



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 08:02 PM UTC

PDB ID : 2INU / pdb_00002inu
Title : Crystal structure of Inulin fructotransferase in the absence of substrate
Authors : Rhee, S.; Jung, W.S.
Deposited on : 2006-10-09
Resolution : 1.80 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

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

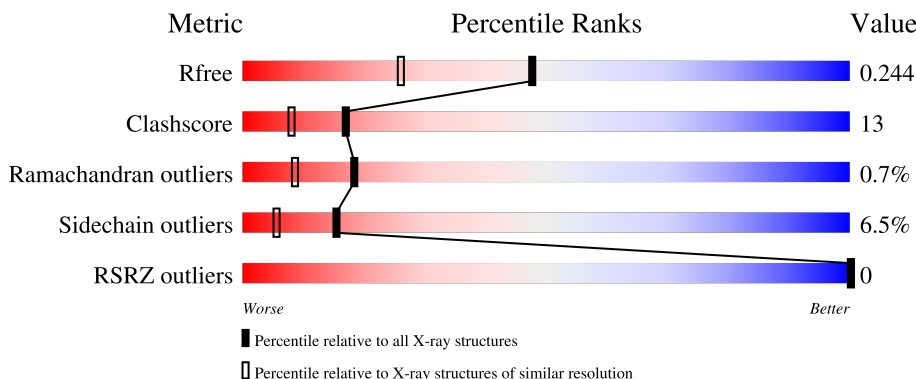
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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 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	410	65% 27% 5% 2% 1%
1	B	410	63% 29% 5% 2% 1%
1	C	410	66% 25% 5% 2% 1%

2 Entry composition [i](#)

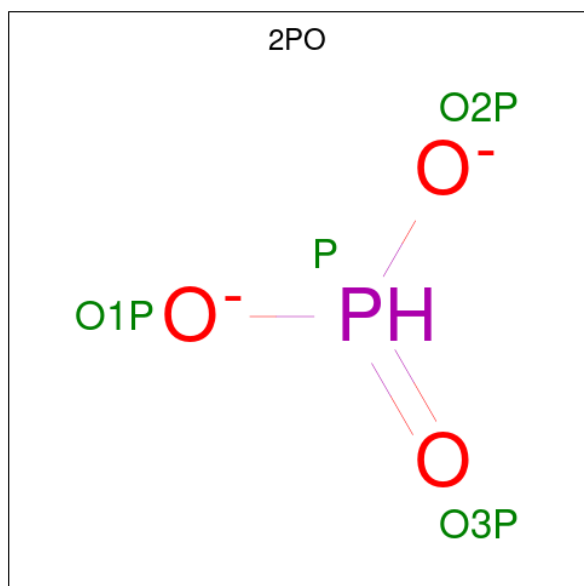
There are 3 unique types of molecules in this entry. The entry contains 9530 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Inulin fructotransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	Se	0	0	0
			2982	1859	535	578	6	4			
1	B	399	Total	C	N	O	S	Se	0	0	0
			2982	1859	535	578	6	4			
1	C	399	Total	C	N	O	S	Se	0	0	0
			2982	1859	535	578	6	4			

- Molecule 2 is PHOSPHONATE (CCD ID: 2PO) (formula: HO_3P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			4	3	1		
2	B	1	Total	O	P	0	0
			4	3	1		

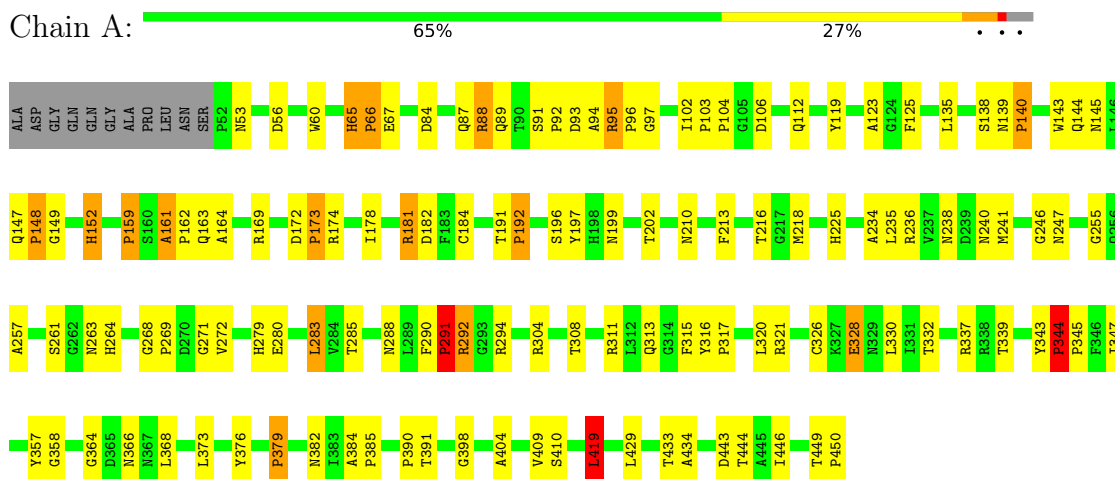
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	185	Total 185	O 185	0	0
3	B	195	Total 195	O 195	0	0
3	C	196	Total 196	O 196	0	0

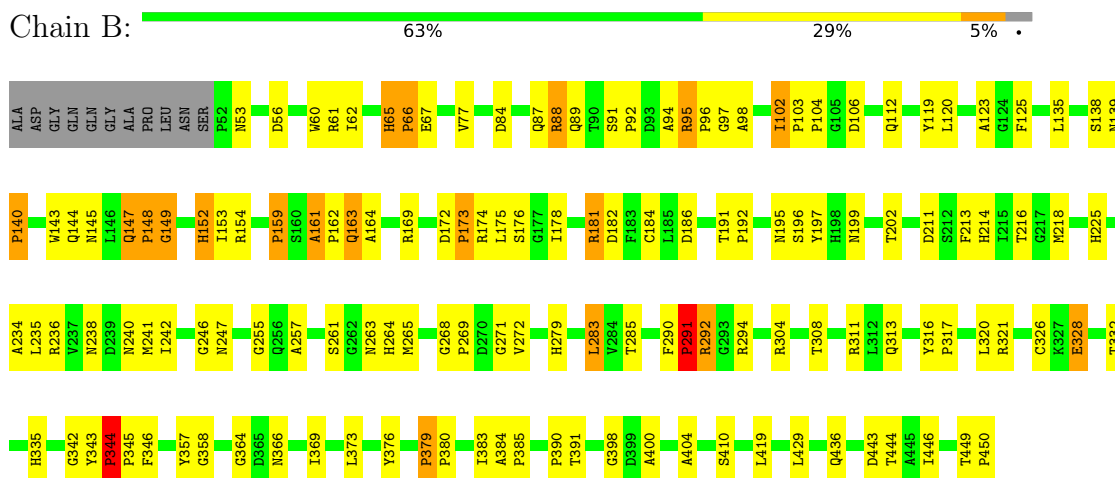
3 Residue-property plots

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.

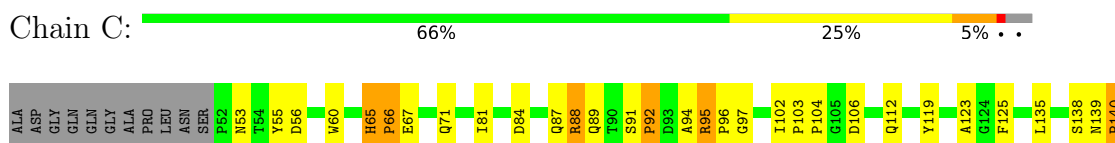
• Molecule 1: Inulin fructotransferase



• Molecule 1: Inulin fructotransferase



• Molecule 1: Inulin fructotransferase



I347	W143	G246	A257	L146	H152	P189	R169	D172	R174	L175	R181	N210	A234	I343
Y357	Q144	N247	T258	Q147	I153	S160	E280	D173	R175	S176	D182	D211	L235	P344
G358	N145	A257	L259	P148	R154	A161	L283	R174	G177	I178	F183	S212	R236	P345
G364	L146	T258	V260	G149		P162	T284	L174	I176		C184	F213	Y237	F346
N365	L147	L259	S261			Q163	T285	L175	S177			H214	R237	
N366	Q148	V260	G262			A164	F290	P291	G177			I215	N238	
N367	P148	S261	N263				P291	R292	I177			T216	D239	
L368	G149	G262	H264				R292	G293	I178			G217	P240	
I369		L368					R294	R294				M218	N240	
S370		S370												
N377		N377												
V378		V378												
P379		P379												
N382		N382												
I383		I383												
A384		A384												
P385		P385												
A388		A388												
Q389		Q389												
P390		P390												
T391		T391												
G398		G398												
D399		D399												
A400		A400												
A404		A404												
D420		D420												
L429		L429												
Q436		Q436												
D443		D443												
T449		T449												
P450		P450												

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	159.14Å 91.91Å 93.02Å 90.00° 124.75° 90.00°	Depositor
Resolution (Å)	30.00 – 1.80 30.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	74.1 (30.00-1.80) 98.4 (30.00-1.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 1.80Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.198 , 0.226 0.218 , 0.244	Depositor DCC
R_{free} test set	10149 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å ²)	13.4	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 25.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.003 for $1/2^*h+1/2^*k+2^*l, 1/2^*h+1/2^*k, -1/2^*h+1/2^*k-l$ 0.011 for $-1/2^*h-3/2^*k-l, -1/2^*h+1/2^*k-l, 1/2^*h+1/2^*k$ 0.012 for $-1/2^*h+3/2^*k-l, 1/2^*h+1/2^*k+l, 1/2^*h-1/2^*k$ 0.018 for $1/2^*h-1/2^*k+2^*l, -1/2^*h+1/2^*k, -1/2^*h-1/2^*k-l$ 0.018 for $-h+k-l, -l, -k$ 0.002 for $-h-k-l, l, k$ 0.019 for $-1/2^*h+1/2^*k+l, 1/2^*h-1/2^*k+l, 1/2^*h+1/2^*k$ 0.003 for $-1/2^*h-1/2^*k+l, -1/2^*h-1/2^*k-l, 1/2^*h-1/2^*k$ 0.489 for $1/2^*h+3/2^*k, 1/2^*h-1/2^*k, -1/2^*h-1/2^*k-l$ 0.489 for $1/2^*h-3/2^*k, -1/2^*h-1/2^*k, -1/2^*h+1/2^*k-l$ 0.013 for $-h-2^*l, -k, l$	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9530	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

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.

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% of the height of the origin peak. No significant pseudotranslation is detected.*

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2PO

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	0.61	7/3042 (0.2%)	1.50	46/4143 (1.1%)
1	B	0.59	6/3042 (0.2%)	1.50	51/4143 (1.2%)
1	C	0.59	6/3042 (0.2%)	1.76	52/4143 (1.3%)
All	All	0.60	19/9126 (0.2%)	1.59	149/12429 (1.2%)

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
1	B	0	1
1	C	0	1
All	All	0	3

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	291	PRO	C-N	9.28	1.46	1.33
1	B	291	PRO	C-N	9.27	1.46	1.33
1	C	291	PRO	C-N	8.39	1.45	1.33
1	A	320	LEU	CB-CG	7.71	1.68	1.53
1	A	419	LEU	CG-CD2	-6.14	1.32	1.52

The worst 5 of 149 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	172	ASP	CA-C-N	47.90	179.72	119.84
1	C	172	ASP	C-N-CA	47.90	179.72	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	291	PRO	O-C-N	-35.10	75.25	122.64
1	C	291	PRO	O-C-N	-34.63	75.89	122.64
1	A	291	PRO	O-C-N	-33.50	77.41	122.64

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	291	PRO	Mainchain
1	B	291	PRO	Mainchain
1	C	291	PRO	Mainchain

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	2982	0	2905	90	0
1	B	2982	0	2905	92	0
1	C	2982	0	2905	87	0
2	A	4	0	1	0	0
2	B	4	0	1	0	0
3	A	185	0	0	2	0
3	B	195	0	0	2	0
3	C	196	0	0	1	0
All	All	9530	0	8717	224	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 224 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:B:283:LEU:HD22	1:B:285:THR:HG23	1.68	0.76
1:B:169:ARG:HH12	1:C:145:ASN:HD21	1.35	0.75
1:A:145:ASN:HD21	1:C:169:ARG:HH12	1.35	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:GLN:HE22	1:B:97:GLY:H	1.35	0.74
1:A:283:LEU:HD22	1:A:285:THR:HG23	1.68	0.74

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	397/410 (97%)	372 (94%)	22 (6%)	3 (1%)	16	6
1	B	397/410 (97%)	372 (94%)	23 (6%)	2 (0%)	24	14
1	C	397/410 (97%)	370 (93%)	24 (6%)	3 (1%)	16	6
All	All	1191/1230 (97%)	1114 (94%)	69 (6%)	8 (1%)	18	8

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	173	PRO
1	A	199	ASN
1	B	199	ASN
1	C	199	ASN
1	B	291	PRO

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	322/325 (99%)	300 (93%)	22 (7%)	14	5
1	B	322/325 (99%)	303 (94%)	19 (6%)	18	7
1	C	322/325 (99%)	300 (93%)	22 (7%)	14	5
All	All	966/975 (99%)	903 (94%)	63 (6%)	15	5

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	159	PRO
1	C	344	PRO
1	B	344	PRO
1	C	320	LEU
1	C	390	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	425	HIS
1	C	247	ASN
1	C	53	ASN
1	C	145	ASN
1	C	264	HIS

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	$\# Z > 2$
2	2PO	A	1002	-	0,3,3	-	-	0,3,3	-	-
2	2PO	B	1001	-	0,3,3	-	-	0,3,3	-	-

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 [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	395/410 (96%)	-1.48	0 100 100	7, 13, 25, 32	0
1	B	395/410 (96%)	-1.48	0 100 100	7, 13, 25, 31	0
1	C	395/410 (96%)	-1.48	0 100 100	6, 13, 24, 31	0
All	All	1185/1230 (96%)	-1.48	0 100 100	6, 13, 25, 32	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 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(Å ²)	Q<0.9
2	2PO	A	1002	4/4	0.96	0.05	56,56,56,56	0
2	2PO	B	1001	4/4	0.99	0.06	57,58,58,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.