8641 (2.10-2.06)
Sidechain outliers	187428	8642 (2.10-2.06)
RSRZ outliers	180081	8177 (2.10-2.06)

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	270	2% 84% 15% .
1	B	270	5% 86% 13% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4658 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 PET hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	0	0	0
			2059	1288	364	397	10			
1	B	270	Total	C	N	O	S	0	0	0
			2059	1288	364	397	10			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Ca 1	0	0
3	B	1	Total 1	Ca 1	0	0

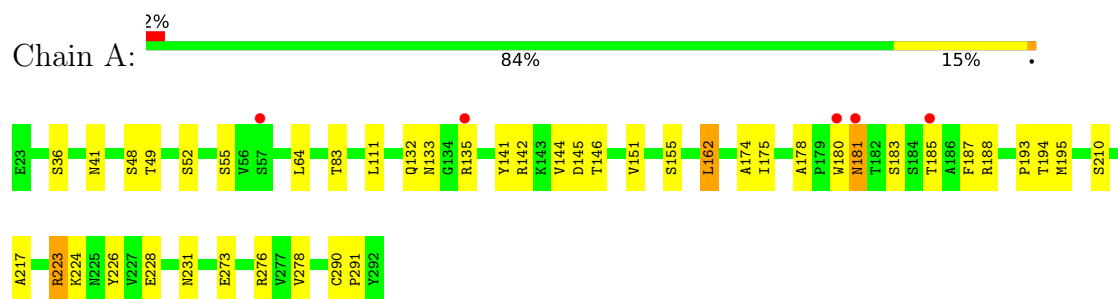
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	284	Total 284	O 284	0	0
4	B	226	Total 226	O 226	0	0

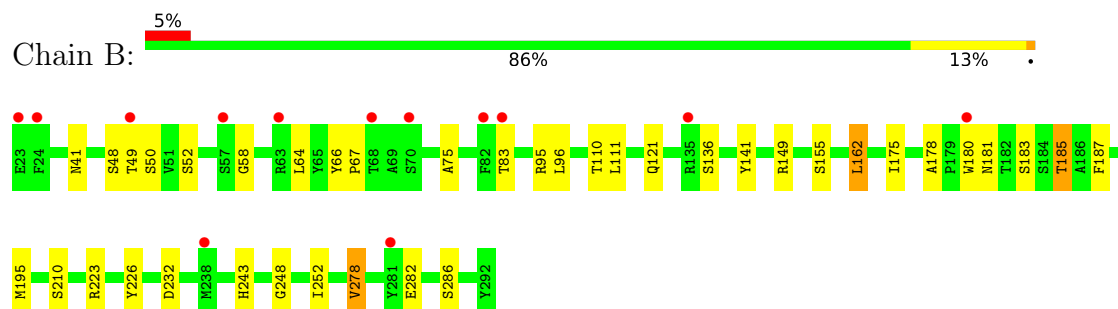
3 Residue-property plots

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: PET hydrolase



• Molecule 1: PET hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	115.36Å 115.36Å 94.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.79 – 2.08 37.79 – 2.08	Depositor EDS
% Data completeness (in resolution range)	100.0 (37.79-2.08) 100.0 (37.79-2.08)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.200 , 0.254 0.207 , 0.257	Depositor DCC
R_{free} test set	2226 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	20.8	Xtriage
Anisotropy	0.438	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 52.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4658	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.33 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.9383e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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, CA

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	1.04	0/2112	1.34	2/2871 (0.1%)
1	B	1.03	0/2112	1.37	2/2871 (0.1%)
All	All	1.04	0/4224	1.35	4/5742 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	145	ASP	CA-C-N	5.31	128.14	120.38
1	A	145	ASP	C-N-CA	5.31	128.14	120.38
1	B	52	SER	CA-C-N	5.20	128.21	120.31
1	B	52	SER	C-N-CA	5.20	128.21	120.31

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	2059	0	1974	24	0
1	B	2059	0	1974	31	0
2	A	14	0	13	0	0
2	B	14	0	13	1	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
4	A	284	0	0	5	0
4	B	226	0	0	5	0
All	All	4658	0	3974	56	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 7.

All (56) 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:B:301:NAG:H82	4:B:560:HOH:O	1.69	0.92
1:A:183:SER:OG	1:A:185:THR:HG22	1.75	0.86
1:B:248:GLY:O	1:B:252:ILE:HG12	1.79	0.82
1:B:162:LEU:HD13	1:B:187:PHE:CD1	2.20	0.77
1:B:41:ASN:HD22	1:B:95:ARG:HE	1.40	0.68
1:B:181:ASN:ND2	4:B:401:HOH:O	2.27	0.68
1:B:181:ASN:ND2	1:B:210:SER:OG	2.28	0.67
1:B:243:HIS:HD2	1:B:282:GLU:OE1	1.80	0.65
1:B:180:TRP:CE3	1:B:181:ASN:N	2.66	0.63
1:A:223:ARG:HD2	1:A:223:ARG:H	1.66	0.59
1:A:231:ASN:ND2	4:A:403:HOH:O	2.35	0.58
1:A:49:THR:HG23	4:A:413:HOH:O	2.04	0.57
1:A:181:ASN:ND2	1:A:210:SER:OG	2.38	0.57
1:B:232:ASP:OD2	1:B:243:HIS:HE1	1.88	0.55
1:B:41:ASN:ND2	1:B:95:ARG:HE	2.06	0.54
1:B:48:SER:HA	1:B:64:LEU:O	2.08	0.54
1:A:146:THR:HG22	4:A:548:HOH:O	2.09	0.52
1:B:83:THR:HA	1:B:111:LEU:HB3	1.92	0.52
1:A:181:ASN:ND2	4:A:408:HOH:O	2.42	0.52
1:B:162:LEU:HD13	1:B:187:PHE:CG	2.45	0.51
1:A:141:TYR:OH	1:A:142:ARG:CZ	2.60	0.50
1:B:96:LEU:HD23	1:B:252:ILE:HD13	1.92	0.50
1:B:183:SER:OG	1:B:185:THR:HG22	2.11	0.50
1:B:181:ASN:CG	4:B:401:HOH:O	2.53	0.50
1:B:232:ASP:OD2	1:B:243:HIS:CE1	2.65	0.49
1:B:155:SER:HA	1:B:178:ALA:O	2.13	0.49
1:A:83:THR:HA	1:A:111:LEU:HB3	1.94	0.48
1:B:95:ARG:HG3	1:B:252:ILE:HD11	1.96	0.48
1:B:226:TYR:O	1:B:286:SER:HA	2.13	0.48
1:A:151:VAL:O	1:A:174:ALA:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:VAL:HG22	1:B:286:SER:HB3	1.95	0.47
1:A:155:SER:HA	1:A:178:ALA:O	2.15	0.46
1:A:290:CYS:HB3	1:A:291:PRO:HA	1.97	0.45
1:A:52:SER:OG	1:A:55:SER:HB3	2.17	0.45
1:A:188:ARG:HA	1:A:217:ALA:O	2.17	0.45
1:B:136:SER:HA	1:B:141:TYR:CG	2.51	0.45
1:A:48:SER:HA	1:A:64:LEU:O	2.17	0.44
1:B:58:GLY:O	1:B:121:GLN:HG2	2.18	0.44
1:B:175:ILE:HA	1:B:195:MET:O	2.18	0.44
1:B:49:THR:HG22	1:B:50:SER:O	2.18	0.44
1:B:162:LEU:HD23	1:B:162:LEU:HA	1.86	0.44
1:A:223:ARG:HD2	4:A:581:HOH:O	2.17	0.43
1:B:181:ASN:HA	4:B:428:HOH:O	2.18	0.43
1:A:183:SER:CB	1:A:185:THR:HG22	2.48	0.43
1:B:180:TRP:HZ2	4:B:604:HOH:O	2.01	0.43
1:B:180:TRP:CG	1:B:181:ASN:H	2.36	0.43
1:A:175:ILE:HA	1:A:195:MET:O	2.19	0.42
1:A:132:GLN:HE22	1:A:135:ARG:NH1	2.17	0.42
1:B:75:ALA:O	1:B:149:ARG:HA	2.21	0.41
1:A:194:THR:O	1:A:224:LYS:HA	2.21	0.41
1:A:162:LEU:HD13	1:A:187:PHE:CD1	2.55	0.41
1:B:66:TYR:HA	1:B:67:PRO:HD3	1.96	0.41
1:A:193:PRO:HA	1:A:223:ARG:O	2.21	0.41
1:B:162:LEU:HB3	1:B:187:PHE:CE1	2.56	0.41
1:A:133:ASN:HB2	1:A:144:VAL:HB	2.02	0.40
1:A:226:TYR:CE2	1:A:228:GLU:HB2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	268/270 (99%)	261 (97%)	6 (2%)	1 (0%)	30	28
1	B	268/270 (99%)	259 (97%)	9 (3%)	0	100	100
All	All	536/540 (99%)	520 (97%)	15 (3%)	1 (0%)	43	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	180	TRP

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	221/221 (100%)	213 (96%)	8 (4%)	31	32
1	B	221/221 (100%)	216 (98%)	5 (2%)	44	49
All	All	442/442 (100%)	429 (97%)	13 (3%)	37	40

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	SER
1	A	41	ASN
1	A	162	LEU
1	A	181	ASN
1	A	223	ARG
1	A	273	GLU
1	A	276	ARG
1	A	278	VAL
1	B	110	THR
1	B	162	LEU
1	B	185	THR
1	B	223	ARG
1	B	278	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	GLN
1	A	181	ASN
1	B	41	ASN
1	B	132	GLN
1	B	181	ASN
1	B	243	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	B	301	1	14,14,15	0.88	0	17,19,21	1.71	5 (29%)
2	NAG	A	301	1	14,14,15	0.47	0	17,19,21	1.10	1 (5%)

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	B	301	1	-	3/6/23/26	0/1/1/1
2	NAG	A	301	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	NAG	C1-C2-N2	-4.22	103.78	110.43
2	B	301	NAG	C3-C4-C5	2.85	115.40	110.23
2	A	301	NAG	O5-C5-C4	-2.30	105.24	110.83
2	B	301	NAG	O5-C1-C2	-2.23	107.84	111.29
2	B	301	NAG	O5-C5-C4	2.16	116.08	110.83
2	B	301	NAG	C1-O5-C5	2.08	114.98	112.19

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	NAG	C4-C5-C6-O6
2	B	301	NAG	O5-C5-C6-O6
2	B	301	NAG	C8-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	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	270/270 (100%)	-0.12	5 (1%) 66 69	15, 22, 39, 53	0
1	B	270/270 (100%)	0.26	13 (4%) 35 37	17, 28, 47, 68	0
All	All	540/540 (100%)	0.07	18 (3%) 49 51	15, 25, 45, 68	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	180	TRP	5.8
1	A	180	TRP	4.0
1	B	63	ARG	3.3
1	B	82	PHE	3.0
1	B	23	GLU	2.8
1	B	24	PHE	2.6
1	B	135	ARG	2.5
1	B	57	SER	2.5
1	B	83	THR	2.5
1	B	238	MET	2.4
1	B	281	TYR	2.3
1	A	185	THR	2.3
1	A	135	ARG	2.3
1	A	57	SER	2.3
1	B	70	SER	2.1
1	B	49	THR	2.1
1	A	181	ASN	2.1
1	B	68	THR	2.1

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	NAG	B	301	14/15	0.80	0.15	50,58,65,68	0
2	NAG	A	301	14/15	0.90	0.10	35,41,49,53	0
3	CA	A	302	1/1	0.99	0.06	37,37,37,37	0
3	CA	B	302	1/1	0.99	0.07	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.