Integrative Structure Validation Report

July 22, 2024 - 03:42 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	8ZZF
PDB-Dev ID	PDBDEV_00000015
Structure Title	Structure of human mitochondrial iron sulfur cluster core complex (NIAUF)2
Structure Authors	Cai K; Frederick RO; Dashti H; Markley JL

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

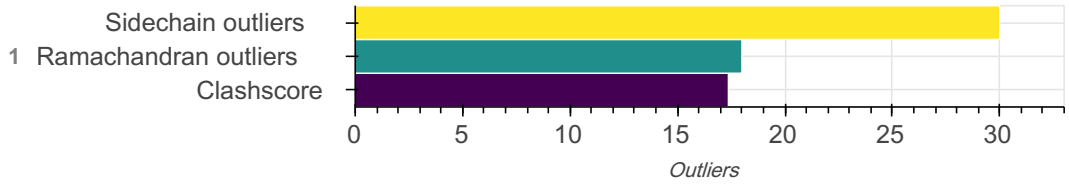
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 16 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 16 flexible or non-rigid units.

Entry composition

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

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	NFS1	A	A	399
1	2	1	NFS1	E	E	401
1	3	2	ISD11	B	B	81
1	4	2	ISD11	F	F	83
1	5	3	Acp	C	C	71
1	6	3	Acp	G	G	70
1	7	4	ISCU	D	D	128
1	8	4	ISCU	H	H	124
1	9	5	FXN	I	I	119
1	10	5	FXN	J	J	119

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	11	6	PYRIDOXAL-5'-PHOSPHATE	K	A	Not available
1	12	6	PYRIDOXAL-5'-PHOSPHATE	N	E	Not available
1	13	7	S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate	L	C	Not available
1	14	7	S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate	O	G	Not available
1	15	8	ZINC ION	M	D	Not available
1	16	8	ZINC ION	P	H	Not available

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	5WLW
2	Experimental model	PDB	1EKG
3	NMR data	BMRB	27171
4	Crosslinking-MS data	PRIDE	PXD006938
5	Crosslinking-MS data	PRIDE	PXD006928

Representation

This entry has only one representation and includes 0 rigid bodies and 16 flexible units

Chain ID	Rigid bodies	Non-rigid segments
A	-	3-401
E	-	3-403
I	-	1-119
J	-	1-119
K	-	None-None
L	-	None-None
M	-	None-None
N	-	None-None
O	-	None-None
P	-	None-None
B	-	5-85
C	-	4-74
D	-	6-133
F	-	3-85
G	-	3-72
H	-	10-133

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	None	None	None	False	False

There is 1 software package reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	HADDOCK	2.2	molecular docking	http://haddock.science.uu.nl/services/HADDOCK/

Data quality

NMR

Validation for this section is under development.

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 397 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	0.98	0.86	207
ND2--HD21	0.98	0.86	4
NE2--HE22	0.98	0.86	4
NE2--HE21	0.98	0.86	2
NE2--HE2	0.98	0.86	4
ND2--HD22	0.98	0.86	6
NE1--HE1	0.98	0.86	6
OH--HH	0.96	0.84	8
OG--HG	0.96	0.84	4
NE--HE	0.98	0.86	2

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
OG1--HG1	0.96	0.84	2
N--H	0.99	0.86	21
OG1--HG1	0.97	0.84	14
ND2--HD21	0.99	0.86	2
NE--HE	0.99	0.86	2
OG--HG	0.97	0.84	16
OH--HH	0.97	0.84	4
NE2--HE21	0.99	0.86	2
OG1--HG1	0.98	0.84	4
OG--HG	0.98	0.84	4
OH--HH	0.98	0.84	2
NH2--HH22	1.00	0.86	4
NH1--HH12	1.00	0.86	4
NH1--HH11	1.00	0.86	2
NH2--HH21	1.00	0.86	2
NH1--HH11	1.01	0.86	2
NZ--HZ1	1.04	0.89	20
NZ--HZ2	1.04	0.89	17
NZ--HZ3	1.04	0.89	18
NZ--HZ2	1.05	0.89	3
NH2--HH21	1.02	0.86	2
NZ--HZ3	1.05	0.89	2
C6--H6	0.93	1.09	1

Standard geometry: angle outliers

There are 1 angle outliers in this entry. A summary is provided below, and a detailed list of outliers can be found here.

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-C	111.00	98.42	1

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	17.37	396

All 396 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	D:115:ILE:HG23	I:76:ARG:NH2	1.351
1	D:42:PRO:HG2	I:62:ASN:OD1	1.250
1	E:221:ARG:NH2	I:35:ASP:OD1	1.247
1	D:115:ILE:CG2	I:76:ARG:HH21	1.220
1	D:115:ILE:CG2	I:76:ARG:NH2	1.121
1	F:6:ARG:NH2	O:1:8Q1:O3	1.111
1	A:221:ARG:NH1	J:36:VAL:O	1.099
1	H:20:ASN:H	H:21:PRO:CD	1.095
1	A:71:ILE:HD12	A:219:ILE:HD12	1.033
1	H:20:ASN:H	H:21:PRO:HD3	1.015
1	H:20:ASN:N	H:21:PRO:CD	0.981
1	A:66:ASP:OD1	A:67:PRO:HD2	0.980
1	D:115:ILE:HG21	I:76:ARG:HE	0.980
1	D:108:PRO:HG3	I:55:VAL:HG11	0.969

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	D:42:PRO:CG	I:62:ASN:OD1	0.967
1	F:44:LYS:O	O:1:8Q1:H35	0.959
1	G:59:ALA:HA	G:62:ILE:HD13	0.951
1	A:220:ARG:HD3	A:223:PRO:HD2	0.943
1	H:20:ASN:O	H:22:ARG:NE	0.941
1	C:59:ALA:HA	C:62:ILE:HD13	0.918
1	D:115:ILE:CG2	I:76:ARG:CZ	0.906
1	D:115:ILE:HG23	I:76:ARG:CZ	0.893
1	A:76:ALA:HB2	A:204:SER:HB2	0.887
1	D:115:ILE:CG2	I:76:ARG:NE	0.887
1	D:115:ILE:CG2	I:76:ARG:HE	0.884
1	H:16:ASP:O	H:20:ASN:HB2	0.882
1	D:108:PRO:CG	I:55:VAL:HG11	0.881
1	A:270:ARG:NH2	A:363:THR:O	0.881
1	E:270:ARG:NH2	E:363:THR:O	0.862
1	A:286:LEU:HD11	A:376:ILE:HA	0.857
1	A:391:MET:O	A:395:GLY:N	0.855
1	A:334:SER:CB	I:40:SER:HB3	0.854
1	D:115:ILE:HG23	I:76:ARG:HH21	0.845
1	D:115:ILE:HG21	I:76:ARG:NE	0.844
1	D:43:ALA:HA	I:61:PRO:HG3	0.822
1	D:38:LEU:HD13	D:49:LYS:HB2	0.802
1	A:221:ARG:HH22	J:35:ASP:HA	0.800

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	D:108:PRO:CB	I:55:VAL:HG11	0.796
1	E:387:PRO:O	E:391:MET:HG3	0.793
1	D:43:ALA:HB2	I:59:GLN:OE1	0.790
1	H:19:GLU:HA	H:21:PRO:HD3	0.772
1	A:341:LEU:O	A:346:THR:HG22	0.766
1	E:315:LEU:O	E:319:LEU:HD12	0.764
1	E:177:TYR:CE2	E:225:VAL:HG13	0.763
1	H:20:ASN:N	H:21:PRO:HD3	0.761
1	D:43:ALA:HA	I:61:PRO:CG	0.760
1	B:41:ARG:NH1	C:35:ASP:OD2	0.757
1	D:8:VAL:HG13	D:9:ASP:H	0.754
1	C:12:GLY:O	C:16:GLY:N	0.746
1	E:247:THR:HB	E:248:PRO:HD3	0.737
1	E:221:ARG:HH12	I:36:VAL:H	0.735
1	L:1:8Q1:N36	L:1:8Q1:O40	0.735
1	B:55:LEU:HB3	L:1:8Q1:O4	0.729
1	D:98:THR:CB	I:74:PRO:HD3	0.725
1	A:56:ARG:NH2	A:70:ILE:O	0.720
1	D:112:HIS:HA	I:66:TRP:CZ3	0.716
1	D:60:ILE:HB	D:85:LYS:O	0.715
1	E:85:LYS:HB2	E:230:LEU:HD11	0.715
1	A:66:ASP:OD1	A:67:PRO:CD	0.709
1	H:65:PHE:CD1	H:67:THR:HG23	0.700

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:315:LEU:O	A:319:LEU:HD12	0.693
1	A:71:ILE:HD12	A:219:ILE:CD1	0.690
1	H:89:VAL:HG13	H:125:LEU:HD22	0.690
1	B:81:LEU:N	B:84:GLU:OE1	0.687
1	A:387:PRO:O	A:391:MET:HG3	0.685
1	A:207:LYS:NZ	K:1:PLP:O3	0.684
1	A:221:ARG:HH12	J:36:VAL:C	0.683
1	A:209:TYR:OH	A:361:ARG:N	0.682
1	D:130:LEU:O	D:130:LEU:HD13	0.681
1	B:39:ALA:HB1	L:1:8Q1:H22	0.680
1	E:84:ILE:HD11	E:108:VAL:HG13	0.679
1	A:221:ARG:NH2	J:35:ASP:HA	0.676
1	A:266:TYR:OH	B:38:ASP:OD2	0.676
1	A:71:ILE:CD1	A:219:ILE:HD12	0.672
1	D:108:PRO:HB2	I:57:ASN:OD1	0.671
1	A:275:SER:OG	A:303:ILE:HD11	0.670
1	D:27:LEU:N	D:51:GLN:OE1	0.669
1	A:341:LEU:HB3	A:346:THR:HG21	0.665
1	B:18:ARG:HG2	C:44:MET:HE3	0.659
1	D:108:PRO:HB3	I:55:VAL:HG11	0.652
1	E:398:LEU:H	E:398:LEU:HD22	0.652
1	D:43:ALA:HB2	I:61:PRO:HG2	0.651
1	E:270:ARG:HH21	E:274:LEU:HD11	0.650

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	E:43:ALA:O	E:47:GLU:HG2	0.646
1	H:36:THR:HG22	H:127:ASP:OD2	0.638
1	A:222:ARG:CB	A:223:PRO:CD	0.636
1	E:69:GLU:OE1	E:220:ARG:HA	0.635
1	A:84:ILE:HD11	A:108:VAL:HG13	0.628
1	E:76:ALA:HB2	E:204:SER:HB2	0.627
1	E:222:ARG:CB	E:223:PRO:CD	0.625
1	H:65:PHE:HD1	H:67:THR:HG23	0.625
1	E:69:GLU:CG	E:221:ARG:HG2	0.624
1	E:97:HIS:C	E:98:LEU:HD12	0.623
1	A:222:ARG:O	J:25:ALA:HB3	0.623
1	A:221:ARG:HH22	J:36:VAL:H	0.623
1	E:275:SER:OG	E:303:ILE:HD11	0.622
1	A:311:GLU:OE1	A:313:GLU:N	0.622
1	D:112:HIS:CB	I:66:TRP:HZ3	0.620
1	A:390:GLU:OE1	D:49:LYS:NZ	0.620
1	A:214:VAL:HB	A:249:LEU:HB3	0.618
1	A:85:LYS:O	A:89:ARG:HG3	0.617
1	D:127:ASP:O	D:131:LYS:HG2	0.616
1	D:46:ASP:OD2	D:112:HIS:NE2	0.616
1	E:314:SER:O	H:18:TYR:OH	0.615
1	D:115:ILE:HG22	I:76:ARG:NH2	0.612
1	A:190:PRO:O	A:191:LEU:HD23	0.611

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:62:ASP:O	B:65:VAL:HG12	0.611
1	D:112:HIS:HA	I:66:TRP:HZ3	0.611
1	B:43:ASN:O	L:1:8Q1:H36	0.611
1	A:221:ARG:HH22	J:35:ASP:CA	0.610
1	D:23:ASN:O	D:64:ARG:HA	0.608
1	C:36:SER:O	C:39:THR:OG1	0.607
1	E:60:ALA:N	E:70:ILE:HD11	0.606
1	G:7:VAL:HG12	G:50:PHE:CZ	0.606
1	H:67:THR:OG1	H:74:ILE:HD13	0.606
1	D:21:PRO:HB2	D:24:VAL:HG21	0.605
1	A:186:VAL:HG21	A:203:ILE:HG12	0.604
1	D:108:PRO:HB3	I:55:VAL:CG1	0.604
1	A:221:ARG:HH12	J:36:VAL:H	0.604
1	E:59:VAL:HB	E:70:ILE:HD13	0.601
1	D:108:PRO:O	I:57:ASN:ND2	0.601
1	A:323:ALA:HB1	E:42:HIS:CG	0.596
1	D:8:VAL:HG13	D:9:ASP:N	0.595
1	D:112:HIS:CA	I:66:TRP:HZ3	0.595
1	D:17:HIS:HB2	D:75:ALA:HB1	0.594
1	D:23:ASN:HB3	D:63:ALA:O	0.594
1	E:60:ALA:CA	E:70:ILE:HD11	0.594
1	H:12:THR:HG23	H:13:GLN:OE1	0.594
1	E:85:LYS:O	E:89:ARG:HG3	0.592

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	C:23:THR:OG1	C:26:ALA:HB2	0.591
1	H:16:ASP:O	H:20:ASN:CB	0.590
1	A:84:ILE:CD1	A:108:VAL:HG13	0.587
1	F:48:ASP:OD1	F:50:VAL:HG12	0.587
1	H:52:ILE:HD11	H:125:LEU:HD23	0.587
1	E:207:LYS:NZ	N:1:PLP:O3	0.587
1	O:1:8Q1:H29	O:1:8Q1:O35	0.587
1	A:291:MET:HA	A:305:LEU:HD23	0.585
1	D:98:THR:CB	I:74:PRO:CD	0.585
1	H:130:LEU:O	H:130:LEU:HD13	0.585
1	F:6:ARG:CZ	O:1:8Q1:O3	0.585
1	E:326:SER:OG	E:354:SER:O	0.584
1	G:59:ALA:HA	G:62:ILE:CD1	0.583
1	D:31:SER:C	D:33:ASN:H	0.576
1	E:138:LEU:O	E:142:ILE:HG13	0.576
1	E:43:ALA:HA	E:46:TRP:CE3	0.574
1	G:58:GLU:O	G:61:LYS:HG2	0.574
1	D:21:PRO:HB2	D:24:VAL:CG2	0.572
1	A:226:ARG:HA	A:226:ARG:HE	0.568
1	G:35:ASP:O	G:39:THR:HG23	0.568
1	H:52:ILE:CD1	H:125:LEU:HD23	0.567
1	E:35:GLY:HA3	E:44:TYR:HB3	0.564
1	D:44:CYS:O	D:46:ASP:N	0.563

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	E:227:VAL:HB	E:240:MET:CE	0.562
1	C:35:ASP:O	C:39:THR:HG23	0.561
1	A:221:ARG:NH2	J:35:ASP:OD1	0.560
1	A:233:GLY:HA2	E:107:CYS:HA	0.559
1	H:52:ILE:HD12	H:60:ILE:CD1	0.557
1	A:306:SER:HA	A:353:SER:O	0.554
1	F:43:ASN:O	O:1:8Q1:H36	0.554
1	H:31:SER:O	H:131:LYS:HE2	0.553
1	D:88:THR:HG22	D:90:GLU:H	0.552
1	E:267:ASP:OD2	E:361:ARG:HD3	0.552
1	C:71:TYR:C	C:73:ASN:H	0.551
1	A:330:CYS:SG	D:44:CYS:HB3	0.548
1	D:108:PRO:C	I:57:ASN:HD21	0.547
1	D:43:ALA:CA	I:61:PRO:CG	0.546
1	A:247:THR:HB	A:248:PRO:HD3	0.544
1	H:17:HIS:O	H:18:TYR:O	0.544
1	A:221:ARG:NH1	J:36:VAL:H	0.540
1	H:20:ASN:N	H:21:PRO:HD2	0.540
1	H:67:THR:HG21	H:77:SER:OG	0.539
1	H:93:LEU:CD1	H:125:LEU:HD13	0.539
1	F:16:MET:O	F:20:SER:OG	0.538
1	A:221:ARG:HH12	J:36:VAL:N	0.535
1	E:166:GLU:HA	E:166:GLU:OE1	0.534

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:221:ARG:NH2	J:36:VAL:H	0.534
1	E:100:THR:OG1	E:104:GLU:HG3	0.533
1	D:8:VAL:HG22	D:9:ASP:N	0.531
1	D:43:ALA:CB	I:61:PRO:HG2	0.531
1	F:66:ILE:HD11	O:1:8Q1:H6	0.530
1	H:39:VAL:HG22	H:116:LEU:HD11	0.528
1	I:43:LEU:HD23	I:56:ILE:HD12	0.527
1	D:43:ALA:CA	I:61:PRO:HG3	0.526
1	H:32:LYS:HA	H:131:LYS:HE3	0.525
1	C:19:GLN:O	C:22:VAL:HG22	0.524
1	E:391:MET:O	E:395:GLY:N	0.523
1	A:24:ASP:CG	B:65:VAL:HG23	0.522
1	D:108:PRO:CB	I:55:VAL:CG1	0.522
1	F:17:LEU:O	F:21:LYS:HG3	0.522
1	E:227:VAL:HB	E:240:MET:HE1	0.521
1	A:12:VAL:HG22	A:358:GLY:HA3	0.520
1	E:177:TYR:HE2	E:225:VAL:HG13	0.520
1	J:43:LEU:HD23	J:56:ILE:HD12	0.520
1	D:40:GLY:HA2	D:47:VAL:HA	0.519
1	G:20:GLU:N	G:20:GLU:OE2	0.519
1	F:23:PHE:CG	F:70:VAL:HG22	0.518
1	A:283:MET:SD	A:289:VAL:HG13	0.517
1	E:200:LEU:HA	E:218:TYR:O	0.517

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:299:TYR:CE2	A:301:GLY:HA3	0.516
1	E:402:LYS:HA	H:40:GLY:O	0.516
1	E:153:THR:HG1	E:180:THR:HG1	0.515
1	A:76:ALA:CB	A:204:SER:HB2	0.510
1	A:246:PRO:CB	A:249:LEU:HD12	0.509
1	D:43:ALA:CB	I:59:GLN:OE1	0.508
1	E:84:ILE:CD1	E:108:VAL:HG13	0.504
1	E:8:LEU:HD22	E:367:GLU:HG2	0.503
1	B:66:ILE:O	B:70:VAL:HG23	0.502
1	C:52:THR:HG23	C:53:GLU:N	0.502
1	E:60:ALA:N	E:70:ILE:CD1	0.502
1	E:222:ARG:O	E:224:ARG:N	0.501
1	D:50:LEU:HD12	D:64:ARG:O	0.496
1	F:6:ARG:NH2	G:36:SER:HB3	0.495
1	E:214:VAL:HB	E:249:LEU:HB3	0.494
1	A:246:PRO:HB2	A:249:LEU:HD12	0.493
1	E:130:SER:HB2	E:294:ASP:HB2	0.493
1	E:355:ILE:HD11	E:357:PHE:CZ	0.493
1	F:13:TYR:OH	G:41:GLU:OE2	0.493
1	A:153:THR:HA	A:164:ILE:HD11	0.492
1	E:299:TYR:CE2	E:301:GLY:HA3	0.492
1	A:221:ARG:HH22	J:36:VAL:N	0.492
1	H:10:LEU:C	H:10:LEU:HD23	0.491

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:24:ASP:OD1	F:76:TYR:OH	0.491
1	A:130:SER:HB2	A:294:ASP:HB2	0.488
1	D:54:VAL:HG13	D:59:LYS:O	0.488
1	E:52:MET:SD	E:245:VAL:HG11	0.487
1	F:34:ARG:CZ	F:34:ARG:HB3	0.486
1	G:42:LEU:C	G:42:LEU:HD23	0.486
1	A:291:MET:HA	A:305:LEU:CD2	0.485
1	H:84:VAL:O	H:84:VAL:HG12	0.484
1	D:41:ALA:N	D:46:ASP:O	0.484
1	A:375:CYS:O	A:379:VAL:HG23	0.483
1	J:12:GLU:HB2	J:116:TYR:HE1	0.482
1	F:16:MET:HE1	O:1:8Q1:H16	0.481
1	I:12:GLU:HB2	I:116:TYR:HE1	0.480
1	D:48:MET:SD	D:77:SER:OG	0.480
1	G:27:SER:O	G:31:ASP:HB2	0.478
1	E:385:MET:HG2	H:24:VAL:HG11	0.477
1	D:43:ALA:CB	I:61:PRO:CG	0.474
1	E:326:SER:HB2	E:355:ILE:HG22	0.474
1	B:80:LYS:HB3	B:84:GLU:OE1	0.473
1	D:108:PRO:C	I:57:ASN:ND2	0.473
1	K:1:PLP:O3P	E:244:THR:HB	0.472
1	E:398:LEU:N	E:398:LEU:HD22	0.472
1	E:177:TYR:CD2	E:225:VAL:HG13	0.471

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	E:13:GLN:NE2	E:302:CYS:HB2	0.470
1	G:63:THR:O	G:63:THR:HG22	0.470
1	A:329:ALA:C	A:331:THR:H	0.470
1	E:368:VAL:O	E:372:VAL:HG23	0.469
1	H:10:LEU:CD2	H:15:VAL:HG23	0.469
1	A:222:ARG:CB	A:223:PRO:HD3	0.468
1	A:107:CYS:HA	E:233:GLY:HA2	0.467
1	H:19:GLU:CA	H:21:PRO:HD3	0.467
1	D:43:ALA:CA	I:61:PRO:HG2	0.466
1	A:32:ASN:ND2	F:76:TYR:O	0.466
1	A:68:ARG:HH22	J:35:ASP:HB2	0.465
1	A:329:ALA:O	A:331:THR:N	0.465
1	I:102:THR:HA	I:107:THR:O	0.464
1	A:305:LEU:O	A:354:SER:HA	0.463
1	J:102:THR:HA	J:107:THR:O	0.463
1	C:14:GLN:CB	C:42:LEU:HD13	0.462
1	E:60:ALA:HB1	E:65:ALA:O	0.462
1	E:291:MET:HA	E:305:LEU:HD23	0.462
1	D:38:LEU:CD1	D:49:LYS:HB2	0.460
1	D:54:VAL:HG12	D:55:ASP:O	0.460
1	E:177:TYR:CE2	E:225:VAL:HG22	0.460
1	E:39:SER:O	E:45:GLY:HA3	0.459
1	E:315:LEU:CD1	E:319:LEU:HD11	0.459

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	H:39:VAL:CG1	H:120:ALA:HB2	0.459
1	H:39:VAL:HG22	H:116:LEU:CD1	0.459
1	E:321:ASP:HB3	F:82:ILE:HD13	0.458
1	H:21:PRO:HG2	H:21:PRO:O	0.458
1	E:334:SER:O	E:335:LEU:C	0.458
1	I:6:TYR:CE2	I:60:THR:HA	0.457
1	H:127:ASP:O	H:131:LYS:HG3	0.456
1	A:301:GLY:O	A:358:GLY:HA2	0.455
1	D:27:LEU:HD13	D:53:GLN:HB2	0.455
1	E:255:ALA:O	E:259:VAL:HG23	0.454
1	J:6:TYR:CE2	J:60:THR:HA	0.454
1	B:39:ALA:CB	L:1:8Q1:H22	0.454
1	A:127:VAL:HG12	A:133:ILE:HG22	0.453
1	E:346:THR:HG22	E:347:ASP:O	0.453
1	H:11:SER:OG	H:14:VAL:HG23	0.453
1	A:6:ARG:HH12	E:47:GLU:CD	0.453
1	J:67:LEU:O	J:74:PRO:HA	0.450
1	I:67:LEU:O	I:74:PRO:HA	0.449
1	A:35:GLY:HA3	A:44:TYR:HB3	0.448
1	A:55:ALA:HA	A:58:GLN:OE1	0.448
1	A:78:GLU:O	A:82:ILE:HG13	0.448
1	A:200:LEU:HA	A:218:TYR:O	0.448
1	F:48:ASP:HB3	F:51:GLU:CG	0.448

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	H:131:LYS:HB2	H:132:GLN:HE21	0.448
1	E:224:ARG:HE	I:22:GLU:HB3	0.448
1	A:22:VAL:O	A:26:MET:HG3	0.447
1	F:27:ASN:N	F:27:ASN:OD1	0.447
1	B:68:ARG:HG2	F:75:LEU:HD22	0.446
1	H:93:LEU:HD12	H:125:LEU:HD13	0.446
1	H:10:LEU:HD23	H:11:SER:O	0.445
1	B:12:LEU:HA	B:12:LEU:HD12	0.444
1	I:102:THR:HG23	I:108:LYS:HA	0.444
1	A:299:TYR:CD1	A:300:PRO:HD2	0.443
1	I:12:GLU:HB2	I:116:TYR:CE1	0.443
1	D:31:SER:O	D:33:ASN:N	0.443
1	D:88:THR:HB	D:91:GLU:H	0.442
1	J:12:GLU:HB2	J:116:TYR:CE1	0.442
1	H:93:LEU:HD12	H:125:LEU:CD1	0.441
1	J:102:THR:HG23	J:108:LYS:HA	0.441
1	A:6:ARG:NH1	E:47:GLU:OE1	0.441
1	J:43:LEU:HB3	J:56:ILE:HB	0.440
1	E:269:LYS:O	E:272:SER:OG	0.440
1	H:50:LEU:C	H:50:LEU:HD23	0.439
1	E:18:LEU:HA	E:18:LEU:HD23	0.438
1	G:72:ILE:O	G:72:ILE:HG22	0.438
1	H:83:TRP:C	H:85:LYS:H	0.437

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:275:SER:HG	A:303:ILE:HD11	0.436
1	D:41:ALA:HB2	D:116:LEU:HD22	0.436
1	B:25:ALA:HB1	B:27:ASN:OD1	0.435
1	F:12:LEU:HA	F:12:LEU:HD12	0.435
1	D:46:ASP:OD2	D:112:HIS:CD2	0.434
1	D:23:ASN:HB2	D:81:THR:OG1	0.433
1	C:14:GLN:HG2	C:42:LEU:HA	0.432
1	G:36:SER:O	G:39:THR:OG1	0.432
1	H:28:ASP:OD1	H:30:THR:OG1	0.432
1	H:11:SER:OG	H:13:GLN:HG2	0.431
1	I:43:LEU:HB3	I:56:ILE:HB	0.431
1	E:227:VAL:O	E:240:MET:HE1	0.430
1	E:12:VAL:HG22	E:358:GLY:HA3	0.429
1	D:115:ILE:HG23	I:76:ARG:NE	0.429
1	C:62:ILE:N	C:62:ILE:HD12	0.428
1	B:23:PHE:O	B:29:ARG:NH1	0.428
1	A:283:MET:HE1	A:289:VAL:O	0.427
1	B:68:ARG:O	B:72:ILE:HG12	0.427
1	E:132:ILE:HD11	E:297:HIS:HB2	0.427
1	E:294:ASP:O	E:298:HIS:HB2	0.427
1	E:375:CYS:O	E:379:VAL:HG23	0.427
1	A:332:SER:O	A:333:ALA:C	0.427
1	H:133:GLU:HA	H:133:GLU:OE2	0.427

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	E:222:ARG:CB	E:223:PRO:HD2	0.426
1	G:22:VAL:O	G:22:VAL:HG12	0.425
1	A:99:ILE:HD11	A:142:ILE:HA	0.424
1	H:23:ASN:HB3	H:63:ALA:O	0.424
1	D:77:SER:O	D:81:THR:HG23	0.423
1	E:39:SER:HB3	E:42:HIS:NE2	0.423
1	E:306:SER:HA	E:353:SER:O	0.423
1	E:362:PHE:HB3	F:27:ASN:HB2	0.423
1	B:76:TYR:OH	E:24:ASP:OD1	0.423
1	F:57:ASN:O	F:61:ARG:HG3	0.422
1	A:43:ALA:O	A:47:GLU:HG2	0.421
1	H:36:THR:O	H:36:THR:HG23	0.421
1	A:69:GLU:OE1	A:218:TYR:HE1	0.421
1	C:4:GLU:CD	C:5:GLU:H	0.420
1	E:168:GLY:HA3	E:197:LYS:HB2	0.420
1	D:56:GLU:O	D:57:LYS:CB	0.420
1	B:10:LEU:HA	B:10:LEU:HD23	0.419
1	H:13:GLN:CD	H:13:GLN:H	0.419
1	H:31:SER:HB3	H:34:VAL:HG23	0.419
1	C:12:GLY:HA2	C:17:VAL:HG12	0.418
1	E:96:LYS:HB3	E:96:LYS:HE2	0.418
1	E:98:LEU:N	E:98:LEU:HD12	0.418
1	H:131:LYS:HB2	H:132:GLN:NE2	0.417

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:244:THR:OG1	N:1:PLP:O3P	0.417
1	A:44:TYR:CD2	E:9:TYR:HD1	0.416
1	E:317:MET:HB2	E:317:MET:HE3	0.416
1	F:59:ALA:HB2	O:1:8Q1:H23	0.416
1	A:267:ASP:O	A:271:ILE:HB	0.415
1	A:391:MET:SD	D:38:LEU:HD21	0.414
1	A:350:LEU:N	A:350:LEU:HD23	0.412
1	A:368:VAL:O	A:372:VAL:HG23	0.412
1	F:23:PHE:CD1	F:70:VAL:HG22	0.411
1	D:43:ALA:HB2	I:61:PRO:CG	0.410
1	H:97:ASN:HB3	H:118:GLU:OE2	0.410
1	A:97:HIS:C	A:98:LEU:HD12	0.409
1	C:40:VAL:O	C:43:VAL:HG22	0.409
1	D:112:HIS:CB	I:66:TRP:CZ3	0.409
1	H:13:GLN:HG3	H:104:LEU:HA	0.408
1	A:55:ALA:O	A:58:GLN:HB2	0.407
1	A:54:ARG:HB2	A:54:ARG:NH1	0.406
1	A:71:ILE:HD13	A:240:MET:CB	0.406
1	A:19:ASP:O	A:22:VAL:N	0.406
1	B:27:ASN:N	B:27:ASN:OD1	0.406
1	E:307:PHE:O	E:353:SER:HB3	0.406
1	A:59:VAL:HG22	A:257:CYS:SG	0.405
1	G:5:GLU:HA	G:5:GLU:OE1	0.405

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	H:84:VAL:O	H:85:LYS:C	0.405
1	H:39:VAL:HG11	H:120:ALA:HB2	0.404
1	A:19:ASP:OD2	A:361:ARG:NH2	0.404
1	A:90:PHE:CZ	A:226:ARG:HB3	0.403
1	D:112:HIS:HB3	I:66:TRP:HZ3	0.403
1	E:19:ASP:O	E:22:VAL:N	0.403
1	A:221:ARG:CZ	J:35:ASP:OD1	0.403
1	E:267:ASP:O	E:271:ILE:HB	0.402
1	H:16:ASP:OD1	H:22:ARG:NH2	0.402
1	H:17:HIS:C	H:18:TYR:O	0.402
1	A:104:GLU:OE1	A:152:MET:HB3	0.401
1	F:53:GLN:HA	F:53:GLN:OE1	0.401
1	F:18:ARG:HA	G:44:MET:HE1	0.401
1	G:54:ILE:HA	G:71:TYR:OH	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	1575	1503	54	18

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	1124	1010	84	30

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	121	GLN
1	A	221	ARG
1	A	226	ARG
1	B	65	VAL
1	C	10	ILE
1	C	36	SER
1	C	52	THR
1	E	92	ARG
1	E	121	GLN
1	F	61	ARG
1	G	20	GLU
1	G	36	SER
1	H	13	GLN
1	H	60	ILE
1	H	77	SER
1	H	133	GLU
1	I	2	ASP
1	I	4	THR
1	I	24	LEU
1	I	30	THR
1	I	44	THR
1	I	50	ASP
1	I	55	VAL

Model ID	Chain	Residue ID	Residue type
1	J	2	ASP
1	J	4	THR
1	J	24	LEU
1	J	30	THR
1	J	44	THR
1	J	50	ASP
1	J	55	VAL

Fit of model to data used for modeling

NMR

Validation for this section is under development.

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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