

# Full wwPDB X-ray Structure Validation Report (i)

#### May 13, 2020 – 10:37 pm BST

PDB ID	:	5NTU
Title	:	Crystal Structure of human Pro-myostatin Precursor at 2.6 A Resolution
Authors	:	Cotton, T.R.; Fischer, G.; Hyvonen, M.
Deposited on	:	2017-04-28
Resolution	:	2.58  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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

:	4.02b-467
:	1.8.5 (274361), CSD as541be (2020)
:	1.13
:	2.11
:	20191225.v01 (using entries in the PDB archive December 25th 2019)
:	5.8.0158
:	7.0.044  (Gargrove)
:	Engh & Huber (2001)
:	Parkinson et al. (1996)
:	2.11

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.58 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$
$R_{free}$	130704	$3676 \ (2.60-2.56)$
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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 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 <=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	А	335	18%		11%	•	8%
1	В	335	10%	8%	·	19%	

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
3	EDO	А	405	-	-	-	Х
3	EDO	В	402	-	-	-	Х
3	EDO	В	415	-	-	-	Х



## 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4520 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.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Δ	308	Total	С	Ν	Ο	$\mathbf{S}$	0	1	0
			2307	1475	386	429	17	0		
1	п	072	Total	С	Ν	0	S	0	0	0
I D	213	2097	1342	349	390	16	U	0	0	

• Molecule 1 is a protein called Growth/differentiation factor 8.

Chain	Residue	Modelled	Actual	$\mathbf{Comment}$	Reference
А	41	GLY	-	expression tag	UNP 014793
А	42	SER	-	expression tag	UNP 014793
A	217	ALA	LYS	engineered mutation	UNP 014793
A	218	ALA	GLN	engineered mutation	UNP 014793
A	220	ALA	GLU	engineered mutation	UNP 014793
А	319	ALA	GLN	engineered mutation	UNP 014793
A	320	ALA	LYS	engineered mutation	UNP 014793
В	41	GLY	-	expression tag	UNP 014793
В	42	SER	-	expression tag	UNP 014793
В	217	ALA	LYS	engineered mutation	UNP 014793
В	218	ALA	GLN	engineered mutation	UNP 014793
В	220	ALA	GLU	engineered mutation	UNP 014793
В	319	ALA	GLN	engineered mutation	UNP 014793
В	320	ALA	LYS	engineered mutation	UNP 014793

There are 14 discrepancies between the modelled and reference sequences:

• Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	1	Total Cl 1 1	0	0
2	А	1	Total Cl 1 1	0	0

• Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	14	Total O 14 14	0	0
4	В	16	Total O 16 16	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 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: Growth/differentiation factor 8



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	$168.16\text{\AA}$ $36.30\text{\AA}$ $120.45\text{\AA}$	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $104.39^{\circ}$ $90.00^{\circ}$	Depositor
$\mathbf{Bosolution} \left( \overset{\circ}{\mathbf{A}} \right)$	28.27 - 2.58	Depositor
	76.27 - 2.58	EDS
$\% { m Data \ completeness}$	97.7(28.27-2.58)	Depositor
(in resolution range)	97.8(76.27-2.58)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.61 (at 2.58 \text{\AA})$	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
D D.	0.215 , $0.260$	Depositor
$\Pi, \Pi_{free}$	0.227 , $0.277$	DCC
$R_{free}$ test set	1127 reflections $(5.01\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	79.3	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.33 , $82.6$	EDS
L-test for twinning <sup>2</sup>	$ \langle L  \rangle = 0.50, \langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4520	wwPDB-VP
Average B, all atoms $(Å^2)$	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.60% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

## 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: EDO, CL

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).

Mal	Chain	Bond	lengths	Bond angles		
	Ullalli	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.48	0/2365	0.34	0/3229	
1	В	0.48	0/2142	0.32	0/2912	
All	All	0.48	0/4507	0.33	0/6141	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

#### 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	А	2307	0	2180	20	0
1	В	2097	0	2003	16	0
2	А	1	0	0	0	0
2	В	1	0	0	0	0
3	А	20	0	30	1	0
3	В	64	0	96	5	0
4	А	14	0	0	0	0
4	В	16	0	0	0	0
All	All	4520	0	4309	34	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.



Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
1:A:242:PRO:HG3	1:A:250:ASN:ND2	2.16	0.61
1:A:190:ARG:HH21	1:A:207:ASP:HB3	1.72	0.54
1:A:158:ILE:HD13	1:A:251:PRO:HB3	1.90	0.54
1:A:171:VAL:HB	1:A:192:LEU:HB2	1.90	0.53
1:B:173:ILE:HG22	1:B:189:ILE:HG23	1.91	0.53
1:A:72:ILE:HD11	1:A:355:GLY:HA2	1.92	0.52
1:B:340:CYS:HB3	3:B:415:EDO:H21	1.92	0.52
1:B:171:VAL:HB	1:B:192:LEU:HB2	1.91	0.52
1:A:146:ILE:H	1:A:146:ILE:HD13	1.76	0.49
1:B:72:ILE:HD11	1:B:355:GLY:HA2	1.93	0.49
1:A:207:ASP:HB2	3:A:405:EDO:H12	1.95	0.48
1:B:347:PRO:HB3	1:B:365:PRO:HA	1.96	0.48
1:B:339:CYS:HB3	1:B:375:SER:OXT	2.13	0.48
1:B:72:ILE:HG22	1:B:77:ILE:HG13	1.95	0.47
1:A:347:PRO:HB3	1:A:365:PRO:HA	1.96	0.47
1:A:121[B]:MET:HE3	1:B:82:PRO:HG3	1.97	0.46
1:A:114:THR:HG23	1:A:259:ASP:HB3	1.97	0.46
1:A:313:CYS:HB3	1:A:338:PRO:HB2	1.97	0.46
1:A:315:PHE:CE1	1:A:337:GLY:HA3	2.51	0.46
1:B:122:PRO:HB3	1:B:138:CYS:HB3	1.98	0.46
1:B:273:ASP:HB2	3:B:402:EDO:H12	1.97	0.45
1:B:56:ILE:HD13	1:B:288:VAL:HG21	1.99	0.45
1:A:322:PRO:HG2	1:A:323:HIS:HD2	1.84	0.43
1:A:158:ILE:HD12	1:A:227:ILE:HG21	2.00	0.43
1:A:203:TRP:CD1	3:B:417:EDO:H21	2.54	0.43
1:A:154:ALA:HB3	1:A:209:LYS:HA	2.00	0.43
1:B:154:ALA:HB3	1:B:209:LYS:HA	2.00	0.42
1:B:94:TYB:HE2	3:B:412:EDO:H22	1.84	0.42
1:A:122:PRO:HD3	1:A:251:PRO:O	2.21	0.41
1:A:78:ARG:O	1:B:247:ASP:HB3	2.20	0.41
1:A:72:ILE:HG22	1:A:77:ILE:HG13	2.01	0.41
1:B:302:LVS:H	3:B:411:EDO:H21	1.86	0.40
1:A:158:ILE:CD1	1:A:251:PRO:HB3	2.51	0.40
1:B:122:PRO:HD3	1:B:251:PRO:O	2.22	0.40

All (34) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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	Perce	entiles
1	А	303/335~(90%)	288~(95%)	12~(4%)	3 (1%)	15	31
1	В	259/335~(77%)	247~(95%)	11 (4%)	1 (0%)	34	55
All	All	562/670~(84%)	535~(95%)	23~(4%)	4 (1%)	22	41

All (4) Ramachandran outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	А	181	LYS
1	А	183	GLY
1	А	109	ASP
1	В	338	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	А	238/297~(80%)	227~(95%)	11 (5%)	27 49
1	В	222/297~(75%)	217 (98%)	5(2%)	50 73
All	All	460/594~(77%)	444 (96%)	16 (4%)	36 59

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	53	ILE
1	А	146	ILE



Mol	Chain	$\mathbf{Res}$	Type
1	А	174	LEU
1	А	192	LEU
1	А	250	ASN
1	А	271	ASP
1	А	274	GLU
1	А	303	ARG
1	А	312	GLU
1	А	331	ASN
1	А	363	LYS
1	В	137	CYS
1	В	187	THR
1	В	189	ILE
1	В	192	LEU
1	В	250	ASN

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Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	323	HIS
1	А	331	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 carbohydrates in this entry.

### 5.6 Ligand geometry (i)

Of 23 ligands modelled in this entry, 2 are monoatomic - leaving 21 for Mogul analysis.

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).

Mal	Tune	Chain	Dog	Tink	B	ond leng	$_{ m gths}$	E	Bond ang	gles
	Type	Chain	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
3	EDO	А	404	-	3,3,3	0.58	0	2,2,2	0.38	0
3	EDO	В	404	-	3,3,3	0.67	0	2,2,2	0.23	0
3	EDO	А	405	-	3,3,3	0.81	0	2,2,2	0.25	0
3	EDO	В	406	-	3,3,3	0.74	0	2,2,2	0.33	0
3	EDO	В	413	-	3,3,3	0.63	0	2,2,2	0.30	0
3	EDO	В	417	-	3,3,3	0.71	0	2,2,2	0.27	0
3	EDO	В	414	-	3,3,3	0.87	0	2,2,2	0.18	0
3	EDO	В	410	-	3,3,3	0.69	0	2,2,2	0.28	0
3	EDO	В	415	-	3,3,3	0.54	0	2,2,2	0.37	0
3	EDO	В	403	-	3,3,3	0.31	0	2,2,2	0.48	0
3	EDO	В	409	-	3,3,3	0.67	0	2,2,2	0.31	0
3	EDO	А	406	-	3,3,3	0.65	0	2,2,2	0.31	0
3	EDO	В	411	-	3,3,3	0.60	0	2,2,2	0.32	0
3	EDO	В	407	-	3,3,3	0.54	0	2,2,2	0.32	0
3	EDO	А	402	-	3,3,3	0.53	0	2,2,2	0.37	0
3	EDO	А	403	-	3,3,3	0.61	0	2,2,2	0.31	0
3	EDO	В	416	-	3,3,3	0.69	0	2,2,2	0.29	0
3	EDO	В	405	-	3,3,3	0.55	0	2,2,2	0.36	0
3	EDO	В	412	-	3,3,3	0.51	0	2,2,2	0.34	0
3	EDO	В	402	-	3,3,3	0.67	0	2,2,2	0.34	0
3	EDO	В	408	-	3,3,3	0.75	0	2,2,2	0.25	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
3	EDO	А	404	-	-	0/1/1/1	-
3	EDO	В	404	-	-	0/1/1/1	-
3	EDO	А	405	-	-	1/1/1/1	-
3	EDO	В	406	-	-	0/1/1/1	-
3	EDO	В	413	-	-	0/1/1/1	-
3	EDO	В	417	-	-	1/1/1/1	-
3	EDO	В	414	-	-	1/1/1/1	-
3	EDO	В	410	-	-	0/1/1/1	-
3	EDO	В	415	-	-	1/1/1/1	-



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Mol	Type	Chain	$\mathbf{Res}$	Link	Chirals	Torsions	Rings		
3	EDO	В	403	-	-	0/1/1/1	-		
3	EDO	В	409	-	-	0/1/1/1	-		
3	EDO	А	406	-	-	1/1/1/1	-		
3	EDO	В	411	-	-	0/1/1/1	-		
3	EDO	В	407	-	-	0/1/1/1	-		
3	EDO	А	402	-	-	0/1/1/1	-		
3	EDO	А	403	-	-	0/1/1/1	-		
3	EDO	В	416	-	-	1/1/1/1	-		
3	EDO	В	405	-	-	0/1/1/1	-		
3	EDO	В	412	-	-	0/1/1/1	-		
3	EDO	В	402	-	-	1/1/1/1	-		
3	EDO	В	408	-	-	0/1/1/1	-		

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There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	В	416	EDO	O1-C1-C2-O2
3	В	415	EDO	O1-C1-C2-O2
3	А	405	EDO	O1-C1-C2-O2
3	В	402	EDO	O1-C1-C2-O2
3	В	414	EDO	O1-C1-C2-O2
3	А	406	EDO	O1-C1-C2-O2
3	В	417	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	А	405	EDO	1	0
3	В	417	EDO	1	0
3	В	415	EDO	1	0
3	В	411	EDO	1	0
3	В	412	EDO	1	0
3	В	402	EDO	1	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, 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	< <b>RSRZ</b> >	#RSRZ>2		$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q < 0.9
1	А	308/335~(91%)	1.16	59 (19%) 1 (	0	56,107,147,163	0
1	В	273/335~(81%)	1.01	35 (12%) 3	2	51,93,157,172	0
All	All	581/670~(86%)	1.09	94 (16%) 1	1	51, 100, 153, 172	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	51	SER	10.9
1	В	176	LEU	10.2
1	А	72	ILE	8.1
1	А	67	GLU	7.2
1	В	142	PHE	5.8
1	А	66	LEU	5.6
1	А	286	LEU	5.3
1	А	275	HIS	5.2
1	В	189	ILE	5.2
1	А	77	ILE	4.7
1	А	336	ALA	4.5
1	В	112	HIS	4.4
1	А	269	GLY	4.4
1	А	288	VAL	4.3
1	В	44	TRP	4.3
1	В	177	ILE	4.2
1	В	111	TYR	4.2
1	А	291	GLU	4.1
1	В	375	SER	4.1
1	A	371	ARG	4.1
1	A	293	PHE	3.9
1	В	158	ILE	3.9
1	A	217	ALA	3.9
1	A	94	TYR	3.8



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Mol	Chain	Res	Type	RSRZ
1	А	366	ALA	3.8
1	В	156	LEU	3.7
1	А	353	PHE	3.7
1	A	270	LEU	3.6
1	А	271	ASP	3.6
1	В	186	TYR	3.6
1	А	295	TRP	3.5
1	В	225	ILE	3.4
1	А	48	THR	3.4
1	В	173	ILE	3.3
1	В	109	ASP	3.3
1	В	143	SER	3.2
1	В	188	GLY	3.2
1	В	118	ILE	3.1
1	В	161	ARG	3.1
1	А	264	SER	3.0
1	А	315	PHE	3.0
1	А	80	LEU	3.0
1	В	270	LEU	3.0
1	В	175	ARG	3.0
1	В	206	ILE	2.9
1	В	107	GLU	2.9
1	А	148	TYR	2.9
1	В	152	VAL	2.8
1	А	139	PHE	2.8
1	А	68	THR	2.8
1	А	194	LEU	2.8
1	А	297	TRP	2.8
1	B	187	THR	2.8
1	A	163	VAL	2.7
1	A	369	VAL	2.7
1	A	59	GLN	2.7
1	A	299	ILE	2.6
1	A	375	SER	2.6
1	A	60	ILE	2.6
1	A	283	ARG	2.6
1	A	189	ILE	2.6
1	A	306	ALA	2.6
1	В	139	PHE	2.6
1	В	192	LEU	2.5
1	В	257	VAL	2.5
1	A	364	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	В	140	PHE	2.4
1	А	87	LEU	2.4
1	А	73	SER	2.4
1	А	75	ASP	2.4
1	А	63	LYS	2.4
1	А	348	ILE	2.4
1	А	290	PHE	2.4
1	А	74	LYS	2.4
1	А	285	PRO	2.4
1	А	282	CYS	2.4
1	В	280	ARG	2.3
1	В	160	LEU	2.3
1	А	317	PHE	2.3
1	А	53	ILE	2.3
1	А	304	TYR	2.3
1	А	192	LEU	2.3
1	А	230	LEU	2.3
1	В	202	ILE	2.2
1	В	204	GLN	2.1
1	В	224	GLY	2.1
1	А	332	PRO	2.1
1	А	64	LEU	2.1
1	А	49	LYS	2.1
1	В	171	VAL	2.0
1	В	60	ILE	2.0
1	А	338	PRO	2.0
1	А	121[A]	MET	2.0
1	А	160	LEU	2.0

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#### 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. The B-factors column lists the minimum,



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(A^2)$	Q<0.9
3	EDO	В	417	4/4	0.49	0.37	$104,\!105,\!106,\!106$	0
3	EDO	А	406	4/4	0.53	0.31	117,118,119,119	0
3	EDO	В	402	4/4	0.54	0.41	80,84,86,87	0
3	EDO	В	414	4/4	0.66	0.36	79,83,83,84	0
3	EDO	В	415	4/4	0.67	0.50	92,92,93,93	0
3	EDO	В	410	4/4	0.68	0.28	95,97,99,100	0
2	CL	А	401	1/1	0.70	0.17	119,119,119,119	0
3	EDO	В	408	4/4	0.70	0.29	81,84,86,87	0
3	EDO	А	403	4/4	0.70	0.19	$103,\!104,\!105,\!105$	0
3	EDO	А	405	4/4	0.70	0.44	85,86,88,89	0
3	EDO	В	405	4/4	0.75	0.31	91,91,92,93	0
3	EDO	В	404	4/4	0.77	0.25	99,99,99,99	0
2	CL	В	401	1/1	0.77	0.26	97,97,97,97	0
3	EDO	В	406	4/4	0.81	0.21	76,80,84,86	0
3	EDO	А	402	4/4	0.82	0.28	89,89,90,91	0
3	EDO	В	416	4/4	0.84	0.24	79,84,87,87	0
3	EDO	В	411	4/4	0.84	0.25	93,94,94,95	0
3	EDO	В	409	4/4	0.86	0.26	92,94,97,100	0
3	EDO	В	412	4/4	0.88	0.39	85,86,88,91	0
3	EDO	В	413	4/4	0.89	0.57	83,86,86,86	0
3	EDO	A	404	4/4	0.90	0.30	87,89,92,93	0
3	EDO	В	403	4/4	0.94	0.39	70,70,71,73	0
3	EDO	В	407	4/4	0.95	0.27	70,71,71,71	0

median,  $95^{th}$  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.

## 6.5 Other polymers (i)

There are no such residues in this entry.

