



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:42 AM UTC

PDB ID : 7ZB6 / pdb_00007zb6
Title : Crystal Structure of SARS-CoV-2 Main Protease (Mpro) variant C44S at 2.12 Å resolution
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Deposited on : 2022-03-23
Resolution : 2.12 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

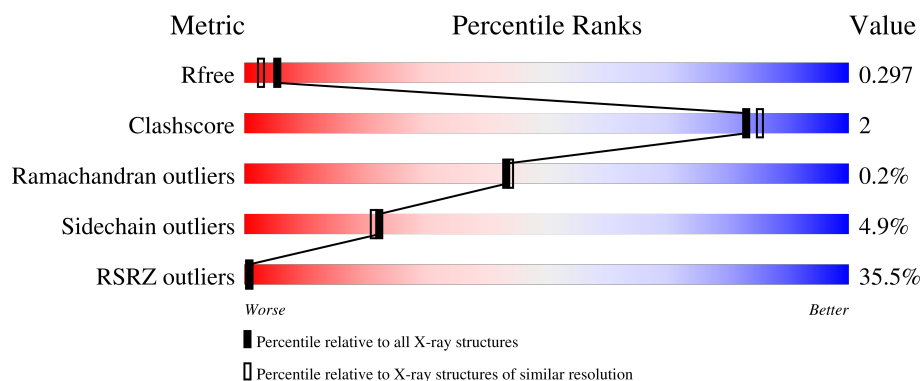
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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	306	34% 90% 9%
1	C	306	37% 90% 9%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9466 atoms, of which 4636 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.

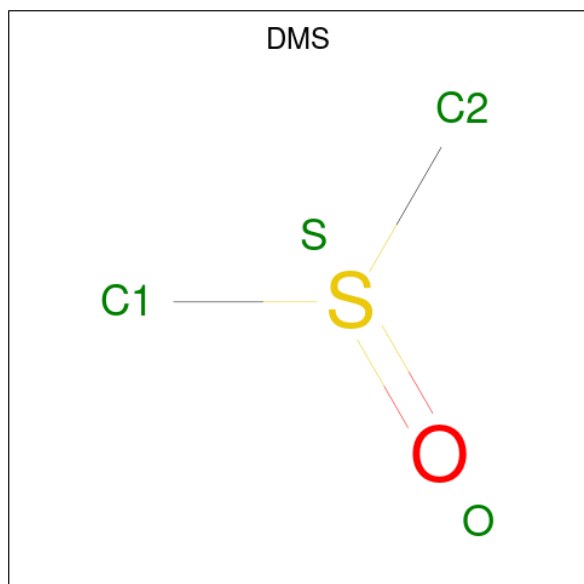
- Molecule 1 is a protein called 3C-like proteinase nsp5.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	306	Total	C	H	N	O	S	0	2	0
			4696	1507	2318	402	447	22			
1	C	306	Total	C	H	N	O	S	0	2	0
			4687	1504	2312	403	446	22			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	SER	CYS	engineered mutation	UNP P0DTD1
C	44	SER	CYS	engineered mutation	UNP P0DTD1

- Molecule 2 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

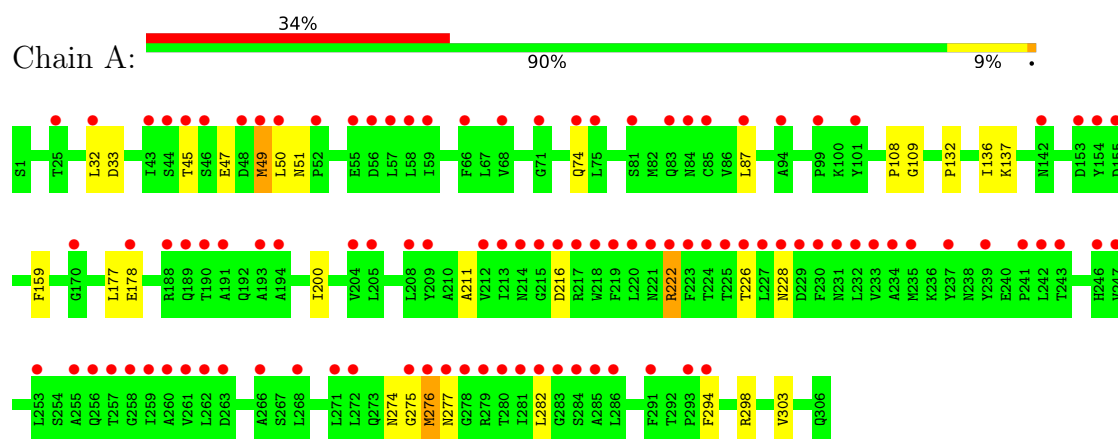
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	34	Total 34	O 34	0	0
3	C	39	Total 39	O 39	0	0

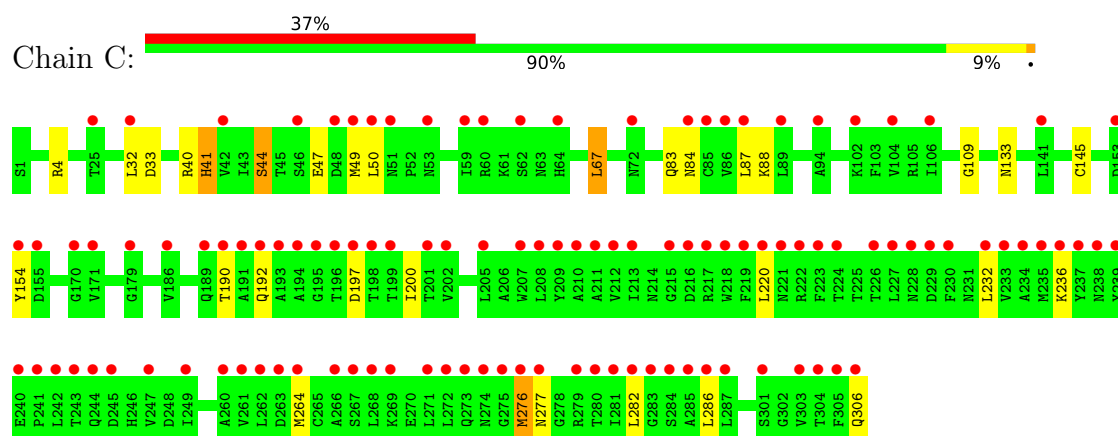
3 Residue-property plots [i](#)

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: 3C-like proteinase nsp5



- Molecule 1: 3C-like proteinase nsp5



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	122.88Å 81.36Å 63.56Å 90.00° 90.04° 90.00°	Depositor
Resolution (Å)	46.39 – 2.12 46.39 – 2.12	Depositor EDS
% Data completeness (in resolution range)	63.5 (46.39-2.12) 63.5 (46.39-2.12)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.12Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.261 , 0.298 0.262 , 0.297	Depositor DCC
R_{free} test set	1153 reflections (3.24%)	wwPDB-VP
Wilson B-factor (Å ²)	47.6	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.020 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9466	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.38% 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: DMS

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	0.14	0/2437	0.29	0/3311
1	C	0.29	1/2433 (0.0%)	0.39	4/3306 (0.1%)
All	All	0.23	1/4870 (0.0%)	0.34	4/6617 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	41	HIS	C-O	-6.15	1.16	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	41	HIS	N-CA-CB	7.89	123.83	110.49
1	C	40	ARG	N-CA-C	-6.98	100.15	110.48
1	C	40	ARG	CA-C-N	5.33	131.72	121.54
1	C	40	ARG	C-N-CA	5.33	131.72	121.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	222	ARG	Peptide

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	2378	2318	2329	14	0
1	C	2375	2312	2318	10	1
2	C	4	6	6	0	0
3	A	34	0	0	1	0
3	C	39	0	0	1	0
All	All	4830	4636	4653	23	1

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 (23) 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:C:44:SER:OG	1:C:49:MET:CE	2.51	0.59
1:A:74:GLN:NE2	3:A:402:HOH:O	2.35	0.59
1:A:276:MET:N	1:A:276:MET:SD	2.73	0.58
1:C:276:MET:SD	1:C:277:ASN:N	2.75	0.55
1:A:274:ASN:OD1	1:A:275:GLY:N	2.43	0.51
1:C:44:SER:OG	1:C:49:MET:SD	2.70	0.49
1:A:211:ALA:O	1:A:216:ASP:N	2.47	0.48
1:A:49:MET:O	1:A:50:LEU:HB3	2.13	0.48
1:A:32:LEU:O	1:A:33:ASP:C	2.57	0.47
1:A:51:ASN:O	1:A:51:ASN:ND2	2.48	0.47
1:A:109:GLY:HA2	1:A:200:ILE:HD13	1.98	0.46
1:C:133:ASN:ND2	1:C:197:ASP:OD1	2.49	0.45
1:C:67:LEU:O	3:C:501:HOH:O	2.20	0.45
1:A:137:LYS:O	1:C:4:ARG:NE	2.40	0.45
1:C:109:GLY:HA2	1:C:200:ILE:HD13	2.00	0.43
1:A:108:PRO:HB3	1:A:132:PRO:HA	2.00	0.43
1:C:83:GLN:HB2	1:C:88:LYS:HE2	2.01	0.43
1:A:276:MET:HG2	1:A:277:ASN:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:PHE:HB3	1:A:177:LEU:HD13	2.02	0.42
1:C:32:LEU:O	1:C:33:ASP:C	2.63	0.42
1:C:190:THR:HG23	1:C:192:GLN:HG3	2.03	0.40
1:A:49:MET:SD	1:A:49:MET:N	2.95	0.40
1:A:298:ARG:HG2	1:A:303:VAL:HB	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:CYS:SG	1:C:306:GLN:C[4_545]	1.79	0.41

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	306/306 (100%)	279 (91%)	27 (9%)	0	100	100
1	C	306/306 (100%)	281 (92%)	24 (8%)	1 (0%)	36	36
All	All	612/612 (100%)	560 (92%)	51 (8%)	1 (0%)	43	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	41	HIS

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	265/263 (101%)	253 (96%)	12 (4%)	24	24
1	C	264/263 (100%)	250 (95%)	14 (5%)	20	18
All	All	529/526 (101%)	503 (95%)	26 (5%)	22	21

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	THR
1	A	47	GLU
1	A	49	MET
1	A	87	LEU
1	A	136	ILE
1	A	178	GLU
1	A	222	ARG
1	A	226	THR
1	A	228	ASN
1	A	276	MET
1	A	282	LEU
1	A	294	PHE
1	C	44	SER
1	C	47	GLU
1	C	50	LEU
1	C	67	LEU
1	C	84	ASN
1	C	87	LEU
1	C	154	TYR
1	C	220	LEU
1	C	232	LEU
1	C	236	LYS
1	C	264	MET
1	C	276	MET
1	C	282	LEU
1	C	286	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	GLN

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Mol	Chain	Res	Type
1	C	51	ASN
1	C	64	HIS
1	C	163	HIS
1	C	246	HIS
1	C	274	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](#)

1 ligand is 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	DMS	C	401	-	3,3,3	0.59	0	3,3,3	0.72	0

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, 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	306/306 (100%)	1.72	104 (33%)	1 1	29, 66, 149, 228	2 (0%)
1	C	306/306 (100%)	1.81	113 (36%)	1 1	20, 66, 142, 206	1 (0%)
All	All	612/612 (100%)	1.76	217 (35%)	1 1	20, 66, 148, 228	3 (0%)

All (217) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	285	ALA	8.4
1	A	45	THR	7.0
1	C	208	LEU	6.6
1	C	286	LEU	6.4
1	C	281	ILE	6.3
1	C	232	LEU	6.0
1	A	44	SER	5.9
1	C	268	LEU	5.8
1	A	285	ALA	5.8
1	A	259	ILE	5.7
1	A	242	LEU	5.6
1	C	234	ALA	5.6
1	A	84	ASN	5.5
1	C	84	ASN	5.4
1	A	50	LEU	5.3
1	C	223	PHE	5.2
1	C	242	LEU	5.2
1	A	230	PHE	5.1
1	A	154	TYR	5.1
1	C	154	TYR	5.0
1	C	218	TRP	4.9
1	A	219	PHE	4.9
1	A	49	MET	4.9
1	A	268	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	219	PHE	4.7
1	A	190	THR	4.7
1	A	218	TRP	4.7
1	A	223	PHE	4.6
1	C	283	GLY	4.5
1	C	205	LEU	4.5
1	C	228	ASN	4.5
1	A	232	LEU	4.4
1	C	179	GLY	4.3
1	C	262	LEU	4.3
1	A	55[A]	GLU	4.3
1	C	230	PHE	4.3
1	A	260	ALA	4.3
1	C	50	LEU	4.2
1	C	280	THR	4.2
1	A	241	PRO	4.2
1	A	276	MET	4.2
1	C	306	GLN	4.2
1	A	208	LEU	4.2
1	C	220	LEU	4.2
1	C	227	LEU	4.2
1	C	305	PHE	4.2
1	C	282	LEU	4.1
1	A	46	SER	4.1
1	C	284	SER	4.1
1	A	71	GLY	4.0
1	A	282	LEU	4.0
1	C	87	LEU	4.0
1	C	275	GLY	4.0
1	A	216	ASP	3.9
1	A	271	LEU	3.9
1	A	277	ASN	3.9
1	A	257	THR	3.9
1	C	155	ASP	3.8
1	A	221	ASN	3.8
1	A	262	LEU	3.8
1	C	221	ASN	3.8
1	A	253	LEU	3.8
1	A	281	ILE	3.7
1	C	249	ILE	3.7
1	C	237	TYR	3.7
1	C	222	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	283	GLY	3.7
1	C	247	VAL	3.7
1	A	214	ASN	3.7
1	C	153	ASP	3.7
1	C	217	ARG	3.7
1	C	190	THR	3.7
1	C	211	ALA	3.7
1	A	213	ILE	3.7
1	C	226	THR	3.7
1	A	278	GLY	3.6
1	A	294	PHE	3.5
1	C	241	PRO	3.5
1	A	205	LEU	3.5
1	C	287	LEU	3.5
1	C	277	ASN	3.5
1	A	235	MET	3.5
1	A	52	PRO	3.5
1	A	81	SER	3.5
1	A	48	ASP	3.5
1	A	258	GLY	3.4
1	A	272	LEU	3.4
1	A	220	LEU	3.4
1	C	272	LEU	3.4
1	C	274	ASN	3.4
1	A	212	VAL	3.4
1	C	261	VAL	3.4
1	A	194	ALA	3.4
1	C	264	MET	3.3
1	C	86	VAL	3.3
1	C	215	GLY	3.3
1	C	192	GLN	3.3
1	C	269	LYS	3.3
1	A	233	VAL	3.3
1	A	59	ILE	3.3
1	C	102	LYS	3.3
1	C	196	THR	3.2
1	C	193	ALA	3.2
1	A	246	HIS	3.2
1	A	193	ALA	3.2
1	A	209	TYR	3.2
1	C	89	LEU	3.2
1	A	153	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	279	ARG	3.1
1	C	195	GLY	3.1
1	C	303	VAL	3.1
1	A	224	THR	3.1
1	A	286	LEU	3.1
1	C	266	ALA	3.1
1	C	171	VAL	3.1
1	A	261	VAL	3.0
1	C	233	VAL	3.0
1	A	222	ARG	3.0
1	A	284	SER	3.0
1	C	49	MET	3.0
1	A	155	ASP	2.9
1	A	189	GLN	2.9
1	C	104	VAL	2.9
1	A	239	TYR	2.9
1	C	64	HIS	2.9
1	C	60	ARG	2.9
1	C	243	THR	2.9
1	A	237	TYR	2.9
1	A	32	LEU	2.8
1	C	25	THR	2.8
1	A	275	GLY	2.8
1	C	207	TRP	2.8
1	C	244	GLN	2.8
1	C	198	THR	2.8
1	C	236	LYS	2.8
1	A	57	LEU	2.7
1	C	239	TYR	2.7
1	A	25	THR	2.7
1	A	56	ASP	2.7
1	C	201	THR	2.7
1	A	43	ILE	2.7
1	A	94	ALA	2.6
1	C	224	THR	2.6
1	C	197	ASP	2.6
1	C	216	ASP	2.6
1	A	68	VAL	2.6
1	A	85	CYS	2.6
1	C	210	ALA	2.6
1	C	202	VAL	2.6
1	A	255	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	74	GLN	2.5
1	C	212	VAL	2.5
1	A	225	THR	2.5
1	C	301	SER	2.5
1	C	240	GLU	2.5
1	C	235	MET	2.5
1	C	72	ASN	2.5
1	A	293	PRO	2.5
1	C	191	ALA	2.5
1	A	87	LEU	2.5
1	C	229	ASP	2.5
1	C	189	GLN	2.5
1	A	227	LEU	2.5
1	C	59	ILE	2.5
1	C	260	ALA	2.4
1	C	271	LEU	2.4
1	A	142	ASN	2.4
1	A	228	ASN	2.4
1	A	247	VAL	2.4
1	A	226	THR	2.4
1	A	243	THR	2.4
1	A	191	ALA	2.4
1	A	204	VAL	2.4
1	A	280	THR	2.4
1	A	99	PRO	2.4
1	A	266	ALA	2.3
1	A	291	PHE	2.3
1	C	32	LEU	2.3
1	A	188	ARG	2.3
1	A	256	GLN	2.3
1	A	215	GLY	2.3
1	C	62	SER	2.3
1	C	106	ILE	2.3
1	C	267	SER	2.2
1	A	66	PHE	2.2
1	A	217	ARG	2.2
1	A	229	ASP	2.2
1	C	85	CYS	2.2
1	A	75	LEU	2.2
1	C	273	GLN	2.2
1	C	53	ASN	2.2
1	C	304	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	101	TYR	2.2
1	C	46	SER	2.2
1	A	279	ARG	2.2
1	C	51	ASN	2.2
1	C	213	ILE	2.2
1	C	141	LEU	2.2
1	C	48	ASP	2.2
1	C	199	THR	2.2
1	C	245	ASP	2.2
1	C	42	VAL	2.1
1	A	83	GLN	2.1
1	C	170	GLY	2.1
1	A	234	ALA	2.1
1	A	231	ASN	2.1
1	A	58	LEU	2.1
1	A	178	GLU	2.1
1	C	194	ALA	2.1
1	A	263	ASP	2.1
1	C	186	VAL	2.0
1	C	276	MET	2.0
1	C	94	ALA	2.0
1	C	238	ASN	2.0
1	C	263	ASP	2.0
1	A	170	GLY	2.0
1	C	209	TYR	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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	DMS	C	401	4/4	0.69	0.21	98,118,120,120	0

6.5 Other polymers [i](#)

There are no such residues in this entry.