



Full wwPDB EM Validation Report ⓘ

Dec 12, 2022 – 09:08 AM EST

PDB ID : 6WDT
EMDB ID : EMD-21648
Title : Enterovirus D68 in complex with human monoclonal antibody EV68-228
Authors : Fu, J.; Vogt, M.R.; Klose, T.; Crowe, J.E.; Rossmann, M.G.; Kuhn, R.J.;
Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2020-04-01
Resolution : 3.10 Å(reported)
Based on initial model : 4WM8

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : **FAILED**
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

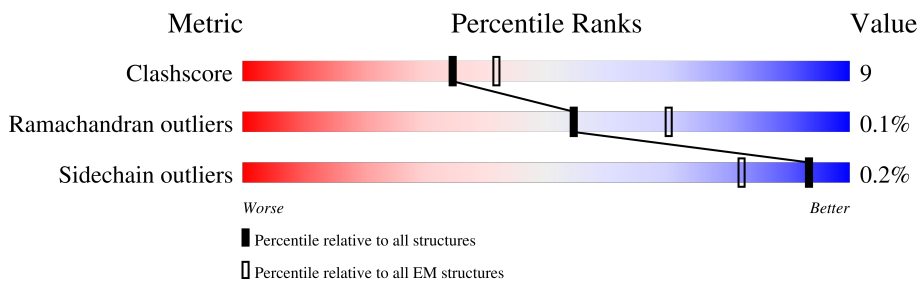
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	297	85% (Green), 15% (Yellow)
2	B	248	76% (Green), 19% (Yellow), 5% (Grey)
3	C	247	78% (Green), 22% (Yellow)
4	D	68	34% (Green), 7% (Yellow), 59% (Grey)
5	H	126	64% (Green), 33% (Yellow), 3% (Grey)
6	L	106	64% (Green), 28% (Yellow), 8% (Grey)

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7979 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 viral protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	296	2312	1469	401	435	7	0	0

- Molecule 2 is a protein called viral protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	237	1863	1188	324	339	12	0	0

- Molecule 3 is a protein called viral protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	247	1895	1198	313	366	18	0	0

- Molecule 4 is a protein called viral protein 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	28	224	143	34	47	0	0

- Molecule 5 is a protein called EV68-228 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	H	122	952	605	155	188	4	0	0

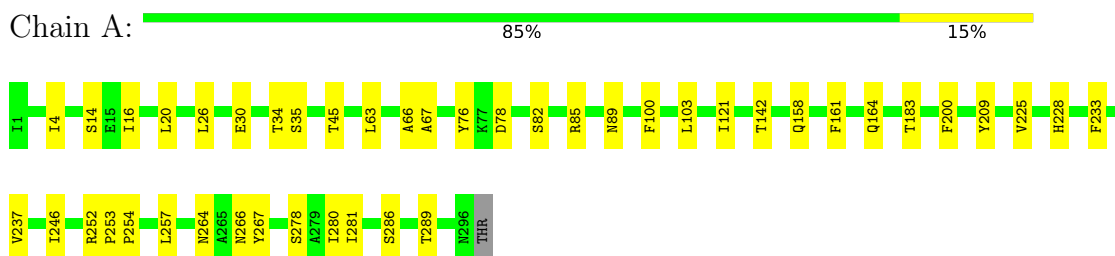
- Molecule 6 is a protein called EV68-228 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	L	98	733	463	124	143	3	0	0

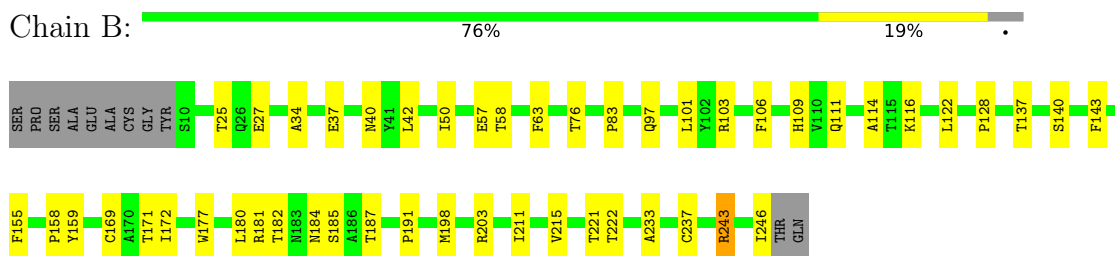
3 Residue-property plots [i](#)

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. 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.

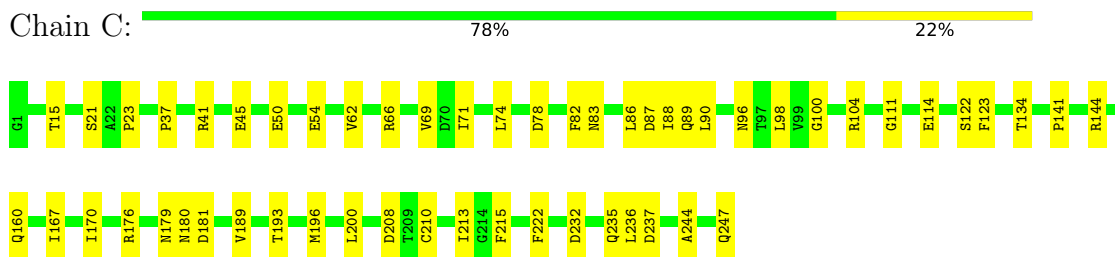
- Molecule 1: viral protein 1



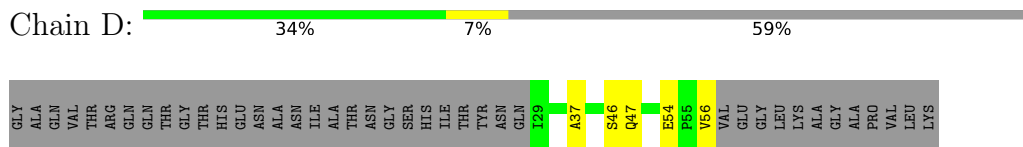
- Molecule 2: viral protein 2



- Molecule 3: viral protein 3



- Molecule 4: viral protein 4



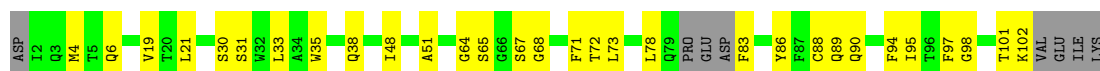
- Molecule 5: EV68-228 heavy chain

Chain H:  64% 33%



- Molecule 6: EV68-228 light chain

Chain L:  64% 28% 8%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	20194	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

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	0.31	0/2365	0.46	0/3218
2	B	0.30	0/1921	0.47	0/2630
3	C	0.30	0/1940	0.46	0/2643
4	D	0.30	0/230	0.42	0/310
5	H	0.32	0/975	0.48	0/1325
6	L	0.29	0/749	0.47	0/1013
All	All	0.30	0/8180	0.47	0/11139

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	2312	0	2308	36	0
2	B	1863	0	1793	37	0
3	C	1895	0	1844	42	0
4	D	224	0	204	5	0
5	H	952	0	908	28	0
6	L	733	0	714	20	0
All	All	7979	0	7771	139	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 9.

All (139) 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)
2:B:34:ALA:HB3	2:B:191:PRO:HD3	1.63	0.81
3:C:87:ASP:HB2	3:C:90:LEU:HG	1.64	0.78
5:H:2:VAL:HG11	5:H:27:TYR:HB2	1.69	0.73
3:C:104:ARG:NH1	3:C:232:ASP:OD1	2.22	0.73
2:B:221:THR:HG22	2:B:222:THR:H	1.55	0.71
6:L:65:SER:HB3	6:L:72:THR:HG22	1.74	0.70
1:A:34:THR:HG23	3:C:50:GLU:HG2	1.75	0.68
3:C:170:ILE:O	3:C:176:ARG:NH2	2.28	0.67
5:H:18:LEU:HD11	5:H:120:VAL:HG11	1.76	0.67
2:B:76:THR:OG1	2:B:155:PHE:O	2.12	0.66
2:B:171:THR:OG1	3:C:50:GLU:O	2.13	0.66
2:B:109:HIS:HD2	2:B:111:GLN:HE21	1.43	0.65
1:A:14:SER:HB2	1:A:45:THR:H	1.60	0.65
5:H:40:GLN:NE2	6:L:38:GLN:OE1	2.27	0.65
6:L:90:GLN:NE2	6:L:94:PHE:O	2.30	0.65
1:A:281:ILE:O	3:C:66:ARG:NH2	2.30	0.65
6:L:4:MET:HB2	6:L:98:GLY:HA3	1.79	0.64
2:B:37:GLU:HG3	3:C:37:PRO:HB3	1.78	0.64
2:B:114:ALA:HB3	2:B:180:LEU:HD13	1.79	0.64
3:C:90:LEU:HD22	3:C:181:ASP:HA	1.80	0.64
5:H:29:ILE:HG23	5:H:72:THR:HG22	1.80	0.63
5:H:48:TRP:O	5:H:61:ASN:ND2	2.31	0.61
2:B:42:LEU:HD13	2:B:103:ARG:NH1	2.16	0.60
3:C:71:ILE:HG13	3:C:200:LEU:HD22	1.83	0.60
5:H:18:LEU:HB3	5:H:81:LEU:HB2	1.84	0.60
5:H:40:GLN:HA	5:H:46:LEU:H	1.68	0.58
5:H:8:GLY:HA3	5:H:20:LEU:HD12	1.85	0.57
6:L:30:SER:OG	6:L:31:SER:N	2.38	0.56
1:A:4:ILE:HA	4:D:46:SER:HA	1.89	0.55
1:A:89:ASN:HB2	1:A:158:GLN:HG2	1.89	0.55
3:C:78:ASP:OD1	3:C:144:ARG:NH2	2.40	0.54
2:B:57:GLU:O	2:B:58:THR:OG1	2.22	0.54
1:A:264:ASN:HD22	2:B:140:SER:HA	1.74	0.53
2:B:83:PRO:HB3	2:B:106:PHE:HZ	1.74	0.53
5:H:66:ILE:HG22	5:H:81:LEU:HD23	1.90	0.53
2:B:109:HIS:HD2	2:B:111:GLN:NE2	2.06	0.53
6:L:65:SER:OG	6:L:71:PHE:HA	2.07	0.53
1:A:266:ASN:ND2	2:B:137:THR:O	2.35	0.53
1:A:4:ILE:HG13	4:D:46:SER:HB3	1.91	0.53
3:C:83:ASN:HB3	3:C:193:THR:HG22	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:244:ALA:HA	3:C:247:GLN:HE21	1.73	0.52
6:L:4:MET:SD	6:L:90:GLN:HB3	2.49	0.52
2:B:181:ARG:HG3	2:B:182:THR:HG23	1.91	0.52
3:C:100:GLY:O	3:C:104:ARG:HG3	2.09	0.52
3:C:134:THR:HG21	3:C:141:PRO:HG3	1.92	0.52
5:H:13:LYS:NZ	5:H:18:LEU:HA	2.25	0.52
3:C:176:ARG:NH1	3:C:189:VAL:HG13	2.25	0.52
5:H:10:GLY:O	5:H:121:THR:N	2.32	0.51
5:H:96:ARG:HG2	5:H:113:ASN:HB2	1.92	0.51
2:B:181:ARG:NH1	3:C:122:SER:O	2.43	0.51
5:H:16:GLU:HG3	5:H:17:THR:N	2.26	0.51
2:B:109:HIS:CD2	2:B:111:GLN:HE21	2.27	0.50
3:C:236:LEU:HB2	5:H:102:ASN:HA	1.91	0.50
1:A:278:SER:HB2	3:C:62:VAL:HG13	1.94	0.49
1:A:100:PHE:HA	3:C:235:GLN:HE22	1.77	0.49
1:A:286:SER:O	1:A:289:THR:HG22	2.12	0.49
2:B:215:VAL:HG23	3:C:213:ILE:HD11	1.94	0.49
6:L:6:GLN:O	6:L:6:GLN:HG2	2.11	0.49
1:A:252:ARG:NH2	2:B:128:PRO:O	2.31	0.49
3:C:237:ASP:N	3:C:237:ASP:OD1	2.46	0.48
3:C:50:GLU:HB3	3:C:215:PHE:HB3	1.95	0.48
6:L:101:THR:OG1	6:L:102:LYS:N	2.46	0.48
1:A:35:SER:OG	3:C:114:GLU:OE1	2.31	0.48
2:B:101:LEU:HB3	2:B:198:MET:HB3	1.96	0.48
1:A:30:GLU:HA	2:B:177:TRP:HB2	1.94	0.48
6:L:35:TRP:HB2	6:L:48:ILE:HG12	1.94	0.48
5:H:55:THR:OG1	5:H:57:ASP:OD2	2.30	0.48
3:C:45:GLU:CD	4:D:47:GLN:HB2	2.34	0.47
6:L:19:VAL:HG12	6:L:78:LEU:HD21	1.96	0.47
6:L:21:LEU:O	6:L:73:LEU:N	2.46	0.47
6:L:90:GLN:HE22	6:L:94:PHE:H	1.63	0.47
2:B:97:GLN:O	2:B:243:ARG:NH1	2.45	0.47
2:B:109:HIS:ND1	2:B:187:THR:OG1	2.46	0.47
5:H:60:TYR:CD1	5:H:66:ILE:HD11	2.50	0.47
2:B:76:THR:HB	2:B:158:PRO:HG3	1.97	0.47
2:B:159:TYR:OH	3:C:54:GLU:OE2	2.17	0.47
6:L:33:LEU:HD11	6:L:88:CYS:SG	2.55	0.47
5:H:89:THR:HG23	5:H:121:THR:HA	1.96	0.47
3:C:176:ARG:HH12	3:C:189:VAL:HG13	1.79	0.46
2:B:103:ARG:O	2:B:237:CYS:HA	2.15	0.46
2:B:50:ILE:O	2:B:50:ILE:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:143:PHE:HZ	2:B:203:ARG:HH21	1.64	0.46
5:H:13:LYS:HZ2	5:H:18:LEU:HA	1.81	0.46
1:A:63:LEU:HB2	1:A:246:ILE:HD13	1.99	0.45
2:B:63:PHE:CD1	2:B:233:ALA:HB2	2.50	0.45
1:A:67:ALA:HB3	1:A:103:LEU:HD22	1.97	0.45
5:H:38:ILE:HD13	6:L:97:PHE:HE2	1.82	0.45
5:H:86:ALA:H	5:H:122:VAL:HG11	1.82	0.45
1:A:281:ILE:HD11	3:C:96:ASN:HB2	1.99	0.45
3:C:208:ASP:OD1	3:C:208:ASP:N	2.48	0.45
1:A:82:SER:HB3	1:A:85:ARG:HH11	1.82	0.45
3:C:179:ASN:O	3:C:180:ASN:HB2	2.17	0.44
6:L:67:SER:OG	6:L:68:GLY:N	2.50	0.44
2:B:172:ILE:HB	3:C:98:LEU:HD11	1.99	0.44
3:C:69:VAL:HG11	3:C:82:PHE:CD2	2.53	0.44
4:D:54:GLU:HG3	4:D:56:VAL:HG22	1.99	0.44
1:A:280:ILE:HG21	3:C:96:ASN:ND2	2.32	0.44
3:C:88:ILE:HG23	3:C:89:GLN:HG3	1.99	0.44
5:H:46:LEU:HD23	5:H:46:LEU:HA	1.86	0.44
2:B:243:ARG:HD3	2:B:243:ARG:H	1.83	0.44
6:L:83:PHE:HA	6:L:102:LYS:NZ	2.32	0.43
5:H:13:LYS:HG3	5:H:84:VAL:HG21	2.00	0.43
1:A:76:TYR:HB3	1:A:233:PHE:HB2	2.00	0.43
1:A:142:THR:HG23	1:A:225:VAL:HB	2.00	0.43
5:H:35:TRP:HB3	5:H:77:PHE:CE1	2.54	0.43
5:H:95:VAL:HB	5:H:111:VAL:HG13	2.01	0.43
6:L:89:GLN:HE21	6:L:95:ILE:HG23	1.84	0.43
1:A:20:LEU:H	1:A:20:LEU:HD23	1.84	0.42
2:B:25:THR:HG21	2:B:185:SER:OG	2.19	0.42
1:A:78:ASP:HB2	1:A:228:HIS:ND1	2.34	0.42
1:A:200:PHE:CE2	1:A:209:TYR:HB2	2.54	0.42
1:A:161:PHE:O	1:A:164:GLN:HG2	2.20	0.42
2:B:122:LEU:HD22	2:B:211:ILE:HG22	2.00	0.42
3:C:23:PRO:HG3	4:D:37:ALA:HB2	2.01	0.42
1:A:253:PRO:HA	1:A:254:PRO:HD3	1.94	0.42
2:B:243:ARG:NH2	2:B:246:ILE:HD11	2.35	0.42
1:A:63:LEU:HD12	1:A:246:ILE:HG21	2.02	0.42
1:A:253:PRO:HB3	2:B:169:CYS:HB2	2.01	0.42
3:C:71:ILE:HG12	3:C:210:CYS:O	2.20	0.41
2:B:27:GLU:HB2	2:B:184:ASN:ND2	2.34	0.41
1:A:183:THR:OG1	3:C:21:SER:HB2	2.20	0.41
1:A:76:TYR:O	1:A:76:TYR:CG	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:111:GLY:HA3	3:C:222:PHE:HA	2.02	0.41
5:H:3:GLN:HB3	5:H:25:SER:HB2	2.02	0.41
1:A:66:ALA:HB3	3:C:15:THR:HB	2.02	0.41
1:A:257:LEU:HD12	1:A:267:TYR:HB2	2.01	0.41
2:B:116:LYS:HD3	3:C:123:PHE:CD2	2.56	0.41
5:H:6:GLU:HA	5:H:22:CYS:HA	2.02	0.41
5:H:84:VAL:HG12	5:H:88:ASP:OD1	2.20	0.41
6:L:51:ALA:O	6:L:64:GLY:HA3	2.21	0.41
2:B:40:ASN:N	2:B:40:ASN:OD1	2.55	0.40
3:C:86:LEU:HD11	3:C:167:ILE:HG12	2.02	0.40
1:A:121:ILE:HG23	1:A:237:VAL:HG13	2.03	0.40
6:L:6:GLN:NE2	6:L:86:TYR:O	2.30	0.40
3:C:74:LEU:HD12	3:C:196:MET:HG3	2.02	0.40
1:A:16:ILE:H	1:A:16:ILE:HD12	1.86	0.40
1:A:26:LEU:HD13	3:C:160:GLN:HB2	2.04	0.40
5:H:30:SER:O	5:H:30:SER:OG	2.32	0.40
1:A:4:ILE:HD12	1:A:4:ILE:H	1.86	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	A	294/297 (99%)	274 (93%)	20 (7%)	0	100	100
2	B	235/248 (95%)	213 (91%)	22 (9%)	0	100	100
3	C	245/247 (99%)	233 (95%)	12 (5%)	0	100	100
4	D	26/68 (38%)	25 (96%)	1 (4%)	0	100	100
5	H	118/126 (94%)	103 (87%)	14 (12%)	1 (1%)	19	54
6	L	94/106 (89%)	80 (85%)	14 (15%)	0	100	100
All	All	1012/1092 (93%)	928 (92%)	83 (8%)	1 (0%)	54	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	H	14	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	A	255/256 (100%)	255 (100%)	0	100	100
2	B	201/209 (96%)	200 (100%)	1 (0%)	88	94
3	C	214/214 (100%)	213 (100%)	1 (0%)	88	94
4	D	25/55 (46%)	25 (100%)	0	100	100
5	H	106/110 (96%)	106 (100%)	0	100	100
6	L	81/89 (91%)	81 (100%)	0	100	100
All	All	882/933 (94%)	880 (100%)	2 (0%)	93	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	243	ARG
3	C	41	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	89	ASN
1	A	162	HIS
1	A	245	HIS
1	A	275	ASN
2	B	55	GLN
2	B	111	GLN
2	B	130	HIS
3	C	39	GLN

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Mol	Chain	Res	Type
3	C	48	GLN
3	C	96	ASN
3	C	235	GLN
3	C	238	HIS
3	C	247	GLN
5	H	31	ASN
5	H	40	GLN
5	H	113	ASN
6	L	37	GLN
6	L	38	GLN
6	L	79	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 monosaccharides 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.