



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:48 PM UTC

PDB ID : 5OFP / pdb_00005ofp
Title : Structure of the antibacterial peptide ABC transporter McjD in an apo inward occluded conformation
Authors : Beis, K.; Choudhury, H.G.
Deposited on : 2017-07-11
Resolution : 4.71 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

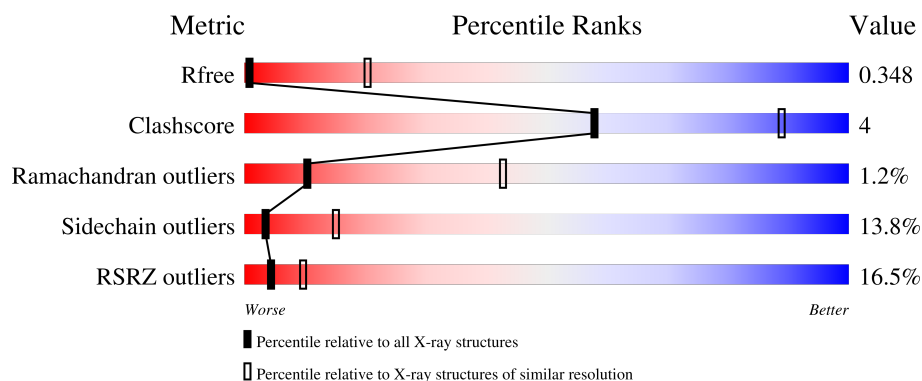
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.71 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	1011 (5.50-3.94)
Clashscore	190562	1009 (5.48-3.96)
Ramachandran outliers	187476	1098 (5.54-3.90)
Sidechain outliers	187428	1079 (5.54-3.90)
RSRZ outliers	180081	1006 (5.50-3.94)

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	580	16% 73% 23% ..

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 4527 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.

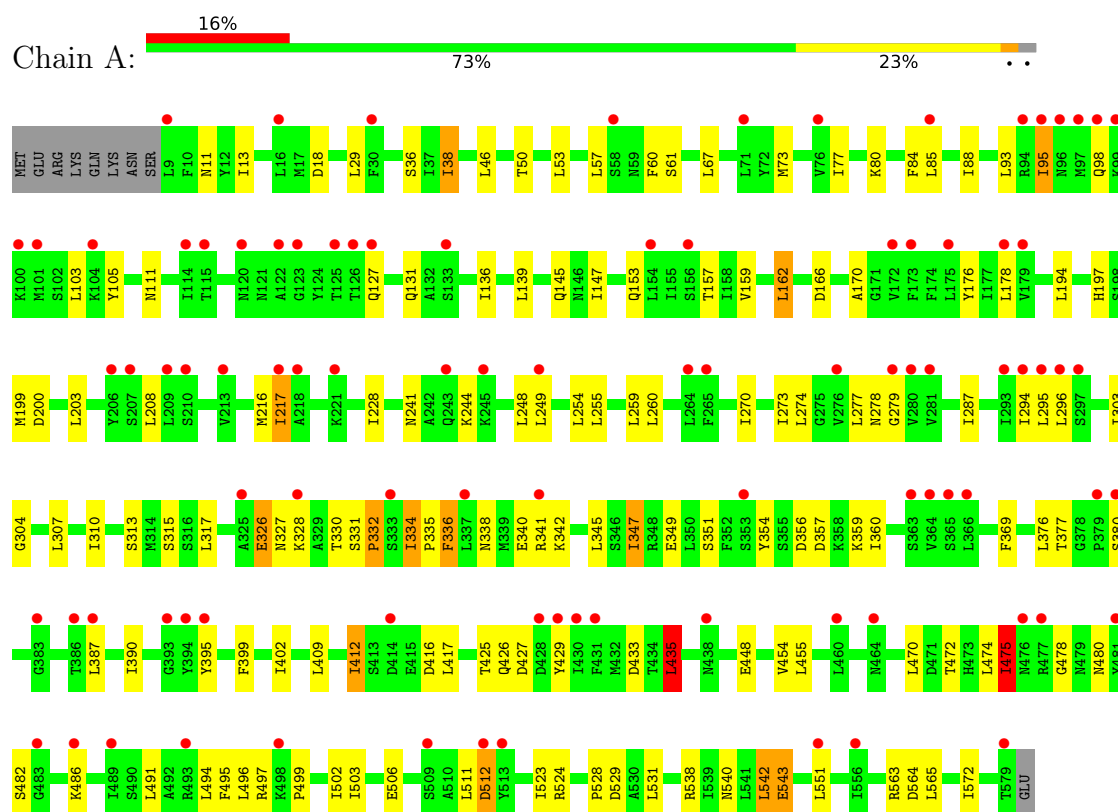
- Molecule 1 is a protein called Microcin-J25 export ATP-binding/permease protein McjD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	571	Total	C	N	O	S	0	0	0
			4527	2920	739	850	18			

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: Microcin-J25 export ATP-binding/permease protein McjD



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 2 2	Depositor
Cell constants a, b, c, α , β , γ	87.85Å 87.85Å 351.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.06 – 4.71 30.06 – 4.71	Depositor EDS
% Data completeness (in resolution range)	98.3 (30.06-4.71) 97.7 (30.06-4.71)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 4.65Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.313 , 0.334 0.361 , 0.348	Depositor DCC
R_{free} test set	376 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	228.3	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 88.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	4527	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% 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

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	0.89	2/4603 (0.0%)	1.41	28/6234 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	334	ILE	CA-C	5.01	1.58	1.52
1	A	326	GLU	CA-C	5.00	1.59	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	369	PHE	CA-C-N	6.75	130.74	120.82
1	A	369	PHE	C-N-CA	6.75	130.74	120.82
1	A	88	ILE	N-CA-C	-6.62	106.12	111.81
1	A	512	ASP	CA-C-N	6.12	128.76	120.38
1	A	512	ASP	C-N-CA	6.12	128.76	120.38
1	A	435	LEU	CA-C-N	5.92	128.48	120.38
1	A	435	LEU	C-N-CA	5.92	128.48	120.38
1	A	166	ASP	CA-C-N	5.77	128.28	120.38
1	A	166	ASP	C-N-CA	5.77	128.28	120.38
1	A	538	ARG	CA-C-N	5.67	128.23	120.46
1	A	538	ARG	C-N-CA	5.67	128.23	120.46
1	A	356	ASP	CA-C-N	5.62	128.58	120.38
1	A	356	ASP	C-N-CA	5.62	128.58	120.38
1	A	18	ASP	CA-CB-CG	5.42	118.02	112.60
1	A	98	GLN	CA-C-N	5.37	127.73	120.65
1	A	98	GLN	C-N-CA	5.37	127.73	120.65
1	A	482	SER	CA-C-N	5.28	125.84	119.98
1	A	482	SER	C-N-CA	5.28	125.84	119.98
1	A	359	LYS	CA-C-N	5.24	127.16	120.56
1	A	359	LYS	C-N-CA	5.24	127.16	120.56
1	A	336	PHE	CA-CB-CG	5.23	119.03	113.80
1	A	336	PHE	CA-C-N	5.20	131.47	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	336	PHE	C-N-CA	5.20	131.47	121.54
1	A	529	ASP	CA-CB-CG	5.18	117.78	112.60
1	A	475	ILE	CA-C-N	5.17	128.19	120.90
1	A	475	ILE	C-N-CA	5.17	128.19	120.90
1	A	95	ILE	CA-C-N	5.03	127.02	120.28
1	A	95	ILE	C-N-CA	5.03	127.02	120.28

There are no chirality outliers.

There are no planarity outliers.

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	4527	0	4639	41	0
All	All	4527	0	4639	41	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 4.

All (41) 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:475:ILE:H	1:A:480:ASN:HB2	1.58	0.68
1:A:200:ASP:HA	1:A:203:LEU:HD12	1.80	0.62
1:A:50:THR:HG21	1:A:287:ILE:HG13	1.82	0.62
1:A:334:ILE:N	1:A:335:PRO:HD2	2.16	0.59
1:A:216:MET:HE1	1:A:228:ILE:HG21	1.86	0.58
1:A:347:ILE:HG12	1:A:402:ILE:HG23	1.86	0.57
1:A:326:GLU:HB3	1:A:327:ASN:HA	1.87	0.56
1:A:304:GLY:HA2	1:A:307:LEU:HD12	1.90	0.53
1:A:454:VAL:HG13	1:A:495:PHE:HB2	1.91	0.53
1:A:478:GLY:HA3	1:A:486:LYS:HD3	1.90	0.52
1:A:13:ILE:HG12	1:A:136:ILE:HG12	1.91	0.51
1:A:435:LEU:HD13	1:A:472:THR:HB	1.93	0.50
1:A:409:LEU:HA	1:A:412:ILE:HD12	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:THR:HG21	1:A:542:LEU:HD21	1.93	0.50
1:A:331:SER:N	1:A:332:PRO:HD3	2.27	0.49
1:A:157:THR:HG21	1:A:296:LEU:HD21	1.95	0.49
1:A:36:SER:HB2	1:A:153:GLN:HG3	1.95	0.48
1:A:351:SER:HB2	1:A:399:PHE:HB2	1.96	0.48
1:A:131:GLN:HG2	1:A:199:MET:HE2	1.96	0.47
1:A:73:MET:HG3	1:A:77:ILE:HD11	1.97	0.47
1:A:127:GLN:HG3	1:A:131:GLN:HE21	1.79	0.47
1:A:341:ARG:HA	1:A:341:ARG:HD3	1.75	0.45
1:A:565:LEU:HB3	1:A:572:ILE:HG13	1.99	0.44
1:A:57:LEU:HA	1:A:61:SER:HB3	2.00	0.44
1:A:270:ILE:O	1:A:274:LEU:HG	2.18	0.44
1:A:354:TYR:HD2	1:A:360:ILE:HG12	1.83	0.44
1:A:162:LEU:HD12	1:A:170:ALA:HB1	2.00	0.43
1:A:217:ILE:H	1:A:217:ILE:HG13	1.65	0.43
1:A:103:LEU:C	1:A:105:TYR:H	2.27	0.43
1:A:176:TYR:HE1	1:A:260:LEU:HB3	1.84	0.43
1:A:494:LEU:HD21	1:A:523:ILE:HG12	1.99	0.43
1:A:543:GLU:HG2	1:A:563:ARG:HH21	1.83	0.42
1:A:565:LEU:HD22	1:A:572:ILE:HG13	2.01	0.42
1:A:80:LYS:HG2	1:A:84:PHE:HE2	1.85	0.42
1:A:499:PRO:HG2	1:A:502:ILE:HG12	2.02	0.41
1:A:38:ILE:H	1:A:38:ILE:HG13	1.50	0.41
1:A:131:GLN:HE22	1:A:203:LEU:HG	1.85	0.41
1:A:334:ILE:N	1:A:335:PRO:CD	2.83	0.41
1:A:335:PRO:HA	1:A:336:PHE:HA	1.60	0.41
1:A:241:ASN:HA	1:A:244:LYS:HD2	2.03	0.40
1:A:313:SER:O	1:A:317:LEU:HB2	2.21	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	569/580 (98%)	509 (90%)	53 (9%)	7 (1%)	10	43

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	332	PRO
1	A	506	GLU
1	A	448	GLU
1	A	278	ASN
1	A	279	GLY
1	A	145	GLN
1	A	528	PRO

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	520/529 (98%)	448 (86%)	72 (14%)	3	15

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	29	LEU
1	A	38	ILE
1	A	46	LEU
1	A	53	LEU
1	A	60	PHE
1	A	67	LEU
1	A	85	LEU
1	A	93	LEU
1	A	95	ILE
1	A	111	ASN
1	A	139	LEU
1	A	147	ILE
1	A	159	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	162	LEU
1	A	178	LEU
1	A	194	LEU
1	A	197	HIS
1	A	208	LEU
1	A	217	ILE
1	A	248	LEU
1	A	249	LEU
1	A	254	LEU
1	A	255	LEU
1	A	259	LEU
1	A	273	ILE
1	A	277	LEU
1	A	294	ILE
1	A	295	LEU
1	A	303	ILE
1	A	310	ILE
1	A	315	SER
1	A	328	LYS
1	A	330	THR
1	A	338	ASN
1	A	340	GLU
1	A	342	LYS
1	A	345	LEU
1	A	347	ILE
1	A	349	GLU
1	A	357	ASP
1	A	376	LEU
1	A	380	SER
1	A	387	LEU
1	A	390	ILE
1	A	395	TYR
1	A	412	ILE
1	A	416	ASP
1	A	417	LEU
1	A	425	THR
1	A	426	GLN
1	A	427	ASP
1	A	429	TYR
1	A	433	ASP
1	A	435	LEU
1	A	455	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	470	LEU
1	A	474	LEU
1	A	475	ILE
1	A	491	LEU
1	A	496	LEU
1	A	497	ARG
1	A	503	ILE
1	A	511	LEU
1	A	512	ASP
1	A	524	ARG
1	A	531	LEU
1	A	540	ASN
1	A	542	LEU
1	A	543	GLU
1	A	551	LEU
1	A	564	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	113	ASN
1	A	120	ASN
1	A	127	GLN
1	A	131	GLN
1	A	134	ASN
1	A	145	GLN
1	A	197	HIS
1	A	223	ASN
1	A	241	ASN
1	A	302	ASN
1	A	338	ASN
1	A	344	ASN
1	A	397	ASN
1	A	476	ASN
1	A	479	ASN
1	A	485	GLN

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](#)

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	571/580 (98%)	0.82	94 (16%) 4 10	24, 94, 127, 165	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	430	ILE	15.4
1	A	94	ARG	12.1
1	A	98	GLN	7.7
1	A	294	ILE	7.6
1	A	394	TYR	7.3
1	A	395	TYR	6.2
1	A	114	ILE	6.1
1	A	556	ILE	5.7
1	A	431	PHE	5.7
1	A	95	ILE	5.6
1	A	364	VAL	5.6
1	A	489	ILE	5.4
1	A	477	ARG	5.2
1	A	126	THR	5.1
1	A	429	TYR	5.1
1	A	279	GLY	5.0
1	A	178	LEU	4.7
1	A	551	LEU	4.6
1	A	97	MET	4.5
1	A	295	LEU	4.5
1	A	217	ILE	4.4
1	A	175	LEU	4.4
1	A	101	MET	4.4
1	A	296	LEU	4.3
1	A	221	LYS	4.2
1	A	265	PHE	4.1
1	A	280	VAL	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	393	GLY	4.0
1	A	513	TYR	3.9
1	A	133	SER	3.8
1	A	481	TYR	3.8
1	A	333	SER	3.8
1	A	366	LEU	3.7
1	A	414	ASP	3.7
1	A	100	LYS	3.7
1	A	365	SER	3.6
1	A	509	SER	3.6
1	A	264	LEU	3.5
1	A	154	LEU	3.5
1	A	173	PHE	3.5
1	A	337	LEU	3.5
1	A	493	ARG	3.4
1	A	476	ASN	3.4
1	A	293	ILE	3.4
1	A	115	THR	3.3
1	A	218	ALA	3.3
1	A	209	LEU	3.3
1	A	213	VAL	3.2
1	A	96	ASN	3.2
1	A	58	SER	3.1
1	A	127	GLN	3.1
1	A	353	SER	3.1
1	A	438	ASN	3.1
1	A	156	SER	3.0
1	A	281	VAL	3.0
1	A	297	SER	3.0
1	A	85	LEU	3.0
1	A	9	LEU	2.9
1	A	464	ASN	2.9
1	A	122	ALA	2.9
1	A	325	ALA	2.8
1	A	363	SER	2.8
1	A	99	LYS	2.8
1	A	341	ARG	2.7
1	A	379	PRO	2.6
1	A	71	LEU	2.6
1	A	172	VAL	2.6
1	A	104	LYS	2.6
1	A	460	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	380	SER	2.5
1	A	483	GLY	2.5
1	A	125	THR	2.5
1	A	123	GLY	2.4
1	A	249	LEU	2.4
1	A	245	LYS	2.4
1	A	276	VAL	2.4
1	A	498	LYS	2.3
1	A	243	GLN	2.3
1	A	386	THR	2.3
1	A	206	TYR	2.3
1	A	30	PHE	2.2
1	A	16	LEU	2.2
1	A	579	THR	2.2
1	A	383	GLY	2.2
1	A	179	VAL	2.2
1	A	76	VAL	2.1
1	A	486	LYS	2.1
1	A	512	ASP	2.1
1	A	120	ASN	2.1
1	A	207	SER	2.1
1	A	428	ASP	2.1
1	A	387	LEU	2.1
1	A	328	LYS	2.0
1	A	210	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 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.