



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:24 PM GMT

PDB ID : 4I84
Title : The crystal structure of the Haemophilus influenzae HxuA secretion domain involved in the two-partner secretion pathway
Authors : Baelen, S.; Dewitte, F.; Clantin, B.; Villeret, V.
Deposited on : 2012-12-03
Resolution : 1.50 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

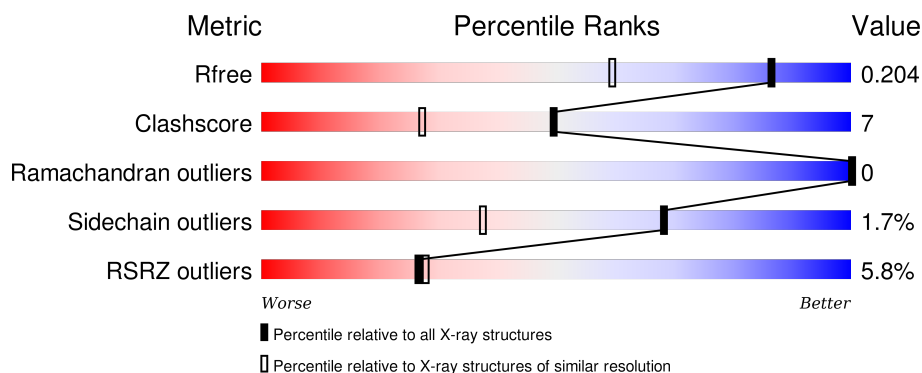
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 1.50 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}	91344	2072 (1.50-1.50)
Clashscore	102246	2274 (1.50-1.50)
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)
RSRZ outliers	91569	2075 (1.50-1.50)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	307	 7% 82% 14% • •
1	B	307	 4% 78% 10% • 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4879 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 Heme/hemopexin-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	15	0
			2292	1422	397	470	3			
1	B	274	Total	C	N	O	S	0	14	0
			2158	1337	380	439	2			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	EXPRESSION TAG	UNP P44602
A	-4	HIS	-	EXPRESSION TAG	UNP P44602
A	-3	HIS	-	EXPRESSION TAG	UNP P44602
A	-2	HIS	-	EXPRESSION TAG	UNP P44602
A	-1	HIS	-	EXPRESSION TAG	UNP P44602
A	0	HIS	-	EXPRESSION TAG	UNP P44602
B	-5	HIS	-	EXPRESSION TAG	UNP P44602
B	-4	HIS	-	EXPRESSION TAG	UNP P44602
B	-3	HIS	-	EXPRESSION TAG	UNP P44602
B	-2	HIS	-	EXPRESSION TAG	UNP P44602
B	-1	HIS	-	EXPRESSION TAG	UNP P44602
B	0	HIS	-	EXPRESSION TAG	UNP P44602

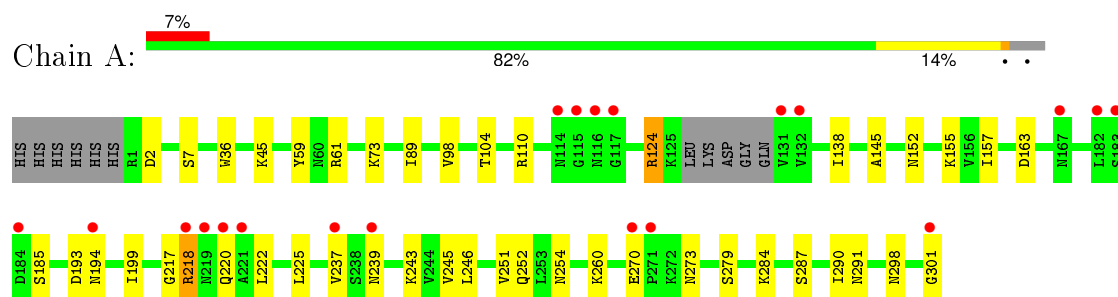
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	258	Total	O	0	0
			258	258		
2	B	171	Total	O	0	0
			171	171		

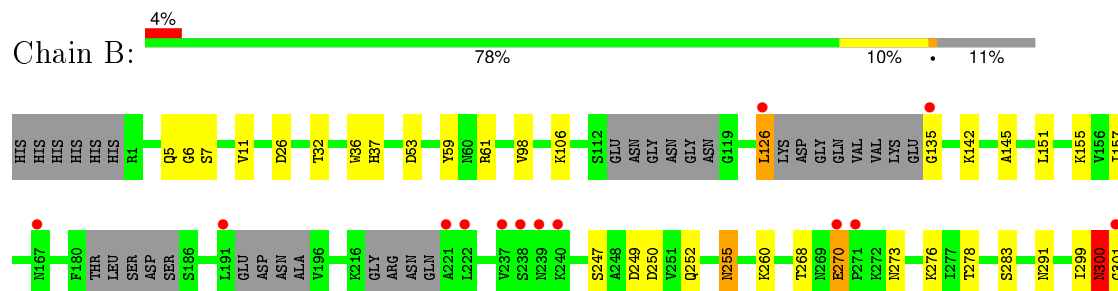
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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: Heme/hemopexin-binding protein



- Molecule 1: Heme/hemopexin-binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	38.99Å 70.84Å 104.98Å 90.00° 98.10° 90.00°	Depositor
Resolution (Å)	41.90 – 1.50 37.97 – 1.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (41.90-1.50) 99.1 (37.97-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.159 , 0.210 0.153 , 0.204	Depositor DCC
R_{free} test set	4488 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	16.7	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.2	EDS
Estimated twinning fraction	0.020 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	9 of 89775 reflections (0.010%)	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4879	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.71% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	1.28	4/2348 (0.2%)	1.22	7/3166 (0.2%)
1	B	1.22	4/2177 (0.2%)	1.07	7/2928 (0.2%)
All	All	1.25	8/4525 (0.2%)	1.15	14/6094 (0.2%)

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	B	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	283	SER	CB-OG	9.30	1.54	1.42
1	A	110	ARG	CB-CG	-6.74	1.34	1.52
1	A	59	TYR	CE1-CZ	6.39	1.46	1.38
1	B	135	GLY	N-CA	6.17	1.55	1.46
1	B	59	TYR	CE1-CZ	5.66	1.46	1.38
1	B	283	SER	CA-CB	5.32	1.60	1.52
1	A	251	VAL	CB-CG2	5.23	1.63	1.52
1	A	279	SER	CA-CB	5.14	1.60	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	ARG	NE-CZ-NH2	-17.79	111.41	120.30
1	A	124	ARG	NE-CZ-NH1	16.57	128.58	120.30
1	A	61	ARG	NE-CZ-NH2	-9.14	115.73	120.30
1	B	61	ARG	NE-CZ-NH2	-6.99	116.81	120.30
1	B	126	LEU	CA-CB-CG	-6.61	100.10	115.30
1	B	53	ASP	CB-CG-OD1	6.39	124.05	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	106	LYS	CD-CE-NZ	-5.93	98.05	111.70
1	B	300	ASN	N-CA-C	-5.66	95.72	111.00
1	A	110	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	A	246	LEU	CB-CG-CD1	-5.59	101.50	111.00
1	A	193	ASP	CB-CG-OD1	5.58	123.32	118.30
1	A	163	ASP	CB-CG-OD1	5.50	123.25	118.30
1	B	151	LEU	CB-CG-CD1	5.50	120.35	111.00
1	B	249	ASP	CB-CG-OD2	-5.08	113.73	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	300	ASN	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	2292	0	2345	46	0
1	B	2158	0	2181	24	0
2	A	258	0	0	12	0
2	B	171	0	0	5	0
All	All	4879	0	4526	64	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 7.

All (64) 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:218:ARG:HH11	1:A:218:ARG:HG2	1.09	1.05
1:A:291:ASN:HD22	1:B:291[A]:ASN:HD22	1.04	0.98
1:A:291:ASN:ND2	1:B:291[A]:ASN:HD22	1.70	0.89
1:A:218:ARG:NH1	1:A:218:ARG:HG2	1.81	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:GLN:HG2	2:B:562:HOH:O	1.72	0.87
1:A:218:ARG:CG	1:A:218:ARG:HH11	1.89	0.85
1:A:291:ASN:HD22	1:B:291[A]:ASN:ND2	1.74	0.83
1:A:194:ASN:HA	1:A:218:ARG:HE	1.46	0.80
1:A:301:GLY:OXT	1:B:301:GLY:O	2.01	0.79
1:A:138[A]:ILE:HD12	1:A:157:ILE:HD12	1.69	0.74
1:A:291:ASN:ND2	1:B:291[A]:ASN:ND2	2.36	0.72
1:A:124:ARG:HD3	2:A:640:HOH:O	1.89	0.72
1:A:252[B]:GLN:HE21	1:A:254:ASN:HD21	1.37	0.71
2:A:658:HOH:O	1:B:301:GLY:HA3	1.90	0.71
1:B:26:ASP:OD2	2:B:570:HOH:O	2.09	0.70
1:B:270:GLU:HB2	1:B:273:ASN:ND2	2.08	0.69
1:A:260:LYS:HE3	2:A:615:HOH:O	1.93	0.68
1:A:89[B]:ILE:HD11	2:A:650:HOH:O	1.93	0.67
1:A:260:LYS:HD2	2:A:561:HOH:O	1.94	0.67
1:B:155:LYS:HE2	1:B:157:ILE:HD11	1.78	0.66
1:A:287:SER:HB3	1:A:290[A]:ILE:CD1	2.28	0.63
1:A:260:LYS:HE2	2:A:633:HOH:O	1.99	0.63
1:A:287:SER:HB3	1:A:290[A]:ILE:HD11	1.81	0.62
1:A:270:GLU:HB2	1:A:273:ASN:ND2	2.15	0.62
1:A:270:GLU:HA	1:A:270:GLU:OE1	1.99	0.62
1:A:138[A]:ILE:HG23	1:A:157:ILE:HB	1.83	0.61
1:A:260:LYS:HG3	2:A:551:HOH:O	2.01	0.60
1:B:299:ILE:HG22	1:B:300:ASN:N	2.19	0.58
1:A:199[A]:ILE:HD13	1:A:225:LEU:HB3	1.88	0.55
1:A:298:ASN:HB3	2:B:501:HOH:O	2.07	0.55
1:A:237:VAL:HG22	2:A:519:HOH:O	2.05	0.54
1:A:298:ASN:ND2	2:A:622:HOH:O	2.19	0.54
1:A:194:ASN:CA	1:A:218:ARG:HE	2.20	0.52
1:A:155:LYS:HE3	1:A:199[A]:ILE:HG21	1.91	0.52
1:A:7:SER:HB3	1:A:36:TRP:CZ3	2.46	0.51
1:B:6:GLY:O	1:B:37[B]:HIS:HD2	1.94	0.50
1:A:218:ARG:O	2:A:571:HOH:O	2.19	0.50
1:A:270:GLU:HG2	1:A:273:ASN:HD22	1.78	0.48
1:B:250:ASP:OD1	1:B:276:LYS:HD3	2.13	0.48
1:A:284:LYS:HG2	1:B:300:ASN:OD1	2.14	0.47
1:A:138[A]:ILE:CD1	1:A:157:ILE:HD12	2.40	0.47
1:B:252:GLN:CG	2:B:562:HOH:O	2.45	0.47
1:A:243:LYS:HE2	1:A:245:VAL:CG2	2.44	0.47
1:B:299:ILE:CG2	1:B:300:ASN:N	2.77	0.47
1:B:126:LEU:HD23	1:B:126:LEU:HA	1.66	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:LYS:CE	2:A:615:HOH:O	2.60	0.46
1:B:98:VAL:O	1:B:145:ALA:HA	2.14	0.46
1:A:218:ARG:HB2	1:A:220:GLN:HG3	1.98	0.45
1:B:7:SER:HB3	1:B:36:TRP:CZ3	2.52	0.45
1:A:217:GLY:C	1:A:218:ARG:NH1	2.70	0.44
1:A:194:ASN:HA	1:A:218:ARG:NE	2.24	0.43
1:A:104:THR:HA	1:A:152:ASN:O	2.19	0.43
1:A:237:VAL:O	1:A:237:VAL:HG23	2.17	0.43
1:A:287:SER:HB3	1:A:290[A]:ILE:HD13	2.00	0.42
1:A:2:ASP:HB3	1:A:45:LYS:HE3	2.01	0.42
1:A:260:LYS:HD2	2:A:551:HOH:O	2.20	0.42
1:A:284:LYS:HB2	1:A:284:LYS:HE2	1.70	0.42
1:B:11:VAL:O	1:B:32[A]:THR:HG23	2.20	0.41
1:A:98:VAL:O	1:A:145:ALA:HA	2.21	0.41
1:A:73:LYS:HE3	1:A:73:LYS:HB3	1.78	0.41
1:B:260:LYS:HG3	2:B:538:HOH:O	2.20	0.41
1:B:278:THR:HA	1:B:300:ASN:O	2.21	0.40
1:B:247:SER:HA	1:B:268:THR:O	2.21	0.40
1:B:255:ASN:H	1:B:255:ASN:HD22	1.69	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	307/307 (100%)	301 (98%)	6 (2%)	0	100	100
1	B	275/307 (90%)	267 (97%)	8 (3%)	0	100	100
All	All	582/614 (95%)	568 (98%)	14 (2%)	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	264/259 (102%)	260 (98%)	4 (2%)	72	44
1	B	245/259 (95%)	241 (98%)	4 (2%)	70	41
All	All	509/518 (98%)	501 (98%)	8 (2%)	68	41

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	185	SER
1	A	218	ARG
1	A	222	LEU
1	A	239	ASN
1	B	5	GLN
1	B	142	LYS
1	B	255	ASN
1	B	270	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	152	ASN
1	A	239	ASN
1	A	273	ASN
1	A	291	ASN
1	A	300	ASN
1	B	15	ASN
1	B	152	ASN
1	B	255	ASN
1	B	273	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	296/307 (96%)	0.36	20 (6%) 20 20	9, 15, 35, 55	0
1	B	274/307 (89%)	0.16	13 (4%) 35 36	12, 20, 35, 47	0
All	All	570/614 (92%)	0.26	33 (5%) 26 28	9, 18, 35, 55	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	219	ASN	9.1
1	B	271	PRO	6.2
1	A	182	LEU	5.6
1	A	183	SER	5.0
1	A	131	VAL	5.0
1	B	237	VAL	4.7
1	B	222	LEU	4.4
1	B	126	LEU	4.4
1	A	221	ALA	4.3
1	B	238	SER	4.1
1	B	221	ALA	4.0
1	B	270	GLU	3.9
1	A	132	VAL	3.7
1	B	239	ASN	3.3
1	A	301	GLY	3.3
1	A	270	GLU	3.0
1	A	115	GLY	3.0
1	B	240	LYS	3.0
1	B	135	GLY	2.8
1	A	117	GLY	2.7
1	A	237	VAL	2.7
1	B	191	LEU	2.7
1	A	271	PRO	2.6
1	A	220	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	167	ASN	2.5
1	A	184	ASP	2.5
1	A	194	ASN	2.5
1	B	167	ASN	2.3
1	A	114	ASN	2.2
1	A	239	ASN	2.2
1	B	301	GLY	2.1
1	A	116	ASN	2.1
1	A	218	ARG	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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.