



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 17, 2025 – 12:28 PM EST

PDB ID : 9YHM / pdb\_00009yhm  
Title : Crystal structure of Chikungunya virus nsP3 macrodomain N24A D31N double mutant (P31 crystal form)  
Authors : Correy, G.J.; Fraser, J.S.  
Deposited on : 2025-09-30  
Resolution : 1.52 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 : 4-5-2 with Phenix2.0  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

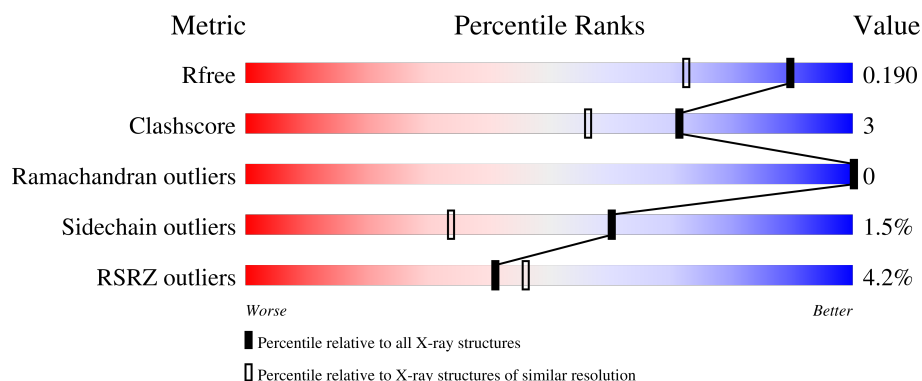
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.52 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))
$R_{free}$	164625	5293 (1.54-1.50)
Clashscore	180529	5759 (1.54-1.50)
Ramachandran outliers	177936	5653 (1.54-1.50)
Sidechain outliers	177891	5650 (1.54-1.50)
RSRZ outliers	164620	5293 (1.54-1.50)

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  $\geq 3$ , 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	168	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; height: 1px; background-color: red;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 5px; left: 89%; width: 10%; text-align: right;">89%</div> <div style="position: absolute; top: 5px; left: 98%; width: 2%; text-align: right;">7%</div> <div style="position: absolute; top: 5px; left: 99%; width: 1px; text-align: center;">•</div> </div> </div>
1	B	168	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; height: 1px; background-color: red;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 5px; left: 88%; width: 10%; text-align: right;">88%</div> <div style="position: absolute; top: 5px; left: 98%; width: 2%; text-align: right;">7%</div> <div style="position: absolute; top: 5px; left: 99%; width: 1px; text-align: center;">•</div> <div style="position: absolute; top: 5px; left: 99.5%; width: 1px; text-align: center;">5%</div> </div> </div>
1	C	168	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; height: 1px; background-color: red;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 5px; left: 91%; width: 10%; text-align: right;">91%</div> <div style="position: absolute; top: 5px; left: 98%; width: 2%; text-align: right;">5%</div> <div style="position: absolute; top: 5px; left: 99%; width: 1px; text-align: center;">•</div> </div> </div>
1	D	168	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; height: 1px; background-color: red;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 5px; left: 90%; width: 10%; text-align: right;">90%</div> <div style="position: absolute; top: 5px; left: 98%; width: 2%; text-align: right;">5%</div> <div style="position: absolute; top: 5px; left: 99%; width: 1px; text-align: center;">•</div> <div style="position: absolute; top: 5px; left: 99.5%; width: 1px; text-align: center;">•</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10594 atoms, of which 5072 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 Non-structural protein 3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	161	Total	C	H	N	O	S	0	10	0
			2575	802	1286	231	247	9			
1	B	160	Total	C	H	N	O	S	0	2	0
			2457	769	1224	216	240	8			
1	C	160	Total	C	H	N	O	S	0	1	0
			2460	770	1228	216	238	8			
1	D	161	Total	C	H	N	O	S	0	18	0
			2670	832	1334	241	255	8			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP Q8JUX6
A	-6	LYS	-	expression tag	UNP Q8JUX6
A	-5	HIS	-	expression tag	UNP Q8JUX6
A	-4	HIS	-	expression tag	UNP Q8JUX6
A	-3	HIS	-	expression tag	UNP Q8JUX6
A	-2	HIS	-	expression tag	UNP Q8JUX6
A	-1	HIS	-	expression tag	UNP Q8JUX6
A	0	HIS	-	expression tag	UNP Q8JUX6
A	24	ALA	ASN	engineered mutation	UNP Q8JUX6
A	31	ASN	ASP	engineered mutation	UNP Q8JUX6
B	-7	MET	-	initiating methionine	UNP Q8JUX6
B	-6	LYS	-	expression tag	UNP Q8JUX6
B	-5	HIS	-	expression tag	UNP Q8JUX6
B	-4	HIS	-	expression tag	UNP Q8JUX6
B	-3	HIS	-	expression tag	UNP Q8JUX6
B	-2	HIS	-	expression tag	UNP Q8JUX6
B	-1	HIS	-	expression tag	UNP Q8JUX6
B	0	HIS	-	expression tag	UNP Q8JUX6
B	24	ALA	ASN	engineered mutation	UNP Q8JUX6
B	31	ASN	ASP	engineered mutation	UNP Q8JUX6
C	-7	MET	-	initiating methionine	UNP Q8JUX6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	LYS	-	expression tag	UNP Q8JUX6
C	-5	HIS	-	expression tag	UNP Q8JUX6
C	-4	HIS	-	expression tag	UNP Q8JUX6
C	-3	HIS	-	expression tag	UNP Q8JUX6
C	-2	HIS	-	expression tag	UNP Q8JUX6
C	-1	HIS	-	expression tag	UNP Q8JUX6
C	0	HIS	-	expression tag	UNP Q8JUX6
C	24	ALA	ASN	engineered mutation	UNP Q8JUX6
C	31	ASN	ASP	engineered mutation	UNP Q8JUX6
D	-7	MET	-	initiating methionine	UNP Q8JUX6
D	-6	LYS	-	expression tag	UNP Q8JUX6
D	-5	HIS	-	expression tag	UNP Q8JUX6
D	-4	HIS	-	expression tag	UNP Q8JUX6
D	-3	HIS	-	expression tag	UNP Q8JUX6
D	-2	HIS	-	expression tag	UNP Q8JUX6
D	-1	HIS	-	expression tag	UNP Q8JUX6
D	0	HIS	-	expression tag	UNP Q8JUX6
D	24	ALA	ASN	engineered mutation	UNP Q8JUX6
D	31	ASN	ASP	engineered mutation	UNP Q8JUX6

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0
2	D	1	Total Cl 1 1	0	0

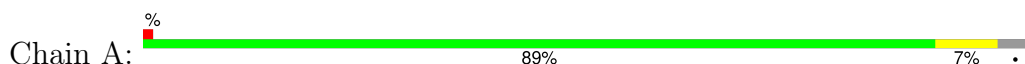
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	153	Total O 154 154	0	2
3	B	95	Total O 95 95	0	1
3	C	66	Total O 67 67	0	3
3	D	114	Total O 114 114	0	8

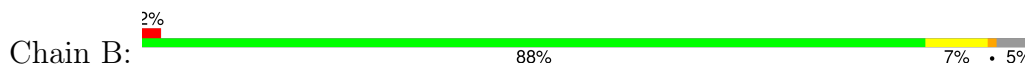
### 3 Residue-property plots [i](#)

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: Non-structural protein 3



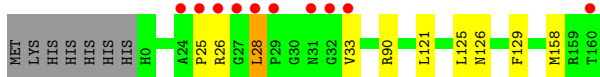
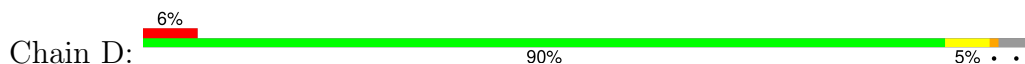
- Molecule 1: Non-structural protein 3



- Molecule 1: Non-structural protein 3



- Molecule 1: Non-structural protein 3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.22Å 87.22Å 85.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.61 – 1.52 43.61 – 1.52	Depositor EDS
% Data completeness (in resolution range)	97.1 (43.61-1.52) 97.1 (43.61-1.52)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.03 (at 1.52Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, $R_{free}$	0.152 , 0.189 0.154 , 0.190	Depositor DCC
$R_{free}$ test set	5708 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.9	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 38.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.009 for -h,-k,l 0.027 for h,-h-k,-l 0.010 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	10594	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	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 21.62 % 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 6.7565e-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:  
CL

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	0.42	0/1338	0.57	0/1810
1	B	0.36	0/1263	0.51	0/1711
1	C	0.34	0/1255	0.51	0/1701
1	D	0.38	0/1388	0.52	0/1882
All	All	0.38	0/5244	0.53	0/7104

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 [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	1289	1286	1253	9	0
1	B	1233	1224	1216	11	0
1	C	1232	1228	1230	5	0
1	D	1336	1334	1315	7	0
2	A	1	0	0	0	0
2	D	1	0	0	0	0
3	A	154	0	0	5	0
3	B	95	0	0	1	0
3	C	67	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	114	0	0	3	0
All	All	5522	5072	5014	32	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 (32) 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:159[B]:ARG:NH2	3:A:301:HOH:O	1.82	1.12
1:C:133:ASP:OD2	1:C:159:ARG:NH2	2.15	0.79
1:A:133:ASP:OD1	3:A:301:HOH:O	1.99	0.79
1:D:126[B]:ASN:ND2	3:D:301:HOH:O	2.30	0.63
1:A:121:LEU:C	1:A:121:LEU:HD23	2.27	0.60
1:C:43:GLU:OE1	1:C:43:GLU:N	2.30	0.60
1:D:25[B]:PRO:HB2	1:D:28[B]:LEU:HD13	1.83	0.59
1:B:7:LYS:HE2	1:B:140:VAL:HG11	1.89	0.54
1:D:121:LEU:C	1:D:121:LEU:HD23	2.34	0.53
1:B:146:LYS:H	1:B:146:LYS:HE2	1.74	0.52
1:A:94:LYS:O	1:A:98[B]:ARG:HG2	2.11	0.51
1:B:121:LEU:C	1:B:121:LEU:HD23	2.36	0.50
1:A:59[A]:MET:HE1	1:A:64:PRO:HG3	1.94	0.49
1:B:146:LYS:H	1:B:146:LYS:CE	2.26	0.49
1:A:5:ARG:HD3	3:A:372:HOH:O	2.13	0.48
1:C:145:ASP:OD1	1:C:147:GLU:N	2.47	0.48
1:D:126[A]:ASN:HB3	3:D:391[A]:HOH:O	2.14	0.47
1:D:90[A]:ARG:HG2	3:D:357:HOH:O	2.15	0.46
1:A:4:TYR:HE1	3:A:301:HOH:O	1.97	0.46
1:A:9:MET:HE3	1:C:42:PRO:HG2	1.99	0.44
1:B:154:GLU:O	1:B:158:MET:HG2	2.17	0.44
1:B:43:GLU:H	1:B:43:GLU:CD	2.26	0.43
1:A:121:LEU:C	1:A:121:LEU:CD2	2.93	0.42
1:D:121:LEU:HD23	1:D:121:LEU:O	2.20	0.41
1:B:55:ALA:HA	1:B:67:HIS:O	2.20	0.41
1:B:128:LEU:HD23	1:B:128:LEU:C	2.46	0.41
1:B:146:LYS:H	1:B:146:LYS:CD	2.33	0.40
1:B:7:LYS:HE3	1:B:142:TYR:OH	2.20	0.40
1:B:31:ASN:ND2	3:B:202:HOH:O	2.54	0.40
1:C:128:LEU:HD23	1:C:128:LEU:C	2.46	0.40
1:D:125:LEU:HG	1:D:129:PHE:CE2	2.57	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	A	168/168 (100%)	166 (99%)	2 (1%)	0	100	100
1	B	160/168 (95%)	156 (98%)	4 (2%)	0	100	100
1	C	159/168 (95%)	156 (98%)	3 (2%)	0	100	100
1	D	177/168 (105%)	176 (99%)	1 (1%)	0	100	100
All	All	664/672 (99%)	654 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	A	142/140 (101%)	140 (99%)	2 (1%)	62	37
1	B	134/140 (96%)	131 (98%)	3 (2%)	47	18
1	C	133/140 (95%)	133 (100%)	0	100	100
1	D	145/140 (104%)	138 (95%)	7 (5%)	21	3
All	All	554/560 (99%)	542 (98%)	12 (2%)	60	18

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	160[A]	THR
1	A	160[B]	THR
1	B	43	GLU
1	B	146	LYS
1	B	159	ARG
1	D	26[A]	ARG
1	D	26[B]	ARG
1	D	28[A]	LEU
1	D	28[B]	LEU
1	D	33[A]	VAL
1	D	33[B]	VAL
1	D	158	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	0	HIS

### 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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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

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 ⓘ

### 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	161/168 (95%)	-0.54	1 (0%)	85 88	11, 26, 46, 72	6 (3%)
1	B	160/168 (95%)	-0.19	3 (1%)	66 71	17, 37, 70, 104	1 (0%)
1	C	160/168 (95%)	0.51	13 (8%)	19 21	20, 48, 83, 95	1 (0%)
1	D	161/168 (95%)	0.07	10 (6%)	28 31	13, 30, 56, 84	15 (9%)
All	All	642/672 (95%)	-0.04	27 (4%)	41 46	11, 34, 70, 104	23 (3%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	28[A]	LEU	14.6
1	D	27[A]	GLY	7.9
1	D	26[A]	ARG	7.6
1	D	29[A]	PRO	6.9
1	D	31[A]	ASN	6.2
1	D	33[A]	VAL	4.3
1	C	160	THR	4.2
1	D	160	THR	3.8
1	D	25[A]	PRO	3.5
1	C	6	VAL	3.4
1	B	160	THR	3.4
1	A	160[A]	THR	3.3
1	C	156	ILE	3.3
1	C	157	GLN	3.2
1	D	24[A]	ALA	3.1
1	B	1	ALA	3.0
1	C	2	PRO	3.0
1	C	7	LYS	2.5
1	C	143	CYS	2.5
1	B	158	MET	2.4
1	C	1	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	146	LYS	2.4
1	C	152	ILE	2.3
1	C	158	MET	2.3
1	D	32[A]	GLY	2.2
1	C	137	ALA	2.1
1	C	13	LYS	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 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
2	CL	A	201	1/1	0.97	0.07	52,52,52,52	0
2	CL	D	201	1/1	0.97	0.08	50,50,50,50	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.