

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	8EM1
Title	:	Type IIS Restriction Endonuclease PaqCI, DNA Unbound
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Deposited on	:	2022-09-26
Resolution	:	2.50 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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
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)	:	2.32.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.50 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}	130704	4661 (2.50-2.50)		
Clashscore	141614	5346 (2.50-2.50)		
Ramachandran outliers	138981	5231 (2.50-2.50)		
Sidechain outliers	138945	5233 (2.50-2.50)		
RSRZ outliers	127900	4559 (2.50-2.50)		

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 of 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	510	80%	14%	•••			
1	В	510	75%	18%	• 5%			



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2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7353 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 PaqCI, DNA Unbound.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Δ	401	Total	С	Ν	0	\mathbf{S}	0	0	0
	491	3696	2363	640	684	9	0	0	0	
1	В	482	Total	С	Ν	0	S	0	0	0
	I D	402	3580	2291	624	655	10	0		

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



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

• Molecule 3 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	38	Total O 38 38	0	0
3	В	31	Total O 31 31	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: PaqCI, DNA Unbound



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants	136.62Å 136.62Å 106.42Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution(A)	49.58 - 2.50	Depositor
Resolution (A)	49.58 - 2.50	EDS
% Data completeness	99.4 (49.58-2.50)	Depositor
(in resolution range)	97.7 (49.58 - 2.50)	EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$5.89 (at 2.51 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20	Depositor
P. P.	0.211 , 0.267	Depositor
n, n_{free}	0.210 , 0.265	DCC
R_{free} test set	2000 reflections $(5.66%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	45.9	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.30 , 37.3	EDS
L-test for $twinning^2$	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7353	wwPDB-VP
Average B, all atoms $(Å^2)$	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 35.55 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.7364e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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: EDO

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		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.47	0/3792	0.66	2/5175~(0.0%)	
1	В	0.45	0/3673	0.63	0/5017	
All	All	0.46	0/7465	0.65	2/10192~(0.0%)	

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	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	81	ILE	CG1-CB-CG2	-6.05	98.09	111.40
1	А	223	ARG	CA-CB-CG	5.18	124.80	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	223	ARG	Sidechain

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	3696	0	3467	49	0
1	В	3580	0	3326	59	0
2	В	8	0	12	1	0
3	А	38	0	0	3	0
3	В	31	0	0	2	0
All	All	7353	0	6805	103	0

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.

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.

All (103) 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:A:75:LYS:HB2	1:A:106:ILE:HG22	1.70	0.71
1:B:293:GLU:HB2	1:B:300:LYS:HD3	1.73	0.71
1:A:306:MET:HE2	1:A:312:ILE:HD13	1.74	0.70
1:A:356:ARG:NH1	3:A:602:HOH:O	2.25	0.68
1:B:359:GLU:HG2	1:B:363:LEU:O	1.93	0.68
1:A:499:TRP:O	1:A:503:VAL:HG23	1.96	0.66
1:B:49:GLY:H	1:B:97:LYS:HE3	1.62	0.65
1:B:76:ARG:HG3	1:B:79:GLU:OE2	1.98	0.64
1:A:293:GLU:HG3	1:A:300:LYS:HE3	1.80	0.64
1:A:81:ILE:HG22	1:B:50:TRP:CZ2	2.33	0.64
1:B:75:LYS:HB2	1:B:106:ILE:HG22	1.79	0.62
1:B:211:PRO:O	1:B:231:ILE:HD11	1.99	0.62
1:B:408:ASN:HB2	1:B:499:TRP:HZ2	1.63	0.62
1:B:394:LEU:HD13	1:B:477:LEU:HD21	1.80	0.62
1:B:235:THR:HG22	1:B:251:TRP:HD1	1.65	0.61
1:A:354:GLN:NE2	3:A:605:HOH:O	2.33	0.60
1:B:133:ILE:O	1:B:157:ARG:NH1	2.33	0.60
1:B:247:TRP:CD2	1:B:345:ARG:HG3	2.37	0.60
1:B:198:VAL:HG12	1:B:246:VAL:HG23	1.83	0.60
1:B:443:GLN:O	1:B:447:THR:HG23	2.01	0.59
1:B:447:THR:HA	1:B:450:THR:HG22	1.84	0.57
1:B:194:ARG:NH2	3:B:703:HOH:O	2.32	0.56
1:B:221:ILE:HG21	1:B:230:PRO:HA	1.87	0.56
1:B:40:SER:OG	1:B:457:ARG:HG3	2.06	0.55
1:A:263:PRO:HB2	1:A:264:TRP:CE3	2.42	0.55
1:B:39:ALA:HA	1:B:58:SER:O	2.07	0.55



	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:446:GLU:O	1:A:450:THR:HG23	2.07	0.55
1:A:4:ASP:HB2	1:A:506:LEU:HD22	1.88	0.54
1:A:73:GLU:OE1	3:A:601:HOH:O	2.19	0.53
1:B:220:ALA:O	1:B:224:LEU:HD12	2.09	0.53
1:B:307:LEU:HD12	1:B:308:ASN:N	2.23	0.53
1:A:214:ARG:NH2	1:A:262:THR:OG1	2.41	0.53
1:A:438:TYR:CZ	1:A:442:LEU:HD11	2.44	0.52
1:A:205:ASP:OD1	1:A:209:PRO:HD3	2.10	0.52
1:B:392:ALA:O	1:B:396:GLN:HG3	2.10	0.52
1:A:81:ILE:HD11	1:A:110:TYR:HB2	1.93	0.51
1:B:221:ILE:HG23	1:B:233:TYR:CD2	2.46	0.50
1:B:449:LEU:HD23	1:B:453:LEU:HD22	1.93	0.50
1:B:295:ARG:O	1:B:300:LYS:HG3	2.11	0.50
1:A:392:ALA:HA	1:A:505:ALA:HB1	1.94	0.50
1:A:81:ILE:HG22	1:B:50:TRP:CH2	2.48	0.49
1:A:306:MET:CE	1:A:312:ILE:HD13	2.40	0.49
1:A:115:THR:HB	1:A:118:GLU:OE1	2.13	0.49
1:B:52:LYS:NZ	3:B:707:HOH:O	2.45	0.49
1:B:410:LEU:HD22	1:B:448:LYS:HG2	1.95	0.49
1:A:424:LYS:HE3	1:A:436:GLU:HB3	1.95	0.49
1:B:110:TYR:HD1	1:B:116:PRO:HG3	1.79	0.48
1:B:435:GLU:OE2	1:B:488:ARG:NH2	2.43	0.47
1:A:414:LYS:HD3	1:A:422:TYR:OH	2.14	0.47
1:A:92:HIS:HD2	1:B:127:ILE:HG22	1.79	0.47
1:A:249:PHE:O	1:A:253:GLU:HB2	2.14	0.47
1:A:11:PHE:CD2	1:A:148:PRO:HG2	2.50	0.47
1:A:313:SER:HB3	1:A:316:GLN:HG3	1.97	0.47
1:A:44:GLU:OE1	1:A:99:TYR:OH	2.17	0.47
1:B:235:THR:HG22	1:B:251:TRP:CD1	2.48	0.46
1:B:292:TRP:CZ2	1:B:337:VAL:HA	2.49	0.46
1:A:403:PHE:CZ	1:A:407:ILE:HD11	2.50	0.46
1:B:60:LEU:HD23	1:B:67:GLN:HB3	1.97	0.46
1:B:15:GLU:OE2	1:B:15:GLU:HA	2.16	0.46
1:A:222:GLY:O	1:A:226:PRO:HA	2.16	0.46
1:B:392:ALA:HA	1:B:505:ALA:HB1	1.99	0.45
1:B:438:TYR:CZ	1:B:442:LEU:HD11	2.51	0.45
1:B:30:ALA:O	1:B:33:LEU:HD12	2.17	0.45
1:B:446:GLU:O	1:B:450:THR:HG22	2.17	0.45
1:A:435:GLU:CD	1:A:488:ARG:HH22	2.21	0.44
1:B:304:ALA:O	1:B:307:LEU:HG	2.17	0.44
1:A:106:ILE:HD11	1:A:117:ALA:HB2	2.00	0.44



A + a 1		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:229:ASP:OD2	1:B:232:GLU:HG3	2.18	0.44
1:A:77:PRO:HA	1:A:110:TYR:CE2	2.53	0.44
1:B:249:PHE:O	1:B:253:GLU:HB2	2.17	0.44
1:A:422:TYR:OH	1:A:444:ASP:OD2	2.26	0.43
1:A:43:TYR:CE2	1:A:180:VAL:HA	2.53	0.43
1:A:106:ILE:HD11	1:A:117:ALA:CA	2.48	0.43
1:B:115:THR:HB	1:B:118:GLU:HB2	2.00	0.43
1:A:410:LEU:HD22	1:A:448:LYS:HG2	2.00	0.43
1:B:49:GLY:N	1:B:97:LYS:HE3	2.32	0.43
1:A:50:TRP:HZ3	1:B:119:TYR:CE2	2.37	0.43
1:A:441:TYR:CZ	1:A:445:LEU:HD11	2.54	0.42
1:B:95:LEU:HD11	1:B:133:ILE:HG13	2.01	0.42
1:B:447:THR:HA	1:B:450:THR:CG2	2.48	0.42
1:A:67:GLN:HB3	1:A:170:PRO:O	2.18	0.42
1:B:256:ALA:HB1	1:B:261:LEU:HD21	2.02	0.42
1:B:356:ARG:HH11	2:B:602:EDO:H21	1.84	0.42
1:A:234:ILE:HD12	1:A:234:ILE:HA	1.87	0.42
1:A:53:ALA:HA	1:A:94:TYR:OH	2.20	0.42
1:B:260:VAL:HG21	1:B:278:THR:HG22	2.00	0.42
1:A:495:ILE:HA	1:A:496:PRO:HD3	1.94	0.42
1:A:53:ALA:HA	1:A:94:TYR:CZ	2.55	0.41
1:A:261:LEU:HD23	1:A:261:LEU:HA	1.93	0.41
1:B:243:LEU:O	1:B:246:VAL:HG12	2.21	0.41
1:B:108:GLY:HA2	1:B:137:SER:HB2	2.02	0.41
1:B:245:LYS:O	1:B:249:PHE:HD1	2.03	0.41
1:A:15:GLU:OE2	1:A:150:ALA:HA	2.20	0.41
1:A:82:HIS:NE2	1:B:86:THR:HG21	2.36	0.41
1:B:106:ILE:O	1:B:137:SER:HA	2.20	0.41
1:A:81:ILE:HD12	1:A:81:ILE:HG23	1.53	0.41
1:B:51:PRO:HD2	1:B:97:LYS:HD2	2.01	0.41
1:B:384:ARG:HA	1:B:384:ARG:HD2	1.88	0.41
1:A:37:ILE:HA	1:A:60:LEU:O	2.21	0.40
1:B:359:GLU:HG2	1:B:359:GLU:H	1.76	0.40
1:A:209:PRO:HB2	1:A:249:PHE:CE2	2.57	0.40
1:A:142:ASP:OD1	1:A:144:THR:HB	2.21	0.40
1:B:377:ARG:HB2	1:B:378:TYR:CD1	2.56	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	А	483/510~(95%)	469 (97%)	12 (2%)	2~(0%)	34	54	
1	В	472/510~(92%)	452 (96%)	19 (4%)	1 (0%)	47	68	
All	All	955/1020~(94%)	921 (96%)	31 (3%)	3 (0%)	41	61	

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	509	ASP
1	В	185	GLY
1	А	170	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	347/408~(85%)	334~(96%)	13~(4%)	34 60		
1	В	327/408~(80%)	313~(96%)	14 (4%)	29 53		
All	All	674/816~(83%)	647~(96%)	27~(4%)	31 56		

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	50	TRP
1	А	113	HIS
1	A	118	GLU



Mol	Chain	Res	Type
1	А	144	THR
1	А	154	GLN
1	А	212	THR
1	А	214	ARG
1	А	229	ASP
1	А	284	ASP
1	А	313	SER
1	А	326	SER
1	А	450	THR
1	А	459	VAL
1	В	29	ASP
1	В	40	SER
1	В	50	TRP
1	В	64	THR
1	В	97	LYS
1	В	106	ILE
1	В	109	ARG
1	В	143	THR
1	В	361	ASP
1	В	370	ARG
1	В	424	LYS
1	В	447	THR
1	В	452	GLU
1	В	485	SER

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

Mol	Chain	Res	Type
1	А	335	GLN
1	В	236	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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).

Mal	True	Chain	Dec	Tinle	Link Bond lengths			Bond angles		
	туре	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	EDO	В	601	-	3,3,3	0.60	0	2,2,2	0.11	0
2	EDO	В	602	-	3,3,3	0.54	0	2,2,2	0.26	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	EDO	В	601	-	-	0/1/1/1	-
2	EDO	В	602	-	-	0/1/1/1	-

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
2	В	602	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^{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	491/510~(96%)	0.05	12 (2%) 59 62	33, 50, 89, 125	0
1	В	482/510~(94%)	0.24	26 (5%) 25 27	33, 54, 97, 120	0
All	All	973/1020~(95%)	0.14	38 (3%) 39 42	33, 52, 96, 125	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ	
1	А	208	ALA	6.0	
1	В	227	GLY	5.4	
1	В	164	GLY	5.4	
1	А	162	ASP	4.7	
1	А	2	PRO	4.5	
1	В	32	SER	4.3	
1	А	168	LEU	4.0	
1	В	162	ASP	3.9	
1	В	204	ALA	3.6	
1	В	186	SER	3.4	
1	В	304	ALA	3.2	
1	В	296	VAL	3.2	
1	В	31	ALA	3.1	
1	А	126	ALA	3.1	
1	В	297	ASN	3.0	
1	В	317	GLY	3.0	
1	В	467	VAL	3.0	
1	А	209	PRO	3.0	
1	В	298	SER	2.8	
1	В	63	GLY	2.7	
1	А	82	HIS	2.7	
1	А	22	ALA	2.6	
1	В	3	TYR	2.6	
1	В	318	TRP	2.6	



Mol	Chain	Res	Type	RSRZ
1	В	184	GLU	2.6
1	В	202	LEU	2.5
1	В	315	ALA	2.5
1	В	427	PRO	2.5
1	А	204	ALA	2.4
1	А	64	THR	2.4
1	В	305	GLY	2.4
1	А	26	LEU	2.3
1	В	308	ASN	2.3
1	А	427	PRO	2.3
1	В	337	VAL	2.3
1	В	299	LEU	2.1
1	В	264	TRP	2.1
1	В	302	THR	2.1

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 monosaccharides 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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
2	EDO	В	602	4/4	0.84	0.57	$53,\!53,\!57,\!61$	0
2	EDO	В	601	4/4	0.87	0.16	$55,\!58,\!59,\!61$	0

6.5 Other polymers (i)

There are no such residues in this entry.

