

Integrative Structure Validation Report

July 22, 2024 - 03:49 PM PDT

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

Python-IHM Version 1.3

MolProbity Version 4.5.2

ATSAS Version 3.2.1 (r14885)

Integrative Modeling Validation Version 1.2

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

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

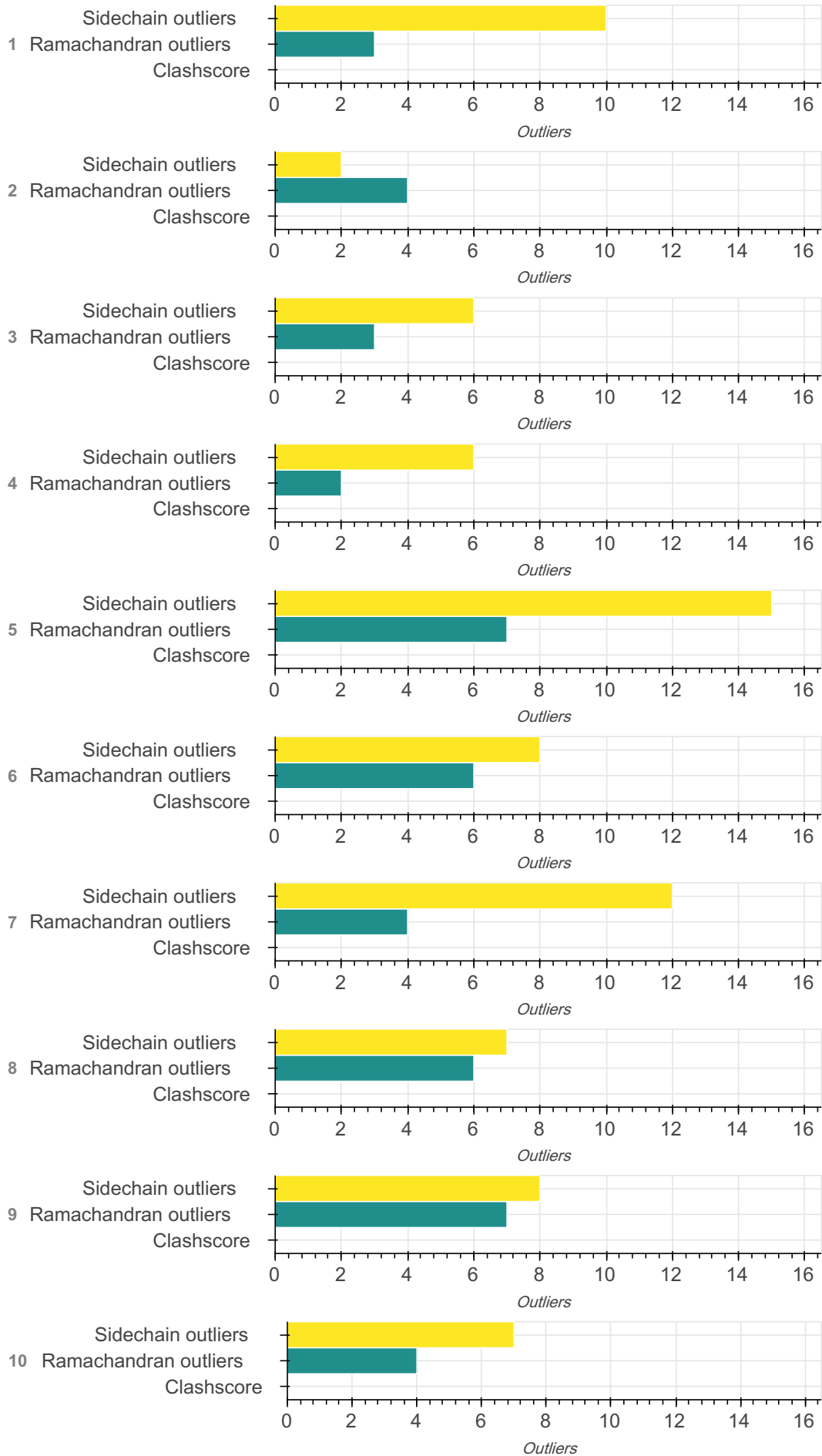
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the  symbol.

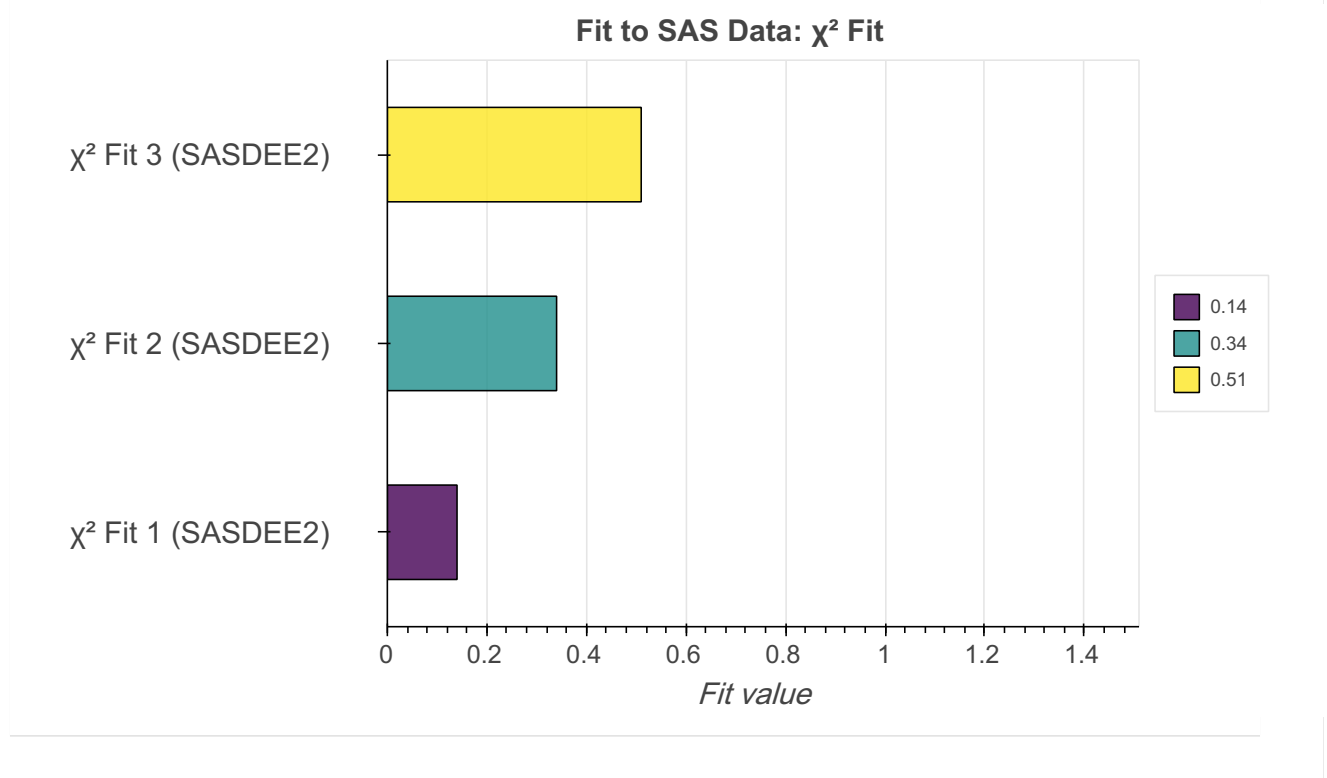
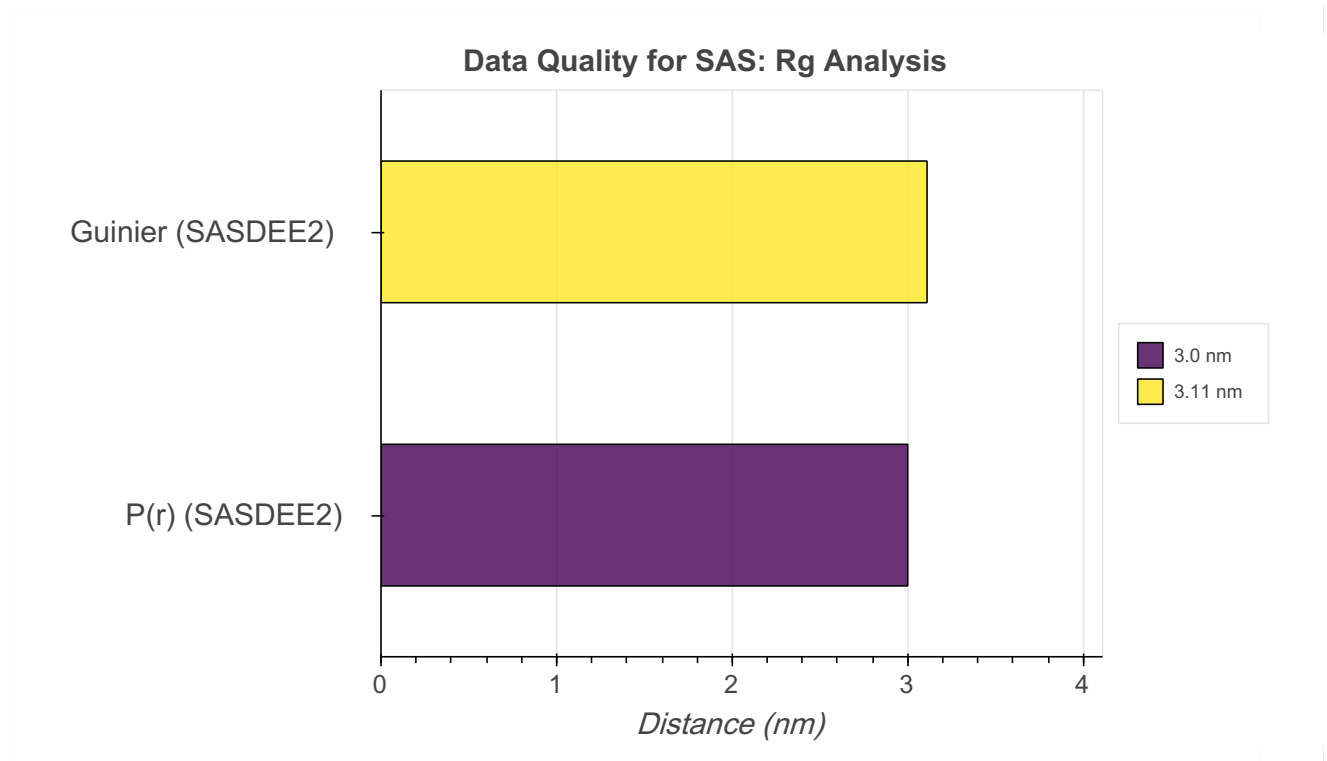
List of references used to build this report is available [here](#).

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 10 unique models, with 1 subunits in each model. A total of 2 datasets or restraints were used to build this entry. Each model is represented by 1 rigid bodies and 0 flexible or non-rigid units.

Entry composition ?

There are 10 unique types of models in this entry. These models are titled None/?, None/?, None/?, None/?, None/?, None/?, None/?, None/?, None/?, None/? respectively.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	Estrogen receptor	A	A	184
2	1	1	Estrogen receptor	A	A	184
3	1	1	Estrogen receptor	A	A	184
4	1	1	Estrogen receptor	A	A	184
5	1	1	Estrogen receptor	A	A	184
6	1	1	Estrogen receptor	A	A	184
7	1	1	Estrogen receptor	A	A	184
8	1	1	Estrogen receptor	A	A	184
9	1	1	Estrogen receptor	A	A	184
10	1	1	Estrogen receptor	A	A	184

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	SASDEE2
2	Other	File	10.1016/j.str.2018.10.026

Representation ?

This entry has only one representation and includes 1 rigid bodies and 0 flexible units

Chain ID	Rigid bodies	Non-rigid segments
A	1-184:None	-

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	iSPOT	Not available	model building	http://www.theyanglab.org/ispot/index.html

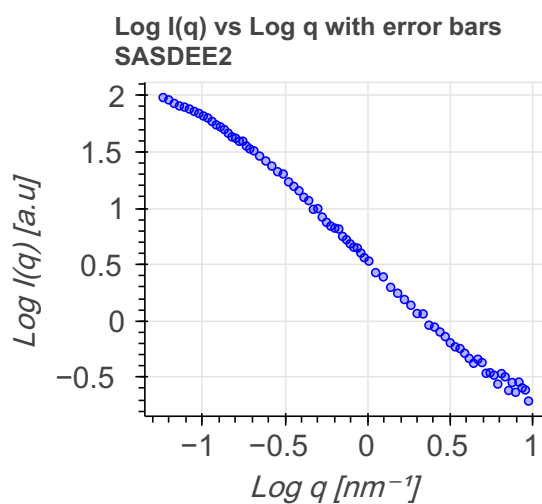
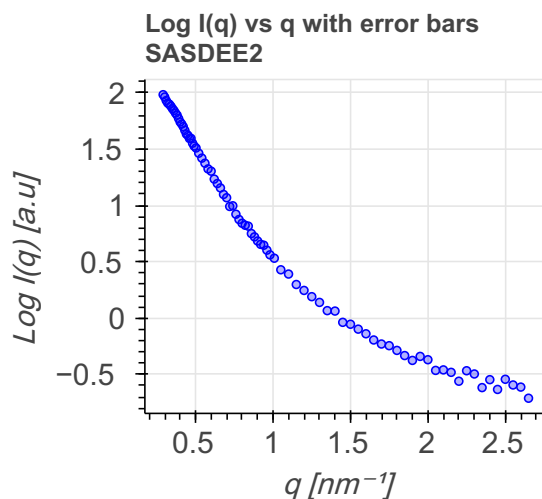
Data quality ?

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.

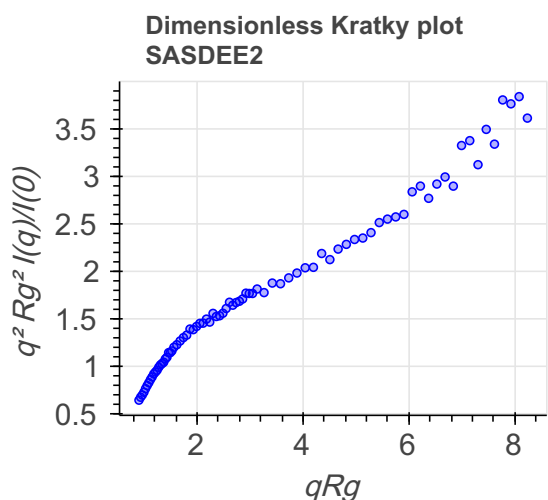
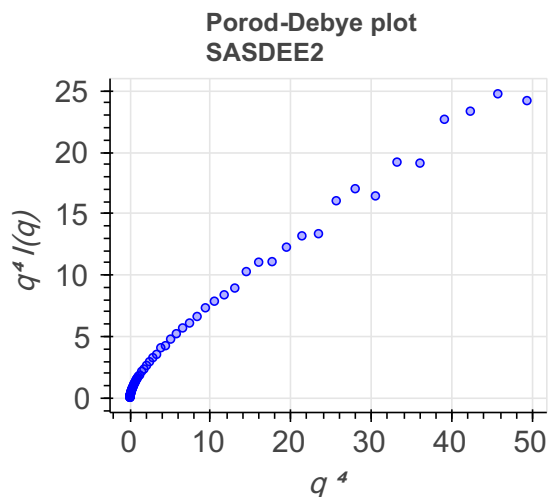
SASDB ID	Chemical composition MW	Standard MW	Porod Volume/MW
SASDEE2	20.2 kDa	N/A	N/A

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	N/A	N/A	N/A	N/A	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.

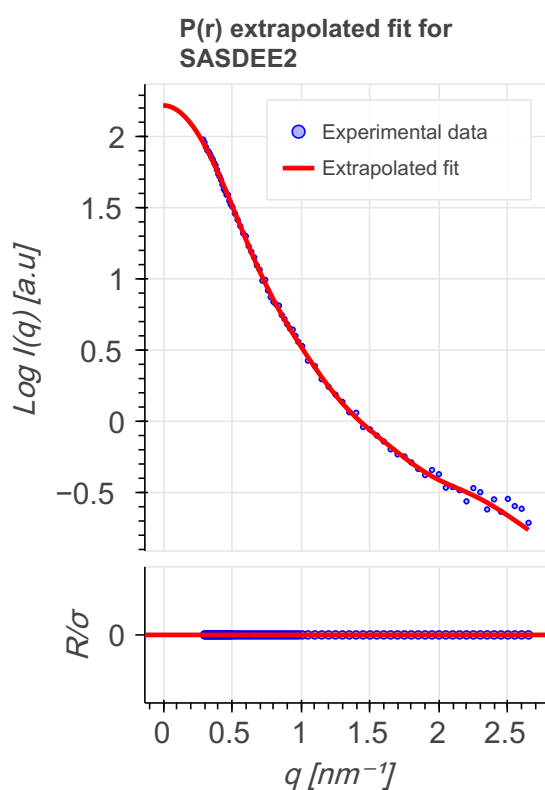
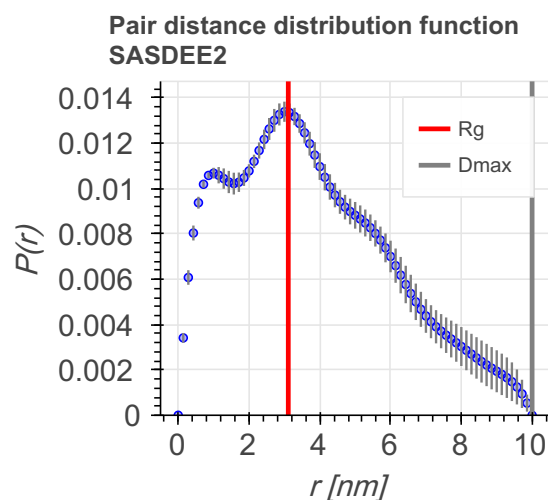


Pair-distance distribution analysis ?

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	Dmax	Dmax error	Rg	Rg error
SASDEE2	GNOM 4.6	10.000 nm	N/A	3.110 nm	N/A

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



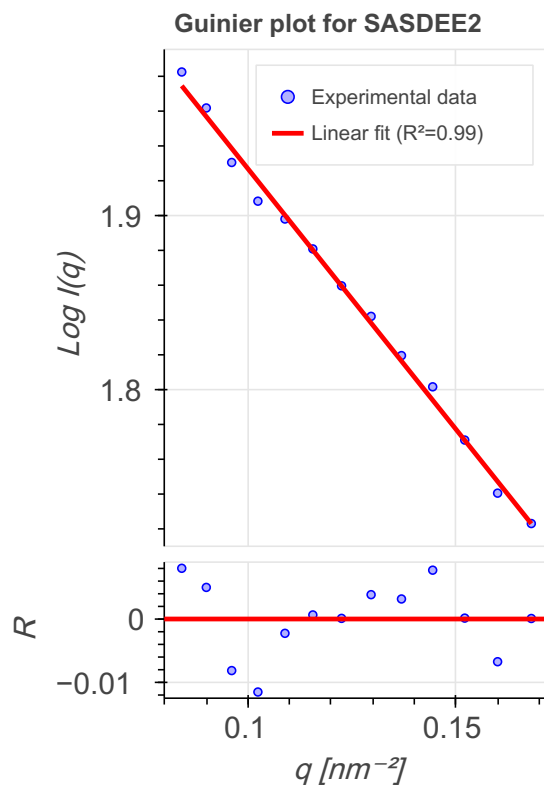
Guinier analysis ?

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	N/A	N/A

Guinier analysis for SASDEE2: 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.



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 13530 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
CB--HB3	1.09	0.97	1510
CB--HB1	1.09	0.97	190
CG--HG2	1.09	0.97	650
CA--HA	1.09	0.97	1660
CB--HB2	1.09	0.97	1510

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CD2--HD22	1.09	0.97	190
CB--HB	1.09	0.97	150
CG2--HG22	1.09	0.97	150
CD1--HD13	1.09	0.97	210
CD2--HD21	1.09	0.97	190
CG1--HG13	1.09	0.97	80
CE--HE1	1.09	0.97	60
CD--HD3	1.09	0.97	360
OG--HG	0.96	0.84	140
CG2--HG23	1.09	0.97	150
CD1--HD11	1.09	0.97	210
CG--HG3	1.09	0.97	650
NZ--HZ2	1.01	0.89	50
CG--HG	1.09	0.97	190
CD--HD2	1.09	0.97	360
CE--HE2	1.09	0.97	110
CA--HA2	1.09	0.97	180
CD1--HD12	1.09	0.97	210
CA--HA3	1.09	0.97	180
CG1--HG11	1.09	0.97	60
NZ--HZ1	1.01	0.89	50
CG2--HG21	1.09	0.97	150
OG1--HG1	0.96	0.84	70

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CD2--HD23	1.09	0.97	190
CE--HE3	1.09	0.97	110
OH--HH	0.96	0.84	110
CG1--HG12	1.09	0.97	80
NZ--HZ3	1.01	0.89	50
N--H2	1.01	0.89	10
N--H1	1.01	0.89	10
N--H3	1.01	0.89	10
NH2--HH22	1.01	0.86	90
CE2--HE2	1.08	0.93	160
N--H	1.01	0.86	1610
NE2--HE21	1.01	0.86	100
CD2--HD2	1.08	0.93	200
ND2--HD22	1.01	0.86	110
NE2--HE2	1.01	0.86	40
CD1--HD1	1.08	0.93	160
CE1--HE1	1.08	0.93	200
ND2--HD21	1.01	0.86	110
NH1--HH11	1.01	0.86	90
NE2--HE22	1.01	0.86	100
NH2--HH21	1.01	0.86	90
NE--HE	1.01	0.86	90
NH1--HH12	1.01	0.86	90

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CZ--HZ	1.08	0.93	50

Standard geometry: angle outliers

There are 1231 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
CA-CB-CG	112.60	122.80	1
CB-CG-CD2	131.20	118.29	1
OE1-CD-NE2	122.60	112.85	1
NE-CZ-NH2	119.20	127.75	1
NE-CZ-NH2	119.20	127.68	1
OE1-CD-NE2	122.60	113.36	1
N-CA-CB	103.00	113.03	1
CB-CG-CD2	131.20	119.43	1
C-CA-CB	110.50	124.01	1
NE-CZ-NH1	121.50	130.44	1
CA-CB-CG	113.80	122.59	1
CA-CB-CG	112.60	121.38	1
C-N-CA	121.70	137.35	1
N-CA-CB	103.00	112.54	1
CA-CB-CG	113.80	105.13	1
CA-CB-CG2	110.50	124.82	1
OD1-CG-ND2	122.60	114.24	1
N-CA-CB	103.00	112.19	1
N-CA-CB	103.00	112.16	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OD1-CG-ND2	122.60	114.32	1
NE-CZ-NH1	121.50	129.74	1
OE1-CD-NE2	122.60	114.37	1
OE1-CD-NE2	122.60	114.47	1
OD1-CG-ND2	122.60	114.49	1
CB-CG-CD2	131.20	120.82	1
N-CA-CB	103.00	111.77	1
OE1-CD-NE2	122.60	114.67	1
N-CA-CB	103.00	111.72	1
OE1-CD-NE2	122.60	114.71	1
OD1-CG-ND2	122.60	114.72	1
O-C-N	123.00	110.55	1
N-CA-CB	103.00	111.55	1
CB-CG-CD2	131.20	121.10	1
CB-CG-CD2	131.20	121.13	1
N-CA-CB	110.40	98.80	1
N-CA-CB	103.00	111.49	1
NE-CZ-NH2	119.20	126.11	1
CB-CG-CD	112.60	125.63	1
ND1-CE1-NE2	108.40	115.99	1
N-CA-CB	103.00	111.35	1
N-CA-CB	103.00	111.32	1
NH1-CZ-NH2	119.30	109.49	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	112.60	120.06	1
OE1-CD-NE2	122.60	115.15	1
OG1-CB-CG2	109.30	94.41	1
N-CA-CB	110.40	99.26	1
NE-CZ-NH2	119.20	112.53	1
CA-CB-CG	113.80	121.16	1
N-CA-CB	103.00	110.98	1
OE1-CD-NE2	122.60	115.35	1
C-N-CA	121.70	134.63	1
N-CA-CB	103.00	110.90	1
OE1-CD-NE2	122.60	115.44	1
CA-CB-CG2	110.40	122.56	1
CA-CB-CG	112.60	105.49	1
NE-CZ-NH1	121.50	128.57	1
CB-CG-CD2	131.20	122.03	1
C-N-CA	121.70	134.38	1
CA-CB-CG2	110.50	122.46	1
OD1-CG-ND2	122.60	115.64	1
NH1-CZ-NH2	119.30	110.27	1
OD1-CG-ND2	122.60	129.54	1
C-N-CA	121.70	134.15	1
N-CA-CB	103.00	110.56	1
CA-C-N	116.90	127.20	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	134.05	1
OE1-CD-NE2	122.60	115.75	1
CA-CB-CG	113.80	120.65	1
C-N-CA	121.70	134.02	1
OE1-CD-NE2	122.60	115.80	1
CB-CG-CD2	131.20	122.36	1
CB-CG-CD2	131.20	122.41	1
CA-CB-CG	112.60	119.36	1
N-CA-CB	103.00	110.41	1
ND1-CG-CD2	106.10	112.84	1
N-CA-CB	103.00	110.39	1
C-N-CA	121.70	133.75	1
CG-CD2-NE2	107.20	100.52	1
C-N-CA	121.70	133.69	1
O-C-N	123.00	112.36	1
CA-CB-OG	111.10	124.40	1
N-CA-CB	103.00	110.31	1
N-CA-CB	103.00	110.29	1
CB-CG-CD2	131.20	122.60	1
CA-CB-CG	113.80	120.41	1
N-CA-CB	110.50	99.27	1
C-N-CA	121.70	133.58	1
OD1-CG-ND2	122.60	116.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	103.00	110.25	1
OD1-CG-ND2	122.60	116.01	1
CG-CD-NE2	116.40	126.28	1
OD1-CG-ND2	122.60	116.02	1
NE-CZ-NH2	119.20	113.28	1
N-CA-CB	110.40	100.62	1
N-CA-CB	103.00	110.17	1
OE1-CD-NE2	122.60	116.10	1
ND1-CE1-NE2	108.40	114.90	1
NE-CZ-NH2	119.20	125.05	1
N-CA-CB	110.40	100.71	1
OD1-CG-ND2	122.60	116.15	1
NE-CZ-NH1	121.50	115.05	1
CA-CB-CG	112.60	106.16	1
CB-CG-ND1	122.70	132.36	1
OD1-CG-ND2	122.60	116.16	1
CB-CG-CD2	131.20	122.85	1
CA-CB-CG	112.60	119.02	1
C-N-CA	121.70	133.26	1
NE-CZ-NH1	121.50	127.92	1
C-N-CA	121.70	133.24	1
C-CA-CB	110.50	120.07	1
ND1-CE1-NE2	108.40	114.74	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O-C-N	123.00	112.86	1
OD1-CG-ND2	122.60	116.28	1
CA-CB-CG	113.80	120.11	1
N-CA-CB	103.00	109.93	1
CA-C-N	116.90	126.31	1
CA-CB-CG	114.10	126.64	1
CA-N-CD	112.00	103.24	1
CA-C-O	120.80	131.38	1
CB-CG-CD	112.60	102.03	1
NH1-CZ-NH2	119.30	111.22	1
NE-CZ-NH1	121.50	127.69	1
CA-CB-CG2	110.50	121.01	1
N-CA-CB	103.00	109.78	1
ND1-CE1-NE2	108.40	114.54	1
OE1-CD-NE2	122.60	116.46	1
C-N-CA	121.70	132.70	1
N-CA-CB	110.50	120.85	1
N-CD-CG	103.20	112.33	1
C-CA-CB	110.10	121.64	1
O-C-N	123.00	113.28	1
ND1-CE1-NE2	108.40	114.46	1
CB-CG-CD	112.60	102.31	1
N-CA-CB	103.00	109.65	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	116.56	1
CA-CB-CG	113.80	119.84	1
ND1-CG-CD2	106.10	112.14	1
OD1-CG-ND2	122.60	116.57	1
OD1-CG-ND2	122.60	128.63	1
N-CA-CB	110.50	100.25	1
NH1-CZ-NH2	119.30	127.13	1
NE-CZ-NH1	121.50	115.48	1
O-C-N	123.00	113.37	1
N-CA-CB	110.50	100.28	1
CA-CB-CG	104.50	93.08	1
OE1-CD-NE2	122.60	116.59	1
NE-CZ-NH2	119.20	124.61	1
C-N-CA	121.70	132.51	1
CD-NE-CZ	124.40	132.80	1
N-CA-CB	110.50	100.37	1
C-CA-CB	110.10	121.42	1
N-CA-CB	110.50	100.39	1
OE1-CD-NE2	122.60	116.67	1
ND1-CG-CD2	106.10	112.02	1
CB-CG-CD2	131.20	123.52	1
N-CD-CG	103.20	112.05	1
C-CA-CB	110.50	101.65	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-O	120.80	110.78	1
N-CA-CB	103.00	109.49	1
CA-CB-CG1	110.40	120.42	1
NE-CZ-NH2	119.20	124.50	1
N-CA-CB	110.40	101.58	1
OE1-CD-NE2	122.60	116.73	1
CA-CB-CG	114.10	102.37	1
O-C-N	123.00	113.62	1
N-CD-CG	103.20	111.96	1
NE-CZ-NH1	121.50	127.33	1
CG-CD-NE	112.00	99.19	1
OD1-CG-ND2	122.60	116.78	1
CA-CB-CG	113.80	107.99	1
N-CA-CB	103.00	109.39	1
ND1-CG-CD2	106.10	111.90	1
C-CA-CB	110.10	121.10	1
C-CA-CB	110.10	121.09	1
N-CA-CB	103.00	109.36	1
CA-CB-CG	113.80	119.57	1
N-CA-CB	103.00	109.35	1
C-N-CA	121.70	132.09	1
N-CD-CG	103.20	111.86	1
NE-CZ-NH2	119.20	124.39	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	103.00	109.34	1
N-CD-CG	103.20	111.85	1
CA-CB-CG	112.60	118.34	1
CA-CB-CG	113.80	119.54	1
O-C-N	123.00	113.82	1
CA-C-N	116.90	125.51	1
O-C-N	123.00	113.85	1
CA-CB-CG	112.60	118.31	1
OE1-CD-NE2	122.60	116.91	1
N-CA-CB	103.00	109.24	1
NE-CZ-NH2	119.20	124.30	1
C-CA-CB	110.10	120.85	1
NE-CZ-NH2	119.20	124.28	1
CA-CB-CG	112.60	106.95	1
C-N-CA	121.70	131.85	1
N-CA-CB	103.00	109.19	1
CA-C-N	116.90	125.33	1
CA-CB-CG	112.60	118.22	1
C-N-CA	121.70	131.81	1
CA-CB-CG	112.60	106.99	1
N-CA-CB	103.00	109.16	1
OE1-CD-NE2	122.60	117.01	1
CA-C-O	120.80	111.31	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-O	120.80	130.28	1
C-N-CA	121.70	131.73	1
C-CA-CB	110.50	118.85	1
NE-CZ-NH2	119.20	124.21	1
CB-CG-CD2	131.20	123.97	1
CA-CB-CG	112.60	118.15	1
CG-CD2-NE2	107.20	101.65	1
OE1-CD-NE2	122.60	117.06	2
O-C-N	123.00	114.14	1
OD1-CG-ND2	122.60	117.07	1
NE-CZ-NH1	121.50	127.03	1
OE1-CD-NE2	122.60	117.07	1
C-N-CA	121.70	131.65	1
CB-CG-ND2	116.40	108.11	1
CA-C-N	116.90	125.18	1
CD2-NE2-CE1	109.00	103.48	1
N-CA-CB	103.00	109.06	1
N-CD-CG	103.20	111.46	1
CA-CB-CG1	110.40	119.76	1
C-N-CA	121.70	131.60	2
NE-CZ-NH2	119.20	114.26	1
O-C-N	123.00	114.22	1
N-CA-CB	103.00	109.04	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-O	120.80	111.48	1
CB-CG-ND1	122.70	130.91	1
NH1-CZ-NH2	119.30	112.19	1
CA-N-CD	112.00	104.36	1
CD2-NE2-CE1	109.00	103.55	1
N-CA-CB	103.00	109.00	1
N-CA-CB	110.50	101.24	1
ND1-CG-CD2	106.10	111.55	1
C-N-CA	121.70	131.50	1
C-CA-CB	110.50	118.66	1
CA-C-N	116.90	125.06	1
ND1-CE1-NE2	108.40	113.84	1
CD1-CG-CD2	110.80	98.88	1
C-CA-CB	110.10	120.39	1
CA-N-CD	112.00	104.43	1
CA-CB-CG	114.10	124.91	1
N-CA-CB	111.50	102.32	1
C-N-CA	121.70	131.41	1
NE-CZ-NH1	121.50	126.87	2
N-CA-CB	103.00	108.91	1
CD1-CG-CD2	110.80	99.00	1
N-CA-CB	103.00	108.89	1
CD2-NE2-CE1	109.00	103.65	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	131.31	3
CA-CB-CG	113.80	108.46	1
CB-CG-CD2	120.70	111.63	1
NE-CZ-NH2	119.20	114.40	1
CA-CB-CG	113.80	119.13	1
N-CD-CG	103.20	111.19	2
O-C-N	123.00	114.48	1
C-N-CA	121.70	131.28	1
CA-CB-CG	112.60	117.92	1
NH1-CZ-NH2	119.30	112.38	1
OD1-CG-ND2	122.60	117.28	1
CA-C-O	120.80	111.77	1
CA-CB-CG	113.90	123.46	1
ND1-CG-CD2	106.10	111.41	1
CG-ND1-CE1	109.30	100.28	1
CB-CG-CD2	131.20	124.31	1
CA-CB-CG	113.80	108.50	1
C-N-CA	121.70	131.22	3
OE1-CD-NE2	122.60	117.31	1
N-CA-CB	103.00	108.81	1
CG-CD1-CE1	121.20	113.27	1
CG-CD-OE2	118.40	106.24	1
CA-CB-CG1	110.40	119.38	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	131.20	2
N-CA-CB	103.00	108.80	1
C-CA-CB	110.10	120.12	1
N-CA-CB	110.50	119.47	1
CA-CB-CG1	110.40	119.36	1
OD1-CG-ND2	122.60	117.33	1
CA-N-CD	112.00	104.64	1
CA-CB-CG1	110.40	119.33	1
CA-C-N	116.20	126.70	1
O-C-N	123.00	114.60	1
CG1-CB-CG2	110.80	99.27	1
NE-CZ-NH1	121.50	126.74	1
CA-CB-CG	113.80	119.04	1
OE1-CD-NE2	122.60	117.36	1
CA-CB-CG	112.60	117.84	1
N-CA-CB	103.00	108.76	1
C-N-CA	121.70	131.13	1
C-CA-CB	110.10	120.04	1
CA-CB-CG2	110.40	119.29	1
CA-CB-CG	112.60	117.83	1
N-CA-CB	110.50	101.62	1
C-N-CA	121.70	131.10	1
C-N-CA	121.70	131.09	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
NH1-CZ-NH2	119.30	112.52	1
N-CA-CB	103.00	108.73	1
C-CA-CB	110.10	119.99	1
N-CD-CG	103.20	111.00	1
N-CA-CB	103.00	108.72	1
NH1-CZ-NH2	119.30	112.55	1
C-N-CA	121.70	131.05	1
O-C-N	123.00	131.30	1
N-CA-CB	110.40	102.62	1
CA-CB-CG	112.60	107.42	1
CG-CD-NE2	116.40	124.17	1
CA-C-N	116.90	124.66	1
N-CD-CG	103.20	110.96	1
C-CA-CB	110.10	119.92	1
OD1-CG-ND2	122.60	117.44	1
N-CA-CB	110.40	102.66	1
N-CA-CB	103.00	108.67	1
CA-CB-CG	112.60	107.45	1
CA-CB-CG	112.60	117.75	1
CA-CB-OG1	109.60	117.32	1
ND1-CG-CD2	106.10	111.24	1
N-CD-CG	103.20	110.91	2
OD1-CG-ND2	122.60	117.47	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.40	102.70	1
C-N-CA	121.70	130.93	1
CA-CB-CG	114.10	103.85	1
CB-CG-CD2	131.20	124.54	1
NE-CZ-NH2	119.20	123.81	1
N-CA-CB	110.40	102.72	1
C-N-CA	121.70	130.90	1
N-CA-CB	110.50	101.81	1
N-CD-CG	103.20	110.86	1
CA-C-N	116.20	126.41	1
C-CA-CB	110.10	119.80	1
N-CA-CB	103.00	108.61	1
N-CA-CB	110.50	101.83	1
C-N-CA	121.70	130.87	2
N-CA-CB	103.00	108.60	2
CA-C-N	116.90	124.54	1
N-CA-CB	110.50	101.85	1
CA-N-CD	112.00	104.88	1
OE1-CD-NE2	122.60	117.52	2
ND1-CG-CD2	106.10	111.17	1
NE-CZ-NH1	121.50	126.57	1
C-N-CA	121.70	130.82	1
OD1-CG-ND2	122.60	117.54	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.50	101.90	1
N-CA-CB	110.40	102.81	1
C-N-CA	121.70	130.80	1
N-CA-CB	103.00	108.54	1
O-C-N	123.00	114.95	1
N-CA-CB	110.50	101.95	1
N-CA-CB	103.00	108.53	1
CA-C-O	120.80	112.25	1
N-CA-CB	110.40	102.86	1
CA-N-CD	112.00	104.97	1
CD2-NE2-CE1	109.00	114.02	1
CA-CB-CG	112.60	117.61	1
C-CA-CB	110.10	119.62	1
C-N-CA	121.70	130.72	1
CB-CG-CD2	120.80	113.29	1
N-CD-CG	103.20	110.71	1
C-N-CA	121.70	130.71	1
C-N-CA	121.70	112.69	1
C-CA-CB	110.10	100.59	1
C-CA-CB	110.50	118.00	1
N-CA-CB	110.50	102.00	1
CA-CB-CG	114.10	104.10	1
CB-CG-CD2	131.20	124.71	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-N	116.90	124.39	1
O-C-N	123.00	130.98	1
OD1-CG-ND2	122.60	117.61	1
C-N-CA	121.70	130.68	1
N-CA-CB	103.00	108.48	1
CA-N-CD	112.00	105.03	1
ND1-CE1-NE2	108.40	113.37	1
CB-CG-CD	112.60	104.15	1
CB-CG-CD2	131.20	124.75	1
NH1-CZ-NH2	119.30	112.86	1
N-CA-CB	110.40	102.97	1
CA-CB-CG	112.60	117.55	1
C-N-CA	121.70	130.61	1
N-CA-CB	103.00	108.45	1
CA-C-N	116.90	124.32	1
O-C-N	123.00	115.09	1
C-CA-CB	110.50	117.91	1
CA-CB-CG	112.60	117.54	1
NE-CZ-NH1	121.50	116.57	1
CD1-CG-CD2	110.80	99.95	1
OE1-CD-NE2	122.60	117.67	1
N-CA-CB	103.00	108.42	1
NE-CZ-NH1	121.50	126.42	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	130.55	1
N-CA-CB	103.00	108.41	1
CA-N-CD	112.00	105.12	1
O-C-N	123.00	115.14	1
NE-CZ-NH2	119.20	123.61	1
CB-CG-CD2	131.20	124.83	2
O-C-N	123.00	130.84	1
C-N-CA	121.70	130.52	1
N-CA-CB	103.00	108.39	1
C-N-CA	121.70	130.51	1
CB-CG-CD1	110.70	125.38	1
N-CA-CB	110.50	102.20	1
O-C-N	123.00	115.20	1
C-N-CA	121.70	130.47	1
CA-C-O	120.80	112.52	1
CB-CG-CD	112.60	104.33	1
CA-C-O	120.80	112.53	1
C-N-CA	121.70	130.46	1
C-CA-CB	110.50	117.80	1
CA-CB-CG	112.60	117.46	1
N-CA-CB	103.00	108.34	1
C-CA-CB	110.10	119.32	1
N-CA-CB	103.00	108.33	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.50	102.26	1
CA-C-N	116.90	124.17	1
O-C-N	123.00	115.25	1
CG-ND1-CE1	109.30	101.07	1
CA-C-O	120.80	112.57	1
C-N-CA	121.70	130.42	1
ND1-CE1-NE2	108.40	113.24	1
OE1-CD-NE2	122.60	117.76	1
CA-CB-CG	114.10	104.43	1
O-C-N	123.00	115.26	1
NH1-CZ-NH2	119.30	113.02	1
C-N-CA	121.70	130.39	1
N-CA-CB	110.50	102.30	1
C-CA-CB	110.10	119.26	1
NE-CZ-NH1	121.50	126.32	1
C-N-CA	121.70	130.35	1
N-CA-CB	110.40	103.20	1
NH1-CZ-NH2	119.30	113.06	1
CA-C-O	120.80	128.95	1
C-N-CA	121.70	130.33	1
NE-CZ-NH1	121.50	126.29	1
C-N-CA	121.70	130.32	1
C-CA-CB	110.10	101.01	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.40	103.23	1
N-CA-CB	110.50	102.37	2
CG-CD2-CE2	121.20	114.04	1
OE1-CD-NE2	122.60	117.83	1
CA-C-O	120.80	112.69	1
CA-CB-CG2	110.50	102.39	1
CA-CB-CG	114.10	104.57	1
CA-CB-CG	112.60	117.37	1
CA-CB-CG	113.80	109.04	1
N-CA-CB	110.40	103.26	2
NE-CZ-NH2	119.20	123.49	1
N-CA-CB	110.50	118.58	1
N-CA-CB	103.00	108.23	1
CG-CD2-NE2	107.20	102.45	1
N-CD-CG	103.20	110.33	1
CA-CB-CG2	110.40	118.47	1
N-CA-CB	103.00	108.22	1
CA-C-O	120.80	112.74	1
CA-CB-CG	112.60	117.34	1
C-N-CA	121.70	130.21	1
C-CA-CB	110.10	119.07	1
C-CA-CB	110.10	101.13	1
N-CA-CB	110.50	102.49	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.40	103.35	1
NE-CZ-NH2	119.20	114.97	1
O-C-N	123.00	115.48	1
CG-CD-NE2	116.40	123.44	1
N-CA-CB	110.40	103.36	1
N-CA-CB	110.50	118.48	1
C-N-CA	121.70	130.14	2
NE-CZ-NH1	121.50	126.19	1
CA-C-N	116.20	125.57	1
NE-CZ-NH2	119.20	114.98	1
OE1-CD-NE2	122.60	117.92	1
CA-C-O	120.80	112.84	1
NE-CZ-NH1	121.50	126.18	1
CA-C-N	116.20	125.56	1
CB-CG-CD2	131.20	125.12	1
OD1-CG-ND2	122.60	117.92	1
CD-NE-CZ	124.40	130.95	1
C-N-CA	121.70	130.11	1
N-CD-CG	103.20	110.20	1
CD2-NE2-CE1	109.00	104.33	1
N-CA-CB	103.00	108.13	1
OD1-CG-ND2	122.60	117.94	1
O-C-N	123.00	115.54	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-O	120.80	128.72	1
C-N-CA	121.70	130.08	1
N-CD-CG	103.20	110.18	1
CA-CB-CG	112.60	117.25	1
CA-C-O	120.80	128.69	1
N-CA-CB	110.50	118.39	1
C-CA-CB	110.10	101.29	1
CA-C-N	116.20	125.47	1
C-CA-CB	110.10	118.91	1
OD1-CG-ND2	122.60	117.97	1
CA-N-CD	112.00	105.52	1
CA-CB-CG1	110.40	118.26	1
CA-CB-CG2	110.40	118.26	1
CA-CB-CG2	110.50	102.64	1
CD1-CG-CD2	110.80	100.63	1
C-CA-CB	110.50	117.43	1
CA-CB-CG	112.60	117.22	1
CD1-CG-CD2	110.80	100.65	1
CA-CB-CG	114.10	104.88	1
CB-CG-CD	112.60	104.78	1
CA-CB-CG	112.60	108.00	1
C-N-CA	121.70	129.98	1
C-CA-CB	110.10	118.81	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OD1-CG-ND2	122.60	118.02	1
O-C-N	123.00	115.67	1
CA-C-O	120.80	113.02	1
C-N-CA	121.70	129.94	1
CA-C-O	120.80	130.40	1
C-CA-CB	110.50	103.64	1
C-CA-CB	110.10	118.78	1
C-CA-CB	110.50	103.65	1
CD1-CG-CD2	110.80	100.76	1
OD1-CG-ND2	122.60	118.04	1
N-CA-CB	103.00	108.02	1
N-CD-CG	103.20	110.04	2
CA-C-O	120.80	113.05	1
O-C-N	123.00	115.71	1
N-CA-CB	110.50	102.76	1
C-N-CA	121.70	129.89	3
CD-NE-CZ	124.40	118.04	1
N-CA-CB	110.50	102.77	2
CB-CG-CD2	131.20	125.29	1
C-CA-CB	110.10	118.73	1
N-CA-CB	110.50	102.78	1
N-CA-CB	103.00	108.00	1
C-CA-CB	110.10	118.72	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	112.60	108.06	1
C-CA-CB	110.10	118.71	1
CA-C-N	116.20	125.25	2
OD1-CG-ND2	122.60	118.07	1
C-N-CA	121.70	129.84	1
C-CA-CB	110.10	101.50	1
N-CA-CB	110.50	102.81	1
CA-C-N	116.90	123.68	1
N-CD-CG	103.20	109.98	1
CG-CD2-NE2	107.20	111.72	1
CB-CG-CD2	120.80	114.03	1
C-CA-CB	110.10	118.67	1
N-CA-CB	110.50	102.83	1
CA-CB-CG1	110.40	102.74	1
CA-CB-CG	113.90	122.01	1
C-N-CA	121.70	129.81	1
O-C-N	123.00	115.81	1
CA-C-N	116.90	123.64	1
N-CD-CG	103.20	109.94	1
C-CA-CB	110.10	101.56	1
OD1-CG-ND2	122.60	118.11	1
C-CA-CB	110.10	118.63	1
CB-CG-CD	112.60	104.97	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O-C-N	123.00	115.82	1
C-N-CA	121.70	129.77	1
CB-CG-ND2	116.40	123.13	1
O-C-N	123.00	115.83	1
CB-CG-CD1	110.70	124.15	1
C-CA-CB	110.50	117.22	1
C-CA-CB	110.10	118.62	1
CA-C-N	116.90	123.62	1
CA-CB-CG	114.10	105.15	1
CA-CB-OG1	109.60	116.31	1
C-N-CA	121.70	129.75	1
C-CA-CB	110.10	118.59	1
C-N-CA	121.70	129.74	1
O-C-N	123.00	115.86	1
CB-CG-OD1	120.80	129.72	1
C-N-CA	121.70	129.73	2
OD1-CG-ND2	122.60	118.14	1
CA-CB-CG	114.10	105.18	1
N-CD-CG	103.20	109.89	1
C-N-CA	121.70	113.68	1
N-CD-CG	103.20	109.88	1
CB-CG-CD1	120.70	128.27	1
C-CA-CB	110.10	118.55	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
ND1-CE1-NE2	108.40	112.85	1
NE-CZ-NH2	119.20	115.20	1
CA-C-N	116.20	125.09	1
CA-C-O	120.80	113.25	1
OD1-CG-ND2	122.60	118.16	1
CA-N-CD	112.00	105.78	1
CA-C-N	116.90	123.56	1
CD-NE-CZ	124.40	130.61	1
CA-C-O	120.80	113.26	1
N-CD-CG	103.20	109.85	1
OD1-CG-ND2	122.60	118.17	1
CG-SD-CE	100.90	91.17	1
NE-CZ-NH1	121.50	125.92	1
CG-ND1-CE1	109.30	101.79	1
NE-CZ-NH2	119.20	115.22	1
CA-CB-CG	113.80	118.22	1
CA-CB-CG	112.60	108.18	1
CA-C-N	116.20	125.03	1
C-N-CA	121.70	129.65	1
CA-CB-OG	111.10	102.27	1
O-C-N	123.00	115.94	1
CB-CG-ND2	116.40	109.78	1
ND1-CG-CD2	106.10	110.51	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-N	116.90	123.51	1
C-N-CA	121.70	129.64	1
CD-NE-CZ	124.40	130.57	1
CB-CG-CD	112.60	120.09	1
NE-CZ-NH2	119.20	123.16	1
CA-C-O	120.80	113.32	1
C-N-CA	121.70	129.62	1
OE1-CD-NE2	122.60	118.20	1
N-CA-CB	103.00	107.84	1
CA-CB-CG	104.50	112.85	1
CA-CB-CG	104.50	96.15	1
C-CA-CB	110.50	117.09	1
CA-C-N	116.90	123.49	2
CA-CB-CG	113.90	105.99	1
CA-C-N	116.20	124.98	2
CA-N-CD	112.00	105.85	1
N-CD-CG	103.20	109.78	1
O-C-N	123.00	115.98	1
CA-CB-CG	114.10	105.33	1
N-CA-CB	110.50	103.05	1
C-CA-CB	110.10	118.42	1
O-C-N	123.00	130.01	1
CA-CB-CG	113.80	109.42	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	118.23	1
N-CA-CB	103.00	107.81	1
CA-C-N	116.90	123.46	1
C-N-CA	121.70	129.57	1
CG-ND1-CE1	109.30	101.87	1
O-C-N	123.00	116.01	1
NH1-CZ-NH2	119.30	113.63	1
O-C-N	123.00	116.02	1
C-N-CA	121.70	129.56	1
C-N-CA	121.70	129.55	1
CA-C-O	120.80	128.21	1
N-CA-CB	103.00	107.79	1
C-CA-CB	110.50	117.03	1
NE-CZ-NH1	121.50	125.86	1
CB-CG-CD	112.60	105.20	1
O-C-N	123.00	116.03	1
CA-CB-CG	114.10	122.80	1
CA-CB-CG	114.10	105.40	1
C-CA-CB	110.10	118.36	1
C-N-CA	121.70	129.52	1
O-C-N	123.00	129.95	1
CA-C-O	120.80	113.41	1
N-CA-CB	110.40	103.88	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	118.26	1
CD1-CG-CD2	118.60	125.11	1
CA-CB-CG	114.10	105.42	1
CA-CB-CG	112.60	116.94	1
C-CA-CB	110.50	117.00	1
CA-C-N	116.90	123.40	2
N-CA-CB	110.50	103.14	1
C-CA-CB	110.50	116.99	2
CD2-NE2-CE1	109.00	104.67	1
CA-CB-CG	112.60	116.93	1
C-N-CA	121.70	129.49	1
C-N-CA	121.70	129.48	1
OD1-CG-ND2	122.60	118.28	1
CA-C-N	116.20	124.84	1
C-CA-CB	110.10	101.89	1
CB-CG-CD	112.60	105.26	1
N-CA-CB	110.50	103.16	1
C-N-CA	121.70	129.46	1
N-CA-CB	103.00	107.74	1
CA-C-N	116.90	123.37	1
OE1-CD-NE2	122.60	118.29	1
CB-CG-CD	111.30	121.21	1
N-CA-CB	110.50	103.17	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.40	103.94	1
CA-CB-CG	113.80	118.11	1
CA-CB-CG1	110.40	117.72	1
CA-C-N	116.20	124.81	1
NE-CZ-NH1	121.50	117.20	1
O-C-N	123.00	116.12	1
N-CA-CB	110.50	103.19	1
CG1-CB-CG2	110.80	101.34	1
CA-C-N	116.20	124.79	1
NH1-CZ-NH2	119.30	113.72	1
O-C-N	123.00	129.87	1
CA-CB-CG	114.10	105.52	1
C-N-CA	121.70	129.42	1
CG-CD-NE2	116.40	122.83	1
NH1-CZ-NH2	119.30	113.73	1
CB-CG-CD2	120.80	114.39	1
CG-ND1-CE1	109.30	102.03	1
ND1-CG-CD2	106.10	110.37	1
N-CA-CB	110.40	103.99	1
CA-C-O	120.80	113.54	1
C-CA-CB	110.10	118.22	1
C-CA-CB	110.10	118.21	1
NH1-CZ-NH2	119.30	113.75	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.50	117.75	1
O-C-N	123.00	116.18	1
CA-C-N	116.20	107.68	1
N-CA-CB	103.00	107.68	1
N-CA-CB	110.40	104.02	1
CG1-CB-CG2	110.80	101.45	1
CA-C-N	116.20	107.71	1
CD1-CG-CD2	110.80	120.14	1
C-N-CA	121.70	129.34	1
NE-CZ-NH2	119.20	123.02	1
C-N-CA	121.70	114.07	1
O-C-N	123.00	116.22	1
NH1-CZ-NH2	119.30	113.79	1
C-N-CA	121.70	129.33	1
OD1-CG-ND2	122.60	118.36	1
NE-CZ-NH1	121.50	125.73	1
C-N-CA	121.70	129.32	1
CA-CB-CG	114.10	105.64	1
CA-C-O	120.80	127.99	1
C-N-CA	121.70	129.31	3
N-CA-CB	103.00	107.65	2
O-C-N	123.00	116.24	1
CG-CD1-CE1	121.20	114.87	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	110.50	116.83	1
NH1-CZ-NH2	119.30	113.82	1
N-CA-CB	110.50	117.67	1
O-C-N	123.00	116.26	2
C-N-CA	121.70	129.28	1
CA-C-O	120.80	113.64	1
OD1-CG-ND2	122.60	118.39	1
CB-CG-ND2	116.40	122.71	1
O-C-N	123.00	129.73	1
C-N-CA	121.70	129.27	1
N-CD-CG	103.20	109.51	1
CD1-CG-CD2	110.80	101.55	1
O-C-N	123.00	116.27	1
CA-CB-CG	114.10	105.69	1
OG1-CB-CG2	109.30	117.71	1
N-CA-CB	103.00	107.62	1
CD-NE-CZ	124.40	130.28	1
C-N-CA	121.70	129.26	1
CD1-CG-CD2	118.60	124.90	1
CA-CB-CG2	110.40	117.54	1
NH1-CZ-NH2	119.30	113.84	1
CA-C-N	116.90	123.20	1
CG-CD1-CE1	121.20	114.90	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	129.25	1
N-CD-CG	103.20	109.49	2
N-CA-CB	111.50	118.63	1
CA-CB-OG1	109.60	103.31	1
CA-CB-CG	104.50	96.54	1
C-N-CA	121.70	129.24	4
C-CA-CB	110.50	116.78	1
C-N-CA	121.70	129.23	1
CA-C-O	120.80	113.69	1
O-C-N	123.00	116.31	1
CB-CG-CD2	120.80	114.53	1
C-N-CA	121.70	129.22	1
CA-CB-CG	114.10	122.45	1
C-CA-CB	110.10	118.03	1
N-CA-CB	103.00	107.59	1
N-CA-CB	111.50	118.59	1
CA-CB-CG	114.10	105.77	1
CA-C-O	120.80	113.72	1
O-C-N	123.00	129.66	1
N-CA-CB	103.00	107.58	1
C-N-CA	121.70	129.19	1
CD2-CE2-CZ	119.60	127.09	1
N-CA-CB	110.40	116.64	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG2	110.50	117.57	1
N-CA-CB	110.50	117.57	1
C-CA-CB	110.50	116.73	1
CA-CB-CG	104.50	112.39	1
C-N-CA	121.70	129.17	1
CA-C-O	120.80	113.74	2
OE1-CD-NE2	122.60	118.45	1
CA-CB-CG	112.60	116.75	1
CA-CB-CG	113.80	109.65	1
CB-CG-CD2	131.20	125.81	1
CB-CG-CD2	110.70	123.14	1
N-CA-CB	110.50	103.45	1
CA-CB-CG	113.90	121.36	1
CD1-CG-CD2	110.80	101.68	1
N-CA-CB	110.50	103.46	1
N-CA-CB	103.00	107.55	1
CA-CB-CG	113.80	109.66	1
CA-C-O	120.80	113.77	1
C-CA-CB	110.10	102.25	1
N-CD-CG	103.20	109.40	1
C-N-CA	121.70	129.14	1
NH1-CZ-NH2	119.30	113.93	1
C-N-CA	121.70	129.13	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.50	117.51	2
CA-C-N	116.20	124.44	1
N-CA-CB	103.00	107.53	1
C-N-CA	121.70	129.11	1
OD1-CG-ND2	122.60	118.48	1
O-C-N	123.00	116.42	1
CA-N-CD	112.00	106.25	1
CA-C-O	120.80	113.82	1
C-CA-CB	110.10	117.90	1
N-CA-CB	110.50	103.52	1
CA-C-N	116.20	124.40	1
CD2-NE2-CE1	109.00	104.90	1
OD1-CG-ND2	122.60	118.50	1
CA-C-N	116.90	123.04	1
NE-CZ-NH2	119.20	115.52	1
NE-CZ-NH2	119.20	122.88	1
CA-CB-CG	114.10	105.91	1
CA-CB-CG	113.80	117.89	1
O-C-N	123.00	116.46	2
CG-CD-NE2	116.40	122.53	1
NH1-CZ-NH2	119.30	113.99	1
N-CA-CB	110.50	103.55	2
C-N-CA	121.70	129.05	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	111.50	104.56	1
CB-CG-CD2	131.20	125.89	1
CA-CB-CG	112.60	116.68	1
C-CA-CB	111.40	103.65	1
N-CA-CB	110.50	103.57	1
CG-ND1-CE1	109.30	102.37	1
C-N-CA	121.70	129.04	1
O-C-N	123.00	129.52	1
CG-CD-OE1	118.40	127.77	1
CG-CD1-CE1	121.20	115.09	1
C-N-CA	121.70	129.03	1
O-C-N	123.00	116.48	1
OE1-CD-NE2	122.60	118.53	1
CA-CB-CG2	110.50	117.42	1
N-CA-C	111.00	122.40	1
CB-CG-CD2	120.80	114.70	1
OG1-CB-CG2	109.30	117.44	1
C-N-CA	121.70	129.02	2
CD-NE-CZ	124.40	130.09	1
O-C-N	123.00	129.50	1
N-CA-CB	110.40	104.31	1
N-CD-CG	103.20	109.29	1
O-C-N	123.00	116.50	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-O	120.80	113.90	1
CB-CG-CD1	120.80	126.89	1
CA-C-O	120.80	113.91	1
CA-CB-CG	112.60	116.65	1
C-CA-CB	110.10	117.80	1
OE1-CD-NE2	122.60	118.55	1
C-N-CA	121.70	128.99	1
O-C-N	123.00	116.52	2
CA-CB-CG	112.60	108.55	1
CA-CB-CG	104.50	112.19	1
N-CA-CB	110.50	103.62	1
CD1-CG-CD2	118.10	124.16	1
C-CA-CB	110.50	116.56	1
N-CD-CG	103.20	109.26	1
C-N-CA	121.70	128.97	2
C-CA-CB	110.10	117.77	1
C-N-CA	121.70	128.96	1
N-CA-CB	110.50	103.64	1
CG-ND1-CE1	109.30	102.44	1
CB-CG-CD2	131.20	125.96	1
N-CA-CB	110.50	103.65	1
ND1-CG-CD2	106.10	110.13	1
CA-CB-CG1	110.40	117.25	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	104.50	96.85	1
C-CA-CB	110.50	116.54	1
O-C-N	123.00	129.44	1
CB-CG-ND2	116.40	122.44	1
N-CA-CB	110.50	117.34	1
C-CA-CB	110.50	116.53	2
OD1-CG-ND2	122.60	118.58	1
C-N-CA	121.70	128.93	2
CB-CG-ND2	116.40	110.37	1
CA-C-O	120.80	113.97	1
CB-CG-CD1	120.80	126.82	1
C-N-CA	121.70	128.92	1
N-CA-CB	110.40	104.38	1
OD1-CG-ND2	122.60	118.59	1
OE1-CD-NE2	122.60	118.59	1
N-CA-CB	111.50	104.68	1
N-CA-CB	110.40	104.39	1
CA-C-N	116.90	122.91	1
NE-CZ-NH2	119.20	122.80	1
CA-C-N	116.20	108.20	1
CB-CG-CD1	120.80	114.80	1
CA-CB-HB2	121.00	109.00	1
CG-CD2-HD22	121.00	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
HB2-CB-HB3	97.99	110.00	1
NZ-CE-HE3	120.02	108.00	1
C-N-H	112.27	124.30	2
C-N-H	112.26	124.30	1
C-N-H	112.25	124.30	1
C-CA-HA	96.95	109.00	1
CA-CB-HB1	121.05	109.00	1
CB-CA-HA	96.94	109.00	1
HA2-CA-HA3	96.94	109.00	1
CG-ND2-HD21	107.93	120.00	1
CA-CB-HB3	96.93	109.00	1
CD-CG-HG3	97.92	110.00	1
CB-CG2-HG23	121.08	109.00	1
HD22-CD2-HD23	97.92	110.00	1
C-N-H	112.22	124.30	1
C-N-H	112.20	124.30	1
HB2-CB-HB3	97.89	110.00	1
CZ-NH2-HH21	107.88	120.00	1
HD12-CD1-HD13	97.87	110.00	1
HA2-CA-HA3	96.87	109.00	1
C-N-H	112.17	124.30	1
C-CA-HA3	96.87	109.00	1
C-CA-HA	96.87	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
HD11-CD1-HD13	97.87	110.00	1
CB-CG-HG2	121.14	109.00	1
HB2-CB-HB3	97.86	110.00	1
N-CA-HA	97.86	110.00	1
C-N-H	112.14	124.30	1
HB2-CB-HB3	97.84	110.00	1
CB-CG-HG2	121.16	109.00	1
CG-CB-HB3	95.83	108.00	1
CB-CG-HG3	121.18	109.00	1
HZ2-NZ-HZ3	121.18	109.00	1
CG-CD-HD3	121.18	109.00	1
C-N-H	112.11	124.30	1
CB-CG2-HG23	97.81	110.00	1
N-CA-HA	97.81	110.00	1
CG-CB-HB2	120.20	108.00	1
C-N-H	112.10	124.30	1
OG-CB-HB3	96.79	109.00	1
N-CA-HA	97.78	110.00	1
HD2-CD-HD3	122.23	110.00	1
HB2-CB-HB3	97.76	110.00	1
CG-CD2-HD23	121.25	109.00	1
HB2-CB-HB3	122.26	110.00	1
CA-N-H	126.27	114.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
HG22-CG2-HG23	96.72	109.00	1
HZ2-NZ-HZ3	96.72	109.00	1
CG2-CB-HB	95.72	108.00	1
CZ-NH1-HH12	107.71	120.00	1
HG2-CG-HG3	97.71	110.00	1
C-N-H	112.01	124.30	1
CA-CB-HB3	121.30	109.00	1
CD2-CG-HG	95.70	108.00	1
CA-CB-HB2	121.30	109.00	1
CG-CD2-HD22	96.70	109.00	1
C-N-H	112.00	124.30	1
HB2-CB-HB3	97.69	110.00	1
C-N-H	111.99	124.30	1
CG-CB-HB3	95.67	108.00	1
CZ-OH-HH	122.33	110.00	1
C-N-H	111.96	124.30	2
C-N-H	111.95	124.30	1
CD-CG-HG3	120.36	108.00	1
HB2-CB-HB3	97.62	110.00	1
C-N-H	111.92	124.30	2
C-N-H	111.91	124.30	1
C-N-H	111.90	124.30	1
CG-CB-HB3	120.41	108.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-HA	96.59	109.00	1
CA-CB-HB3	121.42	109.00	1
C-N-H	111.87	124.30	1
C-N-H	111.86	124.30	1
C-N-H	111.85	124.30	1
N-CD-HD2	121.46	109.00	1
CG-CB-HB3	95.54	108.00	1
HG2-CG-HG3	122.46	110.00	1
CG-CD1-HD12	121.47	109.00	1
N-CA-HA	97.52	110.00	1
HB2-CB-HB3	97.51	110.00	1
C-N-H	111.81	124.30	1
C-N-H	111.80	124.30	1
CG-CB-HB2	95.48	108.00	1
C-N-H	111.78	124.30	1
HB1-CB-HB3	97.47	110.00	1
C-N-H	111.77	124.30	1
N-CD-HD3	121.55	109.00	1
CA-CB-HB3	121.55	109.00	1
CD-CG-HG3	120.56	108.00	1
HG11-CG1-HG13	97.44	110.00	1
C-CA-HA	96.44	109.00	1
C-N-H	111.73	124.30	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-H	111.71	124.30	1
CA-CB-HB3	121.59	109.00	1
CA-N-H	126.60	114.00	1
HG2-CG-HG3	97.40	110.00	1
OG-CB-HB2	121.60	109.00	1
HB2-CB-HB3	97.39	110.00	1
C-N-H	111.69	124.30	1
CG-CB-HB2	95.36	108.00	1
HB2-CB-HB3	97.35	110.00	1
HB1-CB-HB3	97.35	110.00	1
HG11-CG1-HG13	97.34	110.00	1
CA-CB-HB2	121.66	109.00	1
HH11-NH1-HH12	107.33	120.00	1
CA-CB-HB3	121.67	109.00	1
C-CA-HA	96.31	109.00	1
CB-CG2-HG22	97.31	110.00	1
C-N-H	111.61	124.30	1
C-N-H	111.60	124.30	1
CG-CB-HB3	120.71	108.00	1
C-N-H	111.57	124.30	2
HD2-CD-HD3	97.27	110.00	1
HD22-CD2-HD23	97.26	110.00	1
CZ-OH-HH	122.77	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-H	111.53	124.30	1
C-N-H	111.51	124.30	1
CG-CB-HB2	120.79	108.00	1
HB2-CB-HB3	97.20	110.00	1
CG-CB-HB2	120.80	108.00	1
HG11-CG1-HG12	97.19	110.00	1
C-N-H	111.47	124.30	1
HB2-CB-HB3	97.17	110.00	1
CA-N-H	126.83	114.00	1
CZ-CE2-HE2	107.36	120.20	1
HD2-CD-HD3	97.16	110.00	1
CG-CB-HB2	95.14	108.00	1
HB2-CB-HB3	97.12	110.00	1
C-CA-HA	96.10	109.00	1
C-N-H	111.39	124.30	1
HE1-CE-HE3	97.07	110.00	1
C-N-H	111.36	124.30	1
SD-CE-HE2	121.94	109.00	1
C-N-H	111.35	124.30	1
C-N-H	111.32	124.30	1
CA-N-H	126.98	114.00	1
C-N-H	111.31	124.30	1
C-CA-HA	96.01	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
HD21-CD2-HD22	97.00	110.00	1
CA-CB-HB3	95.99	109.00	1
HB1-CB-HB2	96.99	110.00	1
HB1-CB-HB2	123.02	110.00	1
C-N-H	111.27	124.30	1
CG-CB-HB3	121.04	108.00	1
CA-CB-HB3	122.04	109.00	1
C-N-H	111.25	124.30	1
N-CA-HA	96.93	110.00	1
C-N-H	111.23	124.30	1
HB1-CB-HB2	96.92	110.00	1
C-N-H	111.22	124.30	1
HG11-CG1-HG13	96.90	110.00	1
C-N-H	111.18	124.30	2
C-N-H	111.13	124.30	2
HG11-CG1-HG13	96.83	110.00	1
HB2-CB-HB3	123.18	110.00	1
CB-CG2-HG22	122.18	109.00	1
N-CA-HA	96.81	110.00	1
C-N-H	111.11	124.30	1
CA-N-H	127.20	114.00	1
C-N-H	111.10	124.30	2
HB2-CB-HB3	96.80	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
HD2-CD-HD3	96.76	110.00	1
C-N-H	111.06	124.30	1
C-N-H	111.05	124.30	2
CA-N-H	127.25	114.00	1
HB2-CB-HB3	96.75	110.00	1
SD-CE-HE1	95.74	109.00	1
CD-CG-HG2	121.26	108.00	1
C-N-H	111.02	124.30	1
HD21-CD2-HD23	96.71	110.00	1
CA-CB-HB3	95.70	109.00	1
C-N-H	110.99	124.30	2
HZ1-NZ-HZ3	122.37	109.00	1
C-N-H	110.93	124.30	1
C-N-H	110.92	124.30	1
C-N-H	110.91	124.30	1
CB-CG-HG2	95.60	109.00	1
C-N-H	110.88	124.30	1
HG2-CG-HG3	96.56	110.00	1
CG-CB-HB2	94.55	108.00	1
HG22-CG2-HG23	96.55	110.00	1
C-N-H	110.84	124.30	1
C-CA-HA	96.53	110.00	1
HD2-CD-HD3	96.52	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
HB2-CB-HB3	96.52	110.00	1
HE2-CE-HE3	96.47	110.00	1
HB1-CB-HB2	96.46	110.00	1
C-N-H	110.75	124.30	1
C-N-H	110.72	124.30	1
HG2-CG-HG3	96.40	110.00	1
C-N-H	110.70	124.30	1
C-CA-HA	95.40	109.00	1
N-CA-HA2	96.38	110.00	1
HD21-CD2-HD23	96.37	110.00	1
C-CA-HA	95.36	109.00	1
HB2-CB-HB3	96.32	110.00	1
C-N-H	110.61	124.30	1
C-N-H	110.59	124.30	1
CA-N-H	127.71	114.00	1
NZ-CE-HE2	121.71	108.00	1
CB-CA-HA	95.23	109.00	1
C-N-H	110.53	124.30	2
CG-CD2-HD23	95.23	109.00	1
C-N-H	110.51	124.30	2
CB-CG-HG3	122.80	109.00	1
HB2-CB-HB3	96.18	110.00	1
HD2-CD-HD3	96.16	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-HB2	95.16	109.00	1
C-N-H	110.44	124.30	1
C-N-H	110.43	124.30	1
C-N-H	110.42	124.30	1
C-N-H	110.41	124.30	1
HB2-CB-HB3	96.07	110.00	1
HD2-CD-HD3	123.95	110.00	1
CB-CG1-HG11	122.98	109.00	1
C-N-H	110.30	124.30	1
HG22-CG2-HG23	95.99	110.00	1
CB-CA-HA	94.97	109.00	1
C-N-H	110.24	124.30	1
C-N-H	110.20	124.30	1
C-N-H	110.16	124.30	1
CB-CG-HG3	94.84	109.00	1
HB1-CB-HB2	95.84	110.00	1
HG21-CG2-HG23	95.83	110.00	1
C-N-H	110.12	124.30	1
C-N-H	110.10	124.30	1
C-N-H	110.05	124.30	1
C-N-H	110.03	124.30	1
C-N-H	110.01	124.30	1
SD-CE-HE1	94.71	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
HG22-CG2-HG23	123.30	109.00	1
HD11-CD1-HD12	95.70	110.00	1
C-N-H	109.99	124.30	1
HZ1-NZ-HZ3	94.69	109.00	1
HB2-CB-HB3	95.68	110.00	1
C-N-H	109.96	124.30	1
C-N-H	109.92	124.30	1
HB2-CB-HB3	95.59	110.00	1
C-N-H	109.88	124.30	1
C-N-H	109.87	124.30	1
C-N-H	109.84	124.30	1
HD12-CD1-HD13	95.50	110.00	1
C-N-H	109.79	124.30	1
C-N-H	109.75	124.30	1
C-N-H	109.73	124.30	1
HG2-CG-HG3	95.39	110.00	1
C-N-H	109.69	124.30	1
HG2-CG-HG3	95.36	110.00	1
C-N-H	109.64	124.30	1
C-N-H	109.58	124.30	1
CA-CB-HB2	94.28	109.00	1
C-N-H	109.57	124.30	1
C-N-H	109.53	124.30	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-HB3	94.18	109.00	1
C-N-H	109.44	124.30	1
C-N-H	109.40	124.30	2
C-N-H	109.28	124.30	1
C-N-H	109.21	124.30	1
C-N-H	109.18	124.30	1
C-N-H	109.17	124.30	1
CE-NZ-HZ2	94.86	110.00	1
HB2-CB-HB3	94.79	110.00	1
C-N-H	109.09	124.30	1
C-N-H	108.98	124.30	1
CG-CB-HB3	123.36	108.00	1
HB2-CB-HB3	94.59	110.00	1
HB2-CB-HB3	94.58	110.00	1
C-CA-HA	93.56	109.00	1
C-N-H	108.74	124.30	1
HD2-CD-HD3	125.58	110.00	1
HB2-CB-HB3	94.40	110.00	1
C-N-H	108.61	124.30	2
CG-CB-HB3	123.69	108.00	1
HB1-CB-HB2	94.28	110.00	1
C-N-H	108.48	124.30	2
HD21-CD2-HD22	125.82	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-H	108.42	124.30	1
HG2-CG-HG3	125.97	110.00	1
C-N-H	108.30	124.30	1
N-CA-HA	93.60	110.00	1
HB2-CB-HB3	93.46	110.00	1
C-N-H	107.73	124.30	1
HB2-CB-HB3	93.34	110.00	1
HB2-CB-HB3	93.17	110.00	1
CB-CA-HA	92.15	109.00	1
HB2-CB-HB3	93.15	110.00	1
CB-OG1-HG1	93.04	110.00	1
C-N-H	107.24	124.30	1
CA-N-H	131.12	114.00	1
HZ1-NZ-HZ3	91.88	109.00	1
C-N-H	106.95	124.30	1
HB2-CB-HB3	92.45	110.00	1
HG12-CG1-HG13	92.28	110.00	1
C-N-H	106.46	124.30	1
HD22-CD2-HD23	91.61	110.00	1
CG-CB-HB2	128.53	110.00	1
HG2-CG-HG3	128.68	110.00	1
C-N-H	105.54	124.30	1
C-N-H	104.95	124.30	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	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

All 0 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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	150	28	4
3	182	169	10	3
4	182	154	26	2
5	182	161	14	7
6	182	153	23	6
7	182	159	19	4

Model ID	Analyzed	Favored	Allowed	Outliers
8	182	153	23	6
9	182	156	19	7
10	182	155	23	4

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	Analyzed	Favored	Allowed	Outliers
1	147	123	14	10
2	147	133	12	2
3	147	132	9	6
4	147	125	16	6
5	147	108	24	15
6	147	126	13	8
7	147	116	19	12
8	147	119	21	7
9	147	124	15	8
10	147	120	20	7

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	2	THR
1	A	18	ILE
1	A	26	LEU
1	A	72	VAL
1	A	109	MET

Model ID	Chain	Residue ID	Residue type
1	A	116	GLN
1	A	151	ARG
1	A	165	LEU
1	A	168	THR
1	A	184	TYR
2	A	106	SER
2	A	177	GLU
3	A	17	GLN
3	A	26	LEU
3	A	33	ILE
3	A	99	PRO
3	A	102	SER
3	A	140	THR
4	A	12	MET
4	A	51	VAL
4	A	91	SER
4	A	97	PHE
4	A	112	HIS
4	A	140	THR
5	A	14	LEU
5	A	39	LEU
5	A	42	VAL
5	A	43	TYR

Model ID	Chain	Residue ID	Residue type
5	A	60	TYR
5	A	97	PHE
5	A	103	VAL
5	A	117	LEU
5	A	120	PHE
5	A	135	GLU
5	A	154	SER
5	A	164	ARG
5	A	168	THR
5	A	169	ASN
5	A	181	GLU
6	A	4	THR
6	A	52	TYR
6	A	85	GLU
6	A	110	LEU
6	A	134	ASN
6	A	140	THR
6	A	165	LEU
6	A	177	GLU
7	A	1	MET
7	A	4	THR
7	A	31	LEU
7	A	35	LEU

Model ID	Chain	Residue ID	Residue type
7	A	45	ASP
7	A	91	SER
7	A	126	GLN
7	A	128	VAL
7	A	132	LEU
7	A	165	LEU
7	A	180	LYS
7	A	183	ARG
8	A	44	LEU
8	A	72	VAL
8	A	108	LEU
8	A	140	THR
8	A	143	GLU
8	A	159	GLN
8	A	168	THR
9	A	6	HIS
9	A	15	LEU
9	A	19	GLN
9	A	104	SER
9	A	126	GLN
9	A	127	GLN
9	A	174	MET
9	A	178	SER

Model ID	Chain	Residue ID	Residue type
10	A	35	LEU
10	A	39	LEU
10	A	42	VAL
10	A	78	LEU
10	A	100	LEU
10	A	129	PRO
10	A	176	MET

Fit of model to data used for modeling ?

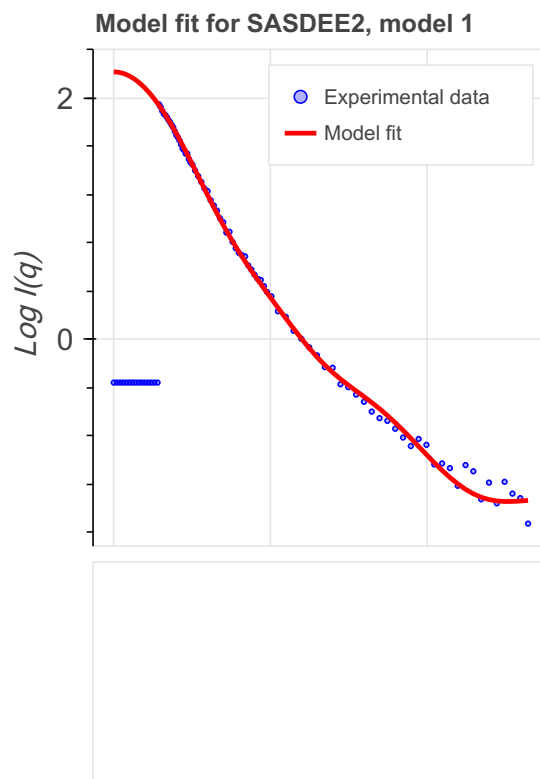
Fit of model(s) to SAS data

χ^2 goodness of fit and cormap analysis ?

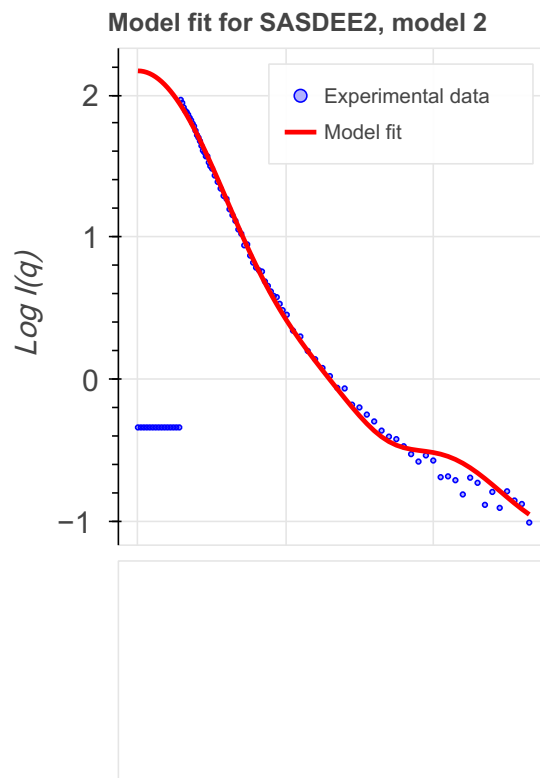
Model and fits displayed below were obtained from SASBDB. χ^2 values are a measure of fit of the model to data. A perfect fit has a χ^2 value of 1.0. ATSAS datcmp was used for hypothesis testing. All data sets are similar (i.e. the fit and the data collected) is the null hypothesis. *p*-value is a measure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

SASDB ID	Model	χ^2	p-value
SASDEE2	1	0.14	2.50E-03
SASDEE2	2	0.34	2.50E-03
SASDEE2	3	0.51	2.50E-03

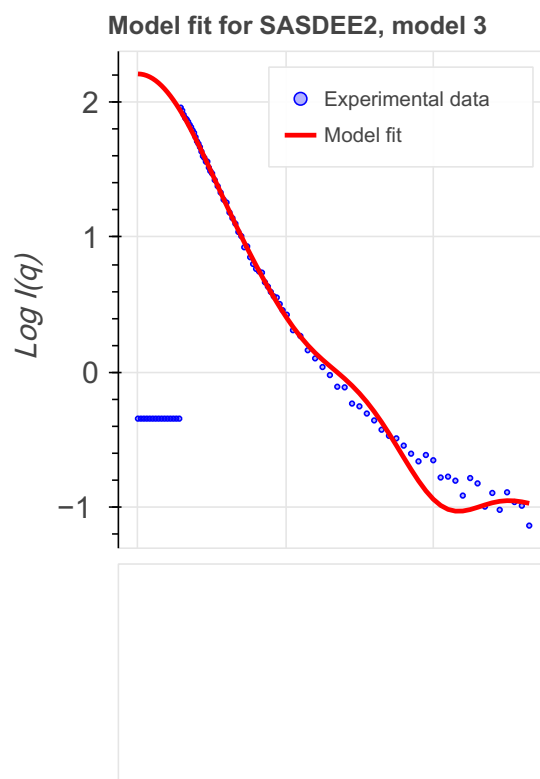
Model fit for SASDEE2 (fit/model number 1): Residual value plot is a measure to assess fit to the data. Residual values should be equally and randomly spaced around the horizontal axis.



Model fit for SASDEE2 (fit/model number 2): Residual value plot is a measure to assess fit to the data. Residual values should be equally and randomly spaced around the horizontal axis.



Model fit for SASDEE2 (fit/model number 3): Residual value plot is a measure to assess fit to the data. Residual values should be equally and randomly spaced around the horizontal axis.



Fit of model to data used for validation ?

Validation for this section is under development.

Acknowledgements

Development of integrative model validation metrics, implementation of a model validation pipeline, and creation of a validation report for integrative structures, are funded by NSF ABI awards (DBI-1756248, DBI-2112966, DBI-2112967, DBI-2112968, and DBI-1756250). The [PDB-Dev team](#) and members of [Sali lab](#) contributed model validation metrics and software packages.

Implementation of validation methods for SAS data and SAS-based models are funded by [RCSB PDB](#) (grant number DBI-1832184). Dr. Stephen Burley, Dr. John Westbrook, and Dr. Jasmine Young from [RCSB PDB](#), Dr. Jill Trehwella, Dr. Dina Schneidman, and members of the [SASBDB](#) repository are acknowledged for their advice and support in implementing SAS validation methods.

Members of the [wwPDB Integrative/Hybrid Methods Task Force](#) provided recommendations and community support for the project.