

Integrative Structure Validation Report ?

March 27, 2025 - 10:03 AM 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	9A1N
PDB-Dev ID	PDBDEV_00000095
Structure Title	Integrative model of the nuclear pore complex with intermediate diameter from energy depleted Schizosaccharomyces pombe
Structure Authors	Christian E. Zimmerli; Matteo Allegretti; Vasileios Rantos; Sara K. Goetz; Agnieszka Obarska-Kosinska; Ievgeniia Zagoriy; Aliaksandr Halavatyi; Gerhard Hummer; Julia Mahamid; Jan Kosinski; Martin Beck
Deposited on	2021-10-20

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

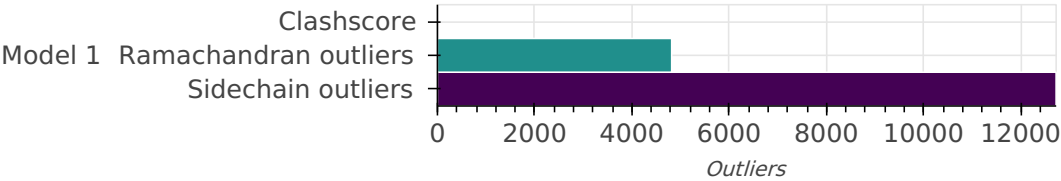
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 1 model(s). A total of 5 datasets were used to build this entry.

Representation ?

This entry has 1 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	10	Nup184	B	1564	1-1564	-	100.00 / 100.00	Atomic
				B1					
				B2					
				B3					
				B4					
				B5					
				B6					
				B7					
				B8					
				B9					
				B10					
				B11					
				B12					
				B13					
				B14					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				B15					
		11	Nup186	C	1647	1-1647	-	100.00 / 100.00	Atomic
				C1					
				C2					
				C3					
				C4					
				C5					
				C6					
				C7					
				C8					
				C9					
				C10					
				C11					
				C12					
				C13					
				C14					
				C15					
		12	Nup155	D	1315	1-1315	-	100.00 / 100.00	Atomic
				D1					
				D2					
				D3					
				D4					
				D5					
				D6					
				D7					
				D8					
				D9					
				D10					
				D11					
				D12					
				D13					
				D14					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				D15					
				D16					
				D17					
				D18					
				D19					
				D20					
				D21					
				D22					
				D23					
				D24					
				D25					
				D26					
				D27					
				D28					
				D29					
				D30					
				D31					
		15	Nup44	H	403	1-403	-	100.00 / 100.00	Atomic
				H1					
				H2					
				H3					
				H4					
				H5					
				H6					
				H7					
				H8					
				H9					
				H10					
				H11					
				H12					
				H13					
				H14					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				H15					
				H16					
				H17					
				H18					
				H19					
				H20					
				H21					
				H22					
				H23					
				H24					
				H25					
				H26					
				H27					
				H28					
				H29					
				H30					
				H31					
		16	Nup45	I	425	1-425	-	100.00 / 100.00	Atomic
				I1					
				I2					
				I3					
				I4					
				I5					
				I6					
				I7					
				I8					
				I9					
				I10					
				I11					
				I12					
				I13					
				I14					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				I15					
				I16					
				I17					
				I18					
				I19					
				I20					
				I21					
				I22					
				I23					
				I24					
				I25					
				I26					
				I27					
				I28					
				I29					
				I30					
				I31					
		14	Nsp1	J	598	1-598	-	100.00 / 100.00	Atomic
				J1					
				J2					
				J3					
				J4					
				J5					
				J6					
				J7					
				J8					
				J9					
				J10					
				J11					
				J12					
				J13					
				J14					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				J15					
				J16					
				J17					
				J18					
				J19					
				J20					
				J21					
				J22					
				J23					
				J24					
				J25					
				J26					
				J27					
				J28					
				J29					
				J30					
				J31					
		1	Nup107	L	813	1-813	-	100.00 / 100.00	Atomic
				L1					
				L2					
				L3					
				L4					
				L5					
				L6					
				L7					
				L8					
				L9					
				L10					
				L11					
				L12					
				L13					
				L14					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				L15					
		6	Nup189c	M	844	1-844	-	100.00 / 100.00	Atomic
				M1					
				M2					
				M3					
				M4					
				M5					
				M6					
				M7					
				M8					
				M9					
				M10					
				M11					
				M12					
				M13					
				M14					
				M15					
				M16					
				M17					
				M18					
				M19					
				M20					
				M21					
				M22					
				M23					
		8	Sec13	N	297	1-297	-	100.00 / 100.00	Atomic
				N1					
				N2					
				N3					
				N4					
				N5					
				N6					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				N7					
				N8					
				N9					
				N10					
				N11					
				N12					
				N13					
				N14					
				N15					
				N16					
				N17					
				N18					
				N19					
				N20					
				N21					
				N22					
				N23					
		7	Seh1	O	339	1-339	-	100.00 / 100.00	Atomic
				O1					
				O2					
				O3					
				O4					
				O5					
				O6					
				O7					
				O8					
				O9					
				O10					
				O11					
				O12					
				O13					
				O14					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				O15					
				O16					
				O17					
				O18					
				O19					
				O20					
				O21					
				O22					
				O23					
		2	Nup85	P	675	1-675	-	100.00 / 100.00	Atomic
				P1					
				P2					
				P3					
				P4					
				P5					
				P6					
				P7					
				P8					
				P9					
				P10					
				P11					
				P12					
				P13					
				P14					
				P15					
				P16					
				P17					
				P18					
				P19					
				P20					
				P21					
				P22					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				P23					
		5	Nup132	Q	1162	1-1162	-	100.00 / 100.00	Atomic
				Q1					
				Q2					
				Q3					
				Q4					
				Q5					
				Q6					
				Q7					
				Q8					
				Q9					
				Q10					
				Q11					
				Q12					
				Q13					
				Q14					
				Q15					
		3	Nup120	R	1136	1-1136	-	100.00 / 100.00	Atomic
				R1					
				R2					
				R3					
				R4					
				R5					
				R6					
				R7					
				R8					
				R9					
				R10					
				R11					
				R12					
				R13					
				R14					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				R15					
				R16					
				R17					
				R18					
				R19					
				R20					
				R21					
				R22					
				R23					
		4	Nup37	S	391	1-391	-	100.00 / 100.00	Atomic
				S1					
				S2					
				S3					
				S4					
				S5					
				S6					
				S7					
				S8					
				S9					
				S10					
				S11					
				S12					
				S13					
				S14					
				S15					
				S16					
				S17					
				S18					
				S19					
				S20					
				S21					
				S22					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				S23					
		9	Ely5	T	298	1-298	-	100.00 / 100.00	Atomic
				T1					
				T2					
				T3					
				T4					
				T5					
				T6					
				T7					
				T8					
				T9					
				T10					
				T11					
				T12					
				T13					
				T14					
				T15					
				T16					
				T17					
				T18					
				T19					
				T20					
				T21					
				T22					
				T23					
		13	Nup97	Y	851	1-851	-	100.00 / 100.00	Atomic
				Y1					
				Y2					
				Y3					
				Y4					
				Y5					
				Y6					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				Y7					
				Y8					
				Y9					
				Y10					
				Y11					
				Y12					
				Y13					
				Y14					
				Y15					
				Y16					
				Y17					
				Y18					
				Y19					
				Y20					
				Y21					
				Y22					
				Y23					
				Y24					
				Y25					
				Y26					
				Y27					
				Y28					
				Y29					
				Y30					
				Y31					

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	3DEM volume	EMDB	EMD-11374

ID	Dataset type	Database name	Data access code
2	3DEM volume	Zenodo	10.5281/zenodo.5585949
3	Integrative model	PDB	9A1M
4	Other	Not available	https://doi.org/10.1038/nsmb1194
5	Other	Not available	https://doi.org/10.1038/nature15381

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	Modeling the full nuclear pore complex at intermediate diameter based on the model of the nuclear pore complex with the normal diameter	Refinement optimization with Assemblin	None	None	False	False

There are 3 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	Assemblin	0.99beta	integrative model building	https://www.embl-hamburg.de/Assemblin/
2	Integrative Modeling Platform (IMP)	2.15.0	integrative model building	https://integrativemodeling.org
3	UCSF Chimera	1.14	rigid body fitting to EM maps	https://www.cgl.ucsf.edu/chimera/

Data quality ?

3DEM volume

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 19104 bond length outliers in this entry (0.99% of 1932384 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)
L5	206	ILE	C-N	113.27	2.91	1.33	1	1
L	206	ILE	C-N	113.26	2.91	1.33	1	1
L2	206	ILE	C-N	113.26	2.91	1.33	1	1
L3	206	ILE	C-N	113.26	2.91	1.33	1	1
L11	206	ILE	C-N	113.24	2.91	1.33	1	1
L10	206	ILE	C-N	113.23	2.91	1.33	1	1
L14	206	ILE	C-N	113.23	2.91	1.33	1	1
L7	206	ILE	C-N	113.23	2.91	1.33	1	1
L6	206	ILE	C-N	113.22	2.91	1.33	1	1
L4	206	ILE	C-N	113.20	2.91	1.33	1	1
L1	206	ILE	C-N	113.19	2.91	1.33	1	1
L8	206	ILE	C-N	113.19	2.91	1.33	1	1
L15	206	ILE	C-N	113.19	2.91	1.33	1	1
L13	206	ILE	C-N	113.18	2.91	1.33	1	1
L9	206	ILE	C-N	113.18	2.91	1.33	1	1
L12	206	ILE	C-N	113.17	2.91	1.33	1	1
L8	725	LEU	C-N	111.23	2.89	1.33	1	1
L9	725	LEU	C-N	111.23	2.89	1.33	1	1
L	725	LEU	C-N	111.22	2.89	1.33	1	1
L6	725	LEU	C-N	111.20	2.89	1.33	1	1
L5	725	LEU	C-N	111.19	2.89	1.33	1	1
L4	725	LEU	C-N	111.18	2.89	1.33	1	1
L14	725	LEU	C-N	111.18	2.89	1.33	1	1
L10	725	LEU	C-N	111.18	2.89	1.33	1	1
L7	725	LEU	C-N	111.17	2.89	1.33	1	1
L2	725	LEU	C-N	111.17	2.89	1.33	1	1
L13	725	LEU	C-N	111.17	2.89	1.33	1	1
L15	725	LEU	C-N	111.16	2.89	1.33	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
L11	725	LEU	C-N	111.16	2.89	1.33	1	1
L3	725	LEU	C-N	111.15	2.89	1.33	1	1
L1	725	LEU	C-N	111.15	2.89	1.33	1	1
L12	725	LEU	C-N	111.13	2.88	1.33	1	1
M17	475	ALA	C-N	108.55	2.85	1.33	1	1
M11	475	ALA	C-N	108.53	2.85	1.33	1	1
M21	475	ALA	C-N	108.52	2.85	1.33	1	1
M23	475	ALA	C-N	108.52	2.85	1.33	1	1
M20	475	ALA	C-N	108.52	2.85	1.33	1	1
M16	475	ALA	C-N	108.52	2.85	1.33	1	1
M22	475	ALA	C-N	108.52	2.85	1.33	1	1
M12	475	ALA	C-N	108.52	2.85	1.33	1	1
M10	475	ALA	C-N	108.52	2.85	1.33	1	1
M19	475	ALA	C-N	108.51	2.85	1.33	1	1
M18	475	ALA	C-N	108.51	2.85	1.33	1	1
M13	475	ALA	C-N	108.51	2.85	1.33	1	1
M1	475	ALA	C-N	108.51	2.85	1.33	1	1
M9	475	ALA	C-N	108.49	2.85	1.33	1	1
M14	475	ALA	C-N	108.47	2.85	1.33	1	1
M15	475	ALA	C-N	108.46	2.85	1.33	1	1
M7	475	ALA	C-N	108.46	2.85	1.33	1	1
M6	475	ALA	C-N	108.45	2.85	1.33	1	1
M8	475	ALA	C-N	108.45	2.85	1.33	1	1
M5	475	ALA	C-N	108.45	2.85	1.33	1	1
M2	475	ALA	C-N	108.44	2.85	1.33	1	1
M	475	ALA	C-N	108.43	2.85	1.33	1	1
M3	475	ALA	C-N	108.43	2.85	1.33	1	1
M4	475	ALA	C-N	108.42	2.85	1.33	1	1
Q4	91	GLN	C-N	107.04	2.83	1.33	1	1
Q3	91	GLN	C-N	107.04	2.83	1.33	1	1
Q	91	GLN	C-N	107.02	2.83	1.33	1	1
Q1	91	GLN	C-N	107.02	2.83	1.33	1	1
Q7	91	GLN	C-N	107.02	2.83	1.33	1	1
Q5	91	GLN	C-N	107.02	2.83	1.33	1	1
Q9	91	GLN	C-N	107.00	2.83	1.33	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
Q2	91	GLN	C-N	106.99	2.83	1.33	1	1
Q14	91	GLN	C-N	106.98	2.83	1.33	1	1
Q6	91	GLN	C-N	106.96	2.83	1.33	1	1
Q13	91	GLN	C-N	106.94	2.83	1.33	1	1
Q15	91	GLN	C-N	106.94	2.83	1.33	1	1
Q12	91	GLN	C-N	106.93	2.83	1.33	1	1
Q10	91	GLN	C-N	106.93	2.83	1.33	1	1
Q8	91	GLN	C-N	106.93	2.83	1.33	1	1
Q11	91	GLN	C-N	106.89	2.83	1.33	1	1
P8	342	CYS	C-N	106.72	2.82	1.33	1	1
P11	342	CYS	C-N	106.72	2.82	1.33	1	1
M10	354	PRO	C-N	106.71	2.82	1.33	1	1
P14	342	CYS	C-N	106.71	2.82	1.33	1	1
P12	342	CYS	C-N	106.68	2.82	1.33	1	1
P10	342	CYS	C-N	106.68	2.82	1.33	1	1
P6	342	CYS	C-N	106.68	2.82	1.33	1	1
P4	342	CYS	C-N	106.68	2.82	1.33	1	1
P3	342	CYS	C-N	106.67	2.82	1.33	1	1
P13	342	CYS	C-N	106.67	2.82	1.33	1	1
P15	342	CYS	C-N	106.67	2.82	1.33	1	1
P9	342	CYS	C-N	106.67	2.82	1.33	1	1
M12	354	PRO	C-N	106.67	2.82	1.33	1	1
M13	354	PRO	C-N	106.66	2.82	1.33	1	1
P17	342	CYS	C-N	106.65	2.82	1.33	1	1
M	354	PRO	C-N	106.65	2.82	1.33	1	1
P23	342	CYS	C-N	106.65	2.82	1.33	1	1
M15	354	PRO	C-N	106.65	2.82	1.33	1	1
P1	342	CYS	C-N	106.64	2.82	1.33	1	1
P20	342	CYS	C-N	106.64	2.82	1.33	1	1
P22	342	CYS	C-N	106.64	2.82	1.33	1	1
P	342	CYS	C-N	106.64	2.82	1.33	1	1
M14	354	PRO	C-N	106.64	2.82	1.33	1	1
M8	354	PRO	C-N	106.64	2.82	1.33	1	1
M9	354	PRO	C-N	106.63	2.82	1.33	1	1
P19	342	CYS	C-N	106.63	2.82	1.33	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
M2	354	PRO	C-N	106.63	2.82	1.33	1	1
M4	354	PRO	C-N	106.63	2.82	1.33	1	1

Standard geometry: angle outliers ?

There are 76991 bond angle outliers in this entry (2.94% of 2619928 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)
B13	777	PHE	CD2-CE2-CZ	58.30	15.06	120.00	1	1
B14	777	PHE	CD2-CE2-CZ	58.30	15.07	120.00	1	1
B8	777	PHE	CD2-CE2-CZ	58.29	15.07	120.00	1	1
B11	777	PHE	CD2-CE2-CZ	58.29	15.07	120.00	1	1
B10	777	PHE	CD2-CE2-CZ	58.29	15.07	120.00	1	1
B15	777	PHE	CD2-CE2-CZ	58.29	15.08	120.00	1	1
B12	777	PHE	CD2-CE2-CZ	58.29	15.09	120.00	1	1
B9	777	PHE	CD2-CE2-CZ	58.27	15.12	120.00	1	1
B3	777	PHE	CD2-CE2-CZ	58.25	15.15	120.00	1	1
B	777	PHE	CD2-CE2-CZ	58.24	15.17	120.00	1	1
B1	777	PHE	CD2-CE2-CZ	58.24	15.18	120.00	1	1
B5	777	PHE	CD2-CE2-CZ	58.22	15.20	120.00	1	1
B4	777	PHE	CD2-CE2-CZ	58.22	15.20	120.00	1	1
B2	777	PHE	CD2-CE2-CZ	58.22	15.20	120.00	1	1
B6	777	PHE	CD2-CE2-CZ	58.22	15.21	120.00	1	1
B7	777	PHE	CD2-CE2-CZ	58.22	15.21	120.00	1	1
D14	231	PHE	CG-CD1-CE1	53.97	28.95	120.70	1	1
D16	231	PHE	CG-CD1-CE1	53.96	28.96	120.70	1	1
D17	231	PHE	CG-CD1-CE1	53.96	28.97	120.70	1	1
D18	231	PHE	CG-CD1-CE1	53.96	28.97	120.70	1	1
D22	231	PHE	CG-CD1-CE1	53.95	28.98	120.70	1	1
D20	231	PHE	CG-CD1-CE1	53.95	28.98	120.70	1	1
D19	231	PHE	CG-CD1-CE1	53.95	28.99	120.70	1	1
D13	231	PHE	CG-CD1-CE1	53.95	28.99	120.70	1	1
D15	231	PHE	CG-CD1-CE1	53.95	28.99	120.70	1	1
D11	231	PHE	CG-CD1-CE1	53.95	28.99	120.70	1	1
D9	231	PHE	CG-CD1-CE1	53.95	28.99	120.70	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
D21	231	PHE	CG-CD1-CE1	53.95	28.99	120.70	1	1
D12	231	PHE	CG-CD1-CE1	53.95	28.99	120.70	1	1
D23	231	PHE	CG-CD1-CE1	53.94	29.00	120.70	1	1
D	231	PHE	CG-CD1-CE1	53.94	29.00	120.70	1	1
D27	231	PHE	CG-CD1-CE1	53.94	29.00	120.70	1	1
D26	231	PHE	CG-CD1-CE1	53.94	29.00	120.70	1	1
D8	231	PHE	CG-CD1-CE1	53.94	29.00	120.70	1	1
D10	231	PHE	CG-CD1-CE1	53.94	29.00	120.70	1	1
D30	231	PHE	CG-CD1-CE1	53.94	29.01	120.70	1	1
D3	231	PHE	CG-CD1-CE1	53.93	29.01	120.70	1	1
D5	231	PHE	CG-CD1-CE1	53.93	29.01	120.70	1	1
D7	231	PHE	CG-CD1-CE1	53.93	29.01	120.70	1	1
D1	231	PHE	CG-CD1-CE1	53.93	29.01	120.70	1	1
D6	231	PHE	CG-CD1-CE1	53.93	29.02	120.70	1	1
D28	231	PHE	CG-CD1-CE1	53.93	29.02	120.70	1	1
D4	231	PHE	CG-CD1-CE1	53.92	29.03	120.70	1	1
D2	231	PHE	CG-CD1-CE1	53.92	29.03	120.70	1	1
D31	231	PHE	CG-CD1-CE1	53.92	29.03	120.70	1	1
D29	231	PHE	CG-CD1-CE1	53.92	29.04	120.70	1	1
D24	231	PHE	CG-CD1-CE1	53.92	29.04	120.70	1	1
D25	231	PHE	CG-CD1-CE1	53.91	29.05	120.70	1	1
D30	985	TYR	CB-CG-CD2	48.65	47.82	120.80	1	1
D28	985	TYR	CB-CG-CD2	48.63	47.85	120.80	1	1
D10	985	TYR	CB-CG-CD2	48.63	47.85	120.80	1	1
D29	985	TYR	CB-CG-CD2	48.63	47.86	120.80	1	1
D26	985	TYR	CB-CG-CD2	48.62	47.86	120.80	1	1
D27	985	TYR	CB-CG-CD2	48.62	47.88	120.80	1	1
D25	985	TYR	CB-CG-CD2	48.61	47.88	120.80	1	1
D11	985	TYR	CB-CG-CD2	48.61	47.88	120.80	1	1
D15	985	TYR	CB-CG-CD2	48.61	47.88	120.80	1	1
D9	985	TYR	CB-CG-CD2	48.61	47.88	120.80	1	1
D14	985	TYR	CB-CG-CD2	48.61	47.88	120.80	1	1
D31	985	TYR	CB-CG-CD2	48.61	47.88	120.80	1	1
D23	985	TYR	CB-CG-CD2	48.61	47.89	120.80	1	1
D21	985	TYR	CB-CG-CD2	48.61	47.89	120.80	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
D24	985	TYR	CB-CG-CD2	48.61	47.89	120.80	1	1
D17	985	TYR	CB-CG-CD2	48.60	47.90	120.80	1	1
D16	985	TYR	CB-CG-CD2	48.60	47.90	120.80	1	1
D22	985	TYR	CB-CG-CD2	48.60	47.90	120.80	1	1
D13	985	TYR	CB-CG-CD2	48.60	47.91	120.80	1	1
D19	985	TYR	CB-CG-CD2	48.59	47.91	120.80	1	1
D7	985	TYR	CB-CG-CD2	48.59	47.91	120.80	1	1
D1	985	TYR	CB-CG-CD2	48.59	47.91	120.80	1	1
D8	985	TYR	CB-CG-CD2	48.59	47.92	120.80	1	1
D12	985	TYR	CB-CG-CD2	48.59	47.92	120.80	1	1
D	985	TYR	CB-CG-CD2	48.58	47.93	120.80	1	1
D6	985	TYR	CB-CG-CD2	48.57	47.94	120.80	1	1
D18	985	TYR	CB-CG-CD2	48.57	47.94	120.80	1	1
D20	985	TYR	CB-CG-CD2	48.57	47.94	120.80	1	1
D4	985	TYR	CB-CG-CD2	48.57	47.94	120.80	1	1
D2	985	TYR	CB-CG-CD2	48.55	47.97	120.80	1	1
D5	985	TYR	CB-CG-CD2	48.55	47.97	120.80	1	1
D3	985	TYR	CB-CG-CD2	48.54	47.99	120.80	1	1
D30	231	PHE	CD1-CG-CD2	48.45	45.93	118.60	1	1
D25	231	PHE	CD1-CG-CD2	48.44	45.93	118.60	1	1
D31	231	PHE	CD1-CG-CD2	48.43	45.95	118.60	1	1
D27	231	PHE	CD1-CG-CD2	48.43	45.95	118.60	1	1
D28	231	PHE	CD1-CG-CD2	48.43	45.96	118.60	1	1
D24	231	PHE	CD1-CG-CD2	48.43	45.96	118.60	1	1
D	231	PHE	CD1-CG-CD2	48.42	45.97	118.60	1	1
D26	231	PHE	CD1-CG-CD2	48.42	45.98	118.60	1	1
D29	231	PHE	CD1-CG-CD2	48.41	45.98	118.60	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
D6	231	PHE	CD1-CG-CD2	48.41	45.99	118.60	1	1
D3	231	PHE	CD1-CG-CD2	48.40	45.99	118.60	1	1
D7	231	PHE	CD1-CG-CD2	48.40	45.99	118.60	1	1
D2	231	PHE	CD1-CG-CD2	48.40	46.00	118.60	1	1
D4	231	PHE	CD1-CG-CD2	48.40	46.00	118.60	1	1
D5	231	PHE	CD1-CG-CD2	48.40	46.01	118.60	1	1
D1	231	PHE	CD1-CG-CD2	48.40	46.01	118.60	1	1
D19	231	PHE	CD1-CG-CD2	48.39	46.01	118.60	1	1
D18	231	PHE	CD1-CG-CD2	48.39	46.02	118.60	1	1
D16	231	PHE	CD1-CG-CD2	48.38	46.03	118.60	1	1
D23	231	PHE	CD1-CG-CD2	48.38	46.03	118.60	1	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

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	231448	214476	12154	4818

There are 4818 unique backbone outliers. Detailed list of outliers are tabulated below. The output is limited to 100 rows.

Chain	Res	Type	Models (Total)
B	2	GLY	1
B	32	ASP	1
B	110	SER	1
B	173	ALA	1
B	174	GLN	1
B	198	PRO	1
B	200	SER	1
B	201	LEU	1
B	203	PHE	1
B	235	VAL	1
B	264	ASP	1
B	299	ASN	1
B	300	PRO	1
B	302	PHE	1
B	360	ILE	1
B	442	ASP	1
B	474	THR	1
B	495	SER	1
B	505	GLU	1
B	510	GLY	1
B	546	SER	1
B	547	VAL	1
B	548	ASP	1
B	549	THR	1
B	579	ILE	1
B	638	ILE	1
B	639	GLU	1
B	675	VAL	1
B	721	PRO	1
B	789	ASN	1
B	833	ILE	1
B	836	THR	1
B	869	LYS	1
B	871	SER	1
B	922	ILE	1

Chain	Res	Type	Models (Total)
B	939	PRO	1
B	995	LEU	1
B	1008	ILE	1
B	1059	GLY	1
B	1104	ASP	1
B	1110	VAL	1
B	1123	ILE	1
B	1264	ILE	1
B	1291	SER	1
B	1314	LEU	1
B	1315	ASN	1
B	1317	LEU	1
B	1332	VAL	1
B	1348	GLU	1
B	1350	ALA	1
B	1353	ASN	1
B	1410	VAL	1
B	1430	SER	1
B	1431	PRO	1
B	1491	ILE	1
B	1516	PRO	1
B	1518	SER	1
B1	2	GLY	1
B1	32	ASP	1
B1	110	SER	1
B1	173	ALA	1
B1	174	GLN	1
B1	198	PRO	1
B1	200	SER	1
B1	201	LEU	1
B1	203	PHE	1
B1	235	VAL	1
B1	264	ASP	1
B1	299	ASN	1
B1	300	PRO	1

Chain	Res	Type	Models (Total)
B1	302	PHE	1
B1	360	ILE	1
B1	442	ASP	1
B1	474	THR	1
B1	495	SER	1
B1	505	GLU	1
B1	510	GLY	1
B1	546	SER	1
B1	547	VAL	1
B1	548	ASP	1
B1	549	THR	1
B1	579	ILE	1
B1	638	ILE	1
B1	639	GLU	1
B1	675	VAL	1
B1	721	PRO	1
B1	789	ASN	1
B1	833	ILE	1
B1	836	THR	1
B1	869	LYS	1
B1	871	SER	1
B1	922	ILE	1
B1	939	PRO	1
B1	995	LEU	1
B1	1008	ILE	1
B1	1059	GLY	1
B1	1104	ASP	1
B1	1110	VAL	1
B1	1123	ILE	1
B1	1264	ILE	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	213160	181318	19117	12725

There are 12725 unique sidechain outliers. Detailed list of outliers are tabulated below. The output is limited to 100 rows.

Chain	Res	Type	Models (Total)
B	12	LEU	1
B	82	ILE	1
B	98	LEU	1
B	135	LYS	1
B	153	LYS	1
B	154	MET	1
B	216	HIS	1
B	238	ASN	1
B	273	LYS	1
B	275	ILE	1
B	281	ILE	1
B	284	ILE	1
B	363	ASN	1
B	365	GLN	1
B	387	ILE	1
B	403	ILE	1
B	416	LYS	1
B	466	LEU	1
B	502	ILE	1
B	520	LEU	1
B	536	LEU	1
B	558	LEU	1
B	572	TYR	1
B	625	ILE	1
B	633	LEU	1
B	655	GLU	1
B	662	THR	1
B	713	ASN	1
B	791	LYS	1
B	802	ILE	1
B	857	LYS	1
B	868	LEU	1
B	888	LEU	1

Chain	Res	Type	Models (Total)
B	909	PRO	1
B	927	ILE	1
B	966	VAL	1
B	978	ARG	1
B	1011	ILE	1
B	1016	PRO	1
B	1049	ILE	1
B	1076	THR	1
B	1096	LYS	1
B	1099	ILE	1
B	1101	PRO	1
B	1107	LYS	1
B	1140	ILE	1
B	1151	LEU	1
B	1177	LYS	1
B	1205	ILE	1
B	1224	LYS	1
B	1238	ILE	1
B	1297	ASN	1
B	1300	MET	1
B	1346	LEU	1
B	1384	LEU	1
B	1448	GLU	1
B	1455	LEU	1
B	1473	ILE	1
B	1496	ARG	1
B	1522	LEU	1
B	1554	LEU	1
B1	12	LEU	1
B1	82	ILE	1
B1	98	LEU	1
B1	135	LYS	1
B1	153	LYS	1
B1	154	MET	1
B1	216	HIS	1

Chain	Res	Type	Models (Total)
B1	238	ASN	1
B1	273	LYS	1
B1	275	ILE	1
B1	281	ILE	1
B1	284	ILE	1
B1	363	ASN	1
B1	365	GLN	1
B1	387	ILE	1
B1	403	ILE	1
B1	416	LYS	1
B1	466	LEU	1
B1	502	ILE	1
B1	520	LEU	1
B1	536	LEU	1
B1	558	LEU	1
B1	572	TYR	1
B1	625	ILE	1
B1	633	LEU	1
B1	655	GLU	1
B1	662	THR	1
B1	713	ASN	1
B1	791	LYS	1
B1	802	ILE	1
B1	857	LYS	1
B1	868	LEU	1
B1	888	LEU	1
B1	909	PRO	1
B1	927	ILE	1
B1	966	VAL	1
B1	978	ARG	1
B1	1011	ILE	1
B1	1016	PRO	1

Fit of model to data used for modeling ?

3DEM volume

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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