

Integrative Structure Validation Report ?

April 09, 2025 - 04:36 PM PDT

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

Integrative Modeling Validation Version 2.0

Python-IHM Version 1.8

MolProbity Version 4.5.2

PDB ID	9A8S
Structure Title	Structure of human myr-Arf1-GTP bound to MSPdH5 nanodisc
Structure Authors	Zhang, Y.; Soubias, O.; Pant, S.; Heinrich, F.; Vogel, A.; Li, J.; Li, Y.; Clifton, L.A.; Daum, S.; Bacia, K.; Huster, D.; Randazzo, P.A.; Losche, M.; Tajkhorshid, E.; Byrd, R.A.
Deposited on	2024-09-05

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

We welcome your comments at helpdesk@pdb-ihm.org

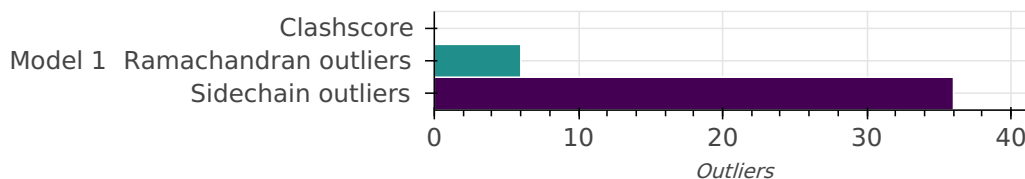
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

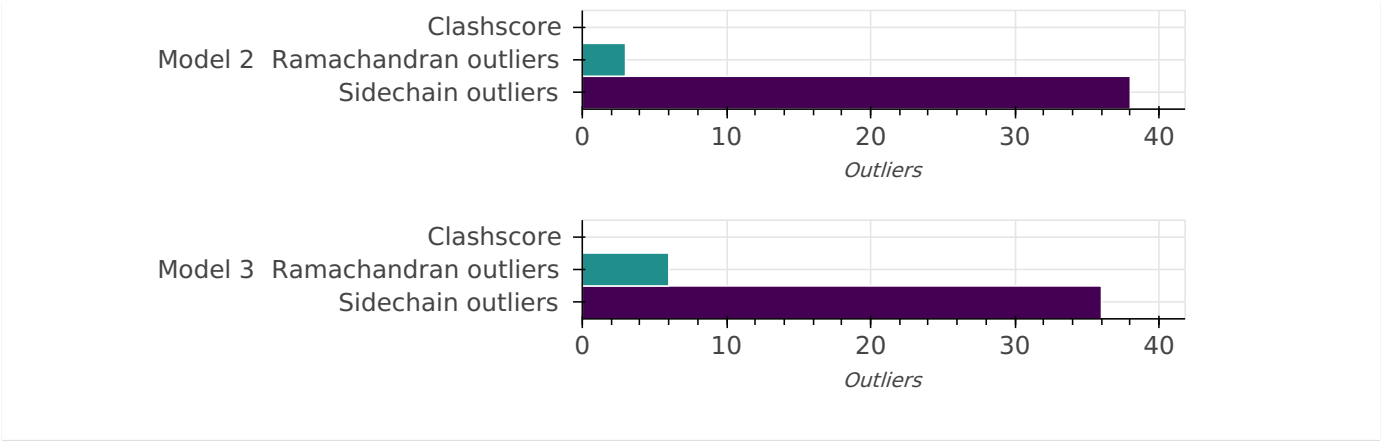
List of references used to build this report is available [here](#).

Overall quality ?

This validation report contains model quality assessments for all structures, data quality and fit to model assessments for SAS and crosslinking-MS 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 3 model(s). A total of 6 datasets were used to build this entry.

Representation ?

This entry has 3 representation(s).

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
1	1	1	Membrane Scaffold Protein (MSP) Apolipoprotein A-I	A	167	-	1-167	100.00 / 100.00	Atomic
				B					
		2	ADP-ribosylation factor 1	C [P]	180	-	1-180	100.00 / 100.00	Atomic
		3	1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine	D [A]	Non-polymeric	-	-	Not available / Not available	Atomic
				E [A]					
				F [A]					
				G [A]					
				H [A]					
				I [A]					
				J [A]					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				K [A]					
				L [A]					
				M [A]					
				N [A]					
				O [A]					
				Q [A]					
				R [A]					
				S [A]					
				T [A]					
				U [A]					
				V [A]					
				W [A]					
				X [A]					
				Y [A]					
				Z [A]					
				AA [A]					
				AC [B]					
				BA [A]					
				BB [B]					
				BC [B]					
				CA [A]					
				CB [B]					
				CC [B]					
				DB [B]					
				DC [P]					
				EA [A]					
				EB [B]					
				EC [P]					
				FA [A]					
				FB [B]					
				FC [P]					
				GA [A]					
				GB [B]					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				GC [P]					
				HA [A]					
				HB [B]					
				HC [P]					
				IA [B]					
				IB [B]					
				IC [P]					
				JA [B]					
				JB [B]					
				JC [P]					
				KA [B]					
				KB [B]					
				KC [P]					
				LA [B]					
				LB [B]					
				LC [P]					
				MB [B]					
				MC [P]					
				NA [B]					
				NB [B]					
				NC [P]					
				OA [B]					
				OB [B]					
				OC [P]					
				PA [B]					
				PB [B]					
				PC [P]					
				QA [B]					
				QB [B]					
				QC [P]					
				RA [B]					
				RB [B]					
				RC [P]					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				SA [B]					
				SB [B]					
				TA [B]					
				TB [B]					
				UA [B]					
				UB [B]					
				UC [P]					
				VA [B]					
				VB [B]					
				VC [P]					
				WA [B]					
				WB [B]					
				WC [P]					
				XA [B]					
				XC [P]					
				YA [B]					
				YB [B]					
				YC [P]					
				ZA [B]					
				ZB [B]					
		4	[(2R)-2-[(E)-octadec-9-enoyl]oxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonooxycyclohexyl]oxy-phosphoryl]oxy-propyl] (E)-octadec-9-enoate	P [A]	Non-polymeric	-	-	Not available / Not available	Atomic
				AB [B]					
				DA [A]					
				MA [B]					
				SC [P]					
				TC [P]					
				XB [B]					
2	2	1	Membrane Scaffold Protein (MSP) Apolipoprotein A-I	A	167	-	1-167	100.00 / 100.00	Atomic
				B					
		2	ADP-ribosylation factor 1	C [P]	180	-	1-180	100.00 / 100.00	Atomic

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
		3	1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine	D [A]	Non-polymeric	-	-	Not available / Not available	Atomic
				E [A]					
				F [A]					
				G [A]					
				H [A]					
				I [A]					
				J [A]					
				K [A]					
				M [A]					
				N [A]					
				O [A]					
				Q [A]					
				R [A]					
				S [A]					
				T [A]					
				V [A]					
				W [A]					
				X [A]					
				Y [A]					
				Z [A]					
				AA [A]					
				AE [A]					
				AG [A]					
				AH [A]					
				AI [A]					
				AJ [A]					
				AK [A]					
				AL [A]					
				AM [A]					
				AN [A]					
				AO [A]					
				AP [A]					
				AQ [A]					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				AR [A]					
				AS [A]					
				AT [B]					
				AW [B]					
				AZ [P]					
				BA [A]					
				BB [B]					
				BD [P]					
				CA [A]					
				CB [B]					
				DB [B]					
				DC [P]					
				EA [A]					
				EB [B]					
				EC [P]					
				FA [A]					
				FB [B]					
				FC [P]					
				GA [A]					
				GB [B]					
				GC [P]					
				HA [A]					
				HB [B]					
				HC [P]					
				IA [B]					
				IB [B]					
				IC [P]					
				JA [B]					
				JB [B]					
				KA [B]					
				KB [B]					
				LA [B]					
				LB [B]					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				LC [P]					
				MB [B]					
				MC [P]					
				NB [B]					
				NC [P]					
				OA [B]					
				OB [B]					
				OC [P]					
				PA [B]					
				PB [B]					
				PC [P]					
				QA [B]					
				QB [B]					
				QC [P]					
				RA [B]					
				RB [B]					
				RC [P]					
				SA [B]					
				TA [B]					
				UA [B]					
				UC [P]					
				VA [B]					
				VC [P]					
				WA [B]					
				WC [P]					
				XA [B]					
				XC [P]					
				YA [B]					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
		4	[(2R)-2-[(E)-octadec-9-enoyl]oxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonooxycyclohexyl]oxyphosphoryl]oxypropyl] (E)-octadec-9-enoate	AD [A]	Non-polymeric	-	-	Not available / Not available	Atomic
				AF [A]					
				AU [B]					
				AV [B]					
				AX [P]					
				AY [P]					
3	3	1	Membrane Scaffold Protein (MSP) Apolipoprotein A-I	A	167	-	1-167	100.00 / 100.00	Atomic
				B					
		2	ADP-ribosylation factor 1	C [P]	180	-	1-180	100.00 / 100.00	Atomic
		3	1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine	D [A]	Non-polymeric	-	-	Not available / Not available	Atomic
				E [A]					
				F [A]					
				G [A]					
				H [A]					
				I [A]					
				J [A]					
				L [A]					
				M [A]					
				N [A]					
				O [A]					
				Q [A]					
				R [A]					
				S [A]					
				T [A]					
				U [A]					
				V [A]					
				W [A]					
				X [A]					
				Y [A]					
				Z [A]					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				AA [A]					
				AE [A]					
				AG [A]					
				AT [B]					
				AW [B]					
				AZ [P]					
				BA [A]					
				BB [B]					
				BD [P]					
				BI [B]					
				BL [P]					
				BM [P]					
				BN [P]					
				BO [P]					
				CA [A]					
				CB [B]					
				DC [P]					
				EA [A]					
				EB [B]					
				EC [P]					
				FA [A]					
				FB [B]					
				FC [P]					
				GA [A]					
				GB [B]					
				GC [P]					
				HA [A]					
				HB [B]					
				HC [P]					
				IA [B]					
				IB [B]					
				IC [P]					
				JA [B]					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				JB [B]					
				JC [P]					
				KA [B]					
				KB [B]					
				KC [P]					
				LA [B]					
				LB [B]					
				LC [P]					
				MB [B]					
				MC [P]					
				NB [B]					
				NC [P]					
				OA [B]					
				OB [B]					
				OC [P]					
				PA [B]					
				PB [B]					
				QA [B]					
				QB [B]					
				QC [P]					
				RB [B]					
				RC [P]					
				SA [B]					
				SB [B]					
				TA [B]					
				TB [B]					
				UA [B]					
				UB [B]					
				UC [P]					
				VA [B]					
				VC [P]					
				WA [B]					
				WB [B]					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				WC [P]					
				XA [B]					
				XC [P]					
				YA [B]					
				YB [B]					
				ZA [B]					
		4	[(2R)-2-[(E)-octadec-9-enoyl]oxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonooxy-cyclohexyl]oxy-phosphoryl]oxy-propyl] (E)-octadec-9-enoate	AU [B]	Non-polymeric	-	-	Not available / Not available	Atomic
				BE [A]					
				BF [B]					
				BG [B]					
				BH [B]					
				BJ [P]					
				BK [P]					

Datasets used for modeling ?

There are 6 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	NMR data	BMRB	27726
2	Experimental model	PDB	3LVQ
3	NMR data	BMRbig	BMRbig101
4	Experimental model	PDB	2N5E
6	Comparative model	Not available	Not available
5	Experimental model	PDB	2KSQ

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	NAMD multi-state modeling	None	True	False
1	1	None	None	NAMD multi-state modeling	None	True	False
1	1	None	None	NAMD multi-state modeling	None	True	False

There are 4 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	NAMD2	Not available	molecular dynamics	http://www.ks.uiuc.edu/Research/namd/
2	CHARMM-GUI	Not available	molecular dynamics simulations	http://www.charmm-gui.org/
3	Swiss-Model	Not available	comparative modeling	https://swissmodel.expasy.org/
4	Visual Molecular Dynamics (VMD)	Not available	model building	https://www.ks.uiuc.edu/Research/vmd/

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 930 bond length outliers in this entry (3.50% of 26552 assessed bonds). A summary is provided below. The output is limited to 100 rows.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
AW	1	LBN	C11-C14	123.35	3.99	1.52	2	2
BD	1	LBN	C11-C14	122.60	3.98	1.52	2	2
AT	1	LBN	C11-C14	122.22	3.97	1.52	2	2
AH	1	LBN	C11-C14	119.75	3.92	1.52	2	1
AJ	1	LBN	C11-C14	119.09	3.90	1.52	2	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
AZ	1	LBN	C11-C14	118.08	3.88	1.52	3	2
BL	1	LBN	C11-C14	117.98	3.88	1.52	3	1
AI	1	LBN	C11-C14	117.90	3.88	1.52	2	1
AG	1	LBN	C11-C14	116.29	3.85	1.52	3	2
AQ	1	LBN	C11-C14	112.83	3.78	1.52	2	1
AE	1	LBN	C11-C14	91.09	3.34	1.52	2	2
AO	1	LBN	C11-C14	87.85	3.28	1.52	2	1
BN	1	LBN	C11-C14	85.52	3.23	1.52	3	1
AK	1	LBN	C11-C14	84.86	3.22	1.52	2	1
AL	1	LBN	C11-C14	84.24	3.21	1.52	2	1
AS	1	LBN	C11-C14	83.77	3.20	1.52	2	1
AP	1	LBN	C11-C14	83.59	3.19	1.52	2	1
AR	1	LBN	C11-C14	80.91	3.14	1.52	2	1
BM	1	LBN	C11-C14	78.44	3.09	1.52	3	1
AM	1	LBN	C11-C14	77.25	3.07	1.52	2	1
BO	1	LBN	C11-C14	73.69	3.00	1.52	3	1
BI	1	LBN	C11-C14	73.38	2.99	1.52	3	1
AN	1	LBN	C11-C14	71.71	2.96	1.52	2	1
OA	1	LBN	C10-C7	8.60	1.69	1.52	1	1
QA	1	LBN	O2-P1	8.30	1.48	1.65	2	1
YB	1	LBN	O2-P1	7.77	1.49	1.65	3	1
PA	1	LBN	O2-P1	7.47	1.50	1.65	3	3
E	1	LBN	O1-P1	7.34	1.49	1.63	1	1
OA	1	LBN	C2-C3	7.30	1.66	1.51	2	1
VA	1	LBN	O1-P1	7.27	1.49	1.63	2	2
LC	1	LBN	C26-C27	7.19	1.66	1.52	1	1
FC	1	LBN	O1-P1	7.12	1.49	1.63	2	1
A	106	LYS	CA-CB	7.10	1.67	1.53	3	3
CB	1	LBN	O2-P1	7.05	1.51	1.65	2	2
YA	1	LBN	C2-C3	7.01	1.65	1.51	1	1
C	178	ARG	C-N	6.95	1.43	1.33	3	1
C	66	TRP	NE1-CE2	6.93	1.45	1.37	3	1
WB	1	LBN	C20-C22	6.91	1.66	1.52	1	1
EB	1	LBN	C2-C3	6.85	1.65	1.51	1	1
C	146	HIS	ND1-CE1	6.82	1.39	1.32	1	1
A	121	THR	C-N	6.80	1.42	1.33	2	3

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
C	137	ALA	C-N	6.76	1.42	1.33	2	3
RB	1	LBN	O1-P1	6.58	1.50	1.63	1	1
O	1	LBN	C11-C8	6.54	1.66	1.53	3	1
C	135	ASN	C-N	6.50	1.42	1.33	1	1
Z	1	LBN	C25-C26	6.50	1.63	1.50	3	1
C	10	LYS	C-N	6.49	1.42	1.33	2	1
C	108	MET	C-N	6.49	1.42	1.33	1	2
UA	1	LBN	O2-P1	6.45	1.52	1.65	3	3
C	36	LYS	C-N	6.43	1.42	1.33	3	1
C	152	ASN	C-N	6.43	1.42	1.33	2	2
A	62	ARG	C-N	6.42	1.42	1.33	2	3
JA	1	LBN	O1-P1	6.42	1.50	1.63	3	1
X	1	LBN	O2-P1	6.39	1.52	1.65	3	2
CB	1	LBN	C40-C41	6.37	1.66	1.53	2	1
K	1	LBN	O1-P1	6.35	1.50	1.63	1	2
B	135	LEU	C-N	6.33	1.42	1.33	2	3
NC	1	LBN	C6-C9	6.33	1.64	1.51	1	1
C	43	VAL	C-N	6.32	1.42	1.33	3	1
C	17	GLU	CA-CB	6.32	1.66	1.53	1	1
C	11	GLY	C-N	6.28	1.24	1.33	3	1
J	1	LBN	C2-C3	6.26	1.64	1.51	3	3
F	1	LBN	O2-P1	6.25	1.53	1.65	2	1
GB	1	LBN	O2-P1	6.23	1.53	1.65	1	2
AP	1	LBN	C1-C2	6.23	1.65	1.52	2	1
AH	1	LBN	C38-C39	6.20	1.65	1.52	2	1
C	174	SER	C-N	6.14	1.41	1.33	1	1
A	17	PHE	C-N	6.13	1.41	1.33	3	3
KB	1	LBN	C2-C3	6.13	1.63	1.51	1	2
DC	1	LBN	C6-C9	6.12	1.63	1.51	1	2
D	1	LBN	C10-C13	6.10	1.65	1.52	1	1
Z	1	LBN	C11-C8	6.07	1.65	1.53	3	1
UC	1	LBN	C19-C21	6.06	1.64	1.52	2	1
G	1	LBN	O1-P1	6.06	1.51	1.63	2	2
WA	1	LBN	O2-P1	6.05	1.53	1.65	1	2
C	150	HIS	ND1-CE1	6.01	1.38	1.32	2	1
C	19	ARG	CD-NE	6.01	1.54	1.46	2	2

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
W	1	LBN	C36-C37	5.99	1.64	1.52	2	1
OA	1	LBN	C36-C37	5.96	1.64	1.52	1	1
MB	1	LBN	C11-C8	5.94	1.65	1.53	1	1
B	37	GLU	CA-CB	5.93	1.65	1.53	2	3
KB	1	LBN	O2-P1	5.93	1.53	1.65	2	2
C	144	GLY	C-N	5.92	1.41	1.33	2	2
A	165	ASN	C-N	5.92	1.41	1.33	2	3
HA	1	LBN	O2-P1	5.91	1.53	1.65	3	1
WB	1	LBN	O1-P1	5.89	1.51	1.63	3	2
QB	1	LBN	O2-P1	5.87	1.53	1.65	1	2
C	168	GLU	C-N	5.87	1.41	1.33	1	1
LB	1	LBN	O2-P1	5.84	1.53	1.65	2	1
OB	1	LBN	C3-O5	5.84	1.54	1.42	3	1
K	1	LBN	O2-P1	5.84	1.53	1.65	2	1
I	1	LBN	O2-P1	5.84	1.53	1.65	2	3
LA	1	LBN	O2-P1	5.83	1.53	1.65	2	1
JB	1	LBN	O2-P1	5.82	1.53	1.65	1	2
A	150	LYS	C-N	5.81	1.41	1.33	1	3
HB	1	LBN	O2-P1	5.81	1.53	1.65	1	1
XC	1	LBN	C2-C3	5.81	1.63	1.51	2	2
GC	1	LBN	O2-P1	5.79	1.53	1.65	2	1
JA	1	LBN	C11-C14	5.78	1.64	1.52	3	1
S	1	LBN	C27-C28	5.78	1.64	1.52	1	1

Standard geometry: angle outliers ?

There are 845 bond angle outliers in this entry (2.62% of 32307 assessed bonds). A summary is provided below. The output is limited to 100 rows.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
C	9	PHE	CA-CB-CG	10.11	103.69	113.80	3	2
C	178	ARG	NE-CZ-NH1	9.26	130.76	121.50	1	1
B	35	ASP	CA-CB-CG	9.12	103.48	112.60	2	3
C	13	PHE	CA-CB-CG	8.80	105.00	113.80	3	2
A	19	ASP	CA-CB-CG	8.74	121.34	112.60	3	3
B	75	ARG	NE-CZ-NH2	8.74	111.34	119.20	3	3
B	75	ARG	NE-CZ-NH1	8.70	130.20	121.50	3	3
B	62	ARG	NE-CZ-NH2	8.67	127.00	119.20	3	3

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
C	151	ARG	NE-CZ-NH2	8.60	126.94	119.20	1	1
C	178	ARG	NH1-CZ-NH2	8.25	108.57	119.30	1	1
C	24	GLY	C-N-CA	8.22	136.50	121.70	3	2
C	135	ASN	C-N-CA	8.21	136.48	121.70	1	1
C	5	PHE	CA-CB-CG	8.01	105.79	113.80	2	1
B	73	ARG	NE-CZ-NH1	7.88	129.38	121.50	3	3
C	172	TRP	CB-CG-CD2	7.83	137.76	126.80	2	1
A	112	ARG	NE-CZ-NH2	7.71	112.26	119.20	1	3
C	103	ALA	N-CA-CB	7.66	121.89	110.40	3	1
C	117	ARG	NE-CZ-NH1	7.62	129.12	121.50	3	1
C	141	ASP	CA-CB-CG	7.47	120.07	112.60	2	1
C	82	PHE	CB-CG-CD2	7.41	108.10	120.70	3	1
C	127	LYS	N-CA-CB	7.39	123.06	110.50	1	2
CA	1	LBN	O1-P1-O2	7.07	114.65	93.45	3	2
C	151	ARG	C-CA-CB	6.98	96.84	110.10	1	1
B	43	VAL	CA-CB-CG2	6.98	98.54	110.40	2	3
A	88	ALA	N-CA-CB	6.93	120.79	110.40	3	3
C	46	ILE	CA-C-O	6.88	109.10	120.80	3	1
C	45	THR	OG1-CB-CG2	6.88	95.55	109.30	1	1
A	142	LEU	N-CA-CB	6.85	122.14	110.50	2	3
C	19	ARG	NE-CZ-NH1	6.79	128.29	121.50	1	2
C	151	ARG	NE-CZ-NH1	6.76	128.26	121.50	2	1
C	44	THR	C-N-CA	6.71	133.78	121.70	1	2
C	125	ALA	C-CA-CB	6.65	120.47	110.50	2	1
C	128	GLN	OE1-CD-NE2	6.63	115.97	122.60	2	2
C	97	ARG	NE-CZ-NH1	6.63	128.13	121.50	3	1
B	101	ARG	NE-CZ-NH1	6.62	128.12	121.50	2	3
C	79	ARG	NE-CZ-NH1	6.52	128.02	121.50	3	1
C	19	ARG	NH1-CZ-NH2	6.49	110.87	119.30	1	2
A	97	ARG	NE-CZ-NH1	6.43	127.93	121.50	2	3
C	75	ARG	CA-C-N	6.40	126.49	116.90	3	2
A	66	GLU	CA-C-N	6.40	126.49	116.90	3	3
C	146	HIS	ND1-CE1-NE2	6.33	114.73	108.40	3	1
C	75	ARG	N-CA-CB	6.28	121.18	110.50	1	1
C	46	ILE	CA-C-N	6.28	126.32	116.90	3	3
C	113	GLU	C-N-CA	6.28	133.00	121.70	3	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
B	143	LEU	CA-C-N	6.27	126.30	116.90	1	3
A	143	LEU	CA-C-N	6.26	126.29	116.90	2	3
RB	1	LBN	O1-P1-O2	6.25	112.20	93.45	1	1
C	175	ASN	OD1-CG-ND2	6.24	116.36	122.60	1	1
C	150	HIS	C-N-CA	6.22	132.90	121.70	3	1
C	146	HIS	CD2-NE2-CE1	6.20	102.80	109.00	3	2
B	101	ARG	NE-CZ-NH2	6.19	113.63	119.20	3	3
A	126	THR	CA-CB-OG1	6.18	118.87	109.60	1	3
B	92	ASP	CA-CB-CG	6.15	106.45	112.60	3	3
A	87	LEU	O-C-N	6.14	113.17	123.00	2	3
C	79	ARG	NE-CZ-NH2	6.14	113.67	119.20	3	1
B	7	ARG	NE-CZ-NH1	6.12	127.62	121.50	2	3
A	108	ASN	OD1-CG-ND2	6.11	116.49	122.60	3	3
B	165	ASN	OD1-CG-ND2	6.10	128.70	122.60	1	3
B	132	LYS	CA-C-N	6.10	126.05	116.90	1	3
C	149	ARG	NH1-CZ-NH2	6.08	111.39	119.30	2	1
C	3	ASN	CA-CB-CG	6.08	118.68	112.60	3	1
C	126	ASN	C-N-CA	6.03	132.56	121.70	1	1
C	18	MET	CG-SD-CE	6.03	87.64	100.90	3	2
B	64	LYS	N-CA-CB	6.01	120.71	110.50	3	3
A	75	ARG	NE-CZ-NH2	5.98	124.58	119.20	3	3
C	135	ASN	OD1-CG-ND2	5.97	128.57	122.60	1	3
C	83	GLN	CA-CB-CG	5.95	125.99	114.10	2	1
A	123	HIS	CD2-NE2-CE1	5.94	103.06	109.00	1	3
C	180	GLN	CB-CG-CD	5.93	122.68	112.60	2	1
B	73	ARG	NH1-CZ-NH2	5.92	111.60	119.30	2	3
C	28	ALA	CA-C-O	5.92	130.86	120.80	3	1
C	38	LYS	C-CA-CB	5.91	98.86	110.10	2	1
C	84	ASN	CA-CB-CG	5.90	106.70	112.60	3	1
C	28	ALA	O-C-N	5.88	113.59	123.00	3	1
A	97	ARG	NH1-CZ-NH2	5.86	111.68	119.30	2	3
C	126	ASN	OD1-CG-ND2	5.85	116.75	122.60	3	1
B	7	ARG	NE-CZ-NH2	5.82	113.96	119.20	2	3
C	175	ASN	CA-CB-CG	5.81	118.41	112.60	2	1
YA	1	LBN	O1-P1-O2	5.80	110.84	93.45	3	2
B	49	ASP	CA-CB-CG	5.77	106.83	112.60	2	3

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
C	151	ARG	NH1-CZ-NH2	5.76	111.81	119.30	1	1
C	28	ALA	C-N-CA	5.75	132.04	121.70	3	1
W	1	LBN	O1-P1-O2	5.74	110.68	93.45	2	2
C	148	LEU	C-N-CA	5.73	132.02	121.70	2	1
C	38	LYS	O-C-N	5.73	113.83	123.00	2	1
UB	1	LBN	C9-O2-P1	5.73	134.76	117.58	3	1
C	117	ARG	C-N-CA	5.72	132.00	121.70	1	1
C	146	HIS	O-C-N	5.72	113.85	123.00	3	1
C	155	ILE	N-CA-CB	5.71	121.20	111.50	3	1
C	156	GLN	OE1-CD-NE2	5.69	116.91	122.60	3	1
C	99	ARG	O-C-N	5.68	113.91	123.00	2	1
C	179	ASN	CA-CB-CG	5.65	106.95	112.60	2	2
C	83	GLN	CB-CG-CD	5.64	122.19	112.60	1	1
A	56	GLU	C-N-CA	5.64	131.84	121.70	1	3
C	101	ASN	OD1-CG-ND2	5.63	116.97	122.60	3	1
C	75	ARG	O-C-N	5.63	114.00	123.00	3	1
C	124	PHE	CA-CB-CG	5.63	108.17	113.80	2	2
B	46	TYR	CA-CB-CG	5.62	124.01	113.90	3	3
C	20	ILE	C-N-CA	5.61	131.80	121.70	2	1
C	172	TRP	CB-CG-CD1	5.60	118.50	126.90	2	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 atomic models in this entry.

Model ID	Clash score	Number of clashes
1	0.00	0
2	0.00	0
3	0.00	0

There are no too-close contacts.

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	507	475	26	6
2	507	477	27	3
3	507	478	23	6

There are 8 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	89	PRO	3
B	109	GLY	3
B	166	THR	3
C	127	LYS	2
C	60	ASN	1
C	75	ARG	1
C	81	TYR	1
C	149	ARG	1

Torsion angles : Protein sidechains ?

In the following table, sidechain rotameric 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	445	350	59	36
2	445	354	53	38
3	445	349	60	36

There are 45 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	6	LEU	3
A	9	GLN	3
A	10	LEU	3
A	24	GLU	3
A	26	GLU	3
A	35	ASP	3
A	43	VAL	3
A	54	TRP	3
A	57	GLU	3
A	59	GLU	3
A	83	LEU	3
A	96	GLN	3
A	103	GLU	3
A	139	ARG	3
A	143	LEU	3
A	154	LEU	3
B	6	LEU	3

Chain	Res	Type	Models (Total)
B	9	GLN	3
B	10	LEU	3
B	24	GLU	3
B	35	ASP	3
B	43	VAL	3
B	59	GLU	3
B	83	LEU	3
B	93	GLU	3
B	96	GLN	3
B	103	GLU	3
B	113	LEU	3
B	126	THR	3
B	135	LEU	3
B	139	ARG	3
B	152	SER	3
C	176	GLN	2
C	4	ILE	1
C	8	LEU	1
C	23	VAL	1
C	45	THR	1
C	55	THR	1
C	73	LYS	1
C	82	PHE	1
C	86	GLN	1
C	92	VAL	1
C	140	THR	1
C	158	THR	1
C	180	GLN	1

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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