



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:53 PM UTC

PDB ID : 8U2X / pdb_00008u2x
Title : Crystal Structure of NendoU (Uridylate-specific endoribonuclease, nsp15) from Betacoronavirus SARS-CoV-2 (H235A mutant)
Authors : Seattle Structural Genomics Center for Infectious Disease; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2023-09-06
Resolution : 2.25 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

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>.

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

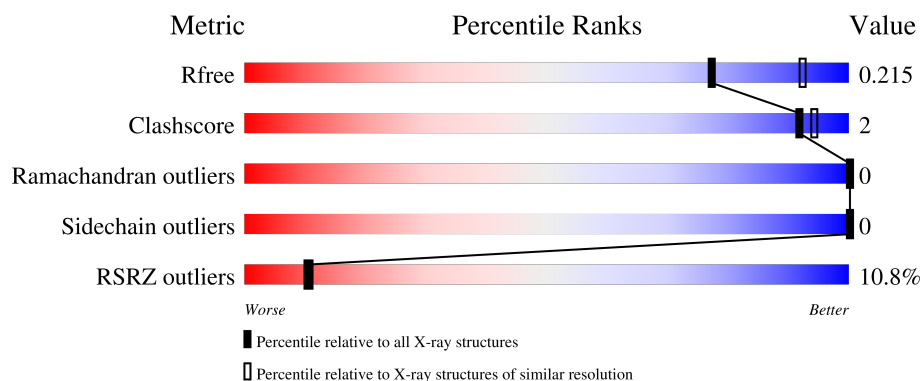
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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 ≥ 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	368	5% 91% 6%
1	B	368	15% 79% 5% 16%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5468 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 Uridylate-specific endoribonuclease nsp15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	S	0	6	0
			2781	1788	453	529	11			
1	B	310	Total	C	N	O	S	0	4	0
			2462	1579	402	472	9			

There are 46 discrepancies between the modelled and reference sequences:

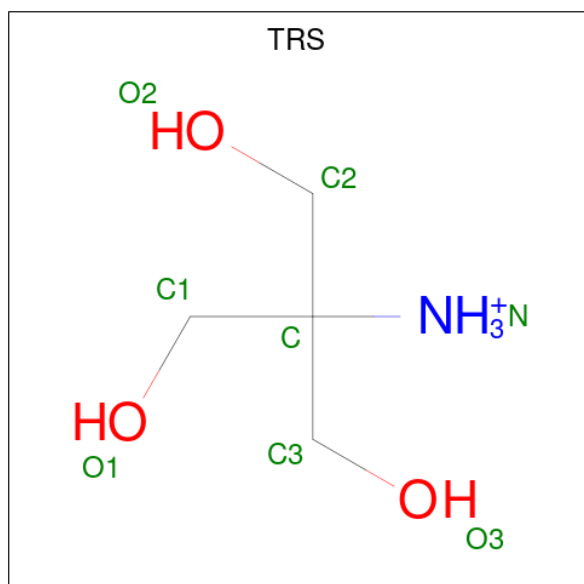
Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP P0DTD1
A	-19	GLY	-	expression tag	UNP P0DTD1
A	-18	SER	-	expression tag	UNP P0DTD1
A	-17	SER	-	expression tag	UNP P0DTD1
A	-16	HIS	-	expression tag	UNP P0DTD1
A	-15	HIS	-	expression tag	UNP P0DTD1
A	-14	HIS	-	expression tag	UNP P0DTD1
A	-13	HIS	-	expression tag	UNP P0DTD1
A	-12	HIS	-	expression tag	UNP P0DTD1
A	-11	HIS	-	expression tag	UNP P0DTD1
A	-10	SER	-	expression tag	UNP P0DTD1
A	-9	SER	-	expression tag	UNP P0DTD1
A	-8	GLY	-	expression tag	UNP P0DTD1
A	-7	GLU	-	expression tag	UNP P0DTD1
A	-6	ASN	-	expression tag	UNP P0DTD1
A	-5	LEU	-	expression tag	UNP P0DTD1
A	-4	TYR	-	expression tag	UNP P0DTD1
A	-3	PHE	-	expression tag	UNP P0DTD1
A	-2	GLN	-	expression tag	UNP P0DTD1
A	-1	GLY	-	expression tag	UNP P0DTD1
A	0	HIS	-	expression tag	UNP P0DTD1
A	1	MET	-	expression tag	UNP P0DTD1
A	235	ALA	HIS	engineered mutation	UNP P0DTD1
B	-20	MET	-	initiating methionine	UNP P0DTD1
B	-19	GLY	-	expression tag	UNP P0DTD1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	SER	-	expression tag	UNP P0DTD1
B	-17	SER	-	expression tag	UNP P0DTD1
B	-16	HIS	-	expression tag	UNP P0DTD1
B	-15	HIS	-	expression tag	UNP P0DTD1
B	-14	HIS	-	expression tag	UNP P0DTD1
B	-13	HIS	-	expression tag	UNP P0DTD1
B	-12	HIS	-	expression tag	UNP P0DTD1
B	-11	HIS	-	expression tag	UNP P0DTD1
B	-10	SER	-	expression tag	UNP P0DTD1
B	-9	SER	-	expression tag	UNP P0DTD1
B	-8	GLY	-	expression tag	UNP P0DTD1
B	-7	GLU	-	expression tag	UNP P0DTD1
B	-6	ASN	-	expression tag	UNP P0DTD1
B	-5	LEU	-	expression tag	UNP P0DTD1
B	-4	TYR	-	expression tag	UNP P0DTD1
B	-3	PHE	-	expression tag	UNP P0DTD1
B	-2	GLN	-	expression tag	UNP P0DTD1
B	-1	GLY	-	expression tag	UNP P0DTD1
B	0	HIS	-	expression tag	UNP P0DTD1
B	1	MET	-	expression tag	UNP P0DTD1
B	235	ALA	HIS	engineered mutation	UNP P0DTD1

- Molecule 2 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			8	4	1	3		
2	B	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cl	0	0
			2	2		

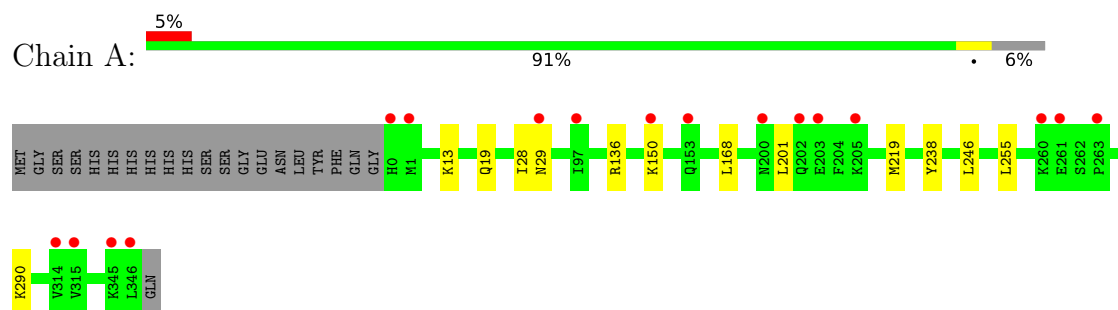
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	117	Total	O	0	0
			117	117		
4	B	90	Total	O	0	0
			90	90		

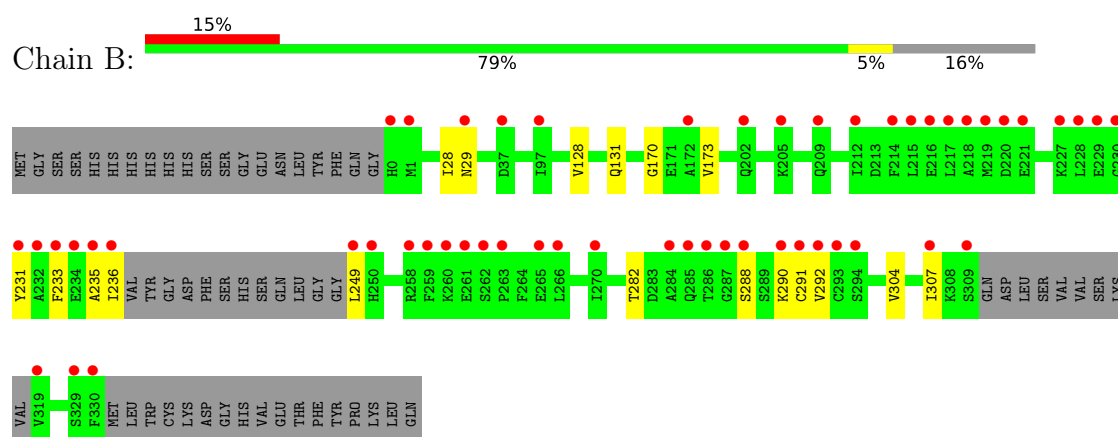
3 Residue-property plots [i](#)

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: Uridylate-specific endoribonuclease nsp15



- Molecule 1: Uridylate-specific endoribonuclease nsp15



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	151.37Å 151.37Å 108.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	65.55 – 2.25 65.55 – 2.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (65.55-2.25) 100.0 (65.55-2.25)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.25Å)	Xtriage
Refinement program	PHENIX (1.21rc1_5057: ???)	Depositor
R, R_{free}	0.187 , 0.213 0.191 , 0.215	Depositor DCC
R_{free} test set	3353 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	44.2	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 52.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.067 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5468	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: CL, TRS

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	0.40	0/2843	0.55	0/3856
1	B	0.37	0/2509	0.53	0/3402
All	All	0.39	0/5352	0.54	0/7258

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	2781	0	2786	7	0
1	B	2462	0	2465	10	0
2	A	8	0	12	0	0
2	B	8	0	12	0	0
3	A	2	0	0	0	0
4	A	117	0	0	0	0
4	B	90	0	0	0	0
All	All	5468	0	5275	17	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 2.

All (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:A:136[A]:ARG:NH2	1:A:150:LYS:O	2.30	0.64
1:B:235:ALA:O	1:B:236:ILE:HG23	2.08	0.54
1:A:219:MET:HG3	1:A:238:TYR:CE2	2.44	0.52
1:A:28[A]:ILE:HG23	1:A:29[A]:ASN:H	1.76	0.50
1:B:304:VAL:O	1:B:307:ILE:HG22	2.12	0.50
1:A:13:LYS:HE3	1:A:19:GLN:HG3	1.95	0.49
1:B:290:LYS:HG2	1:B:291:CYS:N	2.27	0.49
1:B:128:VAL:HB	1:B:131:GLN:HG3	1.94	0.48
1:B:249:LEU:HD12	1:B:292:VAL:HG13	1.96	0.48
1:B:231:TYR:C	1:B:233:PHE:H	2.21	0.47
1:A:201:LEU:HD11	1:A:255:LEU:C	2.40	0.47
1:A:168:LEU:C	1:A:168:LEU:HD12	2.42	0.43
1:B:28[A]:ILE:HG23	1:B:29[A]:ASN:H	1.84	0.43
1:A:246:LEU:O	1:A:290:LYS:HE3	2.19	0.42
1:B:282:THR:HA	1:B:288:SER:O	2.20	0.41
1:B:170:GLY:HA3	1:B:173:VAL:O	2.20	0.40
1:B:28[A]:ILE:HG23	1:B:29[A]:ASN:N	2.36	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	351/368 (95%)	342 (97%)	9 (3%)	0	100	100
1	B	308/368 (84%)	298 (97%)	10 (3%)	0	100	100
All	All	659/736 (90%)	640 (97%)	19 (3%)	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	313/326 (96%)	313 (100%)	0	100	100
1	B	276/326 (85%)	276 (100%)	0	100	100
All	All	589/652 (90%)	589 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	ASN
1	B	83	ASN

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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z > 2$
2	TRS	B	401	-	7,7,7	0.63	0	9,9,9	0.48	0
2	TRS	A	401	-	7,7,7	0.72	0	9,9,9	0.81	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	TRS	B	401	-	-	9/9/9/9	-
2	TRS	A	401	-	-	6/9/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	TRS	C2-C-C1-O1
2	A	401	TRS	C3-C-C1-O1
2	A	401	TRS	C1-C-C3-O3
2	A	401	TRS	C2-C-C3-O3
2	B	401	TRS	C2-C-C1-O1
2	B	401	TRS	C3-C-C1-O1
2	B	401	TRS	N-C-C1-O1
2	B	401	TRS	C1-C-C3-O3
2	B	401	TRS	C2-C-C3-O3
2	A	401	TRS	N-C-C1-O1
2	A	401	TRS	N-C-C3-O3
2	B	401	TRS	C1-C-C2-O2
2	B	401	TRS	N-C-C2-O2
2	B	401	TRS	N-C-C3-O3
2	B	401	TRS	C3-C-C2-O2

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, 95th 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 ²)	Q<0.9
1	A	347/368 (94%)	0.21	17 (4%) 35 34	18, 51, 82, 102	6 (1%)
1	B	310/368 (84%)	0.73	54 (17%) 4 3	20, 54, 130, 152	4 (1%)
All	All	657/736 (89%)	0.45	71 (10%) 11 10	18, 52, 112, 152	10 (1%)

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	249	LEU	9.7
1	A	346	LEU	8.0
1	B	232	ALA	6.1
1	B	236	ILE	6.1
1	B	330	PHE	5.5
1	B	293	CYS	5.2
1	A	0	HIS	5.2
1	B	309	SER	5.1
1	B	235	ALA	4.9
1	B	250	HIS	4.7
1	A	345	LYS	4.6
1	B	319	VAL	4.3
1	B	234	GLU	4.2
1	B	219	MET	4.2
1	B	266	LEU	4.0
1	B	0	HIS	4.0
1	B	231	TYR	3.8
1	B	259	PHE	3.8
1	B	1	MET	3.7
1	A	150	LYS	3.7
1	A	314	VAL	3.6
1	B	285	GLN	3.5
1	B	284	ALA	3.5
1	B	217	LEU	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	214	PHE	3.4
1	B	218	ALA	3.3
1	B	260	LYS	3.3
1	B	258	ARG	3.3
1	B	286	THR	3.2
1	B	227	LYS	3.1
1	B	220	ASP	3.1
1	A	1	MET	3.1
1	B	37	ASP	3.0
1	B	294	SER	2.9
1	B	233	PHE	2.9
1	B	329	SER	2.8
1	A	202	GLN	2.8
1	B	205	LYS	2.8
1	B	202	GLN	2.8
1	B	215	LEU	2.6
1	B	263	PRO	2.6
1	A	203	GLU	2.5
1	B	212	ILE	2.5
1	B	307	ILE	2.5
1	B	172	ALA	2.5
1	B	287	GLY	2.5
1	B	262	SER	2.4
1	A	260	LYS	2.4
1	B	261	GLU	2.4
1	B	288	SER	2.4
1	A	315	VAL	2.4
1	A	97	ILE	2.4
1	B	97	ILE	2.4
1	B	292	VAL	2.3
1	B	290	LYS	2.3
1	B	291	CYS	2.3
1	B	29[A]	ASN	2.2
1	B	229	GLU	2.2
1	A	29[A]	ASN	2.2
1	A	200	ASN	2.2
1	A	153	GLN	2.2
1	B	228	LEU	2.1
1	B	265	GLU	2.1
1	A	261	GLU	2.1
1	B	270	ILE	2.1
1	B	221	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	263	PRO	2.1
1	B	230	GLY	2.0
1	A	205	LYS	2.0
1	B	216	GLU	2.0
1	B	209	GLN	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, 95th 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	TRS	A	401	8/8	0.75	0.22	48,53,63,64	0
2	TRS	B	401	8/8	0.89	0.15	46,54,59,61	0
3	CL	A	403	1/1	0.92	0.17	71,71,71,71	0
3	CL	A	402	1/1	0.96	0.10	78,78,78,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.