



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:51 PM GMT

PDB ID : 1HN0  
Title : CRYSTAL STRUCTURE OF CHONDROITIN ABC LYASE I FROM PROTEUS VULGARIS AT 1.9 ANGSTROMS RESOLUTION  
Authors : Huang, W.; Cygler, M.  
Deposited on : 2000-12-05  
Resolution : 1.90 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](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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865



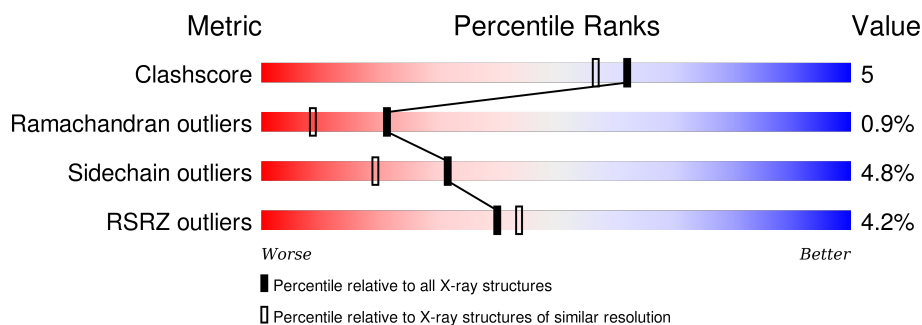
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	1021	



## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9426 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 CHONDROITIN ABC LYASE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	971	Total	C	N	O	S	0	2	0
			7759	4931	1323	1484	21			

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1666	Total	O	0	0
			1666	1666		







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.28 Å 95.14 Å 229.95 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.88 – 1.90 19.90 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.88-1.90) 90.3 (19.90-1.90)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	14.43 (at 1.90 Å)	Xtriage
Refinement program	REFMAC 5.1.08	Depositor
R, $R_{free}$	0.156 , 0.212 0.159 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	16.7	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 62.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 78136 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9426	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA

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	0.75	0/7961	0.83	18/10803 (0.2%)

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	0	1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	906	ASP	CB-CG-OD2	10.59	127.83	118.30
1	A	442	ASP	CB-CG-OD2	7.55	125.10	118.30
1	A	637	ASP	CB-CG-OD2	7.10	124.69	118.30
1	A	311	ASP	CB-CG-OD2	6.59	124.23	118.30
1	A	32	ASP	CB-CG-OD2	6.47	124.12	118.30
1	A	707	ASP	CB-CG-OD1	6.14	123.83	118.30
1	A	406	ASP	CB-CG-OD2	6.01	123.71	118.30
1	A	211	ASP	CB-CG-OD2	5.96	123.67	118.30
1	A	462	ASP	CB-CG-OD2	5.82	123.54	118.30
1	A	525	ASP	CB-CG-OD2	5.78	123.50	118.30
1	A	65	ASP	CB-CG-OD2	5.65	123.39	118.30
1	A	863	ASP	CB-CG-OD1	5.64	123.38	118.30
1	A	987	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	762	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	291	ASP	CB-CG-OD2	5.36	123.12	118.30
1	A	587	ASP	CB-CG-OD2	5.33	123.09	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	705	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	52	ASP	CB-CG-OD2	5.27	123.04	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	958	VAL	Peptide

## 5.2 Too-close contacts ⓘ

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	7759	0	7575	82	0
2	A	1	0	0	0	0
3	A	1666	0	0	37	0
All	All	9426	0	7575	82	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 5.

All (82) 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:272[A]:GLU:HG2	3:A:2547:HOH:O	1.36	1.25
1:A:680:SER:HB2	3:A:3436:HOH:O	1.59	1.00
1:A:406:ASP:OD1	1:A:409:LYS:NZ	1.95	0.98
1:A:343:MET:SD	3:A:3388:HOH:O	2.22	0.95
1:A:597:ILE:HG23	3:A:2941:HOH:O	1.67	0.94
1:A:34:LYS:HG2	3:A:3262:HOH:O	1.77	0.82
1:A:32:ASP:OD1	1:A:33:PRO:HD2	1.82	0.79
1:A:985:SER:HB3	1:A:994:TYR:CE2	2.18	0.79
1:A:409:LYS:HG3	1:A:414:GLN:NE2	1.98	0.78
1:A:97:LYS:HG2	3:A:2446:HOH:O	1.87	0.75
1:A:409:LYS:HG3	1:A:414:GLN:HE21	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:LYS:O	1:A:83:SER:HB3	1.90	0.70
1:A:55:SER:HB3	1:A:61:LEU:HG	1.74	0.69
1:A:340:THR:HA	1:A:343:MET:HE2	1.73	0.69
1:A:715:MET:HE2	3:A:2494:HOH:O	1.93	0.67
1:A:48:ASN:HB3	1:A:51:ALA:HB2	1.75	0.66
1:A:680:SER:CB	3:A:3436:HOH:O	2.28	0.66
1:A:414:GLN:NE2	3:A:2528:HOH:O	2.28	0.65
1:A:985:SER:HB2	3:A:2623:HOH:O	1.98	0.64
1:A:976:ASN:ND2	3:A:2392:HOH:O	2.31	0.63
1:A:270:GLY:C	3:A:2554:HOH:O	2.39	0.60
1:A:252:GLU:HB2	3:A:3415:HOH:O	2.02	0.60
1:A:162:ASP:OD1	1:A:232:ARG:HD3	2.02	0.60
1:A:450:SER:HB2	1:A:519:LEU:HD11	1.84	0.60
1:A:795:ASN:HB3	3:A:2406:HOH:O	2.01	0.60
1:A:303:THR:O	3:A:3387:HOH:O	2.16	0.58
1:A:880:ASP:O	1:A:885:LYS:HE3	2.03	0.57
1:A:212:ARG:HD2	1:A:212:ARG:O	2.05	0.57
1:A:985:SER:CB	3:A:2623:HOH:O	2.51	0.57
1:A:32:ASP:HB3	3:A:3233:HOH:O	2.06	0.55
1:A:854:GLU:HG3	3:A:2415:HOH:O	2.04	0.55
1:A:710:LYS:HE2	3:A:3156:HOH:O	2.06	0.55
1:A:150:THR:CG2	3:A:2638:HOH:O	2.53	0.55
1:A:796:THR:HG22	1:A:805:GLU:OE2	2.06	0.55
1:A:568:LEU:HD23	1:A:597:ILE:CD1	2.37	0.54
1:A:36:LEU:HD11	1:A:94:PRO:HG3	1.89	0.54
1:A:716:GLN:CG	3:A:3239:HOH:O	2.57	0.53
1:A:716:GLN:HG3	3:A:3239:HOH:O	2.08	0.52
1:A:272[A]:GLU:CG	3:A:2547:HOH:O	2.19	0.51
1:A:202:ASN:H	1:A:202:ASN:HD22	1.59	0.51
1:A:867:ARG:HD2	3:A:2453:HOH:O	2.09	0.51
1:A:42:TYR:HB2	1:A:213:ILE:HB	1.93	0.50
1:A:1020:LEU:HD23	1:A:1021:PRO:HD2	1.93	0.50
1:A:967:GLN:NE2	3:A:3123:HOH:O	2.45	0.50
1:A:976:ASN:HB3	3:A:2426:HOH:O	2.12	0.49
1:A:714:LEU:HD11	1:A:716:GLN:NE2	2.28	0.49
1:A:47:ASN:ND2	3:A:2301:HOH:O	2.45	0.49
1:A:257:ILE:HG21	1:A:466:ARG:HD2	1.95	0.48
1:A:42:TYR:CZ	1:A:87:LEU:HD11	2.49	0.48
1:A:677:SER:HB3	1:A:680:SER:HB2	1.97	0.47
1:A:48:ASN:N	1:A:49:PRO:HD3	2.29	0.47
1:A:150:THR:HG23	3:A:2638:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ASP:CG	1:A:33:PRO:HD2	2.35	0.46
1:A:300:ASN:OD1	1:A:300:ASN:N	2.47	0.46
1:A:568:LEU:HD23	1:A:597:ILE:HD11	1.96	0.46
1:A:35:ASN:HB3	3:A:2295:HOH:O	2.15	0.46
1:A:934:TRP:NE1	3:A:3398:HOH:O	2.23	0.45
1:A:810:GLN:NE2	3:A:3420:HOH:O	2.50	0.45
1:A:823:ASN:ND2	3:A:2166:HOH:O	2.37	0.45
1:A:67:ARG:HG2	1:A:152:TRP:CZ2	2.50	0.45
1:A:131:GLU:O	1:A:193:ASP:OD2	2.36	0.44
1:A:311:ASP:O	1:A:314:ILE:HG12	2.18	0.44
1:A:50:LEU:HD21	1:A:63:LEU:HD21	2.00	0.43
1:A:988:LYS:HA	1:A:988:LYS:HD2	1.76	0.43
1:A:734:MET:HA	1:A:758:VAL:O	2.19	0.42
1:A:116:TYR:CZ	1:A:151:GLY:HA2	2.54	0.42
1:A:704:LYS:NZ	3:A:2825:HOH:O	2.53	0.42
1:A:58:ASN:HA	3:A:2510:HOH:O	2.20	0.42
1:A:777:LYS:HB2	1:A:777:LYS:HE3	1.90	0.41
1:A:763:ASN:H	1:A:763:ASN:HD22	1.68	0.41
1:A:995:GLN:HB3	3:A:2826:HOH:O	2.19	0.41
1:A:714:LEU:HD11	1:A:716:GLN:HE21	1.85	0.41
1:A:33:PRO:HA	3:A:2576:HOH:O	2.20	0.41
1:A:985:SER:HB3	1:A:994:TYR:CZ	2.54	0.41
1:A:826:GLY:O	1:A:877:VAL:HA	2.20	0.41
1:A:67:ARG:HD3	1:A:116:TYR:CG	2.56	0.41
1:A:409:LYS:HG2	3:A:3290:HOH:O	2.21	0.41
1:A:645:TYR:CD1	1:A:651:SER:HB3	2.56	0.41
1:A:555:LEU:N	1:A:556:PRO:CD	2.84	0.41
1:A:267:GLU:OE2	1:A:272[B]:GLU:OE1	2.39	0.40
1:A:67:ARG:HD3	1:A:116:TYR:CD1	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	969/1021 (95%)	921 (95%)	38 (4%)	10 (1%)	19 7

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	272[A]	GLU
1	A	272[B]	GLU
1	A	987	ASP
1	A	140	GLN
1	A	988	LYS
1	A	58	ASN
1	A	139	ALA
1	A	990	SER
1	A	57	LYS
1	A	131	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	852/890 (96%)	810 (95%)	42 (5%)	31 18

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	SER
1	A	35	ASN
1	A	55	SER
1	A	56	ASP
1	A	72	ASN
1	A	83	SER
1	A	91	LEU
1	A	119	LYS
1	A	136	THR
1	A	138	GLU
1	A	140	GLN

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Mol	Chain	Res	Type
1	A	150	THR
1	A	165	ASN
1	A	201	SER
1	A	202	ASN
1	A	212	ARG
1	A	213	ILE
1	A	232	ARG
1	A	272[A]	GLU
1	A	272[B]	GLU
1	A	284	SER
1	A	358	GLN
1	A	364	GLN
1	A	413	LEU
1	A	447	ASN
1	A	451	ARG
1	A	505	TYR
1	A	599	ASP
1	A	639	MET
1	A	650	TRP
1	A	667	HIS
1	A	738	ASN
1	A	741	TYR
1	A	742	PRO
1	A	763	ASN
1	A	867	ARG
1	A	884	GLU
1	A	949	GLN
1	A	951	ASP
1	A	966	ARG
1	A	985	SER
1	A	995	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	47	ASN
1	A	72	ASN
1	A	117	ASN
1	A	161	ASN
1	A	202	ASN
1	A	241	HIS

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Mol	Chain	Res	Type
1	A	262	GLN
1	A	266	ASN
1	A	364	GLN
1	A	414	GLN
1	A	447	ASN
1	A	537	ASN
1	A	564	ASN
1	A	656	ASN
1	A	665	GLN
1	A	716	GLN
1	A	744	ASN
1	A	763	ASN
1	A	802	GLN
1	A	896	ASN
1	A	901	GLN
1	A	976	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 ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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

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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	971/1021 (95%)	-0.22	41 (4%) 40 44	8, 18, 49, 70	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	139	ALA	6.6
1	A	299	ALA	6.4
1	A	989	ASN	6.4
1	A	138	GLU	5.5
1	A	165	ASN	5.4
1	A	986	ALA	5.2
1	A	271	GLY	4.3
1	A	56	ASP	3.7
1	A	140	GLN	3.7
1	A	136	THR	3.5
1	A	300	ASN	3.3
1	A	988	LYS	3.2
1	A	987	ASP	3.2
1	A	272[A]	GLU	3.1
1	A	1021	PRO	3.1
1	A	57	LYS	3.1
1	A	204	SER	2.9
1	A	55	SER	2.8
1	A	48	ASN	2.8
1	A	296	HIS	2.8
1	A	135	SER	2.7
1	A	203	VAL	2.7
1	A	132	LYS	2.7
1	A	201	SER	2.6
1	A	82	GLY	2.6
1	A	951	ASP	2.6
1	A	137	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	58	ASN	2.5
1	A	77	TRP	2.4
1	A	81	GLY	2.4
1	A	205	GLN	2.3
1	A	990	SER	2.3
1	A	101	LYS	2.3
1	A	34	LYS	2.2
1	A	72	ASN	2.2
1	A	97	LYS	2.2
1	A	60	ILE	2.2
1	A	47	ASN	2.1
1	A	125	LEU	2.1
1	A	354	LYS	2.1
1	A	131	GLU	2.0

## 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( $\text{\AA}^2$ )	Q<0.9
2	NA	A	1800	1/1	0.80	0.14	-0.23	40,40,40,40	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.