

Integrative Structure Validation Report

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

IHMValidation Version 3.2

Python-IHM Version 2.9

MolProbity Version 4.5.2

PDB ID	9AAB pdb_00009aab
Structure Title	The integrative model of the TRV026-stabilized conformation of AT1R was obtained from experimental DEER distance restraints using a protocol combining AlphaLink, AlphaFold2-Multimer, and short unbiased molecular dynamics simulations in GROMACS.
Structure Authors	Belyaeva, J.; Elgeti, M.
Deposited on	2025-12-16

This is a PDB-IHM Structure Validation Report.

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](#).

1. Overview

1.1. Summary

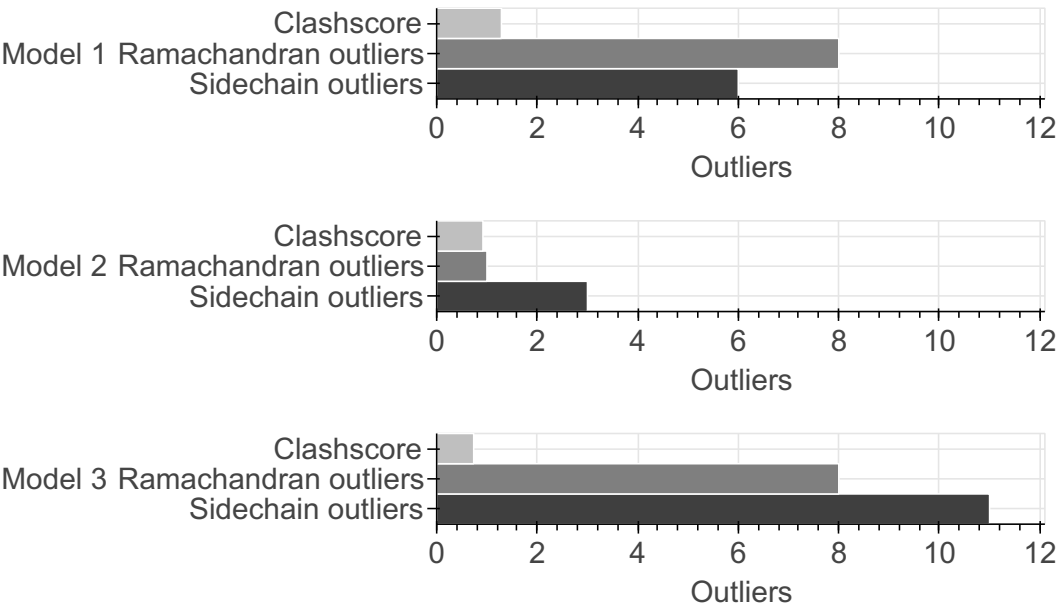
This entry consists of 3 model(s). A total of 4 dataset(s) were used to build this entry.

Name	Type	Count
EPR data	Experimental data	2
Experimental model	Starting model	2

1.2. 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 ?



2. Model Details ?

2.1. Ensemble information ?

This entry consists of 0 distinct ensemble(s).

2.2. 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	1-3	1	Type-1 angiotensin II receptor	A	319	-	1-319	100.00 / 100.00	Atomic
		2	TRV026, beta-arrestin biased peptide	B	8	-	1-8	100.00 / 100.00	Atomic

2.3. Datasets used for modeling ?

There are 4 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	EPR data	Zenodo	10.5281/zenodo.20259483
2	EPR data	Zenodo	10.5281/zenodo.20259483
3	Experimental model	PDB	pdb_00004yay

ID	Dataset type	Database name	Data access code
4	Experimental model	PDB	pdb_00006os2

2.4. 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	Sampling	AlphaLink	AlphaLink builds AT1R models using ten experimental DEER restraints and the AT1R sequence. A total of 2000 models were generated: 1000 with -Neff 5 and 1000 with -Neff 10.	2000	False	False
2	1	Filtering	Filtering: adequacy of models	AlphaLink models were filtered based on per-helix RMSD relative to inactive (PDB: 4YAY) and active (PDB: 6OS2) experimental AT1R structures. Each model was aligned to both references using backbone heavy atoms of TM1-TM7, and RMSD was computed separately for all seven helices. Models were discarded if any TM helix exceeded 4.5 Å RMSD from both reference states, ensuring removal of distorted conformations.	1734	False	False
3	1	Clustering	Clustering of AlphaLink models	AlphaLink models were clustered using three non-correlated Ca-Ca distances: F1.59(55)-R34.56(139), F1.59(55)-D6.31(236), and F1.59(55)-R8.52(311). Clustering was performed with GaussianMixture model, and one representative structure was selected from each cluster.	8	False	False
4	1	Sampling	AlphaFold2-Multimer	AlphaFold2-Multimer (ColabFold version) was used to place TRV026 onto each representative AlphaLink model. Each AlphaFold2-Multimer run used the AlphaLink representative as the main receptor template and the experimental AT1R-TRV026 structure (PDB: 6OS2) as a hypothesis for the peptide pose.	8	False	False
5	1	Sampling	MD simulations in GROMACS	Molecular dynamics simulations were performed in GROMACS. 80 trajectories total, each 500 ns long: 8 systems 5 replicas 2 D3.49(125) protonation variants. Details are available in the manuscript.	80	False	False

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
6	1	Filtering	RMSD-based filtering: ligand and receptor stability	RMSD-based filtering was applied to ensure (i) stability of the AT1R-TRV026 complex and (ii) absence of rapid, non-physical conformational changes in the receptor. Ligand stability: TRV026 heavy-atom RMSD between consecutive frames ≤ 2.0 in at least 95% of frames. Receptor stability: maximum absolute RMSD change of TM6 intracellular part (D6.31-W6.48) within any 50-ns window ≤ 2.0 . Equilibration period was identified using PELT changepoint detection, capped at 75 ns. 39 trajectories passed both filters.	39	False	False
7	1	Analysis	Identification of plateau regions in TM1-TM6 distance	For the 39 filtered trajectories, we identified plateau regions where TM6 adopted stable conformations. DEER distance distributions were simulated for each frame using Off-Rotamer Sampling (chiLife library, V1 spin label, 5000 iterations). Plateaus were identified from TM1-TM6 peak distance time series: smoothed with 25-frame rolling average, local slope calculated over 50-frame windows, slopes $<$ threshold classified as plateaus. Plateaus classified as inactive-like (≤ 32.7 Å), intermediate-like (32.7-38.3 Å), or active-like (≥ 38.3 Å) based on experimental TM1-TM6 distance.	39	False	False
8	1	Analysis	Computing AT1R-TRV026 interactions	Receptor-ligand interactions, hydrogen bonds, salt bridges and pi- or T-stacking, were identified in each frame of the 39 filtered trajectories using MDAnalysis.	39	False	False
9	1	Clustering	Clustering of interactions into binding modes	Interactions were classified as scaffold (constant frequency) or BM-defining (concentrated in specific intervals). Time-lagged Independent Component Analysis (TICA) was applied to reduce dimensionality. K-means clustering (scikit-learn) was performed on TICA-transformed coordinates. Binding mode segments were defined as continuous stretches. Similar BMs were merged using hierarchical clustering. As a result, we obtained 76 binding modes.	76	False	False
10	1	Classification	Classification of binding modes by TM6 conformation	TM6 conformation (inactive/intermediate/active) was assigned to each BM by overlapping with plateau regions. The procedure resulted in seven inactive-like, nine intermediate-like, and 60 active-like BMs. Nine intermediate BMs (INTs) were selected for linear combination analysis.	9	False	False

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
11	1	Validation	Linear combination analysis of intermediate binding modes	For each of the nine intermediate BMs, representative DEER distributions were obtained by averaging over a subset of frames. The optimal percentage (8%) was selected using five-fold leave-one-out cross-validation (LOO-CV). Linear combination coefficients were fitted using SLSQP optimizer (SciPy) with non-negative constraint, sum-to-one constraint, constant offset term. Coefficient uncertainties were estimated by bootstrapping (500 iterations). Final model retained three INTs: INT_2_p, INT_3_p, INT_4_d, representative structures of which were added to the current model.	3	False	False

There are 4 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	AlphaLink	1.00	sampling	https://github.com/lhatsk/AlphaLink
2	AlphaFold2-Multimer	3	sampling	https://colab.research.google.com/github/sokrypton/ColabFold/blob/main/AlphaFold2.ipynb
3	GROMACS	2023	sampling	https://www.gromacs.org/
4	LongDistances	590	data analysis	https://sites.google.com/site/altenbach/labview-programs/epr-programs/long-distances

3. Data quality ?

3.4. EPR ?

Validation for this section is under development.

4. 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.

4.1b. MolProbity Analysis ?

Excluded volume satisfaction for the models in the entry are listed below. The Analysed column shows the number of particle-particle or particle-atom pairs for which excluded volume was analysed.

Standard geometry: bond outliers ?

There are 247 bond length outliers in this entry (3.01% of 8196 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)
A	74	ASP	CG-OD1	9.31	1.37	1.19	3	1
A	125	ASP	CG-OD1	8.80	1.36	1.19	3	2
A	131	VAL	C-N	7.88	1.44	1.33	2	1
A	289	CYS	C-N	7.36	1.43	1.33	1	1
A	266	ILE	C-N	6.91	1.43	1.33	3	1
A	188	ASN	C-N	6.85	1.42	1.33	1	2
A	132	HIS	C-N	6.84	1.45	1.34	3	1
A	101	CYS	CA-CB	6.75	1.66	1.53	2	1
A	125	ASP	CG-OD2	6.68	1.20	1.33	3	2
A	146	LYS	C-N	6.62	1.42	1.33	1	2
A	307	LYS	CA-C	6.60	1.66	1.52	3	1
A	306	GLY	CA-C	6.59	1.40	1.52	3	1
A	219	TRP	C-N	6.56	1.42	1.33	1	1
A	160	SER	C-N	6.47	1.42	1.33	2	1
A	252	SER	C-N	6.39	1.42	1.33	1	1
A	3	LEU	C-N	6.34	1.42	1.33	2	1
B	6	HIS	CE1-NE2	6.21	1.38	1.32	1	2
A	191	LEU	CB-CG	6.12	1.65	1.53	1	1
B	6	HIS	CG-CD2	6.10	1.29	1.35	2	1
A	248	PHE	CA-CB	6.09	1.65	1.53	2	1
A	272	ARG	CD-NE	6.09	1.54	1.46	3	1
A	23	ARG	CZ-NH2	6.09	1.25	1.33	2	1
B	3	VAL	C-N	6.06	1.41	1.33	2	2
A	96	PHE	CG-CD2	6.04	1.51	1.38	2	1
A	272	ARG	CA-CB	6.03	1.65	1.53	2	1
A	173	GLU	C-N	6.00	1.41	1.33	1	1
A	247	LEU	C-N	5.87	1.41	1.33	1	1
A	39	PHE	CA-CB	5.86	1.65	1.53	2	1
A	207	PRO	N-CD	5.84	1.55	1.47	1	1
A	166	HIS	CD2-NE2	5.83	1.44	1.37	3	2
A	195	LEU	C-N	5.82	1.41	1.33	1	2
A	83	LEU	C-N	5.81	1.41	1.33	1	1
A	73	ALA	C-N	5.79	1.41	1.33	3	3
A	4	ASN	C-N	5.77	1.41	1.33	3	1
A	113	TYR	CZ-OH	5.75	1.50	1.38	2	1
A	8	GLU	C-N	5.75	1.41	1.33	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	298	ASN	C-N	5.73	1.43	1.34	3	1
A	204	PHE	CG-CD1	5.72	1.50	1.38	1	1
A	273	ASP	C-N	5.64	1.41	1.33	3	1
A	256	HIS	ND1-CE1	5.63	1.38	1.32	2	1
A	94	TRP	NE1-CE2	5.57	1.31	1.37	2	1
A	225	ALA	CA-C	5.56	1.64	1.52	1	1
A	26	TYR	CA-CB	5.56	1.64	1.53	1	1
A	24	HIS	CE1-NE2	5.55	1.38	1.32	2	1
A	236	ASP	C-N	5.55	1.41	1.33	3	1
A	282	THR	C-N	5.53	1.41	1.33	3	1
A	292	TYR	CZ-OH	5.51	1.49	1.38	1	1
A	143	LEU	C-N	5.46	1.41	1.33	3	2
A	46	ASN	CA-C	5.44	1.64	1.52	1	1
A	285	PRO	CA-CB	5.43	1.64	1.53	3	1
A	308	LYS	CA-CB	5.43	1.64	1.53	1	1
A	264	VAL	C-N	5.40	1.40	1.33	2	1
A	118	LEU	CA-C	5.34	1.64	1.52	1	1
A	58	LYS	C-N	5.33	1.40	1.33	3	1
A	20	LYS	C-N	5.33	1.40	1.33	1	1
A	137	ARG	NE-CZ	5.32	1.38	1.33	1	1
A	302	TYR	CA-CB	5.32	1.64	1.53	1	1
A	120	THR	CB-OG1	5.30	1.52	1.43	2	1
A	209	LEU	C-N	5.30	1.40	1.33	3	1
A	110	PHE	C-N	5.29	1.40	1.33	1	1
A	204	PHE	CA-CB	5.26	1.64	1.53	1	1
A	83	LEU	CA-CB	5.26	1.64	1.53	2	1
A	84	TRP	CZ2-CH2	5.25	1.47	1.37	1	1
A	95	PRO	CA-CB	5.24	1.63	1.53	3	1
B	4	TYR	C-N	5.24	1.40	1.33	1	1
A	166	HIS	ND1-CE1	5.21	1.37	1.32	2	3
A	273	ASP	N-CA	5.20	1.56	1.46	1	1
A	23	ARG	C-N	5.17	1.40	1.33	2	2
A	206	PHE	C-N	5.16	1.26	1.34	2	1
A	139	ARG	CZ-NH2	5.14	1.26	1.33	3	1
A	140	ARG	CD-NE	5.13	1.53	1.46	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	284	MET	CA-CB	5.05	1.63	1.53	2	1
A	314	LEU	C-N	5.05	1.40	1.33	3	1
A	277	ALA	C-N	5.04	1.40	1.33	1	1
A	113	TYR	C-N	5.04	1.40	1.33	2	1
A	17	ASP	CA-CB	5.04	1.63	1.53	2	1
A	41	VAL	C-N	5.02	1.40	1.33	1	1
B	1	SAR	N-CN	5.01	1.54	1.44	2	1
A	82	PRO	C-N	5.01	1.40	1.33	1	1
A	65	VAL	CA-C	4.99	1.42	1.52	3	1
A	253	TRP	NE1-CE2	4.98	1.32	1.37	3	1
A	132	HIS	CG-ND1	4.95	1.43	1.38	1	2
A	26	TYR	C-N	4.95	1.40	1.33	2	1
A	141	THR	C-N	4.93	1.40	1.33	2	1
A	23	ARG	CZ-NH1	4.93	1.25	1.32	3	1
A	118	LEU	CA-CB	4.90	1.63	1.53	1	1
A	234	ARG	CZ-NH2	4.89	1.27	1.33	2	1
A	194	GLY	N-CA	4.88	1.37	1.45	2	1
A	199	LYS	C-N	4.88	1.40	1.33	1	1
A	312	TYR	C-N	4.87	1.40	1.33	3	1
A	7	THR	CA-C	4.86	1.42	1.52	2	1
A	234	ARG	CD-NE	4.85	1.53	1.46	3	1
A	309	PHE	C-N	4.84	1.40	1.33	2	1
A	44	PHE	CA-CB	4.82	1.63	1.53	1	2
A	86	VAL	C-N	4.81	1.40	1.33	1	1
A	245	ILE	C-N	4.81	1.40	1.33	2	1
A	263	ASP	CA-CB	4.79	1.63	1.53	2	1
A	79	LEU	N-CA	4.78	1.55	1.46	3	1
A	163	ALA	C-N	4.78	1.40	1.33	1	1
A	171	PHE	CG-CD1	4.76	1.48	1.38	1	1

Standard geometry: angle outliers ?

There are 543 bond angle outliers in this entry (4.87% of 11139 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)
A	170	PHE	CA-CB-CG	11.33	125.13	113.80	2	2
B	2	ARG	NE-CZ-NH1	10.67	132.17	121.50	3	3

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	46	ASN	CA-CB-CG	9.88	102.72	112.60	3	1
A	200	ASN	CA-CB-CG	8.59	121.19	112.60	2	2
A	191	LEU	CA-C-N	8.37	129.46	116.90	2	3
A	188	ASN	OD1-CG-ND2	8.32	114.28	122.60	1	2
A	273	ASP	CA-CB-CG	8.12	120.72	112.60	1	2
A	174	ASN	CA-CB-CG	8.02	104.58	112.60	1	2
A	248	PHE	CA-CB-CG	7.96	121.76	113.80	3	2
A	236	ASP	CA-CB-CG	7.95	120.55	112.60	1	1
A	311	ARG	NH1-CZ-NH2	7.90	109.03	119.30	2	1
B	6	HIS	ND1-CG-CD2	7.88	113.98	106.10	1	2
A	156	ALA	N-CA-CB	7.83	98.66	110.40	3	1
A	139	ARG	CD-NE-CZ	7.78	135.30	124.40	3	1
A	275	ARG	NE-CZ-NH2	7.69	112.28	119.20	3	2
A	110	PHE	CA-CB-CG	7.56	121.36	113.80	1	3
A	55	PHE	CA-CB-CG	7.49	106.31	113.80	3	2
A	206	PHE	CA-CB-CG	7.46	121.26	113.80	1	3
A	25	ASN	OD1-CG-ND2	7.46	115.14	122.60	2	2
A	208	PHE	CA-CB-CG	7.44	121.24	113.80	3	1
A	74	ASP	CA-CB-CG	7.37	105.23	112.60	2	2
A	126	ARG	CA-CB-CG	7.36	128.81	114.10	1	1
A	183	HIS	ND1-CE1-NE2	7.17	115.57	108.40	3	2
A	31	ILE	CA-C-N	7.11	127.56	116.90	3	3
A	91	GLU	N-CA-CB	7.05	122.48	110.50	3	2
A	175	THR	CA-CB-OG1	7.04	120.16	109.60	3	1
A	259	PHE	CA-CB-CG	7.03	106.77	113.80	3	2
A	295	ASN	CA-CB-CG	6.97	119.57	112.60	3	3
A	187	GLN	OE1-CD-NE2	6.93	129.53	122.60	2	1
A	148	THR	CA-CB-CG2	6.87	122.18	110.50	2	1
A	93	ARG	NE-CZ-NH1	6.85	128.35	121.50	3	2
A	132	HIS	CA-CB-CG	6.85	106.95	113.80	3	2
A	254	ILE	CA-C-N	6.83	127.14	116.90	1	2
A	106	ALA	N-CA-CB	6.81	100.19	110.40	2	2
A	137	ARG	NE-CZ-NH2	6.72	125.25	119.20	2	2
A	256	HIS	ND1-CE1-NE2	6.70	115.10	108.40	3	1
A	183	HIS	CD2-NE2-CE1	6.68	102.32	109.00	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	231	ASN	CA-CB-CG	6.64	119.24	112.60	2	1
A	129	ALA	C-CA-CB	6.57	100.65	110.50	2	1
A	284	MET	CA-C-N	6.56	126.75	116.90	2	2
A	295	ASN	C-N-CA	6.54	133.48	121.70	1	1
A	153	TRP	N-CA-CB	6.53	99.40	110.50	2	1
A	96	PHE	CA-CB-CG	6.51	107.29	113.80	3	2
A	276	ILE	CA-CB-CG1	6.47	121.39	110.40	3	1
A	166	HIS	CA-CB-CG	6.42	107.38	113.80	1	1
A	71	ALA	C-CA-CB	6.41	100.89	110.50	2	1
A	106	ALA	C-N-CA	6.41	133.23	121.70	3	1
A	158	LEU	N-CA-CB	6.41	99.61	110.50	2	1
A	13	ARG	NE-CZ-NH1	6.39	127.89	121.50	3	2
B	5	TYR	CA-CB-CG	6.36	102.45	113.90	1	1
A	290	ILE	CA-CB-CG2	6.32	99.75	110.50	1	1
A	298	ASN	CA-C-N	6.23	126.24	116.90	2	2
A	94	TRP	CA-C-N	6.21	126.22	116.90	2	2
A	26	TYR	CB-CG-CD1	6.15	130.03	120.80	3	1
A	47	SER	O-C-N	6.15	113.16	123.00	3	1
A	177	ILE	O-C-N	6.15	113.17	123.00	1	1
A	17	ASP	C-N-CA	6.13	132.74	121.70	1	1
A	164	ILE	C-N-CA	6.13	132.73	121.70	1	2
A	291	ALA	N-CA-CB	6.12	101.21	110.40	2	1
A	39	PHE	CG-CD2-CE2	6.12	110.29	120.70	1	1
A	137	ARG	C-N-CA	6.07	132.63	121.70	1	1
A	4	ASN	C-CA-CB	6.06	121.61	110.10	1	2
A	275	ARG	NE-CZ-NH1	6.04	127.54	121.50	3	2
A	248	PHE	O-C-N	6.04	113.34	123.00	1	1
A	168	ASN	OD1-CG-ND2	6.03	116.57	122.60	2	1
B	6	HIS	CA-CB-CG	6.02	107.78	113.80	2	1
A	93	ARG	NH1-CZ-NH2	6.00	111.50	119.30	3	1
A	98	ASN	CA-CB-CG	6.00	118.60	112.60	2	1
A	166	HIS	ND1-CE1-NE2	5.97	114.37	108.40	1	1
A	221	ALA	N-CA-CB	5.97	101.45	110.40	2	1
A	159	ALA	N-CA-CB	5.96	101.45	110.40	1	1
A	84	TRP	CE2-CD2-CE3	5.96	124.76	118.80	3	1
A	19	PRO	C-N-CA	5.89	132.31	121.70	2	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	251	PHE	O-C-N	5.89	113.58	123.00	2	1
A	142	MET	C-N-CA	5.88	132.29	121.70	3	1
A	293	PHE	C-CA-CB	5.88	121.27	110.10	2	1
A	117	PHE	CA-CB-CG	5.86	107.94	113.80	1	2
A	96	PHE	C-N-CA	5.85	132.24	121.70	3	1
A	235	ASN	N-CA-CB	5.83	120.41	110.50	1	1
A	172	ILE	CA-CB-CG2	5.81	120.38	110.50	1	1
A	184	TYR	CB-CG-CD2	5.79	112.12	120.80	3	1
A	112	LEU	O-C-N	5.78	113.76	123.00	2	1
A	182	PHE	N-CA-CB	5.77	120.31	110.50	3	1
A	25	ASN	CB-CG-OD1	5.77	132.33	120.80	2	1
A	57	MET	CG-SD-CE	5.76	88.22	100.90	2	1
A	201	ILE	O-C-N	5.76	113.78	123.00	2	1
A	253	TRP	C-CA-CB	5.76	99.16	110.10	3	1
A	6	SER	CA-CB-OG	5.71	122.52	111.10	2	1
A	182	PHE	C-N-CA	5.70	131.97	121.70	1	1
A	216	THR	CA-CB-CG2	5.70	120.19	110.50	2	1
A	294	ASN	C-N-CA	5.68	131.92	121.70	3	1
A	243	MET	CG-SD-CE	5.65	88.46	100.90	3	1
A	220	LYS	CG-CD-CE	5.65	124.29	111.30	2	2
A	58	LYS	C-N-CA	5.64	131.86	121.70	3	1
A	125	ASP	C-N-CA	5.64	131.85	121.70	3	1
A	24	HIS	ND1-CG-CD2	5.61	111.71	106.10	2	2
A	81	LEU	N-CA-C	5.59	126.65	111.00	2	1
A	85	ALA	C-CA-CB	5.58	102.14	110.50	1	1
A	284	MET	O-C-N	5.57	114.08	123.00	2	1
A	141	THR	C-N-CA	5.56	131.71	121.70	3	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	1.29	7
2	0.92	5
3	0.74	4

There are 16 clashes. The table below contains the detailed list of all clashes based on a MolProbity analysis. Bad clashes are ≥ 0.4

Angstrom.

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:206:PHE:CE1	A:210:ILE:HD11	0.66	2	1
A:90:MET:HE2	A:93:ARG:HB2	0.54	2	1
A:168:ASN:HD22	A:183:HIS:CG	0.51	1	1
A:143:LEU:C	A:143:LEU:HD13	0.48	1	1
A:195:LEU:C	A:195:LEU:HD13	0.48	2	1
A:154:LEU:O	A:158:LEU:HB2	0.43	1	1
A:281:ASP:OD2	B:2:ARG:HA	0.43	1	1
A:83:LEU:HD21	A:94:TRP:HH2	0.42	3	1
A:171:PHE:CE1	A:176:ASN:HA	0.42	2	1
A:228:ILE:H	A:228:ILE:HG22	0.42	1	1
A:305:LEU:HA	A:305:LEU:HD12	0.41	2	1
A:263:ASP:CG	B:2:ARG:HH12	0.41	3	1
A:44:PHE:C	A:44:PHE:CD1	0.41	3	1
A:114:ALA:HA	A:152:ILE:CG2	0.41	1	1
A:243:MET:O	A:247:LEU:N	0.41	1	1
A:245:ILE:HD13	A:245:ILE:HG21	0.40	3	1

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	321	296	17	8
2	321	306	14	1
3	321	298	15	8

There are 14 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	91	GLU	2
A	95	PRO	2
A	97	GLY	2
A	2	ILE	1
A	11	ILE	1
A	58	LYS	1
A	59	LEU	1
A	60	LYS	1

Chain	Res	Type	Models (Total)
A	92	TYR	1
A	136	SER	1
A	143	LEU	1
A	230	LYS	1
A	231	ASN	1
A	284	MET	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	292	266	20	6
2	292	271	18	3
3	292	266	15	11

There are 20 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	11	ILE	1
A	19	PRO	1
A	48	LEU	1
A	49	VAL	1
A	67	LEU	1
A	74	ASP	1
A	101	CYS	1
A	125	ASP	1
A	133	PRO	1
A	134	MET	1
A	155	LEU	1
A	162	PRO	1
A	205	LEU	1
A	228	ILE	1
A	230	LYS	1
A	246	VAL	1
A	267	GLN	1
A	286	ILE	1
A	315	GLN	1
B	2	ARG	1

5. Fit to Data Used for Modeling Assessment ?

5.4. EPR ?

Validation for this section is under development.

6. Fit to Data Used for Validation Assessment ?

Validation for this section is under development.

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