wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:40 PM BST

PDB ID	:	3J24
EMDB ID:	:	EMD-5475
Title	:	CryoEM reconstruction of complement decay-accelerating factor
Authors	:	Yoder, J.D.; Hafenstein, S.H.
Deposited on	:	2012-08-17
Resolution	:	9.00 Å(reported)
Based on PDB ID	:	1OJW

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

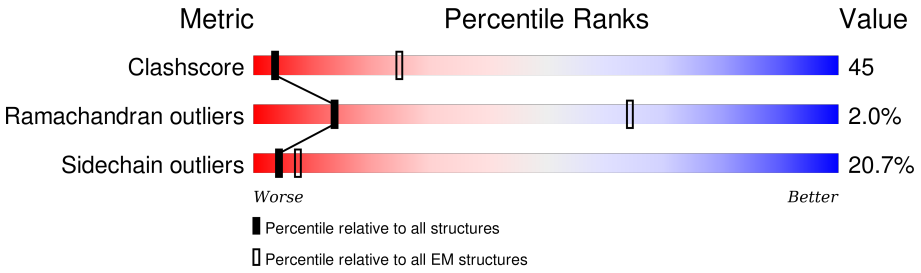
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 9.00 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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 <=5%

Mol	Chain	Length	Quality of chain
1	B	254	39% 44% 15% .

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1946 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 Complement decay-accelerating factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	251	1946	1221	326	382	17	0	0

There are 3 discrepancies between the modelled and reference sequences:

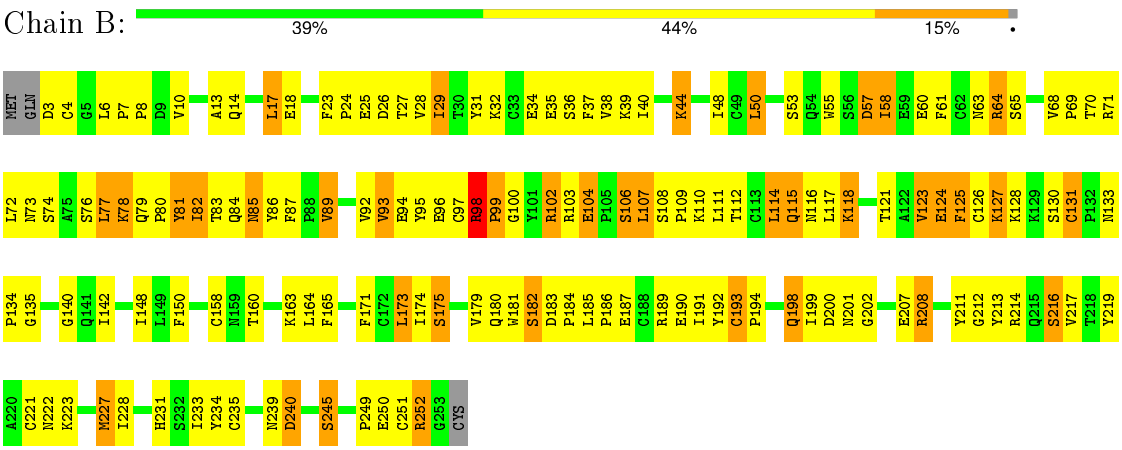
Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	EXPRESSION TAG	UNP P08174
B	2	GLN	-	EXPRESSION TAG	UNP P08174
B	254	CYS	-	EXPRESSION TAG	UNP P08174

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Complement decay-accelerating factor

Chain B:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of images	3010	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	AUTO3DEM	Depositor
Microscope	FEI/PHILIPS CM300FEG/T	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	24.0	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4600	Depositor
Magnification	45000	Depositor
Image detector	KODAK SO-163 FILM	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	B	0.36	0/1999	0.55	2/2719 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	98	ARG	C-N-CD	-11.62	95.03	120.60
1	B	104	GLU	C-N-CD	-7.21	104.74	120.60

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	B	1946	0	1842	169	0
All	All	1946	0	1842	169	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 45.

All (169) 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:252:ARG:HB3	1:B:252:ARG:NH2	1.72	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:ARG:HH21	1:B:252:ARG:HB3	0.94	1.05
1:B:165:PHE:HD2	1:B:189:ARG:HG3	1.29	0.96
1:B:252:ARG:HH21	1:B:252:ARG:CB	1.83	0.91
1:B:163:LYS:HG3	1:B:240:ASP:HB3	1.54	0.89
1:B:191:ILE:CD1	1:B:240:ASP:HA	2.03	0.88
1:B:191:ILE:HD13	1:B:240:ASP:HA	1.56	0.87
1:B:78:LYS:HD3	1:B:96:GLU:HB3	1.57	0.87
1:B:165:PHE:CD2	1:B:189:ARG:HG3	2.13	0.84
1:B:28:VAL:CG2	1:B:48:ILE:HD12	2.08	0.84
1:B:77:LEU:CB	1:B:82:ILE:HD12	2.11	0.81
1:B:89:VAL:HG11	1:B:115:GLN:HA	1.64	0.78
1:B:106:SER:C	1:B:107:LEU:HD23	2.07	0.75
1:B:148:ILE:HG22	1:B:181:TRP:CZ2	2.21	0.75
1:B:217:VAL:CG1	1:B:233:ILE:HG12	2.18	0.74
1:B:171:PHE:HB3	1:B:173:LEU:HD13	1.69	0.73
1:B:227:MET:HE2	1:B:249:PRO:HB2	1.70	0.73
1:B:217:VAL:HG12	1:B:233:ILE:HG12	1.70	0.73
1:B:123:VAL:HG23	1:B:125:PHE:HD2	1.54	0.72
1:B:131:CYS:HB2	1:B:148:ILE:O	1.90	0.72
1:B:28:VAL:HG22	1:B:48:ILE:HD12	1.71	0.71
1:B:10:VAL:HG23	1:B:31:TYR:CE1	2.27	0.70
1:B:23:PHE:HB3	1:B:27:THR:HG21	1.74	0.70
1:B:77:LEU:HB2	1:B:82:ILE:HD12	1.73	0.70
1:B:163:LYS:CG	1:B:240:ASP:HB3	2.23	0.69
1:B:110:LYS:O	1:B:111:LEU:HD23	1.93	0.68
1:B:71:ARG:C	1:B:72:LEU:HD23	2.14	0.68
1:B:227:MET:CE	1:B:249:PRO:HB2	2.23	0.68
1:B:73:ASN:O	1:B:98:ARG:HD2	1.94	0.68
1:B:198:GLN:NE2	1:B:198:GLN:HA	2.09	0.66
1:B:199:ILE:CD1	1:B:202:GLY:HA3	2.26	0.66
1:B:103:ARG:NH2	1:B:107:LEU:O	2.28	0.65
1:B:3:ASP:OD2	1:B:24:PRO:HA	1.95	0.65
1:B:133:ASN:OD1	1:B:134:PRO:HD2	1.96	0.65
1:B:234:TYR:H	1:B:245:SER:HB3	1.62	0.65
1:B:175:SER:HB3	1:B:180:GLN:HB2	1.78	0.65
1:B:40:ILE:HD11	1:B:63:ASN:HB2	1.78	0.65
1:B:69:PRO:HG2	1:B:77:LEU:HD21	1.78	0.64
1:B:68:VAL:HG12	1:B:69:PRO:HD2	1.80	0.64
1:B:77:LEU:HB3	1:B:82:ILE:HD12	1.78	0.63
1:B:48:ILE:CG2	1:B:50:LEU:HD21	2.28	0.63
1:B:191:ILE:HD11	1:B:240:ASP:HA	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:ILE:HG23	1:B:50:LEU:CD2	2.29	0.62
1:B:48:ILE:HG23	1:B:50:LEU:HD21	1.80	0.62
1:B:148:ILE:HG22	1:B:181:TRP:HZ2	1.65	0.62
1:B:94:GLU:HG3	1:B:110:LYS:HG2	1.82	0.61
1:B:207:GLU:HG3	1:B:208:ARG:H	1.66	0.60
1:B:80:PRO:HG2	1:B:84:GLN:OE1	2.02	0.59
1:B:76:SER:O	1:B:96:GLU:HG2	2.03	0.58
1:B:163:LYS:HE3	1:B:165:PHE:CE1	2.37	0.58
1:B:163:LYS:HG3	1:B:240:ASP:CB	2.30	0.58
1:B:208:ARG:HB2	1:B:211:TYR:CZ	2.38	0.58
1:B:25:GLU:O	1:B:26:ASP:HB2	2.03	0.58
1:B:228:ILE:N	1:B:250:GLU:O	2.36	0.57
1:B:148:ILE:HG22	1:B:181:TRP:CH2	2.39	0.57
1:B:199:ILE:HD12	1:B:202:GLY:HA3	1.87	0.57
1:B:93:VAL:HG23	1:B:111:LEU:HB2	1.85	0.57
1:B:77:LEU:HD13	1:B:95:TYR:CE2	2.39	0.57
1:B:190:GLU:HG2	1:B:192:TYR:CE1	2.40	0.56
1:B:107:LEU:N	1:B:107:LEU:HD23	2.20	0.56
1:B:72:LEU:N	1:B:72:LEU:HD23	2.20	0.56
1:B:240:ASP:N	1:B:240:ASP:OD1	2.38	0.55
1:B:81:TYR:HB3	1:B:93:VAL:HG12	1.87	0.55
1:B:34:GLU:O	1:B:37:PHE:HB2	2.06	0.55
1:B:116:ASN:OD1	1:B:118:LYS:HB2	2.07	0.55
1:B:81:TYR:CD2	1:B:93:VAL:HA	2.42	0.54
1:B:92:VAL:HA	1:B:111:LEU:O	2.06	0.54
1:B:148:ILE:CG2	1:B:181:TRP:HZ2	2.20	0.54
1:B:207:GLU:HG3	1:B:208:ARG:N	2.23	0.53
1:B:102:ARG:O	1:B:102:ARG:HG3	2.08	0.53
1:B:219:TYR:CD1	1:B:249:PRO:HD2	2.43	0.53
1:B:38:VAL:HG11	1:B:86:TYR:HA	1.90	0.53
1:B:8:PRO:HD3	1:B:55:TRP:CD1	2.44	0.53
1:B:227:MET:HG2	1:B:231:HIS:CE1	2.44	0.52
1:B:13:ALA:HB1	1:B:31:TYR:HB3	1.91	0.52
1:B:74:SER:C	1:B:98:ARG:HG3	2.30	0.52
1:B:40:ILE:HD12	1:B:61:PHE:O	2.09	0.52
1:B:160:THR:HG22	1:B:213:TYR:CE2	2.45	0.51
1:B:28:VAL:HG23	1:B:48:ILE:HD12	1.90	0.51
1:B:216:SER:HB2	1:B:234:TYR:CD1	2.46	0.51
1:B:17:LEU:O	1:B:18:GLU:HB2	2.11	0.51
1:B:165:PHE:CE2	1:B:189:ARG:HB2	2.46	0.51
1:B:89:VAL:CG1	1:B:115:GLN:HA	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:LEU:CD1	1:B:123:VAL:HB	2.42	0.50
1:B:201:ASN:O	1:B:222:ASN:ND2	2.45	0.50
1:B:14:GLN:OE1	1:B:14:GLN:HA	2.11	0.50
1:B:104:GLU:N	1:B:125:PHE:O	2.42	0.50
1:B:198:GLN:NE2	1:B:198:GLN:CA	2.73	0.49
1:B:180:GLN:OE1	1:B:180:GLN:HA	2.12	0.49
1:B:200:ASP:O	1:B:201:ASN:HB2	2.11	0.49
1:B:68:VAL:HA	1:B:87:PHE:HE1	1.78	0.49
1:B:208:ARG:HB2	1:B:211:TYR:CE1	2.47	0.49
1:B:231:HIS:CD2	1:B:231:HIS:N	2.80	0.49
1:B:165:PHE:CD2	1:B:189:ARG:NH2	2.80	0.49
1:B:109:PRO:HA	1:B:125:PHE:CD1	2.46	0.49
1:B:217:VAL:HG12	1:B:233:ILE:CG1	2.40	0.49
1:B:114:LEU:HB2	1:B:118:LYS:O	2.11	0.49
1:B:116:ASN:OD1	1:B:116:ASN:O	2.30	0.49
1:B:228:ILE:HG13	1:B:252:ARG:HB2	1.94	0.49
1:B:200:ASP:O	1:B:251:CYS:HB2	2.13	0.49
1:B:36:SER:HB3	1:B:117:LEU:CD1	2.43	0.48
1:B:183:ASP:HB3	1:B:184:PRO:HD2	1.94	0.48
1:B:123:VAL:HG23	1:B:125:PHE:CD2	2.43	0.48
1:B:165:PHE:HE2	1:B:189:ARG:HB2	1.78	0.48
1:B:77:LEU:CD1	1:B:95:TYR:CZ	2.96	0.48
1:B:163:LYS:CE	1:B:165:PHE:CE1	2.97	0.48
1:B:82:ILE:HG23	1:B:83:THR:HG23	1.95	0.48
1:B:131:CYS:HA	1:B:179:VAL:HG23	1.94	0.48
1:B:140:GLY:HA2	1:B:158:CYS:HA	1.96	0.48
1:B:191:ILE:HD13	1:B:240:ASP:CA	2.37	0.47
1:B:112:THR:HG22	1:B:114:LEU:CD1	2.45	0.47
1:B:7:PRO:HG3	1:B:29:ILE:HD12	1.96	0.47
1:B:97:CYS:SG	1:B:103:ARG:HG2	2.55	0.47
1:B:130:SER:C	1:B:179:VAL:HG21	2.36	0.47
1:B:217:VAL:O	1:B:217:VAL:HG13	2.14	0.47
1:B:127:LYS:HD2	1:B:127:LYS:HA	1.41	0.46
1:B:208:ARG:HG3	1:B:208:ARG:HH11	1.79	0.46
1:B:79:GLN:OE1	1:B:82:ILE:HG22	2.15	0.46
1:B:107:LEU:HD13	1:B:123:VAL:HB	1.98	0.46
1:B:213:TYR:O	1:B:214:ARG:HB2	2.16	0.46
1:B:219:TYR:CD1	1:B:249:PRO:CD	2.98	0.46
1:B:36:SER:HB3	1:B:117:LEU:HD12	1.99	0.45
1:B:6:LEU:HA	1:B:23:PHE:HE2	1.81	0.45
1:B:198:GLN:HE21	1:B:198:GLN:CA	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:GLU:OE2	1:B:127:LYS:HE2	2.17	0.45
1:B:96:GLU:O	1:B:96:GLU:HG3	2.17	0.45
1:B:69:PRO:HD3	1:B:87:PHE:CE1	2.52	0.45
1:B:135:GLY:O	1:B:142:ILE:HD12	2.17	0.44
1:B:57:ASP:O	1:B:58:ILE:HB	2.17	0.44
1:B:216:SER:CB	1:B:234:TYR:CD1	3.01	0.43
1:B:199:ILE:HD12	1:B:202:GLY:CA	2.47	0.43
1:B:85:ASN:N	1:B:85:ASN:ND2	2.66	0.43
1:B:10:VAL:CG2	1:B:31:TYR:CE1	2.98	0.43
1:B:23:PHE:HA	1:B:24:PRO:HD2	1.89	0.43
1:B:35:GLU:O	1:B:36:SER:HB2	2.18	0.43
1:B:77:LEU:HD13	1:B:95:TYR:CZ	2.53	0.43
1:B:44:LYS:HB3	1:B:44:LYS:HE2	1.62	0.43
1:B:74:SER:O	1:B:98:ARG:HG3	2.18	0.43
1:B:77:LEU:CD1	1:B:95:TYR:CE2	3.01	0.43
1:B:99:PRO:HA	1:B:100:GLY:HA2	1.51	0.43
1:B:231:HIS:H	1:B:231:HIS:CD2	2.37	0.42
1:B:208:ARG:CB	1:B:211:TYR:CE1	3.02	0.42
1:B:199:ILE:HD11	1:B:202:GLY:HA3	2.01	0.42
1:B:212:GLY:O	1:B:235:CYS:HB3	2.20	0.42
1:B:74:SER:OG	1:B:126:CYS:HB2	2.20	0.42
1:B:208:ARG:NH1	1:B:208:ARG:HG3	2.34	0.42
1:B:160:THR:CG2	1:B:213:TYR:CE2	3.02	0.42
1:B:207:GLU:CG	1:B:208:ARG:N	2.82	0.42
1:B:128:LYS:HE2	1:B:150:PHE:O	2.18	0.42
1:B:171:PHE:O	1:B:182:SER:N	2.47	0.42
1:B:125:PHE:N	1:B:125:PHE:CD2	2.88	0.42
1:B:64:ARG:H	1:B:64:ARG:HG3	1.69	0.42
1:B:58:ILE:HG23	1:B:58:ILE:O	2.20	0.42
1:B:68:VAL:CG1	1:B:69:PRO:HD2	2.48	0.41
1:B:252:ARG:CB	1:B:252:ARG:NH2	2.59	0.41
1:B:77:LEU:HA	1:B:77:LEU:HD12	1.82	0.41
1:B:148:ILE:CG2	1:B:181:TRP:CZ2	2.96	0.41
1:B:201:ASN:C	1:B:222:ASN:ND2	2.74	0.41
1:B:185:LEU:HA	1:B:185:LEU:HD12	1.88	0.41
1:B:68:VAL:HA	1:B:87:PHE:CE1	2.56	0.41
1:B:64:ARG:NH2	1:B:115:GLN:O	2.53	0.41
1:B:24:PRO:HG2	1:B:27:THR:HG1	1.86	0.41
1:B:221:CYS:SG	1:B:227:MET:HE3	2.61	0.41
1:B:23:PHE:CD2	1:B:55:TRP:HZ2	2.39	0.41
1:B:85:ASN:N	1:B:85:ASN:HD22	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:CYS:HB3	1:B:194:PRO:HD2	2.03	0.40
1:B:227:MET:HG3	1:B:228:ILE:N	2.35	0.40
1:B:4:CYS:SG	1:B:53:SER:HA	2.62	0.40
1:B:71:ARG:O	1:B:72:LEU:HD23	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 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	B	249/254 (98%)	222 (89%)	22 (9%)	5 (2%)	9 51

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	99	PRO
1	B	98	ARG
1	B	58	ILE
1	B	123	VAL
1	B	186	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 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	B	222/225 (99%)	176 (79%)	46 (21%)	1 10

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	17	LEU
1	B	29	ILE
1	B	32	LYS
1	B	39	LYS
1	B	44	LYS
1	B	50	LEU
1	B	57	ASP
1	B	60	GLU
1	B	64	ARG
1	B	65	SER
1	B	70	THR
1	B	77	LEU
1	B	78	LYS
1	B	81	TYR
1	B	82	ILE
1	B	85	ASN
1	B	89	VAL
1	B	93	VAL
1	B	102	ARG
1	B	106	SER
1	B	107	LEU
1	B	108	SER
1	B	114	LEU
1	B	115	GLN
1	B	118	LYS
1	B	121	THR
1	B	124	GLU
1	B	125	PHE
1	B	127	LYS
1	B	131	CYS
1	B	164	LEU
1	B	173	LEU
1	B	174	ILE
1	B	175	SER
1	B	182	SER
1	B	187	GLU
1	B	193	CYS
1	B	198	GLN

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Mol	Chain	Res	Type
1	B	208	ARG
1	B	216	SER
1	B	223	LYS
1	B	227	MET
1	B	239	ASN
1	B	240	ASP
1	B	245	SER
1	B	252	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	85	ASN
1	B	115	GLN
1	B	159	ASN
1	B	198	GLN
1	B	222	ASN
1	B	231	HIS

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.