



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:57 AM GMT

PDB ID : 2OVM  
Title : Progesterone Receptor with Bound Asoprisnil and a Peptide from the Co-Repressor NCoR  
Authors : Madauss, K.P.; Deng, S.-J.; Short, S.A.; Stewart, E.L.; Williams, S.P.  
Deposited on : 2007-02-14  
Resolution : 2.60 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

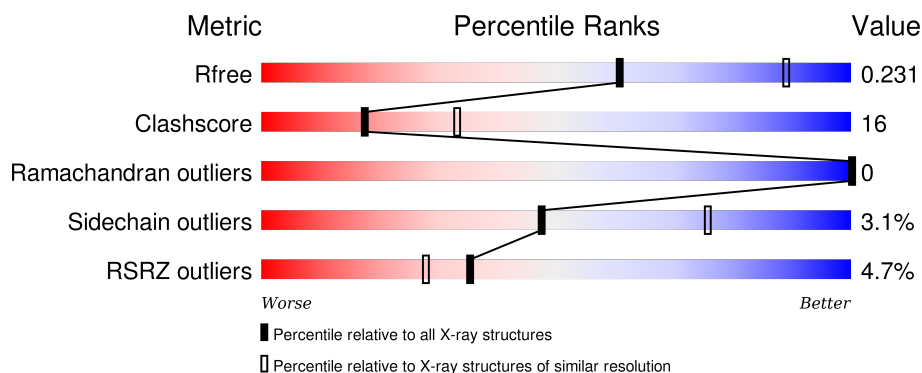
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*



The reported resolution of this entry is 2.60 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))
$R_{free}$	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	256	
2	B	25	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2125 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.

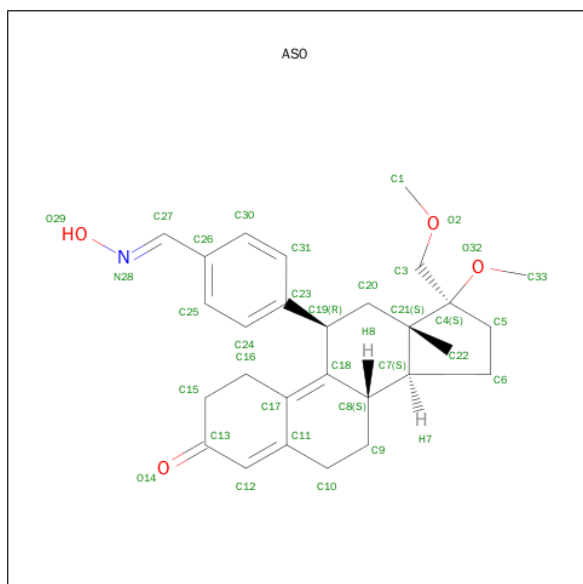
- Molecule 1 is a protein called Progesterone receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	0	0
			1951	1264	327	347	13			

- Molecule 2 is a protein called NCoR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	11	Total	C	N	O	S	0	0	0
			82	52	14	15	1			

- Molecule 3 is 4-[(11BETA,17BETA)-17-METHOXY-17-(METHOXYMETHYL)-3-OXO-ESTRA-4,9-DIEN-11-YL]BENZALDEHYDE OXIME (three-letter code: AS0) (formula: C<sub>28</sub>H<sub>35</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			33	28	1	4		

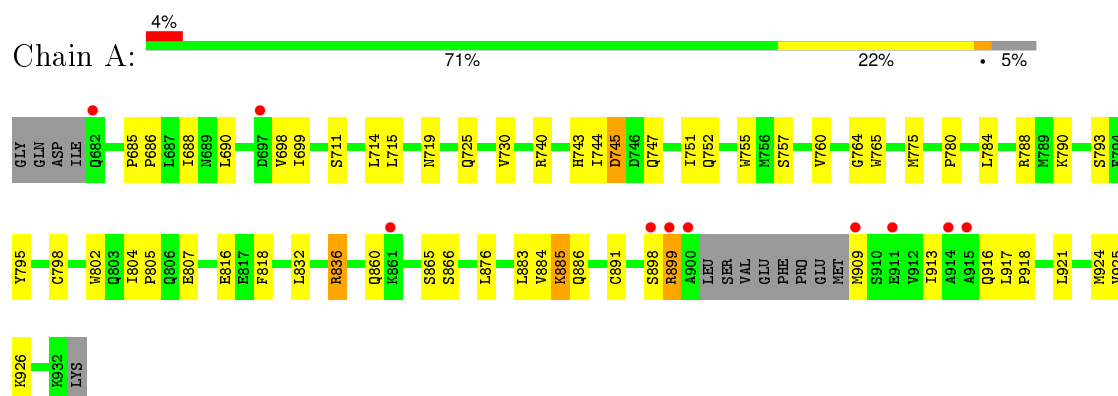
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	57	Total 57	O 57	0	0
4	B	2	Total 2	O 2	0	0

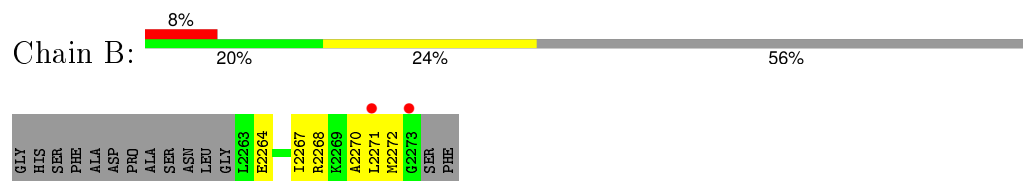
### 3 Residue-property plots

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 ( $RSRZ > 2$ ). 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: Progesterone receptor



#### • Molecule 2: NCoR



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.51Å 87.51Å 90.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.60 19.69 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.6 (20.00-2.60) 97.6 (19.69-2.60)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.00	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.75 (at 2.59Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.219 , 0.244 0.221 , 0.231	Depositor DCC
$R_{free}$ test set	914 reflections (7.39%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.2	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 49.1	EDS
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 12366 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	2125	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.33% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: AS0

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	0.41	1/1991 (0.1%)	0.59	0/2693
2	B	0.35	0/81	0.47	0/107
All	All	0.40	1/2072 (0.0%)	0.59	0/2800

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	755	TRP	NE1-CE2	8.57	1.48	1.37

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	A	1951	0	1994	64	1
2	B	82	0	85	15	0
3	A	33	0	35	4	0
4	A	57	0	0	4	0
4	B	2	0	0	0	0
All	All	2125	0	2114	67	1

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 16.

All (67) 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:752:GLN:NE2	2:B:2264:GLU:HB2	1.70	1.06
1:A:807:GLU:HG2	4:A:38:HOH:O	1.62	0.98
1:A:752:GLN:HE21	2:B:2264:GLU:HB2	1.27	0.92
1:A:743:HIS:HD2	1:A:745:ASP:H	1.21	0.89
1:A:740:ARG:HH11	1:A:747:GLN:HE22	1.25	0.83
1:A:764:GLY:HA2	1:A:805:PRO:HG3	1.61	0.83
1:A:784:LEU:HD23	1:A:788:ARG:HD3	1.65	0.77
1:A:802:TRP:O	1:A:805:PRO:HD2	1.85	0.76
1:A:743:HIS:CD2	1:A:745:ASP:H	2.07	0.72
1:A:686:PRO:HD2	4:A:37:HOH:O	1.90	0.72
1:A:913:ILE:O	1:A:917:LEU:HG	1.94	0.68
1:A:740:ARG:NH1	1:A:747:GLN:HE22	1.93	0.66
1:A:909:MET:O	1:A:913:ILE:HG13	1.97	0.64
2:B:2267:ILE:HG22	2:B:2267:ILE:O	1.98	0.62
1:A:744:ILE:HG12	2:B:2272:MET:CE	2.30	0.61
1:A:688:ILE:HG21	1:A:816:GLU:HG3	1.82	0.61
1:A:917:LEU:N	1:A:918:PRO:HD2	2.16	0.61
1:A:698:VAL:HG13	4:A:15:HOH:O	2.02	0.60
1:A:836:ARG:HG2	1:A:836:ARG:HH11	1.67	0.59
1:A:916:GLN:C	1:A:918:PRO:HD2	2.23	0.59
1:A:836:ARG:CG	1:A:836:ARG:HH11	2.17	0.58
1:A:917:LEU:N	1:A:918:PRO:CD	2.67	0.57
1:A:860:GLN:HG3	1:A:865:SER:HB3	1.84	0.57
1:A:784:LEU:CD2	1:A:788:ARG:HD3	2.35	0.57
1:A:752:GLN:NE2	2:B:2264:GLU:CB	2.60	0.56
1:A:836:ARG:HG2	1:A:836:ARG:NH1	2.22	0.55
1:A:747:GLN:NE2	2:B:2271:LEU:HD22	2.20	0.55
1:A:802:TRP:C	1:A:805:PRO:HD2	2.27	0.55
1:A:698:VAL:HG11	1:A:780:PRO:HG2	1.89	0.55
1:A:760:VAL:HG22	1:A:804:ILE:HD12	1.88	0.55
1:A:876:LEU:HD23	1:A:876:LEU:C	2.28	0.53
2:B:2267:ILE:CG2	2:B:2267:ILE:O	2.58	0.51
1:A:883:LEU:HD23	1:A:883:LEU:C	2.31	0.51
1:A:917:LEU:O	1:A:921:LEU:HB2	2.11	0.50
1:A:751:ILE:HG22	2:B:2267:ILE:HD13	1.92	0.50
1:A:685:PRO:HD2	1:A:688:ILE:HD12	1.94	0.49
1:A:860:GLN:HG2	1:A:866:SER:HA	1.96	0.48
1:A:752:GLN:HE22	2:B:2264:GLU:HB2	1.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:711:SER:O	1:A:715:LEU:HG	2.14	0.47
1:A:798:CYS:O	1:A:802:TRP:HB2	2.14	0.47
1:A:832:LEU:HD23	1:A:926:LYS:HB2	1.95	0.47
1:A:883:LEU:O	1:A:886:GLN:HB2	2.15	0.47
1:A:725:GLN:HE22	3:A:101:AS0:C13	2.29	0.46
1:A:925:VAL:HG22	4:A:6:HOH:O	2.14	0.46
3:A:101:AS0:C23	3:A:101:AS0:H221	2.46	0.46
1:A:690:LEU:HD23	1:A:690:LEU:C	2.36	0.46
1:A:730:VAL:HG11	2:B:2270:ALA:CB	2.46	0.46
1:A:790:LYS:HA	1:A:795:TYR:CD1	2.51	0.45
1:A:743:HIS:HD2	1:A:745:ASP:N	2.02	0.45
1:A:751:ILE:HG21	2:B:2267:ILE:CG2	2.46	0.45
1:A:757:SER:HB3	1:A:884:VAL:HG21	1.99	0.45
1:A:891:CYS:HB2	3:A:101:AS0:H51	2.00	0.44
1:A:804:ILE:HB	1:A:805:PRO:HD3	1.99	0.44
1:A:883:LEU:HD23	1:A:883:LEU:O	2.17	0.44
1:A:747:GLN:HE21	2:B:2271:LEU:HD22	1.80	0.44
1:A:751:ILE:HG21	2:B:2267:ILE:HG23	1.99	0.43
1:A:898:SER:OG	1:A:899:ARG:HD2	2.18	0.43
1:A:765:TRP:HB2	1:A:818:PHE:CE1	2.52	0.43
1:A:744:ILE:HG12	2:B:2272:MET:HE2	1.99	0.42
1:A:711:SER:OG	1:A:793:SER:HB2	2.20	0.42
1:A:685:PRO:HA	1:A:686:PRO:HD3	1.86	0.41
1:A:918:PRO:HA	1:A:924:MET:SD	2.60	0.41
1:A:747:GLN:O	1:A:751:ILE:HG12	2.20	0.41
1:A:885:LYS:HB3	1:A:885:LYS:HE2	1.94	0.40
1:A:714:LEU:HD23	1:A:714:LEU:HA	1.83	0.40
1:A:719:ASN:HA	3:A:101:AS0:H31	2.04	0.40
1:A:730:VAL:HG11	2:B:2270:ALA:HB3	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:886:GLN:NE2	1:A:886:GLN:NE2[6_555]	1.88	0.32

## 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	239/256 (93%)	233 (98%)	6 (2%)	0	100	100
2	B	9/25 (36%)	8 (89%)	1 (11%)	0	100	100
All	All	248/281 (88%)	241 (97%)	7 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	220/238 (92%)	214 (97%)	6 (3%)	52	79
2	B	8/19 (42%)	7 (88%)	1 (12%)	6	10
All	All	228/257 (89%)	221 (97%)	7 (3%)	47	76

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	699	ILE
1	A	745	ASP
1	A	775	MET
1	A	836	ARG
1	A	885	LYS
1	A	899	ARG
2	B	2268	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	725	GLN
1	A	743	HIS
1	A	747	GLN
1	A	752	GLN
1	A	774	GLN
1	A	868	GLN
1	A	897	GLN

### 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](#)

1 ligand is 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	$\# Z  > 2$
3	ASO	A	101	-	35,37,37	2.82	14 (40%)	41,56,56	2.73	13 (31%)

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	AS0	A	101	-	-	0/14/74/74	0/5/5/5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	101	AS0	C8-C18	2.52	1.55	1.52
3	A	101	AS0	C8-C7	2.60	1.60	1.54
3	A	101	AS0	C20-C21	2.61	1.58	1.53
3	A	101	AS0	C31-C30	2.71	1.43	1.38
3	A	101	AS0	C20-C19	3.04	1.58	1.53
3	A	101	AS0	C23-C19	3.05	1.56	1.52
3	A	101	AS0	C17-C11	3.17	1.51	1.44
3	A	101	AS0	C15-C13	3.20	1.53	1.45
3	A	101	AS0	C31-C23	3.23	1.44	1.39
3	A	101	AS0	C24-C23	3.30	1.44	1.39
3	A	101	AS0	C19-C18	3.46	1.56	1.52
3	A	101	AS0	O32-C4	4.04	1.50	1.44
3	A	101	AS0	C16-C17	6.06	1.54	1.40
3	A	101	AS0	C16-C15	10.03	1.57	1.35

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	101	AS0	C16-C15-C13	-4.83	114.37	121.09
3	A	101	AS0	C9-C8-C7	-4.48	104.08	111.33
3	A	101	AS0	C21-C7-C8	-4.44	109.60	113.59
3	A	101	AS0	C22-C21-C4	-3.63	103.10	108.68
3	A	101	AS0	C22-C21-C20	-3.23	106.67	111.14
3	A	101	AS0	C15-C16-C17	-3.07	116.53	121.67
3	A	101	AS0	C30-C26-C25	2.04	120.75	117.64
3	A	101	AS0	O2-C3-C4	2.05	113.95	110.46
3	A	101	AS0	C20-C21-C4	2.99	120.06	117.74
3	A	101	AS0	C12-C11-C17	3.74	124.75	117.37
3	A	101	AS0	C6-C7-C8	5.11	126.05	118.34
3	A	101	AS0	O29-N28-C27	5.37	121.03	111.88
3	A	101	AS0	C4-C21-C7	10.05	107.81	99.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	101	AS0	4	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	243/256 (94%)	-0.32	10 (4%) 41 33	9, 22, 51, 73	0
2	B	11/25 (44%)	1.10	2 (18%) 2 1	51, 53, 65, 66	0
All	All	254/281 (90%)	-0.26	12 (4%) 35 28	9, 22, 57, 73	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	682	GLN	8.2
1	A	900	ALA	4.2
1	A	911	GLU	3.5
2	B	2273	GLY	3.4
1	A	898	SER	3.1
1	A	899	ARG	2.7
1	A	697	ASP	2.5
2	B	2271	LEU	2.4
1	A	914	ALA	2.2
1	A	909	MET	2.1
1	A	861	LYS	2.1
1	A	915	ALA	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. 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( $\text{\AA}^2$ )	Q<0.9
3	AS0	A	101	33/33	0.91	0.18	1.19	27,29,36,37	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.