



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Feb 5, 2020 – 12:35 PM EST

PDB ID : 6V4P
EMDB ID: : EMD-21044
Title : Structure of the integrin AlphaIIbBeta3-Abciximab complex
Authors : Nesic, D.; Zhang, Y.; Spasic, A.; Li, J.; Provasi, D.; Filizola, M.; Walz, T.;
Coller, B.S.
Deposited on : 2019-11-28
Resolution : 2.80 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) : 2.4

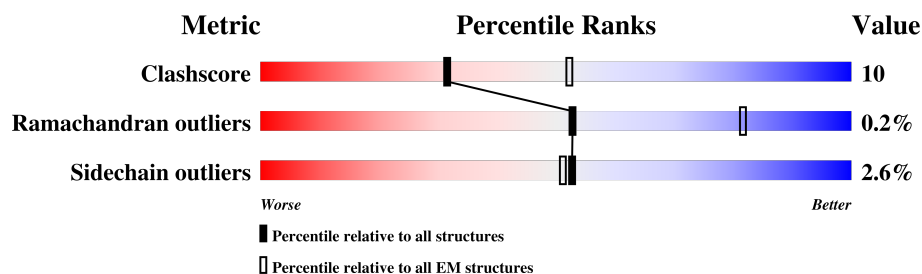
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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	A	963	
2	B	690	
3	C	225	
4	D	214	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9717 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 Integrin alpha-IIb.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	452	Total	C	N	O	S	0	0
			3467	2202	597	660	8		

- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	375	Total	C	N	O	S	0	0
			2927	1840	493	576	18		

- Molecule 3 is a protein called Abciximab, heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	221	Total	C	N	O	S	0	0
			1665	1061	268	328	8		

- Molecule 4 is a protein called Abciximab, light chain.

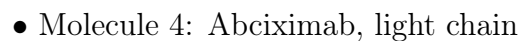
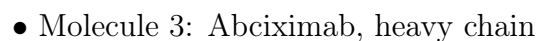
Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	214	Total	C	N	O	S	0	0
			1651	1028	278	338	7		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms		AltConf
5	B	2	Total	Ca	0
			2	2	
5	A	4	Total	Ca	0
			4	4	

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms		AltConf
6	B	1	Total	Mg	0
			1	1	



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	1161396	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, MG

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	A	0.34	0/3563	0.46	0/4855
2	B	0.30	0/2979	0.46	1/4036 (0.0%)
3	C	0.30	0/1709	0.45	0/2333
4	D	0.31	0/1687	0.47	0/2288
All	All	0.32	0/9938	0.46	1/13512 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	375	LEU	CA-CB-CG	-5.44	102.78	115.30

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	3467	0	3299	74	0
2	B	2927	0	2910	67	0
3	C	1665	0	1628	30	0
4	D	1651	0	1587	45	0
5	A	4	0	0	0	0
5	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	1	0	0	0	0
All	All	9717	0	9424	199	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 10.

All (199) 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:D:195:GLU:HG3	4:D:206:THR:HG23	1.26	1.13
1:A:299:ASN:ND2	1:A:332:LEU:HD22	1.64	1.11
4:D:195:GLU:HG3	4:D:206:THR:CG2	1.90	1.01
1:A:299:ASN:HD22	1:A:332:LEU:HD22	1.35	0.86
3:C:174:VAL:HG11	4:D:160:GLN:OE1	1.78	0.82
4:D:195:GLU:CG	4:D:206:THR:HG23	2.10	0.81
2:B:306:LEU:HB3	2:B:328:THR:HG22	1.67	0.77
4:D:78:VAL:HG13	4:D:82:ASP:HB2	1.68	0.74
2:B:417:LYS:NZ	2:B:421:PHE:O	2.20	0.74
3:C:14:PRO:HD2	3:C:118:ALA:HB2	1.73	0.71
3:C:174:VAL:CG1	4:D:160:GLN:OE1	2.40	0.70
4:D:195:GLU:HG2	4:D:197:THR:HG23	1.73	0.70
2:B:300:SER:O	2:B:360:ARG:NH1	2.25	0.70
1:A:59:ARG:NH1	1:A:62:GLY:O	2.24	0.69
1:A:296:THR:OG1	1:A:362:PRO:HB3	1.94	0.66
1:A:262:TRP:HB3	2:B:317:LEU:HD13	1.77	0.66
2:B:360:ARG:HB2	2:B:415:THR:HG23	1.78	0.65
1:A:395:GLN:OE1	1:A:400:ARG:NH1	2.30	0.65
1:A:205:SER:O	1:A:208:ARG:NH1	2.30	0.65
1:A:314:MET:HB3	1:A:322:LEU:HB3	1.80	0.63
3:C:24:ALA:HB1	3:C:27:TYR:HE1	1.64	0.63
3:C:4:LEU:HD21	3:C:98:LEU:HD12	1.81	0.63
1:A:278:HIS:NE2	1:A:340:LEU:O	2.32	0.63
2:B:111:PRO:HB3	2:B:148:ASN:HB3	1.80	0.62
3:C:39:GLN:NE2	4:D:38:GLN:OE1	2.28	0.62
3:C:174:VAL:CG2	4:D:162:SER:HB3	2.29	0.62
2:B:239:ARG:O	2:B:244:HIS:NE2	2.24	0.62
4:D:12:SER:HB3	4:D:107:LYS:HB2	1.82	0.62
1:A:386:ARG:NH2	1:A:409:SER:O	2.33	0.62
2:B:230:THR:HG23	2:B:304:ILE:HD12	1.81	0.61
1:A:107:CYS:HA	1:A:130:CYS:HA	1.82	0.61
1:A:9:THR:HB	1:A:447:VAL:HB	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:305:ASN:HB3	2:B:351:ILE:HD13	1.82	0.61
2:B:249:THR:HG22	2:B:309:ALA:HB3	1.83	0.60
2:B:394:THR:O	2:B:394:THR:HG23	2.01	0.60
4:D:19:VAL:HG21	4:D:78:VAL:HG21	1.84	0.59
4:D:137:ASN:ND2	4:D:138:ASN:OD1	2.35	0.59
4:D:13:VAL:HG11	4:D:19:VAL:HG22	1.84	0.59
2:B:157:VAL:HG21	2:B:213:SER:HB3	1.84	0.58
4:D:31:ASN:O	4:D:50:TYR:HA	2.04	0.58
1:A:296:THR:HG22	1:A:297:ASP:N	2.19	0.58
3:C:173:ALA:HB1	3:C:181:TYR:HB3	1.83	0.58
2:B:417:LYS:NZ	2:B:418:PRO:O	2.36	0.57
2:B:194:LEU:HD13	2:B:206:GLU:HG3	1.86	0.57
3:C:189:VAL:HG22	3:C:190:PRO:HD2	1.86	0.57
4:D:29:ILE:O	4:D:29:ILE:HG13	2.03	0.57
2:B:167:ILE:HD13	2:B:173:LEU:HD21	1.87	0.56
3:C:39:GLN:HB2	3:C:45:LEU:HD23	1.88	0.56
1:A:230:TYR:OH	1:A:279:ARG:NH2	2.34	0.56
1:A:176:THR:HG22	1:A:241:VAL:HG11	1.88	0.56
3:C:164:LEU:HD13	3:C:187:VAL:HG11	1.88	0.56
1:A:22:SER:OG	1:A:94:GLY:O	2.25	0.55
2:B:127:ASP:O	2:B:131:ILE:HG12	2.07	0.54
2:B:134:LEU:O	2:B:204:ASN:ND2	2.41	0.54
1:A:307:LEU:HD21	1:A:399:LEU:HD11	1.90	0.54
1:A:23:LEU:HD13	1:A:436:ILE:HG22	1.90	0.54
4:D:155:GLN:HG2	4:D:179:LEU:HD11	1.90	0.54
4:D:85:MET:HG2	4:D:87:PHE:CZ	2.43	0.54
1:A:436:ILE:HG13	1:A:447:VAL:HG22	1.89	0.53
2:B:202:ARG:NH2	2:B:206:GLU:OE2	2.40	0.53
1:A:390:LEU:HD23	1:A:403:PRO:HG3	1.89	0.53
2:B:342:GLN:NE2	2:B:346:ASP:OD1	2.42	0.53
3:C:38:LYS:HB2	3:C:48:ILE:HD11	1.90	0.53
1:A:299:ASN:HD22	1:A:332:LEU:CD2	2.14	0.53
1:A:311:PRO:HB2	1:A:355:ARG:HG3	1.90	0.53
1:A:117:GLU:HG2	1:A:118:LYS:HD2	1.89	0.53
4:D:39:THR:O	4:D:41:HIS:N	2.39	0.53
2:B:126:ASP:OD1	2:B:126:ASP:N	2.37	0.53
1:A:91:GLN:OE1	1:A:111:GLN:NE2	2.42	0.52
2:B:288:ASP:OD1	2:B:289:TYR:N	2.39	0.52
2:B:141:GLN:HB2	2:B:341:LEU:HD11	1.92	0.52
1:A:259:THR:HA	1:A:263:THR:HA	1.91	0.52
1:A:187:GLY:HA2	1:A:191:PHE:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:140:THR:OG1	3:C:189:VAL:O	2.27	0.51
1:A:25:PHE:CZ	1:A:436:ILE:HD13	2.45	0.51
4:D:115:VAL:HG21	4:D:196:VAL:HG21	1.92	0.51
2:B:126:ASP:HB3	4:D:50:TYR:CG	2.46	0.51
2:B:250:THR:HG22	2:B:310:VAL:HG12	1.93	0.50
4:D:39:THR:HG23	4:D:41:HIS:ND1	2.25	0.50
4:D:19:VAL:CG2	4:D:78:VAL:HG21	2.41	0.50
2:B:180:MET:O	4:D:96:TYR:OH	2.25	0.50
2:B:206:GLU:O	2:B:210:GLN:HG2	2.12	0.50
1:A:421:LEU:HD22	1:A:435:LEU:HD11	1.94	0.50
4:D:13:VAL:HG23	4:D:83:PHE:HE1	1.76	0.50
4:D:39:THR:O	4:D:39:THR:HG23	2.12	0.50
1:A:276:ARG:HD2	1:A:279:ARG:HB2	1.94	0.49
2:B:335:MET:SD	4:D:67:SER:OG	2.66	0.49
2:B:145:LEU:HD13	2:B:348:TYR:HD2	1.77	0.49
1:A:107:CYS:HB3	1:A:170:GLY:HA3	1.95	0.49
1:A:319:ASP:N	1:A:319:ASP:OD1	2.43	0.49
2:B:244:HIS:HB2	2:B:304:ILE:HA	1.93	0.49
2:B:109:ASP:HA	2:B:146:THR:HA	1.95	0.49
2:B:373:THR:HB	2:B:396:SER:HB2	1.95	0.49
3:C:24:ALA:HB1	3:C:27:TYR:CE1	2.45	0.49
3:C:48:ILE:HG21	3:C:81:MET:HE1	1.93	0.49
1:A:84:LEU:HB3	1:A:113:TRP:CH2	2.48	0.49
3:C:168:VAL:HG12	3:C:187:VAL:HG22	1.94	0.48
1:A:26:HIS:HB2	1:A:36:VAL:HG23	1.96	0.48
1:A:427:ILE:HG13	1:A:427:ILE:H	1.40	0.48
2:B:114:ILE:HB	2:B:151:ILE:HG22	1.94	0.48
3:C:160:ASN:HD21	3:C:199:TYR:HA	1.79	0.47
4:D:37:GLN:HB2	4:D:47:LEU:HD11	1.97	0.47
1:A:172:SER:OG	1:A:236:GLY:O	2.27	0.47
2:B:362:LEU:HD12	2:B:363:PRO:HD2	1.97	0.47
4:D:108:ARG:HH12	4:D:111:ALA:HB2	1.80	0.47
4:D:167:ASP:OD1	4:D:168:SER:N	2.41	0.47
4:D:94:TRP:CD2	4:D:95:PRO:HA	2.50	0.47
4:D:141:PRO:HB2	4:D:143:GLU:HG2	1.97	0.47
1:A:292:SER:OG	1:A:357:GLY:O	2.33	0.47
4:D:61:ARG:HD2	4:D:82:ASP:OD2	2.14	0.47
4:D:2:ILE:HD13	4:D:29:ILE:HG22	1.96	0.47
1:A:363:LEU:HD21	1:A:435:LEU:HD13	1.95	0.46
3:C:104:VAL:HG11	4:D:49:LYS:HB2	1.96	0.46
3:C:18:VAL:HG12	3:C:86:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:49:LYS:HG3	4:D:53:GLN:HB2	1.96	0.46
1:A:91:GLN:HB2	1:A:111:GLN:HB2	1.96	0.46
4:D:66:GLY:HA3	4:D:71:PHE:HA	1.98	0.46
1:A:149:ASN:N	1:A:149:ASN:OD1	2.47	0.46
1:A:432:TYR:CZ	1:A:452:PRO:HA	2.51	0.46
2:B:117:LEU:HD11	2:B:225:ALA:HB1	1.98	0.46
1:A:291:HIS:CD2	2:B:258:LEU:HD13	2.51	0.46
2:B:315:VAL:HG21	2:B:332:VAL:HG22	1.98	0.46
2:B:399:ILE:HD13	2:B:416:ILE:HD13	1.97	0.46
1:A:242:GLY:HA3	1:A:295:VAL:HG11	1.98	0.45
2:B:109:ASP:OD2	2:B:147:SER:OG	2.32	0.45
2:B:142:MET:HB3	2:B:149:LEU:HD22	1.96	0.45
3:C:146:LEU:HD13	3:C:148:LYS:HB2	1.97	0.45
2:B:227:MET:SD	2:B:298:LYS:HG3	2.57	0.45
3:C:14:PRO:CD	3:C:118:ALA:HB2	2.45	0.45
2:B:278:ASP:OD1	2:B:278:ASP:N	2.49	0.45
1:A:82:GLN:HE22	1:A:149:ASN:HB2	1.81	0.45
2:B:417:LYS:HB3	2:B:424:SER:HB3	1.99	0.45
3:C:174:VAL:HG21	4:D:162:SER:HB3	1.99	0.45
1:A:248:LEU:HD23	1:A:248:LEU:H	1.81	0.45
1:A:361:ALA:HB2	1:A:421:LEU:HB3	1.98	0.45
4:D:142:ARG:HH21	4:D:163:VAL:HG11	1.82	0.45
4:D:34:HIS:HB3	4:D:46:LEU:HD11	1.99	0.45
2:B:412:LYS:HG3	2:B:431:PHE:HE2	1.82	0.45
2:B:69:LEU:HD11	2:B:103:GLN:HB3	1.99	0.45
2:B:139:ALA:HB2	2:B:200:VAL:HG11	1.99	0.44
1:A:21:PHE:CE2	2:B:266:VAL:HG11	2.51	0.44
2:B:156:PHE:HB3	2:B:225:ALA:HB2	1.99	0.44
1:A:230:TYR:HH	1:A:279:ARG:HH21	1.63	0.44
1:A:377:ALA:HB2	1:A:421:LEU:HD11	2.00	0.44
4:D:78:VAL:HG11	4:D:83:PHE:CE1	2.52	0.44
1:A:368:ARG:HG3	1:A:432:TYR:CE2	2.53	0.44
1:A:2:ASN:OD1	1:A:2:ASN:N	2.50	0.44
2:B:181:LYS:HE2	3:C:59:SER:OG	2.18	0.44
1:A:296:THR:CG2	1:A:297:ASP:N	2.80	0.43
2:B:308:PHE:HB2	2:B:330:VAL:HG22	2.00	0.43
2:B:181:LYS:HB3	3:C:35:HIS:CE1	2.53	0.43
1:A:114:ASN:HB2	1:A:124:LYS:HB2	2.00	0.43
1:A:363:LEU:HD11	1:A:375:ALA:HB2	1.99	0.43
1:A:366:LEU:N	1:A:373:ASP:OD2	2.41	0.43
2:B:74:SER:HB3	2:B:109:ASP:HB3	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:182:THR:HA	3:C:99:TYR:CZ	2.53	0.43
3:C:149:ASP:OD1	3:C:176:GLN:NE2	2.51	0.43
3:C:51:ILE:O	3:C:53:PRO:HD3	2.18	0.43
1:A:86:THR:HG23	1:A:212:LEU:HD13	2.00	0.43
2:B:120:LEU:HA	2:B:120:LEU:HD23	1.81	0.43
1:A:92:GLY:HA3	1:A:110:TRP:CE3	2.53	0.43
3:C:124:PRO:HD2	3:C:210:THR:HG21	2.01	0.43
4:D:119:PRO:HG3	4:D:211:ARG:HD2	2.01	0.43
1:A:335:ARG:H	1:A:335:ARG:HG2	1.59	0.43
1:A:25:PHE:HZ	1:A:436:ILE:HD13	1.84	0.43
2:B:418:PRO:HG2	2:B:421:PHE:HB2	2.01	0.42
1:A:76:THR:O	1:A:77:ARG:HD2	2.19	0.42
1:A:53:VAL:HG21	1:A:106:ALA:CB	2.50	0.42
2:B:184:CYS:HB2	2:B:212:VAL:O	2.19	0.42
4:D:24:ARG:HA	4:D:69:THR:O	2.18	0.42
1:A:121:GLU:HG3	1:A:123:GLU:H	1.84	0.42
1:A:260:TRP:CE3	1:A:266:ALA:HB2	2.54	0.42
2:B:152:GLY:N	2:B:196:LEU:HD23	2.33	0.42
2:B:414:PHE:HE2	2:B:416:ILE:HD11	1.85	0.42
2:B:215:ASN:OD1	2:B:215:ASN:N	2.53	0.42
1:A:132:LEU:HD23	1:A:200:VAL:HG13	2.00	0.42
1:A:58:TRP:CZ3	1:A:447:VAL:HG11	2.55	0.42
2:B:394:THR:O	2:B:394:THR:CG2	2.66	0.42
4:D:151:ASP:H	4:D:191:VAL:HB	1.85	0.42
1:A:395:GLN:NE2	1:A:399:LEU:O	2.53	0.42
2:B:183:THR:HG23	3:C:99:TYR:OH	2.20	0.41
1:A:100:TRP:CG	1:A:101:SER:N	2.89	0.41
1:A:82:GLN:NE2	1:A:149:ASN:HB2	2.36	0.41
1:A:436:ILE:HD11	1:A:447:VAL:HG13	2.03	0.41
2:B:375:LEU:O	2:B:377:ASN:N	2.54	0.41
1:A:195:LEU:HG	1:A:235:TRP:CZ3	2.56	0.41
2:B:142:MET:HG2	2:B:149:LEU:HD13	2.03	0.41
1:A:21:PHE:HE2	2:B:266:VAL:HG11	1.85	0.41
2:B:175:ASN:OD1	2:B:183:THR:HA	2.21	0.41
2:B:188:PHE:CZ	2:B:191:LYS:HE2	2.56	0.41
1:A:1:LEU:HB2	1:A:393:LEU:HD11	2.03	0.40
1:A:24:ASP:OD1	1:A:25:PHE:N	2.47	0.40
4:D:133:VAL:HG22	4:D:178:THR:HG22	2.03	0.40
2:B:219:PRO:HB2	2:B:255:HIS:CE1	2.56	0.40
2:B:319:GLN:O	2:B:323:GLU:HG2	2.22	0.40
1:A:143:TYR:CZ	1:A:145:PRO:HB3	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ALA:HA	1:A:207:TYR:CD2	2.56	0.40
3:C:164:LEU:HD11	3:C:199:TYR:CD1	2.57	0.40
4:D:167:ASP:HB3	4:D:170:ASP:O	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	A	450/963 (47%)	434 (96%)	16 (4%)	0	100	100
2	B	373/690 (54%)	360 (96%)	11 (3%)	2 (0%)	31	65
3	C	219/225 (97%)	211 (96%)	8 (4%)	0	100	100
4	D	212/214 (99%)	195 (92%)	16 (8%)	1 (0%)	31	65
All	All	1254/2092 (60%)	1200 (96%)	51 (4%)	3 (0%)	53	81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	30	SER
2	B	376	ASN
2	B	374	CYS

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	360/799 (45%)	351 (98%)	9 (2%)	50	82
2	B	336/605 (56%)	326 (97%)	10 (3%)	44	78
3	C	187/191 (98%)	183 (98%)	4 (2%)	56	86
4	D	192/192 (100%)	187 (97%)	5 (3%)	49	81
All	All	1075/1787 (60%)	1047 (97%)	28 (3%)	53	81

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	77	ARG
1	A	166	TYR
1	A	270	LEU
1	A	285	MET
1	A	288	TYR
1	A	355	ARG
1	A	413	THR
1	A	427	ILE
2	B	81	THR
2	B	109	ASP
2	B	126	ASP
2	B	127	ASP
2	B	167	ILE
2	B	187	MET
2	B	262	LEU
2	B	294	LEU
2	B	415	THR
2	B	417	LYS
3	C	47	TRP
3	C	81	MET
3	C	98	LEU
3	C	189	VAL
4	D	85	MET
4	D	103	LYS
4	D	119	PRO
4	D	179	LEU
4	D	181	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	85	GLN
2	B	199	GLN
2	B	280	HIS
3	C	3	GLN
4	D	32	ASN
4	D	92	ASN
4	D	124	GLN
4	D	137	ASN
4	D	147	GLN
4	D	155	GLN

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 ⓘ

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.