



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:07 PM UTC

PDB ID : 2V6F / pdb_00002v6f
Title : Structure of Progesterone 5beta-Reductase from Digitalis Lanata
Authors : Thorn, A.; Egerer-Sieber, C.; Jaeger, C.M.; Herl, V.; Mueller-Uri, F.; Kreis, W.; Muller, Y.A.
Deposited on : 2007-07-18
Resolution : 2.40 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
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

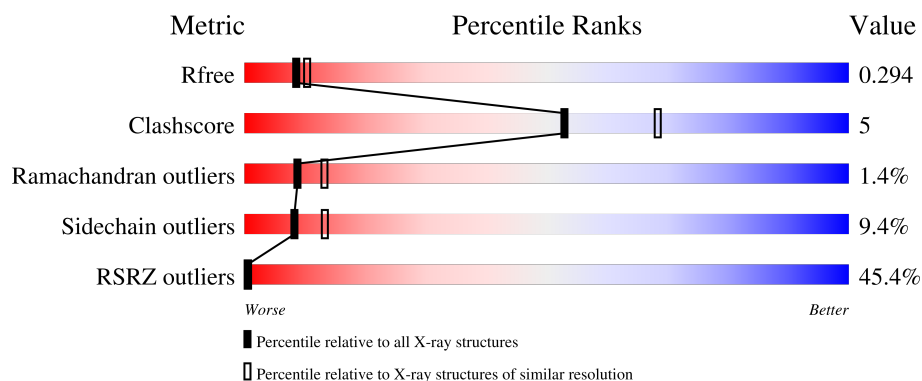
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	364	44% 80% 14% ...

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2927 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 PROGESTERONE 5-BETA-REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	S	0	0	0
			2787	1783	463	524	17			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	298	GLU	GLY	conflict	UNP Q6PQJ9

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

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

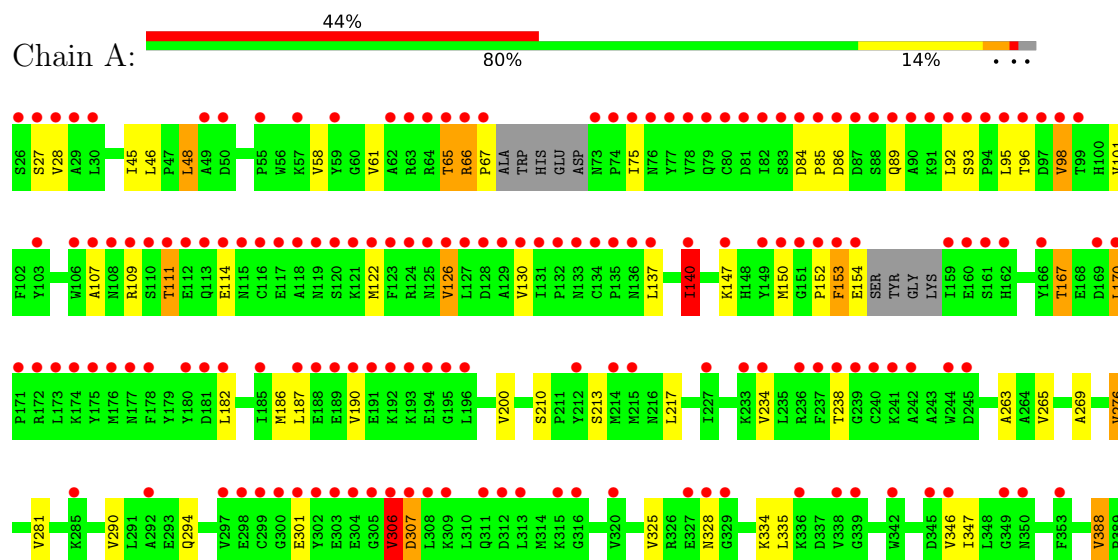
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	139	Total	O	0	0
			139	139		

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: PROGESTERONE 5-BETA-REDUCTASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	78.66Å 78.66Å 180.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.34 – 2.40 39.34 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.34-2.40) 100.0 (39.34-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.45 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.205 , 0.251 0.277 , 0.294	Depositor DCC
R_{free} test set	2313 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.429	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 91.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.29$, $\langle L^2 \rangle = 0.12$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	2927	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.97% 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

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	0.87	6/2864 (0.2%)	0.95	4/3890 (0.1%)

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	85	PRO	C-O	10.57	1.37	1.24
1	A	86	ASP	CG-OD2	10.03	1.44	1.25
1	A	86	ASP	CG-OD1	8.34	1.41	1.25
1	A	85	PRO	C-N	8.09	1.45	1.33
1	A	140	ILE	CA-CB	6.34	1.61	1.54
1	A	84	ASP	C-O	5.60	1.31	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	388	VAL	N-CA-C	-7.28	103.22	109.19
1	A	276	VAL	CB-CA-C	-6.87	102.56	110.73
1	A	388	VAL	CB-CA-C	6.67	115.86	109.33
1	A	388	VAL	N-CA-CB	-5.59	105.66	111.64

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	306	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	2787	0	2648	27	0
2	A	1	0	0	0	0
3	A	139	0	0	2	0
All	All	2927	0	2648	27	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 (27) 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:66:ARG:HB2	1:A:67:PRO:HA	1.73	0.71
1:A:167:THR:O	1:A:170:LEU:HD22	1.98	0.64
1:A:238:THR:HG23	1:A:238:THR:O	1.98	0.64
1:A:153:PHE:CA	1:A:154:GLU:HB2	2.32	0.60
1:A:153:PHE:CA	1:A:154:GLU:CB	2.81	0.59
1:A:150:MET:HE1	3:A:1104:HOH:O	2.02	0.58
1:A:107:ALA:HB1	1:A:109:ARG:NH1	2.19	0.57
1:A:325:VAL:O	1:A:328:ASN:O	2.23	0.56
1:A:95:LEU:O	1:A:98:VAL:HG13	2.09	0.52
1:A:170:LEU:O	1:A:170:LEU:HD23	2.12	0.50
1:A:89:GLN:NE2	1:A:93:SER:OG	2.45	0.49
1:A:306:VAL:HG22	1:A:307:ASP:H	1.77	0.49
1:A:186:MET:O	1:A:190:VAL:HG23	2.12	0.49
1:A:306:VAL:HG22	1:A:307:ASP:N	2.29	0.47
1:A:217:LEU:HD13	1:A:347:ILE:HD12	1.97	0.46
1:A:167:THR:O	1:A:170:LEU:CD2	2.63	0.45
1:A:210:SER:OG	1:A:213:SER:HB2	2.16	0.45
1:A:140:ILE:HD12	1:A:140:ILE:C	2.43	0.44
1:A:290:VAL:O	1:A:294:GLN:HG2	2.17	0.44
1:A:45:ILE:HA	1:A:48:LEU:HD22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:MET:O	1:A:126:VAL:HG13	2.18	0.42
1:A:263:ALA:HA	1:A:269:ALA:CB	2.49	0.42
1:A:334:LYS:NZ	3:A:1099:HOH:O	2.52	0.42
1:A:28:VAL:HB	1:A:98:VAL:HA	2.01	0.42
1:A:186:MET:HE1	1:A:200:VAL:HG22	2.00	0.42
1:A:111:THR:HG23	1:A:114:GLU:CD	2.46	0.41
1:A:130:VAL:HG12	1:A:137:LEU:HD22	2.04	0.40

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	349/364 (96%)	332 (95%)	12 (3%)	5 (1%)	9 13

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	306	VAL
1	A	66	ARG
1	A	65	THR
1	A	153	PHE
1	A	152	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	297/314 (95%)	269 (91%)	28 (9%)	8 13

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	SER
1	A	46	LEU
1	A	48	LEU
1	A	58	VAL
1	A	61	VAL
1	A	65	THR
1	A	75	ILE
1	A	92	LEU
1	A	96	THR
1	A	98	VAL
1	A	101	VAL
1	A	111	THR
1	A	126	VAL
1	A	140	ILE
1	A	147	LYS
1	A	167	THR
1	A	170	LEU
1	A	182	LEU
1	A	187	LEU
1	A	234	VAL
1	A	265	VAL
1	A	276	VAL
1	A	281	VAL
1	A	301	GLU
1	A	307	ASP
1	A	335	LEU
1	A	346	VAL
1	A	388	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	125	ASN
1	A	136	ASN

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](#)

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 [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 ⓘ

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, 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	355/364 (97%)	1.90	161 (45%) 0 0	26, 76, 144, 189	0

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	96	THR	6.8
1	A	176	MET	5.8
1	A	90	ALA	5.3
1	A	174	LYS	5.2
1	A	132	PRO	4.9
1	A	67	PRO	4.8
1	A	307	ASP	4.8
1	A	153	PHE	4.8
1	A	175	TYR	4.8
1	A	85	PRO	4.7
1	A	212	TYR	4.7
1	A	305	GLY	4.6
1	A	306	VAL	4.6
1	A	115	ASN	4.6
1	A	309	LYS	4.6
1	A	304	GLU	4.5
1	A	133	ASN	4.5
1	A	151	GLY	4.5
1	A	173	LEU	4.5
1	A	152	PRO	4.5
1	A	107	ALA	4.4
1	A	308	LEU	4.4
1	A	63	ARG	4.4
1	A	26	SER	4.4
1	A	84	ASP	4.3
1	A	86	ASP	4.3
1	A	83	SER	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	95	LEU	4.2
1	A	299	CYS	4.2
1	A	78	VAL	4.2
1	A	131	ILE	4.1
1	A	94	PRO	4.1
1	A	93	SER	4.1
1	A	190	VAL	4.1
1	A	128	ASP	4.0
1	A	110	SER	4.0
1	A	154	GLU	3.9
1	A	160	GLU	3.9
1	A	129	ALA	3.9
1	A	88	SER	3.9
1	A	113	GLN	3.9
1	A	112	GLU	3.9
1	A	303	GLU	3.9
1	A	300	GLY	3.8
1	A	159	ILE	3.8
1	A	66	ARG	3.8
1	A	124	ARG	3.8
1	A	91	LYS	3.7
1	A	116	CYS	3.7
1	A	161	SER	3.6
1	A	82	ILE	3.6
1	A	242	ALA	3.6
1	A	92	LEU	3.6
1	A	127	LEU	3.6
1	A	118	ALA	3.5
1	A	195	GLY	3.5
1	A	126	VAL	3.5
1	A	302	TYR	3.5
1	A	109	ARG	3.5
1	A	301	GLU	3.5
1	A	135	PRO	3.5
1	A	185	ILE	3.5
1	A	111	THR	3.4
1	A	192	LYS	3.4
1	A	80	CYS	3.4
1	A	59	TYR	3.3
1	A	87	ASP	3.3
1	A	76	ASN	3.2
1	A	117	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	81	ASP	3.2
1	A	297	VAL	3.2
1	A	194	GLU	3.2
1	A	241	LYS	3.2
1	A	234	VAL	3.2
1	A	108	ASN	3.1
1	A	349	GLY	3.1
1	A	134	CYS	3.1
1	A	187	LEU	3.1
1	A	64	ARG	3.1
1	A	89	GLN	3.1
1	A	140	ILE	3.1
1	A	62	ALA	3.0
1	A	178	PHE	3.0
1	A	312	ASP	3.0
1	A	130	VAL	3.0
1	A	170	LEU	3.0
1	A	214	MET	2.9
1	A	180	TYR	2.9
1	A	313	LEU	2.9
1	A	311	GLN	2.9
1	A	298	GLU	2.9
1	A	191	GLU	2.9
1	A	327	GLU	2.9
1	A	121	LYS	2.9
1	A	172	ARG	2.8
1	A	320	VAL	2.8
1	A	171	PRO	2.8
1	A	65	THR	2.8
1	A	239	GLY	2.8
1	A	119	ASN	2.8
1	A	98	VAL	2.8
1	A	29	ALA	2.8
1	A	79	GLN	2.8
1	A	339	GLY	2.8
1	A	136	ASN	2.8
1	A	74	PRO	2.8
1	A	345	ASP	2.8
1	A	342	TRP	2.7
1	A	28	VAL	2.7
1	A	236	ARG	2.7
1	A	97	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	237	PHE	2.7
1	A	120	SER	2.7
1	A	181	ASP	2.6
1	A	27	SER	2.6
1	A	238	THR	2.6
1	A	328	ASN	2.6
1	A	189	GLU	2.6
1	A	188	GLU	2.5
1	A	137	LEU	2.5
1	A	233	LYS	2.5
1	A	123	PHE	2.5
1	A	350	ASN	2.5
1	A	147	LYS	2.5
1	A	193	LYS	2.5
1	A	346	VAL	2.5
1	A	73	ASN	2.5
1	A	99	THR	2.5
1	A	244	TRP	2.4
1	A	245	ASP	2.4
1	A	125	ASN	2.4
1	A	329	GLY	2.4
1	A	162	HIS	2.4
1	A	196	LEU	2.4
1	A	103	TYR	2.4
1	A	57	LYS	2.4
1	A	50	ASP	2.3
1	A	114	GLU	2.3
1	A	55	PRO	2.3
1	A	30	LEU	2.3
1	A	177	ASN	2.3
1	A	182	LEU	2.2
1	A	315	LYS	2.2
1	A	240	CYS	2.2
1	A	150	MET	2.2
1	A	169	ASP	2.2
1	A	292	ALA	2.2
1	A	285	LYS	2.2
1	A	122	MET	2.2
1	A	106	TRP	2.2
1	A	49	ALA	2.2
1	A	338	VAL	2.1
1	A	75	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	149	TYR	2.1
1	A	166	TYR	2.1
1	A	353	PHE	2.1
1	A	316	GLY	2.1
1	A	227	ILE	2.1
1	A	336	LYS	2.0
1	A	77	TYR	2.0
1	A	215	MET	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 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	NA	A	1390	1/1	0.88	0.18	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.