



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:16 AM GMT

PDB ID : 3HS6
Title : X-ray crystal structure of eicosapentaenoic acid bound to the cyclooxygenase channel of cyclooxygenase-2
Authors : Vecchio, A.J.; Simmons, D.M.; Malkowski, M.G.
Deposited on : 2009-06-10
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
<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

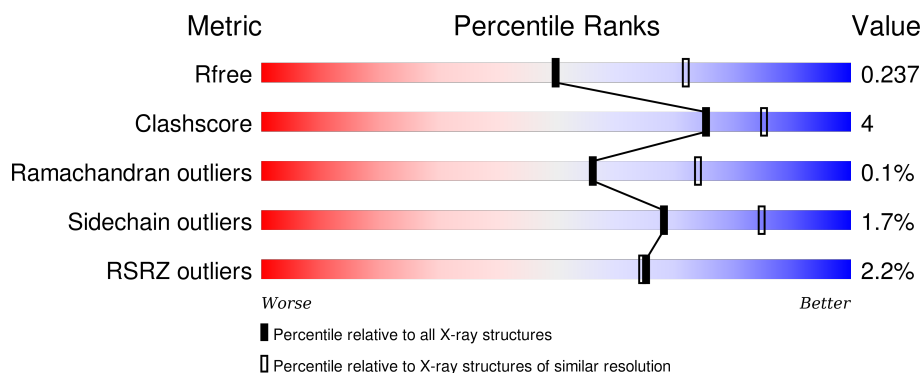
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (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 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	591	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 86%, grey 12%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 86% 6% • 7% </div> </div>
1	B	591	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 1%, green 85%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 3% 85% 7% 7% </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EPA	B	1	-	-	X	X
3	AKR	A	2	-	-	X	X
3	AKR	B	2	-	-	X	-
3	AKR	B	3	-	-	-	X
4	COH	A	619	-	-	-	X
4	COH	B	619	-	-	-	X
5	NAG	A	661	X	-	-	X
7	NAG	A	681	-	-	-	X
7	NAG	B	681	-	-	-	X
9	EDO	A	620	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 9765 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.

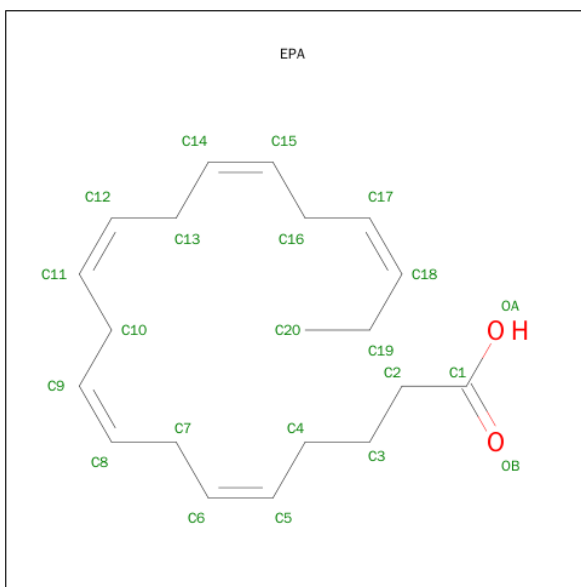
- Molecule 1 is a protein called Prostaglandin G/H synthase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	551	Total	C	N	O	S	0	3	0
			4463	2882	743	813	25			
1	B	551	Total	C	N	O	S	0	3	0
			4442	2868	742	807	25			

There are 14 discrepancies between the modelled and reference sequences:

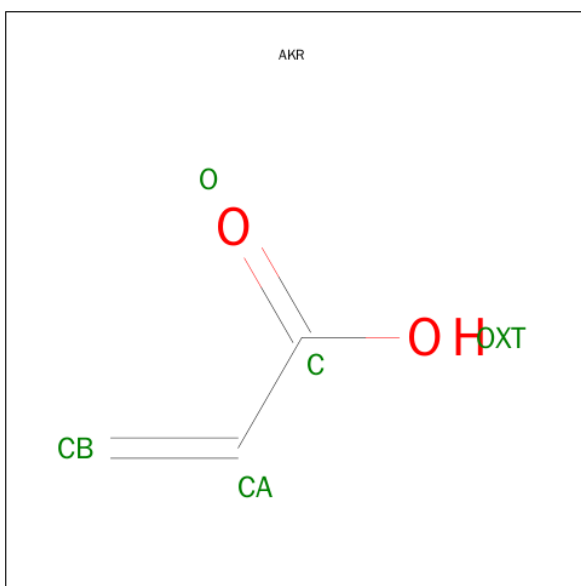
Chain	Residue	Modelled	Actual	Comment	Reference
A	29	HIS	-	EXPRESSION TAG	UNP Q05769
A	30	HIS	-	EXPRESSION TAG	UNP Q05769
A	31	HIS	-	EXPRESSION TAG	UNP Q05769
A	32	HIS	-	EXPRESSION TAG	UNP Q05769
A	33	HIS	-	EXPRESSION TAG	UNP Q05769
A	34	HIS	-	EXPRESSION TAG	UNP Q05769
A	594	ALA	ASN	ENGINEERED	UNP Q05769
B	29	HIS	-	EXPRESSION TAG	UNP Q05769
B	30	HIS	-	EXPRESSION TAG	UNP Q05769
B	31	HIS	-	EXPRESSION TAG	UNP Q05769
B	32	HIS	-	EXPRESSION TAG	UNP Q05769
B	33	HIS	-	EXPRESSION TAG	UNP Q05769
B	34	HIS	-	EXPRESSION TAG	UNP Q05769
B	594	ALA	ASN	ENGINEERED	UNP Q05769

- Molecule 2 is 5,8,11,14,17-EICOSAPENTAENOIC ACID (three-letter code: EPA) (formula: $C_{20}H_{30}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			22	20	2		
2	B	1	Total	C	O	0	0
			22	20	2		

- Molecule 3 is ACRYLIC ACID (three-letter code: AKR) (formula: $C_3H_4O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			5	3	2		
3	A	1	Total	C	O	0	0
			5	3	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 5 3 2	0	0
3	B	1	Total C O 5 3 2	0	0

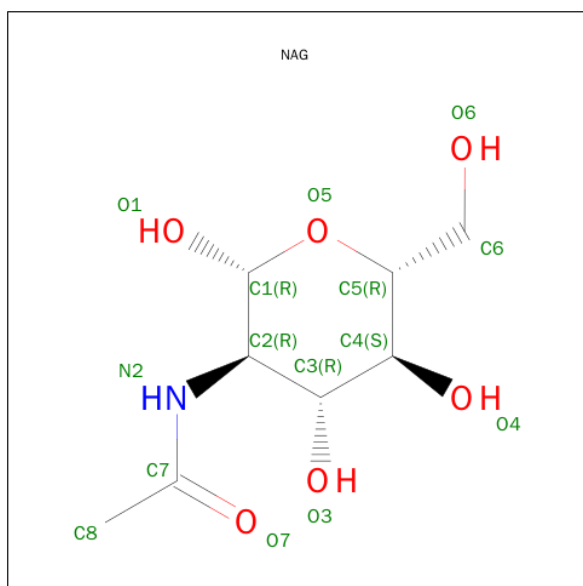
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- The chemical structure shows a central cobalt (Co) atom coordinated by four nitrogen atoms (N) in a corrin-like macrocycle. The macrocycle consists of four pyrrole rings linked by methylene bridges. The nitrogen atoms are labeled NC, NB, ND, and NE. The cobalt atom is coordinated to these nitrogens and two water molecules (O1A and O2A). The side chains are labeled CAA and CBA, and the carboxylic acid groups are labeled C1A and C2A. The structure is shown in a 2D representation with various atoms labeled with their element symbols and coordinates.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	2	Total 28	C 16	N 2	O 10	0	0
5	B	2	Total 28	C 16	N 2	O 10	0	0

- 

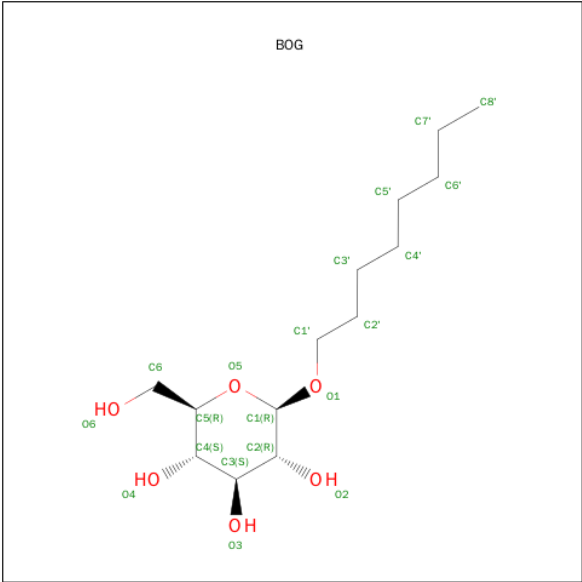
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 7 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



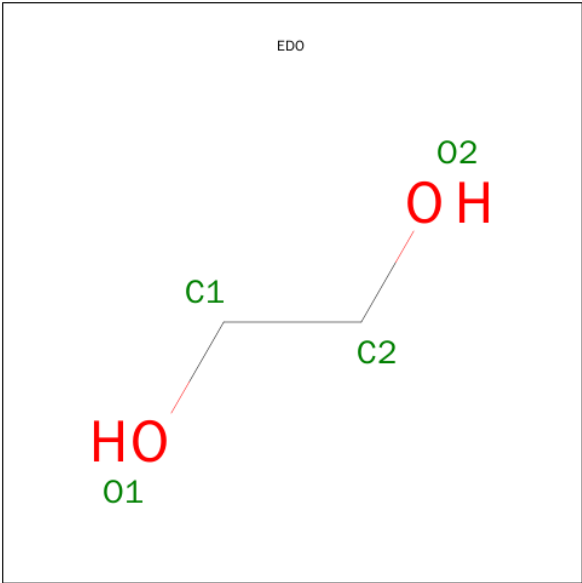
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			20	14	6		
8	B	1	Total	C	O	0	0
			20	14	6		

- Molecule 9 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total 4	C 2	O 2	0	0
9	A	1	Total 4	C 2	O 2	0	0
9	A	1	Total 4	C 2	O 2	0	0
9	B	1	Total 4	C 2	O 2	0	0
9	B	1	Total 4	C 2	O 2	0	0
9	B	1	Total 4	C 2	O 2	0	0

- Molecule 10 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	2	Total 28	C 16	N 2	O 10	0	0

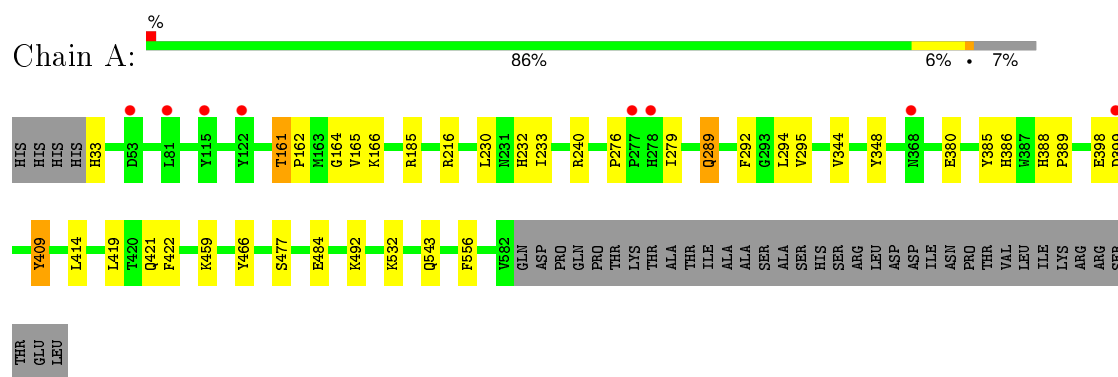
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	258	Total 258	O 258	0	0
11	B	229	Total 229	O 229	0	0

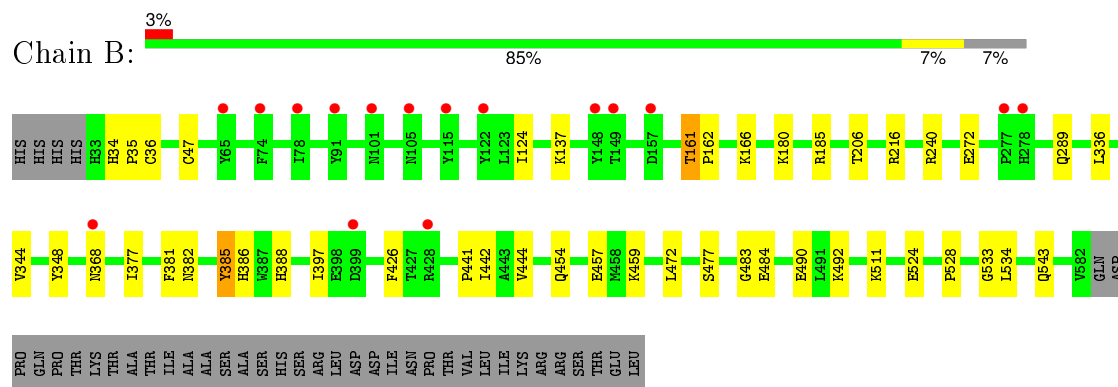
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Prostaglandin G/H synthase 2



• Molecule 1: Prostaglandin G/H synthase 2



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	121.85Å 132.34Å 180.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.95 – 2.40 19.95 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.95-2.40) 99.9 (19.95-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.176 , 0.223 0.189 , 0.237	Depositor DCC
R_{free} test set	2889 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	34.8	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 56978 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9765	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, AKR, EDO, NDG, EPA, COH, BOG, MAN

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	0.44	0/4600	0.53	0/6249
1	B	0.44	0/4578	0.54	0/6218
All	All	0.44	0/9178	0.53	0/12467

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
5	A	2	0

There are no bond length outliers.

There are no bond angle outliers.

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	661	NAG	C5,C1

There are no planarity outliers.

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	4463	0	4295	28	0
1	B	4442	0	4263	42	0
2	A	22	0	29	0	0
2	B	22	0	29	9	0
3	A	10	0	6	5	0
3	B	10	0	6	5	0
4	A	43	0	30	0	0
4	B	43	0	30	0	0
5	A	28	0	25	0	0
5	B	28	0	25	1	0
6	A	39	0	34	3	0
7	A	14	0	13	0	0
7	B	14	0	13	0	0
8	A	20	0	28	1	0
8	B	20	0	28	5	0
9	A	20	0	30	2	0
9	B	12	0	18	2	0
10	B	28	0	25	0	0
11	A	258	0	0	3	0
11	B	229	0	0	1	0
All	All	9765	0	8927	70	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 4.

All (70) 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:533:GLY:HA3	2:B:1:EPA:H181	1.44	0.99
1:A:477:SER:HB2	3:A:2:AKR:HA1	1.51	0.93
1:B:477:SER:HB2	3:B:2:AKR:HA1	1.51	0.90
1:A:216:ARG:HH11	6:A:672:NAG:H83	1.43	0.81
1:B:185:ARG:CZ	8:B:703:BOG:H4'2	2.11	0.81
1:B:36:CYS:HG	1:B:47:CYS:HG	0.91	0.79
1:B:161:THR:HG21	1:B:166:LYS:O	1.84	0.77
1:B:534:LEU:HG	2:B:1:EPA:H171	1.70	0.72
1:B:533:GLY:HA3	2:B:1:EPA:C18	2.19	0.72
1:A:492:LYS:HD3	3:A:2:AKR:HB2	1.72	0.72
1:A:161:THR:HG21	1:A:166:LYS:O	1.91	0.70
1:A:216:ARG:NH1	6:A:672:NAG:H83	2.07	0.70
1:A:532:LYS:HE2	11:A:10:HOH:O	1.93	0.69
1:B:272:GLU:HG3	3:B:3:AKR:HB2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:533:GLY:CA	2:B:1:EPA:H181	2.24	0.66
1:A:216:ARG:HH11	6:A:672:NAG:C8	2.10	0.65
1:A:414:LEU:HD11	1:A:419:LEU:HD12	1.78	0.65
1:A:289:GLN:HG2	1:A:292:PHE:CE1	2.33	0.63
1:A:294:LEU:HG	1:A:295:VAL:HG23	1.81	0.63
1:A:477:SER:CB	3:A:2:AKR:HA1	2.29	0.61
1:B:216:ARG:HG2	5:B:672:NAG:H81	1.83	0.61
1:B:492:LYS:HE2	3:B:2:AKR:HB2	1.81	0.60
1:A:543:GLN:O	1:B:137:LYS:HE2	2.01	0.60
1:B:386:HIS:HB3	1:B:388[B]:HIS:CE1	2.37	0.60
1:A:276:PRO:HD2	1:A:279:ILE:HD12	1.86	0.58
1:A:230:LEU:HD13	1:A:233:ILE:HD12	1.86	0.58
1:B:162:PRO:O	9:B:7:EDO:H12	2.06	0.56
1:B:459:LYS:HA	9:B:7:EDO:H11	1.86	0.56
1:B:180:LYS:HB3	1:B:490:GLU:HG2	1.88	0.56
1:B:454:GLN:HA	1:B:457:GLU:HG2	1.88	0.55
1:B:185:ARG:HG3	8:B:703:BOG:H7'2	1.89	0.54
1:A:459:LYS:HA	9:A:4:EDO:H11	1.88	0.54
1:B:185:ARG:NE	8:B:703:BOG:H5'1	2.24	0.53
1:A:33:HIS:N	11:A:748:HOH:O	2.42	0.53
1:B:124:ILE:HD11	1:B:528:PRO:HB2	1.92	0.52
1:B:483:GLY:HA3	1:B:511:LYS:HD3	1.91	0.52
1:B:382:ASN:O	1:B:386:HIS:HD2	1.93	0.52
1:B:477:SER:HB2	3:B:2:AKR:CA	2.33	0.52
1:B:377:ILE:CD1	2:B:1:EPA:H201	2.40	0.51
11:A:668:HOH:O	1:B:543:GLN:HB2	2.11	0.50
1:B:36:CYS:CB	1:B:47:CYS:HG	2.24	0.49
1:A:386:HIS:HB3	1:A:388[B]:HIS:CE1	2.49	0.48
1:B:206:THR:HG21	1:B:385:TYR:CE2	2.48	0.48
1:B:185:ARG:NH2	8:B:703:BOG:H4'2	2.29	0.47
1:A:161:THR:HG22	1:A:164:GLY:H	1.78	0.47
1:A:230:LEU:HD22	1:A:232:HIS:HE1	1.81	0.46
1:A:161:THR:HG22	1:A:164:GLY:N	2.31	0.46
1:A:380:GLU:HG2	1:A:466:TYR:CE2	2.52	0.45
1:B:381:PHE:HE2	2:B:1:EPA:H192	1.81	0.45
1:A:240:ARG:HH11	3:A:3:AKR:HA1	1.81	0.45
1:B:344:VAL:O	1:B:348:TYR:HB3	2.17	0.44
1:B:441:PRO:HG2	1:B:444:VAL:HG22	1.99	0.44
1:B:161:THR:HG23	11:B:694:HOH:O	2.17	0.43
1:B:161:THR:CG2	1:B:166:LYS:O	2.60	0.43
1:A:344:VAL:HA	1:A:348:TYR:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:ILE:HD11	2:B:1:EPA:H201	2.01	0.43
1:A:162:PRO:O	9:A:4:EDO:H12	2.19	0.42
1:B:385:TYR:OH	2:B:1:EPA:H131	2.19	0.42
1:A:477:SER:HB2	3:A:2:AKR:CA	2.36	0.42
1:A:398:GLU:HB3	1:A:399:ASP:H	1.72	0.42
1:B:381:PHE:HE2	2:B:1:EPA:C19	2.33	0.41
1:B:397:ILE:HD11	1:B:426:PHE:CE1	2.55	0.41
1:B:34:HIS:HA	1:B:35:PRO:HD3	1.92	0.41
1:A:398:GLU:OE1	1:A:421:GLN:HG2	2.20	0.41
8:A:703:BOG:H6'1	8:A:703:BOG:H3'1	1.70	0.41
1:B:240:ARG:NH2	1:B:272:GLU:O	2.33	0.41
1:B:472:LEU:HD21	1:B:524:GLU:HG3	2.02	0.41
1:B:185:ARG:HG3	8:B:703:BOG:H5'1	2.03	0.41
1:B:492:LYS:HD3	3:B:2:AKR:HB2	2.03	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	552/591 (93%)	537 (97%)	13 (2%)	2 (0%)	39	56
1	B	552/591 (93%)	537 (97%)	15 (3%)	0	100	100
All	All	1104/1182 (93%)	1074 (97%)	28 (2%)	2 (0%)	56	69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	409[A]	TYR
1	A	409[B]	TYR

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	484/529 (92%)	474 (98%)	10 (2%)	61	80
1	B	477/529 (90%)	470 (98%)	7 (2%)	72	87
All	All	961/1058 (91%)	944 (98%)	17 (2%)	68	84

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	161	THR
1	A	165	VAL
1	A	185	ARG
1	A	289	GLN
1	A	385	TYR
1	A	409[A]	TYR
1	A	409[B]	TYR
1	A	422	PHE
1	A	484	GLU
1	A	556	PHE
1	B	161	THR
1	B	289	GLN
1	B	336	LEU
1	B	368	ASN
1	B	385	TYR
1	B	442	ILE
1	B	484	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

9 carbohydrates 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	$\# Z > 2$
5	NAG	A	661	1,5	14,14,15	0.58	0	15,19,21	1.24	1 (6%)
5	NAG	A	662	5	14,14,15	0.44	0	15,19,21	1.15	1 (6%)
6	NAG	A	671	1,6	14,14,15	0.55	0	15,19,21	1.20	1 (6%)
6	NAG	A	672	6	14,14,15	0.58	0	15,19,21	0.90	0
6	MAN	A	673	6	11,11,12	0.51	0	14,15,17	1.51	1 (7%)
10	NAG	B	661	1,10	14,14,15	0.57	0	15,19,21	1.00	2 (13%)
10	NDG	B	662	10	14,14,15	0.67	0	15,19,21	0.99	0
5	NAG	B	671	1,5	14,14,15	0.59	0	15,19,21	1.05	1 (6%)
5	NAG	B	672	5	14,14,15	0.53	0	15,19,21	0.76	0

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
5	NAG	A	661	1,5	2/2/5/7	0/6/23/26	0/1/1/1
5	NAG	A	662	5	-	0/6/23/26	0/1/1/1
6	NAG	A	671	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	672	6	-	0/6/23/26	0/1/1/1
6	MAN	A	673	6	-	0/2/19/22	1/1/1/1
10	NAG	B	661	1,10	-	0/6/23/26	0/1/1/1
10	NDG	B	662	10	-	0/6/23/26	0/1/1/1
5	NAG	B	671	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	672	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	661	NAG	C4-C3-C2	2.13	114.54	111.23
5	A	662	NAG	C1-O5-C5	2.30	115.17	112.25
10	B	661	NAG	C1-O5-C5	2.52	115.44	112.25
5	A	661	NAG	C1-O5-C5	3.29	116.43	112.25
5	B	671	NAG	C1-O5-C5	3.70	116.94	112.25
6	A	671	NAG	C1-O5-C5	4.06	117.40	112.25
6	A	673	MAN	C1-O5-C5	4.51	117.97	112.25

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	661	NAG	C5
5	A	661	NAG	C1

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	673	MAN	C1-C2-C3-C4-C5-O5

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	672	NAG	3	0
5	B	672	NAG	1	0

5.6 Ligand geometry

20 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	EPA	A	1	-	18,21,21	0.30	0	18,21,21	0.72	0
3	AKR	A	2	-	1,4,4	1.55	0	0,4,4	0.00	-
3	AKR	A	3	-	1,4,4	1.60	0	0,4,4	0.00	-
9	EDO	A	4	-	3,3,3	0.45	0	2,2,2	0.51	0
9	EDO	A	5	-	3,3,3	0.47	0	2,2,2	0.48	0
9	EDO	A	6	-	3,3,3	0.51	0	2,2,2	0.48	0
4	COH	A	619	1	28,50,50	2.26	9 (32%)	19,82,82	1.34	3 (15%)
9	EDO	A	620	-	3,3,3	0.54	0	2,2,2	0.33	0
7	NAG	A	681	1	14,14,15	0.56	0	15,19,21	1.12	1 (6%)
8	BOG	A	703	-	20,20,20	0.43	0	25,25,25	0.76	1 (4%)
9	EDO	A	8	-	3,3,3	0.45	0	2,2,2	0.51	0
2	EPA	B	1	-	18,21,21	0.24	0	18,21,21	0.88	2 (11%)
3	AKR	B	2	-	1,4,4	1.57	0	0,4,4	0.00	-
3	AKR	B	3	-	1,4,4	1.57	0	0,4,4	0.00	-
4	COH	B	619	1	28,50,50	2.28	9 (32%)	19,82,82	1.66	4 (21%)
9	EDO	B	620	-	3,3,3	0.55	0	2,2,2	0.33	0
9	EDO	B	621	-	3,3,3	0.37	0	2,2,2	0.62	0
7	NAG	B	681	1	14,14,15	0.53	0	15,19,21	0.72	0
9	EDO	B	7	-	3,3,3	0.38	0	2,2,2	0.58	0
8	BOG	B	703	-	20,20,20	0.50	0	25,25,25	0.69	0

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	EPA	A	1	-	-	0/17/19/19	0/0/0/0
3	AKR	A	2	-	-	0/0/2/2	0/0/0/0
3	AKR	A	3	-	-	0/0/2/2	0/0/0/0
9	EDO	A	4	-	-	0/1/1/1	0/0/0/0
9	EDO	A	5	-	-	0/1/1/1	0/0/0/0
9	EDO	A	6	-	-	0/1/1/1	0/0/0/0
4	COH	A	619	1	-	0/6/54/54	0/0/8/8
9	EDO	A	620	-	-	0/1/1/1	0/0/0/0
7	NAG	A	681	1	-	0/6/23/26	0/1/1/1
8	BOG	A	703	-	-	0/11/31/31	0/1/1/1
9	EDO	A	8	-	-	0/1/1/1	0/0/0/0
2	EPA	B	1	-	-	0/17/19/19	0/0/0/0
3	AKR	B	2	-	-	0/0/2/2	0/0/0/0
3	AKR	B	3	-	-	0/0/2/2	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	COH	B	619	1	-	0/6/54/54	0/0/8/8
9	EDO	B	620	-	-	0/1/1/1	0/0/0/0
9	EDO	B	621	-	-	0/1/1/1	0/0/0/0
7	NAG	B	681	1	-	0/6/23/26	0/1/1/1
9	EDO	B	7	-	-	0/1/1/1	0/0/0/0
8	BOG	B	703	-	-	0/11/31/31	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	619	COH	C3B-C2B	-4.41	1.34	1.40
4	A	619	COH	C3C-C2C	-4.32	1.34	1.40
4	B	619	COH	C3B-C2B	-4.29	1.34	1.40
4	B	619	COH	C3C-C2C	-4.24	1.34	1.40
4	B	619	COH	CO-NA	2.11	2.08	1.97
4	A	619	COH	CO-NA	2.31	2.09	1.97
4	A	619	COH	CO-NC	2.42	2.10	1.97
4	B	619	COH	CO-NB	2.48	2.10	1.97
4	A	619	COH	CO-NB	2.69	2.11	1.97
4	B	619	COH	CO-NC	2.77	2.12	1.97
4	A	619	COH	CO-ND	2.99	2.13	1.97
4	B	619	COH	CO-ND	3.31	2.15	1.97
4	B	619	COH	C3B-CAB	3.49	1.55	1.47
4	B	619	COH	C3C-CAC	3.53	1.55	1.47
4	A	619	COH	C3C-CAC	3.55	1.55	1.47
4	A	619	COH	C3B-CAB	3.56	1.55	1.47
4	A	619	COH	C3D-C2D	5.41	1.53	1.37
4	B	619	COH	C3D-C2D	5.59	1.54	1.37

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	619	COH	CBD-CAD-C3D	-3.65	105.99	112.53
4	B	619	COH	C3B-CAB-CBB	-3.07	120.05	126.32
4	B	619	COH	C3C-CAC-CBC	-2.90	120.38	126.32
4	A	619	COH	C3C-CAC-CBC	-2.52	121.17	126.32
4	A	619	COH	CBD-CAD-C3D	-2.51	108.02	112.53
4	A	619	COH	C3B-CAB-CBB	-2.45	121.31	126.32
2	B	1	EPA	C14-C13-C12	-2.22	104.62	112.00
2	B	1	EPA	C17-C16-C15	-2.17	104.78	112.00
4	B	619	COH	CBA-CAA-C2A	-2.16	108.66	112.53
8	A	703	BOG	O1-C1-C2	2.11	110.71	108.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	681	NAG	C1-O5-C5	3.66	116.90	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2	AKR	4	0
3	A	3	AKR	1	0
9	A	4	EDO	2	0
8	A	703	BOG	1	0
2	B	1	EPA	9	0
3	B	2	AKR	4	0
3	B	3	AKR	1	0
9	B	7	EDO	2	0
8	B	703	BOG	5	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 ⓘ

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	551/591 (93%)	-0.26	8 (1%) 76 75	17, 33, 51, 58	0
1	B	551/591 (93%)	-0.14	16 (2%) 55 54	20, 34, 53, 68	1 (0%)
All	All	1102/1182 (93%)	-0.20	24 (2%) 65 64	17, 34, 52, 68	1 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	277	PRO	3.8
1	A	278	HIS	3.6
1	A	81	LEU	3.5
1	B	122	TYR	3.4
1	B	74	PHE	3.3
1	A	399	ASP	3.2
1	A	277	PRO	3.1
1	B	368	ASN	3.0
1	B	157	ASP	3.0
1	A	368	ASN	2.9
1	B	399	ASP	2.6
1	A	122	TYR	2.5
1	B	115	TYR	2.4
1	B	105	ASN	2.3
1	A	53	ASP	2.3
1	B	278	HIS	2.2
1	B	78	ILE	2.2
1	B	91	TYR	2.1
1	B	65	TYR	2.1
1	B	101	ASN	2.1
1	B	149	THR	2.1
1	A	115	TYR	2.1
1	B	148	TYR	2.0
1	B	428	ARG	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](#)

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
5	NAG	A	661	14/15	0.89	0.24	2.85	45,51,54,59	0
5	NAG	B	671	14/15	0.94	0.13	-0.02	30,34,37,41	0
6	NAG	A	671	14/15	0.95	0.10	-0.67	30,36,38,42	0
10	NDG	B	662	14/15	0.79	0.53	-	69,72,73,73	0
6	NAG	A	672	14/15	0.87	0.20	-	46,48,52,56	0
5	NAG	B	672	14/15	0.90	0.27	-	43,46,48,48	0
5	NAG	A	662	14/15	0.75	0.56	-	64,67,68,68	0
6	MAN	A	673	11/12	0.81	0.39	-	60,62,63,63	0
10	NAG	B	661	14/15	0.84	0.32	-	52,57,60,65	0

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
4	COH	A	619	43/43	0.68	0.35	5.47	92,94,96,97	0
4	COH	B	619	43/43	0.64	0.36	4.45	80,85,87,88	0
7	NAG	A	681	14/15	0.86	0.37	3.84	48,52,54,55	0
9	EDO	A	620	4/4	0.93	0.21	2.93	36,36,37,37	0
2	EPA	B	1	22/22	0.87	0.23	2.92	42,45,50,52	0
3	AKR	A	2	5/5	0.92	0.28	2.84	52,52,52,52	0
7	NAG	B	681	14/15	0.85	0.33	2.53	52,56,59,59	0
3	AKR	B	3	5/5	0.79	0.31	2.31	63,63,63,63	0
2	EPA	A	1	22/22	0.90	0.21	1.93	41,43,48,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
9	EDO	B	621	4/4	0.93	0.14	1.88	33,33,34,34	0
9	EDO	B	620	4/4	0.94	0.18	1.86	34,35,36,36	0
9	EDO	A	4	4/4	0.92	0.18	1.82	38,39,41,41	0
9	EDO	A	6	4/4	0.74	0.20	1.39	58,58,58,58	0
3	AKR	B	2	5/5	0.91	0.24	1.10	65,65,66,66	0
9	EDO	A	5	4/4	0.83	0.18	0.62	61,62,62,63	0
3	AKR	A	3	5/5	0.85	0.22	0.45	54,54,54,54	0
8	BOG	B	703	20/20	0.94	0.14	0.06	36,37,37,37	20
8	BOG	A	703	20/20	0.96	0.14	-0.17	22,23,27,27	20
9	EDO	B	7	4/4	0.94	0.12	-0.30	39,39,39,40	0
9	EDO	A	8	4/4	0.94	0.17	-	39,39,41,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.