



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:48 AM UTC

PDB ID : 9HHH / pdb\_00009hhh  
Title : A rare open conformation for Ubl2 domain of papain-like protease C111S of SARS-CoV2  
Authors : Freiherr von Scholley, G.L.; Schaefer, M.; Soler Lopez, M.; Hillig, R.; Mueller-Dieckmann, C.; Kandiah, E.  
Deposited on : 2024-11-21  
Resolution : 1.98 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  
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

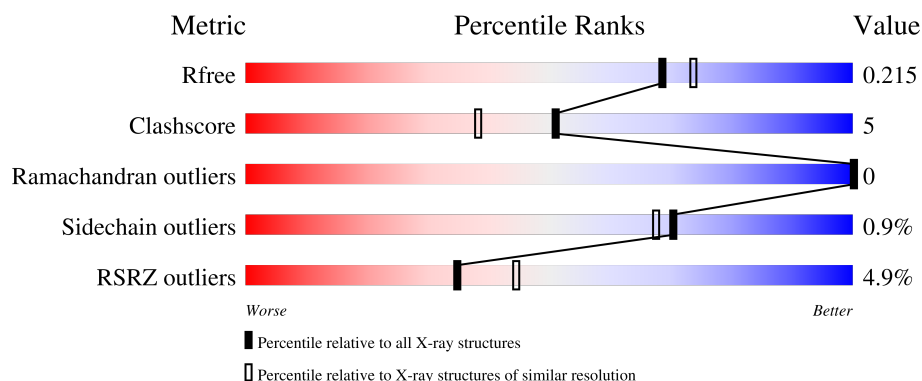
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

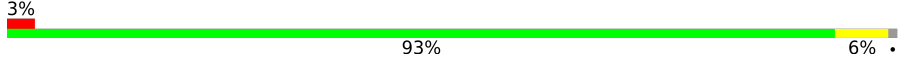
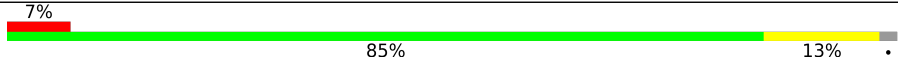
The reported resolution of this entry is 1.98 Å.

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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	322	
1	B	322	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5615 atoms, of which 16 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 Papain-like protease nsp3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	2	0
			2566	1634	424	490	18			
1	B	315	Total	C	N	O	S	0	4	0
			2533	1609	419	487	18			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	111	SER	CYS	engineered mutation	UNP P0DTC1
A	317	GLU	-	expression tag	UNP P0DTC1
A	318	ASN	-	expression tag	UNP P0DTC1
A	319	LEU	-	expression tag	UNP P0DTC1
A	323	TYR	-	expression tag	UNP P0DTC1
A	324	PHE	-	expression tag	UNP P0DTC1
A	325	GLN	-	expression tag	UNP P0DTC1
B	111	SER	CYS	engineered mutation	UNP P0DTC1
B	317	GLU	-	expression tag	UNP P0DTC1
B	318	ASN	-	expression tag	UNP P0DTC1
B	319	LEU	-	expression tag	UNP P0DTC1
B	320	TYR	-	expression tag	UNP P0DTC1
B	321	PHE	-	expression tag	UNP P0DTC1
B	322	GLN	-	expression tag	UNP P0DTC1

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C H O 14 3 8 3	0	0
2	A	1	Total C H O 14 3 8 3	0	0
2	B	1	Total C O 6 3 3	0	0

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

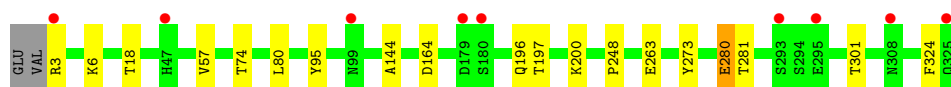
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	272	Total	O	0	0
			272	272		
5	B	188	Total	O	0	0
			188	188		

### 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.

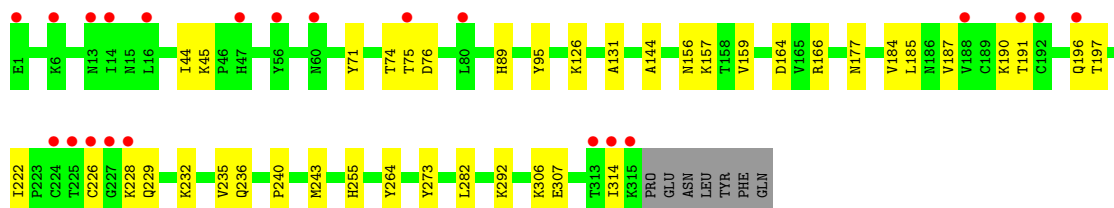
- Molecule 1: Papain-like protease nsp3

Chain A: 



- Molecule 1: Papain-like protease nsp3

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.43Å 106.25Å 72.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.21 – 1.98 72.21 – 1.98	Depositor EDS
% Data completeness (in resolution range)	98.5 (72.21-1.98) 98.5 (72.21-1.98)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.51 (at 1.98Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, $R_{free}$	0.179 , 0.215 0.179 , 0.215	Depositor DCC
$R_{free}$ test set	2982 reflections (3.14%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.6	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 46.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5615	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% 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: SO4, ZN, 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	0.63	1/2628 (0.0%)	0.66	1/3566 (0.0%)
1	B	0.31	0/2592	0.46	0/3517
All	All	0.49	1/5220 (0.0%)	0.57	1/7083 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	324	PHE	C-N	-19.48	1.06	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	GLU	N-CA-C	-5.73	105.18	111.82

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	2566	0	2496	17	0
1	B	2533	0	2468	37	0
2	A	12	16	16	3	0
2	B	6	0	8	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0
5	A	272	0	0	2	0
5	B	188	0	0	4	0
All	All	5599	16	4988	53	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 5.

All (53) 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:B:184:VAL:HG13	1:B:196:GLN:HE21	1.44	0.82
1:B:74:THR:HG22	1:B:76:ASP:H	1.55	0.72
1:B:235:VAL:HG12	1:B:236:GLN:HG3	1.72	0.70
1:B:184:VAL:CG1	1:B:196:GLN:NE2	2.55	0.70
1:B:184:VAL:CG1	1:B:196:GLN:HE21	2.05	0.70
1:A:6:LYS:HE3	1:A:18:THR:HG21	1.75	0.69
1:B:240:PRO:O	1:B:306:LYS:HD2	1.95	0.67
1:A:6:LYS:HE3	1:A:18:THR:CG2	2.25	0.66
1:A:248:PRO:HG3	1:A:301:THR:CG2	2.28	0.64
1:B:126:LYS:HG2	5:B:523:HOH:O	1.97	0.63
1:A:200:LYS:HD2	1:B:156:ASN:ND2	2.14	0.63
1:B:196:GLN:HG2	1:B:197:THR:N	2.15	0.59
1:B:273:TYR:OH	2:B:401:GOL:H12	2.03	0.59
1:B:44:ILE:HG22	1:B:45:LYS:O	2.05	0.57
1:B:185:LEU:O	1:B:196:GLN:HG3	2.05	0.56
1:A:200:LYS:HE2	5:B:536:HOH:O	2.07	0.55
1:B:191:THR:HG23	1:B:228:LYS:NZ	2.23	0.54
1:B:184:VAL:HG11	1:B:196:GLN:NE2	2.21	0.54
1:A:164:ASP:OD1	2:A:402:GOL:H32	2.08	0.53
1:B:74:THR:HG22	1:B:76:ASP:N	2.21	0.53
1:B:71:TYR:CD2	1:B:131:ALA:HB2	2.44	0.53
1:B:126:LYS:HE2	1:B:177:ASN:ND2	2.26	0.51
1:B:228:LYS:HG2	1:B:229:GLN:H	1.76	0.50
1:B:306:LYS:HD2	1:B:307:GLU:H	1.78	0.49
1:B:191:THR:HG23	1:B:228:LYS:HZ3	1.77	0.49
1:B:95:TYR:CD1	1:B:144:ALA:HB3	2.48	0.49
1:B:191:THR:CB	1:B:228:LYS:HZ3	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:TYR:CE2	1:B:131:ALA:HB2	2.48	0.48
1:A:57:VAL:O	1:A:80:LEU:HD13	2.13	0.48
1:B:74:THR:CG2	1:B:76:ASP:H	2.23	0.48
1:A:164:ASP:OD1	2:A:402:GOL:H12	2.14	0.48
1:B:166:ARG:HA	1:B:243:MET:HE1	1.95	0.48
1:B:187:VAL:HG22	1:B:232:LYS:HB2	1.96	0.47
1:B:191:THR:CG2	1:B:228:LYS:HZ3	2.28	0.47
1:B:264:TYR:CZ	2:B:401:GOL:H11	2.50	0.47
1:A:248:PRO:HG3	1:A:301:THR:HG22	1.95	0.47
1:A:3:ARG:N	5:A:513:HOH:O	2.49	0.46
1:A:74:THR:HA	2:A:401:GOL:H2	1.97	0.46
1:A:196:GLN:NE2	5:A:512:HOH:O	2.49	0.46
1:B:190:LYS:HB2	1:B:228:LYS:HZ1	1.82	0.45
1:A:248:PRO:HG3	1:A:301:THR:HG21	1.98	0.45
1:B:196:GLN:CG	1:B:197:THR:N	2.81	0.44
1:B:292:LYS:NZ	5:B:507:HOH:O	2.47	0.44
1:B:164:ASP:OD1	2:B:401:GOL:H2	2.17	0.44
1:B:255:HIS:HB2	5:B:641:HOH:O	2.18	0.44
1:B:89:HIS:HB2	1:B:159:VAL:HG21	2.00	0.43
1:B:126:LYS:HG3	1:B:177:ASN:HB3	2.00	0.43
1:A:6:LYS:HE3	1:A:18:THR:HG23	1.99	0.43
1:B:157:LYS:HE3	1:B:157:LYS:HB3	1.85	0.42
1:A:280:GLU:HG2	1:A:281:THR:N	2.34	0.42
1:A:95:TYR:CD1	1:A:144:ALA:HB3	2.55	0.42
1:B:255:HIS:HA	1:B:282:LEU:HD21	2.01	0.41
1:A:263:GLU:O	1:A:273:TYR:HA	2.21	0.41

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	320/322 (99%)	312 (98%)	8 (2%)	0	100	100
1	B	317/322 (98%)	306 (96%)	11 (4%)	0	100	100
All	All	637/644 (99%)	618 (97%)	19 (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	282/282 (100%)	281 (100%)	1 (0%)	84	82
1	B	279/282 (99%)	275 (99%)	4 (1%)	59	54
All	All	561/564 (100%)	556 (99%)	5 (1%)	70	67

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	197	THR
1	B	75	THR
1	B	222	ILE
1	B	226	CYS
1	B	314	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	A	186	ASN
1	A	194	GLN
1	A	308	ASN
1	B	15	ASN
1	B	97	GLN
1	B	99	ASN
1	B	156	ASN

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Mol	Chain	Res	Type
1	B	196	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](#)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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	$\# Z  > 2$
4	SO4	B	404	-	4,4,4	0.72	0	6,6,6	0.24	0
4	SO4	A	405	-	4,4,4	0.81	0	6,6,6	0.22	0
2	GOL	A	402	-	5,5,5	0.19	0	5,5,5	0.85	0
4	SO4	A	404	-	4,4,4	0.62	0	6,6,6	0.04	0
4	SO4	B	403	-	4,4,4	0.69	0	6,6,6	0.11	0
2	GOL	B	401	-	5,5,5	0.36	0	5,5,5	0.42	0
2	GOL	A	401	-	5,5,5	0.28	0	5,5,5	0.29	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	402	-	-	4/4/4/4	-
2	GOL	A	401	-	-	0/4/4/4	-
2	GOL	B	401	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	402	GOL	C1-C2-C3-O3
2	B	401	GOL	C1-C2-C3-O3
2	A	402	GOL	O2-C2-C3-O3
2	B	401	GOL	O2-C2-C3-O3
2	A	402	GOL	O1-C1-C2-O2
2	A	402	GOL	O1-C1-C2-C3

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	402	GOL	2	0
2	B	401	GOL	3	0
2	A	401	GOL	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	324:PHE	C	325:GLN	N	1.06

## 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	320/322 (99%)	-0.08	9 (2%) 55 65	8, 20, 38, 57	2 (0%)
1	B	315/322 (97%)	0.35	22 (6%) 22 30	9, 26, 52, 75	4 (1%)
All	All	635/644 (98%)	0.13	31 (4%) 35 44	8, 22, 46, 75	6 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	314	ILE	4.7
1	B	196	GLN	3.9
1	B	47	HIS	3.7
1	B	224	CYS	3.5
1	B	228	LYS	3.5
1	B	225	THR	3.5
1	B	313	THR	3.4
1	B	226	CYS	3.3
1	A	3	ARG	3.1
1	A	180	SER	3.1
1	B	191	THR	3.0
1	A	308	ASN	2.8
1	B	192	CYS	2.7
1	A	179	ASP	2.6
1	B	16	LEU	2.6
1	B	60	ASN	2.6
1	B	227	GLY	2.5
1	B	1	GLU	2.4
1	B	14	ILE	2.4
1	B	315	LYS	2.4
1	B	13	ASN	2.3
1	B	188	VAL	2.3
1	B	75	THR	2.2
1	B	80	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	6	LYS	2.1
1	A	325	GLN	2.1
1	A	295	GLU	2.0
1	A	293	SER	2.0
1	A	47	HIS	2.0
1	A	99	ASN	2.0
1	B	56	TYR	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	GOL	A	401	6/6	0.75	0.15	42,53,68,68	0
2	GOL	A	402	6/6	0.83	0.18	36,61,75,75	0
4	SO4	A	405	5/5	0.85	0.11	30,33,60,88	0
2	GOL	B	401	6/6	0.86	0.14	28,36,39,42	0
4	SO4	B	404	5/5	0.90	0.18	27,39,46,46	0
3	ZN	B	402	1/1	0.93	0.12	73,73,73,73	0
4	SO4	B	403	5/5	0.97	0.07	30,33,40,43	0
4	SO4	A	404	5/5	0.97	0.10	26,27,29,31	0
3	ZN	A	403	1/1	0.99	0.03	26,26,26,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.