



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 07:52 PM UTC

PDB ID : 9HUB / pdb\_00009hub  
Title : D11 mAbs bound to alpha-Bungarotoxin at pH 7.5  
Authors : Wade, J.W.; Bohn, M.F.; Laustsen, A.H.; Morth, J.P.  
Deposited on : 2024-12-21  
Resolution : 1.33 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

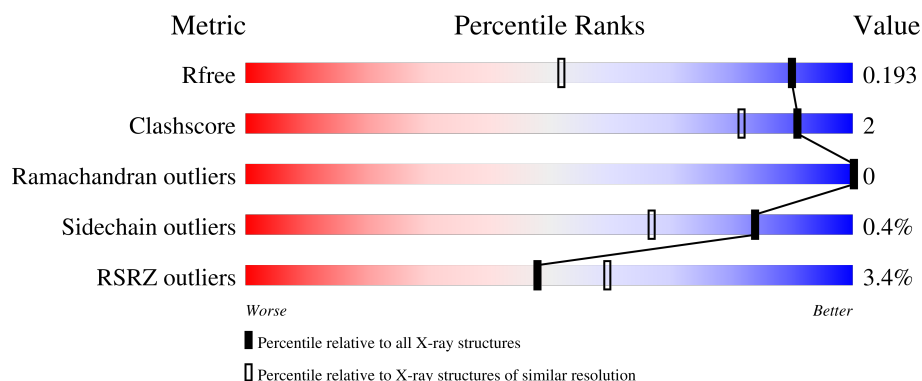
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.33 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))
$R_{free}$	180053	2194 (1.36-1.32)
Clashscore	190562	2222 (1.36-1.32)
Ramachandran outliers	187476	2197 (1.36-1.32)
Sidechain outliers	187428	2197 (1.36-1.32)
RSRZ outliers	180081	2193 (1.36-1.32)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	C	121	<div> <div>2%</div> <div>96%</div> <div>2%</div> </div>
1	M	121	<div> <div>0%</div> <div>91%</div> <div>8%</div> </div>
2	X	95	<div> <div>0%</div> <div>74%</div> <div>23%</div> </div>
2	Z	95	<div> <div>0%</div> <div>77%</div> <div>22%</div> </div>
3	B	144	<div> <div>3%</div> <div>90%</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
3	I	144	<div><div></div><div>8%</div><div>88%</div><div>5%</div><div>8%</div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10953 atoms, of which 4864 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 heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	C	119	Total	C	H	N	O	S	0	6	0
			1814	574	880	160	197	3			
1	M	120	Total	C	H	N	O	S	0	6	0
			1811	574	871	160	201	5			

- Molecule 2 is a protein called Alpha-bungarotoxin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	X	73	Total	C	H	N	O	S	0	1	0
			1081	338	532	96	104	11			
2	Z	74	Total	C	H	N	O	S	0	1	0
			1098	343	538	98	108	11			

- Molecule 3 is a protein called light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	I	133	Total	C	H	N	O	S	0	8	0
			2082	669	1011	183	211	8			
3	B	133	Total	C	H	N	O	S	0	10	0
			2036	655	990	172	211	8			

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	H	O	0	0
			10	2	6	2		
4	X	1	Total	C	H	O	0	0
			10	2	6	2		
4	X	1	Total	C	H	O	0	0
			10	2	6	2		
4	M	1	Total	C	H	O	0	0
			10	2	6	2		
4	M	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	157	Total	O	0	0
			157	157		
5	X	104	Total	O	0	0
			104	104		
5	Z	108	Total	O	0	0
			108	108		
5	I	179	Total	O	0	0
			179	179		
5	M	192	Total	O	0	0
			192	192		

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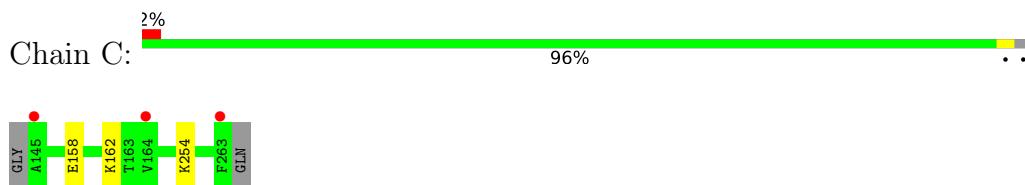
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	221	Total 221	O 221	0	0

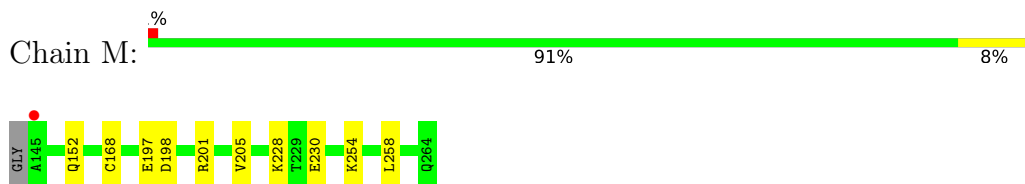
### 3 Residue-property plots [i](#)

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.

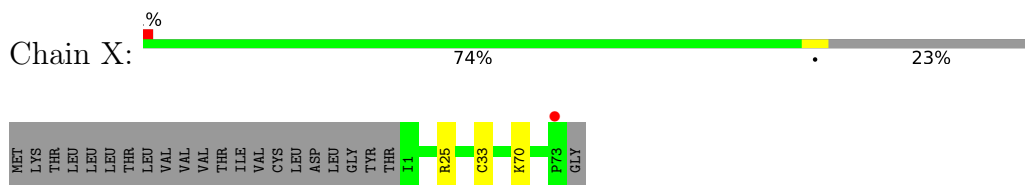
- Molecule 1: heavy chain



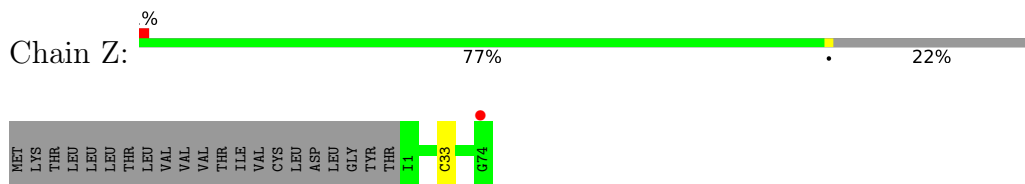
- Molecule 1: heavy chain



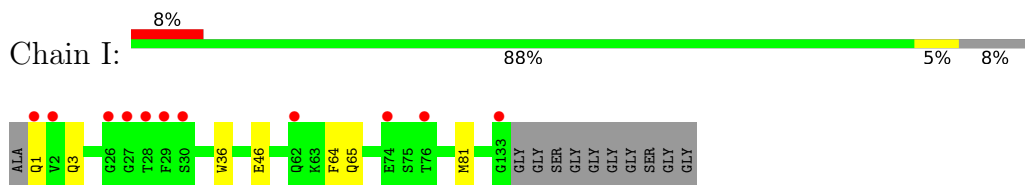
- Molecule 2: Alpha-bungarotoxin



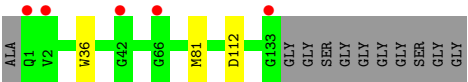
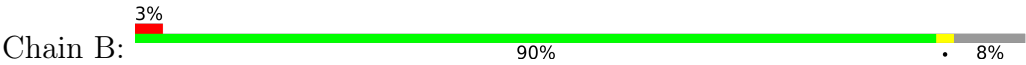
- Molecule 2: Alpha-bungarotoxin



- Molecule 3: light chain



- Molecule 3: light chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.05Å 84.73Å 102.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.38 – 1.33 22.38 – 1.33	Depositor EDS
% Data completeness (in resolution range)	99.6 (22.38-1.33) 90.6 (22.38-1.33)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.30 (at 1.33Å)	Xtriage
Refinement program	PHENIX 1.21rc1_5156	Depositor
R, $R_{free}$	0.159 , 0.195 0.158 , 0.193	Depositor DCC
$R_{free}$ test set	8021 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.6	Xtriage
Anisotropy	0.452	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.44 , 56.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	10953	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	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 23.88 % 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 4.2774e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: 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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	C	0.34	0/979	0.54	0/1330
1	M	0.40	0/984	0.57	0/1334
2	X	0.40	0/566	0.62	0/770
2	Z	0.41	0/574	0.62	0/779
3	B	0.39	0/1114	0.61	0/1508
3	I	0.38	0/1103	0.55	0/1490
All	All	0.38	0/5320	0.58	0/7211

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
2	X	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	X	25	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 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	C	934	880	856	2	0
1	M	940	871	841	7	0
2	X	549	532	534	2	0
2	Z	560	538	537	0	0
3	B	1046	990	947	2	0
3	I	1071	1011	1009	5	0
4	B	8	12	12	0	0
4	C	4	6	6	0	0
4	M	8	12	12	1	0
4	X	8	12	12	0	0
5	B	221	0	0	1	5
5	C	157	0	0	1	1
5	I	179	0	0	1	2
5	M	192	0	0	1	0
5	X	104	0	0	0	2
5	Z	108	0	0	0	4
All	All	6089	4864	4766	17	7

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 2.

The worst 5 of 17 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:M:254:LYS:NZ	5:M:401:HOH:O	1.81	1.10
1:M:152:GLN:HG2	1:M:168[A]:CYS:SG	2.08	0.94
3:I:1:GLN:HE21	3:I:3:GLN:HG3	1.62	0.65
1:C:254:LYS:NZ	5:C:402:HOH:O	2.38	0.57
1:M:228:LYS:HE3	1:M:230:GLU:OE1	2.05	0.56

The worst 5 of 7 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)
5:C:505:HOH:O	5:X:203:HOH:O[3_545]	1.90	0.30
5:Z:189:HOH:O	5:B:397:HOH:O[3_555]	1.94	0.26
5:Z:192:HOH:O	5:B:440:HOH:O[2_445]	1.95	0.25
5:I:259:HOH:O	5:B:468:HOH:O[2_445]	1.97	0.23
5:Z:160:HOH:O	5:B:479:HOH:O[3_555]	1.98	0.22

## 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	C	123/121 (102%)	119 (97%)	4 (3%)	0	100	100
1	M	124/121 (102%)	120 (97%)	4 (3%)	0	100	100
2	X	72/95 (76%)	71 (99%)	1 (1%)	0	100	100
2	Z	73/95 (77%)	72 (99%)	1 (1%)	0	100	100
3	B	141/144 (98%)	137 (97%)	4 (3%)	0	100	100
3	I	139/144 (96%)	132 (95%)	7 (5%)	0	100	100
All	All	672/720 (93%)	651 (97%)	21 (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	C	112/107 (105%)	112 (100%)	0	100	100
1	M	113/107 (106%)	113 (100%)	0	100	100
2	X	66/85 (78%)	65 (98%)	1 (2%)	57	22
2	Z	66/85 (78%)	65 (98%)	1 (2%)	57	22
3	B	115/108 (106%)	115 (100%)	0	100	100
3	I	113/108 (105%)	113 (100%)	0	100	100
All	All	585/600 (98%)	583 (100%)	2 (0%)	84	70

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	X	33	CYS
2	Z	33	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
3	B	100	ASN
3	B	39	GLN
3	I	100	ASN
3	I	59	ASN
1	M	185	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

7 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	$\# Z  > 2$
4	EDO	M	302	-	3,3,3	0.27	0	2,2,2	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	EDO	C	301	-	3,3,3	0.26	0	2,2,2	0.26	0
4	EDO	M	301	-	3,3,3	0.24	0	2,2,2	0.25	0
4	EDO	X	101	-	3,3,3	0.27	0	2,2,2	0.06	0
4	EDO	B	201	-	3,3,3	0.23	0	2,2,2	0.52	0
4	EDO	X	102	-	3,3,3	0.28	0	2,2,2	0.38	0
4	EDO	B	202	-	3,3,3	0.25	0	2,2,2	0.33	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
4	EDO	M	302	-	-	1/1/1/1	-
4	EDO	C	301	-	-	0/1/1/1	-
4	EDO	M	301	-	-	0/1/1/1	-
4	EDO	X	101	-	-	0/1/1/1	-
4	EDO	B	201	-	-	0/1/1/1	-
4	EDO	X	102	-	-	0/1/1/1	-
4	EDO	B	202	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	202	EDO	O1-C1-C2-O2
4	M	302	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	302	EDO	1	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	C	119/121 (98%)	0.14	3 (2%) 58 68	17, 29, 51, 73	3 (2%)
1	M	120/121 (99%)	-0.05	1 (0%) 82 89	11, 27, 48, 56	3 (2%)
2	X	73/95 (76%)	-0.17	1 (1%) 73 82	13, 24, 41, 60	1 (1%)
2	Z	74/95 (77%)	-0.19	1 (1%) 73 82	14, 22, 39, 66	1 (1%)
3	B	133/144 (92%)	-0.31	5 (3%) 44 56	10, 21, 35, 86	5 (3%)
3	I	133/144 (92%)	0.18	11 (8%) 17 24	12, 25, 63, 88	7 (5%)
All	All	652/720 (90%)	-0.05	22 (3%) 48 59	10, 25, 51, 88	20 (3%)

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	145	ALA	6.1
1	C	263	PHE	5.0
3	I	29	PHE	4.7
3	I	133	GLY	4.3
3	I	27	GLY	4.2

### 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 oligosaccharides 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<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	B-factors(Å <sup>2</sup> )	Q<0.9
4	EDO	M	302	4/4	0.82	0.16	43,55,88,88	0
4	EDO	M	301	4/4	0.85	0.12	41,50,54,54	0
4	EDO	C	301	4/4	0.85	0.13	36,44,68,82	0
4	EDO	X	102	4/4	0.90	0.11	31,44,63,76	0
4	EDO	X	101	4/4	0.92	0.11	29,53,66,66	0
4	EDO	B	202	4/4	0.94	0.08	32,57,79,94	0
4	EDO	B	201	4/4	0.96	0.06	24,28,32,32	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.