

Full wwPDB X-ray Structure Validation Report (i)

May 16, 2020 – 12:53 am BST

PDB ID	:	5WIZ
Title	:	Phosphotriesterase variant S5
Authors	:	Miton, C.M.; Campbell, E.C.; Jackson, C.J.; Tokuriki, N.
Deposited on	:	2017-07-21
Resolution	:	1.96 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:

$\operatorname{MolProbity}$:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11
Ideal geometry (proteins) Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)	: : :	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 1.96 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	$2580 \ (1.96-1.96)$
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 $(1.96-1.96)$
Sidechain outliers	138945	2678(1.96-1.96)
RSRZ outliers	127900	2539(1.96-1.96)

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	333	84%	9%	• 7%
1	G	333	87%	7%	6%

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	MPD	G	2403	-	-	-	Х



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4982 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 Phosphotriesterase.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Δ	211	Total	С	Ν	Ο	S	0	5	0
	I A	911	2392	1514	424	448	6	0		
1	C	212	Total	С	Ν	Ο	S	0	4	0
I G	616	2408	1522	428	452	6	0	4	U	

Chain	Residue	Modelled	Actual	Comment	Reference
А	216	LEU	PHE	$\operatorname{conflict}$	UNP A0A060GYS1
А	233	ALA	ASP	conflict	UNP A0A060GYS1
A	254	SER	HIS	$\operatorname{conflict}$	UNP A0A060GYS1
А	271	HIS	LEU	conflict	UNP A0A060GYS1
A	293	THR	MET	$\operatorname{conflict}$	UNP A0A060GYS1
А	306	ILE	PHE	conflict	UNP A0A060GYS1
А	320	GLY	VAL	$\operatorname{conflict}$	UNP A0A060GYS1
G	216	LEU	PHE	conflict	UNP A0A060GYS1
G	233	ALA	ASP	conflict	UNP A0A060GYS1
G	254	SER	HIS	$\operatorname{conflict}$	UNP A0A060GYS1
G	271	HIS	LEU	conflict	UNP A0A060GYS1
G	293	THR	MET	$\operatorname{conflict}$	UNP A0A060GYS1
G	306	ILE	PHE	$\operatorname{conflict}$	UNP A0A060GYS1
G	320	GLY	VAL	conflict	UNP A0A060GYS1

There are 14 discrepancies between the modelled and reference sequences:

• Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	2	Total Zn 2 2	0	0
2	А	2	Total Zn 2 2	0	0

• Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:



 $\mathrm{C}_{6}\mathrm{H}_{14}\mathrm{O}_{2}\big).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 8 & 6 & 2 \end{array}$	0	0
3	G	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 8 6 2 \end{array}$	0	0
3	G	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 8 6 2 \end{array}$	0	0

• Molecule 4 is CACODYLATE ION (three-letter code: CAC) (formula: $C_2H_6AsO_2$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	$\begin{array}{cccc} \text{Total} & \text{As} & \text{C} & \text{O} \\ 5 & 1 & 2 & 2 \end{array}$	0	0
4	G	1	$\begin{array}{cccc} \text{Total} & \text{As} & \text{C} & \text{O} \\ 5 & 1 & 2 & 2 \end{array}$	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	75	Total O 75 75	0	0
5	G	69	Total O 69 69	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: Phosphotriesterase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants	85.25Å 85.69Å 88.48Å	Deneiten
$\mathrm{a,b,c,\alpha,\beta,\gamma}$	90.00° 90.00° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	28.95 - 1.96	Depositor
Resolution (A)	28.95 - 1.96	EDS
% Data completeness	99.3 (28.95 - 1.96)	Depositor
(in resolution range)	99.3 (28.95 - 1.96)	EDS
R_{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.49 (at 1.96 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
D D .	0.212 , 0.233	Depositor
n, n_{free}	0.210 , 0.232	DCC
R_{free} test set	2436 reflections $(5.19%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	26.6	Xtriage
Anisotropy	0.823	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.38 , 49.3	EDS
L-test for $twinning^2$	$< L > = 0.50, < L^2 > = 0.33$	Xtriage
	0.010 for -h,l,k	
	0.016 for -l,-k,-h	
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
	0.000 for k,l,h	
	0.000 for l,h,k	
F_o, F_c correlation	0.95	EDS
Total number of atoms	4982	wwPDB-VP
Average B, all atoms $(Å^2)$	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.64% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities 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: CAC, ZN, MPD, KCX

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		
	Cham	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.27	0/2428	0.45	0/3300	
1	G	0.26	0/2444	0.46	0/3319	
All	All	0.27	0/4872	0.46	0/6619	

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	А	0	2
1	G	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	169	KCX	Mainchain
1	G	169	KCX	Mainchain

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	2392	0	2432	15	0
1	G	2408	0	2440	10	0
2	А	2	0	0	0	0
2	G	2	0	0	0	0
3	А	8	0	14	2	0
3	G	16	0	28	1	0
4	А	5	0	0	0	0
4	G	5	0	0	0	0
5	А	75	0	0	1	0
5	G	69	0	0	0	0
All	All	4982	0	4914	26	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 3.

All (26) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:G:173:THR:HG23	1:G:180:GLN:HE22	1.58	0.69
1:G:294:LYS:O	1:G:356[B]:ARG:NH2	2.25	0.68
1:A:170[B]:VAL:HG11	1:A:184:LEU:HD13	1.77	0.66
3:A:2403:MPD:H12	3:A:2403:MPD:O4	2.01	0.60
1:G:333:ILE:HG23	1:G:346:LEU:HD13	1.87	0.55
1:A:207:ARG:NH1	1:A:236:ASP:OD2	2.38	0.54
1:A:170[A]:VAL:HG12	1:A:183:VAL:HG12	1.92	0.51
3:A:2403:MPD:O2	3:A:2403:MPD:H53	2.12	0.50
1:G:132:LEU:HD13	3:G:2404:MPD:H52	1.94	0.49
1:G:169:KCX:OQ1	1:G:201:HIS:HB2	2.13	0.49
1:A:67:ARG:NH2	1:A:111[B]:SER:OG	2.46	0.48
1:A:152:ARG:NH2	5:A:2503:HOH:O	2.40	0.48
1:G:258:SER:OG	1:G:280:ARG:NE	2.48	0.44
1:G:302:TRP:CH2	1:G:321:ASN:HB3	2.53	0.44
1:A:175:LYS:HA	1:A:211:GLN:HE21	1.83	0.44
1:A:131:TRP:CG	1:A:132:LEU:N	2.86	0.44
1:G:131:TRP:CG	1:G:132:LEU:N	2.86	0.44
1:A:143:VAL:HB	1:A:182:LEU:HD22	2.02	0.42
1:G:311:THR:O	1:G:312:ASN:HB2	2.19	0.42
1:A:353:ASN:HB2	1:A:354:PRO:HD3	2.01	0.42
1:A:152:ARG:HG3	1:G:71[B]:GLU:OE1	2.21	0.41
1:A:302:TRP:CH2	1:A:321:ASN:HB3	2.55	0.41
1:A:217:GLU:OE2	1:A:246:ARG:NH2	2.51	0.40
1:A:106:LEU:HA	1:A:106:LEU:HD23	1.94	0.40

Continued on next page...



Atom-1 Atom-2		Interatomic distance (Å)	Clash overlap (Å)
1:A:207:ARG:HG2	1:A:239:TYR:CD1	2.57	0.40
1:A:333:ILE:HB	1:A:334:PRO:HD3	2.03	0.40

Continued from previous page...

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	ntiles	
1	А	311/333~(93%)	301~(97%)	9~(3%)	1 (0%)	41	30
1	G	312/333~(94%)	301~(96%)	11 (4%)	0	100	100
All	All	623/666~(94%)	602 (97%)	20(3%)	1 (0%)	47	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	176	VAL

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	Perce	ntiles
1	А	254/264~(96%)	246~(97%)	8 (3%)	40	28
1	G	254/264~(96%)	248~(98%)	6(2%)	49	40
All	All	508/528~(96%)	494 (97%)	14 (3%)	46	33



Mol	Chain	\mathbf{Res}	Type
1	А	51	PHE
1	А	67	ARG
1	А	77	LYS
1	А	184	LEU
1	А	202	THR
1	А	222[A]	SER
1	А	222[B]	SER
1	А	294	LYS
1	G	47	SER
1	G	51	PHE
1	G	206	GLN
1	G	299	SER
1	G	338	GLU
1	G	362	LEU

All (14) residues with a non-rotameric sidechain are listed below:

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

2 non-standard protein/DNA/RNA residues 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).

Mal	Mol Tune Chain Bog Link		B	Bond lengths			ond ang	gles		
	Type	Chain	nes	LINK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	KCX	А	169	1,2	7,11,12	0.67	0	4,12,14	0.64	0
1	KCX	G	169	1,2	7,11,12	0.68	0	4,12,14	0.63	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
1	KCX	А	169	1,2	-	0/7/10/12	-
1	KCX	G	169	1,2	-	0/7/10/12	-

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	169	KCX	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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 True		Chain	Chain	Chain	Chain	Chain	nin Dog	Tinle	B	Bond lengths			Bond angles		
	101 Type Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2						
4	CAC	А	2404	2	$0,\!4,\!4$	0.00	-	$0,\!6,\!6$	0.00	-					
3	MPD	А	2403	-	7,7,7	0.25	0	9,10,10	0.23	0					
3	MPD	G	2403	-	7,7,7	0.56	0	9,10,10	0.39	0					
3	MPD	G	2404	-	7,7,7	0.57	0	9,10,10	0.37	0					
4	CAC	G	2405	2	0,4,4	0.00	-	0,6,6	0.00	-					

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	MPD	А	2403	-	-	1/5/5/5	-
3	MPD	G	2403	-	-	1/5/5/5	-
3	MPD	G	2404	-	-	1/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	2404	MPD	C1-C2-C3-C4
3	G	2403	MPD	O2-C2-C3-C4
3	А	2403	MPD	C2-C3-C4-O4

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	А	2403	MPD	2	0
3	G	2404	MPD	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, 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	А	310/333~(93%)	0.50	22 (7%) 16 24	19, 28, 44, 51	0
1	G	312/333~(93%)	0.66	36 (11%) 4 8	21, 35, 52, 68	0
All	All	622/666~(93%)	0.58	58 (9%) 8 14	19, 32, 49, 68	0

All (58) RSRZ outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	RSRZ
1	G	362	LEU	8.6
1	G	35	ASP	5.9
1	А	259	ALA	3.9
1	G	258	SER	3.9
1	G	206	GLN	3.8
1	А	298[A]	VAL	3.8
1	G	170[A]	VAL	3.7
1	G	34	GLY	3.7
1	А	362	LEU	3.6
1	А	53	LEU	3.5
1	G	228	ILE	3.4
1	G	316	VAL	3.4
1	G	361	THR	3.4
1	А	316	VAL	3.3
1	А	170[A]	VAL	3.3
1	G	98	ILE	3.2
1	G	338	GLU	3.1
1	G	125	VAL	3.1
1	А	338	GLU	3.1
1	G	156	TYR	3.0
1	G	99	VAL	3.0
1	G	199	THR	3.0
1	A	258	SER	3.0
1	G	198	VAL	3.0

Continued on next page...



Mol	Chain	\mathbf{Res}	Type	RSRZ
1	G	167	ILE	2.9
1	G	168	ILE	2.9
1	G	337	ARG	2.8
1	A	167	ILE	2.8
1	А	99	VAL	2.8
1	G	335	PHE	2.8
1	G	259	ALA	2.7
1	А	198	VAL	2.6
1	А	312	ASN	2.6
1	А	168	ILE	2.6
1	G	173	THR	2.6
1	G	312	ASN	2.5
1	А	46	ILE	2.4
1	А	207	ARG	2.4
1	G	44	ILE	2.4
1	А	118	ARG	2.4
1	G	227	CYS	2.3
1	G	174	GLY	2.3
1	A	130	LEU	2.3
1	G	36	ARG	2.3
1	G	339	LYS	2.3
1	G	297	LEU	2.2
1	А	252	LEU	2.2
1	А	297	LEU	2.2
1	A	278	GLN	2.2
1	G	341	ILE	2.2
1	G	129	GLY	2.2
1	G	89	ARG	2.1
1	А	199	THR	2.1
1	G	45	THR	2.1
1	G	175	LYS	2.1
1	G	53	LEU	2.1
1	G	204	ALA	2.0
1	А	227	CYS	2.0

Continued from previous page...

6.2 Non-standard residues in protein, DNA, RNA chains (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, 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.



Mol	Type	Chain	Res	Atoms	RSCC	RSR	${f B}$ -factors(Å ²)	Q<0.9
1	KCX	G	169	12/13	0.87	0.22	$26,\!29,\!31,\!31$	0
1	KCX	А	169	12/13	0.92	0.19	$21,\!22,\!26,\!26$	0

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, 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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} extsf{-}\mathbf{B} extsf{-}\mathbf{factors}(\mathbf{A}^2)$	Q<0.9
3	MPD	G	2403	8/8	0.69	0.42	49,50,50,51	0
3	MPD	G	2404	8/8	0.77	0.18	40,41,42,43	8
3	MPD	А	2403	8/8	0.78	0.25	44,44,45,45	0
4	CAC	G	2405	5/5	0.88	0.21	16,37,63,67	5
4	CAC	А	2404	5/5	0.97	0.16	17,26,32,35	5
2	ZN	G	2402	1/1	0.99	0.07	$31,\!31,\!31,\!31$	1
2	ZN	А	2402	1/1	0.99	0.09	27,27,27,27	1
2	ZN	G	2401	1/1	1.00	0.07	29, 29, 29, 29, 29	0
2	ZN	A	2401	1/1	1.00	0.07	20,20,20,20	1

6.5 Other polymers (i)

There are no such residues in this entry.

