



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:44 AM GMT

PDB ID : 3POR  
Title : PORIN CONFORMATION IN THE ABSENCE OF CALCIUM; REFINED  
STRUCTURE AT 2.5 ANGSTROMS RESOLUTION  
Authors : Weiss, M.S.; Schulz, G.E.  
Deposited on : 1992-11-09  
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](mailto: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.

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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

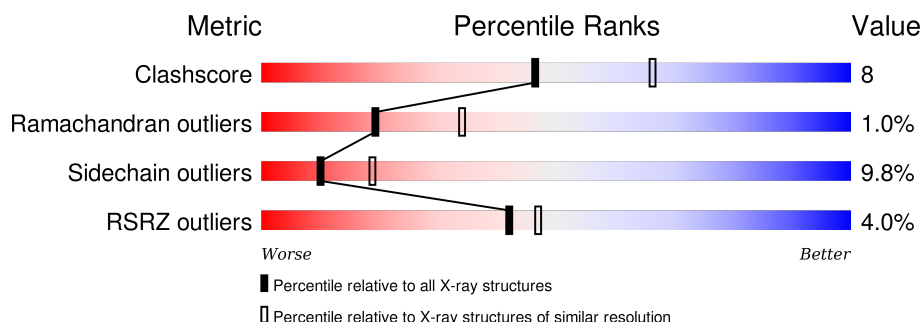
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	301	

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	C8E	A	545	-	-	-	X
3	TRS	A	700	-	-	-	X

## 2 Entry composition [i](#)

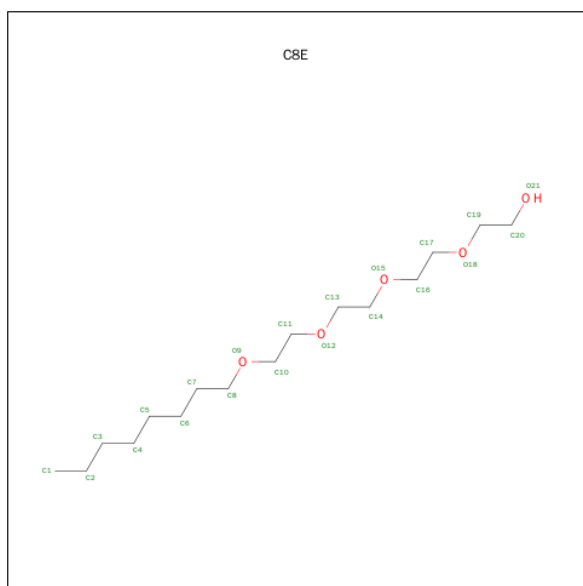
There are 4 unique types of molecules in this entry. The entry contains 2325 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PORIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	301	Total	C	N	O	S	0	0	0
			2219	1389	348	473	9			

- Molecule 2 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: C<sub>16</sub>H<sub>34</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			21	16	5		

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C<sub>4</sub>H<sub>12</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	4	1	3		

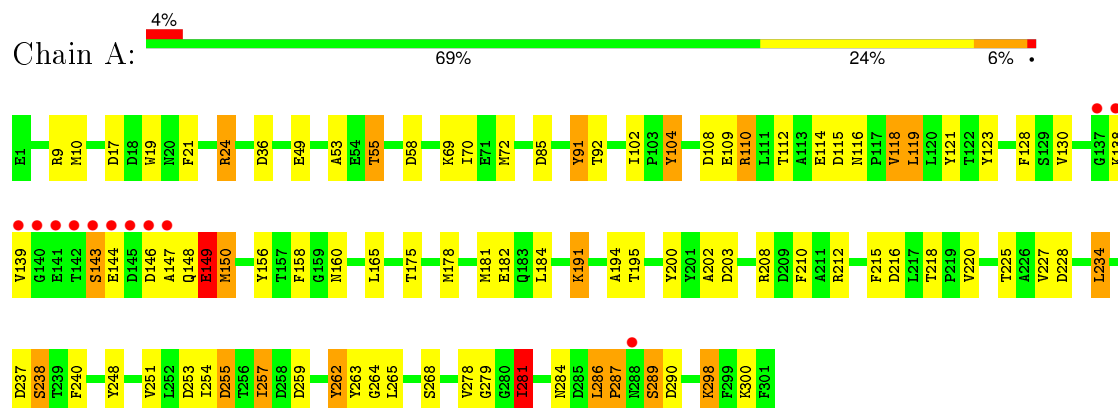
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	77	Total	O	0	0
			77	77		

### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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: PORIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.30 Å 95.30 Å 146.80 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.50 27.66 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.50) 95.2 (27.66-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.188 , (Not available) 0.178 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	39.7	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 97.2	EDS
Estimated twinning fraction	0.066 for h,-h-k,-l	Xtriage
L-test for twinning <sup>1</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 16568 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	2325	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.52% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Theoretical 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: TRS, C8E

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	1.15	2/2258 (0.1%)	1.86	53/3061 (1.7%)

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	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	49	GLU	CA-CB	-5.59	1.41	1.53
1	A	70	ILE	CA-CB	-5.35	1.42	1.54

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	263	TYR	CB-CG-CD2	-12.04	113.78	121.00
1	A	289	SER	CA-C-N	-8.65	98.17	117.20
1	A	19	TRP	CG-CD2-CE3	8.10	141.19	133.90
1	A	104	TYR	CB-CG-CD1	-8.10	116.14	121.00
1	A	200	TYR	CB-CG-CD2	-7.87	116.28	121.00
1	A	10	MET	CA-CB-CG	7.74	126.45	113.30
1	A	10	MET	CG-SD-CE	-7.58	88.07	100.20
1	A	55	THR	CA-CB-CG2	-7.53	101.85	112.40
1	A	253	ASP	CB-CG-OD1	7.46	125.02	118.30
1	A	257	ILE	CA-C-N	7.08	132.76	117.20
1	A	19	TRP	CE2-CD2-CG	-6.97	101.72	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	123	TYR	CB-CG-CD1	-6.96	116.83	121.00
1	A	19	TRP	CD1-CG-CD2	6.95	111.86	106.30
1	A	19	TRP	CB-CG-CD1	-6.67	118.33	127.00
1	A	130	VAL	CA-CB-CG1	-6.56	101.06	110.90
1	A	298	LYS	N-CA-CB	-6.50	98.91	110.60
1	A	289	SER	CA-C-O	6.44	133.62	120.10
1	A	259	ASP	CB-CG-OD1	6.44	124.09	118.30
1	A	216	ASP	N-CA-CB	-6.40	99.07	110.60
1	A	91	TYR	CB-CG-CD2	-6.36	117.18	121.00
1	A	268	SER	CB-CA-C	-6.32	98.09	110.10
1	A	149	GLU	CA-C-N	6.29	131.03	117.20
1	A	150	MET	CG-SD-CE	6.25	110.20	100.20
1	A	156	TYR	CB-CG-CD1	-6.21	117.27	121.00
1	A	212	ARG	NE-CZ-NH2	6.06	123.33	120.30
1	A	200	TYR	CB-CG-CD1	6.04	124.62	121.00
1	A	147	ALA	CA-C-N	-6.01	103.98	117.20
1	A	119	LEU	CA-C-N	5.81	129.97	117.20
1	A	36	ASP	CA-C-N	5.77	129.89	117.20
1	A	9	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	A	165	LEU	CA-CB-CG	5.74	128.51	115.30
1	A	268	SER	N-CA-CB	5.68	119.02	110.50
1	A	118	VAL	CA-CB-CG1	-5.65	102.43	110.90
1	A	289	SER	N-CA-CB	-5.63	102.05	110.50
1	A	289	SER	N-CA-C	5.59	126.10	111.00
1	A	225	THR	CA-CB-CG2	-5.55	104.64	112.40
1	A	110	ARG	CA-CB-CG	-5.54	101.20	113.40
1	A	279	GLY	CA-C-N	5.53	127.27	116.20
1	A	150	MET	CA-CB-CG	5.45	122.56	113.30
1	A	281	ILE	CB-CG1-CD1	-5.40	98.78	113.90
1	A	121	TYR	CB-CG-CD2	-5.35	117.79	121.00
1	A	146	ASP	CA-CB-CG	5.35	125.16	113.40
1	A	21	PHE	CB-CG-CD2	-5.23	117.14	120.80
1	A	149	GLU	O-C-N	-5.21	114.37	122.70
1	A	92	THR	CA-C-N	5.19	128.61	117.20
1	A	265	LEU	CA-CB-CG	5.19	127.23	115.30
1	A	69	LYS	CA-CB-CG	5.17	124.77	113.40
1	A	146	ASP	CA-C-N	-5.16	105.85	117.20
1	A	24	ARG	CB-CG-CD	-5.15	98.20	111.60
1	A	85	ASP	O-C-N	-5.10	114.54	122.70
1	A	130	VAL	CA-CB-CG2	5.06	118.50	110.90
1	A	181	MET	CG-SD-CE	-5.06	92.11	100.20
1	A	55	THR	CA-CB-OG1	5.00	119.50	109.00



There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	286	LEU	Peptide

## 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	2219	0	2072	33	0
2	A	21	0	34	1	0
3	A	8	0	12	1	0
4	A	77	0	0	2	0
All	All	2325	0	2118	33	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 8.

All (33) 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:A:112:THR:HG21	1:A:149:GLU:HG3	1.67	0.77
1:A:138:LYS:HA	1:A:144:GLU:O	1.87	0.73
1:A:215:PHE:HE2	1:A:254:ILE:HD12	1.64	0.62
1:A:191:LYS:HE3	4:A:933:HOH:O	2.01	0.61
1:A:108:ASP:CG	1:A:109:GLU:H	2.04	0.61
1:A:116:ASN:HA	1:A:118:VAL:HG13	1.84	0.60
1:A:148:GLN:OE1	1:A:148:GLN:HA	2.02	0.59
1:A:53:ALA:HA	1:A:58:ASP:O	2.01	0.59
1:A:112:THR:O	1:A:115:ASP:HB2	2.05	0.56
1:A:175:THR:HA	1:A:178:MET:O	2.06	0.56
1:A:210:PHE:HZ	2:A:545:C8E:H42	1.71	0.55
1:A:234:LEU:O	1:A:248:TYR:HA	2.06	0.55
1:A:278:VAL:HG21	1:A:298:LYS:HD3	1.92	0.52
1:A:108:ASP:CG	1:A:109:GLU:N	2.65	0.50
1:A:194:ALA:O	1:A:238:SER:HA	2.13	0.49
1:A:264:GLY:HA2	1:A:281:ILE:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:VAL:HG21	1:A:257:ILE:HD12	1.95	0.47
1:A:138:LYS:HB3	1:A:143:SER:HA	1.96	0.47
1:A:208:ARG:HD3	1:A:208:ARG:HH11	1.61	0.46
1:A:24:ARG:HH22	3:A:700:TRS:H31	1.81	0.46
1:A:262:TYR:HB3	1:A:284:ASN:HB3	1.99	0.45
1:A:104:TYR:HB2	1:A:110:ARG:NE	2.31	0.45
1:A:208:ARG:NE	1:A:220:VAL:HG22	2.32	0.44
1:A:286:LEU:HA	1:A:287:PRO:HD2	1.79	0.44
1:A:228:ASP:O	1:A:255:ASP:HB3	2.18	0.44
1:A:184:LEU:O	1:A:202:ALA:HA	2.19	0.42
1:A:109:GLU:HG2	4:A:927:HOH:O	2.18	0.42
1:A:215:PHE:CE2	1:A:254:ILE:HD12	2.51	0.42
1:A:72:MET:HE2	1:A:119:LEU:HD13	2.02	0.41
1:A:138:LYS:HD3	1:A:144:GLU:O	2.21	0.41
1:A:102:ILE:HB	1:A:104:TYR:CE2	2.56	0.41
1:A:139:VAL:HB	1:A:144:GLU:HB3	2.02	0.41
1:A:195:THR:HA	1:A:237:ASP:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	299/301 (99%)	284 (95%)	12 (4%)	3 (1%)	19	34

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	287	PRO
1	A	143	SER
1	A	289	SER

### 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	224/224 (100%)	202 (90%)	22 (10%)	10	19

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ASP
1	A	55	THR
1	A	91	TYR
1	A	114	GLU
1	A	128	PHE
1	A	149	GLU
1	A	150	MET
1	A	158	PHE
1	A	160	ASN
1	A	182	GLU
1	A	191	LYS
1	A	203	ASP
1	A	218	THR
1	A	234	LEU
1	A	238	SER
1	A	240	PHE
1	A	251	VAL
1	A	255	ASP
1	A	262	TYR
1	A	281	ILE
1	A	290	ASP
1	A	300	LYS

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 [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](#)

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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	C8E	A	545	-	20,20,20	0.82	0	19,19,19	1.82	6 (31%)
3	TRS	A	700	-	7,7,7	1.95	3 (42%)	9,9,9	2.45	6 (66%)

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	C8E	A	545	-	-	0/18/18/18	0/0/0/0
3	TRS	A	700	-	-	0/9/9/9	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	700	TRS	C-N	-3.26	1.45	1.50
3	A	700	TRS	C1-C	2.30	1.57	1.53
3	A	700	TRS	C3-C	2.37	1.57	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	A	700	TRS	C3-C-N	-2.44	103.65	108.09
3	A	700	TRS	C2-C-N	-2.27	103.96	108.09
2	A	545	C8E	O12-C11-C10	2.38	120.95	110.36
2	A	545	C8E	O9-C8-C7	2.43	119.60	109.87
3	A	700	TRS	O3-C3-C	2.44	116.12	111.18
2	A	545	C8E	O18-C19-C20	2.45	121.70	110.43
3	A	700	TRS	C3-C-C2	2.53	116.27	110.78
2	A	545	C8E	O9-C10-C11	2.69	122.32	110.36
3	A	700	TRS	C1-C-N	3.26	114.02	108.09
2	A	545	C8E	O18-C17-C16	3.53	126.06	110.36
2	A	545	C8E	O15-C16-C17	3.57	126.23	110.36
3	A	700	TRS	O1-C1-C	4.02	119.32	111.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	545	C8E	1	0
3	A	700	TRS	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	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	301/301 (100%)	-0.62	12 (3%)	42 47	12, 30, 64, 121	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	139	VAL	7.4
1	A	142	THR	6.4
1	A	143	SER	6.3
1	A	144	GLU	6.2
1	A	141	GLU	5.0
1	A	140	GLY	4.2
1	A	145	ASP	3.1
1	A	288	ASN	3.1
1	A	138	LYS	2.8
1	A	146	ASP	2.8
1	A	147	ALA	2.4
1	A	137	GLY	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 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. 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	TRS	A	700	8/8	0.80	0.21	11.04	56,63,65,65	0
2	C8E	A	545	21/21	0.89	0.24	4.17	35,57,114,118	0

## 6.5 Other polymers

There are no such residues in this entry.