



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 25, 2023 – 03:36 PM EDT

PDB ID : 2Z58
Title : Crystal structure of G56W-propeptide:S324A-subtilisin complex
Authors : Pulido, M.A.; Tanaka, S.; Sringiew, C.; You, D.J.; Matsumura, H.; Koga, Y.;
Takano, K.; Kanaya, S.
Deposited on : 2007-06-29
Resolution : 1.88 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

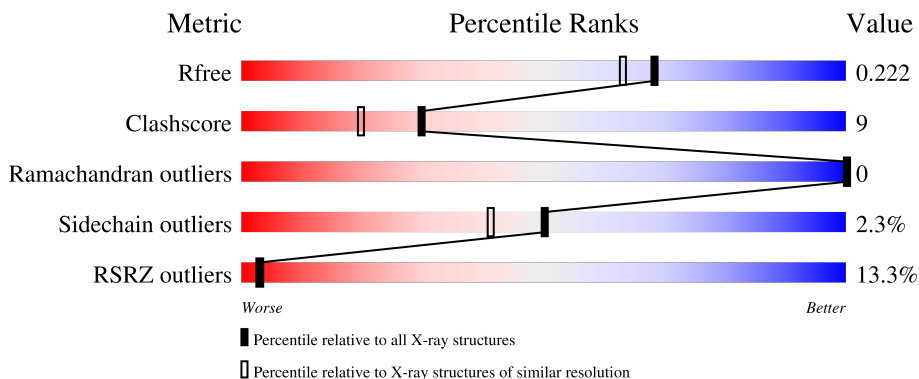
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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}	130704	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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	318	
2	B	66	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CA	A	1002	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3010 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 Tk-subtilisin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	318	2314	1452	384	472	6	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	324	ALA	SER	engineered mutation	UNP P58502

- Molecule 2 is a protein called Tk-subtilisin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	66	518	342	88	87	1	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	56	TRP	GLY	engineered mutation	UNP P58502

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
3	A	7	7	7	0	0

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

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

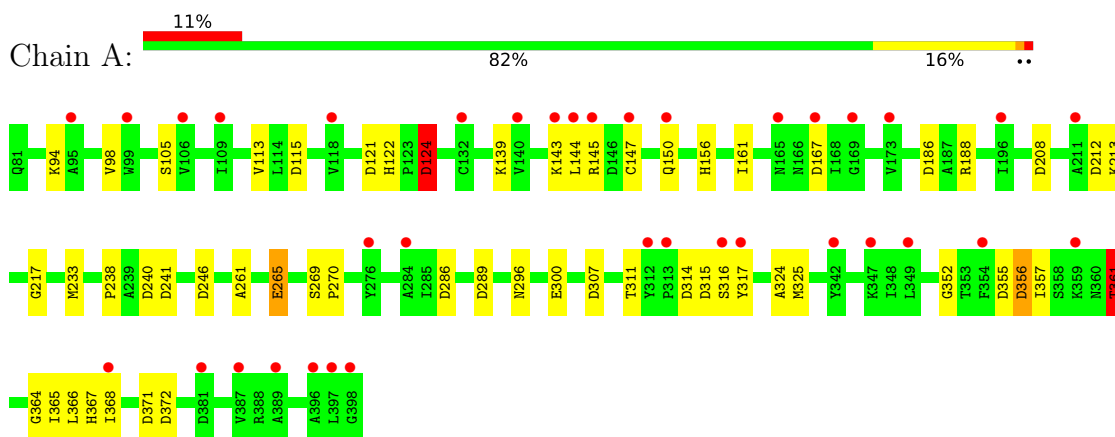
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	150	Total 150	O 150	0	0
5	B	20	Total 20	O 20	0	0

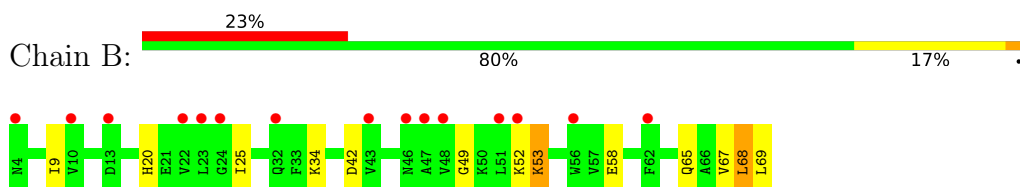
3 Residue-property plots [i](#)

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: Tk-subtilisin



- Molecule 2: Tk-subtilisin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.84Å 67.34Å 74.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.88 49.82 – 1.88	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-1.88) 99.0 (49.82-1.88)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 1.88Å)	Xtrriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.195 , 0.226 0.195 , 0.222	Depositor DCC
R_{free} test set	1343 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	22.5	Xtrriage
Anisotropy	0.158	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.016 for k,h,-l	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	3010	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.20% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, ZN

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	1.31	8/2361 (0.3%)	1.14	14/3235 (0.4%)
2	B	1.20	2/530 (0.4%)	1.02	1/719 (0.1%)
All	All	1.29	10/2891 (0.3%)	1.12	15/3954 (0.4%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	361	THR	CB-CG2	-8.86	1.23	1.52
1	A	233	MET	SD-CE	-7.55	1.35	1.77
1	A	113	VAL	CB-CG2	-7.17	1.37	1.52
2	B	34	LYS	CE-NZ	5.91	1.63	1.49
1	A	98	VAL	CB-CG2	-5.55	1.41	1.52
1	A	265	GLU	CD-OE2	5.42	1.31	1.25
2	B	67	VAL	CB-CG1	-5.28	1.41	1.52
1	A	265	GLU	CG-CD	5.25	1.59	1.51
1	A	317	TYR	CD1-CE1	5.04	1.47	1.39
1	A	365	ILE	C-O	5.02	1.32	1.23

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	356	ASP	CB-CG-OD2	9.59	126.93	118.30
1	A	372	ASP	CB-CG-OD1	8.53	125.97	118.30
1	A	124	ASP	CB-CG-OD1	8.48	125.93	118.30
2	B	42	ASP	CB-CG-OD2	7.49	125.04	118.30
1	A	241	ASP	CB-CG-OD2	7.36	124.93	118.30
1	A	115	ASP	CB-CG-OD1	6.56	124.20	118.30
1	A	167	ASP	CB-CG-OD2	6.21	123.89	118.30
1	A	240	ASP	CB-CG-OD2	6.06	123.75	118.30
1	A	289	ASP	CB-CG-OD2	5.61	123.35	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	366	LEU	CB-CG-CD1	-5.38	101.85	111.00
1	A	233	MET	CG-SD-CE	-5.24	91.82	100.20
1	A	355	ASP	CB-CG-OD2	5.18	122.97	118.30
1	A	161	ILE	CG1-CB-CG2	-5.15	100.08	111.40
1	A	212	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	286	ASP	CB-CG-OD2	5.08	122.87	118.30

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	2314	0	2239	37	2
2	B	518	0	547	17	0
3	A	7	0	0	2	0
4	B	1	0	0	0	0
5	A	150	0	0	11	0
5	B	20	0	0	4	0
All	All	3010	0	2786	53	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 (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:A:94:LYS:NZ	5:A:1071:HOH:O	1.94	0.99
1:A:361:THR:HG22	1:A:364:GLY:H	1.30	0.93
2:B:53:LYS:HD2	2:B:53:LYS:N	1.89	0.87
3:A:1002:CA:CA	5:A:1097:HOH:O	1.58	0.81
2:B:68:LEU:HD12	2:B:68:LEU:O	1.81	0.80
1:A:314:ASP:OD2	5:A:1008:HOH:O	1.98	0.79
1:A:246:ASP:OD1	5:A:1019:HOH:O	2.05	0.73
2:B:58:GLU:OE1	5:B:277:HOH:O	2.05	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:PRO:HD2	5:B:270:HOH:O	1.88	0.72
1:A:122:HIS:HD2	1:A:124:ASP:H	1.39	0.70
1:A:307:ASP:OD2	5:A:1060:HOH:O	2.09	0.69
1:A:105:SER:OG	5:A:1156:HOH:O	2.12	0.68
2:B:52:LYS:C	2:B:53:LYS:HD2	2.14	0.66
1:A:371:ASP:OD1	5:A:1081:HOH:O	2.14	0.65
1:A:356:ASP:O	1:A:367:HIS:HD2	1.80	0.64
1:A:357:ILE:HB	1:A:368:ILE:HD11	1.79	0.64
2:B:68:LEU:HD12	2:B:68:LEU:C	2.18	0.63
1:A:122:HIS:HE1	1:A:316:SER:O	1.84	0.60
1:A:121:ASP:OD1	3:A:1002:CA:CA	1.78	0.60
1:A:300:GLU:OE2	1:A:367:HIS:HE1	1.85	0.59
2:B:49:GLY:HA2	2:B:52:LYS:HE2	1.84	0.58
1:A:357:ILE:CB	1:A:368:ILE:HD11	2.34	0.57
1:A:144:LEU:HA	1:A:147:CYS:SG	2.46	0.56
1:A:208:ASP:OD2	1:A:213:LYS:HD2	2.05	0.56
1:A:139:LYS:HE3	5:A:1062:HOH:O	2.04	0.56
1:A:356:ASP:OD1	1:A:361:THR:HG21	2.07	0.55
2:B:9:ILE:HD12	2:B:9:ILE:N	2.23	0.54
1:A:150:GLN:HG3	5:A:1076:HOH:O	2.09	0.53
1:A:324:ALA:HB2	2:B:69:LEU:C	2.29	0.52
2:B:53:LYS:N	2:B:53:LYS:CD	2.70	0.51
2:B:20:HIS:CE1	5:B:278:HOH:O	2.65	0.50
1:A:265:GLU:H	1:A:296:ASN:HD21	1.58	0.50
2:B:25:ILE:C	2:B:25:ILE:HD12	2.33	0.48
1:A:352:GLY:HA3	1:A:361:THR:HG23	1.94	0.48
2:B:20:HIS:HE1	5:B:278:HOH:O	1.97	0.48
2:B:52:LYS:HE3	2:B:53:LYS:HZ3	1.78	0.47
1:A:186:ASP:OD2	1:A:188:ARG:NH1	2.48	0.47
1:A:300:GLU:OE2	1:A:367:HIS:CE1	2.66	0.47
1:A:361:THR:CG2	1:A:364:GLY:H	2.15	0.47
2:B:68:LEU:C	2:B:68:LEU:CD1	2.84	0.46
1:A:269:SER:HB2	1:A:270:PRO:CD	2.46	0.46
1:A:357:ILE:CA	1:A:368:ILE:HD11	2.45	0.46
1:A:265:GLU:H	1:A:296:ASN:ND2	2.13	0.46
1:A:213:LYS:HE2	5:A:1043:HOH:O	2.15	0.45
1:A:186:ASP:OD2	1:A:188:ARG:CZ	2.64	0.45
1:A:213:LYS:CE	5:A:1043:HOH:O	2.65	0.44
1:A:361:THR:HG22	1:A:364:GLY:N	2.13	0.44
1:A:352:GLY:HA3	1:A:361:THR:CG2	2.48	0.44
1:A:261:ALA:HB3	2:B:69:LEU:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:HIS:HA	1:A:311:THR:O	2.19	0.43
1:A:368:ILE:HG23	1:A:368:ILE:HD12	1.71	0.42
2:B:65:GLN:HE21	2:B:65:GLN:HB3	1.57	0.42
2:B:49:GLY:O	2:B:53:LYS:HD3	2.21	0.41

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:145:ARG:NH2	1:A:217:GLY:O[4_455]	1.28	0.92
1:A:145:ARG:NH2	1:A:217:GLY:C[4_455]	2.19	0.01

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	316/318 (99%)	302 (96%)	14 (4%)	0	100	100
2	B	64/66 (97%)	64 (100%)	0	0	100	100
All	All	380/384 (99%)	366 (96%)	14 (4%)	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	242/242 (100%)	237 (98%)	5 (2%)	53	45
2	B	57/57 (100%)	55 (96%)	2 (4%)	36	24
All	All	299/299 (100%)	292 (98%)	7 (2%)	50	41

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	ASP
1	A	143	LYS
1	A	315	ASP
1	A	325	MET
1	A	361	THR
2	B	53	LYS
2	B	68	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	HIS
1	A	150	GLN
1	A	178	GLN
1	A	290	ASN
1	A	296	ASN
1	A	343	GLN
1	A	367	HIS
2	B	65	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 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	318/318 (100%)	0.64	36 (11%) 5 5	15, 21, 32, 48	0
2	B	66/66 (100%)	1.31	15 (22%) 0 0	20, 28, 45, 51	0
All	All	384/384 (100%)	0.76	51 (13%) 3 3	15, 22, 37, 51	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	48	VAL	7.2
1	A	398	GLY	6.9
2	B	46	ASN	6.4
1	A	99	TRP	6.3
2	B	56	TRP	5.2
2	B	4	ASN	4.4
1	A	313	PRO	4.0
1	A	144	LEU	3.9
2	B	51	LEU	3.9
1	A	150	GLN	3.8
1	A	368	ILE	3.7
1	A	147	CYS	3.7
1	A	396	ALA	3.6
1	A	349	LEU	3.6
1	A	132	CYS	3.5
1	A	173	VAL	3.4
1	A	381	ASP	3.4
2	B	62	PHE	3.2
1	A	145	ARG	3.2
1	A	143	LYS	3.1
2	B	43	VAL	3.1
2	B	22	VAL	3.0
1	A	389	ALA	3.0
2	B	23	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	312	TYR	2.9
1	A	165	ASN	2.8
1	A	359	LYS	2.8
1	A	167	ASP	2.7
1	A	397	LEU	2.7
2	B	32	GLN	2.7
1	A	196	ILE	2.6
1	A	387	VAL	2.6
1	A	140	VAL	2.5
1	A	169	GLY	2.5
1	A	276	TYR	2.4
1	A	347	LYS	2.4
2	B	10	VAL	2.4
1	A	342	TYR	2.3
2	B	52	LYS	2.3
1	A	316	SER	2.3
2	B	13	ASP	2.3
1	A	118	VAL	2.2
1	A	354	PHE	2.2
1	A	211	ALA	2.2
1	A	284	ALA	2.2
1	A	106	VAL	2.2
1	A	109	ILE	2.1
2	B	47	ALA	2.1
1	A	95	ALA	2.1
1	A	317	TYR	2.0
2	B	24	GLY	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(\AA^2)	Q<0.9
4	ZN	B	263	1/1	0.95	0.05	31,31,31,31	0
3	CA	A	1007	1/1	0.96	0.05	19,19,19,19	0
3	CA	A	1002	1/1	0.98	0.15	14,14,14,14	0
3	CA	A	1006	1/1	0.99	0.08	16,16,16,16	0
3	CA	A	1001	1/1	0.99	0.04	19,19,19,19	0
3	CA	A	1005	1/1	0.99	0.15	10,10,10,10	0
3	CA	A	1003	1/1	1.00	0.18	9,9,9,9	0
3	CA	A	1004	1/1	1.00	0.07	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.