



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 19, 2022 – 01:09 pm BST

PDB ID : 7R1E  
Title : Mosquitocidal Cry11Ba determined at pH 10.4 from naturally-occurring nanocrystals by Serial femtosecond crystallography  
Authors : Colletier, J.-P.; Sawaya, M.R.; Schibrowsky, N.A.; Cascio, D.; Rodriguez, J.A.  
Deposited on : 2022-02-02  
Resolution : 2.65 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

<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	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

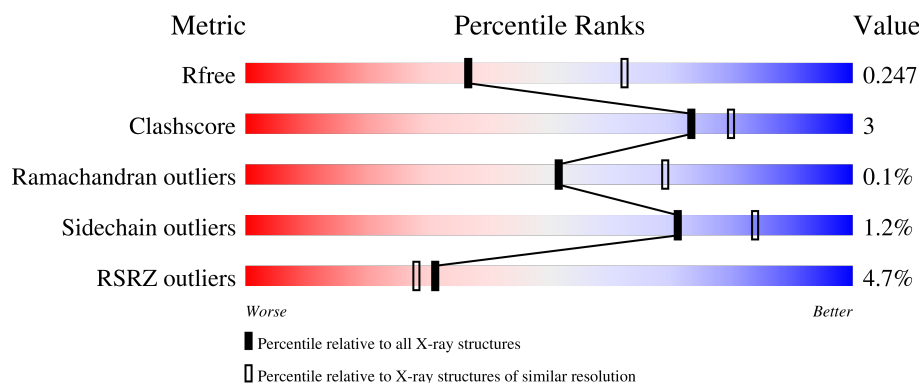
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	A	724	<div> <div>5%</div> <div> <div></div> <div>77%</div> <div>9%</div> <div>14%</div> </div> </div>
1	B	724	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>9%</div> <div>14%</div> </div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10031 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 Pesticidal crystal protein Cry11Ba.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	626	Total	C	N	O	S	0	0	0
			4968	3196	823	937	12			
1	B	621	Total	C	N	O	S	0	0	0
			4932	3168	819	934	11			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		

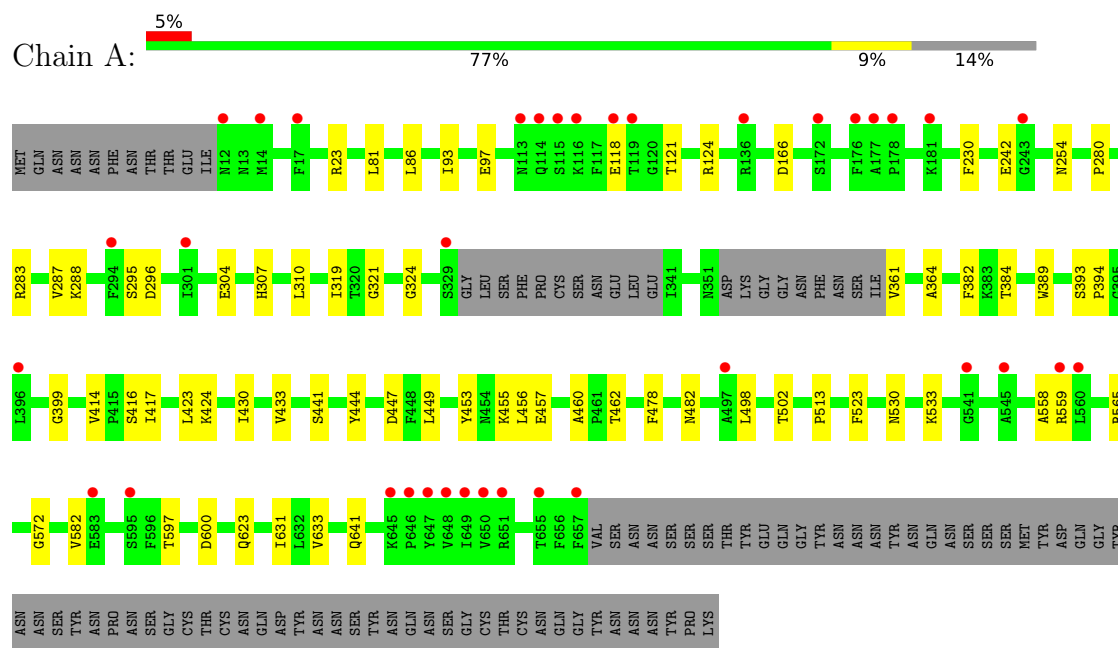
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	67	Total 67	O 67	0	0
3	B	52	Total 52	O 52	0	0

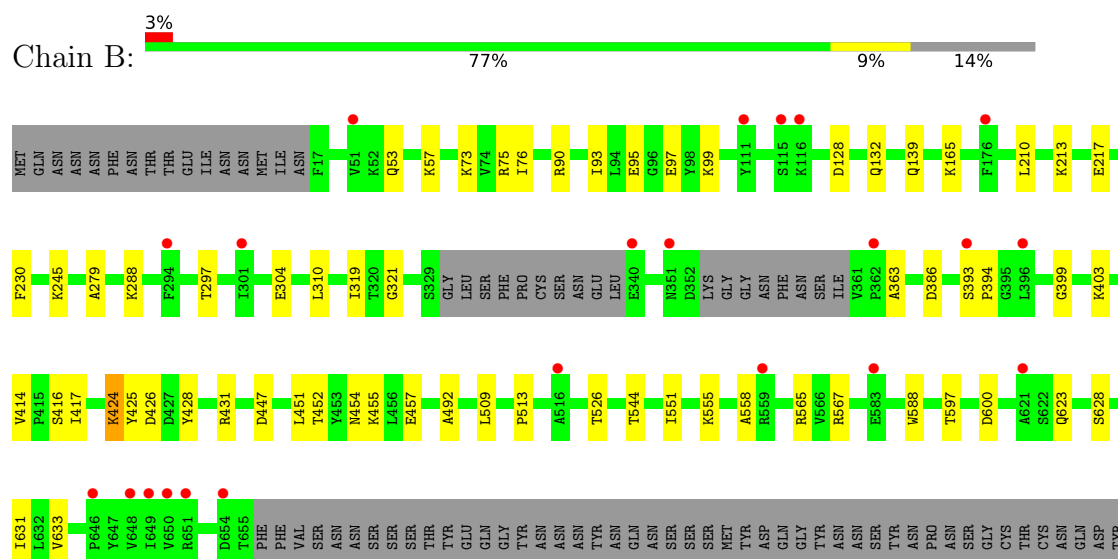
### 3 Residue-property plots [i](#)

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: Pesticidal crystal protein Cry11Ba



#### • Molecule 1: Pesticidal crystal protein Cry11Ba



ASN
ASN
SER
TYR
ASN
GLN
ASN
SER
GLY
CYS
THR
CYS
ASN
GLN
GLY
TYR
ASN
ASN
ASN
TYR
PRO
LYS

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	167.50Å 157.99Å 57.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.72 – 2.65 35.72 – 2.65	Depositor EDS
% Data completeness (in resolution range)	100.0 (35.72-2.65) 100.0 (35.72-2.65)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.23 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.20_4459	Depositor
R, $R_{free}$	0.236 , 0.247 0.237 , 0.247	Depositor DCC
$R_{free}$ test set	4525 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.0	Xtriage
Anisotropy	0.308	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	10031	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	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 68.36 % 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 4.4242e-06. 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL

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	0.25	0/5089	0.45	0/6918
1	B	0.24	0/5051	0.46	0/6866
All	All	0.24	0/10140	0.46	0/13784

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

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	4968	0	4888	33	0
1	B	4932	0	4857	33	0
2	A	12	0	16	0	0
3	A	67	0	0	0	0
3	B	52	0	0	1	0
All	All	10031	0	9761	64	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 3.

All (64) 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:307:HIS:HA	1:A:462:THR:HG23	1.79	0.64
1:A:296:ASP:HB2	1:A:361:VAL:HG23	1.83	0.61
1:A:242:GLU:OE1	1:A:641:GLN:NE2	2.33	0.60
1:B:304:GLU:HB2	1:B:399:GLY:HA2	1.82	0.59
1:A:304:GLU:HB2	1:A:399:GLY:HA2	1.86	0.57
1:A:288:LYS:HB2	1:A:310:LEU:HB3	1.88	0.55
1:B:73:LYS:HD2	1:B:76:ILE:HD11	1.90	0.53
1:A:572:GLY:HA2	1:B:567:ARG:HH22	1.76	0.50
1:B:165:LYS:NZ	3:B:808:HOH:O	2.44	0.50
1:A:287:VAL:HG21	1:A:433:VAL:HB	1.96	0.48
1:B:95:GLU:HG2	1:B:99:LYS:HE2	1.96	0.48
1:B:319:ILE:HG23	1:B:455:LYS:HA	1.95	0.48
1:B:321:GLY:HA3	1:B:457:GLU:HB3	1.95	0.48
1:A:324:GLY:HA2	1:A:460:ALA:HB3	1.96	0.47
1:A:280:PRO:HB2	1:A:498:LEU:HB3	1.97	0.46
1:A:23:ARG:NH2	1:A:81:LEU:O	2.49	0.46
1:A:319:ILE:HG23	1:A:455:LYS:HA	1.98	0.46
1:A:523:PHE:CD1	1:A:530:ASN:HB3	2.51	0.46
1:A:597:THR:HG23	1:A:600:ASP:H	1.80	0.46
1:B:597:THR:HG23	1:B:600:ASP:H	1.80	0.45
1:B:544:THR:O	1:B:597:THR:OG1	2.35	0.45
1:A:559:ARG:HG3	1:A:582:VAL:O	2.16	0.45
1:B:90:ARG:HH12	1:B:139:GLN:HG3	1.81	0.44
1:A:121:THR:HG23	1:A:124:ARG:HH22	1.82	0.44
1:B:558:ALA:HB3	1:B:623:GLN:HA	1.99	0.44
1:B:93:ILE:O	1:B:97:GLU:HG2	2.18	0.43
1:A:393:SER:OG	1:A:394:PRO:HD3	2.19	0.43
1:B:386:ASP:HB3	1:B:403:LYS:HB3	2.00	0.43
1:A:93:ILE:O	1:A:97:GLU:HG2	2.19	0.43
1:B:393:SER:OG	1:B:394:PRO:HD3	2.18	0.43
1:B:452:THR:O	1:B:454:ASN:N	2.51	0.43
1:A:502:THR:HG22	1:A:533:LYS:HB2	2.01	0.43
1:B:210:LEU:HD13	1:B:217:GLU:HG2	2.00	0.43
1:A:295:SER:HB3	1:A:364:ALA:HB3	2.00	0.43
1:A:384:THR:HG22	1:A:424:LYS:HB2	2.00	0.43
1:A:121:THR:HG23	1:A:124:ARG:NH2	2.34	0.42
1:A:449:LEU:HD22	1:A:456:LEU:HD12	2.01	0.42
1:A:631:ILE:HG22	1:A:633:VAL:HG13	2.00	0.42
1:B:414:VAL:HG12	1:B:416:SER:H	1.83	0.42
1:A:558:ALA:HB3	1:A:623:GLN:HA	2.01	0.42
1:B:451:LEU:HD21	1:B:509:LEU:HB2	2.02	0.42
1:B:551:ILE:HB	1:B:631:ILE:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:ALA:O	1:B:431:ARG:NH1	2.47	0.42
1:B:297:THR:HA	1:B:363:ALA:HB2	2.02	0.42
1:B:631:ILE:HG22	1:B:633:VAL:HG13	2.01	0.42
1:A:118:GLU:OE1	1:A:121:THR:N	2.53	0.42
1:A:478:PHE:O	1:A:482:ASN:N	2.46	0.42
1:B:128:ASP:O	1:B:132:GLN:HB2	2.20	0.42
1:B:424:LYS:NZ	1:B:426:ASP:OD1	2.51	0.42
1:B:288:LYS:HB2	1:B:310:LEU:HB3	2.00	0.42
1:B:588:TRP:CZ3	1:B:628:SER:HB2	2.55	0.41
1:B:53:GLN:O	1:B:57:LYS:HG3	2.20	0.41
1:B:425:TYR:HB2	1:B:428:TYR:HB2	2.01	0.41
1:A:382:PHE:HB2	1:A:430:ILE:HB	2.03	0.41
1:A:414:VAL:HG12	1:A:416:SER:H	1.85	0.41
1:A:572:GLY:HA2	1:B:567:ARG:NH2	2.35	0.41
1:B:245:LYS:HB2	1:B:492:ALA:HB3	2.02	0.41
1:A:441:SER:HB3	1:A:444:TYR:CE2	2.56	0.40
1:B:213:LYS:HE3	1:B:217:GLU:OE1	2.21	0.40
1:A:321:GLY:HA3	1:A:457:GLU:HB3	2.02	0.40
1:B:230:PHE:CE2	1:B:513:PRO:HB2	2.56	0.40
1:A:230:PHE:CE2	1:A:513:PRO:HB2	2.57	0.40
1:A:254:ASN:HD22	1:A:423:LEU:HD22	1.87	0.40
1:B:555:LYS:HE3	1:B:588:TRP:CE2	2.56	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	620/724 (86%)	604 (97%)	15 (2%)	1 (0%)	47	64
1	B	615/724 (85%)	597 (97%)	18 (3%)	0	100	100
All	All	1235/1448 (85%)	1201 (97%)	33 (3%)	1 (0%)	51	69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	453	TYR

### 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	543/635 (86%)	536 (99%)	7 (1%)	69	82
1	B	540/635 (85%)	534 (99%)	6 (1%)	73	85
All	All	1083/1270 (85%)	1070 (99%)	13 (1%)	71	84

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	LEU
1	A	166	ASP
1	A	283	ARG
1	A	389	TRP
1	A	417	ILE
1	A	447	ASP
1	A	565	ARG
1	B	75	ARG
1	B	417	ILE
1	B	424	LYS
1	B	447	ASP
1	B	526	THR
1	B	565	ARG

Sometimes 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 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	GOL	A	802	-	5,5,5	0.93	0	5,5,5	1.00	0
2	GOL	A	801	-	5,5,5	0.92	0	5,5,5	0.99	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	GOL	A	802	-	-	0/4/4/4	-
2	GOL	A	801	-	-	0/4/4/4	-

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.

No monomer is involved in short contacts.

## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	626/724 (86%)	0.31	36 (5%)	23 19	26, 42, 77, 132	0
1	B	621/724 (85%)	0.21	22 (3%)	44 40	24, 42, 67, 113	0
All	All	1247/1448 (86%)	0.26	58 (4%)	31 28	24, 42, 73, 132	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	648	VAL	6.0
1	A	650	VAL	4.9
1	B	650	VAL	4.7
1	B	621	ALA	4.4
1	B	559	ARG	4.3
1	A	655	THR	4.2
1	A	14	MET	4.2
1	A	645	LYS	4.0
1	B	396	LEU	3.8
1	A	176	PHE	3.5
1	A	559	ARG	3.5
1	A	646	PRO	3.5
1	A	647	TYR	3.4
1	A	115	SER	3.4
1	A	294	PHE	3.3
1	A	178	PRO	3.3
1	B	111	TYR	3.2
1	A	119	THR	3.2
1	A	136	ARG	3.1
1	B	646	PRO	3.1
1	A	12	ASN	3.1
1	A	113	ASN	3.0
1	B	294	PHE	3.0
1	B	362	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	583	GLU	3.0
1	A	118	GLU	2.9
1	A	545	ALA	2.9
1	B	648	VAL	2.9
1	B	651	ARG	2.8
1	B	649	ILE	2.8
1	B	516	ALA	2.7
1	A	301	ILE	2.7
1	A	649	ILE	2.7
1	B	340	GLU	2.6
1	B	654	ASP	2.6
1	A	657	PHE	2.6
1	A	17	PHE	2.5
1	A	497	ALA	2.5
1	B	583	GLU	2.5
1	A	172	SER	2.5
1	A	116	LYS	2.4
1	B	393	SER	2.4
1	A	114	GLN	2.4
1	A	595	SER	2.4
1	B	176	PHE	2.3
1	A	243	GLY	2.3
1	A	329	SER	2.3
1	A	541	GLY	2.3
1	A	651	ARG	2.3
1	B	115	SER	2.2
1	B	351	ASN	2.2
1	A	560	LEU	2.2
1	B	116	LYS	2.2
1	A	396	LEU	2.1
1	A	177	ALA	2.1
1	A	181	LYS	2.1
1	B	51	VAL	2.0
1	B	301	ILE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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<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( $\text{\AA}^2$ )	Q<0.9
2	GOL	A	802	6/6	0.86	0.27	44,54,56,61	0
2	GOL	A	801	6/6	0.93	0.29	55,64,67,71	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.