



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:06 AM GMT

PDB ID : 3H52
Title : Crystal structure of the antagonist form of human glucocorticoid receptor
Authors : Schoch, G.A.; Benz, J.; D'Arcy, B.; Stihle, M.; Burger, D.; Thoma, R.; Ruf, A.
Deposited on : 2009-04-21
Resolution : 2.80 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

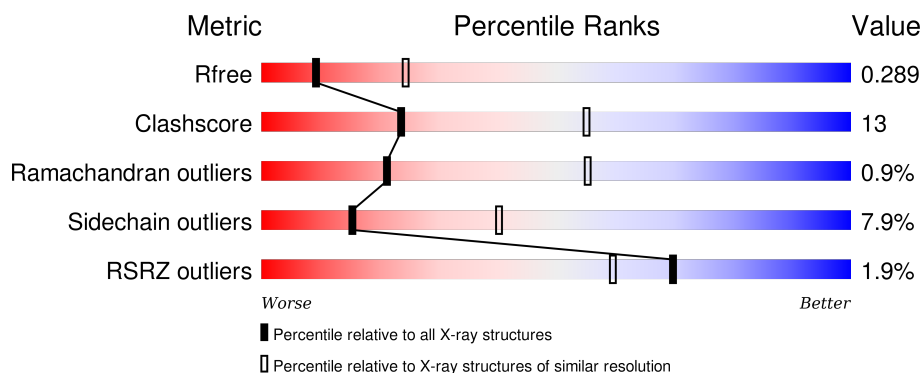
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	254	<div> <div>0%</div> <div> <div></div> <div>70%</div> <div>24%</div> <div>• •</div> </div> </div>
1	B	254	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>21%</div> <div>• •</div> </div> </div>
1	C	254	<div> <div>3%</div> <div> <div></div> <div>66%</div> <div>26%</div> <div>• 7%</div> </div> </div>
1	D	254	<div> <div>2%</div> <div> <div></div> <div>65%</div> <div>25%</div> <div>• 8%</div> </div> </div>
2	M	19	<div> <div></div> <div> <div>26%</div> <div>26%</div> <div>47%</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	N	19	 A horizontal bar chart showing the quality of chain N. The bar is divided into five segments: a small red segment at the beginning labeled '5%', followed by a large green segment labeled '63%', then a yellow segment labeled '11%', an orange segment labeled '5%', and a grey segment at the end labeled '21%'.

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7989 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 Glucocorticoid receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	247	Total	C	N	O	S	0	0	0
			1964	1265	325	357	17			
1	B	249	Total	C	N	O	S	0	0	0
			1986	1279	327	363	17			
1	C	237	Total	C	N	O	S	0	0	0
			1845	1180	314	336	15			
1	D	234	Total	C	N	O	S	0	0	0
			1855	1193	308	338	16			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	524	GLY	-	EXPRESSION TAG	UNP P04150
A	525	SER	-	EXPRESSION TAG	UNP P04150
A	526	HIS	-	EXPRESSION TAG	UNP P04150
A	527	MET	-	EXPRESSION TAG	UNP P04150
A	602	SER	PHE	ENGINEERED	UNP P04150
A	638	ASP	CYS	ENGINEERED	UNP P04150
A	684	ALA	GLU	ENGINEERED	UNP P04150
A	688	ALA	GLU	ENGINEERED	UNP P04150
A	712	SER	TRP	ENGINEERED	UNP P04150
B	524	GLY	-	EXPRESSION TAG	UNP P04150
B	525	SER	-	EXPRESSION TAG	UNP P04150
B	526	HIS	-	EXPRESSION TAG	UNP P04150
B	527	MET	-	EXPRESSION TAG	UNP P04150
B	602	SER	PHE	ENGINEERED	UNP P04150
B	638	ASP	CYS	ENGINEERED	UNP P04150
B	684	ALA	GLU	ENGINEERED	UNP P04150
B	688	ALA	GLU	ENGINEERED	UNP P04150
B	712	SER	TRP	ENGINEERED	UNP P04150
C	524	GLY	-	EXPRESSION TAG	UNP P04150
C	525	SER	-	EXPRESSION TAG	UNP P04150
C	526	HIS	-	EXPRESSION TAG	UNP P04150

Continued on next page...

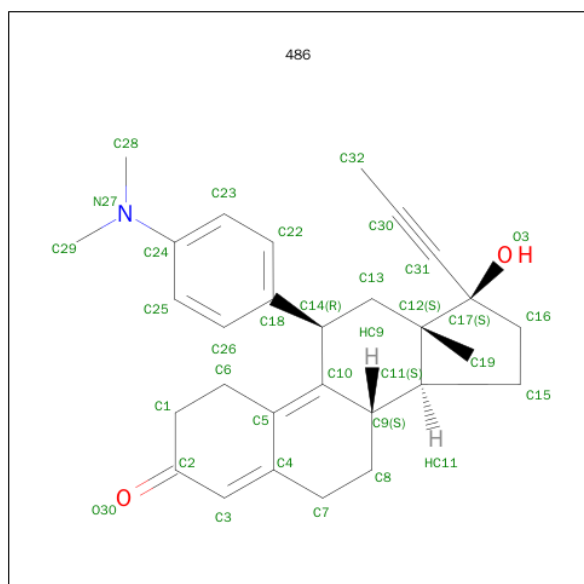
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	527	MET	-	EXPRESSION TAG	UNP P04150
C	602	SER	PHE	ENGINEERED	UNP P04150
C	638	ASP	CYS	ENGINEERED	UNP P04150
C	684	ALA	GLU	ENGINEERED	UNP P04150
C	688	ALA	GLU	ENGINEERED	UNP P04150
C	712	SER	TRP	ENGINEERED	UNP P04150
D	524	GLY	-	EXPRESSION TAG	UNP P04150
D	525	SER	-	EXPRESSION TAG	UNP P04150
D	526	HIS	-	EXPRESSION TAG	UNP P04150
D	527	MET	-	EXPRESSION TAG	UNP P04150
D	602	SER	PHE	ENGINEERED	UNP P04150
D	638	ASP	CYS	ENGINEERED	UNP P04150
D	684	ALA	GLU	ENGINEERED	UNP P04150
D	688	ALA	GLU	ENGINEERED	UNP P04150
D	712	SER	TRP	ENGINEERED	UNP P04150

- Molecule 2 is a protein called Nuclear receptor corepressor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	15	Total	C	N	O	S	0	0	0
			106	66	19	20	1			
2	M	10	Total	C	N	O	S	0	0	0
			72	44	14	13	1			

- Molecule 3 is 11-(4-DIMETHYLAMINO-PHENYL)-17-HYDROXY-13-METHYL-17-PRO P-1-YNYL-1,2,6,7,8,11,12,13,14,15,16,17-DODEC AHYDRO-CYCLOPENTA[A]PHENAN THREN-3-ONE (three-letter code: 486) (formula: $C_{29}H_{35}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			32	29	1	2		
3	B	1	Total	C	N	O	0	0
			32	29	1	2		
3	C	1	Total	C	N	O	0	0
			32	29	1	2		
3	D	1	Total	C	N	O	0	0
			32	29	1	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	8	Total	O	0	0
			8	8		
5	B	4	Total	O	0	0
			4	4		
5	C	1	Total	O	0	0
			1	1		
5	D	11	Total	O	0	0
			11	11		
5	N	2	Total	O	0	0
			2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	M	1	Total	O	0	0
			1	1		



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	99.53Å 99.53Å 252.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.10 – 2.80 43.10 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (43.10-2.80) 99.8 (43.10-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.226 , 0.283 0.232 , 0.289	Depositor DCC
R_{free} test set	1830 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	66.3	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 68.0	EDS
Estimated twinning fraction	0.034 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 36497 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7989	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, 486

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	0.46	0/2004	0.58	0/2711
1	B	0.45	0/2028	0.58	0/2746
1	C	0.41	0/1880	0.56	0/2547
1	D	0.43	0/1891	0.58	0/2556
2	M	0.55	0/71	0.63	0/92
2	N	0.49	0/105	0.68	0/138
All	All	0.44	0/7979	0.58	0/10790

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.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	616	SER	Peptide

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	1964	0	1965	53	0
1	B	1986	0	1987	60	0
1	C	1845	0	1816	47	0
1	D	1855	0	1848	54	0
2	M	72	0	75	3	0
2	N	106	0	108	7	0
3	A	32	0	35	5	0
3	B	32	0	35	9	0
3	C	32	0	35	7	0
3	D	32	0	35	14	0
4	B	6	0	8	0	0
5	A	8	0	0	0	0
5	B	4	0	0	0	0
5	C	1	0	0	0	0
5	D	11	0	0	1	0
5	M	1	0	0	1	0
5	N	2	0	0	0	0
All	All	7989	0	7947	210	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 210 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:D:685:LEU:HD13	1:D:689:ILE:HD11	1.41	1.02
1:A:652:GLU:HG2	1:A:721:LEU:HD13	1.46	0.98
1:A:571:VAL:HG22	1:A:604:MET:HE1	1.46	0.95
1:A:634:MET:HE1	1:A:647:LEU:HD11	1.50	0.93
1:A:670:LEU:HD13	1:A:722:LEU:HD22	1.48	0.93

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	243/254 (96%)	222 (91%)	19 (8%)	2 (1%)	24	58
1	B	247/254 (97%)	221 (90%)	22 (9%)	4 (2%)	12	38
1	C	233/254 (92%)	215 (92%)	16 (7%)	2 (1%)	21	55
1	D	228/254 (90%)	214 (94%)	13 (6%)	1 (0%)	39	74
2	M	8/19 (42%)	7 (88%)	1 (12%)	0	100	100
2	N	13/19 (68%)	11 (85%)	2 (15%)	0	100	100
All	All	972/1054 (92%)	890 (92%)	73 (8%)	9 (1%)	21	55

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	528	LEU
1	B	769	ILE
1	C	764	TYR
1	D	679	GLY
1	A	530	PRO

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	215/231 (93%)	201 (94%)	14 (6%)	21	52
1	B	219/231 (95%)	202 (92%)	17 (8%)	16	41
1	C	196/231 (85%)	179 (91%)	17 (9%)	13	35
1	D	202/231 (87%)	187 (93%)	15 (7%)	17	43
2	M	7/15 (47%)	5 (71%)	2 (29%)	0	1
2	N	10/15 (67%)	8 (80%)	2 (20%)	1	5
All	All	849/954 (89%)	782 (92%)	67 (8%)	15	40

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	776	GLN
1	C	640	TYR
1	D	758	THR
1	C	535	LEU
1	C	613	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	731	ASN
1	C	683	GLN
1	D	775	HIS
1	B	776	GLN
1	C	570	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

5 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	486	A	3	-	36,36,36	0.62	0	48,56,56	1.66	10 (20%)
3	486	B	1	-	36,36,36	0.93	2 (5%)	48,56,56	2.24	13 (27%)
4	GOL	B	778	-	5,5,5	0.30	0	5,5,5	0.56	0
3	486	C	4	-	36,36,36	0.77	1 (2%)	48,56,56	1.80	7 (14%)
3	486	D	2	-	36,36,36	0.90	1 (2%)	48,56,56	2.00	12 (25%)

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	486	A	3	-	-	0/8/72/72	0/5/5/5
3	486	B	1	-	-	0/8/72/72	0/5/5/5
4	GOL	B	778	-	-	0/4/4/4	0/0/0/0
3	486	C	4	-	-	0/8/72/72	0/5/5/5
3	486	D	2	-	-	0/8/72/72	0/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1	486	C12-C17	-3.87	1.51	1.56
3	D	2	486	C12-C17	-3.42	1.52	1.56
3	C	4	486	C12-C17	-3.02	1.52	1.56
3	B	1	486	C3-C2	-2.20	1.40	1.45

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1	486	C12-C11-C9	-8.06	106.35	113.59
3	C	4	486	C12-C11-C9	-6.63	107.63	113.59
3	B	1	486	C16-C17-C12	-6.62	98.45	102.91
3	D	2	486	C12-C11-C9	-6.46	107.79	113.59
3	A	3	486	C12-C11-C9	-5.49	108.65	113.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3	486	5	0
3	B	1	486	9	0
3	C	4	486	7	0
3	D	2	486	14	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	247/254 (97%)	-0.25	2 (0%) 87 81	33, 43, 69, 76	0
1	B	249/254 (98%)	-0.34	5 (2%) 68 58	37, 47, 69, 75	0
1	C	237/254 (93%)	-0.03	7 (2%) 54 41	34, 50, 69, 80	0
1	D	234/254 (92%)	-0.25	4 (1%) 73 63	25, 43, 55, 74	0
2	M	10/19 (52%)	-0.18	0 100 100	32, 34, 37, 38	0
2	N	15/19 (78%)	-0.27	1 (6%) 21 12	45, 50, 58, 58	0
All	All	992/1054 (94%)	-0.22	19 (1%) 70 59	25, 46, 68, 80	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	635	THR	7.4
1	D	739	THR	4.0
1	C	637	PRO	3.3
1	B	711	ASN	2.9
1	C	764	TYR	2.9

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, 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	LLDF	B-factors(Å ²)	Q<0.9
3	486	C	4	32/32	0.95	0.26	1.27	43,48,54,54	0
3	486	A	3	32/32	0.97	0.22	1.09	32,39,41,41	0
3	486	B	1	32/32	0.96	0.18	0.42	29,40,43,45	0
3	486	D	2	32/32	0.96	0.15	-0.54	31,34,35,36	0
4	GOL	B	778	6/6	0.91	0.11	-1.23	80,80,81,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.