



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 20, 2017 – 02:46 PM EDT

PDB ID : 3D0I  
Title : Crystal structure of spike protein receptor-binding domain from the 2005-2006 SARS coronavirus civet strain complexed with human-civet chimeric receptor ACE2  
Authors : Li, F.  
Deposited on : 2008-05-01  
Resolution : 2.90 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

<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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029077  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20029077

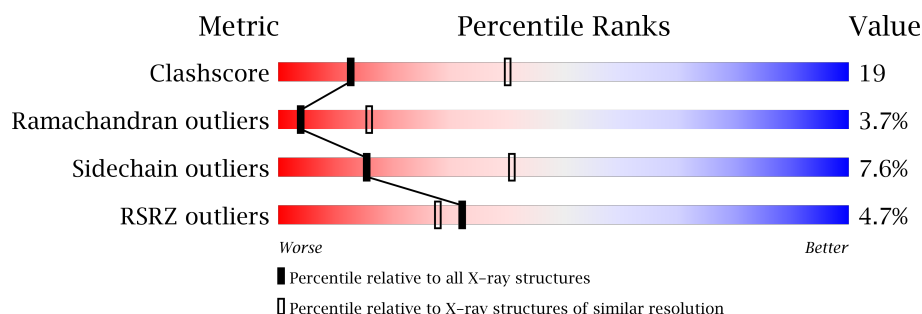
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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	597	<div> <div>6%</div> <div>56%</div> <div>40%</div> <div>.</div> </div>
1	B	597	<div> <div>4%</div> <div>59%</div> <div>37%</div> <div>.</div> </div>
2	E	179	<div> <div>4%</div> <div>64%</div> <div>28%</div> <div>.</div> <div>.</div> </div>
2	F	179	<div> <div>4%</div> <div>62%</div> <div>28%</div> <div>6%</div> <div>.</div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12639 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 Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	597	Total	C	N	O	S	0	0	0
			4864	3110	803	922	29			
1	B	597	Total	C	N	O	S	0	0	0
			4864	3110	803	922	29			

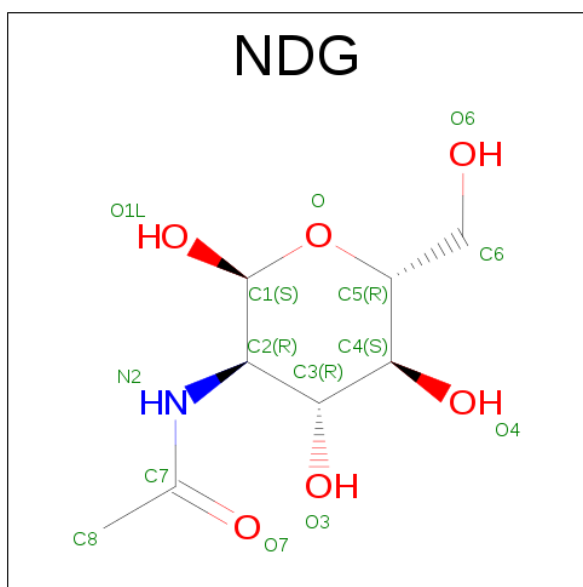
- Molecule 2 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	173	Total	C	N	O	S	0	0	0
			1395	905	229	255	6			
2	F	173	Total	C	N	O	S	0	0	0
			1395	905	229	255	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	479	ARG	ASN	conflict	UNP P59594
E	480	GLY	ASP	conflict	UNP P59594
E	487	SER	THR	conflict	UNP P59594
F	479	ARG	ASN	conflict	UNP P59594
F	480	GLY	ASP	conflict	UNP P59594
F	487	SER	THR	conflict	UNP P59594

- Molecule 3 is 2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE (three-letter code: NDG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			15	8	1	6		
3	B	1	Total	C	N	O	0	0
			15	8	1	6		
3	B	1	Total	C	N	O	0	0
			15	8	1	6		
3	B	1	Total	C	N	O	0	0
			15	8	1	6		
3	B	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cl	0	0
			1	1		
5	A	1	Total	Cl	0	0
			1	1		

- Molecule 6 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

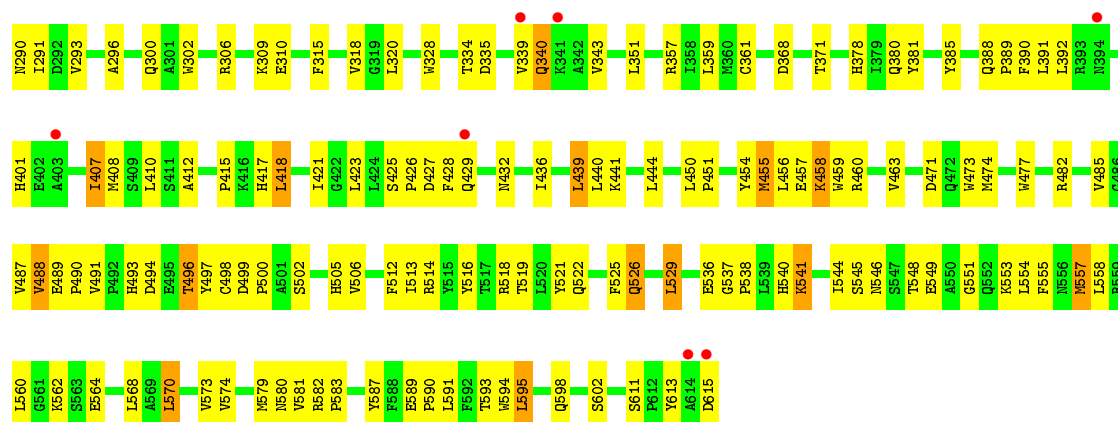


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	E	1	Total	C	N	O	0	0
			15	8	1	6		

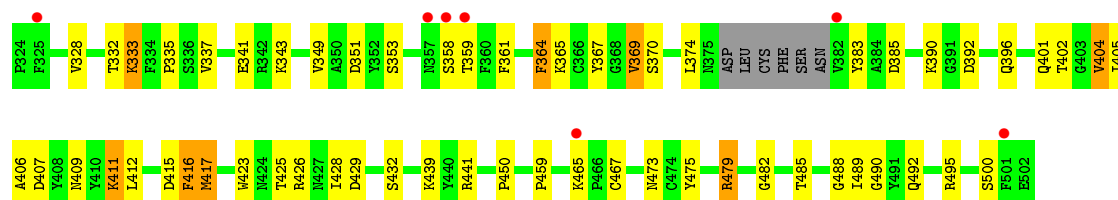
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	21	Total	O	0	0
			21	21		
7	F	6	Total	O	0	0
			6	6		

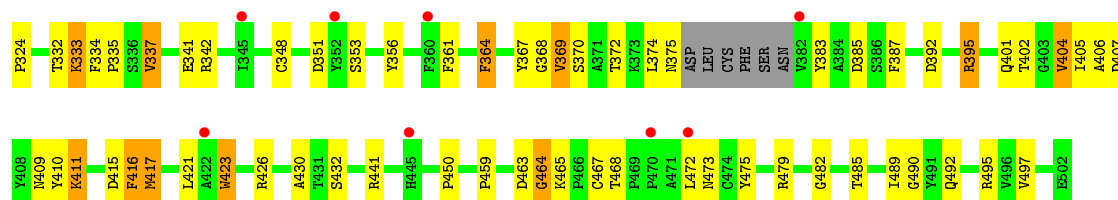




• Molecule 2: Spike glycoprotein



• Molecule 2: Spike glycoprotein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.42Å 119.82Å 109.77Å 90.00° 95.50° 90.00°	Depositor
Resolution (Å)	36.47 – 2.90 36.47 – 2.89	Depositor EDS
% Data completeness (in resolution range)	89.9 (36.47-2.90) 89.3 (36.47-2.89)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.71 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.224 , 0.278 0.243 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	75.7	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 44.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	12639	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% 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, 0.333 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: ZN, NAG, NDG, 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	0.53	1/5000 (0.0%)	0.60	0/6796
1	B	0.53	0/5000	0.62	0/6796
2	E	0.55	0/1440	0.61	0/1958
2	F	0.54	0/1440	0.61	0/1958
All	All	0.53	1/12880 (0.0%)	0.61	0/17508

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	300	GLN	CD-OE1	6.23	1.37	1.24

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	4864	0	4638	187	0
1	B	4864	0	4638	197	0
2	E	1395	0	1329	34	0
2	F	1395	0	1329	48	0
3	A	15	0	15	4	0
3	B	60	0	60	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	1	0
6	E	15	0	15	2	0
7	B	21	0	0	1	0
7	F	6	0	0	1	0
All	All	12639	0	12024	458	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 19.

The worst 5 of 458 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)
2:E:409:ASN:HD21	2:E:441:ARG:H	1.13	0.96
1:B:546:ASN:HD21	3:B:619:NDG:H1	1.35	0.90
1:A:574:VAL:HG23	1:A:576:ALA:H	1.35	0.89
1:A:47:SER:HA	1:A:62:MET:HG3	1.56	0.88
1:A:474:MET:HE2	1:A:499:ASP:H	1.38	0.88

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	595/597 (100%)	524 (88%)	52 (9%)	19 (3%)	5	19
1	B	595/597 (100%)	528 (89%)	50 (8%)	17 (3%)	5	21
2	E	169/179 (94%)	138 (82%)	21 (12%)	10 (6%)	2	6
2	F	169/179 (94%)	141 (83%)	17 (10%)	11 (6%)	1	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1528/1552 (98%)	1331 (87%)	140 (9%)	57 (4%)	4	16

5 of 57 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	PRO
1	A	212	VAL
1	A	289	PRO
1	A	340	GLN
1	A	614	ALA

### 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	527/527 (100%)	491 (93%)	36 (7%)	18	47
1	B	527/527 (100%)	484 (92%)	43 (8%)	13	37
2	E	150/156 (96%)	137 (91%)	13 (9%)	12	34
2	F	150/156 (96%)	139 (93%)	11 (7%)	16	43
All	All	1354/1366 (99%)	1251 (92%)	103 (8%)	15	41

5 of 103 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	250	ASN
1	B	418	LEU
2	F	369	VAL
1	B	254	SER
1	B	371	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	49	ASN
1	B	139	GLN
2	E	409	ASN
1	B	63	ASN
1	B	149	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 for Mogul analysis.

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	NDG	A	616	-	15,15,15	0.50	0	21,21,21	0.64	0
3	NDG	B	616	-	15,15,15	0.61	0	21,21,21	0.62	0
3	NDG	B	617	-	15,15,15	0.55	0	21,21,21	1.27	2 (9%)
3	NDG	B	618	-	15,15,15	0.74	0	21,21,21	1.08	1 (4%)
3	NDG	B	619	-	15,15,15	0.65	0	21,21,21	1.12	2 (9%)
6	NAG	E	91	-	15,15,15	0.77	0	21,21,21	1.34	2 (9%)

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	NDG	A	616	-	-	1/6/26/26	0/1/1/1
3	NDG	B	616	-	-	0/6/26/26	0/1/1/1
3	NDG	B	617	-	-	0/6/26/26	0/1/1/1
3	NDG	B	618	-	-	1/6/26/26	0/1/1/1
3	NDG	B	619	-	-	0/6/26/26	0/1/1/1
6	NAG	E	91	-	-	0/6/26/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	619	NDG	C1-O-C5	2.16	117.29	113.39
3	B	619	NDG	O-C5-C4	2.30	113.89	109.66
3	B	617	NDG	C4-C3-C2	2.75	114.41	110.33
3	B	618	NDG	O-C1-C2	2.87	112.40	109.52
6	E	91	NAG	O5-C1-C2	3.07	112.60	109.52

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	618	NDG	O7-C7-N2-C2
3	A	616	NDG	C1-C2-N2-C7

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	616	NDG	4	0
3	B	616	NDG	1	0
3	B	617	NDG	1	0
3	B	619	NDG	5	0
6	E	91	NAG	2	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	A	597/597 (100%)	0.31	34 (5%) 24 19	47, 80, 130, 154	0
1	B	597/597 (100%)	0.18	23 (3%) 40 35	38, 74, 130, 156	0
2	E	173/179 (96%)	0.30	7 (4%) 39 34	56, 89, 132, 134	0
2	F	173/179 (96%)	0.28	8 (4%) 33 28	58, 90, 131, 134	0
All	All	1540/1552 (99%)	0.25	72 (4%) 32 28	38, 80, 131, 156	0

The worst 5 of 72 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	615	ASP	6.9
1	A	290	ASN	6.8
1	A	105	SER	5.4
1	A	106	SER	4.7
1	A	302	TRP	4.6

### 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
5	CL	A	902	1/1	0.93	0.20	-0.36	84,84,84,84	0
3	NDG	A	616	15/15	0.92	0.12	-1.52	109,113,114,114	0
5	CL	B	902	1/1	0.95	0.17	-2.86	73,73,73,73	0
4	ZN	A	901	1/1	0.84	0.43	-	123,123,123,123	0
3	NDG	B	618	15/15	0.75	0.23	-	111,113,114,114	0
6	NAG	E	91	15/15	0.65	0.28	-	137,140,141,142	0
3	NDG	B	617	15/15	0.82	0.29	-	126,128,129,129	0
3	NDG	B	619	15/15	0.82	0.18	-	72,76,81,81	0
4	ZN	B	901	1/1	0.93	0.29	-	131,131,131,131	0
3	NDG	B	616	15/15	0.79	0.35	-	123,125,125,126	0

## 6.5 Other polymers

There are no such residues in this entry.