



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:31 PM UTC

PDB ID : 4MGF / pdb_00004mgf
Title : Crystal structure of apo-PhuS, a heme-binding protein from *Pseudomonas aeruginosa*
Authors : Lee, M.J.Y.; Jia, Z.; Montreal-Kingston Bacterial Structural Genomics Initiative (BSGI)
Deposited on : 2013-08-28
Resolution : 2.00 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
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

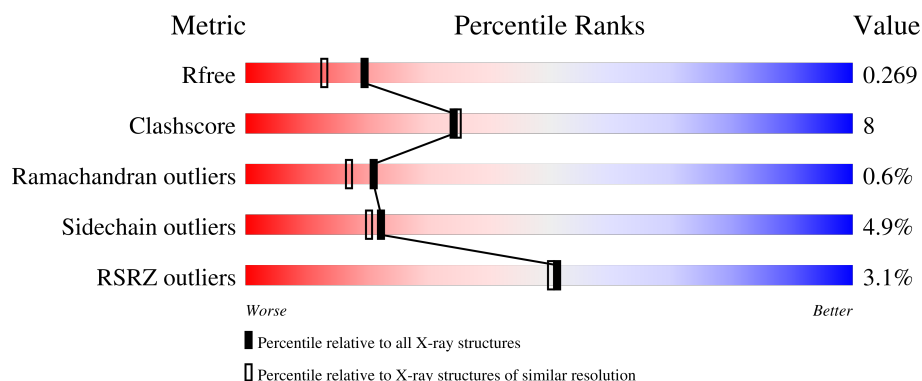
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	360	2% 78% 16% • 5%
1	B	360	4% 80% 12% •• 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5847 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 Hemin degrading factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	0	0
			2676	1696	486	488	6			
1	B	341	Total	C	N	O	S	0	0	0
			2669	1691	488	484	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP O68880
A	-4	HIS	-	expression tag	UNP O68880
A	-3	HIS	-	expression tag	UNP O68880
A	-2	HIS	-	expression tag	UNP O68880
A	-1	HIS	-	expression tag	UNP O68880
A	0	HIS	-	expression tag	UNP O68880
B	-5	HIS	-	expression tag	UNP O68880
B	-4	HIS	-	expression tag	UNP O68880
B	-3	HIS	-	expression tag	UNP O68880
B	-2	HIS	-	expression tag	UNP O68880
B	-1	HIS	-	expression tag	UNP O68880
B	0	HIS	-	expression tag	UNP O68880

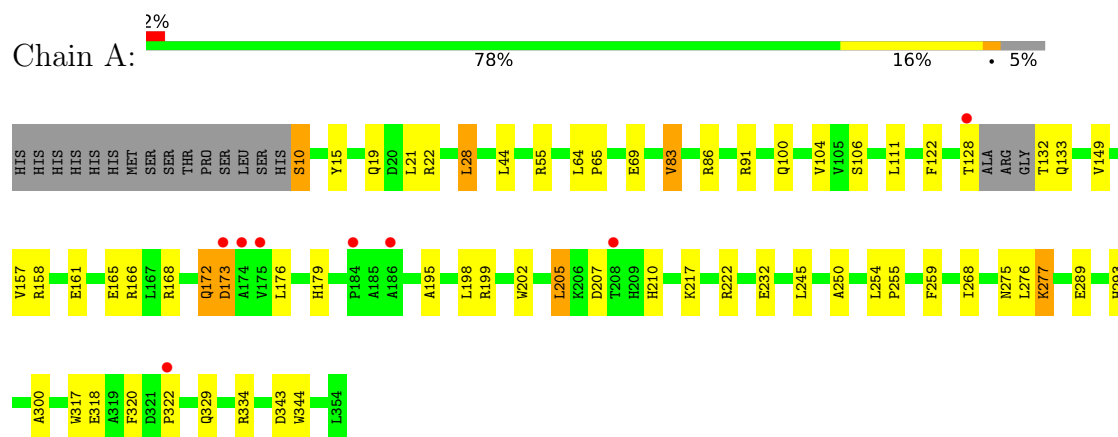
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	249	Total	O	0	0
			249	249		
2	B	253	Total	O	0	0
			253	253		

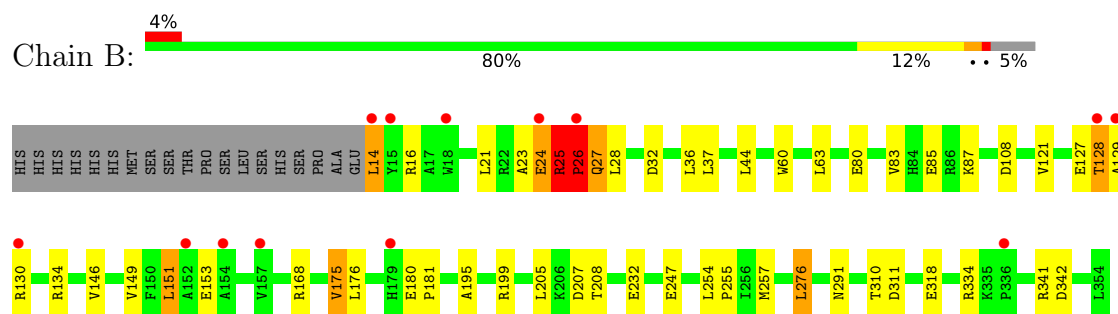
3 Residue-property plots

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: Hemin degrading factor



- Molecule 1: Hemin degrading factor



4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	186.50Å 186.50Å 41.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.70 – 2.00 41.70 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.0 (41.70-2.00) 99.0 (41.70-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.208 , 0.266 0.211 , 0.269	Depositor DCC
R_{free} test set	2445 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	27.7	Xtriage
Anisotropy	0.626	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.017 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5847	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.49% 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](#)

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	0.48	0/2738	0.81	1/3724 (0.0%)
1	B	0.56	2/2731 (0.1%)	0.88	8/3714 (0.2%)
All	All	0.52	2/5469 (0.0%)	0.84	9/7438 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	24	GLU	C-O	-5.10	1.18	1.24
1	B	25	ARG	CA-C	5.09	1.59	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	27	GLN	N-CA-C	-7.54	103.01	114.16
1	B	24	GLU	N-CA-C	7.32	118.90	111.07
1	B	25	ARG	N-CA-C	6.01	123.10	109.81
1	B	26	PRO	CA-N-CD	-5.91	103.73	112.00
1	B	146	VAL	N-CA-C	-5.59	106.75	111.56
1	A	268	ILE	CB-CA-C	-5.48	102.33	110.33
1	B	175	VAL	N-CA-C	5.46	116.85	111.67
1	B	25	ARG	CA-C-N	-5.12	113.44	119.84
1	B	25	ARG	C-N-CA	-5.12	113.44	119.84

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	2676	0	2639	44	0
1	B	2669	0	2638	37	0
2	A	249	0	0	19	0
2	B	253	0	0	14	0
All	All	5847	0	5277	81	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 8.

All (81) 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:B:26:PRO:HD2	1:B:28:LEU:HB2	1.56	0.86
1:B:207:ASP:OD1	2:B:645:HOH:O	1.92	0.85
1:A:161:GLU:OE1	2:A:634:HOH:O	1.99	0.81
1:A:166:ARG:NH1	2:A:565:HOH:O	2.13	0.81
1:A:21:LEU:HD21	1:A:28:LEU:HD23	1.65	0.79
1:B:199:ARG:NH2	1:B:232:GLU:OE1	2.15	0.79
1:A:168:ARG:HD2	2:A:532:HOH:O	1.85	0.75
1:B:342:ASP:OD1	2:B:626:HOH:O	2.05	0.74
1:A:199:ARG:NH2	1:A:232:GLU:OE2	2.21	0.73
1:B:27:GLN:OE1	2:B:643:HOH:O	2.07	0.72
1:A:10:SER:N	2:A:450:HOH:O	2.27	0.68
1:B:318:GLU:OE2	2:B:445:HOH:O	2.11	0.67
1:B:87:LYS:NZ	2:B:534:HOH:O	2.28	0.66
1:B:232:GLU:OE2	2:B:617:HOH:O	2.14	0.66
1:A:173:ASP:OD1	2:A:542:HOH:O	2.14	0.65
1:A:83:VAL:HG13	1:A:293:HIS:HB2	1.79	0.65
1:B:25:ARG:NE	1:B:25:ARG:O	2.32	0.62
1:A:158:ARG:NE	2:A:639:HOH:O	2.26	0.62
1:A:172:GLN:HG3	2:A:628:HOH:O	1.99	0.61
1:A:55:ARG:NH1	2:A:558:HOH:O	2.32	0.61
1:B:128:THR:O	1:B:130:ARG:N	2.24	0.60
1:A:277:LYS:HG2	2:B:469:HOH:O	2.03	0.59
1:B:181:PRO:O	2:B:509:HOH:O	2.16	0.59
1:A:217:LYS:NZ	2:A:647:HOH:O	2.19	0.59
1:A:195:ALA:O	1:A:199:ARG:HG3	2.03	0.58
1:B:24:GLU:OE2	1:B:37:LEU:HD11	2.03	0.58
1:A:100:GLN:NE2	2:A:619:HOH:O	2.29	0.56
1:B:257:MET:HE1	2:B:556:HOH:O	2.06	0.55
1:B:175:VAL:HG13	1:B:176:LEU:N	2.23	0.54
1:B:23:ALA:HB3	2:B:552:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:ASP:OD2	1:A:344:TRP:N	2.41	0.54
1:B:26:PRO:CD	1:B:28:LEU:HB2	2.35	0.53
1:A:318:GLU:OE2	2:A:574:HOH:O	2.19	0.53
1:A:161:GLU:HB3	2:A:634:HOH:O	2.08	0.53
1:B:14:LEU:HD22	1:B:16:ARG:HB2	1.90	0.53
1:A:254:LEU:HD12	1:A:255:PRO:HD2	1.91	0.52
1:B:180:GLU:HG3	1:B:181:PRO:HD2	1.91	0.51
1:A:86:ARG:HD2	1:A:289:GLU:O	2.10	0.51
1:A:259:PHE:HB2	1:A:329:GLN:HB2	1.93	0.50
1:B:195:ALA:O	1:B:199:ARG:HG3	2.12	0.50
1:B:134:ARG:HB2	1:B:151:LEU:HG	1.93	0.50
1:A:277:LYS:NZ	2:A:485:HOH:O	2.42	0.49
1:A:173:ASP:CG	2:A:542:HOH:O	2.53	0.49
1:A:245:LEU:HD22	1:A:317:TRP:CE3	2.48	0.49
1:B:28:LEU:HD21	1:B:36:LEU:HD12	1.93	0.49
1:B:28:LEU:HG	1:B:32:ASP:HB2	1.94	0.48
1:A:207:ASP:OD2	1:A:210:HIS:NE2	2.45	0.48
1:B:108:ASP:HB2	2:B:468:HOH:O	2.13	0.48
1:A:91:ARG:O	1:A:106:SER:HB3	2.14	0.48
1:B:26:PRO:HD2	1:B:28:LEU:H	1.79	0.47
1:A:276:LEU:C	1:A:277:LYS:HD2	2.40	0.47
1:B:127:GLU:O	1:B:128:THR:C	2.56	0.46
1:B:60:TRP:NE1	2:B:537:HOH:O	2.03	0.46
1:A:55:ARG:HG3	1:A:122:PHE:CE2	2.50	0.46
1:B:334:ARG:NH2	2:B:648:HOH:O	2.14	0.45
1:A:222:ARG:HG2	1:A:320:PHE:HE2	1.80	0.45
1:B:153:GLU:H	1:B:153:GLU:CD	2.24	0.45
1:B:255:PRO:HG2	1:B:341:ARG:HH12	1.81	0.45
1:B:254:LEU:HD12	1:B:255:PRO:HD2	1.99	0.45
1:B:80:GLU:OE1	2:B:624:HOH:O	2.21	0.44
1:A:15:TYR:O	1:A:19:GLN:HG2	2.18	0.44
1:A:202:TRP:HA	1:A:205:LEU:HD22	1.98	0.44
1:A:334:ARG:NH2	2:A:516:HOH:O	2.50	0.44
1:A:275:ASN:ND2	2:A:464:HOH:O	2.38	0.44
1:A:199:ARG:HD3	2:A:590:HOH:O	2.17	0.43
1:B:85:GLU:HB2	1:B:291:ASN:HB2	2.00	0.43
1:A:250:ALA:HB2	1:A:276:LEU:HD21	2.00	0.43
1:A:165:GLU:HA	1:A:168:ARG:HG3	2.01	0.43
1:A:254:LEU:HD21	1:A:344:TRP:HA	2.00	0.43
1:A:28:LEU:HA	1:A:28:LEU:HD12	1.72	0.42
1:A:133:GLN:HA	2:A:602:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:LEU:HB2	1:A:65:PRO:HD3	2.01	0.42
1:A:222:ARG:HG2	1:A:320:PHE:CE2	2.53	0.42
1:A:104:VAL:HB	1:A:111:LEU:HB2	2.02	0.42
1:B:247:GLU:HA	1:B:276:LEU:HD23	2.01	0.42
1:A:300:ALA:HB2	1:A:322:PRO:HG3	2.01	0.42
1:B:128:THR:C	1:B:130:ARG:H	2.20	0.42
1:A:22:ARG:NH1	2:A:635:HOH:O	2.51	0.41
1:B:310:THR:HG23	1:B:311:ASP:OD1	2.20	0.41
1:B:25:ARG:O	1:B:25:ARG:CD	2.69	0.40
1:B:21:LEU:HB2	1:B:44:LEU:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	338/360 (94%)	324 (96%)	12 (4%)	2 (1%)	21	17
1	B	339/360 (94%)	317 (94%)	20 (6%)	2 (1%)	21	17
All	All	677/720 (94%)	641 (95%)	32 (5%)	4 (1%)	21	17

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	129	ALA
1	A	173	ASP
1	B	26	PRO
1	A	176	LEU

5.3.2 Protein sidechains ⓘ

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	269/285 (94%)	255 (95%)	14 (5%)	21	18
1	B	267/285 (94%)	255 (96%)	12 (4%)	24	23
All	All	536/570 (94%)	510 (95%)	26 (5%)	22	20

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

Mol	Chain	Res	Type
1	A	10	SER
1	A	28	LEU
1	A	44	LEU
1	A	69	GLU
1	A	83	VAL
1	A	128	THR
1	A	132	THR
1	A	149	VAL
1	A	157	VAL
1	A	172	GLN
1	A	179	HIS
1	A	198	LEU
1	A	205	LEU
1	A	277	LYS
1	B	14	LEU
1	B	25	ARG
1	B	63	LEU
1	B	83	VAL
1	B	121	VAL
1	B	128	THR
1	B	149	VAL
1	B	151	LEU
1	B	168	ARG
1	B	205	LEU
1	B	208	THR
1	B	276	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	133	GLN
1	B	133	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 oligosaccharides 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	342/360 (95%)	-0.11	8 (2%) 61 60	8, 22, 44, 69	0
1	B	341/360 (94%)	0.06	13 (3%) 44 43	8, 22, 45, 67	0
All	All	683/720 (94%)	-0.02	21 (3%) 51 50	8, 22, 44, 69	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	129	ALA	3.9
1	B	14	LEU	3.8
1	B	15	TYR	3.4
1	B	128	THR	3.2
1	B	26	PRO	3.1
1	A	174	ALA	2.9
1	B	24	GLU	2.9
1	A	322	PRO	2.8
1	A	173	ASP	2.7
1	A	186	ALA	2.7
1	A	184	PRO	2.6
1	A	128	THR	2.6
1	A	175	VAL	2.6
1	A	208	THR	2.5
1	B	18	TRP	2.4
1	B	152	ALA	2.3
1	B	157	VAL	2.3
1	B	336	PRO	2.2
1	B	130	ARG	2.2
1	B	179	HIS	2.1
1	B	154	ALA	2.1

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.