PROTEIN DATA BANK

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

### Aug 18, 2018 – 11:53 AM EDT

This is a Preliminary Full wwPDB X-ray Structure Validation Report.

This report is produced by the standalone wwPDB validation server. The structure in question has not been deposited to the wwPDB. This report should not be submitted to journals.

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:

MolProbity	: /	4.02b-467
Mogul	;/	1.7.3 (157068), CSD as 539 be (2018)
Xtriage (Phenix)	/:	1.13
EDS	:	rb-20031172
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20031172
	MolProbity Mogul Xtriage (Phenix) EDS Percentile statistics Refmac CCP4 Ideal geometry (proteins) Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)	MolProbity : Mogul : Mogul : Xtriage (Phenix) : EDS : Percentile statistics : Refmac : CCP4 : Ideal geometry (proteins) : Ideal geometry (DNA, RNA) : Validation Pipeline (wwPDB-VP) :

## 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 2.10 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.



Motrie	Whole archive	Similar resolution				
IVIETIC	$(\# \mathbf{Entries})$	(#Entries, resolution range(Å))				
$R_{free}$	111664	4608 (2.10-2.10)				
Clashscore	122126	5109(2.10-2.10)				
Ramachandran outliers	120053	5059(2.10-2.10)				
Sidechain outliers	120020	5060 (2.10-2.10)				
RSRZ outliers	108989	4497(2.10-2.10)				

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 <=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	Ą	461	13%	85%	15%
2	В	3	33%	100%	

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:



## 2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 3987 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	А	461	Total 3563	C 2396	N 552	O 598	S 17	0	0	0

• Molecule 2 is a protein called PHE-ALA-THR.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
2	В	3	Total         C         N           24         16         3	O 5	0	0	0

• Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



	Mol	Chain	Residues	Ato	oms		ZeroOcc	AltConf
	3	С	1	Total 5	O $4$	Р 1	0	0
/	3	С	1	Total 5	0 4	Р 1	0	0



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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	С	1	TotalO54	Р 1	0	0

• Molecule 4 is SODIUM ION (three-letter code: NA) (formula; Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	С	1	Total Na 1 1	0	0

• Molecule 5 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula:  $C_{10}H_{22}O_6$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	С	/1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 10  6  4 \end{array}$	0	0

• Molecule 6 is (2R)-2,3-DIHYDROXYPROPYL(7Z)-PENTADEC-7-ENOATE (three-letter code: 78N) (formula: C<sub>18</sub>H<sub>34</sub>O<sub>4</sub>).





Conf	AltC	ZeroOcc		oms	At	Residues	Chain	Mol
0		0	0 /	С	Total	1	р	6
0		0	4	18	22	1		0
0	0	0	0	С	Total	1	D	6
			4	18	22	-		
0	0 / 0	<b>0</b>	0	C	Total	1	D	6
-	/		4	$\frac{18}{3}$	22			
0	0	0	0	C	Total	1	D	6
		Y/	4	18	22			
0	0	0	0-		Total	1	D	6
			4	18				
0	0	0		10		1 /	D	6
			$\frac{4}{0}$	$\frac{10}{C}$	ZZ Tofal			
0	0	0		18	10ta1	1	D	6
			$\frac{4}{0}$	$\frac{10}{C}$	Total			
0	0	0		18	10tal 22	1	D	6
			<u>4</u>	$\frac{10}{C}$	Total			
0	0	0	4	18	22		D	6
			- <u>+</u>	C	Total		/	
0	0	0	4	18	22	1	D	6
(	(	0	4 0 4	18 C 18	22 Total 22		D D	6 6

• Molecule 7 is (2S)-2,3-DIHYDROXYPROPYL(7Z)-PENTADEC-7-ENOATE (three-letter code: 78M) (formula:  $C_{18}H_{34}O_4$ ).





Mol	Chain	Residues	Atoms	ZeroOcc AltConf
7	D	1	Total         C         O           22         18         4	0 0
7	D	1	Total         C         O           22         18         4	0 0
7	D	1	$\begin{array}{c cc} Total & C & O \\ 22 & 18 & 4 \end{array}$	0 0

• Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	$\mathbf{S}$	88	Total O 88 88	0	0

• Molecule 1:

## 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.

13% Chain A: 85% 15% • Molecule 2: PHE-ALA-THR 100% Chain B: 67% 33%

### 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	101.02Å $108.05$ Å $110.50$ Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
$\mathbf{B}_{\mathrm{esolution}}(\mathbf{\hat{A}})$	48.53 - 2.10	Depositor
nesolution (A)	48.53 - 2.10	EDS
$\% { m Data \ completeness}$	99.6 (48.53-2.10)	Depositor
(in resolution range)	99.6 (48.53-2.10)	EDS
$R_{merge}$	(Not available)	Depositor
$\mathrm{R}_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.00 (at 2,10Å)	Xtriage
Refinement program	PHENIX (1.11/1_2575: ???)	Depositor
R R.	0.205 , $0.247$	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.205 , $0.248$	DCC
$R_{free}$ test set	1762 reflections $(5.00%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	46.7	Xtriage
Anisotropy	0.529	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.35, 62.5	EDS
L-test for $twinning^2$	$ < L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3987	wwPDB-VP
Average B, all atoms $(Å^2)$	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.59% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>1</sup>Intensities estimated from amplitudes.

<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.



## 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: 78M, NA, PO4, 78N, 1PE

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
	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5/
1	А	0.39	0/3669	0.52	0/5003
2	В	0.43	0/24	0.56	0/30
All	All	0.39	0/3693	0.52	0/5033

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	3563	0	3647	49	0
2	B	24 📥	0	23	2	0
3	C	15	0	0	0	0
4	Ø	1	0	0	0	0
5	/C	10	0	13	1	0
6	D	220	0	340	15	0
7 /	D	66	0	102	4	0
8	S	88	0	0	1	0
All	All	3987	0	4125	55	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 7.



A 4 a ma 1	A 4 0	Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
1:A:386:PRO:HB2	6:D:4:78N:H71	1.72	0.71	<b>`</b>
1:A:248:ALA:HA	6:D:8:78N:H172	1.76	0.68	
1:A:248:ALA:HB2	6:D:8:78N:H191	1.77	0.67	
1:A:284:SER:HB2	1:A:475:ILE:HG23	1.77	0.66	1
1:A:6:LYS:HG2	1:A:13:LEU:HD21	1.78	0.65	
1:A:391:GLY:HA3	7:D:3:78M:H122	1.81	0.62	
1:A:85:ARG:HH21	6:D:9:78N:H191	1.66	0.60	
1:A:224:VAL:HG21	6:D:10:78N:H101	1.86	0.58	7
1:A:74:GLY:HA3	1:A:123:GLY:O	2.04	0.57	1
1:A:378:TYR:CE2	7:D:3:78M:H202	2.41	0.55	
1:A:459:LEU:HD13	7:D:13:78M:H22C	1.88	0.55	]
1:A:77:VAL:HG11	1:A:124:PHE:HE1	1.72	0.54	]
1:A:352:SER:HB2	1:A:354:PRO:HD2	1.90	0.53	]
1:A:473:LYS:HG2	6:D:12:78N:H192	1.90	0.53	]
1:A:85:ARG:NH2	6:D:9:78N:H191	2.24	0.52	
1:A:261:PRO:HG2	1:A:433:VAL:HG21	1.92	0.51	]
1:A:284:SER:O	1:A:287:PRO:HD2	2.12	0.50	1
1:A:407:GLY:HA3	1:A:427:TRP:CH2	2.47	0.50	]
1:A:378:TYR:CZ	7:D:3:78M:H202	2.49	0.48	]
1:A:236:VAL:O	1:A:240:LEU:HG	2.14	0.47	]
1:A:473:LYS:HA	1:A:473:LYS:HD3	1.72	0.47	]
5:C:5:1PE:H262	8:S:51:HOH:O	2.15	0.46	]
1:A:59:ILE:HD11	1:A:246:LEU:HD21	1.96	0.46	]
1:A:358:ALA:O	1:A:362:MET:HG3	2.16	0.46	]
1:A:68:TYR:HE1	2:B:3:THR:HG22	1.80	0.46	
1:A:11:GLN:OE1	1:A:143:ARG:HB3	2.16	0.45	
1:A:251:ASN:HD22	6:D:8:78N:C17	2.29	0.45	
1:A:77:VAL:HG11	1:A:124:PHE:CE1	2.51	0.45	
1:A:425:SER:HA	1:A:428:PHE:HD2	1.81	0.45	
1:A:278:GLU:O	1:A:282:VAL:HG23	2.17	0.45	
1:A:286:ILE:HB	1:A:287:PRO:HD3	1.99	0.45	]
6:D:2:78N:H71	6:D:2:78N:H42C	1.56	0.45	
1:A:258:ILE:O	1:A:261:PRO:HD2	2.17	0.44	
1:A:298:ILE:HD11	1:A:461:SER:OG	2.18	0.44	
1:A:426:MET:HA	1:A:429:LEU:HB2	1.98	0.44	
1:A:474:ARG:O	1:A:478:LEU:HD12	2.18	0.43	
1:A:22:GLU:OE1	1:A:22:GLU:HA	2.18	0.43	
1:A:68:TYR:OH	1:A:300:GLU:OE2	2.09	0.43	
1:A:78:ALA:HB1	1:A:84:ALA:HA	2.01	0.43	
1·A·22·GLU·HC2	$1 \cdot A \cdot 129 \cdot VAI \cdot HC21$	2.01	0.43	1

All (55) 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)
6:D:9:78N:H2	6:D:9:78N:H102	1.90	0.43
1:A:269:ILE:HD11	1:A:282:VAL:HG12	2.01	0.42
1:A:296:TRP:CH2	2:B:2:ALA:HA	2.54	0.42
1:A:332:ILE:O	1:A:336:THR:HG23	2.19	0.42
1:A:194:TYR:CZ	1:A:198:LYS:HE3	2.55	0.42
1:A:336:THR:HG22	1:A:401:MET:HE1	2.01	0.42
1:A:422:GLN:CD	1:A:422:GLN:H	2.24	0.42
1:A:345:ALA:O	1:A:347:LYS:HG2	2.19	0.41
6:D:10:78N:H141	6:D:10:78N:H111	1.27	0.41
1:A:473:LYS:HG2	6:D:12:78N:C19	2.50	0.41
1:A:251:ASN:HD22	6:D:8:78N:H171	1.84	0.41
1:A:14:GLY:HA2	1:A:200:THR:HB	2.02	0.41
6:D:5:78N:H52C	6:D:5:78N:H2	1.86	0.41
1:A:373:ILE:N	1:A:374:PRO:HD2	2.37	0.40
6:D:10:78N:H31C	6:D:10:78N:H92C	1.80	0.40

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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	455/461 (99%)	449 (99%)	5(1%)	1 (0%)	49 51
2	В	1/3~(33%)	1 (100%)	0	0	100 100
All	All	456/464~(98%)	450 (99%)	5 (1%)	1 (0%)	49 51

All (1) Ramachandran outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type
/ 1		346	TRP



#### 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	Analysed Rotameric Outliers		Perce	ntiles
1	А	372/372~(100%)	367~(99%)	5 (1%)	71	78
2	В	2/2~(100%)	2(100%)	0	100	100
All	All	374/374~(100%)	369~(99%)	5 (1%)	71	78

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	22	GLU
1	А	130	SER
1	А	142	ARG
1	А	350	GLN
1	А	393	TRP

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)

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 18 ligands modelled in this entry, 1 is monoatomic - leaving 17 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	Tuno	Chain	Dog	Tink	Bo	ond leng	gths /	B	ond ang	les
	туре	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
3	PO4	С	1	-	4,4,4	0.87	0	6,6,6	0.28	0
3	PO4	С	2	-	4,4,4	0.74	0	6,6,6	0.46	0
3	PO4	С	4	-	$4,\!4,\!4$	0.68	0	6,6,6	0.53	0
5	1PE	С	5	-	$9,\!9,\!15$	0.51	0	8,8,14	0.51	0
6	78N	D	1	-	21,21,21	0.91	1 (4%)	22,22,22	1.08	1 (4%)
6	78N	D	10	-	21, 21, 21	0.96	1 (4%)	22,22,22	1.00	1 (4%)
6	78N	D	11	-	21,21,21	0.97	1 (4%)	22,22,22	1.08	1 (4%)
6	78N	D	12	-	21,21,21	0.96	1 (4%)	22,22,22	1.06	1 (4%)
7	78M	D	13	-	21,21,21	1.20	1 (4%)	22,22,22	0.96	1 (4%)
6	78N	D	2	-	21,21,21	0.88	1 (4%)	22,22,22	1.11	2 (9%)
7	78M	D	3	-	21,21,21	1.12	1 (4%)	22,22,22	0.98	1 (4%)
6	78N	D	4	- /	21,21,21	0.95	1 (4%)	22,22,22	1.21	1 (4%)
6	78N	D	5	-	21,21,21	0.95	2 (9%)	22,22,22	1.22	2 (9%)
6	78N	D	6	/ -	21,21,21	0.96	1 (4%)	22,22,22	1.03	1 (4%)
7	78M	D	7 /	-	21,21,21	1.17	1 (4%)	22,22,22	1.09	1 (4%)
6	78N	D	8	-	21,21,21	0.94	1 (4%)	22,22,22	1.13	1 (4%)
6	78N	D	9	4	21,21,21	0.95	1 (4%)	22,22,22	1.14	1 (4%)

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	$\mathbf{Res}$	Link	Chirals	Torsions	Rings
3	PO4	C	1	<u> </u>	-	0/0/0/0	0/0/0/0
3	/PO4	C	2	_	-	0/0/0/0	0/0/0/0
3	PO4	С	4 /	-	-	0/0/0/0	0/0/0/0
5	1PE	C	5	-	-	0/7/7/13	0/0/0/0
6	78N	D	/1	-	-	0/21/21/21	0/0/0/0
6	78N	D	10	-	-	0/21/21/21	0/0/0/0
6	78N	D /	11	-	-	0/21/21/21	0/0/0/0
6	78N	D	12	_	-	0/21/21/21	0/0/0/0



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Mol	Type	Chain	Res	$\mathbf{Link}$	Chirals	Torsions	Rings
7	78M	D	13	-	-	0/21/21/21	0/0/0/0
6	78N	D	2	-	-	0/21/21/21	0/0/0/0
7	78M	D	3	-	-	0/21/21/21	0/0/0/0
6	78N	D	4	-	-	0/21/21/21	0/0/0/0
6	78N	D	5	-	-	0/21/21/21	0/0/0/0
6	78N	D	6	-	-	0/21/21/21	0/0/0/0
7	78M	D	7	-	-	0/21/21/21	0/0/0/0
6	78N	D	8	-	-	0/21/21/21	0/0/0/0
6	78N	D	9	-	-	0/21/21/21	0/0/0/0

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All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	5	78N	O16-C17	-2.33	1.40	1.45
6	D	5	78N	O16-C8	2.60	1.40	1.33
6	D	2	78N	O16-C8	2.63	1.40	1.33
6	D	10	78N	O16-C8	2.82	1.41	1.33
6	D	8	78N	O16-C8	2.87	1.41	1.33
6	D	1	78N	O16-C8	2.87	1.41	1.33
6	D	9	78N	O16-C8	2.89	1.41	1.33
6	D	6	78N	O16-C8	2.96	1.41	1.33
6	D	11	78N	O16-C8	2.99	1.42	1.33
6	D	4	78N	Ø16-C8	3.01	1.42	1.33
6	D	12	78N	O16-C8	3.03	1.42	1.33
7	D	3	78M	O2-C1	3.20	1.42	1.33
7	D	7	78M	O2-C1	3.39	1.43	1.33
7	D	13	78 M	O2-C1	3.48	1.43	1.33

All (15) bond angle outliers are listed below;

	Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
	6	D	5	78N	C6-C7-C8	-2.27	105.42	113.60
	6	D	2	78N	C6-C7-C8	-2.10	106.03	113.60
	7	D	3	78M	O2-C1-C2	2.63	119.53	111.92
	6	Ď	1	78N	O16-C8-C7	2.70	119.73	111.92
	6	D	2	<b>7</b> 8N	Ó16-C8-C7	2.77	119.93	111.92
	6	D	10	78N	O16-C8-C7	2.84	120.13	111.92
	6	D	6	78N	O16-C8-C7	3.00	120.59	111.92
	6	D	12	78N	O16-C8-C7	3.01	120.63	111.92
	7	D	13	78M	O2-C1-C2	3.05	120.74	111.92
/	6	D	8	78N	O16-C8-C7	3.12	120.94	111.92
	6	D	11/	78N	O16-C8-C7	3.19	121.13	111.92
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Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
6	D	9	78N	O16-C8-C7	3.20	121.17	111.92
6	D	5	78N	O16-C8-C7	3.20	121.18	111.92
7	D	7	78M	O2-C1-C2	3.29	121.42	1/11.92
6	D	4	78N	O16-C8-C7	3.44	121.87	/111.92

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There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	С	5	1PE	1	0
6	D	10	78N	3	0
6	D	12	78N	2	0
7	D	13	78M	1	
6	D	2	78N	1	0
7	D	3	78M	3	0
6	D	4	78N	1 /	0
6	D	5	78N	1 /	0
6	D	8	78N	4	0
6	D	9	78N	3	0

### 5.7 Other polymers (i

There are no such residues in this entry.

#### 5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2
	/	

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	271:SER	С	277:THR	Ν	10.61
1	A	412:THR	С	421:SER	Ν	9.18



### 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,  $95^{th}$  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	$461/461 \ (100\%)$	0.53	60 (13%) 3 4	40,51,93,115	0
2	В	3/3~(100%)	3.34	3 (100%) 0 0	73, 73, 81, 87	0
All	All	464/464~(100%)	0.54	63 (13%) 3 4	40, 52, 93, 115	0

All (63) RSRZ outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	RSRZ
1	А	280	LEU	12.1
1	А	140	HIS	10.5
1	А	269	ILE	8.5
1	А	279	HIS	7.7
1	А	349	ASN	7.3
1	А	278	GLU	7.3
1	А	348	LYS	7.3
1	А	347	LY/S	6.7
1	А	267	TRP	6.2
1	А	142	ARG	5.2
1	А	346	TRP	5.1
1	А	138	ASP	4.7
1	А	281	ARG	4.6
1	A	268	MET	4.5
1	A /	203	PRO	4.3
1	A	270	SER	4.3
2	/B	1	PHE	<i>A</i> .2
1	A	139	GLU	3.8
1	A	410	VAL	3.8
1/	A	422	GLN	3.8
1	A	265	РНЕ	3.6
2	В	3	THR	3.4
1	А	141	ASP	3.4
1	A	350	GLN	3.4



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Mol	Chain	$\mathbf{Res}$	Type	RSRZ
1	А	5	GLY	3.4
1	A	266	ALA	3.4
1	А	13	LEU	3.3
1	А	50	HIS	3.3
1	А	137	TYR	3.1
1	А	341	TRP	3.1
1	А	411	THR	3.1
1	А	285	TYR	3.0
1	А	345	ALA	3.0
1	А	338	PHE	3.0
1	А	7	THR	2.9
1	А	283	VAL	2.9
1	А	475	ILE	2.7
1	А	284	SER	2.6
1	А	344	THR	2.5
1	А	243	TRP	2.4
1	А	165	ILE	2.4
1	А	412	THR	2.4
1	А	64	ALA	2.4
1	А	204	HIS	2.4
1	А	161	ILE	2.4
1	А	263	PHE	2.3
1	А	159	ALA	2.3
1	А	271	SER	2.3
2	В	2	ALA/	2.3
1	А	10	GLY	2.3
1	А	423	MÉT	2.3
1	А	287	PRO	2.3
1	А	282	VAL	2.3
1	А	155	ILE	2.3
1	А	264	TYR	2.3
1	А	/277	THR	2.2
1	A /	34	ALA	2.2
1	A	199	LYS	2.2
1	A	200	THR	2.2
1	A	164	LEU	2.1
1	A	30	TYR	2.1
1 /	A	162	ALA	2.0
1/	A	456	TYR	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 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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
7	78M	D	3	22/?	0.64	0.19	69,76,86,93	0
5	1PE	С	5	10/?	0.67	0.20	71,74,80,83	0
6	78N	D	8	22/?	0.68	0.27	72,79,83,93	0
7	78M	D	13	22/?	0.74	0.58	$84,\!89,\!99,\!100$	0
7	78M	D	7	22/?	0.74	0.25	$88,\!96,\!107,\!109$	0
6	78N	D	9	22/?	0.80	0.19	$67,\!75,\!86,\!87$	0
6	78N	D	11	22/?	0.82	0.25	76,83,88,96	0
6	78N	D	6	22/?	0.82	0.38	$72,\!79,\!86,\!93$	0
6	78N	D	10	22/?	0.83	0.26	$74,\!80,\!86,\!88$	0
6	78N	D	2	22/?	0.83	0.38	76,86,94,96	0
6	78N	D	4	22/?	0.84	0.20	$76,\!81,\!85,\!94$	0
3	PO4	С	4	5/?	0.86	0.15	$91,\!96,\!100,\!102$	0
6	78N	D	5	22/?	0.87	0.25	$65,\!75,\!82,\!86$	0
6	78N	D	12	22/?	0.89	0.20	$79,\!84,\!87,\!91$	0
6	78N	D	1	22/?	0.91	0.19	$56,\!66,\!76,\!85$	0
3	PO4		1	5/?	0.94	0.16	82,84,89,96	0
3	PO4	C	2	5/?	0.96	0.20	$8\overline{3,\!86,\!91,\!95}$	0
4	NA	С	3	1/?	0.97	0.20	$5\overline{4,}54,54,54$	0

#### 6.5 Other polymers (i

There are no such residues in this entry.

