



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Nov 19, 2018 – 09:38 AM EST

PDB ID : 6CX1
EMDB ID: : EMD-7772
Title : Cryo-EM structure of Seneca Valley Virus-Anthrax Toxin Receptor 1 complex
Authors : Jayawardena, N.; Burga, L.; Easingwood, R.; Takizawa, Y.; Wolf, M.; Bostina, M.
Deposited on : 2018-04-02
Resolution : 3.80 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031633

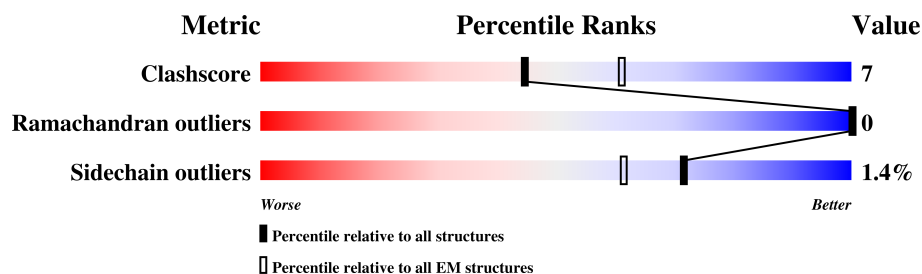
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	E	182	76% 23% .
2	A	258	80% 19% .
3	C	268	76% 23% .
4	B	238	81% 19%
5	D	58	57% . 41%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7732 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Anthrax toxin receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	182	Total	C	N	O	S	0	0
			1483	946	253	279	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	177	ALA	CYS	conflict	UNP Q9H6X2

- Molecule 2 is a protein called Capsid protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	258	Total	C	N	O	S	0	0
			2015	1295	345	371	4		

- Molecule 3 is a protein called Capsid protein VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	268	Total	C	N	O	S	0	0
			2105	1333	357	407	8		

- Molecule 4 is a protein called Capsid protein VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	238	Total	C	N	O	S	0	0
			1855	1199	294	351	11		

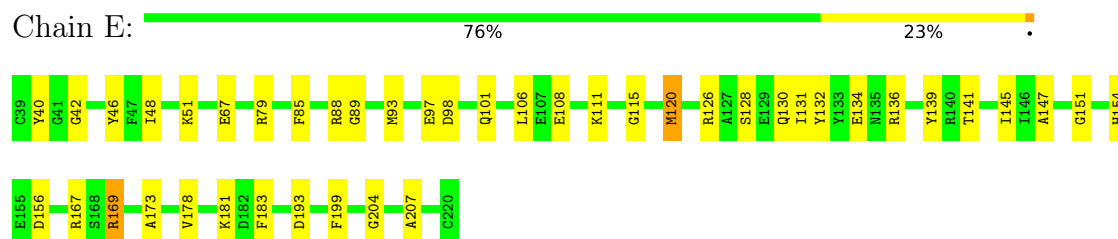
- Molecule 5 is a protein called Capsid protein VP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	34	Total	C	N	O	S	0	0
			274	172	46	55	1		

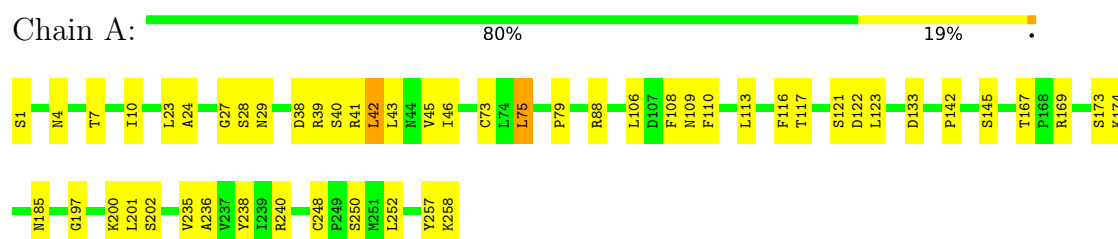
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

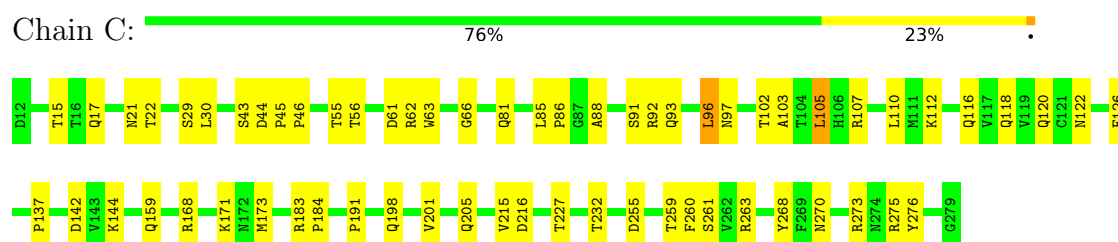
- Molecule 1: Anthrax toxin receptor 1



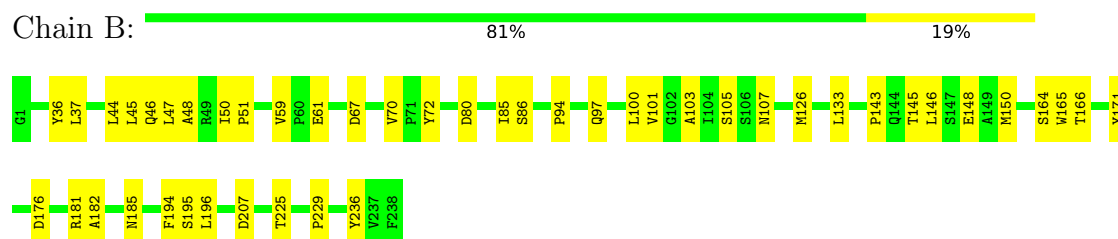
- Molecule 2: Capsid protein VP1



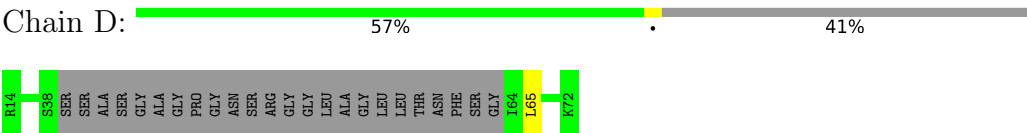
- Molecule 3: Capsid protein VP2



- Molecule 4: Capsid protein VP3



- Molecule 5: Capsid protein VP4



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	6782	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	39	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	73000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	E	0.33	0/1516	0.63	0/2043
2	A	0.42	0/2078	0.70	3/2833 (0.1%)
3	C	0.40	0/2164	0.71	2/2963 (0.1%)
4	B	0.43	0/1915	0.68	2/2636 (0.1%)
5	D	0.36	0/279	0.59	0/375
All	All	0.40	0/7952	0.68	7/10850 (0.1%)

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	E	0	1
3	C	0	2
All	All	0	3

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	255	ASP	CB-CG-OD1	6.41	124.07	118.30
2	A	43	LEU	CA-CB-CG	5.82	128.68	115.30
4	B	196	LEU	CA-CB-CG	5.78	128.59	115.30
4	B	207	ASP	CB-CG-OD1	5.64	123.38	118.30
2	A	75	LEU	CA-CB-CG	5.58	128.14	115.30
2	A	133	ASP	CB-CG-OD1	5.30	123.07	118.30
3	C	96	LEU	CA-CB-CG	5.11	127.06	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	144	LYS	Peptide
3	C	61	ASP	Peptide
1	E	154	HIS	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	E	1483	0	1433	24	0
2	A	2015	0	1951	36	0
3	C	2105	0	2030	37	0
4	B	1855	0	1815	35	0
5	D	274	0	251	1	0
All	All	7732	0	7480	113	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 (113) 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)
4:B:44:LEU:O	4:B:47:LEU:HB3	1.76	0.85
2:A:167:THR:HG23	2:A:169:ARG:HH22	1.53	0.72
2:A:42:LEU:HA	2:A:238:TYR:HA	1.70	0.72
3:C:110:LEU:HB2	3:C:270:ASN:HB3	1.72	0.70
3:C:205:GLN:NE2	3:C:216:ASP:O	2.28	0.67
2:A:46:ILE:HD11	2:A:73:CYS:HB2	1.78	0.64
4:B:101:VAL:O	4:B:105:SER:HB3	1.97	0.64
1:E:89:GLY:H	1:E:126:ARG:HH12	1.45	0.62
2:A:4:ASN:HA	4:B:164:SER:HB3	1.81	0.62
2:A:41:ARG:HH22	2:A:110:PHE:HB2	1.64	0.62
4:B:146:LEU:O	4:B:150:MET:HB2	1.99	0.62
3:C:116:GLN:HB2	3:C:263:ARG:HB3	1.81	0.60
3:C:103:ALA:O	3:C:107:ARG:NH1	2.34	0.60
1:E:169:ARG:HA	1:E:173:ALA:H	1.65	0.60
1:E:79:ARG:HH22	1:E:97:GLU:HA	1.67	0.59
2:A:167:THR:O	2:A:169:ARG:NH2	2.35	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:98:ASP:O	1:E:101:GLN:NE2	2.36	0.59
3:C:81:GLN:NE2	3:C:159:GLN:O	2.35	0.59
2:A:200:LYS:NZ	2:A:202:SER:O	2.34	0.58
3:C:102:THR:HA	3:C:105:LEU:HD23	1.85	0.58
2:A:79:PRO:HB3	2:A:106:LEU:HD12	1.86	0.57
2:A:7:THR:HA	3:C:30:LEU:HD21	1.87	0.57
2:A:121:SER:OG	2:A:122:ASP:N	2.37	0.57
2:A:252:LEU:HD22	4:B:103:ALA:HB1	1.87	0.56
2:A:38:ASP:OD1	2:A:240:ARG:NH1	2.39	0.56
3:C:120:GLN:HG3	3:C:259:THR:HG23	1.88	0.55
1:E:48:ILE:HB	1:E:147:ALA:HA	1.89	0.55
1:E:178:VAL:HG12	1:E:199:PHE:HB2	1.87	0.55
2:A:41:ARG:NH2	2:A:109:ASN:OD1	2.31	0.55
3:C:168:ARG:NH2	4:B:67:ASP:OD2	2.40	0.55
1:E:108:GLU:HA	1:E:111:LYS:HD3	1.90	0.54
4:B:143:PRO:HB3	4:B:148:GLU:HB3	1.90	0.53
3:C:66:GLY:HA3	3:C:96:LEU:HB2	1.90	0.53
2:A:257:TYR:HE1	4:B:97:GLN:HG3	1.74	0.53
4:B:145:THR:OG1	4:B:146:LEU:N	2.42	0.52
3:C:201:VAL:HA	4:B:50:ILE:HG21	1.92	0.52
1:E:98:ASP:OD1	1:E:101:GLN:NE2	2.40	0.52
3:C:142:ASP:OD1	3:C:142:ASP:N	2.41	0.51
4:B:94:PRO:HA	4:B:97:GLN:HE21	1.76	0.50
1:E:156:ASP:N	1:E:156:ASP:OD1	2.42	0.50
4:B:46:GLN:HE21	5:D:65:LEU:HB3	1.76	0.50
2:A:7:THR:HG22	3:C:30:LEU:HD11	1.94	0.49
1:E:51:LYS:O	1:E:115:GLY:N	2.45	0.49
3:C:173:MET:HE1	3:C:191:PRO:HD2	1.95	0.49
2:A:75:LEU:HD13	2:A:123:LEU:HD11	1.94	0.48
2:A:117:THR:OG1	2:A:248:CYS:SG	2.54	0.47
1:E:89:GLY:N	1:E:126:ARG:HH12	2.12	0.47
2:A:108:PHE:O	4:B:236:TYR:OH	2.31	0.47
1:E:40:TYR:HD2	1:E:42:GLY:HA3	1.79	0.47
2:A:28:SER:OG	2:A:29:ASN:N	2.48	0.47
3:C:29:SER:OG	3:C:30:LEU:N	2.47	0.47
4:B:133:LEU:HD12	4:B:194:PHE:HZ	1.79	0.47
3:C:43:SER:OG	3:C:44:ASP:N	2.48	0.46
1:E:139:TYR:HB3	1:E:141:THR:HG23	1.96	0.46
4:B:101:VAL:O	4:B:105:SER:CB	2.63	0.46
4:B:45:LEU:HD13	4:B:48:ALA:HB3	1.96	0.46
3:C:110:LEU:HB3	3:C:227:THR:HG21	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:46:TYR:HB2	1:E:145:ILE:HG12	1.97	0.46
1:E:132:TYR:O	1:E:136:ARG:NH2	2.49	0.46
4:B:164:SER:OG	4:B:165:TRP:N	2.48	0.46
1:E:181:LYS:HE2	1:E:183:PHE:HA	1.97	0.46
2:A:46:ILE:N	2:A:235:VAL:O	2.47	0.46
2:A:88:ARG:NH2	3:C:171:LYS:O	2.49	0.46
1:E:151:GLY:HA3	1:E:181:LYS:HD3	1.97	0.46
3:C:259:THR:OG1	3:C:260:PHE:N	2.49	0.46
3:C:88:ALA:HA	3:C:93:GLN:HE22	1.81	0.46
4:B:59:VAL:O	4:B:61:GLU:N	2.44	0.45
3:C:126:PHE:HE1	4:B:126:MET:HG3	1.81	0.45
3:C:22:THR:HG21	3:C:63:TRP:H	1.81	0.45
4:B:146:LEU:O	4:B:150:MET:CB	2.64	0.45
3:C:21:ASN:OD1	3:C:62:ARG:NH2	2.50	0.45
1:E:67:GLU:HG3	1:E:106:LEU:HD21	1.99	0.45
1:E:204:GLY:HA2	1:E:207:ALA:HB3	1.98	0.45
2:A:185:ASN:OD1	2:A:185:ASN:N	2.50	0.44
2:A:113:LEU:HD23	4:B:107:ASN:HD21	1.82	0.44
3:C:198:GLN:HE22	4:B:100:LEU:HG	1.83	0.44
2:A:117:THR:HG21	3:C:137:PRO:HG2	1.98	0.44
4:B:70:VAL:HG22	4:B:72:TYR:H	1.83	0.44
3:C:85:LEU:HD12	3:C:86:PRO:HA	2.00	0.44
2:A:173:SER:OG	2:A:174:LYS:N	2.51	0.44
2:A:197:GLY:HA2	3:C:232:THR:HG22	2.00	0.44
1:E:128:SER:HA	1:E:131:ILE:HB	2.00	0.43
2:A:45:VAL:HA	2:A:236:ALA:HA	1.99	0.43
4:B:171:TYR:OH	4:B:176:ASP:O	2.27	0.43
3:C:92:ARG:HG3	3:C:97:ASN:HB3	1.99	0.43
1:E:193:ASP:N	1:E:193:ASP:OD1	2.51	0.43
3:C:55:THR:OG1	3:C:56:THR:N	2.49	0.43
3:C:91:SER:OG	3:C:93:GLN:OE1	2.26	0.43
3:C:45:PRO:HA	3:C:46:PRO:HD3	1.84	0.43
1:E:130:GLN:O	1:E:134:GLU:HB2	2.18	0.43
2:A:201:LEU:HD11	3:C:276:TYR:HE1	1.83	0.43
4:B:85:ILE:O	4:B:195:SER:HA	2.19	0.42
2:A:40:SER:HA	2:A:240:ARG:HB2	2.02	0.42
3:C:15:THR:HG22	3:C:17:GLN:HG3	2.02	0.42
2:A:142:PRO:O	2:A:145:SER:OG	2.35	0.42
4:B:94:PRO:HA	4:B:97:GLN:HG2	2.02	0.42
4:B:86:SER:HA	4:B:194:PHE:O	2.19	0.42
2:A:116:PHE:O	2:A:250:SER:OG	2.33	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:122:ASN:N	3:C:122:ASN:OD1	2.53	0.42
2:A:39:ARG:HH22	4:B:229:PRO:HD2	1.85	0.41
2:A:27:GLY:H	4:B:225:THR:HG21	1.85	0.41
3:C:183:ARG:HD2	3:C:184:PRO:HD2	2.02	0.41
2:A:1:SER:H1	4:B:166:THR:HB	1.85	0.41
2:A:10:ILE:HD11	4:B:51:PRO:HG3	2.03	0.41
2:A:23:LEU:HD22	2:A:24:ALA:H	1.86	0.41
4:B:182:ALA:HB1	4:B:185:ASN:HA	2.03	0.41
4:B:36:TYR:CZ	4:B:37:LEU:HD23	2.56	0.41
3:C:118:GLN:O	3:C:261:SER:OG	2.34	0.41
3:C:112:LYS:HB3	3:C:268:TYR:HB2	2.02	0.41
4:B:44:LEU:HB2	4:B:47:LEU:HD23	2.03	0.40
1:E:85:PHE:CE2	1:E:120:MET:HB3	2.56	0.40
1:E:131:ILE:HD13	1:E:131:ILE:HA	1.95	0.40
4:B:80:ASP:OD1	4:B:80:ASP:N	2.55	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 PDB entries followed by that with respect to all EM entries.

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	E	180/182 (99%)	161 (89%)	19 (11%)	0	100	100
2	A	256/258 (99%)	231 (90%)	25 (10%)	0	100	100
3	C	266/268 (99%)	234 (88%)	32 (12%)	0	100	100
4	B	236/238 (99%)	210 (89%)	26 (11%)	0	100	100
5	D	30/58 (52%)	26 (87%)	4 (13%)	0	100	100
All	All	968/1004 (96%)	862 (89%)	106 (11%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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	E	158/158 (100%)	153 (97%)	5 (3%)	42	72
2	A	216/216 (100%)	214 (99%)	2 (1%)	81	91
3	C	235/235 (100%)	231 (98%)	4 (2%)	63	84
4	B	213/213 (100%)	212 (100%)	1 (0%)	90	96
5	D	30/44 (68%)	30 (100%)	0	100	100
All	All	852/866 (98%)	840 (99%)	12 (1%)	71	86

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	88	ARG
1	E	93	MET
1	E	120	MET
1	E	167	ARG
1	E	169	ARG
2	A	42	LEU
2	A	258	LYS
3	C	105	LEU
3	C	215	VAL
3	C	273	ARG
3	C	275	ARG
4	B	181	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	110	GLN
2	A	243	ASN
3	C	120	GLN
3	C	192	ASN
3	C	198	GLN
4	B	46	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	B	97	GLN
4	B	110	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.