Integrative Structure Validation Report

July 22, 2024 - 04:20 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	9A13
PDB-Dev ID	PDBDEV_00000075
Structure Title	Model of the vaccinia virus DNA polymerase: complex between A20-Cter and E9
Structure Authors	Bersch B; Tarbouriech N; Burmeister WP; Iseni F

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

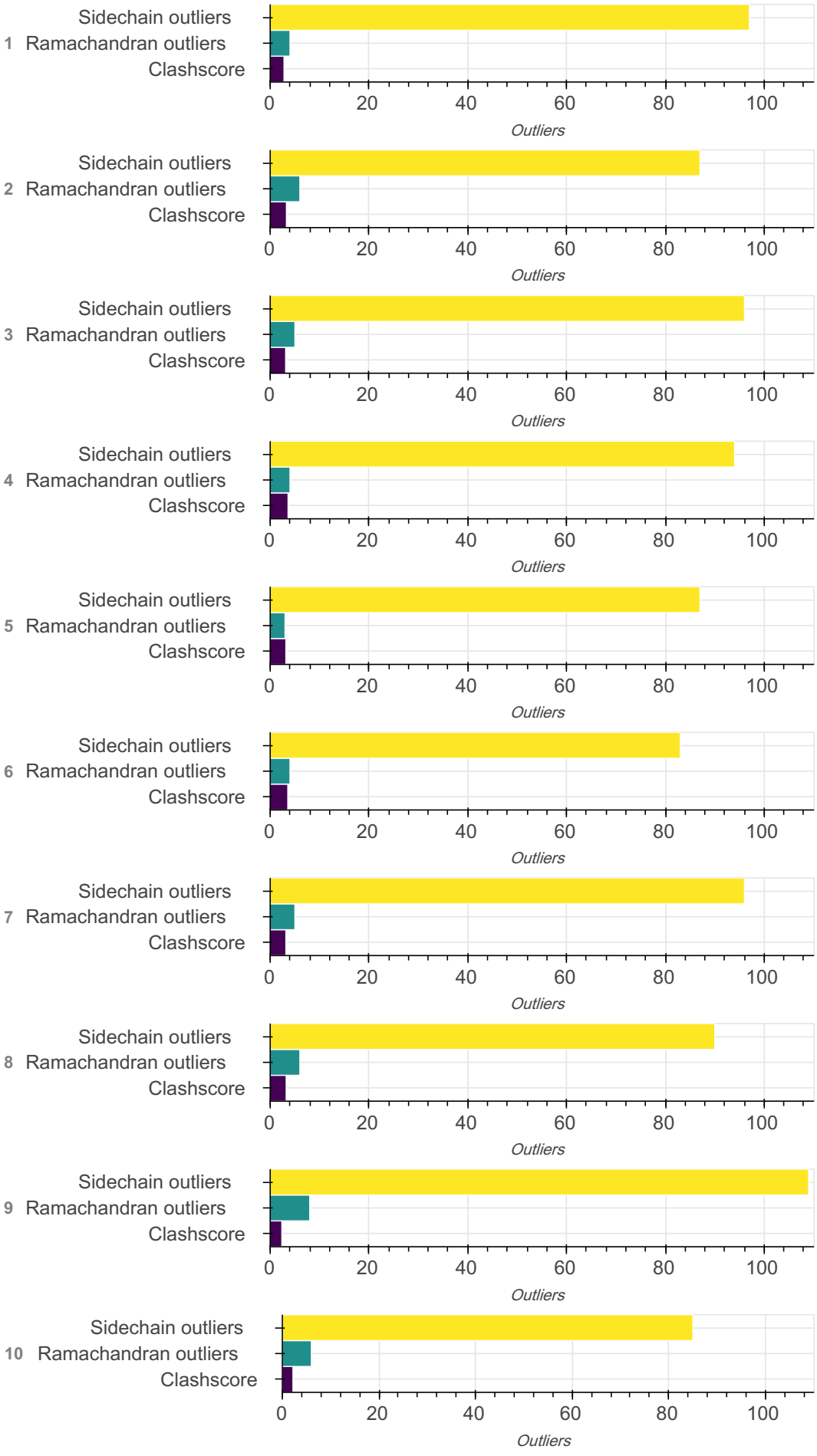
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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


1
Sidechain outliers
Ramachandran outliers
Clashscore
0
20
40
60
80
100
Outliers
2
Sidechain outliers
Ramachandran outliers
Clashscore
0
20
40
60
80
100
Outliers
3
Sidechain outliers
Ramachandran outliers
Clashscore
0
20
40
60
80
100
Outliers
4
Sidechain outliers
Ramachandran outliers
Clashscore
0
20
40
60
80
100
Outliers
5
Sidechain outliers
Ramachandran outliers
Clashscore
0
20
40
60
80
100
Outliers
6
Sidechain outliers
Ramachandran outliers
Clashscore
0
20
40
60
80
100
Outliers
7
Sidechain outliers
Ramachandran outliers
Clashscore
0
20
40
60
80
100
Outliers
8
Sidechain outliers
Ramachandran outliers
Clashscore
0
20
40
60
80
100
Outliers
9
Sidechain outliers
Ramachandran outliers
Clashscore
0
20
40
60
80
100
Outliers
10
Sidechain outliers
Ramachandran outliers
Clashscore
0
20
40
60
80
100
Outliers

Ensemble information

This entry consists of 0 distinct ensemble(s).

Summary

This entry consists of 10 unique models, with 2 subunits in each model. A total of 5 datasets or restraints were used to build this entry. Each model is represented by 0 rigid bodies and 2 flexible or non-rigid units.

Entry composition

There are 10 unique types of models in this entry.These models are titled None, None, None, None, None, None, None, None, None, None respectively.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	DNA polymerase processivity factor component A20	A	A	124
1	2	2	DNA polymerase	B	B	1010
2	1	1	DNA polymerase processivity factor component A20	A	A	124
2	2	2	DNA polymerase	B	B	1010
3	1	1	DNA polymerase processivity factor component A20	A	A	124
3	2	2	DNA polymerase	B	B	1010
4	1	1	DNA polymerase processivity factor component A20	A	A	124
4	2	2	DNA polymerase	B	B	1010
5	1	1	DNA polymerase processivity factor component A20	A	A	124
5	2	2	DNA polymerase	B	B	1010

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
6	1	1	DNA polymerase processivity factor component A20	A	A	124
6	2	2	DNA polymerase	B	B	1010
7	1	1	DNA polymerase processivity factor component A20	A	A	124
7	2	2	DNA polymerase	B	B	1010
8	1	1	DNA polymerase processivity factor component A20	A	A	124
8	2	2	DNA polymerase	B	B	1010
9	1	1	DNA polymerase processivity factor component A20	A	A	124
9	2	2	DNA polymerase	B	B	1010
10	1	1	DNA polymerase processivity factor component A20	A	A	124
10	2	2	DNA polymerase	B	B	1010

Datasets used for modeling

There are 5 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Experimental model	PDB	6ZXP
2	Experimental model	PDB	5N2E
3	NMR data	BMRB	34544
4	NMR data	BMRB	34545
5	Other	File	None

Representation

This entry has only one representation and includes 0 rigid bodies and 2 flexible units

Chain ID	Rigid bodies	Non-rigid segments
A	-	1-124
B	-	1-1010

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	Docking	None	None	_	False	False

There is 1 software package reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	HADDOCK	Not available	model building	http://haddock.science.uu.nl/services/HADDOCK/

Data quality

NMR

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 90490 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

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CB--HB	1.07	0.97	7
CD--HD3	1.07	0.97	6
CB--HB3	1.07	0.97	7
CA--HA	1.07	0.97	2
CG--HG2	1.07	0.97	1
CB--HB2	1.07	0.97	1
CB--HB3	1.08	0.97	8573
CB--HB2	1.08	0.97	8579
CA--HA	1.08	0.97	10678
CD--HD3	1.08	0.97	1854
CE--HE2	1.08	0.97	1100
CG1--HG11	1.08	0.97	640
CB--HB	1.08	0.97	2093
CD2--HD22	1.08	0.97	1030
CD--HD2	1.08	0.97	1860
CG--HG2	1.08	0.97	3139
CG2--HG21	1.08	0.97	2100
CD1--HD13	1.08	0.97	1860
CG--HG3	1.08	0.97	3140
CG1--HG12	1.08	0.97	1470
CG--HG	1.08	0.97	1030
CD1--HD11	1.08	0.97	1860
CD2--HD21	1.08	0.97	1030

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CG2--HG22	1.08	0.97	2100
CE--HE3	1.08	0.97	1100
CA--HA2	1.08	0.97	440
CG2--HG23	1.08	0.97	2100
CB--HB1	1.08	0.97	430
CD2--HD23	1.08	0.97	1030
CD1--HD12	1.08	0.97	1860
CA--HA3	1.08	0.97	440
CE--HE1	1.08	0.97	290
CG1--HG13	1.08	0.97	1470
N--H	0.97	0.86	5
NE2--HE22	0.97	0.86	2
N--H	0.98	0.86	9924
NE2--HE22	0.98	0.86	235
ND2--HD22	0.98	0.86	772
NE2--HE21	0.98	0.86	199
ND2--HD21	0.98	0.86	685
NE1--HE1	0.98	0.86	51
NE2--HE2	0.98	0.86	80
ND1--HD1	0.98	0.86	17
OH--HH	0.96	0.84	233
NE--HE	0.98	0.86	327
OG1--HG1	0.96	0.84	227

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
OG--HG	0.96	0.84	279
SG--HG	1.32	1.20	26
N--H	0.99	0.86	761
NE2--HE21	0.99	0.86	41
OG--HG	0.97	0.84	490
OG1--HG1	0.97	0.84	391
NE--HE	0.99	0.86	304
ND2--HD21	0.99	0.86	115
OH--HH	0.97	0.84	352
ND2--HD22	0.99	0.86	28
SG--HG	1.33	1.20	252
ND1--HD1	0.99	0.86	8
NE2--HE2	0.99	0.86	20
NE1--HE1	0.99	0.86	9
NE2--HE22	0.99	0.86	3
NE--HE	1.00	0.86	9
ND1--HD1	1.00	0.86	5
OG1--HG1	0.98	0.84	12
SG--HG	1.34	1.20	2
OH--HH	0.98	0.84	25
OG--HG	0.98	0.84	51
NZ--HZ1	1.04	0.89	770
CZ2--HZ2	1.08	0.93	60

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NZ--HZ3	1.04	0.89	766
NZ--HZ2	1.04	0.89	758
CE3--HE3	1.08	0.93	60
CD2--HD2	1.08	0.93	1370
CE1--HE1	1.08	0.93	1370
CE2--HE2	1.08	0.93	1250
N--H2	1.04	0.89	19
N--H3	1.04	0.89	19
CD1--HD1	1.08	0.93	1310
CZ--HZ	1.08	0.93	640
N--H1	1.04	0.89	20
CH2--HH2	1.08	0.93	60
CZ3--HZ3	1.08	0.93	60
NZ--HZ2	1.05	0.89	52
NZ--HZ3	1.05	0.89	44
N--H2	1.05	0.89	1
NZ--HZ1	1.05	0.89	40
N--H3	1.05	0.89	1
NH1--HH12	1.04	0.86	454
NH1--HH11	1.04	0.86	456
NH2--HH21	1.04	0.86	417
NH2--HH22	1.04	0.86	381
NH2--HH22	1.05	0.86	242

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NH1--HH11	1.05	0.86	169
NH1--HH12	1.05	0.86	168
NH2--HH21	1.05	0.86	212
NH2--HH21	1.06	0.86	11
NH1--HH11	1.06	0.86	15
NH1--HH12	1.06	0.86	18
NH2--HH22	1.06	0.86	17

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	2.79	51
2	3.28	60
3	3.12	57
4	3.61	66
5	3.17	58
6	3.56	65
7	3.17	58
8	3.23	59
9	2.35	43
10	2.19	40

All 557 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	B:841:ARG:CZ	B:841:ARG:HA	0.649
1	B:273:HIS:HA	B:277:LEU:HD12	0.582
1	A:77:ILE:HD12	B:590:ILE:HG12	0.572
1	B:689:TYR:CZ	B:693:LYS:HD2	0.559
1	B:224:ALA:HB2	B:457:LEU:HD11	0.538
1	B:132:CYS:SG	B:163:ARG:HA	0.535
1	B:373:VAL:HG13	B:375:GLU:H	0.531
1	B:631:ILE:HB	B:632:PRO:HD3	0.525
1	B:841:ARG:HA	B:841:ARG:NH1	0.524
1	B:494:TYR:CG	B:509:VAL:HB	0.521
1	B:913:ASN:N	B:914:PRO:HD2	0.517
1	B:408:ASP:OD1	B:839:THR:HB	0.511
1	B:258:GLN:O	B:262:LEU:HG	0.498
1	B:856:THR:O	B:860:GLU:HG3	0.496
1	B:988:VAL:HG21	B:937:TYR:HA	0.478
1	B:900:LEU:O	A:46:ILE:HG12	0.475
1	A:42:VAL:O	B:666:TYR:CD1	0.473
1	B:486:LYS:HE2	B:887:GLU:OE2	0.473
1	B:887:GLU:HA	B:373:VAL:HG12	0.468
1	B:372:GLY:O	B:229:CYS:O	0.457
1	B:225:VAL:HA	B:265:ASP:HB2	0.457
1	B:169:SER:O	B:335:ILE:HD12	0.455
1	B:266:TYR:CE1	B:225:VAL:HG23	0.454

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:221:ILE:O	B:374:ARG:H	0.451
1	B:373:VAL:HG22	B:129:PRO:O	0.444
1	B:13:CYS:HB2	B:509:VAL:HG22	0.443
1	B:506:ALA:HA	B:595:LEU:HG	0.442
1	B:591:ASN:O	B:742:LYS:HD2	0.442
1	B:719:MET:SD	A:103:ARG:HG3	0.441
1	A:99:GLU:O	B:387:LYS:HA	0.441
1	B:382:ASP:OD2	B:731:TYR:O	0.439
1	B:728:ASN:HB3	B:472:CYS:SG	0.433
1	B:399:THR:HG21	B:749:TYR:HB2	0.432
1	B:746:PRO:O	B:518:LEU:HG	0.431
1	B:514:LEU:O	B:32:CYS:SG	0.430
1	B:11:VAL:HG12	B:733:ASP:HB2	0.426
1	B:728:ASN:HB2	B:742:LYS:HE2	0.426
1	B:718:GLY:O	B:345:LYS:HG3	0.418
1	B:341:SER:O	B:61:PRO:HD3	0.415
1	B:60:PRO:HA	B:376:MET:SD	0.413
1	B:371:ARG:HA	B:571:LEU:HD12	0.413
1	B:566:CYS:HA	B:563:PRO:HD3	0.412
1	B:562:TYR:HB2	B:872:VAL:HG22	0.409
1	B:861:MET:SD	B:723:ALA:HB2	0.406
1	B:712:GLY:HA3	B:327:HIS:NE2	0.406
1	B:325:THR:HB	B:374:ARG:N	0.405

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:373:VAL:HG13	B:932:LEU:HA	0.403
1	B:904:HIS:ND1	B:337:PHE:O	0.403
1	B:268:VAL:HA	B:153:PRO:HB3	0.402
1	B:42:PHE:CE2	B:242:ARG:HG3	0.402
2	B:230:LEU:HD22	B:194:THR:HG22	0.650
2	B:175:ILE:HG22	B:282:ASN:HB3	0.593
2	B:186:VAL:HG11	B:509:VAL:HG22	0.558
2	B:506:ALA:HA	B:229:CYS:O	0.547
2	B:225:VAL:HA	A:46:ILE:HG12	0.543
2	A:42:VAL:O	B:983:LEU:HA	0.528
2	B:847:HIS:CE1	B:632:PRO:HD3	0.525
2	B:631:ILE:HB	B:693:LYS:HD2	0.516
2	B:689:TYR:CZ	B:373:VAL:HG12	0.497
2	B:372:GLY:O	B:796:LYS:HG2	0.495
2	B:795:PHE:C	B:874:ILE:HG12	0.494
2	B:870:ASN:O	B:914:PRO:HD2	0.494
2	B:913:ASN:N	B:409:ILE:HD13	0.489
2	B:406:ASP:HB3	B:221:ILE:HD13	0.488
2	B:213:GLU:HG2	B:616:LEU:HD23	0.486
2	B:583:THR:HG23	B:102:PRO:HD3	0.484
2	B:63:PHE:HB2	B:877:LEU:HB2	0.483
2	B:873:CYS:O	A:67:ILE:HG13	0.476
2	A:63:GLU:O	B:899:MET:SD	0.476

Model ID	Atom-1	Atom-2	Clash overlap (Å)
2	B:896:GLU:HA	B:476:TYR:N	0.472
2	B:475:GLN:HG3	B:631:ILE:HD12	0.470
2	B:573:PRO:HD3	B:374:ARG:N	0.468
2	B:373:VAL:HG13	B:327:HIS:HB2	0.467
2	B:308:TYR:CZ	B:327:HIS:CD2	0.466
2	B:310:ARG:HG3	B:884:LEU:HG	0.466
2	B:880:LEU:O	B:522:LYS:HE3	0.458
2	B:70:LYS:O	B:795:PHE:O	0.456
2	B:791:LEU:HB3	B:693:LYS:HG3	0.451
2	B:689:TYR:O	B:591:ASN:ND2	0.450
2	B:83:ASN:HA	B:592:ASN:HB2	0.447
2	B:588:GLU:O	B:32:CYS:HB3	0.445
2	B:8:ASP:HB3	B:375:GLU:H	0.441
2	B:373:VAL:HG13	B:996:LEU:HD23	0.440
2	B:873:CYS:SG	B:77:ASP:HB2	0.438
2	B:75:ASP:OD2	B:563:PRO:HD3	0.437
2	B:562:TYR:HB2	B:711:ASN:HB2	0.437
2	B:707:GLU:O	A:92:CYS:SG	0.436
2	A:87:ILE:HD11	B:302:ALA:HA	0.435
2	B:294:PHE:O	B:283:ARG:NH2	0.432
2	B:190:PRO:HB3	B:147:CYS:HA	0.430
2	B:39:PHE:O	B:374:ARG:H	0.430
2	B:373:VAL:HG22	B:473:LEU:HG	0.427

Model ID	Atom-1	Atom-2	Clash overlap (Å)
2	B:469:HIS:O	B:670:ILE:HG12	0.427
2	B:666:TYR:O	B:747:ILE:HA	0.426
2	B:717:ASN:O	B:767:ILE:O	0.425
2	B:551:ASN:HB3	B:776:ILE:HG13	0.424
2	B:772:VAL:O	B:534:PHE:CE2	0.420
2	B:532:GLN:HB3	B:816:THR:HB	0.420
2	B:815:THR:O	A:84:ASN:HB3	0.419
2	A:76:LYS:HB3	B:418:ILE:HG23	0.418
2	B:394:ALA:HB1	B:564:ASN:HB2	0.418
2	B:560:SER:O	B:591:ASN:ND2	0.417
2	B:587:GLU:HB3	B:280:ILE:HG13	0.414
2	B:276:ASP:O	B:616:LEU:HD12	0.414
2	B:613:LEU:HB2	B:797:ILE:HG23	0.414
2	B:791:LEU:HD11	B:518:LEU:HG	0.413
2	B:514:LEU:O	B:429:CYS:SG	0.410
2	B:376:MET:HB2	B:851:ILE:HG22	0.404
2	B:848:LYS:HA	B:897:LEU:O	0.404
3	B:844:SER:HB3	B:841:ARG:HA	0.590
3	B:841:ARG:CZ	B:594:LEU:HB3	0.570
3	B:84:LEU:HD22	B:782:LEU:HG	0.555
3	B:778:ILE:O	B:168:ARG:HA	0.554
3	B:31:ARG:NH2	B:525:LEU:HB3	0.542
3	B:76:ILE:HD13	B:914:PRO:HD2	0.529

Model ID	Atom-1	Atom-2	Clash overlap (Å)
3	B:913:ASN:N	B:475:GLN:HG2	0.524
3	B:472:CYS:O	B:588:GLU:OE1	0.517
3	B:585:ARG:HD3	B:945:ASN:OD1	0.511
3	B:943:PRO:HB2	B:632:PRO:HD3	0.508
3	B:631:ILE:HB	B:307:ILE:HB	0.507
3	B:278:ARG:NH2	B:693:LYS:HD2	0.505
3	B:689:TYR:CZ	B:344:GLN:HB2	0.502
3	B:340:TYR:O	B:580:VAL:HA	0.496
3	B:81:SER:O	B:750:ARG:HA	0.496
3	B:715:LEU:O	B:733:ASP:OD1	0.495
3	B:728:ASN:HB2	A:67:ILE:HG13	0.492
3	A:63:GLU:O	B:355:ASP:OD1	0.489
3	B:353:LYS:HB3	B:731:TYR:O	0.489
3	B:728:ASN:HB3	B:288:THR:O	0.478
3	B:285:GLU:HA	B:155:ASN:HB2	0.473
3	B:152:ASP:CG	B:282:ASN:HB3	0.468
3	B:186:VAL:HG11	B:581:VAL:O	0.465
3	B:82:TYR:HA	B:872:VAL:HG22	0.465
3	B:861:MET:SD	B:509:VAL:HG22	0.464
3	B:506:ALA:HA	B:584:ASN:HB2	0.459
3	A:70:VAL:HG21	B:632:PRO:HD2	0.449
3	B:629:GLY:C	B:885:ARG:HG3	0.442
3	B:881:GLU:O	B:850:MET:HB2	0.441

Model ID	Atom-1	Atom-2	Clash overlap (Å)
3	B:846:PHE:O	B:156:CYS:SG	0.440
3	B:140:LEU:HG	B:862:LEU:HG	0.438
3	B:858:LEU:O	B:497:PRO:HB3	0.435
3	B:16:TRP:HB2	B:443:LYS:HG2	0.434
3	B:355:ASP:OD2	B:926:ASN:HB2	0.433
3	B:922:TYR:O	B:996:LEU:HD23	0.432
3	B:873:CYS:SG	B:262:LEU:HG	0.431
3	B:258:GLN:O	B:832:ILE:O	0.429
3	B:815:THR:HA	B:733:ASP:HB2	0.428
3	B:728:ASN:HB2	B:29:LYS:HB3	0.426
3	B:15:ASN:HB3	B:897:LEU:HA	0.424
3	B:845:LYS:HB3	A:88:GLU:OE1	0.422
3	A:74:ARG:HD2	B:661:TYR:CE2	0.422
3	B:657:GLU:HB3	B:784:ARG:HD3	0.418
3	B:781:GLU:OE1	B:302:ALA:HA	0.415
3	B:294:PHE:O	B:194:THR:HG23	0.413
3	B:175:ILE:HG22	B:221:ILE:HG13	0.412
3	B:217:THR:O	B:475:GLN:HE22	0.410
3	B:199:ILE:HD11	B:877:LEU:HB2	0.408
3	B:873:CYS:O	B:979:TYR:CZ	0.408
3	B:898:PHE:HB3	B:747:ILE:O	0.408
3	B:717:ASN:HA	B:666:TYR:CD1	0.407
3	B:486:LYS:HE2	B:534:PHE:CZ	0.407

Model ID	Atom-1	Atom-2	Clash overlap (Å)
3	B:532:GLN:HB3	B:102:PRO:HD3	0.403
3	B:101:GLU:HA	B:936:TYR:OH	0.402
3	B:902:ARG:HD2	B:660:ILE:HD13	0.401
3	B:485:THR:HG22	B:183:PHE:O	0.401
4	B:182:LYS:HE2	B:912:ASP:N	0.633
4	B:908:TYR:HH	B:932:LEU:HA	0.555
4	B:904:HIS:ND1	A:9:VAL:HG22	0.534
4	A:8:LYS:O	B:265:ASP:HA	0.526
4	B:29:LYS:NZ	B:509:VAL:HG22	0.513
4	B:506:ALA:HA	A:111:ILE:HG23	0.509
4	A:17:LEU:HD21	B:564:ASN:HB2	0.505
4	B:560:SER:O	B:675:VAL:HG21	0.505
4	B:635:LEU:HD21	B:914:PRO:HD2	0.504
4	B:913:ASN:N	B:29:LYS:HB3	0.502
4	B:15:ASN:HB3	B:475:GLN:HG2	0.500
4	B:472:CYS:O	B:632:PRO:HD3	0.493
4	B:631:ILE:HB	B:375:GLU:H	0.490
4	B:373:VAL:HG13	B:262:LEU:HG	0.487
4	B:258:GLN:O	B:153:PRO:HG2	0.485
4	B:125:ASN:ND2	B:989:ASN:HB2	0.485
4	B:985:SER:O	B:56:GLN:HG2	0.484
4	B:52:ASP:O	B:678:LEU:HG	0.484
4	B:674:SER:O	A:46:ILE:HG12	0.480

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	A:42:VAL:O	B:563:PRO:HD3	0.479
4	B:562:TYR:HB2	B:590:ILE:HG12	0.477
4	A:77:ILE:HD12	B:998:ILE:HG13	0.477
4	B:994:LYS:O	B:841:ARG:NE	0.474
4	B:841:ARG:HA	B:32:CYS:HB3	0.469
4	B:8:ASP:HB3	B:632:PRO:HD2	0.458
4	B:629:GLY:C	B:988:VAL:HG22	0.457
4	B:984:THR:O	B:595:LEU:HG	0.456
4	B:591:ASN:O	B:428:LEU:O	0.453
4	B:411:CYS:HB3	B:255:ILE:HG13	0.452
4	B:251:VAL:O	A:4:LYS:HB3	0.451
4	A:3:GLY:O	B:776:ILE:HG13	0.446
4	B:772:VAL:O	B:147:CYS:HA	0.445
4	B:39:PHE:O	B:860:GLU:HG3	0.438
4	B:856:THR:O	B:276:ASP:OD2	0.435
4	B:175:ILE:HG12	B:265:ASP:HB2	0.434
4	B:169:SER:O	B:838:GLU:HG3	0.432
4	B:838:GLU:H	B:534:PHE:O	0.430
4	B:534:PHE:HD1	B:355:ASP:OD1	0.429
4	B:353:LYS:HB3	B:584:ASN:HB2	0.425
4	A:70:VAL:HG21	B:30:SER:HB2	0.425
4	B:11:VAL:HB	B:519:LEU:HG	0.425
4	B:515:LEU:O	B:374:ARG:N	0.425

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	B:373:VAL:HG13	B:181:LYS:H	0.421
4	B:180:ASP:CG	B:709:VAL:HG23	0.419
4	B:705:TYR:O	B:912:ASP:HB2	0.419
4	B:908:TYR:CE1	B:827:SER:OG	0.416
4	B:823:SER:HB3	B:302:ALA:HA	0.414
4	B:294:PHE:O	B:899:MET:SD	0.414
4	B:896:GLU:HA	B:227:ARG:HD2	0.413
4	B:223:GLU:OE2	B:135:LEU:O	0.412
4	B:9:PRO:HB3	B:28:LEU:HD13	0.412
4	B:16:TRP:CE2	B:373:VAL:HG12	0.412
4	B:372:GLY:O	B:670:ILE:HG12	0.412
4	B:666:TYR:O	B:210:LEU:HB2	0.410
4	B:194:THR:OG1	B:418:ILE:HG23	0.410
4	B:394:ALA:HB1	B:876:ILE:HG22	0.410
4	B:872:VAL:O	A:59:LEU:HD13	0.408
4	A:59:LEU:HA	B:491:ALA:HB1	0.408
4	B:129:PRO:HB2	B:175:ILE:HG13	0.408
4	B:175:ILE:O	B:60:PRO:HD3	0.406
4	B:59:SER:CB	B:830:GLU:HB3	0.406
4	B:818:LYS:HB3	B:484:GLU:HB2	0.404
4	B:478:TRP:HE1	B:756:VAL:HG21	0.403
4	B:549:PHE:HZ	A:45:LYS:HB2	0.401
5	A:41:THR:O	B:841:ARG:HA	0.638

Model ID	Atom-1	Atom-2	Clash overlap (Å)
5	B:841:ARG:CZ	B:418:ILE:HG23	0.624
5	B:394:ALA:HB1	B:457:LEU:HD11	0.603
5	B:224:ALA:HB2	B:693:LYS:HD2	0.588
5	B:689:TYR:CZ	B:750:ARG:HA	0.571
5	B:715:LEU:O	B:595:LEU:HG	0.559
5	B:591:ASN:O	B:914:PRO:HD2	0.552
5	B:913:ASN:N	A:67:ILE:HG13	0.540
5	A:63:GLU:O	B:509:VAL:HG22	0.537
5	B:506:ALA:HA	B:632:PRO:HD3	0.531
5	B:631:ILE:HB	B:635:LEU:HD13	0.523
5	B:563:PRO:HA	B:337:PHE:O	0.518
5	B:268:VAL:HA	B:373:VAL:HG12	0.504
5	B:372:GLY:O	B:375:GLU:H	0.502
5	B:373:VAL:HG13	B:271:ASN:HB3	0.499
5	B:270:PHE:O	B:229:CYS:O	0.498
5	B:225:VAL:HA	B:679:MET:SD	0.496
5	B:676:TYR:HA	B:899:MET:O	0.489
5	B:841:ARG:HD3	B:168:ARG:HA	0.480
5	B:31:ARG:NH2	B:32:CYS:HB3	0.479
5	B:8:ASP:HB3	B:327:HIS:HB2	0.477
5	B:308:TYR:CZ	A:46:ILE:HG12	0.470
5	A:42:VAL:O	B:170:TYR:CZ	0.468
5	B:168:ARG:HB2	B:862:LEU:HG	0.466

Model ID	Atom-1	Atom-2	Clash overlap (Å)
5	B:858:LEU:O	B:787:ASN:HB2	0.460
5	B:783:GLU:O	B:899:MET:SD	0.457
5	B:896:GLU:HA	B:168:ARG:HA	0.456
5	B:31:ARG:HH21	B:45:TYR:CE2	0.454
5	B:43:PRO:HB2	B:935:ARG:HG2	0.453
5	B:903:MET:SD	B:740:ILE:HA	0.451
5	B:720:LEU:O	B:936:TYR:OH	0.448
5	B:902:ARG:HD2	B:584:ASN:HB2	0.443
5	A:70:VAL:HG21	B:32:CYS:SG	0.439
5	B:11:VAL:HG12	B:29:LYS:HB3	0.437
5	B:15:ASN:HB3	B:133:TYR:CE1	0.437
5	B:127:ILE:HG23	B:861:MET:HG3	0.433
5	B:857:ARG:O	B:563:PRO:HD3	0.428
5	B:562:TYR:HB2	B:819:TYR:CE1	0.428
5	B:804:LYS:HD3	B:961:ILE:HB	0.428
5	B:922:TYR:CD2	B:389:LYS:HB3	0.423
5	B:364:CYS:SG	B:580:VAL:HA	0.422
5	B:81:SER:O	B:796:LYS:HG2	0.422
5	B:795:PHE:C	B:877:LEU:HB2	0.422
5	B:873:CYS:O	B:262:LEU:HG	0.420
5	B:258:GLN:O	A:119:LYS:HE2	0.418
5	A:116:THR:HG23	B:91:CYS:SG	0.415
5	B:74:ILE:HG12	B:225:VAL:HG23	0.411

Model ID	Atom-1	Atom-2	Clash overlap (Å)
5	B:221:ILE:O	B:140:LEU:HG	0.410
5	B:136:ASP:O	B:260:LEU:HG	0.410
5	B:256:ALA:O	B:410:ILE:HG22	0.409
5	B:402:TYR:HD1	B:302:ALA:HA	0.408
5	B:294:PHE:O	B:687:TYR:HB2	0.408
5	B:681:PHE:O	B:101:GLU:OE2	0.407
5	B:62:PRO:HA	B:61:PRO:HD3	0.405
5	B:60:PRO:HA	B:472:CYS:SG	0.403
5	B:399:THR:HG21	B:375:GLU:N	0.402
5	B:373:VAL:HG13	B:91:CYS:HA	0.401
5	B:73:THR:O	B:650:LYS:HG3	0.401
6	B:646:LYS:O	B:374:ARG:H	0.630
6	B:373:VAL:HG13	B:912:ASP:N	0.603
6	B:908:TYR:HH	B:750:ARG:HA	0.583
6	B:715:LEU:O	B:491:ALA:HB1	0.574
6	B:129:PRO:HB2	B:899:MET:SD	0.561
6	B:896:GLU:HA	A:53:ASP:HB2	0.546
6	A:50:SER:OG	B:418:ILE:HG23	0.545
6	B:394:ALA:HB1	B:526:VAL:O	0.530
6	B:75:ASP:HA	B:491:ALA:HB3	0.528
6	B:130:ASP:HB3	B:590:ILE:HG13	0.523
6	B:586:LEU:O	B:463:MET:HE3	0.522
6	B:448:LEU:HD22	B:594:LEU:HB2	0.516

Model ID	Atom-1	Atom-2	Clash overlap (Å)
6	B:590:ILE:O	B:229:CYS:O	0.510
6	B:225:VAL:HA	B:693:LYS:HD2	0.509
6	B:689:TYR:CZ	B:632:PRO:HD3	0.508
6	B:631:ILE:HB	B:509:VAL:HG22	0.491
6	B:506:ALA:HA	B:581:VAL:O	0.488
6	B:82:TYR:HA	B:668:TYR:CE1	0.482
6	B:950:LYS:HB3	B:884:LEU:HG	0.477
6	B:641:GLU:HG2	B:586:LEU:HB3	0.474
6	B:880:LEU:O	B:56:GLN:HG2	0.469
6	B:584:ASN:OD1	A:67:ILE:HG13	0.467
6	B:52:ASP:O	B:651:GLN:CD	0.466
6	A:63:GLU:O	B:459:ILE:HB	0.464
6	B:648:MET:HA	B:29:LYS:HB3	0.462
6	B:456:ASN:ND2	B:476:TYR:CD2	0.462
6	B:15:ASN:HB3	B:679:MET:HG3	0.461
6	B:396:VAL:HG13	B:667:THR:HG21	0.459
6	B:675:VAL:O	B:374:ARG:N	0.456
6	B:490:GLY:HA2	A:92:CYS:SG	0.455
6	B:373:VAL:HG22	B:680:GLY:HA3	0.453
6	A:72:ASN:HB2	B:915:ASN:ND2	0.451
6	B:536:TYR:CD2	B:914:PRO:HD2	0.446
6	B:912:ASP:HA	B:147:CYS:HA	0.444
6	B:913:ASN:N	B:475:GLN:OE1	0.441

Model ID	Atom-1	Atom-2	Clash overlap (Å)
6	B:39:PHE:O	B:877:LEU:HB2	0.440
6	B:205:ARG:HD2	B:616:LEU:HD13	0.438
6	B:873:CYS:O	B:687:TYR:CZ	0.434
6	B:581:VAL:HB	B:632:PRO:HD2	0.433
6	B:682:ARG:HG3	B:225:VAL:HG23	0.431
6	B:629:GLY:C	B:374:ARG:N	0.429
6	B:221:ILE:O	B:534:PHE:CE2	0.429
6	B:373:VAL:HG13	B:841:ARG:HA	0.428
6	B:532:GLN:HB3	B:784:ARG:HD3	0.424
6	B:841:ARG:CZ	B:660:ILE:HG12	0.423
6	B:781:GLU:OE1	B:963:ASP:HB3	0.422
6	B:656:THR:O	B:451:MET:HB2	0.418
6	B:922:TYR:OH	B:867:MET:SD	0.417
6	B:447:ASP:O	B:932:LEU:HD21	0.416
6	B:862:LEU:HA	B:475:GLN:HG2	0.415
6	B:447:ASP:HB3	B:703:ILE:HG12	0.413
6	B:472:CYS:O	B:522:LYS:O	0.411
6	B:699:GLY:O	B:337:PHE:O	0.411
6	B:72:ARG:HG2	B:255:ILE:HG13	0.409
6	B:268:VAL:HA	B:503:GLU:OE2	0.409
6	B:251:VAL:O	B:919:VAL:HG21	0.409
6	B:310:ARG:HD2	B:497:PRO:HB3	0.407
6	B:904:HIS:CD2	B:841:ARG:HG2	0.406

Model ID	Atom-1	Atom-2	Clash overlap (Å)
6	B:16:TRP:HB2	B:792:PHE:HB3	0.405
6	B:840:ARG:HG2	B:683:ASN:HB2	0.403
6	B:735:ARG:HD3	B:840:ARG:HD3	0.403
6	B:681:PHE:CE2	B:733:ASP:HB2	0.402
6	B:408:ASP:OD2	B:327:HIS:HB2	0.401
7	B:728:ASN:HB2	B:375:GLU:H	0.736
7	B:308:TYR:CZ	B:586:LEU:H	0.692
7	B:373:VAL:HG13	B:585:ARG:HB3	0.687
7	A:70:VAL:HG11	B:984:THR:HG22	0.650
7	A:70:VAL:HG12	B:509:VAL:HG22	0.627
7	B:880:LEU:HD21	B:731:TYR:O	0.595
7	B:506:ALA:HA	B:163:ARG:HA	0.581
7	B:728:ASN:HB3	B:586:LEU:HB3	0.579
7	B:132:CYS:SG	B:756:VAL:HG13	0.532
7	B:584:ASN:OD1	B:425:VAL:HG21	0.530
7	B:545:LYS:HB2	B:632:PRO:HD3	0.525
7	B:413:VAL:HG13	B:451:MET:HB2	0.518
7	B:631:ILE:HB	B:38:VAL:HG23	0.483
7	B:447:ASP:O	B:420:GLU:H	0.483
7	B:32:CYS:SG	A:46:ILE:HG12	0.474
7	B:419:TRP:CD1	B:428:LEU:HA	0.474
7	A:42:VAL:O	B:100:GLU:O	0.472
7	B:374:ARG:O	B:678:LEU:HG	0.469

Model ID	Atom-1	Atom-2	Clash overlap (Å)
7	B:63:PHE:HB3	B:586:LEU:N	0.465
7	B:674:SER:O	B:463:MET:SD	0.461
7	A:70:VAL:HG11	B:437:TYR:CE2	0.460
7	B:193:HIS:HE1	B:740:ILE:HG23	0.459
7	B:434:ASN:HB2	B:271:ASN:HB3	0.456
7	B:721:ARG:HG2	B:595:LEU:HG	0.456
7	B:270:PHE:O	B:852:LYS:HB2	0.455
7	B:591:ASN:O	B:983:LEU:HA	0.449
7	B:848:LYS:O	A:58:CYS:SG	0.447
7	B:847:HIS:CE1	B:756:VAL:HG11	0.443
7	A:20:LYS:HG3	A:75:PHE:CZ	0.441
7	B:549:PHE:HZ	B:94:ALA:O	0.441
7	A:70:VAL:HG13	B:632:PRO:HD2	0.440
7	B:70:LYS:HA	B:750:ARG:HA	0.440
7	B:629:GLY:C	B:766:GLU:OE1	0.439
7	B:715:LEU:O	B:255:ILE:HG13	0.436
7	B:754:ARG:HD3	B:373:VAL:HG12	0.436
7	B:251:VAL:O	B:787:ASN:HB2	0.435
7	B:372:GLY:O	B:416:LYS:HD3	0.433
7	B:783:GLU:O	B:711:ASN:HB2	0.431
7	B:413:VAL:HG11	B:601:PRO:HD3	0.426
7	B:707:GLU:O	B:816:THR:HB	0.424
7	B:600:PRO:HA	B:914:PRO:HD3	0.424

Model ID	Atom-1	Atom-2	Clash overlap (Å)
7	B:815:THR:O	B:686:LEU:O	0.418
7	B:913:ASN:HB2	B:111:THR:O	0.415
7	B:679:MET:HA	B:61:PRO:HD3	0.415
7	B:49:VAL:HB	B:28:LEU:HD13	0.414
7	B:59:SER:O	B:34:ASN:OD1	0.414
7	B:16:TRP:CE2	B:437:TYR:CZ	0.411
7	B:32:CYS:HB2	B:862:LEU:HG	0.408
7	B:434:ASN:HB2	B:829:PRO:HG3	0.405
7	B:858:LEU:O	B:484:GLU:HB2	0.405
7	B:819:TYR:CZ	B:148:TYR:O	0.404
7	B:478:TRP:NE1	B:483:VAL:HG21	0.404
7	B:40:ILE:HA	B:616:LEU:HB2	0.402
7	B:339:LEU:HD21	B:138:GLN:HB2	0.402
7	B:611:PRO:HB3	B:663:SER:OG	0.401
7	B:136:ASP:OD1	B:602:PRO:HA	0.401
7	B:485:THR:HB	A:88:GLU:OE1	0.400
8	B:601:PRO:CB	B:374:ARG:H	0.762
8	A:74:ARG:HD3	B:163:ARG:HA	0.635
8	B:373:VAL:HG13	A:118:VAL:HG23	0.571
8	B:132:CYS:SG	B:265:ASP:HB2	0.568
8	A:114:VAL:O	B:840:ARG:NE	0.560
8	B:169:SER:O	A:67:ILE:HG13	0.520
8	B:840:ARG:HA	B:693:LYS:HD2	0.517

Model ID	Atom-1	Atom-2	Clash overlap (Å)
8	A:63:GLU:O	B:28:LEU:HD13	0.516
8	B:689:TYR:CZ	B:867:MET:SD	0.502
8	B:16:TRP:CE2	B:731:TYR:O	0.498
8	B:862:LEU:HA	B:153:PRO:HG2	0.487
8	B:728:ASN:HB3	B:632:PRO:HD3	0.484
8	B:125:ASN:ND2	B:246:LEU:HD23	0.481
8	B:631:ILE:HB	B:959:GLU:HG2	0.480
8	B:211:ILE:HB	B:897:LEU:HD13	0.479
8	B:940:TYR:CE1	B:94:ALA:O	0.472
8	B:894:PRO:HD2	B:509:VAL:HG22	0.471
8	B:70:LYS:HA	B:387:LYS:HA	0.470
8	B:506:ALA:HA	B:717:ASN:HB2	0.470
8	B:382:ASP:OD1	B:872:VAL:HG23	0.470
8	B:716:SER:O	B:32:CYS:HB3	0.467
8	B:868:ASN:O	B:155:ASN:HB2	0.460
8	B:8:ASP:HB3	B:563:PRO:HD3	0.460
8	B:152:ASP:CG	B:733:ASP:HB2	0.457
8	B:562:TYR:HB2	B:282:ASN:HB3	0.453
8	B:728:ASN:HB2	B:581:VAL:O	0.451
8	B:186:VAL:HG11	B:194:THR:HG22	0.449
8	B:82:TYR:HA	B:337:PHE:O	0.447
8	B:175:ILE:HG22	B:147:CYS:HA	0.444
8	B:268:VAL:HA	B:750:ARG:HA	0.442

Model ID	Atom-1	Atom-2	Clash overlap (Å)
8	B:39:PHE:O	A:66:PHE:HB2	0.441
8	B:715:LEU:O	B:266:TYR:CD2	0.440
8	A:62:PRO:O	B:475:GLN:HG2	0.439
8	B:265:ASP:HB3	B:268:VAL:HB	0.437
8	B:472:CYS:O	A:46:ILE:HG12	0.434
8	B:172:PHE:CD1	B:286:LEU:HD22	0.432
8	A:42:VAL:O	B:832:ILE:HD11	0.432
8	B:187:PHE:HA	B:616:LEU:HD23	0.430
8	B:818:LYS:HB2	B:229:CYS:O	0.429
8	B:583:THR:HG23	B:265:ASP:HA	0.429
8	B:225:VAL:HA	B:632:PRO:HD2	0.426
8	B:29:LYS:NZ	B:590:ILE:HG12	0.425
8	B:629:GLY:C	B:242:ARG:HG3	0.425
8	A:77:ILE:HD12	B:276:ASP:HB2	0.424
8	B:230:LEU:HD22	B:767:ILE:O	0.424
8	B:272:GLY:HA2	B:227:ARG:HD2	0.419
8	B:551:ASN:HB3	B:280:ILE:HG13	0.414
8	B:223:GLU:OE2	B:595:LEU:HB2	0.413
8	B:276:ASP:O	B:709:VAL:HG23	0.411
8	B:591:ASN:O	B:286:LEU:CD2	0.409
8	B:705:TYR:O	B:338:ASP:HA	0.409
8	B:187:PHE:HA	B:261:GLU:HB2	0.406
8	B:269:THR:O	B:58:LEU:HG	0.406

Model ID	Atom-1	Atom-2	Clash overlap (Å)
8	B:257:LYS:O	B:95:ASP:OD2	0.404
8	B:54:ILE:O	B:518:LEU:HG	0.404
8	B:70:LYS:HG3	B:29:LYS:HB3	0.402
8	B:514:LEU:O	B:866:ARG:HD3	0.401
8	B:15:ASN:HB3	B:924:LYS:H	0.400
9	B:864:GLU:OE2	B:374:ARG:H	0.647
9	B:922:TYR:C	A:12:ALA:HA	0.568
9	B:373:VAL:HG13	B:731:TYR:O	0.540
9	A:6:PHE:O	B:389:LYS:HE3	0.539
9	B:728:ASN:HB3	B:461:LEU:HG	0.532
9	B:363:SER:O	B:496:LEU:HD21	0.526
9	B:457:LEU:O	B:693:LYS:HD2	0.518
9	B:116:LEU:HD13	B:32:CYS:HA	0.512
9	B:689:TYR:CZ	B:842:ASP:HB3	0.512
9	B:10:ASP:O	B:163:ARG:HA	0.505
9	B:838:GLU:HA	B:632:PRO:HD3	0.505
9	B:132:CYS:SG	B:983:LEU:HA	0.492
9	B:631:ILE:HB	B:594:LEU:HD21	0.491
9	B:847:HIS:CE1	B:418:ILE:HG23	0.482
9	A:80:CYS:SG	B:229:CYS:O	0.473
9	B:394:ALA:HB1	B:914:PRO:HD2	0.471
9	B:225:VAL:HA	B:56:GLN:HG2	0.470
9	B:913:ASN:N	B:58:LEU:HG	0.463

Model ID	Atom-1	Atom-2	Clash overlap (Å)
9	B:52:ASP:O	B:265:ASP:HB2	0.462
9	B:54:ILE:O	A:12:ALA:HB2	0.454
9	B:169:SER:O	B:512:GLY:HA3	0.450
9	A:8:LYS:HA	B:965:SER:H	0.443
9	B:494:TYR:O	B:374:ARG:N	0.436
9	B:963:ASP:CG	B:733:ASP:HB2	0.432
9	B:373:VAL:HG22	B:109:ASN:N	0.428
9	B:728:ASN:HB2	B:150:CYS:O	0.423
9	B:108:GLN:HG2	B:998:ILE:HG13	0.421
9	B:43:PRO:HD3	A:46:ILE:HG12	0.420
9	B:449:ALA:HB3	B:841:ARG:HA	0.418
9	B:994:LYS:O	B:295:ARG:NH1	0.417
9	A:42:VAL:O	B:840:ARG:HD3	0.414
9	B:841:ARG:CZ	B:833:ASN:OD1	0.414
9	B:293:ILE:HB	B:431:THR:HB	0.413
9	B:840:ARG:C	B:740:ILE:HB	0.413
9	B:815:THR:HB	B:245:VAL:HG12	0.412
9	B:373:VAL:O	B:60:PRO:HD3	0.410
9	B:738:ASN:ND2	B:980:PHE:CE2	0.408
9	B:230:LEU:HB3	A:73:MET:HG3	0.406
9	B:59:SER:HB2	B:148:TYR:O	0.405
9	B:976:TYR:HB3	B:525:LEU:HB3	0.404
9	A:69:LEU:O	B:670:ILE:HG12	0.402

Model ID	Atom-1	Atom-2	Clash overlap (Å)
10	B:40:ILE:HA	B:375:GLU:H	0.729
10	B:1002:GLU:O	B:221:ILE:HD12	0.707
10	B:76:ILE:HD13	B:416:LYS:HD3	0.541
10	B:666:TYR:O	B:194:THR:HG23	0.531
10	B:373:VAL:HG13	B:666:TYR:CD1	0.517
10	B:218:GLU:HA	B:914:PRO:HD2	0.505
10	B:413:VAL:HG11	B:632:PRO:HD3	0.504
10	B:175:ILE:HG22	A:92:CYS:SG	0.502
10	B:486:LYS:HE2	B:884:LEU:HG	0.497
10	B:913:ASN:N	B:996:LEU:HD23	0.494
10	B:631:ILE:HB	B:337:PHE:O	0.493
10	A:72:ASN:HB2	B:511:LYS:HD3	0.493
10	B:880:LEU:O	A:66:PHE:HB2	0.488
10	B:873:CYS:SG	B:933:GLY:HA2	0.484
10	B:268:VAL:HA	B:742:LYS:HD2	0.467
10	B:114:GLU:O	A:46:ILE:HG12	0.462
10	A:62:PRO:O	B:138:GLN:HB3	0.460
10	B:903:MET:SD	B:276:ASP:HA	0.458
10	B:719:MET:SD	B:221:ILE:HG13	0.456
10	A:42:VAL:O	B:834:LYS:HD2	0.454
10	B:136:ASP:OD1	B:632:PRO:HD2	0.451
10	B:175:ILE:HD11	B:937:TYR:HA	0.446
10	B:217:THR:O	B:750:ARG:HA	0.444

Model ID	Atom-1	Atom-2	Clash overlap (Å)
10	B:814:TYR:CE2	B:816:THR:HG21	0.431
10	B:629:GLY:C	B:473:LEU:HG	0.427
10	B:900:LEU:O	B:512:GLY:HA3	0.427
10	B:715:LEU:O	B:990:LEU:HG	0.419
10	B:803:TYR:CD2	B:680:GLY:HA3	0.414
10	B:469:HIS:O	A:9:VAL:HB	0.413
10	B:494:TYR:O	B:61:PRO:HD3	0.413
10	B:986:GLU:O	B:168:ARG:HA	0.410
10	B:1002:GLU:O	B:899:MET:SD	0.410
10	B:536:TYR:CD2	B:660:ILE:HG12	0.409
10	A:8:LYS:O	B:883:ASP:HB2	0.409
10	B:60:PRO:HA	B:584:ASN:HB2	0.406
10	B:31:ARG:NH2	B:60:PRO:HD3	0.405
10	B:896:GLU:HA	A:101:ILE:HG12	0.404
10	B:656:THR:O	B:798:GLU:HB2	0.404
10	B:879:SER:O	B:797:ILE:HG23	0.402

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	1115	1048	63	4
2	1115	1049	60	6
3	1115	1046	64	5
4	1115	1048	63	4

Model ID	Analyzed	Favored	Allowed	Outliers
5	1115	1040	72	3
6	1115	1040	71	4
7	1115	1050	60	5
8	1115	1054	55	6
9	1115	1045	62	8
10	1115	1048	61	6

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	1036	834	105	97
2	1036	838	111	87
3	1036	838	102	96
4	1036	843	99	94
5	1036	834	115	87
6	1036	838	115	83
7	1036	829	111	96
8	1036	826	120	90
9	1036	807	120	109
10	1036	831	120	85

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	11	SER
1	A	20	LYS

Model ID	Chain	Residue ID	Residue type
1	A	32	LEU
1	A	37	ASN
1	A	41	THR
1	A	50	SER
1	A	59	LEU
1	A	66	PHE
1	A	77	ILE
1	A	90	THR
1	A	92	CYS
1	A	117	ASP
1	A	119	LYS
1	B	19	SER
1	B	22	GLU
1	B	31	ARG
1	B	33	ARG
1	B	57	SER
1	B	59	SER
1	B	73	THR
1	B	77	ASP
1	B	106	SER
1	B	108	GLN
1	B	113	ASP
1	B	114	GLU

Model ID	Chain	Residue ID	Residue type
1	B	147	CYS
1	B	169	SER
1	B	173	LEU
1	B	176	GLU
1	B	177	CYS
1	B	180	ASP
1	B	181	LYS
1	B	204	LYS
1	B	209	THR
1	B	217	THR
1	B	223	GLU
1	B	245	VAL
1	B	248	SER
1	B	263	THR
1	B	269	THR
1	B	288	THR
1	B	298	ASP
1	B	300	LYS
1	B	306	CYS
1	B	324	THR
1	B	325	THR
1	B	346	SER
1	B	365	MET

Model ID	Chain	Residue ID	Residue type
1	B	373	VAL
1	B	381	ASP
1	B	389	LYS
1	B	407	GLU
1	B	411	CYS
1	B	432	LEU
1	B	435	ASP
1	B	439	LEU
1	B	459	ILE
1	B	470	ASP
1	B	488	ASP
1	B	499	SER
1	B	507	SER
1	B	508	THR
1	B	530	THR
1	B	534	PHE
1	B	572	SER
1	B	593	GLN
1	B	606	THR
1	B	618	SER
1	B	655	SER
1	B	656	THR
1	B	691	SER

Model ID	Chain	Residue ID	Residue type
1	B	696	THR
1	B	700	ARG
1	B	707	GLU
1	B	708	SER
1	B	716	SER
1	B	744	SER
1	B	755	SER
1	B	759	ASP
1	B	762	SER
1	B	805	ASN
1	B	820	SER
1	B	822	SER
1	B	825	SER
1	B	836	THR
1	B	838	GLU
1	B	841	ARG
1	B	892	SER
1	B	929	THR
1	B	957	THR
1	B	965	SER
1	B	975	PHE
1	B	984	THR
1	B	1008	LYS

Model ID	Chain	Residue ID	Residue type
2	A	11	SER
2	A	17	LEU
2	A	20	LYS
2	A	32	LEU
2	A	38	LYS
2	A	47	LYS
2	A	49	GLN
2	A	50	SER
2	A	59	LEU
2	A	74	ARG
2	A	81	LYS
2	A	87	ILE
2	A	90	THR
2	B	13	CYS
2	B	18	GLU
2	B	19	SER
2	B	20	HIS
2	B	30	SER
2	B	59	SER
2	B	73	THR
2	B	77	ASP
2	B	83	ASN
2	B	88	ASP

Model ID	Chain	Residue ID	Residue type
2	B	92	SER
2	B	106	SER
2	B	108	GLN
2	B	120	TRP
2	B	150	CYS
2	B	161	ILE
2	B	166	ILE
2	B	173	LEU
2	B	217	THR
2	B	248	SER
2	B	252	LEU
2	B	263	THR
2	B	269	THR
2	B	281	THR
2	B	285	GLU
2	B	325	THR
2	B	328	VAL
2	B	350	ASP
2	B	353	LYS
2	B	364	CYS
2	B	373	VAL
2	B	384	THR
2	B	408	ASP

Model ID	Chain	Residue ID	Residue type
2	B	411	CYS
2	B	431	THR
2	B	452	TYR
2	B	475	GLN
2	B	485	THR
2	B	499	SER
2	B	507	SER
2	B	530	THR
2	B	534	PHE
2	B	536	TYR
2	B	572	SER
2	B	583	THR
2	B	585	ARG
2	B	592	ASN
2	B	606	THR
2	B	618	SER
2	B	641	GLU
2	B	656	THR
2	B	674	SER
2	B	700	ARG
2	B	708	SER
2	B	714	GLU
2	B	716	SER

Model ID	Chain	Residue ID	Residue type
2	B	744	SER
2	B	765	THR
2	B	800	GLU
2	B	822	SER
2	B	837	SER
2	B	838	GLU
2	B	840	ARG
2	B	866	ARG
2	B	869	SER
2	B	879	SER
2	B	890	SER
2	B	957	THR
2	B	963	ASP
2	B	965	SER
2	B	973	ARG
2	B	982	ARG
2	B	1001	PHE
3	A	6	PHE
3	A	8	LYS
3	A	11	SER
3	A	28	THR
3	A	50	SER
3	A	66	PHE

Model ID	Chain	Residue ID	Residue type
3	A	75	PHE
3	A	90	THR
3	A	100	THR
3	A	117	ASP
3	B	19	SER
3	B	20	HIS
3	B	30	SER
3	B	31	ARG
3	B	59	SER
3	B	75	ASP
3	B	95	ASP
3	B	113	ASP
3	B	116	LEU
3	B	141	THR
3	B	156	CYS
3	B	166	ILE
3	B	169	SER
3	B	173	LEU
3	B	192	SER
3	B	217	THR
3	B	223	GLU
3	B	226	ASP
3	B	234	SER

Model ID	Chain	Residue ID	Residue type
3	B	235	LEU
3	B	247	CYS
3	B	248	SER
3	B	263	THR
3	B	265	ASP
3	B	285	GLU
3	B	309	GLU
3	B	350	ASP
3	B	353	LYS
3	B	364	CYS
3	B	365	MET
3	B	381	ASP
3	B	404	THR
3	B	411	CYS
3	B	417	ASP
3	B	485	THR
3	B	488	ASP
3	B	493	THR
3	B	499	SER
3	B	507	SER
3	B	508	THR
3	B	527	ARG
3	B	528	SER

Model ID	Chain	Residue ID	Residue type
3	B	530	THR
3	B	534	PHE
3	B	548	MET
3	B	558	TYR
3	B	572	SER
3	B	583	THR
3	B	585	ARG
3	B	595	LEU
3	B	606	THR
3	B	618	SER
3	B	641	GLU
3	B	655	SER
3	B	682	ARG
3	B	688	SER
3	B	691	SER
3	B	701	ARG
3	B	744	SER
3	B	765	THR
3	B	768	ASP
3	B	773	ASP
3	B	820	SER
3	B	823	SER
3	B	825	SER

Model ID	Chain	Residue ID	Residue type
3	B	837	SER
3	B	838	GLU
3	B	840	ARG
3	B	844	SER
3	B	853	THR
3	B	854	TYR
3	B	858	LEU
3	B	868	ASN
3	B	877	LEU
3	B	881	GLU
3	B	899	MET
3	B	929	THR
3	B	952	LEU
3	B	957	THR
3	B	960	THR
3	B	965	SER
3	B	970	SER
3	B	995	VAL
4	A	7	SER
4	A	8	LYS
4	A	9	VAL
4	A	32	LEU
4	A	41	THR

Model ID	Chain	Residue ID	Residue type
4	A	66	PHE
4	A	90	THR
4	A	97	SER
4	A	99	GLU
4	A	105	PHE
4	A	113	ASN
4	A	119	LYS
4	B	18	GLU
4	B	19	SER
4	B	30	SER
4	B	31	ARG
4	B	59	SER
4	B	73	THR
4	B	77	ASP
4	B	84	LEU
4	B	95	ASP
4	B	103	LYS
4	B	141	THR
4	B	165	ASP
4	B	173	LEU
4	B	176	GLU
4	B	194	THR
4	B	206	LEU

Model ID	Chain	Residue ID	Residue type
4	B	217	THR
4	B	223	GLU
4	B	246	LEU
4	B	248	SER
4	B	258	GLN
4	B	269	THR
4	B	273	HIS
4	B	288	THR
4	B	300	LYS
4	B	339	LEU
4	B	365	MET
4	B	373	VAL
4	B	411	CYS
4	B	417	ASP
4	B	454	ASP
4	B	470	ASP
4	B	485	THR
4	B	492	SER
4	B	499	SER
4	B	507	SER
4	B	508	THR
4	B	520	GLU
4	B	525	LEU

Model ID	Chain	Residue ID	Residue type
4	B	529	GLU
4	B	530	THR
4	B	532	GLN
4	B	534	PHE
4	B	548	MET
4	B	557	ASP
4	B	572	SER
4	B	588	GLU
4	B	594	LEU
4	B	606	THR
4	B	649	LEU
4	B	656	THR
4	B	679	MET
4	B	691	SER
4	B	708	SER
4	B	727	SER
4	B	743	THR
4	B	744	SER
4	B	755	SER
4	B	760	THR
4	B	820	SER
4	B	822	SER
4	B	825	SER

Model ID	Chain	Residue ID	Residue type
4	B	836	THR
4	B	838	GLU
4	B	844	SER
4	B	859	SER
4	B	892	SER
4	B	929	THR
4	B	932	LEU
4	B	957	THR
4	B	965	SER
4	B	970	SER
4	B	975	PHE
4	B	982	ARG
4	B	989	ASN
4	B	991	LEU
4	B	995	VAL
4	B	999	SER
4	B	1001	PHE
5	A	11	SER
5	A	28	THR
5	A	32	LEU
5	A	41	THR
5	A	66	PHE
5	A	90	THR

Model ID	Chain	Residue ID	Residue type
5	A	97	SER
5	A	124	GLU
5	B	14	ILE
5	B	18	GLU
5	B	19	SER
5	B	24	ARG
5	B	57	SER
5	B	59	SER
5	B	103	LYS
5	B	113	ASP
5	B	120	TRP
5	B	166	ILE
5	B	173	LEU
5	B	181	LYS
5	B	194	THR
5	B	217	THR
5	B	223	GLU
5	B	235	LEU
5	B	248	SER
5	B	252	LEU
5	B	263	THR
5	B	285	GLU
5	B	288	THR

Model ID	Chain	Residue ID	Residue type
5	B	300	LYS
5	B	301	GLU
5	B	325	THR
5	B	356	SER
5	B	358	SER
5	B	373	VAL
5	B	411	CYS
5	B	417	ASP
5	B	435	ASP
5	B	485	THR
5	B	488	ASP
5	B	492	SER
5	B	493	THR
5	B	499	SER
5	B	529	GLU
5	B	530	THR
5	B	534	PHE
5	B	572	SER
5	B	583	THR
5	B	606	THR
5	B	618	SER
5	B	641	GLU
5	B	653	THR

Model ID	Chain	Residue ID	Residue type
5	B	655	SER
5	B	656	THR
5	B	674	SER
5	B	688	SER
5	B	695	CYS
5	B	716	SER
5	B	724	ASN
5	B	744	SER
5	B	759	ASP
5	B	770	GLN
5	B	796	LYS
5	B	822	SER
5	B	836	THR
5	B	838	GLU
5	B	853	THR
5	B	854	TYR
5	B	859	SER
5	B	877	LEU
5	B	892	SER
5	B	897	LEU
5	B	903	MET
5	B	932	LEU
5	B	949	THR

Model ID	Chain	Residue ID	Residue type
5	B	957	THR
5	B	963	ASP
5	B	965	SER
5	B	975	PHE
5	B	984	THR
5	B	986	GLU
5	B	1001	PHE
5	B	1007	SER
5	B	1008	LYS
6	A	11	SER
6	A	17	LEU
6	A	41	THR
6	A	47	LYS
6	A	49	GLN
6	A	53	ASP
6	A	59	LEU
6	A	75	PHE
6	A	82	VAL
6	A	90	THR
6	B	19	SER
6	B	59	SER
6	B	71	MET
6	B	77	ASP

Model ID	Chain	Residue ID	Residue type
6	B	88	ASP
6	B	92	SER
6	B	95	ASP
6	B	108	GLN
6	B	117	ASN
6	B	151	ASP
6	B	168	ARG
6	B	173	LEU
6	B	180	ASP
6	B	206	LEU
6	B	223	GLU
6	B	226	ASP
6	B	237	GLU
6	B	245	VAL
6	B	248	SER
6	B	269	THR
6	B	288	THR
6	B	300	LYS
6	B	309	GLU
6	B	324	THR
6	B	351	SER
6	B	356	SER
6	B	381	ASP

Model ID	Chain	Residue ID	Residue type
6	B	383	THR
6	B	428	LEU
6	B	432	LEU
6	B	434	ASN
6	B	435	ASP
6	B	459	ILE
6	B	462	ASP
6	B	470	ASP
6	B	473	LEU
6	B	485	THR
6	B	499	SER
6	B	507	SER
6	B	508	THR
6	B	529	GLU
6	B	530	THR
6	B	534	PHE
6	B	572	SER
6	B	593	GLN
6	B	594	LEU
6	B	606	THR
6	B	620	ILE
6	B	655	SER
6	B	665	GLN

Model ID	Chain	Residue ID	Residue type
6	B	674	SER
6	B	708	SER
6	B	716	SER
6	B	727	SER
6	B	738	ASN
6	B	744	SER
6	B	759	ASP
6	B	765	THR
6	B	806	LEU
6	B	836	THR
6	B	838	GLU
6	B	843	VAL
6	B	844	SER
6	B	870	ASN
6	B	877	LEU
6	B	886	SER
6	B	892	SER
6	B	949	THR
6	B	960	THR
6	B	991	LEU
6	B	1008	LYS
7	A	4	LYS
7	A	11	SER

Model ID	Chain	Residue ID	Residue type
7	A	17	LEU
7	A	18	THR
7	A	28	THR
7	A	30	ASP
7	A	32	LEU
7	A	39	SER
7	A	41	THR
7	A	50	SER
7	A	55	SER
7	A	57	GLU
7	A	74	ARG
7	A	90	THR
7	A	112	PHE
7	A	113	ASN
7	A	119	LYS
7	A	120	LYS
7	B	18	GLU
7	B	19	SER
7	B	20	HIS
7	B	24	ARG
7	B	59	SER
7	B	92	SER
7	B	106	SER

Model ID	Chain	Residue ID	Residue type
7	B	108	GLN
7	B	141	THR
7	B	181	LYS
7	B	185	SER
7	B	194	THR
7	B	217	THR
7	B	226	ASP
7	B	235	LEU
7	B	248	SER
7	B	263	THR
7	B	273	HIS
7	B	285	GLU
7	B	300	LYS
7	B	325	THR
7	B	346	SER
7	B	350	ASP
7	B	363	SER
7	B	369	LEU
7	B	373	VAL
7	B	377	THR
7	B	381	ASP
7	B	399	THR
7	B	418	ILE

Model ID	Chain	Residue ID	Residue type
7	B	431	THR
7	B	432	LEU
7	B	434	ASN
7	B	454	ASP
7	B	458	ASN
7	B	475	GLN
7	B	485	THR
7	B	488	ASP
7	B	499	SER
7	B	507	SER
7	B	530	THR
7	B	534	PHE
7	B	558	TYR
7	B	572	SER
7	B	606	THR
7	B	674	SER
7	B	681	PHE
7	B	708	SER
7	B	716	SER
7	B	727	SER
7	B	743	THR
7	B	744	SER
7	B	755	SER

Model ID	Chain	Residue ID	Residue type
7	B	760	THR
7	B	765	THR
7	B	793	ASN
7	B	820	SER
7	B	822	SER
7	B	823	SER
7	B	825	SER
7	B	836	THR
7	B	837	SER
7	B	838	GLU
7	B	844	SER
7	B	853	THR
7	B	859	SER
7	B	866	ARG
7	B	889	ASP
7	B	897	LEU
7	B	929	THR
7	B	957	THR
7	B	965	SER
7	B	970	SER
7	B	973	ARG
7	B	1001	PHE
7	B	1007	SER

Model ID	Chain	Residue ID	Residue type
8	A	8	LYS
8	A	17	LEU
8	A	25	GLU
8	A	29	VAL
8	A	41	THR
8	A	50	SER
8	A	81	LYS
8	A	87	ILE
8	A	90	THR
8	A	113	ASN
8	A	117	ASP
8	B	19	SER
8	B	20	HIS
8	B	59	SER
8	B	75	ASP
8	B	87	LYS
8	B	95	ASP
8	B	144	ASN
8	B	173	LEU
8	B	181	LYS
8	B	194	THR
8	B	217	THR
8	B	223	GLU

Model ID	Chain	Residue ID	Residue type
8	B	241	GLU
8	B	263	THR
8	B	291	LYS
8	B	325	THR
8	B	339	LEU
8	B	351	SER
8	B	360	ASN
8	B	364	CYS
8	B	365	MET
8	B	381	ASP
8	B	389	LYS
8	B	399	THR
8	B	414	ILE
8	B	432	LEU
8	B	437	TYR
8	B	461	LEU
8	B	462	ASP
8	B	474	CYS
8	B	485	THR
8	B	486	LYS
8	B	499	SER
8	B	508	THR
8	B	530	THR

Model ID	Chain	Residue ID	Residue type
8	B	534	PHE
8	B	565	VAL
8	B	572	SER
8	B	583	THR
8	B	606	THR
8	B	618	SER
8	B	653	THR
8	B	665	GLN
8	B	700	ARG
8	B	704	LEU
8	B	716	SER
8	B	724	ASN
8	B	727	SER
8	B	743	THR
8	B	744	SER
8	B	756	VAL
8	B	759	ASP
8	B	765	THR
8	B	797	ILE
8	B	805	ASN
8	B	820	SER
8	B	825	SER
8	B	836	THR

Model ID	Chain	Residue ID	Residue type
8	B	838	GLU
8	B	840	ARG
8	B	844	SER
8	B	848	LYS
8	B	859	SER
8	B	864	GLU
8	B	866	ARG
8	B	869	SER
8	B	903	MET
8	B	918	LEU
8	B	924	LYS
8	B	926	ASN
8	B	929	THR
8	B	949	THR
8	B	952	LEU
8	B	957	THR
8	B	965	SER
8	B	1008	LYS
9	A	4	LYS
9	A	8	LYS
9	A	11	SER
9	A	17	LEU
9	A	28	THR

Model ID	Chain	Residue ID	Residue type
9	A	30	ASP
9	A	32	LEU
9	A	41	THR
9	A	50	SER
9	A	74	ARG
9	A	75	PHE
9	A	82	VAL
9	A	90	THR
9	A	93	LEU
9	A	117	ASP
9	B	10	ASP
9	B	14	ILE
9	B	19	SER
9	B	20	HIS
9	B	22	GLU
9	B	31	ARG
9	B	51	THR
9	B	73	THR
9	B	75	ASP
9	B	77	ASP
9	B	79	THR
9	B	88	ASP
9	B	117	ASN

Model ID	Chain	Residue ID	Residue type
9	B	141	THR
9	B	173	LEU
9	B	180	ASP
9	B	192	SER
9	B	194	THR
9	B	204	LYS
9	B	207	LEU
9	B	213	GLU
9	B	217	THR
9	B	226	ASP
9	B	235	LEU
9	B	248	SER
9	B	252	LEU
9	B	263	THR
9	B	285	GLU
9	B	288	THR
9	B	300	LYS
9	B	306	CYS
9	B	340	TYR
9	B	363	SER
9	B	365	MET
9	B	383	THR
9	B	389	LYS

Model ID	Chain	Residue ID	Residue type
9	B	399	THR
9	B	408	ASP
9	B	411	CYS
9	B	475	GLN
9	B	499	SER
9	B	507	SER
9	B	508	THR
9	B	522	LYS
9	B	529	GLU
9	B	530	THR
9	B	532	GLN
9	B	534	PHE
9	B	537	GLU
9	B	572	SER
9	B	575	THR
9	B	588	GLU
9	B	610	GLU
9	B	641	GLU
9	B	656	THR
9	B	683	ASN
9	B	686	LEU
9	B	697	SER
9	B	701	ARG

Model ID	Chain	Residue ID	Residue type
9	B	716	SER
9	B	727	SER
9	B	743	THR
9	B	755	SER
9	B	759	ASP
9	B	760	THR
9	B	762	SER
9	B	800	GLU
9	B	820	SER
9	B	822	SER
9	B	823	SER
9	B	825	SER
9	B	837	SER
9	B	838	GLU
9	B	839	THR
9	B	844	SER
9	B	867	MET
9	B	869	SER
9	B	877	LEU
9	B	879	SER
9	B	892	SER
9	B	929	THR
9	B	931	GLU

Model ID	Chain	Residue ID	Residue type
9	B	957	THR
9	B	963	ASP
9	B	973	ARG
9	B	975	PHE
9	B	989	ASN
9	B	999	SER
9	B	1007	SER
9	B	1008	LYS
10	A	11	SER
10	A	17	LEU
10	A	32	LEU
10	A	41	THR
10	A	74	ARG
10	A	90	THR
10	A	97	SER
10	A	100	THR
10	A	113	ASN
10	A	122	LEU
10	B	19	SER
10	B	40	ILE
10	B	50	VAL
10	B	57	SER
10	B	79	THR

Model ID	Chain	Residue ID	Residue type
10	B	95	ASP
10	B	151	ASP
10	B	173	LEU
10	B	176	GLU
10	B	180	ASP
10	B	223	GLU
10	B	226	ASP
10	B	234	SER
10	B	248	SER
10	B	269	THR
10	B	275	PHE
10	B	285	GLU
10	B	288	THR
10	B	293	ILE
10	B	300	LYS
10	B	325	THR
10	B	328	VAL
10	B	339	LEU
10	B	359	LYS
10	B	365	MET
10	B	369	LEU
10	B	373	VAL
10	B	397	LEU

Model ID	Chain	Residue ID	Residue type
10	B	404	THR
10	B	408	ASP
10	B	411	CYS
10	B	417	ASP
10	B	485	THR
10	B	487	THR
10	B	499	SER
10	B	507	SER
10	B	508	THR
10	B	522	LYS
10	B	526	VAL
10	B	528	SER
10	B	530	THR
10	B	534	PHE
10	B	559	ASN
10	B	572	SER
10	B	575	THR
10	B	606	THR
10	B	656	THR
10	B	674	SER
10	B	734	ASP
10	B	743	THR
10	B	744	SER

Model ID	Chain	Residue ID	Residue type
10	B	760	THR
10	B	823	SER
10	B	825	SER
10	B	827	SER
10	B	837	SER
10	B	844	SER
10	B	848	LYS
10	B	850	MET
10	B	866	ARG
10	B	867	MET
10	B	883	ASP
10	B	889	ASP
10	B	892	SER
10	B	929	THR
10	B	949	THR
10	B	952	LEU
10	B	960	THR
10	B	963	ASP
10	B	965	SER
10	B	984	THR
10	B	999	SER
10	B	1007	SER

Fit of model to data used for modeling

NMR

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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