

# Integrative Structure Validation Report ?

March 27, 2025 - 09:57 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*

*ATSAS Version 3.2.1 (r14885)*

PDB ID	8ZZR
PDB-Dev ID	PDBDEV_00000027
Structure Title	A metastable contact and structural disorder in the estrogen receptor transactivation domain
Structure Authors	Peng Y; Cao S; Kiselar J; Xiao X; Du Z; Hsien A; Ko S; Chen Y; Agrawal P; Zheng W; Shi W; Jiang W; Yang L; Chance MR; Surewicz WK; Buck M; Yang S
Deposited on	2018-09-26

*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](mailto:helpdesk@pdb-ihm.org)*

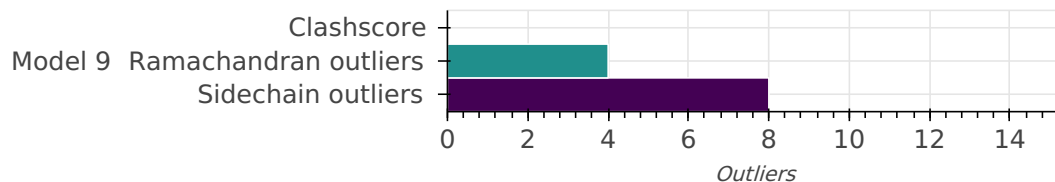
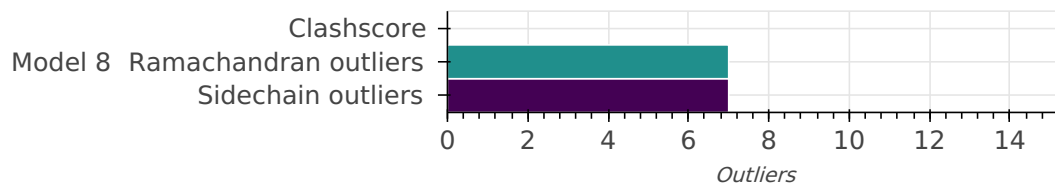
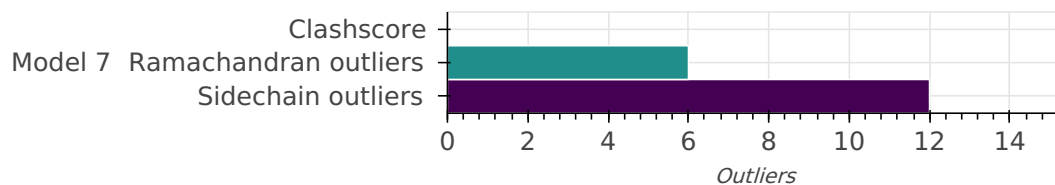
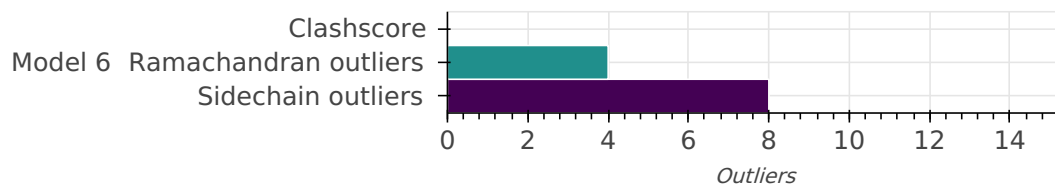
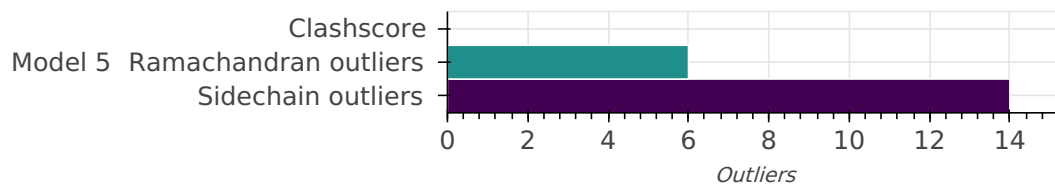
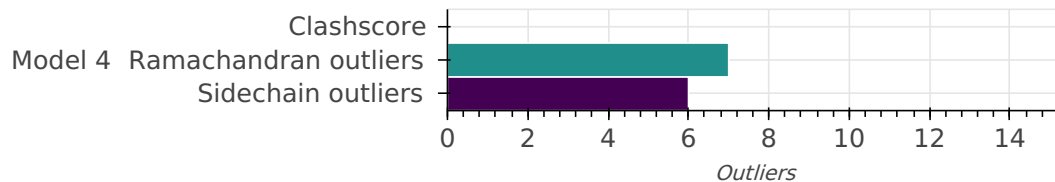
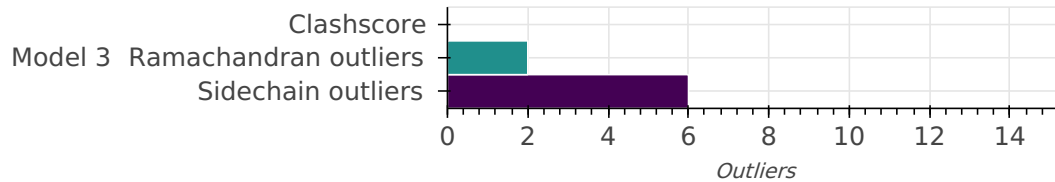
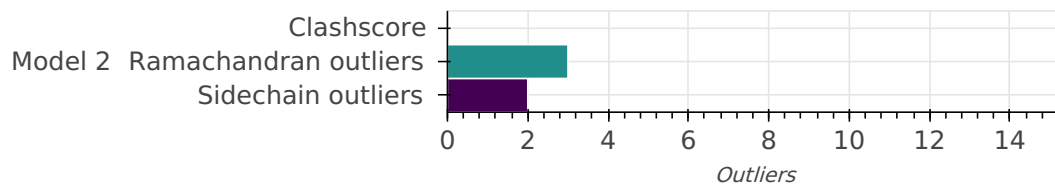
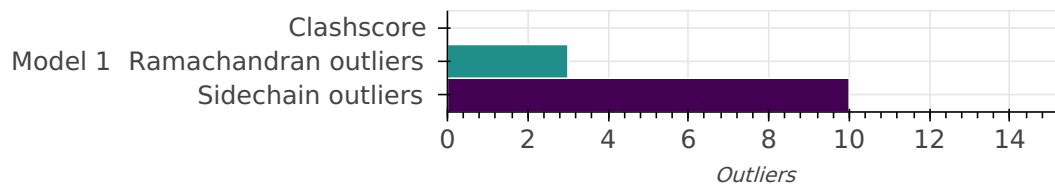
*A user guide is available at [https://pdb-ihm.org/validation\\_help.html](https://pdb-ihm.org/validation_help.html) with specific help available everywhere you see the ? symbol.*

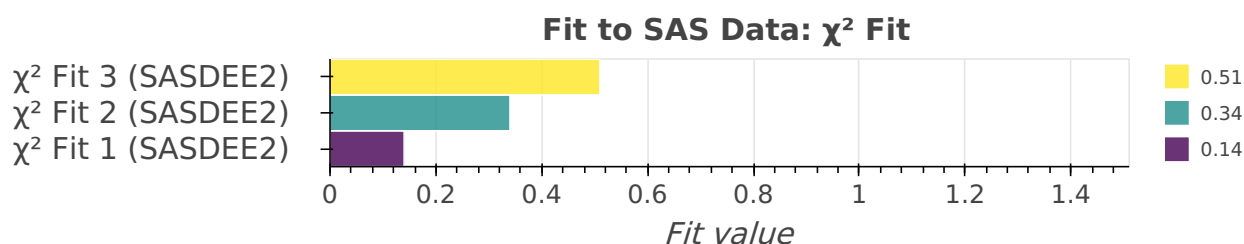
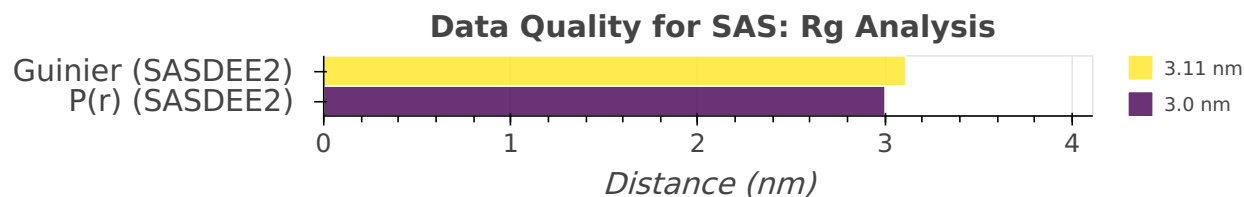
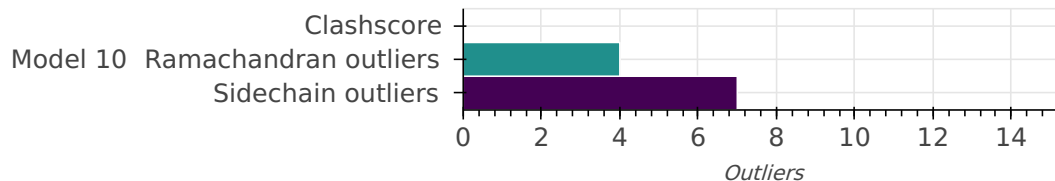
*List of references used to build this report is available [here](#).*

## 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 10 model(s). A total of 2 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	1	Estrogen receptor	A	184	1-184	-	100.00 / 0.00	Atomic

## Datasets used for modeling ?

There are 2 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	SAS data	SASBDB	<a href="#">SASDEE2</a>
2	Hydroxyl radical footprinting data	Not available	<a href="#">10.1016/j.str.2018.10.026</a>

## 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 estrogen receptor N-terminal domain	–	None	None	False	False

There is 1 software package reported in this entry.

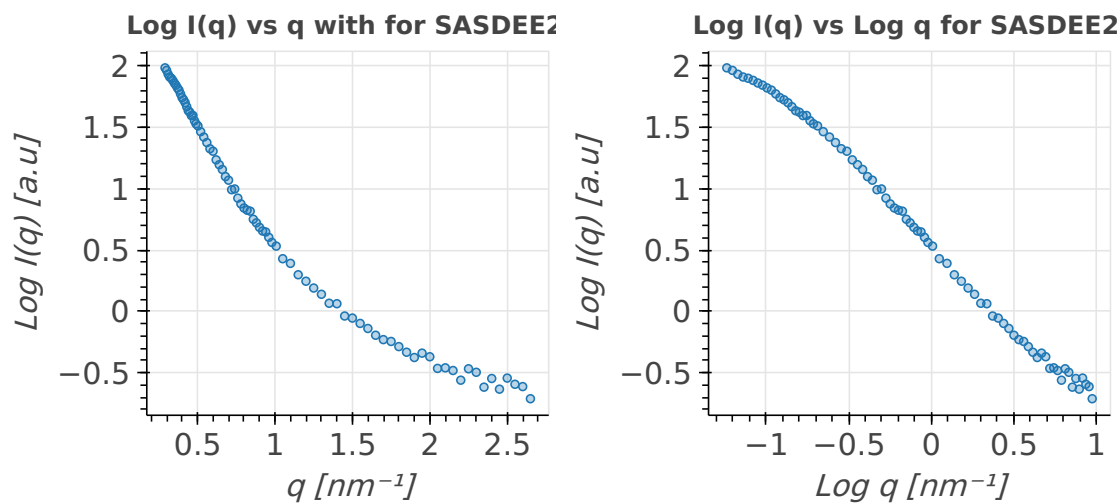
ID	Software name	Software version	Software classification	Software location
1	<a href="#">iSPOT</a>	Not available	model building	<a href="http://www.theyanglab.org/ispot/index.html">http://www.theyanglab.org/ispot/index.html</a>

## Data quality ?

### Scattering profile ?

SAS data used in this integrative model was obtained from 1 deposited SASBDB entry (entries).

Scattering profile for [SASDEE2](#): data from solutions of biological macromolecules are presented as both log I(q) vs q and log I(q) vs log (q) based on [SAS validation task force \(SASvtf\) recommendations](#). I(q) is the intensity (in arbitrary units) and q is the modulus of the scattering vector.



Key experimental estimates ?

Molecular weight (MW) estimates from experiments and analysis: true molecular weight can be compared to the Porod estimate from scattering profiles.

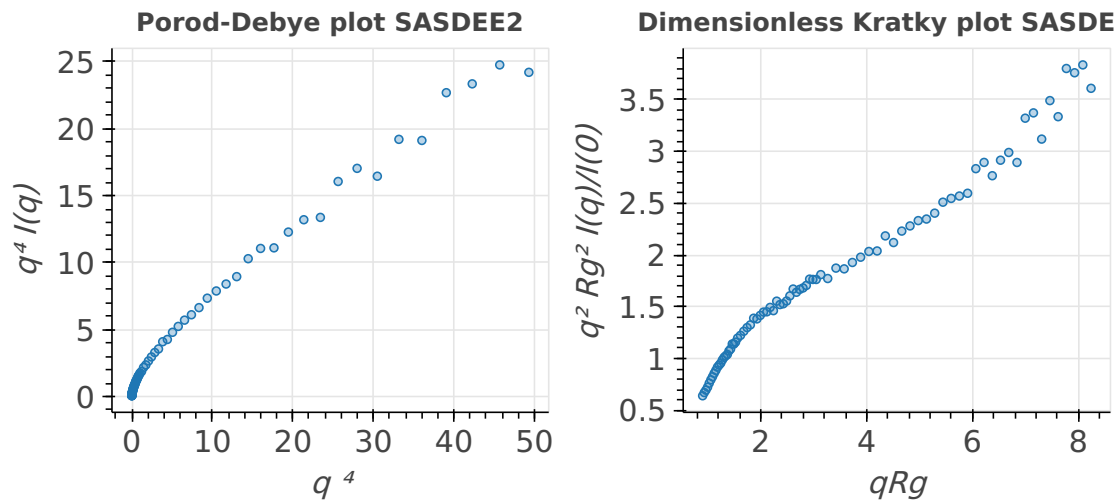
SASDB ID	Chemical composition MW	Standard MW	Porod Volume/MW
SASDEE2	20.2 kDa	Not available	Not available

Volume estimates from experiments and analysis: estimated volume can be compared to Porod volume obtained from scattering profiles.

SASDB ID	Estimated Volume	Porod Volume	Specific Volume	Sample Contrast	Sample Concentration
SASDEE2	Not available	Not available	Not available	Not available	2.50 mg/mL

Flexibility analysis ?

Flexibility analysis for SASDEE2: In a Porod-Debye plot, a clear plateau is observed for globular (partial or fully folded) domains, whereas, fully unfolded domains are devoid of any discernable plateau. For details, refer to Figure 5 in Rambo and Tainer, 2011. In a Kratky plot, a parabolic shape is observed for globular (partial or fully folded) domains and a hyperbolic shape is observed for fully unfolded domains.

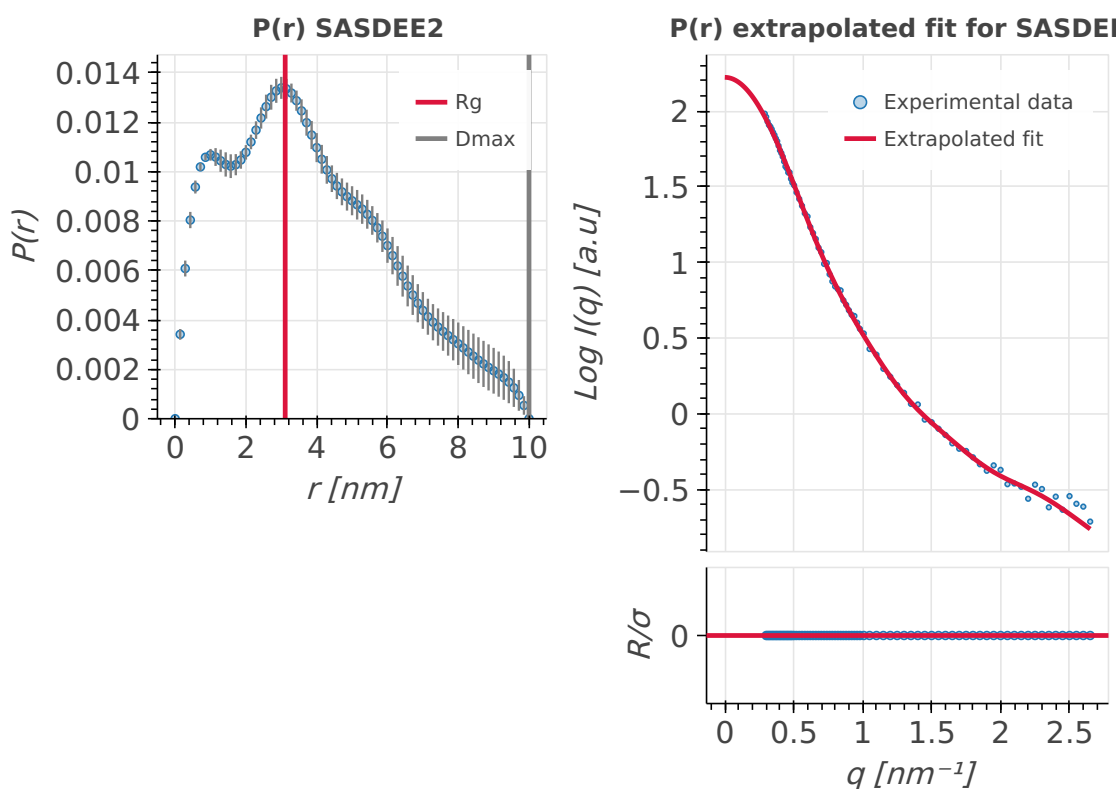


## Pair-distance distribution analysis ?

**P(r) analysis:**  $P(r)$  represents the distribution of distances between all pairs of atoms within the particle weighted by the respective electron densities.  $P(r)$  is the Fourier transform of  $I(s)$  (and vice versa).  $R_g$  can be estimated from integrating the  $P(r)$  function. Agreement between the  $P(r)$  and Guinier-determined  $R_g$  (table below) is a good measure of the self-consistency of the SAS profile.  $R_g$  is a measure for the overall size of a macromolecule; e.g. a protein with a smaller  $R_g$  is more compact than a protein with a larger  $R_g$ , provided both have the same molecular weight (MW). The point where  $P(r)$  is decaying to zero is called  $D_{\max}$  and represents the maximum size of the particle.

SASDB ID	Software used	$D_{\max}$	$D_{\max}$ error	$R_g$	$R_g$ error
SASDEE2	GNOM 4.6	10.000 nm	Not available	3.110 nm	Not available

**P(r) for SASDEE2:** The value of  $P(r)$  should be zero beyond  $r=D_{\max}$ .



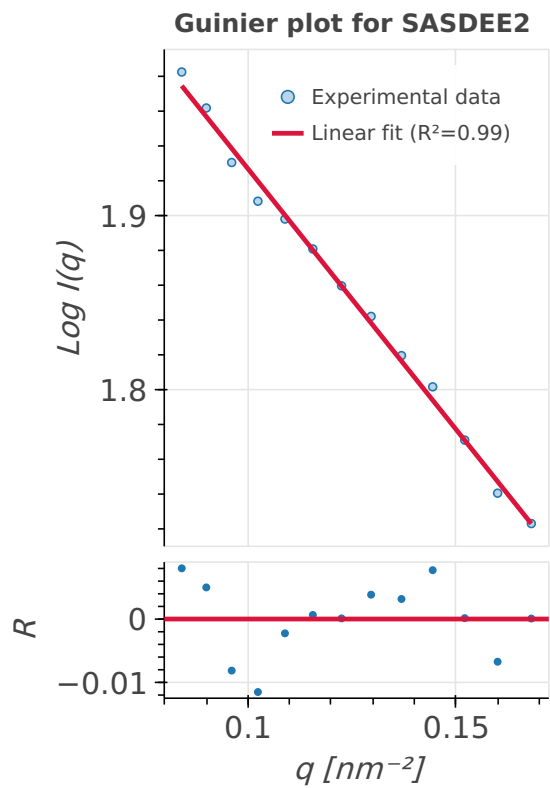
## Guinier analysis ?

**Guinier analysis:** agreement between the  $P(r)$  and Guinier-determined  $R_g$  (table below) is a good measure of the self-consistency of the SAS profile. Molecular weight estimates can also be compared to Porod and sample molecular weights for consistency.

SASDB ID	$R_g$	$R_g$ error	MW	MW error
SASDEE2	3.00 nm	0.16 nm	Not available	Not available

**Guinier analysis:** the linearity of the Guinier plot is a sensitive indicator of the quality of the experimental SAS data; a linear Guinier plot is a necessary but not sufficient demonstration that a solution contains monodisperse particles of the same size. Deviations from linearity usually point to strong interference effects, polydispersity of the samples or improper background subtraction. Residual value plot and

coefficient of determination ( $R^2$ ) are measures to assess linear fit to the data. A perfect fit has an  $R^2$  value of 1. Residual values should be equally and randomly spaced around the horizontal axis.



Hydroxyl radical footprinting

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 247 bond length outliers in this entry (1.71% of 14440 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	142	ARG	CZ-NH2	10.91	1.19	1.33	3	4
A	112	HIS	CG-ND1	9.68	1.48	1.38	8	3
A	112	HIS	CE1-NE2	7.47	1.40	1.32	7	2
A	112	HIS	ND1-CE1	7.39	1.39	1.32	5	7
A	147	PRO	CA-CB	7.27	1.68	1.53	10	1
A	109	MET	C-N	7.20	1.43	1.33	10	2

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	162	ARG	CD-NE	7.01	1.56	1.46	3	1
A	129	PRO	N-CD	6.72	1.38	1.47	1	1
A	16	HIS	CE1-NE2	6.61	1.39	1.32	7	4
A	89	PHE	C-N	6.41	1.42	1.33	6	1
A	124	HIS	ND1-CE1	6.37	1.38	1.32	5	1
A	28	ARG	NE-CZ	6.27	1.39	1.33	7	2
A	16	HIS	ND1-CE1	6.22	1.38	1.32	4	6
A	158	ARG	NE-CZ	6.17	1.39	1.33	10	3
A	37	ARG	CZ-NH2	6.17	1.25	1.33	9	1
A	175	ALA	C-N	6.12	1.41	1.33	9	2
A	124	HIS	CG-ND1	6.06	1.44	1.38	10	3
A	38	PRO	N-CA	6.04	1.38	1.47	2	1
A	34	PRO	C-N	6.02	1.41	1.33	1	1
A	127	GLN	C-N	5.98	1.41	1.33	5	1
A	59	ALA	CA-C	5.92	1.65	1.52	9	1
A	124	HIS	CE1-NE2	5.91	1.38	1.32	8	3
A	151	ARG	CZ-NH2	5.89	1.25	1.33	6	2
A	98	PRO	N-CA	5.84	1.38	1.47	2	1
A	148	ALA	C-N	5.79	1.41	1.33	10	1
A	119	PRO	N-CA	5.76	1.38	1.47	6	2
A	115	PRO	N-CD	5.67	1.39	1.47	5	2
A	2	THR	CB-OG1	5.62	1.34	1.43	8	2
A	84	SER	CB-OG	5.59	1.53	1.42	9	1
A	96	GLY	N-CA	5.59	1.54	1.45	10	2
A	146	PRO	N-CD	5.57	1.40	1.47	2	2
A	141	VAL	C-N	5.51	1.41	1.33	9	1
A	51	VAL	C-N	5.51	1.41	1.33	1	1
A	29	PRO	N-CA	5.50	1.55	1.47	3	1
A	89	PHE	CA-CB	5.49	1.64	1.53	9	1
A	79	PRO	N-CA	5.47	1.55	1.47	5	3
A	135	GLU	CA-C	5.47	1.64	1.52	1	1
A	7	THR	CB-OG1	5.44	1.35	1.43	7	3
A	6	HIS	CG-CD2	5.44	1.41	1.35	7	3
A	6	HIS	CG-ND1	5.44	1.44	1.38	1	2
A	74	GLY	C-N	5.35	1.40	1.33	10	1



Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	36	GLU	C-N	5.26	1.40	1.33	2	2
A	182	THR	CB-OG1	5.22	1.35	1.43	2	1
A	66	ALA	C-N	5.21	1.40	1.33	2	2
A	144	ALA	CA-C	5.18	1.63	1.52	7	1
A	123	PRO	N-CA	5.17	1.39	1.47	6	1
A	105	PRO	N-CD	5.13	1.54	1.47	6	3
A	76	THR	CB-OG1	5.12	1.35	1.43	1	1
A	158	ARG	CZ-NH2	5.12	1.26	1.33	7	1
A	136	PRO	N-CD	5.10	1.40	1.47	6	1
A	37	ARG	NE-CZ	5.09	1.38	1.33	4	1
A	17	GLN	N-CA	5.09	1.55	1.46	6	1
A	37	ARG	CD-NE	5.07	1.53	1.46	8	1
A	28	ARG	CZ-NH2	5.06	1.26	1.33	3	2
A	98	PRO	C-N	5.05	1.42	1.34	4	1
A	157	ARG	NE-CZ	5.05	1.38	1.33	4	1
A	28	ARG	CZ-NH1	5.05	1.25	1.32	6	1
A	154	SER	C-N	5.04	1.40	1.33	6	2
A	60	TYR	CA-C	5.00	1.63	1.52	2	1
A	9	ALA	C-N	4.99	1.26	1.33	7	1
A	34	PRO	N-CD	4.99	1.40	1.47	7	2
A	178	SER	N-CA	4.98	1.55	1.46	2	1
A	107	PRO	N-CD	4.97	1.40	1.47	2	1
A	68	ALA	C-N	4.97	1.26	1.33	3	1
A	20	GLY	CA-C	4.96	1.43	1.52	8	2
A	23	LEU	CA-C	4.93	1.63	1.52	7	1
A	140	THR	C-N	4.93	1.40	1.33	2	1
A	6	HIS	CE1-NE2	4.89	1.37	1.32	7	1
A	104	SER	CB-OG	4.88	1.32	1.42	1	1
A	4	THR	CB-OG1	4.86	1.36	1.43	5	1
A	151	ARG	NE-CZ	4.86	1.38	1.33	9	1
A	45	ASP	C-N	4.85	1.40	1.33	4	1
A	133	GLU	C-N	4.83	1.40	1.33	10	1
A	2	THR	C-N	4.82	1.26	1.33	5	1
A	162	ARG	CZ-NH2	4.80	1.27	1.33	10	2
A	105	PRO	N-CA	4.80	1.39	1.47	2	2

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	131	TYR	C-N	4.78	1.40	1.33	5	1
A	16	HIS	CG-ND1	4.78	1.43	1.38	1	2
A	112	HIS	CD2-NE2	4.77	1.43	1.37	1	1
A	126	GLN	C-N	4.76	1.40	1.33	4	1
A	157	ARG	CZ-NH1	4.76	1.26	1.32	9	1
A	163	GLU	N-CA	4.75	1.55	1.46	6	2
A	79	PRO	N-CD	4.75	1.41	1.47	6	1
A	111	LEU	C-N	4.75	1.40	1.33	5	1
A	183	ARG	CA-CB	4.75	1.62	1.53	6	2
A	105	PRO	C-N	4.73	1.26	1.33	2	1
A	152	PRO	C-N	4.72	1.40	1.33	10	1
A	131	TYR	N-CA	4.71	1.55	1.46	5	1
A	80	TYR	CG-CD1	4.71	1.49	1.39	3	1
A	171	LYS	CA-CB	4.70	1.62	1.53	1	1
A	139	TYR	C-N	4.66	1.26	1.33	7	1
A	152	PRO	N-CD	4.66	1.41	1.47	6	1
A	22	GLU	CA-CB	4.64	1.62	1.53	1	1
A	86	ALA	C-N	4.64	1.39	1.33	2	1
A	113	PRO	N-CD	4.63	1.41	1.47	4	3
A	39	LEU	C-N	4.63	1.39	1.33	1	1
A	151	ARG	CZ-NH1	4.60	1.26	1.32	4	1
A	179	ALA	C-N	4.57	1.39	1.33	7	1
A	163	GLU	CA-C	4.57	1.62	1.52	5	1
A	52	TYR	CB-CG	4.54	1.61	1.51	3	1

### Standard geometry: angle outliers ?

There are 915 bond angle outliers in this entry (4.65% of 19680 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	63	ASN	CA-CB-CG	10.20	122.80	112.60	3	3
A	124	HIS	CB-CG-CD2	9.93	118.29	131.20	4	6
A	159	GLN	OE1-CD-NE2	9.75	112.85	122.60	6	2
A	28	ARG	NE-CZ-NH2	9.51	127.75	119.20	1	3
A	142	ARG	NE-CZ-NH2	9.42	127.68	119.20	6	4

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	75	GLN	OE1-CD-NE2	9.24	113.36	122.60	8	6
A	119	PRO	N-CA-CB	9.12	113.03	103.00	1	6
A	6	HIS	CB-CG-CD2	9.06	119.43	131.20	2	5
A	166	ALA	C-CA-CB	9.01	124.01	110.50	5	1
A	37	ARG	NE-CZ-NH1	8.94	130.44	121.50	2	3
A	120	PHE	CA-CB-CG	8.79	122.59	113.80	7	4
A	92	ASN	CA-CB-CG	8.78	121.38	112.60	1	3
A	31	LEU	C-N-CA	8.69	137.35	121.70	3	3
A	146	PRO	N-CA-CB	8.67	112.54	103.00	6	2
A	140	THR	CA-CB-CG2	8.43	124.82	110.50	9	1
A	156	ASN	OD1-CG-ND2	8.36	114.24	122.60	2	4
A	49	PRO	N-CA-CB	8.36	112.19	103.00	4	3
A	38	PRO	N-CA-CB	8.33	112.16	103.00	7	6
A	101	ASN	OD1-CG-ND2	8.28	114.32	122.60	8	5
A	122	GLN	OE1-CD-NE2	8.23	114.37	122.60	9	6
A	17	GLN	OE1-CD-NE2	8.13	114.47	122.60	3	4
A	21	ASN	OD1-CG-ND2	8.11	114.49	122.60	3	2
A	99	PRO	N-CA-CB	7.97	111.77	103.00	7	3
A	30	GLN	OE1-CD-NE2	7.93	114.67	122.60	10	6
A	25	PRO	N-CA-CB	7.93	111.72	103.00	7	4
A	27	ASN	OD1-CG-ND2	7.88	114.72	122.60	2	4
A	16	HIS	O-C-N	7.78	110.55	123.00	2	1
A	55	PRO	N-CA-CB	7.77	111.55	103.00	7	4
A	112	HIS	CB-CG-CD2	7.74	121.13	131.20	2	4
A	175	ALA	N-CA-CB	7.73	98.80	110.40	4	3
A	79	PRO	N-CA-CB	7.72	111.49	103.00	7	5
A	126	GLN	CB-CG-CD	7.66	125.63	112.60	9	1
A	16	HIS	ND1-CE1-NE2	7.59	115.99	108.40	5	3
A	107	PRO	N-CA-CB	7.59	111.35	103.00	10	5
A	152	PRO	N-CA-CB	7.57	111.32	103.00	2	3
A	142	ARG	NH1-CZ-NH2	7.54	109.49	119.30	6	3
A	156	ASN	CA-CB-CG	7.46	120.06	112.60	2	2
A	71	GLN	OE1-CD-NE2	7.45	115.15	122.60	6	4

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	140	THR	OG1-CB-CG2	7.45	94.41	109.30	9	1
A	166	ALA	N-CA-CB	7.43	99.26	110.40	5	2
A	37	ARG	NE-CZ-NH2	7.41	112.53	119.20	2	2
A	62	PHE	CA-CB-CG	7.36	121.16	113.80	9	4
A	126	GLN	OE1-CD-NE2	7.25	115.35	122.60	6	5
A	56	GLU	C-N-CA	7.18	134.63	121.70	8	2
A	82	PRO	N-CA-CB	7.18	110.90	103.00	9	2
A	72	VAL	CA-CB-CG2	7.15	122.56	110.40	8	2
A	21	ASN	CA-CB-CG	7.11	105.49	112.60	7	2
A	158	ARG	NE-CZ-NH1	7.07	128.57	121.50	7	5
A	16	HIS	CB-CG-CD2	7.06	122.03	131.20	7	8
A	109	MET	C-N-CA	7.04	134.38	121.70	6	4
A	76	THR	CA-CB-CG2	7.04	122.46	110.50	3	2
A	153	ASN	OD1-CG-ND2	6.96	115.64	122.60	6	2
A	158	ARG	NH1-CZ-NH2	6.95	110.27	119.30	5	4
A	43	TYR	C-N-CA	6.92	134.15	121.70	6	1
A	34	PRO	N-CA-CB	6.88	110.56	103.00	5	4
A	97	PHE	CA-C-N	6.87	127.20	116.90	6	2
A	124	HIS	C-N-CA	6.86	134.05	121.70	4	1
A	45	ASP	CA-CB-CG	6.76	119.36	112.60	7	3
A	124	HIS	ND1-CG-CD2	6.74	112.84	106.10	7	2
A	34	PRO	C-N-CA	6.69	133.75	121.70	9	2
A	6	HIS	CG-CD2-NE2	6.68	100.52	107.20	4	2
A	47	SER	C-N-CA	6.66	133.69	121.70	6	1
A	6	HIS	O-C-N	6.65	112.36	123.00	1	1
A	47	SER	CA-CB-OG	6.65	124.40	111.10	2	1
A	29	PRO	N-CA-CB	6.64	110.31	103.00	4	5
A	112	HIS	CA-CB-CG	6.61	120.41	113.80	10	2
A	26	LEU	N-CA-CB	6.60	99.27	110.50	6	1
A	168	THR	C-N-CA	6.60	133.58	121.70	8	1
A	134	ASN	OD1-CG-ND2	6.60	116.00	122.60	10	3
A	53	ASN	OD1-CG-ND2	6.59	116.01	122.60	4	5
A	30	GLN	CG-CD-NE2	6.58	126.28	116.40	10	1
A	151	ARG	NE-CZ-NH2	6.58	113.28	119.20	3	3

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	86	ALA	N-CA-CB	6.52	100.62	110.40	2	1
A	124	HIS	ND1-CE1-NE2	6.50	114.90	108.40	10	3
A	164	ARG	NE-CZ-NH2	6.50	125.05	119.20	1	6
A	87	ALA	N-CA-CB	6.46	100.71	110.40	8	1
A	183	ARG	NE-CZ-NH1	6.45	115.05	121.50	1	3
A	112	HIS	CB-CG-ND1	6.44	132.36	122.70	2	1
A	63	ASN	OD1-CG-ND2	6.44	116.16	122.60	2	5
A	125	GLY	C-N-CA	6.42	133.26	121.70	5	2
A	171	LYS	C-N-CA	6.41	133.24	121.70	6	2
A	67	ALA	C-CA-CB	6.38	120.07	110.50	1	1
A	112	HIS	ND1-CE1-NE2	6.34	114.74	108.40	1	2
A	164	ARG	O-C-N	6.34	112.86	123.00	1	2
A	69	ASN	OD1-CG-ND2	6.32	116.28	122.60	6	2
A	6	HIS	CA-CB-CG	6.31	120.11	113.80	10	3
A	147	PRO	N-CA-CB	6.30	109.93	103.00	7	3
A	98	PRO	CA-C-N	6.27	126.31	116.90	1	2
A	177	GLU	CA-CB-CG	6.27	126.64	114.10	1	1
A	107	PRO	CA-N-CD	6.25	103.24	112.00	6	2
A	67	ALA	CA-C-O	6.22	131.38	120.80	8	1
A	24	GLU	CB-CG-CD	6.22	102.03	112.60	3	2
A	37	ARG	NH1-CZ-NH2	6.22	111.22	119.30	6	2
A	28	ARG	NE-CZ-NH1	6.19	127.69	121.50	9	3
A	162	ARG	C-N-CA	6.11	132.70	121.70	6	2
A	35	LEU	N-CA-CB	6.09	120.85	110.50	7	2
A	99	PRO	N-CD-CG	6.09	112.33	103.20	5	4
A	12	MET	C-CA-CB	6.07	121.64	110.10	6	2
A	76	THR	O-C-N	6.07	113.28	123.00	5	1
A	143	GLU	CB-CG-CD	6.05	102.31	112.60	9	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
4	0.00	0
5	0.00	0
6	0.00	0
7	0.00	0
8	0.00	0
9	0.00	0
10	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	182	147	32	3
2	182	169	10	3
3	182	154	26	2
4	182	161	14	7
5	182	153	23	6
6	182	159	19	4
7	182	153	23	6
8	182	156	19	7
9	182	155	23	4
10	182	150	28	4

There are 33 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	55	PRO	10
A	57	GLY	2
A	70	ALA	2
A	126	GLN	2
A	144	ALA	2
A	10	SER	1
A	11	GLY	1

Chain	Res	Type	Models (Total)
A	14	LEU	1
A	21	ASN	1
A	32	LYS	1
A	35	LEU	1
A	42	VAL	1
A	44	LEU	1
A	47	SER	1
A	69	ASN	1
A	72	VAL	1
A	74	GLY	1
A	76	THR	1
A	79	PRO	1
A	86	ALA	1
A	88	ALA	1
A	90	GLY	1
A	96	GLY	1
A	99	PRO	1
A	103	VAL	1
A	110	LEU	1
A	117	LEU	1
A	124	HIS	1
A	129	PRO	1
A	136	PRO	1
A	141	VAL	1
A	146	PRO	1
A	163	GLU	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	147	123	14	10
2	147	133	12	2
3	147	132	9	6
4	147	126	15	6
5	147	109	24	14

Model ID	Analysed	Favored	Allowed	Outliers
6	147	126	13	8
7	147	117	18	12
8	147	120	20	7
9	147	125	14	8
10	147	120	20	7

*There are 63 unique sidechain outliers. Detailed list of outliers are tabulated below.*

Chain	Res	Type	Models (Total)
A	140	THR	4
A	165	LEU	3
A	168	THR	3
A	4	THR	2
A	26	LEU	2
A	35	LEU	2
A	39	LEU	2
A	42	VAL	2
A	72	VAL	2
A	91	SER	2
A	97	PHE	2
A	126	GLN	2
A	177	GLU	2
A	1	MET	1
A	2	THR	1
A	6	HIS	1
A	12	MET	1
A	14	LEU	1
A	15	LEU	1
A	17	GLN	1
A	18	ILE	1
A	19	GLN	1
A	31	LEU	1
A	33	ILE	1
A	43	TYR	1
A	44	LEU	1
A	45	ASP	1



Chain	Res	Type	Models (Total)
A	51	VAL	1
A	52	TYR	1
A	60	TYR	1
A	78	LEU	1
A	85	GLU	1
A	99	PRO	1
A	100	LEU	1
A	102	SER	1
A	103	VAL	1
A	104	SER	1
A	106	SER	1
A	108	LEU	1
A	109	MET	1
A	110	LEU	1
A	112	HIS	1
A	116	GLN	1
A	117	LEU	1
A	120	PHE	1
A	127	GLN	1
A	128	VAL	1
A	129	PRO	1
A	132	LEU	1
A	134	ASN	1
A	143	GLU	1
A	151	ARG	1
A	154	SER	1
A	159	GLN	1
A	164	ARG	1
A	169	ASN	1
A	174	MET	1
A	176	MET	1
A	178	SER	1
A	180	LYS	1
A	181	GLU	1
A	183	ARG	1

Chain	Res	Type	Models (Total)
A	184	TYR	1

Fit of model to data used for modeling ?

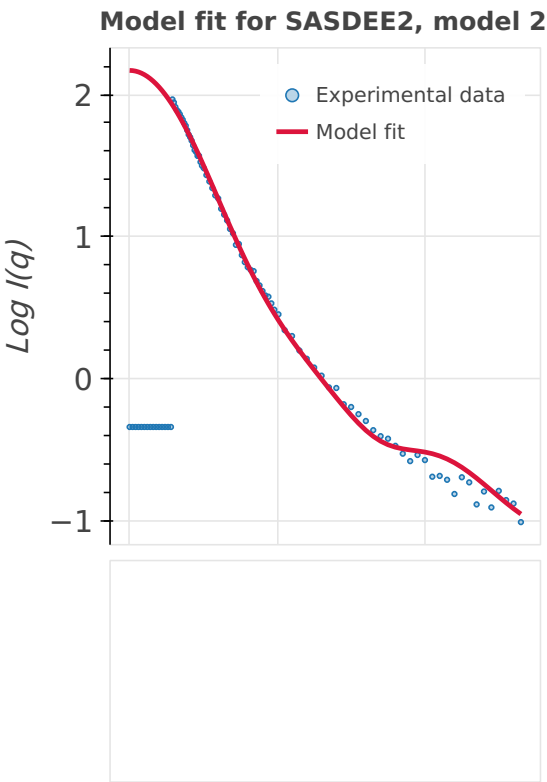
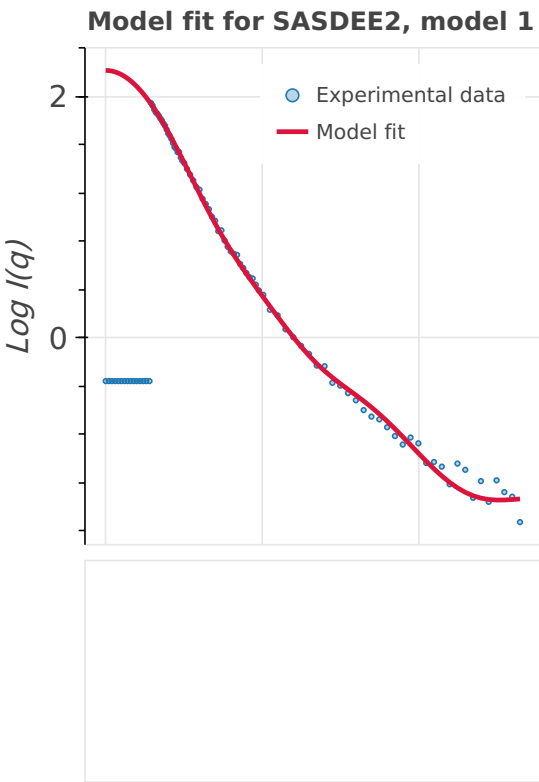
Fit of model(s) to SAS data

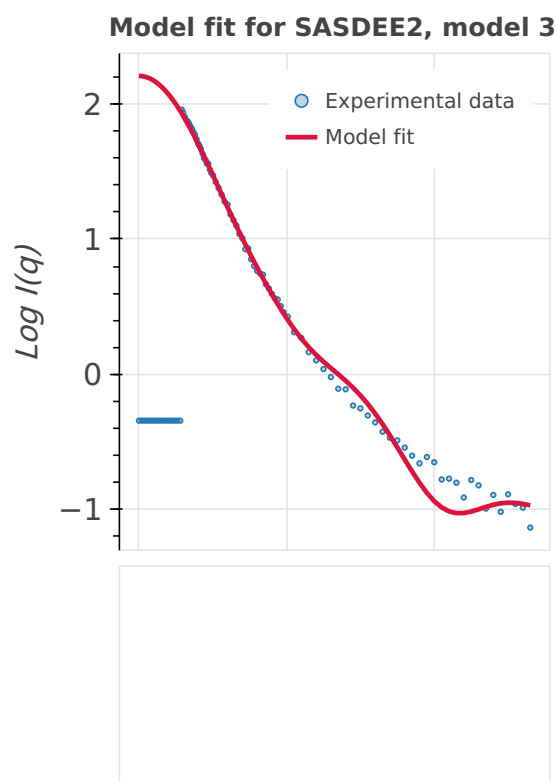
$\chi^2$  goodness of fit and cormap analysis ?

Model and fits displayed below were obtained from SASBDB.  $\chi^2$  values are a measure of fit of the model to data. A perfect fit has a  $\chi^2$  value of 1.0. ATSAS DATCMP was used for hypothesis testing. All data sets are similar (i.e. the fit and the data collected) is the null hypothesis.  $p$ -value is a measure of evidence against the null hypothesis, smaller the value, the stronger the evidence that you should reject the null hypothesis.

SASDB ID	Model	$\chi^2$	p-value
SASDEE2	1	0.14	0.00
SASDEE2	2	0.34	0.00
SASDEE2	3	0.51	0.00

Model fit(s): Residual value plot is a measure to assess fit to the data. Residual values should be equally and randomly spaced around the horizontal axis.





### Hydroxyl radical footprinting

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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