



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 06:06 am GMT

PDB ID : 4JMQ
Title : Crystal structure of pb9: The Dit of bacteriophage T5.
Authors : Flayhan, A.; Vellieux, F.M.D.; Girard, E.; Maury, O.; Boulanger, P.; Breyton, C.
Deposited on : 2013-03-14
Resolution : 1.90 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	:	trunk28620
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)	:	recalc28949

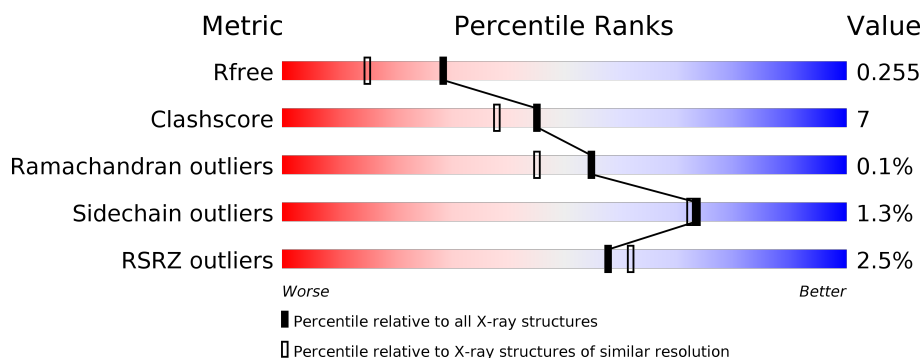
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)

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	217	<div> <div></div> <div>74%13%12%</div> </div>
1	B	217	<div> <div>%</div> <div>72%15%13%</div> </div>
1	C	217	<div> <div>3%</div> <div>74%17%7%</div> </div>
1	D	217	<div> <div>4%</div> <div>78%9%13%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6935 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 Bacteriophage T5 distal tail protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	190	Total	C	N	O	S	0	1	0
			1505	964	246	293	2			
1	B	189	Total	C	N	O	S	0	1	0
			1493	956	242	293	2			
1	C	201	Total	C	N	O	S	0	1	0
			1608	1029	269	307	3			
1	D	189	Total	C	N	O	S	0	2	0
			1500	961	243	294	2			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	205	GLU	-	EXPRESSION TAG	UNP Q6QGE8
A	206	ASN	-	EXPRESSION TAG	UNP Q6QGE8
A	207	LEU	-	EXPRESSION TAG	UNP Q6QGE8
A	208	TYR	-	EXPRESSION TAG	UNP Q6QGE8
A	209	PHE	-	EXPRESSION TAG	UNP Q6QGE8
A	210	GLN	-	EXPRESSION TAG	UNP Q6QGE8
A	211	GLY	-	EXPRESSION TAG	UNP Q6QGE8
A	212	HIS	-	EXPRESSION TAG	UNP Q6QGE8
A	213	HIS	-	EXPRESSION TAG	UNP Q6QGE8
A	214	HIS	-	EXPRESSION TAG	UNP Q6QGE8
A	215	HIS	-	EXPRESSION TAG	UNP Q6QGE8
A	216	HIS	-	EXPRESSION TAG	UNP Q6QGE8
A	217	HIS	-	EXPRESSION TAG	UNP Q6QGE8
B	205	GLU	-	EXPRESSION TAG	UNP Q6QGE8
B	206	ASN	-	EXPRESSION TAG	UNP Q6QGE8
B	207	LEU	-	EXPRESSION TAG	UNP Q6QGE8
B	208	TYR	-	EXPRESSION TAG	UNP Q6QGE8
B	209	PHE	-	EXPRESSION TAG	UNP Q6QGE8
B	210	GLN	-	EXPRESSION TAG	UNP Q6QGE8
B	211	GLY	-	EXPRESSION TAG	UNP Q6QGE8
B	212	HIS	-	EXPRESSION TAG	UNP Q6QGE8

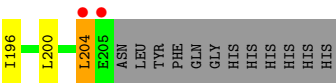
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Chain	Residue	Modelled	Actual	Comment	Reference
B	213	HIS	-	EXPRESSION TAG	UNP Q6QGE8
B	214	HIS	-	EXPRESSION TAG	UNP Q6QGE8
B	215	HIS	-	EXPRESSION TAG	UNP Q6QGE8
B	216	HIS	-	EXPRESSION TAG	UNP Q6QGE8
B	217	HIS	-	EXPRESSION TAG	UNP Q6QGE8
C	205	GLU	-	EXPRESSION TAG	UNP Q6QGE8
C	206	ASN	-	EXPRESSION TAG	UNP Q6QGE8
C	207	LEU	-	EXPRESSION TAG	UNP Q6QGE8
C	208	TYR	-	EXPRESSION TAG	UNP Q6QGE8
C	209	PHE	-	EXPRESSION TAG	UNP Q6QGE8
C	210	GLN	-	EXPRESSION TAG	UNP Q6QGE8
C	211	GLY	-	EXPRESSION TAG	UNP Q6QGE8
C	212	HIS	-	EXPRESSION TAG	UNP Q6QGE8
C	213	HIS	-	EXPRESSION TAG	UNP Q6QGE8
C	214	HIS	-	EXPRESSION TAG	UNP Q6QGE8
C	215	HIS	-	EXPRESSION TAG	UNP Q6QGE8
C	216	HIS	-	EXPRESSION TAG	UNP Q6QGE8
C	217	HIS	-	EXPRESSION TAG	UNP Q6QGE8
D	205	GLU	-	EXPRESSION TAG	UNP Q6QGE8
D	206	ASN	-	EXPRESSION TAG	UNP Q6QGE8
D	207	LEU	-	EXPRESSION TAG	UNP Q6QGE8
D	208	TYR	-	EXPRESSION TAG	UNP Q6QGE8
D	209	PHE	-	EXPRESSION TAG	UNP Q6QGE8
D	210	GLN	-	EXPRESSION TAG	UNP Q6QGE8
D	211	GLY	-	EXPRESSION TAG	UNP Q6QGE8
D	212	HIS	-	EXPRESSION TAG	UNP Q6QGE8
D	213	HIS	-	EXPRESSION TAG	UNP Q6QGE8
D	214	HIS	-	EXPRESSION TAG	UNP Q6QGE8
D	215	HIS	-	EXPRESSION TAG	UNP Q6QGE8
D	216	HIS	-	EXPRESSION TAG	UNP Q6QGE8
D	217	HIS	-	EXPRESSION TAG	UNP Q6QGE8

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	215	Total O 215 215	0	0
2	B	212	Total O 212 212	0	0
2	C	191	Total O 191 191	0	0
2	D	211	Total O 211 211	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.66Å 70.03Å 71.01Å 91.05° 107.66° 112.03°	Depositor
Resolution (Å)	27.69 – 1.90 66.91 – 1.89	Depositor EDS
% Data completeness (in resolution range)	95.4 (27.69-1.90) 91.7 (66.91-1.89)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.19	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 1.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.203 , 0.252 0.206 , 0.255	Depositor DCC
R_{free} test set	3547 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	20.8	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6935	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.10% 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	0.37	0/1545	0.55	0/2100
1	B	0.38	0/1532	0.56	0/2082
1	C	0.39	0/1656	0.60	0/2251
1	D	0.35	0/1542	0.55	0/2096
All	All	0.37	0/6275	0.57	0/8529

There are no bond length outliers.

There are no bond angle outliers.

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	1505	0	1475	23	0
1	B	1493	0	1460	23	0
1	C	1608	0	1549	32	0
1	D	1500	0	1470	14	0
2	A	215	0	0	7	0
2	B	212	0	0	8	0
2	C	191	0	0	5	0
2	D	211	0	0	5	0
All	All	6935	0	5954	89	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 (89) 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:43:ILE:N	2:B:505:HOH:O	1.97	0.97
1:A:43:ILE:N	2:A:464:HOH:O	1.97	0.97
1:A:108:GLN:NE2	2:A:366:HOH:O	1.94	0.94
1:C:60:ASP:OD1	2:C:460:HOH:O	1.91	0.86
1:A:170:GLY:O	2:A:495:HOH:O	2.00	0.80
1:C:19:SER:HB3	1:C:53:SER:HB2	1.71	0.73
1:C:25:ASN:C	1:C:27:PRO:HD2	2.11	0.71
1:B:174:ARG:NH2	1:B:203:SER:O	2.24	0.70
1:B:68:ARG:NH1	2:B:348:HOH:O	2.18	0.70
1:D:182:SER:O	2:D:437:HOH:O	2.09	0.70
1:A:18:GLU:OE1	2:A:496:HOH:O	2.12	0.67
1:D:163:SER:OG	2:D:462:HOH:O	2.11	0.67
1:B:201:ARG:NH2	2:B:318:HOH:O	2.28	0.65
1:C:108:GLN:OE1	2:C:430:HOH:O	2.15	0.65
1:B:178:MET:SD	1:B:201:ARG:NH2	2.70	0.64
1:B:185:SER:HB2	1:B:196:ILE:HD11	1.80	0.63
1:C:208:TYR:CG	1:C:209:PHE:HB3	2.34	0.62
1:B:94:ASP:OD1	1:B:96:LYS:HG2	2.02	0.60
1:D:3:LEU:HD12	1:D:4:PRO:HD2	1.84	0.59
1:B:3:LEU:HD12	1:B:4:PRO:HD2	1.86	0.57
1:A:181:ASP:HB2	1:B:201:ARG:HH21	1.70	0.56
1:C:24:ASP:O	1:D:108[B]:GLN:NE2	2.37	0.56
1:C:187:LEU:HG	1:C:191:GLY:HA2	1.88	0.56
1:A:124:GLY:HA2	1:A:137:LYS:HE3	1.88	0.55
1:C:188[A]:ASN:ND2	1:C:194:SER:OG	2.39	0.55
1:B:18:GLU:OE1	2:B:503:HOH:O	2.17	0.55
1:B:100:ILE:HG12	1:B:111:LEU:HB3	1.88	0.55
1:C:3:LEU:HD12	1:C:4:PRO:HD2	1.88	0.55
1:D:105:LYS:HE3	2:D:431:HOH:O	2.06	0.55
1:A:100:ILE:HG12	1:A:111:LEU:HB3	1.89	0.53
1:B:14:GLY:HA3	2:B:313:HOH:O	2.07	0.53
1:C:26:ASP:N	1:C:27:PRO:HD2	2.23	0.53
1:B:1:MET:HE1	1:B:71:GLU:HG2	1.90	0.53
1:A:185:SER:HB2	1:A:196:ILE:HD11	1.88	0.53
1:B:78:TYR:CD1	1:B:176:LYS:HE3	2.44	0.53
1:A:81:VAL:HG21	1:A:200:LEU:HD13	1.90	0.52
1:D:89:PHE:HE1	2:D:477:HOH:O	1.92	0.52
1:A:174[B]:ARG:HH12	1:A:205:GLU:HA	1.73	0.52
1:D:7:TYR:HE2	1:D:84:PRO:HG3	1.73	0.52
1:C:78:TYR:OH	1:C:205:GLU:OE2	2.21	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174[B]:ARG:HH22	1:A:205:GLU:H	1.58	0.51
1:A:3:LEU:HD12	1:A:4:PRO:HD2	1.94	0.50
1:B:77:ASP:OD1	1:B:78:TYR:N	2.40	0.50
1:D:81:VAL:HG21	1:D:200:LEU:HD13	1.93	0.49
1:A:174[B]:ARG:NH2	1:A:205:GLU:H	2.10	0.49
1:C:107:SER:HB3	1:C:155:ASP:OD1	2.13	0.49
1:C:208:TYR:CD1	1:C:209:PHE:HB3	2.47	0.49
1:B:128:LYS:HE2	1:B:133:PRO:HA	1.94	0.48
1:A:174[B]:ARG:HH22	1:A:205:GLU:N	2.11	0.48
1:C:64:PHE:O	1:C:68:ARG:HG2	2.14	0.48
1:C:209:PHE:C	1:C:211:GLY:H	2.17	0.47
1:D:57:LEU:HD12	1:D:196:ILE:HD12	1.95	0.47
1:A:26:ASP:N	1:A:26:ASP:OD1	2.48	0.46
1:C:26:ASP:HB3	1:D:108[B]:GLN:NE2	2.31	0.46
1:B:137:LYS:HE2	2:B:497:HOH:O	2.15	0.46
1:B:90:ARG:HD3	1:B:122:LYS:HE3	1.97	0.46
1:C:158:ILE:HG22	2:C:451:HOH:O	2.14	0.46
1:D:133:PRO:HG2	1:D:204:LEU:HD21	1.97	0.46
1:C:133:PRO:HG2	1:C:204:LEU:CD2	2.46	0.45
1:C:95:THR:HG22	1:C:117:LEU:HD21	1.98	0.45
1:C:179:ASN:HB2	1:C:182:SER:OG	2.17	0.45
1:C:56:GLU:HG2	1:C:56:GLU:O	2.17	0.45
1:C:19:SER:N	2:C:383:HOH:O	2.50	0.44
1:A:141:PHE:N	2:A:410:HOH:O	2.20	0.44
1:C:185:SER:HA	2:C:423:HOH:O	2.17	0.44
1:C:82:LEU:O	1:C:84:PRO:HD3	2.17	0.44
1:C:133:PRO:HG2	1:C:204:LEU:HD22	2.00	0.44
1:D:68:ARG:NH1	2:D:359:HOH:O	2.50	0.44
1:C:209:PHE:O	1:C:211:GLY:N	2.48	0.43
1:D:183:PHE:CG	1:D:184:GLY:N	2.86	0.43
1:C:187:LEU:HA	1:C:187:LEU:HD12	1.87	0.43
1:C:210:GLN:C	1:C:212:HIS:H	2.22	0.43
1:A:109:ILE:CG2	1:A:150:ILE:HB	2.49	0.43
1:A:120:GLN:OE1	2:A:501:HOH:O	2.22	0.43
1:A:78:TYR:CE1	1:A:176:LYS:HE2	2.54	0.42
1:A:177:LEU:HA	1:A:200:LEU:HD23	2.01	0.42
1:C:109:ILE:HG22	1:C:150:ILE:HB	2.00	0.42
1:B:121:PRO:O	2:B:340:HOH:O	2.21	0.42
1:B:56:GLU:OE2	2:B:350:HOH:O	2.21	0.42
1:C:4:PRO:HG3	1:C:68:ARG:HG3	2.01	0.42
1:A:72:TYR:CD1	1:A:79:LEU:HG	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:LYS:HE2	1:C:133:PRO:HA	2.01	0.41
1:B:178:MET:SD	1:B:201:ARG:CZ	3.08	0.41
1:A:204:LEU:HD23	2:A:481:HOH:O	2.20	0.41
1:A:174[B]:ARG:NH2	1:A:203:SER:O	2.53	0.40
1:B:131:THR:OG1	1:B:164:GLU:HG3	2.21	0.40
1:B:174:ARG:NH1	1:B:205:GLU:O	2.47	0.40
1:C:27:PRO:HA	1:C:28:MET:HA	1.49	0.40
1:D:99:THR:HB	1:D:112:ASN:HB3	2.03	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	187/217 (86%)	184 (98%)	3 (2%)	0	100	100
1	B	186/217 (86%)	184 (99%)	2 (1%)	0	100	100
1	C	198/217 (91%)	190 (96%)	7 (4%)	1 (0%)	32	20
1	D	187/217 (86%)	183 (98%)	4 (2%)	0	100	100
All	All	758/868 (87%)	741 (98%)	16 (2%)	1 (0%)	55	45

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	27	PRO

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	169/193 (88%)	168 (99%)	1 (1%)	89	90
1	B	168/193 (87%)	165 (98%)	3 (2%)	64	60
1	C	179/193 (93%)	175 (98%)	4 (2%)	57	51
1	D	169/193 (88%)	168 (99%)	1 (1%)	89	90
All	All	685/772 (89%)	676 (99%)	9 (1%)	73	72

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	ILE
1	B	109	ILE
1	B	204	LEU
1	B	205	GLU
1	C	56	GLU
1	C	60	ASP
1	C	72	TYR
1	C	208	TYR
1	D	204	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	190/217 (87%)	-0.12	1 (0%) 90 92	21, 32, 60, 97	0
1	B	189/217 (87%)	-0.12	2 (1%) 80 83	19, 31, 57, 83	0
1	C	201/217 (92%)	0.11	7 (3%) 44 48	19, 33, 79, 105	0
1	D	189/217 (87%)	0.15	9 (4%) 31 35	19, 37, 85, 104	0
All	All	769/868 (88%)	0.01	19 (2%) 58 62	19, 32, 72, 105	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	209	PHE	5.9
1	C	208	TYR	5.0
1	C	186	THR	4.5
1	D	186	THR	3.9
1	C	185	SER	3.9
1	C	211	GLY	3.4
1	D	183	PHE	2.7
1	D	204	LEU	2.7
1	D	190	ASN	2.6
1	B	204	LEU	2.6
1	C	58	PHE	2.4
1	D	191	GLY	2.4
1	A	204	LEU	2.3
1	B	43	ILE	2.1
1	D	185	SER	2.1
1	D	58	PHE	2.1
1	C	210	GLN	2.1
1	D	205	GLU	2.0
1	D	19	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 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.