

Integrative Structure Validation Report

July 22, 2024 - 05:27 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	9A3T
PDB-Dev ID	PDBDEV_00000214
Structure Title	Bovine adenylyl cyclase 8 in complex with the G protein heterodimer G beta gamma
Structure Authors	Schuster, D.; Khanppnavar, B.; Korkhov, V.M.

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

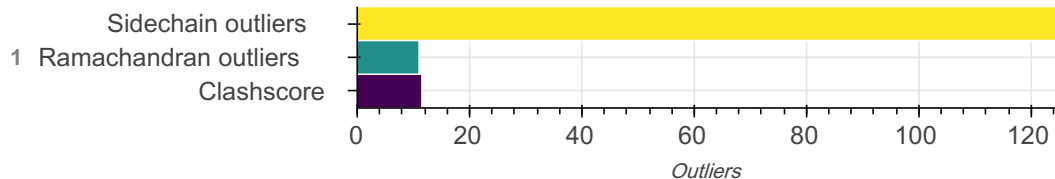
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the  symbol.

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 3 subunits in each model. A total of 3 datasets or restraints were used to build this entry. Each model is represented by 0 rigid bodies and 3 flexible or non-rigid units.

Entry composition ?

There is 1 unique type of models in this entry. This model is titled None/None.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	Adenylate cyclase type 8	A	A	890
1	2	2	Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1	B	B	339
1	3	3	Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2	C	C	46

Datasets used for modeling ?

There are 3 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
3	Crosslinking-MS data	PRIDE	PXD040374
1	Experimental model	PDB	1XHM
2	Experimental model	PDB	8BUZ

ID	Dataset type	Database name	Data access code
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Representation ?

This entry has only one representation and includes 0 rigid bodies and 3 flexible units

Chain ID	Rigid bodies	Non-rigid segments
A	-	1-890
B	-	1-339
C	-	1-46

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	Crosslinked residues were identified from the acquired mass spectrometry data based on the presence of heavy/light pairs of linked peptides.	Identification of crosslinked residues	None	None	False	False

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
2	1	<p>Accessible interaction space was assessed with DisVis, solvent accessible residues were determined with GetArea.</p> <p>The information from these steps was used for docking with HADDOCK.</p>	Docking	None	1	False	False

There are 4 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	xQuest	2.1.5	crosslink identification	https://gitlab.ethz.ch/leitner_lab/xquest_xprophet
4	HADDOCK	2.4	docking	https://wenmr.science.uu.nl/haddock2.4/
2	DisVis	Not available	assessing of accessible interaction space	https://wenmr.science.uu.nl/disvis/
3	GetArea	Not available	calculation of solvent accessible surface area and residues	https://curie.utmb.edu/getarea.html

Data quality ?

Crosslinking-MS

Validation for this section is under development.

Model quality ?

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

Standard geometry: bond outliers

There are 2273 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	0.96	0.86	1
N--H	0.97	0.86	30
ND2--HD22	0.97	0.86	3
NE2--HE21	0.97	0.86	3
ND2--HD21	0.97	0.86	1
NE2--HE2	0.97	0.86	1
NE2--HE22	0.97	0.86	1
N--H	0.98	0.86	1123
ND2--HD21	0.98	0.86	45
NE2--HE21	0.98	0.86	38
ND1--HD1	0.98	0.86	11
NE2--HE22	0.98	0.86	43
ND2--HD22	0.98	0.86	44
NE2--HE2	0.98	0.86	20
NE--HE	0.98	0.86	56
OH--HH	0.96	0.84	32
NE1--HE1	0.98	0.86	15
OG1--HG1	0.96	0.84	41
OG--HG	0.96	0.84	49
SG--HG	1.32	1.20	7

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
OG--HG	0.97	0.84	28
N--H	0.99	0.86	93
SG--HG	1.33	1.20	23
OG1--HG1	0.97	0.84	22
NE2--HE2	0.99	0.86	7
NE2--HE21	0.99	0.86	4
NE1--HE1	0.99	0.86	3
NE--HE	0.99	0.86	14
ND2--HD21	0.99	0.86	6
OH--HH	0.97	0.84	6
ND2--HD22	0.99	0.86	5
NE2--HE22	0.99	0.86	2
ND1--HD1	0.99	0.86	2
NE2--HE21	1.00	0.86	1
OG1--HG1	0.98	0.84	8
NE--HE	1.00	0.86	7
OH--HH	0.98	0.84	3
ND1--HD1	1.00	0.86	5
OG--HG	0.98	0.84	8
NZ--HZ3	1.03	0.89	2
NZ--HZ2	1.03	0.89	2
NZ--HZ3	1.04	0.89	45
NZ--HZ2	1.04	0.89	43

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
OG--HG	0.99	0.84	1
NZ--HZ1	1.04	0.89	41
NZ--HZ2	1.05	0.89	6
NZ--HZ1	1.05	0.89	9
NZ--HZ3	1.05	0.89	4
NZ--HZ1	1.06	0.89	1
NH1--HH11	1.03	0.86	1
NH1--HH12	1.03	0.86	1
NH2--HH21	1.03	0.86	1
NH1--HH12	1.04	0.86	57
NH2--HH22	1.04	0.86	58
NH2--HH21	1.04	0.86	57
NH1--HH11	1.04	0.86	61
NH1--HH12	1.05	0.86	11
NH2--HH22	1.05	0.86	13
NH2--HH21	1.05	0.86	13
NH1--HH11	1.05	0.86	9
NH1--HH11	1.06	0.86	6
NH2--HH21	1.06	0.86	6
NH2--HH22	1.06	0.86	6
NH1--HH12	1.06	0.86	8

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	11.51	232

All 232 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:461:ASP:HB3	A:464:PHE:HB2	0.921
1	B:293:CYS:HB2	B:307:LEU:HB2	0.825
1	B:50:LEU:HB2	B:335:LEU:HB2	0.781
1	B:46:THR:HG21	B:336:LYS:HE2	0.739
1	A:424:GLU:HA	A:427:ILE:HG12	0.736
1	A:251:VAL:HG21	A:353:VAL:HG22	0.706
1	B:309:GLY:HA3	B:338:TRP:HH2	0.701
1	B:319:VAL:HG13	B:326:VAL:HG22	0.701
1	B:120:CYS:HB3	B:138:LEU:HB2	0.687
1	A:147:VAL:HG13	A:148:ILE:HG13	0.686
1	A:460:ARG:HD2	A:532:GLU:OE2	0.686
1	B:94:LEU:HD13	B:99:VAL:HG21	0.686
1	B:24:CYS:HA	C:23:LYS:HE3	0.674
1	A:514:GLU:HA	A:524:ARG:HG2	0.640
1	A:50:LYS:HG2	A:102:TYR:HB3	0.637
1	B:50:LEU:HD23	B:86:THR:HG23	0.637
1	A:358:LEU:HD22	C:32:MET:HE2	0.634
1	C:29:ALA:HA	C:11:GLU:OE1	0.631
1	C:8:LYS:HD3	A:210:ARG:HH21	0.625

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:206:GLN:HG3	A:427:ILE:CG1	0.625
1	A:424:GLU:HA	C:23:LYS:CE	0.617
1	B:24:CYS:HA	A:283:ARG:HD2	0.614
1	A:279:GLU:OE2	A:104:LEU:HD22	0.606
1	A:34:LEU:HD23	A:519:LEU:HD23	0.605
1	A:516:TYR:HB3	B:198:PHE:HB3	0.602
1	B:191:LEU:HD23	A:650:LEU:HD13	0.600
1	A:582:LEU:HD22	B:80:ILE:HG12	0.600
1	B:70:VAL:HG12	A:310:PRO:HD3	0.595
1	A:309:LEU:HB3	A:409:LYS:HE2	0.591
1	A:409:LYS:HA	A:540:ILE:HD12	0.588
1	A:530:ILE:HG21	A:141:GLN:HE21	0.584
1	A:112:VAL:HG21	A:340:HIS:H	0.576
1	A:339:LYS:HG3	A:699:ARG:HG3	0.575
1	A:694:PHE:HA	B:179:PHE:HB2	0.569
1	A:717:ALA:HA	A:420:ILE:HA	0.566
1	B:165:CYS:HB2	A:484:LEU:HD11	0.563
1	A:405:GLU:O	A:645:TYR:HB3	0.560
1	A:161:ALA:HB2	B:259:GLU:OE1	0.555
1	A:122:MET:HE1	A:438:GLU:HB2	0.552
1	B:250:ARG:HD3	A:148:ILE:HD11	0.551
1	A:435:LEU:HA	A:28:VAL:HG12	0.549
1	A:99:GLY:HA2	A:492:PRO:HD3	0.548

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:25:VAL:O	A:79:TYR:HB2	0.547
1	A:491:MET:HB2	A:97:ALA:HB1	0.546
1	A:71:ARG:HG2	A:387:ILE:HG22	0.546
1	A:53:LEU:HD13	A:640:LEU:HD11	0.546
1	A:346:ILE:HB	B:323:GLY:HA2	0.545
1	A:593:LEU:HB3	A:377:LYS:HE3	0.540
1	B:319:VAL:HG12	C:32:MET:HG3	0.540
1	A:376:ASN:OD1	A:122:MET:HG2	0.537
1	C:28:ALA:O	A:102:TYR:O	0.536
1	A:19:SER:HB2	B:314:VAL:HG21	0.535
1	A:98:ALA:HA	B:274:SER:HA	0.529
1	B:293:CYS:SG	B:276:SER:HA	0.528
1	B:230:ALA:HB2	A:440:ILE:HG12	0.527
1	B:232:CYS:SG	B:86:THR:OG1	0.525
1	A:435:LEU:HD12	A:541:ILE:HG12	0.524
1	B:48:ARG:HD2	A:335:ARG:HG2	0.523
1	A:537:ARG:O	A:15:GLN:HG2	0.521
1	A:331:ILE:O	A:638:MET:HE2	0.521
1	A:11:TYR:O	B:294:ASN:HB2	0.517
1	A:635:LEU:HA	A:569:PHE:CZ	0.515
1	B:288:TYR:HE1	A:91:MET:HE2	0.514
1	A:109:ILE:HB	A:275:ARG:HH21	0.514
1	A:88:TRP:HA	A:497:PHE:HE2	0.514

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:272:GLU:HG3	A:698:ASP:OD1	0.514
1	A:479:THR:HA	A:342:VAL:HG23	0.513
1	A:697:LYS:HG2	A:577:THR:HG22	0.513
1	A:335:ARG:HH22	A:6:ARG:HH21	0.512
1	A:474:VAL:HG21	B:81:TRP:HH2	0.512
1	A:3:ASP:HA	A:596:MET:HE2	0.510
1	B:52:GLY:HA3	B:254:LEU:HD22	0.509
1	A:592:VAL:HG22	B:75:ASP:OD1	0.508
1	B:209:LEU:HD22	A:17:ARG:HB2	0.504
1	B:73:SER:HB3	A:372:VAL:HG22	0.504
1	A:13:LEU:O	B:339:ASN:OD1	0.504
1	A:369:SER:O	C:21:ARG:HB3	0.504
1	B:47:ARG:HG3	A:267:THR:OG1	0.502
1	B:24:CYS:SG	A:527:CYS:SG	0.502
1	A:264:LEU:HA	A:417:LYS:NZ	0.501
1	A:514:GLU:HB3	A:105:LEU:HD23	0.499
1	A:378:LEU:HA	A:272:GLU:OE1	0.497
1	A:105:LEU:H	A:704:LEU:HD22	0.497
1	A:269:SER:HB3	B:275:VAL:HG23	0.497
1	A:275:ARG:HA	A:425:HIS:HB2	0.496
1	B:232:CYS:HB2	A:365:PHE:CZ	0.493
1	A:422:ARG:O	A:509:LEU:HG	0.493
1	A:355:CYS:HB2	A:581:PHE:HA	0.491

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:506:ALA:O	B:146:SER:O	0.491
1	A:467:ASN:HD21	A:581:PHE:HA	0.488
1	B:101:THR:HB	A:576:VAL:HG12	0.487
1	A:467:ASN:ND2	B:338:TRP:CH2	0.487
1	A:573:LEU:O	A:13:LEU:HB2	0.484
1	B:309:GLY:HA3	B:210:TRP:HB2	0.484
1	A:9:GLN:O	B:242:THR:HG22	0.484
1	B:198:PHE:CE2	B:134:VAL:HG22	0.482
1	B:231:ILE:HD11	A:91:MET:HG2	0.480
1	B:123:TYR:CE2	A:236:LEU:HD23	0.479
1	A:87:THR:O	B:242:THR:HG22	0.477
1	A:361:ARG:HH22	A:558:TRP:HE3	0.476
1	A:236:LEU:H	B:233:PHE:CE2	0.475
1	B:231:ILE:CD1	B:216:MET:H	0.475
1	A:489:ARG:HG3	A:164:VAL:HG23	0.470
1	B:199:VAL:HG23	A:558:TRP:CE3	0.470
1	B:214:GLU:HG3	A:536:ALA:HB1	0.470
1	A:160:VAL:O	C:22:ILE:HB	0.470
1	A:489:ARG:HG3	A:486:PRO:HD2	0.467
1	A:530:ILE:HD13	A:21:VAL:HG23	0.466
1	B:255:ARG:HB3	A:76:SER:H	0.466
1	A:485:LEU:HD13	A:137:THR:HB	0.465
1	A:17:ARG:O	A:520:PRO:HD2	0.465

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:74:THR:HG22	A:414:PHE:HD1	0.464
1	A:116:LEU:HD13	A:80:LEU:HD22	0.462
1	A:519:LEU:HD13	A:113:LEU:HD12	0.462
1	A:412:ASN:HB3	B:336:LYS:HG2	0.461
1	A:17:ARG:HH11	B:108:GLY:HA2	0.460
1	A:110:GLY:HA2	B:260:LEU:HD11	0.460
1	B:49:THR:HG23	A:438:GLU:OE1	0.457
1	B:104:TYR:CE1	A:583:ARG:HG3	0.455
1	B:253:ASP:HB2	B:7:ARG:HD2	0.455
1	A:434:LYS:HE2	B:215:GLY:HA2	0.455
1	A:461:ASP:OD2	A:185:ARG:HG3	0.454
1	B:4:ASP:HA	A:481:ILE:HG12	0.453
1	B:179:PHE:HE2	A:439:HIS:H	0.453
1	A:181:ASP:O	A:463:VAL:HG13	0.452
1	A:477:PHE:O	B:262:THR:HG23	0.451
1	A:438:GLU:HB3	A:532:GLU:HA	0.450
1	A:462:GLU:HG2	A:378:LEU:HD12	0.448
1	B:248:THR:HB	A:523:LEU:HD22	0.448
1	A:460:ARG:CG	B:274:SER:HA	0.448
1	A:375:ALA:HA	C:23:LYS:HE2	0.448
1	A:519:LEU:HD12	A:379:GLU:HG2	0.446
1	B:230:ALA:CB	C:41:GLU:OE2	0.446
1	B:23:ALA:O	B:209:LEU:HD11	0.444

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:345:ARG:HG3	A:334:VAL:HG12	0.443
1	C:40:LYS:HE3	A:545:ILE:HG13	0.443
1	B:197:LEU:HB3	B:189:LEU:HD23	0.443
1	A:331:ILE:O	B:313:ARG:HG3	0.442
1	A:541:ILE:O	A:37:LEU:HD21	0.439
1	B:189:LEU:HA	B:184:GLY:O	0.437
1	B:289:ASP:HA	A:393:THR:HB	0.436
1	A:34:LEU:HD12	B:84:TYR:HD1	0.436
1	B:163:THR:HG23	B:316:CYS:HA	0.436
1	A:389:ILE:HD12	B:134:VAL:HG22	0.435
1	B:67:ARG:HG3	B:160:SER:HA	0.434
1	B:274:SER:OG	A:50:LYS:HG3	0.433
1	A:295:ARG:O	A:617:ASN:OD1	0.433
1	B:123:TYR:HE2	B:132:VAL:HG22	0.433
1	B:144:TYR:O	A:79:TYR:CB	0.431
1	A:47:ASP:OD2	A:64:ILE:HG13	0.430
1	A:614:ARG:HA	B:126:LYS:HG2	0.430
1	B:125:LEU:HA	A:515:ASP:OD1	0.429
1	A:71:ARG:HG2	A:539:VAL:HG12	0.428
1	A:60:ILE:O	A:20:GLU:OE2	0.427
1	B:109:ASN:OD1	A:53:LEU:HD23	0.423
1	A:465:LYS:NZ	B:215:GLY:HA2	0.423
1	A:536:ALA:O	A:645:TYR:HB3	0.422

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:17:ARG:HD2	A:286:ARG:HD3	0.422
1	A:53:LEU:HA	A:495:ILE:HG12	0.421
1	B:179:PHE:CE2	A:657:ASP:OD2	0.421
1	A:122:MET:CE	B:227:ASP:HA	0.421
1	A:283:ARG:HA	B:331:TRP:HB2	0.421
1	A:491:MET:O	A:381:GLY:H	0.420
1	A:654:ALA:HA	A:329:LYS:HG2	0.419
1	B:203:CYS:HA	A:31:LYS:HG2	0.418
1	B:312:ASN:OD1	A:368:TRP:CH2	0.418
1	A:379:GLU:C	A:662:VAL:HG23	0.418
1	A:325:LEU:O	A:105:LEU:HD22	0.417
1	A:27:ASP:O	B:162:ASP:HA	0.416
1	A:358:LEU:HG	B:288:TYR:HA	0.414
1	A:658:PHE:O	A:667:GLU:OE1	0.414
1	A:50:LYS:HE2	B:193:PRO:HD2	0.413
1	A:313:ARG:HG3	A:342:VAL:CG2	0.413
1	B:271:GLY:O	A:321:VAL:HG12	0.412
1	A:198:ARG:HD2	A:523:LEU:HD13	0.412
1	B:192:ALA:HB1	B:256:ALA:HB3	0.412
1	A:335:ARG:HH22	B:123:TYR:HE1	0.412
1	A:318:HIS:HA	A:310:PRO:CD	0.411
1	A:520:PRO:HG2	B:327:ALA:HB2	0.411
1	B:253:ASP:HB3	B:307:LEU:HD11	0.411

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:113:CYS:SG	B:294:ASN:HB2	0.411
1	A:309:LEU:HB3	A:671:MET:HG3	0.411
1	B:62:TRP:CZ2	A:102:TYR:CB	0.409
1	B:285:LEU:HD23	A:378:LEU:HB2	0.409
1	B:288:TYR:CE1	A:393:THR:HB	0.409
1	A:667:GLU:O	C:44:LEU:HD22	0.409
1	A:722:PHE:CZ	A:520:PRO:HD2	0.408
1	A:50:LYS:HG2	A:565:GLU:H	0.407
1	A:375:ALA:O	C:24:VAL:HG23	0.407
1	A:389:ILE:CD1	A:302:CYS:HB3	0.406
1	B:44:MET:HE2	A:554:LEU:HD11	0.406
1	A:519:LEU:CD1	B:328:THR:HG22	0.406
1	A:565:GLU:CD	C:11:GLU:HB2	0.406
1	B:24:CYS:O	A:547:ILE:HG21	0.405
1	A:299:LEU:HG	B:4:ASP:HB2	0.405
1	A:497:PHE:CD1	A:210:ARG:NH2	0.404
1	B:317:LEU:HB2	A:320:CYS:SG	0.404
1	C:7:ARG:O	A:309:LEU:HD22	0.404
1	A:504:HIS:HB2	C:23:LYS:HE3	0.404
1	B:1:SER:HB3	B:212:VAL:HG23	0.404
1	A:206:GLN:HG3	A:438:GLU:OE1	0.402
1	A:252:SER:HB2	A:580:VAL:HG22	0.401
1	A:306:VAL:HG21	B:129:GLU:H	0.401

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	C:23:LYS:HA	B:308:ALA:HB3	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	1263	1161	91	11

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	1099	820	154	125

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	17	ARG
1	A	41	LEU
1	A	49	LEU
1	A	58	THR
1	A	72	LYS
1	A	128	THR
1	A	155	SER
1	A	168	CYS
1	A	171	THR
1	A	190	GLU
1	A	194	CYS
1	A	196	GLU

Model ID	Chain	Residue ID	Residue type
1	A	209	GLU
1	A	222	LEU
1	A	224	MET
1	A	229	THR
1	A	234	GLU
1	A	262	THR
1	A	265	SER
1	A	267	THR
1	A	268	LEU
1	A	278	ASN
1	A	299	LEU
1	A	343	ASP
1	A	350	SER
1	A	352	SER
1	A	369	SER
1	A	390	SER
1	A	393	THR
1	A	397	LEU
1	A	407	HIS
1	A	413	GLU
1	A	422	ARG
1	A	431	SER
1	A	433	ASP

Model ID	Chain	Residue ID	Residue type
1	A	434	LYS
1	A	437	ARG
1	A	446	MET
1	A	450	SER
1	A	451	SER
1	A	453	GLU
1	A	468	LEU
1	A	484	LEU
1	A	485	LEU
1	A	498	SER
1	A	500	LEU
1	A	515	ASP
1	A	526	THR
1	A	532	GLU
1	A	544	SER
1	A	550	LEU
1	A	562	SER
1	A	565	GLU
1	A	576	VAL
1	A	586	SER
1	A	605	GLU
1	A	616	ASP
1	A	618	LEU

Model ID	Chain	Residue ID	Residue type
1	A	620	HIS
1	A	656	LEU
1	A	657	ASP
1	A	678	ASN
1	A	688	SER
1	A	700	ASP
1	A	724	ASP
1	A	727	SER
1	A	733	ASN
1	A	755	GLU
1	A	756	ASP
1	A	760	ASP
1	A	762	GLU
1	A	765	LYS
1	A	769	SER
1	A	775	SER
1	A	792	SER
1	A	797	GLU
1	A	803	ASN
1	A	806	SER
1	A	820	SER
1	A	852	SER
1	A	856	GLN

Model ID	Chain	Residue ID	Residue type
1	A	857	VAL
1	A	861	THR
1	A	865	LEU
1	A	883	ILE
1	B	8	GLN
1	B	30	SER
1	B	37	ASP
1	B	51	ARG
1	B	64	THR
1	B	69	LEU
1	B	97	SER
1	B	125	LEU
1	B	126	LYS
1	B	127	THR
1	B	128	ARG
1	B	135	SER
1	B	142	THR
1	B	145	LEU
1	B	146	SER
1	B	153	ASP
1	B	159	SER
1	B	160	SER
1	B	176	THR

Model ID	Chain	Residue ID	Residue type
1	B	183	THR
1	B	185	ASP
1	B	186	VAL
1	B	188	SER
1	B	195	THR
1	B	212	VAL
1	B	222	THR
1	B	231	ILE
1	B	233	PHE
1	B	266	ASP
1	B	269	ILE
1	B	270	CYS
1	B	273	THR
1	B	274	SER
1	B	315	SER
1	B	319	VAL
1	B	324	MET
1	B	333	SER
1	C	2	SER
1	C	7	ARG
1	C	23	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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