



Full wwPDB X-ray Structure Validation Report ⓘ

May 3, 2025 – 03:35 PM EDT

PDB ID : 3HJR / pdb_00003hjr
Title : Crystal structure of serine protease of *Aeromonas sobria*
Authors : Utsunomiya, H.; Tsuge, H.; Kobayashi, H.; Okamoto, K.
Deposited on : 2009-05-22
Resolution : 1.65 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 Phenix2.0rc1
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

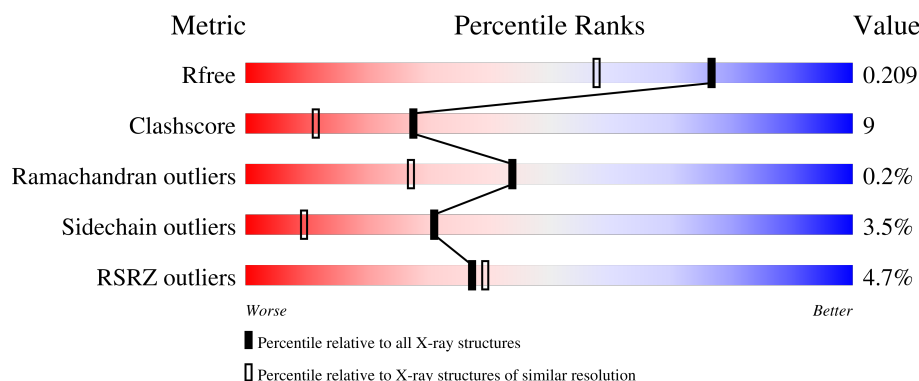
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	2328 (1.66-1.66)
Clashscore	180529	2515 (1.66-1.66)
Ramachandran outliers	177936	2475 (1.66-1.66)
Sidechain outliers	177891	2475 (1.66-1.66)
RSRZ outliers	164620	2328 (1.66-1.66)

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	600	<div> <div>5%</div> <div>86%</div> <div>11%</div> <div>..</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5161 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 Extracellular serine protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	593	Total	C	N	O	S	0	0	0
			4458	2747	808	887	16			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	70	GLN	HIS	SEE REMARK 999	UNP Q9L5A4
A	114	ALA	GLY	SEE REMARK 999	UNP Q9L5A4
A	176	GLN	HIS	SEE REMARK 999	UNP Q9L5A4
A	179	GLY	ARG	SEE REMARK 999	UNP Q9L5A4

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

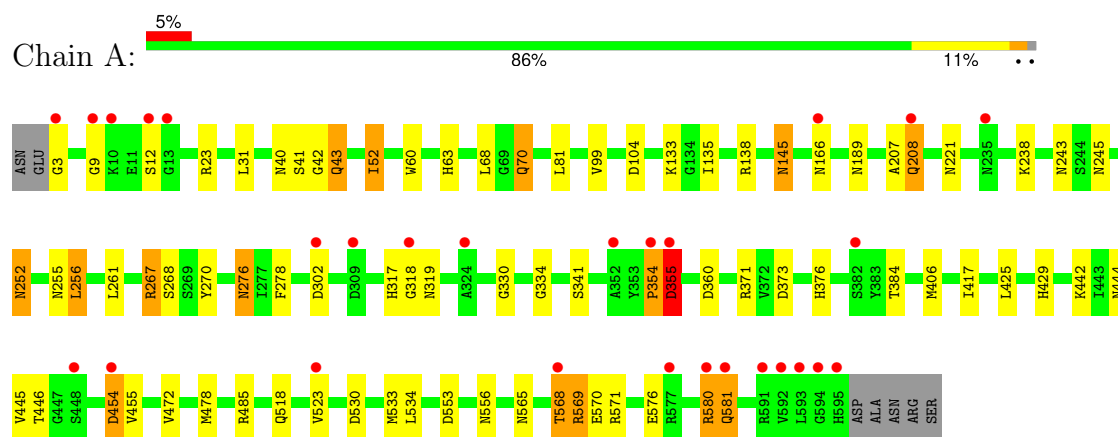
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	700	Total	O	0	0
			700	700		

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: Extracellular serine protease



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.82Å 112.06Å 51.88Å 90.00° 110.75° 90.00°	Depositor
Resolution (Å)	43.02 – 1.65 43.02 – 1.65	Depositor EDS
% Data completeness (in resolution range)	98.7 (43.02-1.65) 98.6 (43.02-1.65)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.41 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.168 , 0.202 0.178 , 0.209	Depositor DCC
R_{free} test set	3172 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	13.1	Xtriage
Anisotropy	0.562	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5161	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.12% 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: CA

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	0.83	5/4541 (0.1%)	0.98	9/6180 (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	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	267	ARG	CD-NE	-6.10	1.37	1.46
1	A	533	MET	SD-CE	-5.47	1.65	1.79
1	A	417	ILE	CA-CB	5.41	1.60	1.54
1	A	52	ILE	CA-CB	5.24	1.60	1.54
1	A	355	ASP	CA-C	5.18	1.60	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	ARG	NE-CZ-NH2	-7.91	112.08	119.20
1	A	354	PRO	CA-C-N	-6.54	113.06	123.91
1	A	354	PRO	C-N-CA	-6.54	113.06	123.91
1	A	454	ASP	N-CA-C	6.41	118.80	111.11
1	A	267	ARG	NE-CZ-NH1	6.28	127.78	121.50
1	A	207	ALA	CA-C-N	-5.91	111.34	122.27
1	A	207	ALA	C-N-CA	-5.91	111.34	122.27
1	A	568	THR	N-CA-C	-5.32	99.11	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	319	ASN	N-CA-C	5.00	117.74	107.69

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	208	GLN	Peptide
1	A	318	GLY	Peptide
1	A	355	ASP	Peptide
1	A	9	GLY	Peptide

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	4458	0	4344	78	2
2	A	3	0	0	0	0
3	A	700	0	0	30	1
All	All	5161	0	4344	78	2

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 9.

All (78) 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:384:THR:HB	3:A:1171:HOH:O	1.04	1.20
1:A:454:ASP:O	1:A:553:ASP:OD2	1.60	1.17
1:A:454:ASP:O	1:A:553:ASP:CG	2.04	0.99
1:A:3:GLY:HA2	3:A:1258:HOH:O	1.66	0.95
1:A:208:GLN:HG2	1:A:208:GLN:O	1.69	0.90
1:A:267:ARG:HD2	1:A:268:SER:O	1.72	0.89
1:A:569:ARG:N	3:A:1172:HOH:O	2.05	0.87
1:A:302:ASP:HB2	3:A:1070:HOH:O	1.75	0.85
1:A:276:ASN:HD22	1:A:276:ASN:H	1.27	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:GLN:HE21	1:A:70:GLN:H	1.26	0.82
1:A:99:VAL:H	1:A:145:ASN:HD21	1.26	0.82
1:A:317:HIS:HE1	1:A:330:GLY:H	1.31	0.78
1:A:580:ARG:HB3	3:A:1053:HOH:O	1.84	0.76
1:A:68:LEU:H	1:A:70:GLN:HE22	1.36	0.73
1:A:208:GLN:O	1:A:208:GLN:CG	2.37	0.72
1:A:243:ASN:HD22	1:A:245:ASN:H	1.37	0.72
1:A:355:ASP:HA	3:A:1176:HOH:O	1.91	0.70
1:A:70:GLN:H	1:A:70:GLN:NE2	1.90	0.69
1:A:565:ASN:HB3	1:A:568:THR:O	1.94	0.68
1:A:454:ASP:HA	3:A:1235:HOH:O	1.95	0.66
1:A:3:GLY:N	3:A:1221:HOH:O	2.29	0.65
1:A:238:LYS:HE3	3:A:664:HOH:O	1.95	0.65
1:A:568:THR:C	3:A:1172:HOH:O	2.35	0.65
1:A:252:ASN:HD21	1:A:255:ASN:H	1.47	0.63
1:A:99:VAL:N	1:A:145:ASN:HD21	1.98	0.62
1:A:99:VAL:H	1:A:145:ASN:ND2	1.96	0.61
1:A:63:HIS:HE1	1:A:135:ILE:O	1.83	0.61
1:A:166:ASN:HB3	3:A:1087:HOH:O	1.99	0.61
1:A:189:ASN:OD1	1:A:478:MET:HE1	2.01	0.60
1:A:270:TYR:CE1	1:A:334:GLY:HA2	2.36	0.60
1:A:12:SER:HB2	3:A:954:HOH:O	2.01	0.59
1:A:40:ASN:HD22	1:A:42:GLY:H	1.49	0.59
1:A:256:LEU:HD13	1:A:278:PHE:HB3	1.84	0.58
1:A:384:THR:CB	3:A:1171:HOH:O	1.89	0.57
1:A:568:THR:CA	3:A:1172:HOH:O	2.51	0.57
1:A:221:ASN:HD21	1:A:238:LYS:NZ	2.01	0.57
1:A:354:PRO:O	1:A:355:ASP:HB2	2.05	0.57
1:A:145:ASN:H	1:A:145:ASN:HD22	1.54	0.56
1:A:267:ARG:CD	1:A:268:SER:O	2.52	0.56
1:A:41:SER:OG	1:A:43:GLN:HG3	2.07	0.55
1:A:376:HIS:HE1	3:A:629:HOH:O	1.89	0.55
1:A:454:ASP:CA	3:A:1235:HOH:O	2.52	0.55
1:A:570:GLU:HG3	3:A:1238:HOH:O	2.07	0.54
1:A:580:ARG:HA	3:A:1037:HOH:O	2.07	0.54
1:A:371:ARG:NE	3:A:1300:HOH:O	2.35	0.53
1:A:406:MET:HG2	3:A:1083:HOH:O	2.07	0.53
1:A:373:ASP:O	1:A:376:HIS:HD2	1.91	0.53
1:A:360:ASP:OD2	1:A:429:HIS:HE1	1.93	0.52
1:A:243:ASN:ND2	1:A:245:ASN:H	2.08	0.51
1:A:518:GLN:NE2	3:A:715:HOH:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ASN:ND2	1:A:42:GLY:H	2.08	0.51
1:A:523:VAL:HG12	3:A:986:HOH:O	2.11	0.50
1:A:565:ASN:O	1:A:568:THR:O	2.30	0.49
1:A:384:THR:HG23	3:A:1143:HOH:O	2.12	0.49
1:A:40:ASN:HD22	1:A:40:ASN:C	2.19	0.49
1:A:384:THR:CG2	3:A:1171:HOH:O	2.45	0.49
1:A:454:ASP:CB	3:A:1235:HOH:O	2.60	0.49
1:A:478:MET:HE2	1:A:530:ASP:O	2.13	0.48
1:A:568:THR:C	1:A:570:GLU:H	2.21	0.48
1:A:221:ASN:HD21	1:A:238:LYS:HZ1	1.60	0.48
1:A:568:THR:O	1:A:568:THR:OG1	2.31	0.48
1:A:581:GLN:NE2	3:A:1261:HOH:O	2.45	0.48
1:A:104:ASP:HB3	3:A:1103:HOH:O	2.13	0.47
1:A:145:ASN:HD22	1:A:145:ASN:N	2.13	0.46
1:A:70:GLN:HG2	1:A:138:ARG:NH1	2.30	0.45
1:A:252:ASN:ND2	1:A:255:ASN:H	2.13	0.45
1:A:571:ARG:NE	3:A:1011:HOH:O	2.27	0.45
1:A:454:ASP:O	1:A:553:ASP:CB	2.66	0.43
1:A:245:ASN:HD21	1:A:534:LEU:H	1.67	0.42
1:A:276:ASN:HD22	1:A:276:ASN:N	2.02	0.41
1:A:302:ASP:OD2	3:A:1217:HOH:O	2.22	0.41
1:A:442:LYS:HE3	1:A:444:ASN:OD1	2.19	0.41
1:A:485:ARG:HD2	1:A:576:GLU:HB3	2.02	0.41
1:A:23:ARG:HG3	1:A:60:TRP:CD1	2.55	0.41
1:A:135:ILE:CD1	1:A:341:SER:HA	2.51	0.41
1:A:276:ASN:H	1:A:276:ASN:ND2	2.07	0.40
1:A:63:HIS:CD2	1:A:133:LYS:NZ	2.89	0.40
1:A:371:ARG:NH2	3:A:711:HOH:O	2.54	0.40

All (2) 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:A:166:ASN:ND2	3:A:1204:HOH:O[1_554]	1.87	0.33
1:A:12:SER:OG	1:A:446:THR:OG1[2_545]	1.89	0.31

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	591/600 (98%)	572 (97%)	18 (3%)	1 (0%)	44	27

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	569	ARG

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	484/490 (99%)	467 (96%)	17 (4%)	31	9

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LEU
1	A	43	GLN
1	A	52	ILE
1	A	70	GLN
1	A	81	LEU
1	A	145	ASN
1	A	252	ASN
1	A	256	LEU
1	A	261	LEU
1	A	276	ASN

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Mol	Chain	Res	Type
1	A	425	LEU
1	A	445	VAL
1	A	455	VAL
1	A	472	VAL
1	A	556	ASN
1	A	580	ARG
1	A	581	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	55	ASN
1	A	58	ASN
1	A	63	HIS
1	A	70	GLN
1	A	73	ASN
1	A	91	ASN
1	A	145	ASN
1	A	150	ASN
1	A	153	GLN
1	A	155	GLN
1	A	166	ASN
1	A	175	ASN
1	A	193	GLN
1	A	208	GLN
1	A	221	ASN
1	A	243	ASN
1	A	245	ASN
1	A	252	ASN
1	A	276	ASN
1	A	314	ASN
1	A	317	HIS
1	A	376	HIS
1	A	429	HIS
1	A	518	GLN
1	A	556	ASN

5.3.3 RNA ⓘ

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 3 ligands modelled in this entry, 3 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 [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	593/600 (98%)	0.24	28 (4%) 37 39	3, 9, 16, 24	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	9	GLY	5.3
1	A	580	ARG	4.6
1	A	12	SER	3.9
1	A	3	GLY	3.9
1	A	166	ASN	3.8
1	A	208	GLN	3.5
1	A	302	ASP	3.4
1	A	454	ASP	3.4
1	A	318	GLY	3.4
1	A	568	THR	3.2
1	A	355	ASP	3.0
1	A	235	ASN	2.5
1	A	593	LEU	2.4
1	A	354	PRO	2.4
1	A	324	ALA	2.4
1	A	594	GLY	2.4
1	A	577	ARG	2.4
1	A	309	ASP	2.4
1	A	352	ALA	2.3
1	A	581	GLN	2.3
1	A	592	VAL	2.3
1	A	10	LYS	2.2
1	A	591	ARG	2.2
1	A	595	HIS	2.2
1	A	13	GLY	2.1
1	A	523	VAL	2.0
1	A	382	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	448	SER	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 monosaccharides 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(Å ²)	Q<0.9
2	CA	A	601	1/1	0.96	0.07	22,22,22,22	0
2	CA	A	603	1/1	0.96	0.13	27,27,27,27	0
2	CA	A	602	1/1	0.98	0.20	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.