Integrative Structure Validation Report

July 22, 2024 - 03:51 PM PDT

The following software was used in the production of this report:

Python-IHM Version 1.3
MolProbity Version 4.5.2
Integrative Modeling Validation Version 1.2

PDB ID	8ZZU
PDB-Dev ID	PDBDEV_00000030
Structure Title	Molecular Architecture of Human Fibrin Clots
Structure Authors	Oleg Klykov; Carmen van der Zwaan; Albert J.R. Heck; Alexander B. Meijer; Richard A. Scheltema

This is a PDB-Dev IM Structure Validation Report for a publicly released PDB-Dev entry.

We welcome your comments at pdb-dev@mail.wwpdb.org

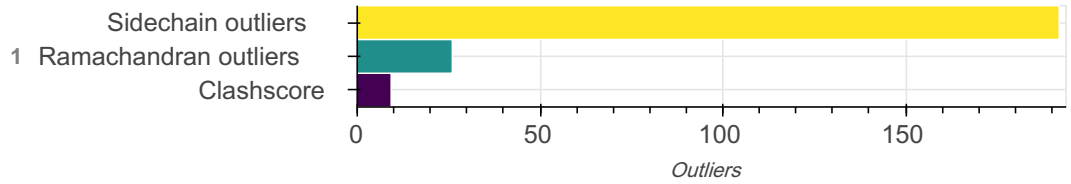
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

List of references used to build this report is available here.

Overall quality

This validation report contains model quality assessments for all structures, data quality assessment for SAS datasets and fit to model assessments for SAS datasets. Data quality and fit to model assessments for other datasets and model uncertainty are under development. Number of plots is limited to 256.

Model Quality: MolProbity Analysis



Ensemble information

This entry consists of 0 distinct ensemble(s).

Summary

This entry consists of 1 unique models, with 13 subunits in each model. A total of 9 datasets or restraints were used to build this entry. Each model is represented by 14 rigid bodies and 7 flexible or non-rigid units.

Entry composition

There is 1 unique type of models in this entry. This model is titled ?/Best scoring model.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	RGD-containing Alpha Domain Alpha_558-620	A	I	63
1	2	2	Subunit Alpha_46-219	B	A	174
1	3	3	Subunit Alpha_220-249	C	Z	30
1	4	4	Subunit Beta	D	B	401
1	5	5	Subunit Gamma	E	C	381
1	6	6	Interactive Alpha Domain Alpha_432-491	F	H	60
1	7	2	Subunit Alpha_46-219	G	D	174
1	8	3	Subunit Alpha_220-249	H	Y	30
1	9	7	Beta N-term Beta_55-84	I	K	34
1	10	4	Subunit Beta	J	E	401

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	11	5	Subunit Gamma	K	F	381
1	12	6	Interactive Alpha Domain Alpha_432-491	L	G	60
1	13	1	RGD-containing Alpha Domain Alpha_558-620	M	J	63

Datasets used for modeling

There are 9 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Experimental model	PDB	3GHG
2	De Novo model	Not available	Not available
3	De Novo model	Not available	Not available
4	De Novo model	Not available	Not available
5	De Novo model	Not available	Not available
6	Crosslinking-MS data	PRIDE	PXD011680
7	De Novo model	Not available	Not available
8	De Novo model	Not available	Not available
9	De Novo model	Not available	Not available

Representation

This entry has only one representation and includes 14 rigid bodies and 7 flexible units

Chain ID	Rigid bodies	Non-rigid segments
A	-	1-12, 36-52

Chain ID	Rigid bodies	Non-rigid segments
B	13-35, 53-6313-35, 53-63	-
C	-	-
D	1-1741-174	-
E	1-301-30	-
F	-	1-28
G	1-4011-401	-
H	-	-
I	-	1-34
J	1-3811-381	-
K	29-6029-60	-
L	-	1-28
M	-	1-12, 36-52

Methodology and software

This entry is a result of 1 distinct protocol(s).

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
1	1	_	_	None	_	False	False

There are 8 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	ThreaDomEx	Not available	None	https://zhanglab.ccmb.med.umich.edu/ThreaDomEx/
2	Robetta	Not available	model building	http://robetta.bakerlab.org

ID	Software name	Software version	Software classification	Software location
3	HHalign-Kbest	Not available	model building	http://bioserv.rpbs.univ-paris-diderot.fr/services/HHalign-Kbest/
4	I-TASSER	Not available	model building	https://zhanglab.ccmb.med.umich.edu/I-TASSER/
5	RaptorX	Not available	model building	http://raptorx.uchicago.edu
6	HADDOCK	2.2	model building	https://haddock.science.uu.nl
7	CPORT	Not available	None	https://milou.science.uu.nl/services/CPORT/
8	DisVis	Not available	None	https://milou.science.uu.nl/cgi/services/DISVIS/disvis/

Data quality

Crosslinking-MS

Validation for this section is under development.

Model quality

For models with atomic structures, molprobity analysis is performed. For models with coarse-grained or multi-scale structures, excluded volume analysis is performed.

Standard geometry: bond outliers

There are 4278 bond outliers in this entry. A summary is provided below, and a detailed list of outliers can be found here.

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
N--H	0.97	0.86	2
N--H	0.98	0.86	2001
ND2--HD22	0.98	0.86	127
ND2--HD21	0.98	0.86	110

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NE2--HE22	0.98	0.86	109
NE2--HE21	0.98	0.86	105
NE1--HE1	0.98	0.86	36
OH--HH	0.96	0.84	31
NE2--HE2	0.98	0.86	20
OG--HG	0.96	0.84	71
OG1--HG1	0.96	0.84	56
NE--HE	0.98	0.86	38
ND1--HD1	0.98	0.86	10
NE2--HE21	0.99	0.86	10
N--H	0.99	0.86	154
NE2--HE22	0.99	0.86	6
OG1--HG1	0.97	0.84	81
NE--HE	0.99	0.86	59
OG--HG	0.97	0.84	105
OH--HH	0.97	0.84	58
ND2--HD21	0.99	0.86	23
ND1--HD1	0.99	0.86	8
SG--HG	1.33	1.20	6
NE1--HE1	0.99	0.86	16
ND2--HD22	0.99	0.86	7
NE2--HE2	0.99	0.86	6
NE--HE	1.00	0.86	7

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
OG--HG	0.98	0.84	8
OG1--HG1	0.98	0.84	2
OH--HH	0.98	0.84	4
ND2--HD21	1.00	0.86	1
NH2--HH21	1.00	0.86	65
NH1--HH12	1.00	0.86	76
NH1--HH11	1.00	0.86	74
NH2--HH22	1.00	0.86	68
NZ--HZ2	1.03	0.89	1
NZ--HZ3	1.03	0.89	1
NH2--HH21	1.01	0.86	37
NH2--HH22	1.01	0.86	32
NH1--HH11	1.01	0.86	29
NH1--HH12	1.01	0.86	28
NZ--HZ3	1.04	0.89	172
NZ--HZ1	1.04	0.89	169
NZ--HZ2	1.04	0.89	164
NZ--HZ2	1.05	0.89	30
NZ--HZ3	1.05	0.89	22
NH2--HH22	1.02	0.86	4
NH1--HH11	1.02	0.86	1
NZ--HZ1	1.05	0.89	26
NH2--HH21	1.02	0.86	2

Standard geometry: angle outliers

Bond angle outliers do not exist or can not be evaluated for this model

Too-close contacts

The following all-atom clashscore is based on a MolProbity analysis. All-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The table below contains clashscores for all the models in this entry.

Model ID	Clash score	Number of clashes
1	9.27	327

All 327 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:63:LYS:C	I:3:ARG:HD3	1.582
1	A:63:LYS:HG3	I:3:ARG:CD	1.523
1	A:63:LYS:CG	I:3:ARG:HD2	1.506
1	A:60:HIS:CB	I:3:ARG:HH21	1.506
1	A:60:HIS:HB3	I:3:ARG:NH2	1.421
1	A:61:SER:C	I:3:ARG:HH12	1.309
1	A:63:LYS:O	I:3:ARG:HD3	1.242
1	A:62:THR:N	I:3:ARG:HH12	1.196
1	A:63:LYS:C	I:3:ARG:CD	1.191
1	A:63:LYS:CG	I:3:ARG:CD	1.162
1	A:60:HIS:C	I:3:ARG:NH2	1.153
1	A:63:LYS:O	I:3:ARG:CD	1.149
1	A:62:THR:N	I:3:ARG:NH1	1.096
1	A:61:SER:C	I:3:ARG:NH1	1.033
1	A:12:GLU:HG3	H:18:PHE:CE1	1.027
1	A:63:LYS:CB	I:3:ARG:HD2	1.008

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:61:SER:OG	H:24:LYS:NZ	0.985
1	A:63:LYS:HG2	I:3:ARG:HD2	0.975
1	C:14:VAL:HG13	C:15:PRO:HD3	0.973
1	A:61:SER:N	I:3:ARG:NH2	0.960
1	A:63:LYS:CA	I:3:ARG:HD3	0.933
1	A:60:HIS:CA	I:3:ARG:NH2	0.930
1	A:62:THR:H	I:3:ARG:HH22	0.894
1	A:60:HIS:CB	I:3:ARG:NH2	0.889
1	A:60:HIS:HB3	I:3:ARG:CZ	0.882
1	A:60:HIS:CA	I:3:ARG:HH21	0.870
1	A:63:LYS:HG3	I:3:ARG:CG	0.847
1	A:60:HIS:C	I:3:ARG:CZ	0.844
1	A:61:SER:N	I:3:ARG:HH22	0.839
1	A:62:THR:H	I:3:ARG:NH2	0.827
1	C:25:VAL:HB	C:26:PRO:HD3	0.825
1	D:237:LEU:HB3	D:242:ILE:HD11	0.825
1	K:238:GLU:HB3	K:368:LYS:HB2	0.818
1	A:63:LYS:HE3	I:3:ARG:O	0.797
1	A:60:HIS:HB2	I:3:ARG:HE	0.790
1	A:63:LYS:CA	I:3:ARG:CD	0.788
1	A:63:LYS:HG2	I:3:ARG:CD	0.785
1	J:328:TRP:HB2	J:349:ARG:HA	0.751
1	E:237:LEU:HB3	E:366:MET:HE2	0.747

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	L:25:THR:HG21	A:22:TYR:C	0.745
1	D:210:ASP:HB3	D:211:PRO:HD3	0.740
1	A:62:THR:N	I:3:ARG:CZ	0.740
1	F:10:GLU:HA	F:20:SER:HA	0.738
1	J:199:GLN:HA	J:392:LYS:HG2	0.738
1	D:70:LYS:HD3	C:12:ASP:HB2	0.734
1	L:25:THR:CG2	A:22:TYR:C	0.733
1	J:258:GLU:HB3	J:392:LYS:HB2	0.733
1	D:311:THR:HB	D:352:ALA:HB2	0.720
1	J:125:LEU:HD23	K:111:LEU:HD13	0.703
1	A:62:THR:N	I:3:ARG:HH22	0.699
1	L:25:THR:HG21	A:22:TYR:N	0.697
1	A:60:HIS:CB	I:3:ARG:CZ	0.690
1	J:341:ASP:HA	J:376:ASP:HB2	0.690
1	D:94:LEU:HD13	J:102:SER:HB3	0.688
1	A:63:LYS:CB	I:3:ARG:CD	0.683
1	J:246:THR:HB	J:273:THR:HA	0.683
1	A:62:THR:N	I:3:ARG:NH2	0.682
1	E:374:ILE:HG12	E:375:PRO:HD2	0.681
1	K:105:ASN:HA	K:108:ILE:HD12	0.679
1	D:90:GLU:O	D:94:LEU:HG	0.670
1	A:60:HIS:NE2	H:17:ASN:HA	0.666
1	I:21:TYR:HB3	I:24:ARG:HB2	0.663

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:60:HIS:CE1	H:17:ASN:HA	0.661
1	D:198:ARG:HB3	D:393:MET:HB3	0.660
1	A:48:ASP:HA	A:54:ALA:HB2	0.658
1	E:243:ARG:HG2	G:28:LEU:HD22	0.656
1	K:247:ALA:HB2	K:273:ALA:HB3	0.655
1	B:25:MET:HE1	E:13:ALA:HB3	0.651
1	A:60:HIS:HB3	I:3:ARG:HH21	0.650
1	A:63:LYS:HG2	I:3:ARG:NE	0.649
1	J:99:THR:HA	J:103:ASN:HB2	0.648
1	D:69:GLN:HB3	C:14:VAL:HG21	0.644
1	K:291:PHE:HB3	K:325:LYS:HB3	0.642
1	J:34:ARG:HB2	J:35:PRO:HD3	0.636
1	A:63:LYS:CD	I:3:ARG:HA	0.631
1	D:82:VAL:HA	C:4:LEU:HD12	0.628
1	A:60:HIS:CB	I:3:ARG:HE	0.626
1	K:179:THR:HB	K:373:ILE:HG13	0.626
1	G:24:ARG:O	G:28:LEU:HG	0.624
1	J:355:PRO:HA	J:378:VAL:HG13	0.623
1	J:104:ILE:HB	J:105:PRO:HD3	0.617
1	B:64:ILE:O	B:68:LEU:HG	0.615
1	A:63:LYS:CG	I:3:ARG:NE	0.614
1	D:341:ASP:HA	D:376:ASP:HB2	0.612
1	K:330:HIS:O	K:354:ILE:HA	0.611

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	J:243:SER:HA	J:274:VAL:HB	0.610
1	J:268:HIS:HB3	J:289:ARG:HG3	0.605
1	A:20:SER:HB2	H:26:PRO:HB3	0.604
1	A:60:HIS:HB2	I:3:ARG:NE	0.603
1	J:316:MET:HG3	J:348:ASN:HB2	0.602
1	C:15:PRO:HD2	C:18:PHE:HB3	0.600
1	E:236:GLU:HG2	E:246:THR:HG23	0.599
1	F:9:LYS:HG3	F:10:GLU:OE1	0.593
1	K:302:TRP:HB3	K:315:GLU:HA	0.589
1	E:53:LEU:HD12	J:127:SER:HB3	0.588
1	F:6:LYS:HB2	F:48:THR:HG21	0.588
1	K:245:SER:HB2	K:273:ALA:HB2	0.587
1	A:60:HIS:CB	I:3:ARG:NE	0.586
1	L:29:SER:HB3	H:28:GLU:HG3	0.586
1	D:81:VAL:HG13	D:82:VAL:HG23	0.585
1	J:88:GLU:O	J:89:LEU:HG	0.585
1	A:63:LYS:O	I:3:ARG:NH1	0.582
1	A:12:GLU:HG3	H:18:PHE:HE1	0.578
1	J:237:LEU:HD23	J:242:ILE:HG12	0.578
1	K:343:LYS:HG3	K:363:TRP:HE1	0.578
1	D:258:GLU:HB3	D:392:LYS:HB2	0.573
1	D:34:ARG:HB3	D:35:PRO:HD3	0.569
1	K:36:GLN:HG3	K:40:LYS:HE3	0.569

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	E:309:PHE:HB2	E:313:CYS:SG	0.568
1	J:58:PHE:HE1	K:41:THR:HA	0.567
1	J:204:ASP:HB3	J:207:ARG:HH21	0.566
1	J:358:ARG:N	J:377:GLY:HA2	0.562
1	J:98:GLU:O	J:102:SER:HB2	0.559
1	L:25:THR:HG23	A:22:TYR:C	0.558
1	A:63:LYS:HD2	I:3:ARG:HA	0.557
1	G:11:SER:O	G:14:ASP:HB2	0.557
1	D:148:VAL:HG11	E:215:LEU:HA	0.555
1	B:139:CYS:HB3	D:136:CYS:HA	0.553
1	E:63:PRO:HG3	J:116:GLU:HB2	0.553
1	C:14:VAL:CG1	C:15:PRO:HD3	0.546
1	D:156:GLU:O	D:160:LYS:HG3	0.542
1	A:63:LYS:HG3	I:3:ARG:HA	0.538
1	G:139:CYS:HB3	J:136:CYS:HA	0.538
1	J:338:SER:HB3	J:347:TYR:CE2	0.538
1	D:260:TRP:HB3	I:1:LYS:HD3	0.537
1	E:312:ASN:HB3	E:315:GLU:HB2	0.537
1	G:25:MET:HG3	K:9:THR:HG22	0.537
1	D:196:GLN:HG3	D:236:TRP:HE3	0.535
1	A:63:LYS:CG	I:3:ARG:HA	0.534
1	L:25:THR:HG21	A:22:TYR:CA	0.530
1	J:58:PHE:CE1	K:41:THR:HA	0.530

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	K:321:TRP:HB3	K:323:MET:HE3	0.530
1	G:146:GLU:HG2	C:15:PRO:HB3	0.529
1	J:107:ASN:HA	J:110:VAL:HG12	0.529
1	G:121:MET:HE1	J:125:LEU:HD22	0.528
1	J:198:ARG:HB2	J:393:MET:HB3	0.527
1	J:210:ASP:HB3	J:211:PRO:HD3	0.527
1	G:136:ARG:HD3	J:202:SER:OG	0.526
1	D:156:GLU:HG2	D:159:ARG:NH2	0.521
1	G:43:LEU:HG	K:30:LEU:HD23	0.521
1	K:170:GLU:HB2	K:178:TRP:HB2	0.520
1	D:223:THR:HB	D:226:LYS:HB2	0.519
1	D:354:ASN:O	D:378:VAL:HA	0.519
1	E:243:ARG:HD3	G:28:LEU:HD13	0.519
1	J:197:ASN:O	J:234:GLU:HA	0.518
1	D:74:GLN:HB2	C:10:VAL:HB	0.517
1	D:316:MET:HG3	D:348:ASN:HB2	0.517
1	D:155:GLU:HG2	D:401:PHE:HE2	0.515
1	J:93:GLN:O	J:97:ASP:HB2	0.515
1	J:112:ARG:HD3	J:116:GLU:OE1	0.514
1	J:161:GLY:HA3	K:197:GLN:HG2	0.514
1	K:237:LEU:HD23	K:366:MET:HG3	0.514
1	J:60:TYR:O	J:63:LEU:HG	0.513
1	K:291:PHE:HB3	K:325:LYS:CB	0.513

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	J:265:VAL:HB	J:291:THR:O	0.512
1	F:38:VAL:HB	F:46:GLU:HB3	0.511
1	E:239:ASP:OD2	E:243:ARG:HB2	0.510
1	E:185:LEU:HG	E:212:GLU:HG2	0.509
1	F:28:ARG:O	F:54:SER:HA	0.508
1	D:161:GLY:HA3	E:197:GLN:HG2	0.505
1	F:36:LYS:HE2	F:38:VAL:HG22	0.505
1	E:181:PHE:HE2	E:373:ILE:HG23	0.503
1	E:83:TYR:O	E:87:ILE:HG12	0.499
1	H:2:LEU:N	H:3:PRO:HD2	0.494
1	G:92:ARG:HG3	G:93:ILE:HG13	0.493
1	J:120:SER:O	J:123:GLN:HG3	0.493
1	J:354:ASN:O	J:378:VAL:HA	0.493
1	L:25:THR:HG23	A:23:SER:N	0.492
1	E:292:THR:HB	E:328:ALA:HB2	0.491
1	D:245:LEU:HA	D:248:MET:HE2	0.490
1	J:72:GLN:O	J:76:LYS:HB2	0.490
1	L:28:ARG:H	L:52:VAL:HG11	0.490
1	D:26:GLN:O	D:30:LEU:HG	0.489
1	J:169:LEU:HD22	K:166:LEU:HD12	0.489
1	J:272:PHE:HE1	J:283:ILE:HD11	0.489
1	L:25:THR:HG21	A:21:SER:C	0.488
1	E:282:PHE:HA	G:12:ASP:HB2	0.488

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	J:196:GLN:HG3	J:236:TRP:HE3	0.488
1	K:300:SER:HA	K:306:ASN:HB2	0.487
1	K:356:TRP:HD1	K:359:TRP:HB2	0.487
1	L:38:VAL:HB	L:46:GLU:HB3	0.487
1	B:127:ASP:O	B:131:LYS:HG2	0.486
1	E:271:GLY:O	G:5:SER:HA	0.484
1	B:135:CYS:HB3	B:139:CYS:SG	0.482
1	D:73:LYS:HG3	C:14:VAL:HG23	0.481
1	B:151:ASP:HA	K:63:PRO:HG3	0.480
1	G:168:LEU:N	G:169:PRO:HD3	0.479
1	D:94:LEU:CD1	J:102:SER:HB3	0.476
1	F:27:ARG:HB2	F:52:VAL:HG11	0.474
1	J:379:VAL:HG22	J:389:SER:HA	0.473
1	J:380:TRP:CD1	J:383:TRP:HB2	0.473
1	K:199:LYS:HA	K:217:ASN:HB2	0.473
1	E:203:GLY:HA3	E:213:PHE:HA	0.472
1	K:282:PHE:HZ	K:328:ALA:HA	0.471
1	A:63:LYS:HG3	I:3:ARG:HD2	0.470
1	B:143:LEU:HD23	B:145:ARG:HD2	0.468
1	E:13:ALA:HB2	E:16:LEU:HB3	0.467
1	B:86:SER:HB3	C:5:ILE:HG23	0.466
1	E:255:GLY:O	E:261:TYR:HA	0.466
1	G:93:ILE:HG12	G:96:LEU:HB2	0.466

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	E:193:LYS:HB3	E:197:GLN:HB2	0.465
1	K:43:GLU:O	K:47:LEU:HG	0.465
1	E:243:ARG:HA	J:3:PRO:HG2	0.464
1	J:258:GLU:HG3	J:264:LYS:HG2	0.464
1	K:178:TRP:CZ3	K:234:ARG:HD2	0.464
1	E:136:THR:HG23	E:155:PHE:HB3	0.462
1	K:33:ILE:O	K:37:VAL:HG23	0.462
1	G:48:PHE:HD1	G:52:LYS:HE3	0.461
1	D:154:CYS:HA	D:157:ILE:HD12	0.460
1	K:218:GLU:O	K:222:LEU:HG	0.460
1	D:320:THR:HG22	D:344:GLY:HA3	0.458
1	E:28:GLN:HA	E:31:GLU:HG2	0.455
1	J:326:ASP:HB2	J:336:GLN:HE21	0.454
1	H:10:VAL:HG13	H:13:LEU:HG	0.453
1	J:358:ARG:H	J:377:GLY:HA2	0.453
1	B:154:ASP:HA	B:157:LYS:HE3	0.451
1	E:193:LYS:HB3	E:197:GLN:CB	0.451
1	K:331:LEU:HA	K:354:ILE:HG23	0.451
1	F:2:LEU:HD13	F:11:LEU:HD22	0.450
1	J:280:LYS:HB3	J:325:ASN:HD21	0.450
1	B:10:CYS:O	K:270:GLY:HA3	0.450
1	D:25:LEU:O	D:29:LEU:HG	0.448
1	D:148:VAL:HG22	E:205:LEU:HG	0.448

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	I:10:ARG:HA	I:10:ARG:NE	0.448
1	G:124:LEU:HG	G:128:ILE:HD11	0.446
1	J:328:TRP:HH2	J:335:LYS:HE3	0.446
1	E:241:ASN:HB3	E:243:ARG:HG3	0.445
1	D:154:CYS:SG	D:193:THR:HG23	0.444
1	D:195:ILE:HG23	D:242:ILE:HD13	0.444
1	D:258:GLU:HA	D:263:ASP:O	0.444
1	D:281:TYR:HB2	D:318:PHE:HB2	0.444
1	G:122:LYS:HE2	J:369:MET:HE2	0.444
1	A:60:HIS:O	I:3:ARG:CZ	0.444
1	J:77:ASP:O	J:80:ASN:HB3	0.443
1	A:63:LYS:O	I:3:ARG:CG	0.443
1	B:168:LEU:N	B:169:PRO:HD3	0.442
1	K:273:ALA:HA	K:359:TRP:CD1	0.442
1	D:192:TRP:HB3	D:396:LYS:HB3	0.441
1	G:118:LEU:HD12	J:118:LEU:HD21	0.441
1	J:89:LEU:HD23	J:92:HIS:HB2	0.440
1	D:153:GLU:OE2	D:155:GLU:HB3	0.438
1	D:240:ASP:HA	D:243:SER:OG	0.438
1	D:56:SER:O	D:59:GLN:HG3	0.437
1	D:161:GLY:HA3	E:197:GLN:CG	0.437
1	E:237:LEU:O	E:244:THR:HA	0.437
1	L:31:SER:HA	L:52:VAL:O	0.436

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	D:198:ARG:HD3	D:359:TYR:HD2	0.435
1	D:303:LEU:HB3	D:307:ASN:HB3	0.435
1	H:11:PRO:HA	H:14:VAL:HB	0.435
1	J:12:ASP:HA	J:13:PRO:HD3	0.435
1	K:140:CYS:SG	K:179:THR:HG23	0.435
1	D:378:VAL:O	D:389:SER:HA	0.434
1	G:126:VAL:O	G:130:ILE:HG13	0.434
1	E:24:ASP:O	E:28:GLN:HB2	0.432
1	G:174:GLN:HB3	H:1:HIS:HB3	0.432
1	H:3:PRO:HG3	H:11:PRO:HD3	0.432
1	I:15:PRO:HA	I:25:PRO:HB3	0.432
1	J:223:THR:HG23	J:231:LEU:HG	0.432
1	B:132:ILE:HG23	D:132:GLN:HG2	0.431
1	D:85:TYR:CD1	C:5:ILE:HB	0.431
1	G:127:ASP:O	G:131:LYS:HG2	0.431
1	D:12:ASP:OD1	D:14:ASP:HB3	0.430
1	A:61:SER:N	I:3:ARG:CZ	0.430
1	E:135:ILE:HD12	E:154:TYR:HE2	0.429
1	J:115:LEU:HD21	K:100:ILE:HB	0.429
1	D:147:PRO:HA	E:203:GLY:O	0.428
1	G:141:ARG:HG2	G:142:ALA:N	0.428
1	K:140:CYS:HB3	K:169:CYS:HB3	0.428
1	B:97:LYS:HA	B:100:VAL:HG12	0.427

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	J:223:THR:HB	J:226:LYS:HG3	0.427
1	K:255:GLY:O	K:261:TYR:HA	0.427
1	K:181:PHE:HE2	K:373:ILE:HG23	0.424
1	D:12:ASP:HA	D:13:PRO:HD3	0.423
1	A:63:LYS:HG3	I:3:ARG:CB	0.422
1	D:213:LYS:HB2	D:240:ASP:OD1	0.422
1	D:259:ASP:CG	D:261:LYS:H	0.422
1	H:16:GLY:O	H:19:LYS:HG2	0.421
1	K:27:LEU:O	K:31:GLU:HG2	0.421
1	D:208:LYS:O	D:211:PRO:HD2	0.420
1	D:73:LYS:CB	C:14:VAL:HA	0.419
1	D:185:MET:HA	D:190:GLY:CA	0.419
1	J:294:ASN:HD21	J:297:MET:HB3	0.419
1	J:56:SER:O	J:59:GLN:HG2	0.418
1	B:21:SER:HB2	D:19:CYS:SG	0.417
1	C:25:VAL:HB	C:26:PRO:CD	0.417
1	J:271:GLY:O	J:285:VAL:HA	0.417
1	D:231:LEU:HD12	D:232:PRO:HD2	0.416
1	J:147:PRO:HA	K:203:GLY:O	0.416
1	J:148:VAL:HG22	K:205:LEU:HG	0.416
1	D:73:LYS:HB2	C:14:VAL:HA	0.415
1	D:337:CYS:HB3	D:350:CYS:HB3	0.415
1	E:18:THR:HA	K:242:GLY:HA3	0.415

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	J:60:TYR:HD1	J:63:LEU:HD21	0.415
1	D:85:TYR:CE2	C:1:HIS:HA	0.414
1	H:10:VAL:HA	H:11:PRO:HD3	0.414
1	A:22:TYR:HB2	A:45:LYS:HB3	0.413
1	K:374:ILE:HG13	K:375:PRO:HD2	0.413
1	E:346:THR:HB	E:348:ASN:OD1	0.413
1	C:26:PRO:HB2	C:27:PRO:HD3	0.412
1	E:282:PHE:HE1	E:292:THR:HG21	0.412
1	K:153:LEU:HG	K:207:PRO:HG3	0.412
1	D:252:GLU:HG2	D:398:ARG:O	0.411
1	J:148:VAL:HG11	K:215:LEU:HA	0.411
1	D:72:GLN:HB2	D:72:GLN:HE21	0.411
1	D:316:MET:HE2	D:347:TYR:O	0.409
1	K:237:LEU:O	K:244:THR:HA	0.409
1	B:47:LEU:HA	B:47:LEU:HD13	0.408
1	D:104:ILE:N	D:105:PRO:HD2	0.408
1	E:199:LYS:HA	E:217:ASN:HB2	0.408
1	J:158:ILE:HG13	J:163:GLU:HA	0.408
1	D:85:TYR:HE2	C:1:HIS:HA	0.407
1	E:49:LYS:HE2	J:134:GLU:HG2	0.407
1	G:64:ILE:HA	G:67:ILE:HG12	0.407
1	D:200:ASP:HA	D:359:TYR:CZ	0.406
1	D:398:ARG:HA	D:399:PRO:HD3	0.406

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	G:47:LEU:HA	G:47:LEU:HD22	0.406
1	D:160:LYS:HD3	E:200:GLU:HB3	0.405
1	G:159:LEU:HA	G:159:LEU:HD22	0.404
1	J:286:ASN:HA	J:297:MET:HE2	0.404
1	K:265:TYR:HE2	K:295:ASN:HB2	0.402
1	G:155:GLN:HB2	G:155:GLN:HE21	0.402
1	E:117:GLN:O	E:121:GLN:HG3	0.401
1	E:265:TYR:HE2	E:295:ASN:HB2	0.401
1	K:321:TRP:CE3	K:332:ASN:HB2	0.401
1	E:139:ASP:H	E:142:ASP:HB3	0.401
1	D:217:GLY:HA3	D:235:TYR:HA	0.400
1	J:398:ARG:HA	J:399:PRO:HD3	0.400

Torsion angles: Protein backbone

In the following table, Ramachandran outliers are listed. The Analysed column shows the number of residues for which the backbone conformation was analysed.

Model ID	Analyzed	Favored	Allowed	Outliers
1	2226	2036	164	26

Detailed list of outliers are tabulated below.

Torsion angles: Protein sidechains

In the following table, sidechain outliers are listed. The Analysed column shows the number of residues for which the sidechain conformation was analysed.

Model ID	Analyzed	Favored	Allowed	Outliers
1	1982	1573	217	192

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	2	GLU

Model ID	Chain	Residue ID	Residue type
1	A	3	SER
1	A	15	SER
1	A	21	SER
1	A	23	SER
1	A	29	SER
1	A	38	THR
1	A	49	GLU
1	A	52	SER
1	A	53	GLU
1	A	61	SER
1	B	10	CYS
1	B	13	GLU
1	B	14	ASP
1	B	18	LYS
1	B	34	GLN
1	B	45	ASN
1	B	47	LEU
1	B	58	HIS
1	B	86	SER
1	B	140	SER
1	B	146	GLU
1	B	158	GLN
1	B	166	ASP

Model ID	Chain	Residue ID	Residue type
1	C	4	LEU
1	C	8	LYS
1	C	14	VAL
1	C	20	SER
1	D	21	THR
1	D	31	GLN
1	D	53	THR
1	D	63	LEU
1	D	65	LYS
1	D	72	GLN
1	D	77	ASP
1	D	78	ASN
1	D	83	ASN
1	D	86	SER
1	D	87	SER
1	D	89	LEU
1	D	92	HIS
1	D	99	THR
1	D	106	THR
1	D	124	LYS
1	D	125	LEU
1	D	153	GLU
1	D	156	GLU

Model ID	Chain	Residue ID	Residue type
1	D	163	GLU
1	D	164	THR
1	D	174	SER
1	D	175	SER
1	D	213	LYS
1	D	223	THR
1	D	245	LEU
1	D	259	ASP
1	D	291	THR
1	D	319	SER
1	D	330	THR
1	D	335	LYS
1	D	336	GLN
1	D	366	THR
1	D	371	LYS
1	D	374	THR
1	D	376	ASP
1	D	386	SER
1	D	397	ILE
1	D	400	PHE
1	E	9	THR
1	E	18	THR
1	E	28	GLN

Model ID	Chain	Residue ID	Residue type
1	E	60	SER
1	E	80	ILE
1	E	89	THR
1	E	124	GLU
1	E	129	THR
1	E	139	ASP
1	E	170	GLU
1	E	172	ASP
1	E	174	SER
1	E	182	GLN
1	E	185	LEU
1	E	188	SER
1	E	208	THR
1	E	210	THR
1	E	241	ASN
1	E	243	ARG
1	E	257	GLU
1	E	284	ASP
1	E	287	SER
1	E	301	THR
1	E	304	ASN
1	E	310	GLU
1	E	319	SER

Model ID	Chain	Residue ID	Residue type
1	E	346	THR
1	E	351	ASP
1	E	358	THR
1	E	377	ASN
1	E	380	THR
1	F	1	LYS
1	F	13	THR
1	F	22	SER
1	F	25	THR
1	F	33	THR
1	F	54	SER
1	G	13	GLU
1	G	14	ASP
1	G	18	LYS
1	G	43	LEU
1	G	47	LEU
1	G	48	PHE
1	G	59	SER
1	G	88	ASP
1	G	92	ARG
1	G	110	LEU
1	G	113	ASN
1	G	125	GLU

Model ID	Chain	Residue ID	Residue type
1	G	140	SER
1	G	145	ARG
1	G	152	TYR
1	G	155	GLN
1	G	158	GLN
1	G	159	LEU
1	H	12	ASP
1	H	13	LEU
1	H	20	SER
1	I	8	SER
1	I	17	SER
1	I	31	THR
1	J	33	GLU
1	J	53	THR
1	J	63	LEU
1	J	72	GLN
1	J	77	ASP
1	J	94	LEU
1	J	112	ARG
1	J	123	GLN
1	J	124	LYS
1	J	138	THR
1	J	153	GLU

Model ID	Chain	Residue ID	Residue type
1	J	164	THR
1	J	175	SER
1	J	187	THR
1	J	221	THR
1	J	223	THR
1	J	259	ASP
1	J	285	VAL
1	J	309	THR
1	J	319	SER
1	J	331	SER
1	J	366	THR
1	J	374	THR
1	J	376	ASP
1	J	386	SER
1	K	9	THR
1	K	20	GLN
1	K	59	GLU
1	K	60	SER
1	K	89	THR
1	K	136	THR
1	K	172	ASP
1	K	182	GLN
1	K	188	SER

Model ID	Chain	Residue ID	Residue type
1	K	206	SER
1	K	208	THR
1	K	210	THR
1	K	244	THR
1	K	245	SER
1	K	246	THR
1	K	253	LYS
1	K	264	THR
1	K	287	SER
1	K	300	SER
1	K	315	GLU
1	K	340	THR
1	K	342	SER
1	K	358	THR
1	K	369	THR
1	L	22	SER
1	L	26	THR
1	L	29	SER
1	L	35	THR
1	L	48	THR
1	L	53	THR
1	M	2	GLU
1	M	3	SER

Model ID	Chain	Residue ID	Residue type
1	M	15	SER
1	M	23	SER
1	M	37	SER
1	M	38	THR
1	M	46	MET
1	M	62	THR
1	M	63	LYS

Fit of model to data used for modeling

Crosslinking-MS

Validation for this section is under development.

Fit of model to data used for validation

Validation for this section is under development.

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