



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2017 – 02:10 PM EDT

PDB ID : 2NS7
Title : How an in vitro selected peptide mimics the antibiotic tetracycline to induce TET repressor
Authors : Luckner, S.R.; Klotzsche, M.; Berens, C.; Hillen, W.; Muller, Y.A.
Deposited on : unknown
Resolution : 2.40 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030345

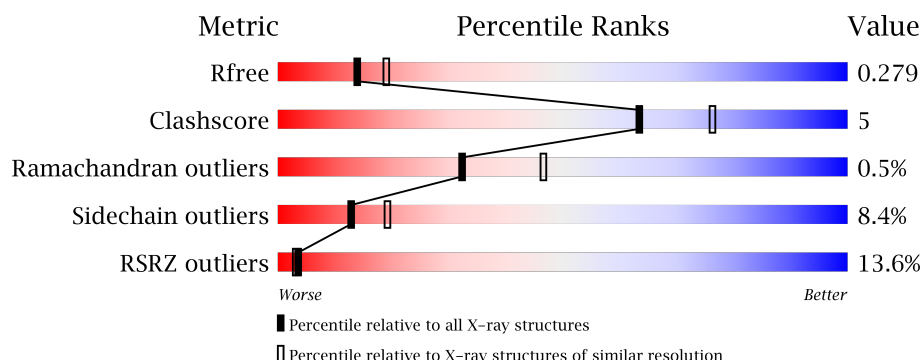
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


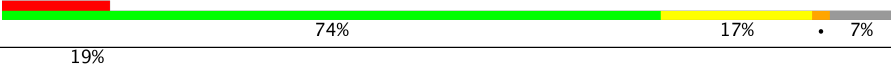


The reported resolution of this entry is 2.40 Å.

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}	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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	208	
1	B	208	
1	C	208	
1	D	208	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6027 atoms, of which 0 are hydrogens and 0 are deuteriums.

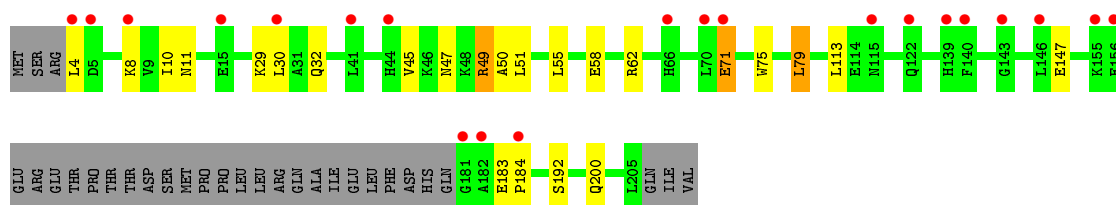
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tetracycline repressor protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	196	Total	C	N	O	S	0	0	0
			1558	987	276	293	2			
1	B	194	Total	C	N	O	S	0	0	0
			1546	980	276	288	2			
1	C	190	Total	C	N	O	S	0	0	0
			1511	957	268	284	2			
1	D	178	Total	C	N	O	S	0	0	0
			1412	896	250	265	1			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	68	SER	CYS	ENGINEERED	UNP P04483
A	88	ASN	CYS	ENGINEERED	UNP P04483
A	121	THR	CYS	ENGINEERED	UNP P04483
A	144	SER	CYS	ENGINEERED	UNP P04483
B	68	SER	CYS	ENGINEERED	UNP P04483
B	88	ASN	CYS	ENGINEERED	UNP P04483
B	121	THR	CYS	ENGINEERED	UNP P04483
B	144	SER	CYS	ENGINEERED	UNP P04483
C	68	SER	CYS	ENGINEERED	UNP P04483
C	88	ASN	CYS	ENGINEERED	UNP P04483
C	121	THR	CYS	ENGINEERED	UNP P04483
C	144	SER	CYS	ENGINEERED	UNP P04483
D	68	SER	CYS	ENGINEERED	UNP P04483
D	88	ASN	CYS	ENGINEERED	UNP P04483
D	121	THR	CYS	ENGINEERED	UNP P04483
D	144	SER	CYS	ENGINEERED	UNP P04483



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	107.91Å 107.91Å 303.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.04 – 2.40 37.05 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (37.04-2.40) 98.5 (37.05-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.90 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.230 , 0.277 0.237 , 0.279	Depositor DCC
R_{free} test set	3302 reflections (8.70%)	DCC
Wilson B-factor (Å ²)	52.6	Xtriage
Anisotropy	0.540	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 82.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6027	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.60 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.2720e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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	0.52	0/1588	0.63	0/2147
1	B	0.65	1/1576 (0.1%)	0.68	0/2129
1	C	0.61	2/1541 (0.1%)	0.59	1/2084 (0.0%)
1	D	0.46	0/1438	0.57	0/1942
All	All	0.57	3/6143 (0.0%)	0.62	1/8302 (0.0%)

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	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	128	GLU	CD-OE1	14.10	1.41	1.25
1	B	37	GLU	CD-OE2	13.57	1.40	1.25
1	C	128	GLU	CD-OE2	8.06	1.34	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	128	GLU	OE1-CD-OE2	5.48	129.88	123.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	35	GLY	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	1558	0	1548	21	0
1	B	1546	0	1539	17	0
1	C	1511	0	1496	14	0
1	D	1412	0	1407	15	0
All	All	6027	0	5990	59	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 5.

All (59) 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:D:29:LYS:HA	1:D:32:GLN:HE21	1.52	0.75
1:A:16:LEU:O	1:A:20:VAL:HG22	1.95	0.67
1:A:180:GLN:OE1	1:B:132:TYR:OH	2.14	0.66
1:A:97:ALA:H	1:A:149:GLN:HE22	1.47	0.63
1:A:177:PHE:CD2	1:B:131:LEU:HD11	2.35	0.62
1:D:11:ASN:ND2	1:D:62:ARG:HH22	1.97	0.62
1:D:45:VAL:HG11	1:D:51:LEU:HB2	1.83	0.59
1:D:47:ASN:HD22	1:D:49:ARG:H	1.51	0.58
1:A:67:PHE:HA	1:A:82:ASN:ND2	2.17	0.58
1:C:21:GLY:HA2	1:C:94:ARG:HD2	1.89	0.54
1:B:49:ARG:O	1:B:49:ARG:HD3	2.08	0.54
1:C:139:HIS:NE2	1:D:147:GLU:OE1	2.30	0.53
1:C:166:MET:CE	1:C:171:ARG:HA	2.39	0.52
1:B:14:LEU:HG	1:B:93:HIS:CE1	2.44	0.52
1:C:64:HIS:NE2	1:C:82:ASN:ND2	2.57	0.52
1:D:10:ILE:HG21	1:D:58:GLU:HG2	1.92	0.51
1:D:11:ASN:ND2	1:D:62:ARG:NH2	2.59	0.50
1:B:75:TRP:HB3	1:B:123:GLN:HG3	1.94	0.49
1:B:178:ASP:OD1	1:B:179:HIS:N	2.45	0.49
1:A:180:GLN:O	1:A:181:GLY:O	2.31	0.49
1:C:80:ARG:HG3	1:C:194:ILE:CD1	2.43	0.48
1:A:180:GLN:HB2	1:A:184:PRO:HG2	1.94	0.48
1:C:64:HIS:CE1	1:C:86:PHE:HB2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:TRP:HB3	1:C:123:GLN:HG3	1.96	0.47
1:D:45:VAL:CG1	1:D:51:LEU:HB2	2.44	0.47
1:B:15:GLU:O	1:B:19:GLU:HG3	2.16	0.46
1:A:104:ARG:NH2	1:B:154:ALA:HB2	2.30	0.46
1:D:183:GLU:N	1:D:184:PRO:CD	2.79	0.46
1:D:47:ASN:ND2	1:D:49:ARG:H	2.14	0.45
1:A:131:LEU:HD11	1:B:177:PHE:CE1	2.52	0.45
1:A:192:SER:OG	1:B:200:GLN:NE2	2.49	0.45
1:A:166:MET:HB2	1:A:167:PRO:CD	2.47	0.45
1:A:70:LEU:O	1:A:73:GLU:CB	2.65	0.45
1:C:196:GLY:HA3	1:D:192:SER:O	2.16	0.45
1:B:24:GLY:O	1:B:29:LYS:HD2	2.17	0.44
1:D:11:ASN:HD22	1:D:62:ARG:HH22	1.66	0.44
1:A:170:LEU:HD13	1:B:113:LEU:HD22	2.00	0.44
1:C:16:LEU:HD23	1:C:25:LEU:HD12	2.00	0.43
1:A:90:LEU:O	1:A:96:GLY:HA3	2.19	0.42
1:B:197:PHE:HA	1:B:200:GLN:HE21	1.84	0.42
1:D:49:ARG:HG2	1:D:50:ALA:N	2.35	0.42
1:A:153:VAL:O	1:A:155:LYS:N	2.52	0.42
1:C:10:ILE:HG22	1:C:14:LEU:HD22	2.01	0.42
1:D:75:TRP:HE3	1:D:79:LEU:HD22	1.83	0.42
1:A:200:GLN:HE22	1:A:206:GLN:HA	1.84	0.42
1:B:10:ILE:HG22	1:B:14:LEU:HD22	2.02	0.42
1:A:126:SER:H	1:A:206:GLN:NE2	2.18	0.42
1:C:69:PRO:HG3	1:C:119:PHE:CG	2.55	0.42
1:C:167:PRO:HD2	1:C:170:LEU:HD23	2.02	0.41
1:D:47:ASN:HD22	1:D:49:ARG:N	2.15	0.41
1:B:112:THR:O	1:B:116:GLN:HG3	2.20	0.41
1:A:146:LEU:O	1:A:150:GLU:HB2	2.20	0.41
1:B:80:ARG:HG3	1:B:194:ILE:HD13	2.02	0.41
1:A:129:ASN:HD22	1:A:206:GLN:NE2	2.18	0.41
1:A:59:MET:HE3	1:A:92:SER:OG	2.20	0.41
1:C:67:PHE:HB2	1:C:112:THR:HG21	2.01	0.41
1:A:14:LEU:HG	1:A:93:HIS:CE1	2.55	0.41
1:B:63:HIS:HB2	1:B:89:ALA:HA	2.02	0.40
1:C:176:LEU:O	1:C:180:GLN:HG2	2.20	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	192/208 (92%)	185 (96%)	4 (2%)	3 (2%)	11	15
1	B	190/208 (91%)	187 (98%)	3 (2%)	0	100	100
1	C	186/208 (89%)	184 (99%)	2 (1%)	0	100	100
1	D	174/208 (84%)	169 (97%)	4 (2%)	1 (1%)	28	41
All	All	742/832 (89%)	725 (98%)	13 (2%)	4 (0%)	32	46

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	154	ALA
1	A	181	GLY
1	D	71	GLU
1	A	179	HIS

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	167/179 (93%)	154 (92%)	13 (8%)	15	23
1	B	165/179 (92%)	146 (88%)	19 (12%)	6	9
1	C	162/179 (90%)	149 (92%)	13 (8%)	14	21
1	D	150/179 (84%)	141 (94%)	9 (6%)	22	35
All	All	644/716 (90%)	590 (92%)	54 (8%)	13	19

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	30	LEU
1	A	55	LEU
1	A	79	LEU
1	A	105	PRO
1	A	108	LYS
1	A	113	LEU
1	A	131	LEU
1	A	162	THR
1	A	176	LEU
1	A	177	PHE
1	A	200	GLN
1	A	201	LEU
1	B	8	LYS
1	B	14	LEU
1	B	49	ARG
1	B	70	LEU
1	B	71	GLU
1	B	79	LEU
1	B	94	ARG
1	B	104	ARG
1	B	108	LYS
1	B	113	LEU
1	B	127	LEU
1	B	131	LEU
1	B	147	GLU
1	B	150	GLU
1	B	155	LYS
1	B	176	LEU
1	B	178	ASP
1	B	180	GLN
1	B	201	LEU
1	C	14	LEU
1	C	30	LEU
1	C	47	ASN
1	C	55	LEU
1	C	68	SER
1	C	71	GLU
1	C	98	LYS
1	C	115	ASN
1	C	131	LEU
1	C	155	LYS

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Mol	Chain	Res	Type
1	C	169	LEU
1	C	172	GLN
1	C	178	ASP
1	D	4	LEU
1	D	8	LYS
1	D	30	LEU
1	D	49	ARG
1	D	55	LEU
1	D	71	GLU
1	D	79	LEU
1	D	113	LEU
1	D	200	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	88	ASN
1	A	93	HIS
1	A	122	GLN
1	A	149	GLN
1	A	151	HIS
1	A	200	GLN
1	A	206	GLN
1	B	63	HIS
1	B	93	HIS
1	B	109	GLN
1	B	115	ASN
1	B	122	GLN
1	B	152	GLN
1	B	200	GLN
1	C	82	ASN
1	C	129	ASN
1	D	11	ASN
1	D	32	GLN
1	D	47	ASN
1	D	88	ASN
1	D	123	GLN
1	D	152	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 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	196/208 (94%)	0.69	17 (8%) 11 10	58, 63, 77, 88	0
1	B	194/208 (93%)	0.90	25 (12%) 4 3	54, 62, 76, 88	0
1	C	190/208 (91%)	1.22	40 (21%) 1 1	52, 62, 74, 80	0
1	D	178/208 (85%)	0.85	21 (11%) 5 4	56, 64, 73, 86	0
All	All	758/832 (91%)	0.92	103 (13%) 3 3	52, 63, 76, 88	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	72	GLY	9.1
1	A	164	ASP	7.2
1	B	72	GLY	7.2
1	C	117	LEU	6.9
1	B	110	TYR	6.6
1	A	163	THR	6.3
1	C	118	ALA	5.9
1	B	155	LYS	5.4
1	D	41	LEU	5.3
1	D	5	ASP	4.8
1	D	181	GLY	4.8
1	A	5	ASP	4.7
1	A	179	HIS	4.6
1	A	180	GLN	4.2
1	A	165	SER	4.0
1	C	71	GLU	4.0
1	D	70	LEU	4.0
1	D	44	HIS	4.0
1	C	193	LEU	3.9
1	B	5	ASP	3.9
1	C	70	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	162	THR	3.8
1	C	140	PHE	3.7
1	B	70	LEU	3.7
1	C	163	THR	3.6
1	D	115	ASN	3.6
1	C	143	GLY	3.5
1	C	122	GLN	3.5
1	C	127	LEU	3.5
1	A	174	ILE	3.5
1	C	190	LEU	3.4
1	A	177	PHE	3.4
1	D	66	HIS	3.4
1	C	110	TYR	3.3
1	A	176	LEU	3.2
1	B	153	VAL	3.2
1	D	30	LEU	3.2
1	A	155	LYS	3.1
1	C	113	LEU	3.1
1	C	141	THR	3.0
1	D	184	PRO	3.0
1	D	146	LEU	3.0
1	A	166	MET	2.9
1	B	204	LEU	2.9
1	C	136	ALA	2.9
1	D	139	HIS	2.9
1	C	32	GLN	2.9
1	D	8	LYS	2.8
1	C	142	LEU	2.8
1	C	120	LEU	2.8
1	B	136	ALA	2.8
1	C	189	GLY	2.8
1	B	203	ALA	2.8
1	C	201	LEU	2.8
1	A	153	VAL	2.7
1	B	141	THR	2.7
1	D	71	GLU	2.7
1	B	140	PHE	2.7
1	C	194	ILE	2.6
1	B	152	GLN	2.6
1	C	144	SER	2.6
1	D	143	GLY	2.6
1	B	154	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	155	LYS	2.6
1	C	155	LYS	2.6
1	D	182	ALA	2.5
1	D	4	LEU	2.5
1	C	51	LEU	2.5
1	C	164	ASP	2.5
1	C	146	LEU	2.4
1	C	186	PHE	2.4
1	C	125	PHE	2.4
1	C	19	GLU	2.4
1	A	140	PHE	2.4
1	B	3	ARG	2.3
1	C	185	ALA	2.3
1	B	144	SER	2.3
1	B	189	GLY	2.3
1	B	104	ARG	2.3
1	C	69	PRO	2.2
1	C	168	PRO	2.2
1	D	140	PHE	2.2
1	C	109	GLN	2.2
1	D	156	GLU	2.2
1	D	122	GLN	2.2
1	C	138	GLY	2.2
1	B	185	ALA	2.2
1	C	53	ASP	2.2
1	B	193	LEU	2.2
1	C	73	GLU	2.2
1	B	143	GLY	2.2
1	C	137	VAL	2.1
1	B	196	GLY	2.1
1	A	144	SER	2.1
1	B	139	HIS	2.1
1	B	192	SER	2.1
1	D	15	GLU	2.1
1	B	145	VAL	2.1
1	B	101	LEU	2.1
1	C	131	LEU	2.1
1	A	6	LYS	2.0
1	C	119	PHE	2.0
1	A	114	GLU	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.