

Integrative Structure Validation Report

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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	9A1K
PDB-Dev ID	PDBDEV_00000092
Structure Title	Integrative structure of the COX-AIFM1 complex
Structure Authors	Johannes F. Hevler; Albert J.R. Heck

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

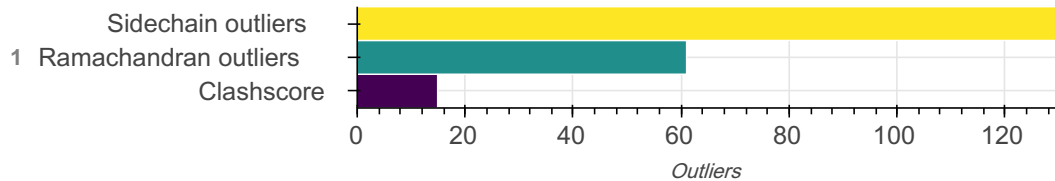
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the  symbol.

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 32 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/None.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	Cytochrome c oxidase polypeptide I	A	A	513
1	2	2	Cytochrome c oxidase polypeptide II	B	B	226
1	3	3	Cytochrome c oxidase polypeptide III	C	C	259
1	4	4	Cytochrome c oxidase subunit IV isoform 1	D	D	144
1	5	5	Cytochrome c oxidase polypeptide Va	E	E	109
1	6	6	Cytochrome c oxidase polypeptide Vb	F	F	98
1	7	7	Cytochrome c oxidase polypeptide VIa-heart	G	G	83

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	8	8	Cytochrome c oxidase polypeptide VIb	H	H	86
1	9	9	Cytochrome c oxidase polypeptide VIc	I	I	72
1	10	10	Cytochrome c oxidase polypeptide VIIa-heart	J	J	58
1	11	11	Cytochrome c oxidase polypeptide VIIb	K	K	49
1	12	12	Cytochrome c oxidase polypeptide VIIc	L	L	46
1	13	13	Cytochrome c oxidase polypeptide VIII-heart	M	M	43
1	14	14	Cytochrome c oxidase subunit NDUFA4	N	N	80
1	15	15	Apoptosis inducing factor 1	O	O	559
1	16	15	Apoptosis inducing factor 1	P	P	559

Datasets used for modeling

There are 32 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Crosslinking-MS data	PRIDE	PXD025102
2	Comparative model	Not available	Not available
3	Comparative model	Not available	Not available
4	Comparative model	Not available	Not available
5	Comparative model	Not available	Not available
6	De Novo model	Not available	Not available

ID	Dataset type	Database name	Data access code
7	Experimental model	PDB	1V54
8	Experimental model	PDB	1OCC
9	Experimental model	PDB	2Y69
10	Experimental model	PDB	3J9M
11	Experimental model	PDB	4G23
12	Experimental model	PDB	4G26
13	Experimental model	PDB	4LEU
14	Experimental model	PDB	5DIZ
15	Experimental model	PDB	5FT9
16	Experimental model	PDB	5IWB
17	Experimental model	PDB	5ORM
18	Experimental model	PDB	5Z62
19	Experimental model	PDB	6F5D
20	Experimental model	PDB	6GAW
21	Experimental model	PDB	6GAZ
22	Experimental model	PDB	6HU9
23	Experimental model	PDB	6LVR
24	Experimental model	PDB	2LQT
25	Experimental model	PDB	5JJ4
26	Experimental model	PDB	5Z62
27	Experimental model	PDB	6NL3
28	Experimental model	PDB	6PCE
29	Experimental model	PDB	6PCF

ID	Dataset type	Database name	Data access code
30	Experimental model	PDB	6TDV
31	Experimental model	PDB	6X89
32	Experimental model	PDB	4BUR

Representation

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

Chain ID	Rigid bodies	Non-rigid segments
E	-	1-109
P	-	1-559
H	-	1-86
I	-	1-72
O	-	1-559
N	-	1-80
B	-	1-226
A	-	1-513
C	-	1-259
D	-	1-144
F	-	1-98
G	-	1-83
J	-	1-58
K	-	1-49
L	-	1-46
M	-	1-43

Methodology and software ?

This entry is a result of 3 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 are 5 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
2	trRosetta	Not available	model building	https://yanglab.nankai.edu.cn/trRosetta/
1	Robetta	Not available	model building	http://robetta.bakerlab.org
3	DisVis	Not available	prediction of protein-protein interface residues and restraint validation	https://wenmr.science.uu.nl/disvis/
4	Haddock	2.4	Structural docking of protein complexes	https://wenmr.science.uu.nl/haddock2.4/
5	Naccess	Not available	prediction of solvent accessible residues	http://www.bioinf.manchester.ac.uk/naccess/

Data quality ?

Crosslinking-MS

Validation for this section is under development.

Model quality ?

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

Standard geometry: bond outliers ?

There are 3016 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	6
OG1--HG1	0.95	0.84	1
OG--HG	0.95	0.84	5
NE1--HE1	0.97	0.86	1
NE2--HE2	0.97	0.86	1
ND1--HD1	0.97	0.86	1
NE--HE	0.97	0.86	1
OG--HG	0.96	0.84	113
N--H	0.98	0.86	1736
OH--HH	0.96	0.84	76
NE2--HE21	0.98	0.86	42
NE1--HE1	0.98	0.86	58
NE2--HE2	0.98	0.86	46
OG1--HG1	0.96	0.84	120
NE--HE	0.98	0.86	65
ND2--HD22	0.98	0.86	66
ND2--HD21	0.98	0.86	66
NE2--HE22	0.98	0.86	42
ND1--HD1	0.98	0.86	21
SG--HG	1.32	1.20	6
SG--HG	1.33	1.20	8
N--H	0.99	0.86	5
OG1--HG1	0.97	0.84	1

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
OG--HG	0.97	0.84	1
NZ--HZ1	1.03	0.89	1
NZ--HZ3	1.03	0.89	2
NZ--HZ2	1.04	0.89	87
NZ--HZ3	1.04	0.89	85
NZ--HZ1	1.04	0.89	87
NZ--HZ2	1.05	0.89	1
NZ--HZ3	1.05	0.89	1
NH1--HH11	1.04	0.86	66
NH2--HH22	1.04	0.86	66
NH1--HH12	1.04	0.86	66
NH2--HH21	1.04	0.86	66

Standard geometry: angle outliers

There are 137 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
O-C-N	123.00	161.30	1
O-C-N	123.00	161.21	1
C-N-CA	121.70	164.16	1
CA-C-N	116.20	80.31	1
CA-C-N	116.20	80.34	1
CA-C-O	119.00	80.90	1
CA-C-O	119.00	81.01	1
N-CA-CB	110.40	94.02	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CD	125.00	84.74	1
CA-C-O	120.80	105.50	1
C-CA-CB	110.10	125.83	1
N-CA-C	112.10	132.62	1
CA-C-O	120.80	107.65	1
C-N-CA	121.70	107.84	1
N-CA-C	111.00	132.43	1
C-N-CA	121.70	108.13	1
CA-C-O	120.80	108.12	1
O-C-N	123.00	111.08	1
C-N-CA	121.70	135.10	1
CA-C-O	120.80	108.28	1
CA-C-O	120.80	108.91	1
O-C-N	123.00	134.08	1
CA-C-O	120.80	109.05	1
O-C-N	123.00	133.94	1
O-C-N	123.00	133.92	1
O-C-N	123.00	133.86	1
CA-C-O	120.80	109.35	1
O-C-N	123.00	133.74	1
C-N-CA	121.70	133.69	1
O-C-N	123.00	133.51	1
O-C-N	123.00	133.42	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-O	120.80	109.79	1
CA-C-O	120.80	109.86	1
CA-C-O	120.80	109.95	1
O-C-N	123.00	133.16	1
O-C-N	123.00	132.99	2
CA-C-O	120.80	110.19	1
CA-C-O	120.80	110.26	1
CA-C-O	120.80	110.27	1
C-N-CA	121.70	110.59	1
CA-C-O	120.80	110.31	1
CA-C-O	120.80	110.38	1
CA-C-O	120.80	110.39	1
O-C-N	123.00	132.79	1
O-C-N	123.00	132.73	1
O-C-N	123.00	132.70	1
CA-C-O	120.80	110.50	1
CA-C-O	120.80	131.00	1
CA-C-O	120.80	110.61	1
O-C-N	123.00	132.56	1
O-C-N	123.00	132.52	1
O-C-N	123.00	132.50	2
CA-C-O	120.80	110.75	1
O-C-N	123.00	132.41	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O-C-N	123.00	132.37	1
O-C-N	123.00	132.36	1
O-C-N	123.00	132.35	1
O-C-N	123.00	132.33	1
CA-C-O	120.80	110.94	1
C-N-CA	121.70	132.14	1
O-C-N	123.00	132.20	1
CA-C-O	120.80	111.09	1
O-C-N	123.00	132.12	1
CA-C-O	120.80	111.11	1
CA-C-O	120.80	111.14	2
CA-C-O	120.80	111.16	1
O-C-N	123.00	132.04	1
O-C-N	123.00	132.01	1
NE-CZ-NH1	121.50	115.90	1
N-CA-C	111.00	126.66	1
CA-C-O	120.80	111.30	1
O-C-N	123.00	131.93	1
CA-C-O	120.80	111.32	1
O-C-N	123.00	131.91	1
O-C-N	123.00	131.90	2
NE-CZ-NH1	121.50	115.95	1
CA-C-O	120.80	111.36	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O-C-N	123.00	131.79	1
CA-C-O	120.80	111.49	1
CA-C-O	120.80	111.52	1
CA-C-N	116.90	125.08	1
O-C-N	123.00	131.70	1
CA-C-O	120.80	111.57	1
O-C-N	123.00	131.68	1
CA-C-O	120.80	111.60	1
O-C-N	123.00	131.62	1
CA-C-O	120.80	111.66	1
CA-C-O	120.80	111.71	1
O-C-N	123.00	131.39	1
O-C-N	123.00	131.36	1
C-N-CA	121.70	112.34	1
O-C-N	123.00	131.32	1
O-C-N	123.00	131.24	1
O-C-N	123.00	131.19	1
O-C-N	123.00	131.13	1
C-CA-CB	110.10	100.52	1
CA-CB-CG	112.60	117.64	1
C-CA-CB	110.50	118.01	1
CA-C-O	120.80	112.29	1
O-C-N	123.00	130.98	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-O	120.80	112.34	1
C-CA-CB	111.40	120.81	1
CA-C-O	120.80	110.42	1
O-C-N	123.00	130.90	1
CA-CB-CG	112.60	117.53	1
C-N-CA	121.70	113.00	1
N-CD-CG	103.20	110.38	1
CA-C-N	116.90	124.06	1
C-N-CA	121.70	113.16	1
CA-CB-CG	113.80	118.51	1
CA-C-O	120.80	112.88	1
CA-C-O	120.80	112.95	1
CD2-NE2-CE1	109.00	104.42	1
CA-C-O	120.80	113.01	1
O-C-N	123.00	130.32	1
CA-C-O	120.80	113.03	1
N-CA-CB	110.50	118.23	1
N-CA-C	111.00	123.63	1
CA-C-O	120.80	113.13	1
O-C-N	123.00	130.20	1
C-N-CA	121.70	113.60	1
N-CA-C	113.30	100.30	1
CA-C-O	120.80	111.43	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	113.80	118.11	1
CA-CB-CG	113.80	118.04	1
CA-C-O	120.80	113.64	1
C-N-CD	125.00	107.83	1
CA-C-N	116.90	110.64	1
CA-C-O	120.80	113.79	1
CA-CB-CG	112.60	116.67	1
CA-CB-CG	112.60	116.66	1
CA-C-N	116.90	122.97	1
CA-C-N	116.90	122.96	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	14.89	667

All 667 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	P:75:PRO:C	P:75:PRO:HA	1.542
1	P:75:PRO:C	P:75:PRO:CA	1.480
1	B:115:LEU:CD2	P:192:ASN:O	1.383
1	P:76:SER:H	P:160:ALA:CB	1.366
1	B:115:LEU:HD23	P:192:ASN:O	1.264
1	B:113:GLU:CG	P:178:LYS:HD3	1.207

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	P:76:SER:N	P:174:LEU:HD21	1.204
1	P:75:PRO:CA	P:160:ALA:HB2	1.143
1	P:75:PRO:HA	P:160:ALA:HB2	1.119
1	B:113:GLU:CD	P:178:LYS:HD3	1.109
1	B:113:GLU:HG3	P:178:LYS:HD3	1.104
1	P:76:SER:HA	P:106:LEU:CD2	1.098
1	P:77:HIS:N	P:106:LEU:HD11	1.090
1	B:220:LYS:HD3	P:178:LYS:NZ	1.080
1	P:76:SER:N	P:160:ALA:HB1	1.056
1	P:76:SER:H	P:160:ALA:HB1	1.050
1	B:220:LYS:HD3	P:178:LYS:HZ2	1.049
1	P:76:SER:N	P:160:ALA:CB	1.045
1	B:220:LYS:HG3	P:351:GLU:OE2	1.041
1	P:76:SER:HA	P:106:LEU:HD22	1.031
1	P:75:PRO:HA	P:160:ALA:CB	1.002
1	P:75:PRO:HB2	P:173:VAL:H	0.941
1	B:104:TYR:HB2	B:225:MET:SD	0.939
1	B:119:SER:HB3	B:225:MET:HB2	0.933
1	B:141:VAL:HB	P:79:PRO:HD3	0.927
1	P:78:VAL:HG13	P:178:LYS:HZ2	0.925
1	B:220:LYS:CD	B:153:VAL:HA	0.916
1	A:482:LEU:HD21	B:138:ASP:HB3	0.910
1	B:98:THR:HG22	B:178:LEU:HD21	0.903

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:124:THR:HA	P:178:LYS:CD	0.897
1	B:152:LEU:HD13	P:173:VAL:N	0.891
1	B:113:GLU:HG3	B:226:LEU:HB3	0.889
1	P:75:PRO:HB2	A:431:GLY:HA3	0.873
1	B:105:TRP:CD1	P:172:ALA:HB1	0.873
1	A:369:THR:HB	P:106:LEU:HD22	0.870
1	P:75:PRO:HB3	A:497:CYS:HB3	0.847
1	P:76:SER:N	P:178:LYS:NZ	0.838
1	B:59:GLU:HB3	B:224:SER:HA	0.806
1	A:398:LEU:HA	B:211:GLU:HB3	0.806
1	A:513:LYS:H	P:106:LEU:CD2	0.801
1	B:220:LYS:CD	B:152:LEU:HD12	0.800
1	A:444:ASP:HB2	B:156:GLU:HB2	0.799
1	B:117:PHE:CG	P:192:ASN:O	0.799
1	B:142:VAL:HG23	B:150:ARG:HB2	0.796
1	P:76:SER:CA	P:106:LEU:HD11	0.794
1	B:97:LYS:HG3	B:226:LEU:HA	0.789
1	B:101:HIS:HB3	P:174:LEU:HD21	0.787
1	B:115:LEU:HD22	P:159:SER:HA	0.778
1	B:92:PRO:HG3	P:79:PRO:HD3	0.773
1	P:77:HIS:HA	P:160:ALA:HB2	0.771
1	B:107:TYR:HB2	P:5:PRO:HB2	0.768
1	P:75:PRO:C	B:191:TYR:HB3	0.768

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	P:75:PRO:HG3	B:3:PRO:CD	0.765
1	P:78:VAL:CG1	B:226:LEU:HD13	0.759
1	P:75:PRO:C	P:174:LEU:CD2	0.757
1	B:63:ILE:HD11	P:172:ALA:HB1	0.756
1	B:166:SER:HB2	B:138:ASP:H	0.752
1	B:2:TYR:HB2	P:178:LYS:HB3	0.747
1	B:98:THR:HB	A:139:GLY:HA3	0.743
1	P:75:PRO:C	B:224:SER:HA	0.743
1	P:75:PRO:CB	P:106:LEU:CD2	0.738
1	B:137:VAL:HG22	B:105:TRP:HB2	0.736
1	B:113:GLU:CD	P:174:LEU:CD2	0.734
1	A:118:GLU:HG3	B:3:PRO:HD2	0.728
1	B:117:PHE:HB2	P:5:PRO:HB2	0.728
1	P:76:SER:N	P:192:ASN:C	0.720
1	B:100:GLY:HA2	A:181:PRO:HG2	0.718
1	P:76:SER:N	P:178:LYS:CD	0.714
1	A:513:LYS:HG2	P:160:ALA:HB2	0.706
1	B:2:TYR:HB2	P:160:ALA:CA	0.697
1	B:63:ILE:CD1	B:158:VAL:HA	0.696
1	B:115:LEU:CD2	P:160:ALA:HB1	0.695
1	A:85:MET:HB3	P:106:LEU:HD21	0.694
1	A:411:ILE:HG12	P:106:LEU:HD11	0.686
1	B:113:GLU:CD	B:224:SER:HA	0.682

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:141:VAL:HG23	P:160:ALA:CB	0.682
1	P:75:PRO:N	P:106:LEU:HD22	0.680
1	B:131:GLU:HA	B:139:ASN:H	0.678
1	P:75:PRO:HA	A:237:PHE:HA	0.673
1	A:130:PRO:HD2	P:5:PRO:HB2	0.673
1	P:76:SER:CA	B:136:GLU:HG2	0.673
1	P:76:SER:CA	P:78:VAL:HG12	0.672
1	P:77:HIS:CA	P:106:LEU:HD21	0.670
1	B:180:GLN:H	P:79:PRO:HD3	0.669
1	B:117:PHE:CB	B:211:GLU:HB3	0.668
1	P:75:PRO:C	P:160:ALA:CB	0.668
1	P:76:SER:CA	P:76:SER:N	0.668
1	B:137:VAL:HG13	P:178:LYS:HD3	0.668
1	B:97:LYS:HB3	P:5:PRO:CB	0.664
1	C:152:GLY:HA3	C:259:SER:HB3	0.664
1	A:197:SER:HB2	B:221:TRP:CZ2	0.657
1	B:63:ILE:CG1	A:85:MET:HE3	0.656
1	B:130:GLY:HA2	B:213:VAL:HG22	0.651
1	P:77:HIS:O	B:128:LYS:H	0.649
1	P:76:SER:HA	P:106:LEU:HD21	0.644
1	P:78:VAL:CB	P:178:LYS:CD	0.638
1	B:142:VAL:CG2	P:5:PRO:HB2	0.632
1	P:75:PRO:CA	P:10:ILE:C	0.631

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	P:75:PRO:HA	D:1:SER:HA	0.627
1	B:113:GLU:OE2	B:109:TYR:HD2	0.627
1	A:31:ALA:HB3	B:223:ALA:HB1	0.626
1	B:63:ILE:HD11	A:17:LEU:HD12	0.622
1	C:258:GLY:O	P:178:LYS:HB3	0.622
1	B:142:VAL:HG12	A:254:SER:HB3	0.617
1	A:81:LEU:HB3	B:3:PRO:HD3	0.616
1	B:142:VAL:CG1	B:146:GLU:HG3	0.614
1	B:127:LEU:HD13	B:149:ILE:HG23	0.613
1	B:225:MET:HA	A:244:ILE:HD12	0.609
1	A:444:ASP:HB2	B:215:LEU:HD23	0.609
1	P:77:HIS:H	B:97:LYS:HD3	0.608
1	A:46:LEU:HD11	P:160:ALA:CA	0.606
1	B:113:GLU:CG	B:137:VAL:HG23	0.605
1	B:63:ILE:HG12	P:106:LEU:CD1	0.605
1	A:482:LEU:HD22	B:174:ILE:HG12	0.603
1	P:9:LYS:O	P:158:VAL:O	0.602
1	A:483:THR:HB	P:79:PRO:CD	0.601
1	B:96:VAL:HG13	P:174:LEU:HD21	0.597
1	B:139:ASN:HD22	B:225:MET:SD	0.596
1	A:14:ILE:HA	B:191:TYR:HB3	0.595
1	B:113:GLU:OE1	B:226:LEU:HD12	0.591
1	A:182:LEU:HD13	P:178:LYS:NZ	0.590

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:445:ALA:HA	P:106:LEU:HD11	0.590
1	B:145:MET:HG3	B:214:PRO:HG3	0.588
1	B:94:LEU:HB3	C:37:SER:H	0.588
1	A:241:GLU:HA	A:484:VAL:HB	0.586
1	B:144:PRO:HB3	B:3:PRO:HD2	0.586
1	B:96:VAL:C	B:138:ASP:N	0.584
1	P:76:SER:H	P:63:ALA:C	0.582
1	B:121:MET:HA	B:224:SER:CA	0.581
1	P:77:HIS:N	B:211:GLU:C	0.581
1	A:228:ILE:HD11	B:195:CYS:HB2	0.581
1	P:75:PRO:HB3	A:111:LEU:HD13	0.580
1	B:131:GLU:HA	B:150:ARG:HD2	0.578
1	P:78:VAL:HG13	A:214:LEU:HD12	0.575
1	P:76:SER:CA	A:246:ILE:HG22	0.575
1	B:118:ASP:HA	C:95:PHE:HD2	0.575
1	B:166:SER:CB	P:192:ASN:O	0.575
1	A:488:THR:HB	A:511:ASN:O	0.574
1	B:107:TYR:HD1	B:212:LEU:HD13	0.573
1	B:220:LYS:CB	P:106:LEU:HD21	0.570
1	P:77:HIS:H	C:35:PHE:HD2	0.569
1	B:145:MET:HG2	A:56:VAL:HG12	0.566
1	C:32:TRP:HA	A:131:LEU:HG	0.566
1	A:259:TYR:OH	B:142:VAL:N	0.565

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:2:TYR:CB	A:269:TYR:HE2	0.564
1	B:190:LEU:HD12	B:117:PHE:HE1	0.564
1	B:137:VAL:HG22	P:172:ALA:HB1	0.563
1	A:403:THR:HG21	B:105:TRP:CB	0.562
1	P:62:SER:O	C:221:LEU:HA	0.561
1	B:117:PHE:HB2	B:212:LEU:HD22	0.559
1	B:142:VAL:HA	B:138:ASP:HB3	0.558
1	B:105:TRP:HH2	B:115:LEU:HG	0.557
1	A:67:PHE:HE2	P:106:LEU:CD1	0.556
1	B:95:THR:HG23	A:20:LEU:HG	0.553
1	C:2:GLN:HE22	A:71:PRO:HD3	0.552
1	A:210:THR:HG22	A:228:ILE:HB	0.551
1	A:243:TYR:HA	P:172:ALA:HB1	0.549
1	C:92:PHE:HA	A:446:TYR:HD2	0.547
1	B:115:LEU:HD21	B:218:PHE:HB3	0.547
1	A:174:ALA:HB1	P:174:LEU:HD23	0.547
1	B:143:LEU:HD12	B:127:LEU:HD12	0.545
1	P:77:HIS:N	A:205:ILE:HB	0.543
1	C:31:MET:HA	P:7:GLY:H	0.543
1	A:53:TYR:O	A:242:VAL:HG22	0.542
1	A:123:THR:HG22	B:177:ARG:HD3	0.542
1	A:458:PHE:HB3	B:226:LEU:HD12	0.539
1	B:141:VAL:HG22	A:470:ILE:HG22	0.537

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:182:LEU:HG	B:105:TRP:HB3	0.537
1	B:107:TYR:HB3	B:207:PRO:HG2	0.536
1	C:153:ASP:HB2	B:214:PRO:HB3	0.536
1	P:75:PRO:CA	A:396:PHE:HB2	0.534
1	B:100:GLY:HA2	B:207:PRO:HB3	0.534
1	C:154:ARG:HH12	P:192:ASN:HB2	0.533
1	B:211:GLU:C	B:128:LYS:N	0.533
1	B:124:THR:CA	A:479:ARG:HE	0.528
1	A:295:GLY:HA2	B:208:ILE:HD12	0.528
1	B:110:THR:HA	A:55:VAL:HG23	0.527
1	P:76:SER:HA	P:395:ARG:NH2	0.527
1	A:16:THR:O	P:106:LEU:HD21	0.526
1	A:70:MET:HB2	B:213:VAL:HG13	0.525
1	A:226:ASP:OD1	C:71:PRO:HD2	0.524
1	C:222:LYS:HG2	A:83:PRO:HD3	0.522
1	P:75:PRO:C	B:72:LEU:HD22	0.522
1	A:443:PRO:HD2	P:5:PRO:CB	0.522
1	B:215:LEU:HA	A:446:TYR:CD2	0.521
1	P:75:PRO:C	A:411:ILE:HD12	0.520
1	A:480:GLU:HB2	B:3:PRO:HD2	0.520
1	B:125:SER:H	B:45:LEU:HG	0.519
1	B:131:GLU:HG2	B:213:VAL:HG22	0.519
1	A:146:ILE:HG23	B:208:ILE:HG12	0.519

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	P:5:PRO:C	B:143:LEU:HG	0.518
1	A:239:HIS:O	B:226:LEU:HD23	0.517
1	B:174:ILE:HD13	A:397:PRO:HD2	0.516
1	B:107:TYR:CD1	B:225:MET:HE2	0.516
1	A:404:LEU:HB3	P:172:ALA:CB	0.516
1	B:101:HIS:H	A:359:ASN:HA	0.515
1	B:135:LEU:HA	P:178:LYS:HZ1	0.515
1	B:144:PRO:HA	B:224:SER:HB2	0.515
1	A:392:PHE:O	A:60:HIS:CE1	0.514
1	B:194:GLN:HE21	A:240:PRO:HD3	0.514
1	B:115:LEU:HD21	A:80:TRP:HB2	0.511
1	B:127:LEU:HD13	B:106:SER:HA	0.511
1	A:510:VAL:HG12	A:493:TRP:HH2	0.510
1	B:141:VAL:HG23	B:211:GLU:HA	0.510
1	A:403:THR:HG23	P:160:ALA:CA	0.510
1	B:208:ILE:H	B:213:VAL:HG13	0.509
1	A:51:GLN:O	P:178:LYS:HZ3	0.509
1	O:359:GLU:OE1	A:355:ILE:HG23	0.508
1	P:76:SER:C	P:351:GLU:CD	0.508
1	B:142:VAL:CG2	A:198:LEU:HD11	0.507
1	C:70:THR:HB	B:97:LYS:N	0.507
1	B:225:MET:O	B:139:ASN:OD1	0.504
1	A:82:VAL:HB	P:178:LYS:HB3	0.502

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:309:MET:HB3	P:178:LYS:CG	0.499
1	B:63:ILE:CD1	A:106:PRO:HD3	0.498
1	B:117:PHE:CZ	B:152:LEU:HB2	0.496
1	A:443:PRO:HD2	O:78:VAL:HG13	0.495
1	A:408:TRP:HA	C:247:TRP:HE1	0.491
1	B:2:TYR:CD1	P:178:LYS:CD	0.491
1	B:41:ILE:O	P:43:GLU:OE2	0.490
1	B:142:VAL:HG13	A:67:PHE:HD2	0.489
1	B:162:TRP:CD1	A:234:PHE:CZ	0.489
1	B:142:VAL:C	C:96:PHE:HB2	0.489
1	B:105:TRP:CD2	C:206:VAL:HG23	0.489
1	A:396:PHE:N	P:7:GLY:N	0.488
1	B:106:SER:HB3	B:226:LEU:HB3	0.487
1	P:75:PRO:HB3	P:178:LYS:CB	0.486
1	A:305:THR:HG23	P:73:ARG:N	0.486
1	B:127:LEU:HB2	B:157:ASP:OD2	0.485
1	B:220:LYS:CD	B:171:THR:HB	0.485
1	B:139:ASN:ND2	B:209:VAL:HB	0.484
1	A:33:SER:HB3	B:213:VAL:HG23	0.484
1	A:239:HIS:HB3	A:479:ARG:HB2	0.482
1	A:76:GLY:O	B:212:LEU:HA	0.482
1	B:99:MET:HB2	B:224:SER:HB3	0.480
1	A:397:PRO:HG2	C:78:ARG:HG3	0.480

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:189:GLY:O	B:104:TYR:N	0.479
1	P:76:SER:N	B:225:MET:CB	0.479
1	B:142:VAL:HG22	P:178:LYS:NZ	0.479
1	B:220:LYS:CB	A:427:GLN:HB2	0.478
1	A:309:MET:HG2	B:151:MET:HE1	0.478
1	B:220:LYS:HG3	B:211:GLU:O	0.477
1	A:156:SER:HB2	C:108:PRO:HD2	0.477
1	B:97:LYS:HD3	P:74:ILE:HD12	0.477
1	B:141:VAL:CB	P:160:ALA:HB2	0.477
1	B:119:SER:HB2	P:172:ALA:CB	0.476
1	B:133:ARG:HB2	A:424:PHE:HD1	0.475
1	B:113:GLU:OE2	P:160:ALA:HB2	0.474
1	B:113:GLU:OE2	P:160:ALA:HB1	0.474
1	A:105:PRO:HB2	B:117:PHE:N	0.472
1	B:58:GLN:HA	B:213:VAL:HG22	0.472
1	B:97:LYS:HA	C:258:GLY:C	0.472
1	B:225:MET:C	P:174:LEU:HD22	0.472
1	A:46:LEU:O	P:174:LEU:HD22	0.471
1	O:78:VAL:O	A:71:PRO:O	0.470
1	A:488:THR:O	B:225:MET:HE3	0.470
1	C:132:THR:HA	B:215:LEU:CD2	0.470
1	B:113:GLU:OE2	P:160:ALA:CB	0.470
1	P:39:LYS:NZ	A:498:PRO:HD3	0.469

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:63:VAL:HA	B:194:GLN:O	0.469
1	A:126:THR:HA	B:148:THR:OG1	0.468
1	C:93:THR:OG1	B:178:LEU:HD12	0.467
1	C:202:HIS:O	C:110:LEU:HD11	0.467
1	P:5:PRO:C	C:259:SER:N	0.467
1	B:105:TRP:CG	P:174:LEU:HD23	0.467
1	B:113:GLU:CD	B:107:TYR:HA	0.466
1	P:72:VAL:HG22	P:160:ALA:HB3	0.466
1	B:101:HIS:HB2	P:106:LEU:CD2	0.466
1	B:153:VAL:HG21	C:90:LEU:HB3	0.465
1	B:140:ARG:CB	B:64:TRP:CE3	0.465
1	B:213:VAL:O	B:72:LEU:HG	0.465
1	B:141:VAL:HG23	B:173:ALA:HB3	0.465
1	A:403:THR:HG22	C:71:PRO:CD	0.465
1	B:143:LEU:H	P:178:LYS:HZ3	0.463
1	B:221:TRP:NE1	B:224:SER:CB	0.461
1	A:508:THR:HG22	B:170:LYS:HA	0.461
1	B:208:ILE:HA	B:207:PRO:CG	0.459
1	B:118:ASP:C	B:177:ARG:O	0.459
1	C:74:GLN:O	P:516:ASP:C	0.459
1	B:104:TYR:CD1	P:106:LEU:HD22	0.458
1	B:119:SER:HB3	C:127:VAL:H	0.458
1	B:220:LYS:HB3	B:206:MET:HE3	0.457

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:424:PHE:HA	O:516:ASP:C	0.457
1	B:107:TYR:CE1	O:532:PRO:CD	0.456
1	B:142:VAL:HA	A:428:HIS:HB2	0.455
1	C:107:THR:HB	P:160:ALA:HA	0.455
1	P:74:ILE:N	B:136:GLU:HG2	0.453
1	P:76:SER:N	B:214:PRO:HG3	0.453
1	P:75:PRO:C	P:532:PRO:CD	0.453
1	A:382:MET:HE3	A:310:ILE:HG13	0.452
1	P:74:ILE:C	B:179:ASN:O	0.452
1	P:76:SER:CB	B:174:ILE:C	0.452
1	B:32:LEU:HD11	B:177:ARG:HB3	0.452
1	B:117:PHE:CD1	C:83:LEU:HG	0.452
1	B:142:VAL:HG11	B:225:MET:O	0.451
1	C:253:SER:HB3	B:219:GLU:HG2	0.450
1	P:74:ILE:HG22	A:286:VAL:HG22	0.449
1	B:140:ARG:HH22	A:494:LEU:HD13	0.449
1	P:74:ILE:CG2	B:212:LEU:CD1	0.449
1	A:18:TYR:HB3	B:224:SER:HA	0.448
1	B:118:ASP:HA	P:73:ARG:H	0.446
1	B:144:PRO:HB3	A:105:PRO:HD3	0.445
1	P:74:ILE:C	B:3:PRO:CD	0.445
1	A:401:GLY:HA3	B:109:TYR:HB3	0.445
1	B:163:ALA:HB3	P:106:LEU:CD1	0.445

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:92:PRO:HA	C:259:SER:C	0.444
1	B:127:LEU:HB2	B:41:ILE:HG13	0.443
1	B:154:SER:HB2	B:68:PRO:HD3	0.443
1	C:106:PRO:HB3	B:219:GLU:O	0.443
1	C:253:SER:HB3	A:481:VAL:HG21	0.442
1	P:75:PRO:CA	A:360:SER:HB2	0.441
1	B:98:THR:HA	C:242:PHE:HE1	0.441
1	P:74:ILE:O	B:156:GLU:HG2	0.440
1	P:77:HIS:H	A:56:VAL:HG21	0.439
1	A:199:PRO:HB2	B:86:MET:HB2	0.439
1	A:320:PHE:HB3	P:160:ALA:HB1	0.439
1	B:68:PRO:O	B:154:SER:HB3	0.438
1	B:160:HIS:HB2	A:439:TYR:CZ	0.436
1	C:70:THR:HB	B:115:LEU:HD13	0.436
1	A:43:PRO:HB3	B:154:SER:HB3	0.435
1	B:220:LYS:HB3	A:493:TRP:CD1	0.434
1	B:117:PHE:HB2	C:246:VAL:HG23	0.433
1	B:162:TRP:O	P:160:ALA:CA	0.433
1	B:108:GLU:OE2	A:442:TYR:HD2	0.432
1	B:135:LEU:HA	B:225:MET:HE3	0.431
1	B:154:SER:HA	B:3:PRO:HD2	0.430
1	P:515:ARG:O	B:225:MET:HE2	0.429
1	P:75:PRO:C	B:138:ASP:CB	0.429

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	C:126:GLU:HB3	C:213:LEU:HD22	0.429
1	B:199:CYS:SG	P:160:ALA:CA	0.429
1	O:515:ARG:O	B:171:THR:CB	0.428
1	O:531:MET:N	C:254:ILE:HG22	0.428
1	A:425:PHE:O	C:5:ALA:H	0.428
1	P:75:PRO:C	C:259:SER:HA	0.427
1	B:130:GLY:CA	P:173:VAL:O	0.427
1	B:145:MET:CG	A:322:TRP:CE3	0.426
1	P:531:MET:N	A:420:VAL:HG22	0.426
1	A:306:SER:O	C:206:VAL:HG21	0.426
1	B:152:LEU:HA	P:192:ASN:C	0.425
1	B:155:SER:HB3	B:209:VAL:HB	0.423
1	B:174:ILE:HB	C:89:VAL:HG23	0.422
1	C:79:TYR:O	B:172:ASP:HB2	0.421
1	B:107:TYR:HB3	P:180:VAL:HG22	0.421
1	B:127:LEU:HB2	P:106:LEU:CG	0.420
1	B:216:LYS:O	P:359:GLU:OE1	0.420
1	A:282:LEU:O	B:144:PRO:HD2	0.419
1	A:487:THR:HB	O:338:ASP:HB2	0.419
1	B:143:LEU:HD12	A:212:ARG:HD2	0.418
1	B:117:PHE:CD2	B:209:VAL:HG12	0.417
1	C:222:LYS:HE2	B:165:PRO:HB3	0.416
1	P:72:VAL:HG22	C:15:PRO:HB3	0.415

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:104:LEU:HB2	P:338:ASP:HB2	0.415
1	B:2:TYR:CB	C:8:MET:HE3	0.415
1	B:96:VAL:HA	O:119:PRO:CD	0.415
1	P:77:HIS:H	B:142:VAL:CB	0.415
1	C:96:PHE:HA	A:177:GLN:HE22	0.414
1	B:37:VAL:O	A:205:ILE:HG12	0.414
1	B:67:LEU:HB3	P:9:LYS:N	0.414
1	B:113:GLU:HB2	P:173:VAL:O	0.414
1	A:397:PRO:HB2	B:137:VAL:HG23	0.413
1	A:397:PRO:HG3	C:221:LEU:HD12	0.412
1	A:301:ARG:HD2	P:245:GLU:OE2	0.412
1	C:205:HIS:HD2	B:138:ASP:HA	0.411
1	B:99:MET:HB3	B:147:MET:H	0.411
1	A:35:LEU:HB2	P:70:PRO:HD2	0.411
1	B:83:LEU:HA	P:74:ILE:HD12	0.411
1	P:76:SER:HB3	A:436:PRO:HD3	0.410
1	B:98:THR:O	B:142:VAL:HB	0.410
1	A:436:PRO:HG2	C:24:LEU:HG	0.410
1	B:115:LEU:N	A:489:THR:HG21	0.409
1	B:99:MET:SD	B:5:GLN:HB3	0.409
1	A:492:GLU:HG2	B:187:ARG:NH1	0.409
1	C:242:PHE:O	C:61:ARG:HD2	0.409
1	P:75:PRO:CA	P:119:PRO:CD	0.409

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:40:LEU:HD22	P:160:ALA:HA	0.409
1	B:117:PHE:O	A:314:PRO:CD	0.408
1	B:2:TYR:CG	A:412:HIS:HE1	0.408
1	B:108:GLU:OE1	B:116:SER:N	0.408
1	B:106:SER:CB	A:493:TRP:CH2	0.407
1	B:124:THR:HA	A:464:VAL:HG23	0.407
1	C:161:LEU:HD11	B:45:LEU:HD22	0.407
1	P:75:PRO:C	C:258:GLY:HA2	0.407
1	B:153:VAL:HG21	O:245:GLU:OE2	0.407
1	C:250:LEU:O	A:362:LEU:HD23	0.406
1	C:4:HIS:HB2	C:222:LYS:HB2	0.406
1	C:253:SER:HB3	B:225:MET:HE1	0.405
1	P:75:PRO:HD2	B:142:VAL:HG23	0.405
1	A:319:VAL:HA	A:411:ILE:HG13	0.404
1	A:416:MET:O	A:470:ILE:HG13	0.404
1	C:171:PHE:CE2	P:372:GLU:OE1	0.404
1	A:269:TYR:HD1	B:115:LEU:HD13	0.403
1	B:115:LEU:HD21	A:507:PRO:HD2	0.402
1	B:140:ARG:HB2	A:470:ILE:HD11	0.401
1	C:85:ILE:O	C:194:THR:HB	0.401
1	A:294:VAL:HA	B:116:SER:H	0.401
1	B:113:GLU:OE2	A:227:PRO:HD3	0.400
1	P:77:HIS:H	B:156:GLU:HB2	0.400

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	O:395:ARG:NH2	C:157:MET:HE3	0.400
1	B:143:LEU:CB	B:142:VAL:N	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	Analysed	Favored	Allowed	Outliers
1	2805	2544	200	61

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	Analysed	Favored	Allowed	Outliers
1	2393	2142	121	130

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	5	TRP
1	A	9	THR
1	A	13	ASP
1	A	52	ILE
1	A	80	TRP
1	A	90	ASP
1	A	179	GLN
1	A	182	LEU
1	A	211	ASP
1	A	265	GLU

Model ID	Chain	Residue ID	Residue type
1	A	300	THR
1	A	365	VAL
1	A	406	ASP
1	A	428	HIS
1	A	430	LEU
1	A	432	LEU
1	A	441	ASP
1	A	444	ASP
1	A	480	GLU
1	A	497	CYS
1	A	510	VAL
1	A	512	LEU
1	B	2	TYR
1	B	59	GLU
1	B	63	ILE
1	B	87	ASP
1	B	88	GLU
1	B	97	LYS
1	B	98	THR
1	B	104	TYR
1	B	105	TRP
1	B	108	GLU
1	B	109	TYR

Model ID	Chain	Residue ID	Residue type
1	B	110	THR
1	B	115	LEU
1	B	117	PHE
1	B	119	SER
1	B	122	ILE
1	B	127	LEU
1	B	128	LYS
1	B	134	LEU
1	B	136	GLU
1	B	138	ASP
1	B	139	ASN
1	B	140	ARG
1	B	141	VAL
1	B	142	VAL
1	B	143	LEU
1	B	153	VAL
1	B	157	ASP
1	B	159	LEU
1	B	171	THR
1	B	210	LEU
1	B	211	GLU
1	B	215	LEU
1	B	217	TYR

Model ID	Chain	Residue ID	Residue type
1	B	218	PHE
1	B	220	LYS
1	B	221	TRP
1	C	2	GLN
1	C	4	HIS
1	C	64	THR
1	C	93	THR
1	C	126	GLU
1	C	188	ASP
1	C	256	TRP
1	C	257	TRP
1	D	2	VAL
1	D	3	VAL
1	D	18	ASP
1	D	55	GLU
1	D	68	MET
1	D	109	GLU
1	D	110	GLU
1	D	111	GLU
1	D	112	TRP
1	D	117	THR
1	D	123	MET
1	E	10	GLU

Model ID	Chain	Residue ID	Residue type
1	E	31	LYS
1	E	66	ARG
1	E	73	ASP
1	E	107	ASP
1	E	108	LYS
1	E	109	VAL
1	F	6	VAL
1	F	61	ILE
1	F	65	ASP
1	F	92	VAL
1	G	16	ARG
1	G	32	LEU
1	G	41	ARG
1	G	56	THR
1	G	67	THR
1	G	81	TYR
1	H	1	MET
1	H	3	GLU
1	H	28	ARG
1	H	30	CYS
1	H	85	LYS
1	H	86	ILE
1	I	3	LEU

Model ID	Chain	Residue ID	Residue type
1	I	7	GLN
1	I	9	ARG
1	I	14	ARG
1	I	67	ILE
1	I	68	PHE
1	I	69	GLN
1	I	70	SER
1	I	72	LYS
1	J	2	GLU
1	J	50	LEU
1	K	3	ASP
1	K	47	GLU
1	L	3	GLU
1	L	10	ILE
1	L	23	MET
1	L	40	ARG
1	L	45	LYS
1	L	46	LYS
1	M	8	THR
1	M	13	LYS
1	M	37	LEU
1	M	42	LYS
1	N	2	GLN

Model ID	Chain	Residue ID	Residue type
1	N	3	ILE
1	N	32	THR
1	N	58	ASN
1	N	60	GLN
1	N	73	LEU

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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