Integrative Structure Validation Report ?

July 22, 2024 - 05:39 PM PDT

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

Python-IHM Version 1.3
MolProbity Version 4.5.2
Integrative Modeling Validation Version 1.2

PDB ID	9A84
PDB-Dev ID	PDBDEV_00000369
Structure Title	52-mer bacterial gasdermin pore model from Vitiosangium sp.
Structure Authors	Johnson, A.G.; Mayer, M.L.; Schaefer, S.L.; McNamara-Bordewick, N.K.; Hummer, G.; Kranzusch, P.J.

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

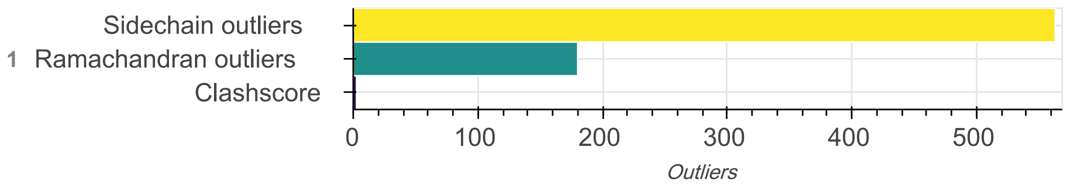
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 1 unique models, with 52 subunits in each model. A total of 2 datasets or restraints were used to build this entry. Each model is represented by 0 rigid bodies and 52 flexible or non-rigid units.

Entry composition

There is 1 unique type of models in this entry. This model is titled None/None.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	Gasdermin bGSDM	AA	a	234
1	2	1	Gasdermin bGSDM	BA	b	234
1	3	1	Gasdermin bGSDM	CA	c	234
1	4	1	Gasdermin bGSDM	DA	d	234
1	5	1	Gasdermin bGSDM	EA	e	234
1	6	1	Gasdermin bGSDM	FA	f	234
1	7	1	Gasdermin bGSDM	GA	g	234

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	8	1	Gasdermin bGSDM	HA	h	234
1	9	1	Gasdermin bGSDM	IA	i	234
1	10	1	Gasdermin bGSDM	JA	j	234
1	11	1	Gasdermin bGSDM	KA	k	234
1	12	1	Gasdermin bGSDM	LA	l	234
1	13	1	Gasdermin bGSDM	MA	m	234
1	14	1	Gasdermin bGSDM	NA	n	234
1	15	1	Gasdermin bGSDM	OA	o	234
1	16	1	Gasdermin bGSDM	PA	p	234
1	17	1	Gasdermin bGSDM	QA	q	234
1	18	1	Gasdermin bGSDM	RA	r	234
1	19	1	Gasdermin bGSDM	SA	s	234
1	20	1	Gasdermin bGSDM	TA	t	234
1	21	1	Gasdermin bGSDM	UA	u	234
1	22	1	Gasdermin bGSDM	VA	v	234

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	23	1	Gasdermin bGSDM	WA	w	234
1	24	1	Gasdermin bGSDM	XA	x	234
1	25	1	Gasdermin bGSDM	YA	y	234
1	26	1	Gasdermin bGSDM	ZA	z	234
1	27	1	Gasdermin bGSDM	A	A	234
1	28	1	Gasdermin bGSDM	B	B	234
1	29	1	Gasdermin bGSDM	C	C	234
1	30	1	Gasdermin bGSDM	D	D	234
1	31	1	Gasdermin bGSDM	E	E	234
1	32	1	Gasdermin bGSDM	F	F	234
1	33	1	Gasdermin bGSDM	G	G	234
1	34	1	Gasdermin bGSDM	H	H	234
1	35	1	Gasdermin bGSDM	I	I	234
1	36	1	Gasdermin bGSDM	J	J	234
1	37	1	Gasdermin bGSDM	K	K	234

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	38	1	Gasdermin bGSDM	L	L	234
1	39	1	Gasdermin bGSDM	M	M	234
1	40	1	Gasdermin bGSDM	N	N	234
1	41	1	Gasdermin bGSDM	O	O	234
1	42	1	Gasdermin bGSDM	P	P	234
1	43	1	Gasdermin bGSDM	Q	Q	234
1	44	1	Gasdermin bGSDM	R	R	234
1	45	1	Gasdermin bGSDM	S	S	234
1	46	1	Gasdermin bGSDM	T	T	234
1	47	1	Gasdermin bGSDM	U	U	234
1	48	1	Gasdermin bGSDM	V	V	234
1	49	1	Gasdermin bGSDM	W	W	234
1	50	1	Gasdermin bGSDM	X	X	234
1	51	1	Gasdermin bGSDM	Y	Y	234
1	52	1	Gasdermin bGSDM	Z	Z	234

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
2	2DEM class average	File	10.5281/zenodo.10570209
1	Experimental model	PDB	8sl0

Representation ?

This entry has only one representation and includes 0 rigid bodies and 52 flexible units

Chain ID	Rigid bodies	Non-rigid segments
AA	-	1-234
BA	-	1-234
CA	-	1-234
DA	-	1-234
EA	-	1-234
FA	-	1-234
GA	-	1-234
HA	-	1-234
IA	-	1-234
JA	-	1-234
KA	-	1-234
LA	-	1-234
MA	-	1-234
NA	-	1-234
OA	-	1-234

Chain ID	Rigid bodies	Non-rigid segments
PA	-	1-234
QA	-	1-234
RA	-	1-234
SA	-	1-234
TA	-	1-234
UA	-	1-234
VA	-	1-234
WA	-	1-234
XA	-	1-234
YA	-	1-234
ZA	-	1-234
A	-	1-234
B	-	1-234
C	-	1-234
D	-	1-234
E	-	1-234
F	-	1-234
G	-	1-234
H	-	1-234
I	-	1-234
J	-	1-234
K	-	1-234
L	-	1-234

Chain ID	Rigid bodies	Non-rigid segments
M	-	1-234
N	-	1-234
O	-	1-234
P	-	1-234
Q	-	1-234
R	-	1-234
S	-	1-234
T	-	1-234
U	-	1-234
V	-	1-234
W	-	1-234
X	-	1-234
Y	-	1-234
Z	-	1-234

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

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
1	1	None	None	To make the 52-mer pore model, protomer models (PDB 8SL0) were realigned using a custom script and a geometric model based on the number of protomers observed in the major 2D classes (52). Protomers were realigned to preserve the inter-subunit hydrogen bonding pattern observed in the slinky-like oligomer.	None	False	False

There are 2 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	Python	v3.9.7	model building	https://www.python.org/
2	MDAnalysis	v2.4.2	model building	https://www.mdanalysis.org/

Data quality ?

2DEM class average

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 93184 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

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CA--HA	1.07	0.97	1564
CA--HA1	1.07	0.97	170
CA--HA2	1.07	0.97	181
N--HN2	0.99	0.89	9
N--HN1	0.99	0.89	7
CA--HA	1.08	0.97	8210
CA--HA1	1.08	0.97	957
N--HN1	1.00	0.89	41
CA--HA2	1.08	0.97	937
N--HN2	1.00	0.89	38
OG1--HG1	0.95	0.84	77
OH--HH	0.95	0.84	43
SG--HG1	1.31	1.20	1
OH--HH	0.96	0.84	285
CA--HA2	1.09	0.97	130
CA--HA	1.09	0.97	1042
OG1--HG1	0.96	0.84	385
CA--HA1	1.09	0.97	121
N--HN2	1.01	0.89	5
SG--HG1	1.32	1.20	28
N--HN1	1.01	0.89	4
N--HN	0.98	0.86	3
OH--HH	0.97	0.84	36

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
N--HN	0.99	0.86	4238
OG1--HG1	0.97	0.84	58
SG--HG1	1.33	1.20	23
CD2--HD22	1.10	0.97	125
CG2--HG23	1.10	0.97	280
CD1--HD13	1.10	0.97	130
ND1--HD1	0.99	0.86	10
NE2--HE22	0.99	0.86	125
CD--HD2	1.10	0.97	228
CB--HB	1.10	0.97	242
NE2--HE21	0.99	0.86	128
CB--HB2	1.10	0.97	833
CG--HG	1.10	0.97	107
CG--HG1	1.10	0.97	304
CD--HD3	1.10	0.97	92
CG1--HG11	1.10	0.97	182
CD--HD1	1.10	0.97	229
ND2--HD21	0.99	0.86	80
CB--HB1	1.10	0.97	798
NH1--HH11	0.99	0.86	59
CG2--HG22	1.10	0.97	238
CG1--HG12	1.10	0.97	187
NH2--HH21	0.99	0.86	60

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NE--HE	0.99	0.86	56
NH2--HH22	0.99	0.86	59
NH1--HH12	0.99	0.86	69
CD2--HD23	1.10	0.97	111
CD1--HD12	1.10	0.97	121
CD2--HD21	1.10	0.97	103
CG2--HG21	1.10	0.97	236
CG--HG2	1.10	0.97	314
ND2--HD22	0.99	0.86	76
CD1--HD11	1.10	0.97	99
CE--HE1	1.10	0.97	91
CE--HE2	1.10	0.97	93
CB--HB3	1.10	0.97	80
CG1--HG13	1.10	0.97	104
CE--HE3	1.10	0.97	6
CD--HD2	1.11	0.97	1933
CB--HB1	1.11	0.97	6297
CG2--HG22	1.11	0.97	1855
CG2--HG21	1.11	0.97	1828
CB--HB2	1.11	0.97	6366
CD2--HD23	1.11	0.97	912
CG1--HG11	1.11	0.97	1507
CG1--HG13	1.11	0.97	882

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CD2--HD21	1.11	0.97	960
CG--HG2	1.11	0.97	2725
CD1--HD13	1.11	0.97	885
CD2--HD22	1.11	0.97	889
CB--HB3	1.11	0.97	720
CG--HG1	1.11	0.97	2752
CD--HD1	1.11	0.97	1939
CD--HD3	1.11	0.97	554
CE--HE3	1.11	0.97	38
CG2--HG23	1.11	0.97	1837
CB--HB	1.11	0.97	1887
CD1--HD11	1.11	0.97	923
CG1--HG12	1.11	0.97	1473
CD1--HD12	1.11	0.97	907
CE--HE2	1.11	0.97	662
ND2--HD22	1.00	0.86	404
NE2--HE22	1.00	0.86	674
N--HN	1.00	0.86	7084
NH1--HH11	1.00	0.86	318
NH2--HH21	1.00	0.86	313
NH2--HH22	1.00	0.86	316
NE2--HE21	1.00	0.86	678
NE--HE	1.00	0.86	318

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NH1--HH12	1.00	0.86	293
CE--HE1	1.11	0.97	667
CG--HG	1.11	0.97	921
ND2--HD21	1.00	0.86	390
ND1--HD1	1.00	0.86	35
CE1--HE1	1.07	0.93	116
NZ--HZ1	1.03	0.89	119
CE2--HE2	1.07	0.93	121
NZ--HZ3	1.03	0.89	105
NZ--HZ2	1.03	0.89	113
CD2--HD2	1.07	0.93	122
CZ--HZ	1.07	0.93	72
CD1--HD1	1.07	0.93	120
N--H1	1.03	0.89	13
N--H3	1.03	0.89	8
N--H2	1.03	0.89	9
NZ--HZ2	1.04	0.89	635
NZ--HZ3	1.04	0.89	652
CZ--HZ	1.08	0.93	399
CE2--HE2	1.08	0.93	662
NZ--HZ1	1.04	0.89	633
CG1--HG11	1.12	0.97	235
CE--HE2	1.12	0.97	129

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CD2--HD22	1.12	0.97	182
CD--HD2	1.12	0.97	387
CG--HG	1.12	0.97	168
CG2--HG22	1.12	0.97	351
CB--HB1	1.12	0.97	1277
CD1--HD11	1.12	0.97	174
CE--HE1	1.12	0.97	126
CB--HB	1.12	0.97	315
CD--HD3	1.12	0.97	134
CG--HG2	1.12	0.97	497
CD1--HD12	1.12	0.97	168
CB--HB3	1.12	0.97	136
CG1--HG13	1.12	0.97	158
CG2--HG23	1.12	0.97	327
CG--HG1	1.12	0.97	480
CB--HB2	1.12	0.97	1173
CG1--HG12	1.12	0.97	264
CD--HD1	1.12	0.97	380
CD2--HD21	1.12	0.97	133
CG2--HG21	1.12	0.97	380
CD2--HD23	1.12	0.97	173
CD1--HD13	1.12	0.97	181
NE2--HE21	1.01	0.86	78

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
ND1--HD1	1.01	0.86	7
CE1--HE1	1.08	0.93	701
CD2--HD2	1.08	0.93	703
CD1--HD1	1.08	0.93	673
NH1--HH11	1.01	0.86	39
N--HN	1.01	0.86	167
ND2--HD22	1.01	0.86	40
NH1--HH12	1.01	0.86	54
NE2--HE22	1.01	0.86	85
N--H3	1.04	0.89	36
NH2--HH21	1.01	0.86	43
NE--HE	1.01	0.86	42
ND2--HD21	1.01	0.86	50
NH2--HH22	1.01	0.86	41
N--H1	1.04	0.89	37
CE--HE3	1.12	0.97	8
N--H2	1.04	0.89	38
NZ--HZ2	1.05	0.89	84
N--H3	1.05	0.89	8
NZ--HZ1	1.05	0.89	80
NZ--HZ3	1.05	0.89	75
CE1--HE1	1.09	0.93	116
CD1--HD1	1.09	0.93	91

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CE2--HE2	1.09	0.93	101
CD2--HD2	1.09	0.93	111
CZ--HZ	1.09	0.93	49
N--H2	1.05	0.89	5
N--H1	1.05	0.89	2
CE1--HE1	1.10	0.93	3

Standard geometry: angle outliers ?

There are 655 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	121.82	1
CA-CB-CG	112.60	119.97	1
CA-CB-CG	112.60	119.28	1
CA-CB-CG	112.60	119.21	1
CA-CB-CG	112.60	118.98	1
CA-CB-CG	112.60	118.96	2
CA-CB-CG	112.60	118.95	1
CA-CB-CG	112.60	118.90	1
CA-CB-CG	112.60	118.87	1
CA-CB-CG	112.60	118.85	1
CA-CB-CG	112.60	118.78	1
CA-CB-CG	112.60	118.76	1
CA-CB-CG	112.60	118.67	1
CA-CB-CG	112.60	118.65	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	112.60	118.64	2
CA-CB-CG	112.60	118.63	1
CA-CB-CG	112.60	118.57	1
CA-CB-CG	112.60	118.55	1
CA-CB-CG	112.60	118.54	2
CA-CB-CG	112.60	118.52	1
CA-CB-CG	112.60	118.50	1
CA-CB-CG	112.60	118.49	1
CA-CB-CG	112.60	118.48	1
CA-CB-CG	112.60	118.45	1
CA-CB-CG	112.60	118.44	1
CA-CB-CG	112.60	118.40	1
CA-CB-CG	112.60	118.38	3
CA-CB-CG	112.60	118.37	1
CA-CB-CG	112.60	118.36	1
CA-CB-CG	112.60	118.35	1
CA-CB-CG	112.60	118.34	1
CA-CB-CG	112.60	118.33	2
CA-CB-CG	112.60	118.32	2
CA-CB-CG	112.60	118.31	2
CA-CB-CG	112.60	118.30	1
CA-CB-CG	112.60	118.29	2
CA-CB-CG	112.60	118.27	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	112.60	118.26	1
CA-CB-CG	112.60	118.25	2
CA-CB-CG	112.60	118.24	1
CA-CB-CG	112.60	118.20	1
CA-CB-CG	112.60	118.19	2
CA-CB-CG	112.60	118.18	2
CA-CB-CG	112.60	118.14	1
CA-CB-CG	112.60	118.12	1
CA-CB-CG	112.60	118.10	1
CA-CB-CG	112.60	118.09	2
CA-CB-CG	112.60	118.08	1
CA-CB-CG	112.60	118.07	1
CA-CB-CG	112.60	118.05	3
C-N-CA	121.70	131.45	1
CA-CB-CG	112.60	118.01	1
CA-CB-CG	112.60	118.00	1
CA-CB-CG	112.60	117.99	1
CA-CB-CG	112.60	117.98	3
CA-CB-CG	112.60	117.97	2
CA-CB-CG	112.60	117.92	2
CA-CB-CG	112.60	117.90	1
CA-CB-CG	112.60	117.88	2
CA-CB-CG	112.60	117.87	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	112.60	117.86	1
N-CA-CB	110.50	119.44	1
CA-CB-CG	112.60	117.84	3
CA-CB-CG	112.60	117.81	2
CA-CB-CG	112.60	117.79	1
CA-CB-CG	112.60	117.78	1
C-N-CA	121.70	131.02	1
N-CA-CB	110.50	119.29	1
CA-CB-CG	112.60	117.76	3
N-CA-CB	110.50	119.26	1
CA-CB-CG	112.60	117.72	1
C-N-CA	121.70	130.88	1
CA-CB-CG	112.60	117.68	2
N-CA-CB	110.50	119.12	1
N-CA-CB	110.50	119.11	1
CA-CB-CG	112.60	117.66	1
CA-CB-CG	112.60	117.65	1
CA-CB-CG	112.60	117.64	2
N-CA-CB	110.50	119.07	1
NH1-CZ-NH2	119.30	112.75	1
CA-CB-CG	112.60	117.61	1
CA-CB-CG	112.60	117.60	2
C-N-CA	121.70	130.70	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.50	118.98	1
CA-CB-CG	112.60	117.58	3
N-CA-CB	110.50	118.97	1
N-CA-CB	110.50	118.96	3
CA-CB-CG	112.60	117.57	1
N-CA-CB	110.50	118.94	1
N-CA-CB	110.50	118.93	1
CA-CB-CG	112.60	117.56	2
N-CA-CB	110.50	118.92	2
CA-CB-CG	112.60	117.55	1
N-CA-CB	110.50	118.91	2
N-CA-CB	110.50	118.88	2
N-CA-CB	110.50	118.85	1
C-N-CA	121.70	130.54	1
CA-CB-CG	112.60	117.51	1
CA-CB-CG	112.60	117.50	4
N-CA-CB	110.50	118.84	1
C-N-CA	121.70	130.50	2
N-CA-CB	110.50	118.79	1
CA-CB-CG	112.60	117.47	1
N-CA-CB	110.50	118.77	1
N-CA-CB	110.50	118.76	1
CA-CB-CG	112.60	117.46	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.50	118.74	1
N-CA-CB	110.50	118.73	3
C-N-CA	121.70	130.41	1
CA-CB-CG	112.60	117.44	2
CA-CB-CG	112.60	117.43	2
C-N-CA	121.70	130.39	1
CA-CB-CG	112.60	117.42	2
N-CA-CB	110.50	118.69	1
C-N-CA	121.70	130.37	1
CA-CB-CG	112.60	117.41	2
CA-CB-CG	112.60	117.40	1
C-N-CA	121.70	130.35	1
CA-CB-CG	113.80	109.00	1
N-CA-CB	110.50	118.66	1
C-N-CA	121.70	130.33	1
CA-CB-CG	113.80	109.01	1
NE-CZ-NH1	121.50	126.29	1
CA-CB-CG	112.60	117.39	3
N-CA-CB	110.50	118.63	1
CA-CB-CG	112.60	117.38	1
N-CA-CB	110.50	118.62	2
NE-CZ-NH1	121.50	126.27	1
C-N-CA	121.70	130.29	3

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.50	118.61	2
CA-CB-CG	112.60	117.37	2
NE-CZ-NH1	121.50	126.26	1
C-N-CA	121.70	130.26	1
CA-CB-CG	112.60	117.35	1
N-CA-CB	110.50	118.57	1
CA-CB-CG	112.60	117.34	1
C-N-CA	121.70	130.24	1
CA-CB-CG	113.80	109.06	2
C-N-CA	121.70	130.23	1
NE-CZ-NH1	121.50	126.24	1
C-N-CA	121.70	130.22	1
N-CA-CB	110.50	118.54	1
NE-CZ-NH1	121.50	126.23	1
CG1-CB-CG2	110.80	121.20	1
C-N-CA	121.70	130.21	1
CA-CB-CG	112.60	117.32	1
CA-C-O	120.80	128.82	1
C-N-CA	121.70	130.16	1
CA-C-O	120.80	128.79	1
C-N-CA	121.70	130.15	1
CA-CB-CG	112.60	117.29	1
N-CA-CB	110.50	118.47	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	112.60	117.28	3
C-N-CA	121.70	130.13	1
CA-CB-CG	113.80	109.13	1
CA-CB-CG	112.60	117.27	3
NE-CZ-NH2	119.20	115.00	1
CA-CB-CG	112.60	117.26	2
N-CA-CB	110.50	118.42	1
CA-CB-CG	113.80	109.14	1
CG1-CB-CG2	110.80	121.04	1
C-N-CA	121.70	130.07	1
CA-CB-CG	112.60	117.25	1
CA-CB-CG	112.60	117.24	1
N-CA-CB	110.50	118.39	3
C-N-CA	121.70	130.04	1
CA-CB-CG	113.80	109.16	1
CA-C-N	116.90	123.84	1
C-N-CA	121.70	130.03	1
CA-CB-CG	112.60	117.23	1
N-CA-CB	110.50	118.36	1
CA-C-N	116.90	123.83	2
N-CA-CB	110.50	118.35	1
C-N-CA	121.70	130.01	1
CG1-CB-CG2	110.80	120.94	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	112.60	117.21	1
SG-C7-C8	109.23	95.42	1
N-CA-CB	110.50	118.32	2
C-N-CA	121.70	129.98	1
CA-C-N	116.90	123.79	1
N-CA-CB	110.50	118.31	1
CA-CB-CG	112.60	117.19	1
C-N-CA	121.70	129.96	1
NE-CZ-NH1	121.50	126.09	1
CA-C-N	116.90	123.75	1
CA-CB-CG	112.60	117.17	1
CA-CB-CG	112.60	117.16	1
NH1-CZ-NH2	119.30	113.37	1
C-N-CA	121.70	129.90	1
CA-C-N	116.90	123.73	2
CA-CB-CG	113.80	109.24	2
CA-CB-CG	112.60	117.15	1
CA-CB-CG	113.80	109.25	1
CA-CB-CG	112.60	117.14	3
C-N-CA	121.70	129.88	1
CA-C-N	116.90	123.71	2
N-CA-CB	110.50	118.22	1
C-CA-CB	111.40	120.02	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-N	116.90	123.70	1
NH1-CZ-NH2	119.30	113.41	1
N-CA-CB	110.50	118.21	1
C-N-CA	121.70	129.86	1
C-CA-CB	111.40	120.01	1
CA-CB-CG	112.60	117.13	1
C-N-CA	121.70	129.85	1
CA-CB-CG	112.60	117.12	2
CA-C-N	116.90	123.67	1
CA-CB-CG	112.60	117.11	2
CG1-CB-CG2	110.80	120.70	1
CA-CB-CG	113.80	109.30	1
CA-CB-CG	112.60	117.10	1
CA-CB-CG	112.60	117.09	1
CA-CB-CG	113.80	109.31	2
C-N-CA	121.70	129.78	1
C-N-CA	121.70	129.77	1
CA-CB-CG	112.60	117.08	1
CA-C-O	120.80	128.42	1
CA-C-N	116.90	123.62	1
CA-CB-CG	112.60	117.07	2
CA-C-N	116.90	123.60	1
CA-C-N	116.90	123.59	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	112.60	117.06	3
CA-CB-CG	113.80	109.35	1
C-N-CA	121.70	129.71	2
CA-C-N	116.90	123.57	1
CA-CB-CG	112.60	117.05	1
CA-CB-CG	112.60	117.04	1
C-N-CA	121.70	129.69	1
CA-C-N	116.90	123.54	1
CA-CB-CG	112.60	117.02	1
O-C-N	123.00	115.92	1
CA-C-O	120.80	128.32	1
SG-C7-C8	109.23	95.97	1
CA-CB-CG	113.80	109.38	1
C-N-CA	121.70	129.65	1
CA-C-N	116.90	123.52	2
C-N-CA	121.70	129.64	1
O-C-N	123.00	115.94	1
CA-CB-CG	113.80	109.39	1
CA-C-N	116.90	123.51	1
C-N-CA	121.70	129.63	1
CA-CB-CG	113.80	109.40	1
C-N-CA	121.70	129.62	2
N-CA-CB	110.50	117.98	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-O	120.80	128.27	1
C-N-CA	121.70	129.61	1
CA-CB-CG	112.60	116.99	2
CA-CB-CG	113.80	109.41	1
CA-C-N	116.90	123.48	1
CG1-CB-CG2	110.80	120.45	1
C-N-CA	121.70	129.59	1
SG-C7-C8	109.23	96.08	1
NE-CZ-NH1	121.50	125.88	1
C-N-CA	121.70	129.58	1
CA-CB-CG	112.60	116.98	1
CA-C-N	116.90	123.46	1
CA-CB-OG1	109.60	116.16	1
C-N-CA	121.70	129.56	3
CA-CB-CG	113.80	109.44	1
NH1-CZ-NH2	119.30	113.63	1
NE-CZ-NH1	121.50	125.86	1
C-N-CA	121.70	129.54	1
CA-C-O	120.80	128.20	1
CA-C-N	116.90	123.43	1
C-CA-CB	111.40	119.67	1
C-N-CA	121.70	129.52	1
CA-CB-CG	113.80	109.45	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	129.51	1
C-CA-CB	111.40	119.65	1
CA-CB-CG	112.60	116.94	1
CA-CB-CG	112.60	116.93	3
C-N-CA	121.70	129.50	1
CA-C-N	116.90	123.39	1
CA-CB-CG	112.60	116.92	4
CG1-CB-CG2	110.80	120.31	1
CA-CB-CG	113.80	109.48	2
N-CA-C	111.00	98.92	1
C-N-CA	121.70	129.46	1
CA-CB-CG	112.60	116.91	1
CA-CB-CG	113.80	109.50	2
CA-CB-CG	112.60	116.90	2
C-CA-CB	111.40	119.58	1
CA-C-N	116.90	123.36	1
NE-CZ-NH1	121.50	125.80	1
CA-C-O	120.80	128.11	1
CA-C-N	116.90	123.35	1
C-CA-CB	111.40	119.57	1
C-N-CA	121.70	129.44	1
C-N-CA	121.70	129.43	1
CA-CB-CG	112.60	116.89	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	111.40	119.56	1
CA-C-N	116.90	123.33	1
CA-CB-CG	113.80	109.51	1
CA-C-N	116.90	123.32	2
C-N-CA	121.70	129.41	1
CA-CB-CG	113.80	109.52	2
CG1-CB-CG2	110.80	120.21	1
C-CA-CB	111.40	119.53	1
CA-C-N	116.90	123.31	1
SG-C7-C8	109.23	96.40	1
N-CA-C	111.00	99.03	1
SG-C7-C8	109.23	96.41	1
CA-CB-CG	112.60	116.87	3
CA-CB-CG	113.80	109.53	1
O-C-N	123.00	116.18	1
C-CA-CB	111.40	119.49	1
CA-CB-CG	112.60	116.86	1
CG1-CB-CG2	110.80	120.17	1
CA-C-N	116.90	123.28	1
CG1-CB-CG2	110.80	120.16	1
CA-CB-CG	113.80	109.55	2
CG1-CB-CG2	110.80	120.15	2
C-N-CA	121.70	129.35	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-N	116.90	123.27	1
C-N-CA	121.70	129.34	2
NE-CZ-NH1	121.50	125.75	1
C-CA-CB	111.40	119.46	1
CA-C-N	116.90	123.26	2
CG1-CB-CG2	110.80	120.13	1
CA-CB-CG	113.80	109.57	1
C-CA-CB	111.40	119.44	1
O-C-N	123.00	116.23	1
C-N-CA	121.70	129.32	1
CA-CB-CG	112.60	116.83	1
CG1-CB-CG2	110.80	120.09	1
C-N-CA	121.70	129.30	2
CA-CB-CG	112.60	116.82	4
CA-CB-CG	113.80	109.58	1
C-N-CA	121.70	129.29	1
CA-CB-CG	113.80	109.59	3
C-CA-CB	111.40	119.40	1
CA-CB-CG	112.60	116.80	2
CA-C-N	116.90	123.19	3
N-CA-CB	110.50	117.62	1
CA-CB-CG	112.60	116.79	1
C-N-CA	121.70	129.23	1

Angle type	**Observed angle (°)**	**Ideal angle (°)**	**Number of outliers**
CA-CB-CG	112.60	116.78	2
N-CA-C	111.00	99.29	1
N-CA-C	111.00	99.30	1
CA-C-N	116.90	123.17	1
CA-C-N	116.90	123.16	1
CA-CB-CG	112.60	116.77	1
O-C-N	123.00	116.33	1
CA-C-N	116.90	123.15	1
C-N-CA	121.70	129.19	1
CA-CB-CG	112.60	116.76	5
N-CA-CB	110.50	117.58	1
CG1-CB-CG2	110.80	119.95	1
NE-CZ-NH1	121.50	125.66	1
CA-C-N	116.90	123.13	1
O-C-N	123.00	116.35	1
CA-CB-CG	112.60	116.75	3
C-N-CA	121.70	129.17	1
C-CA-CB	111.40	119.28	1
CG1-CB-CG2	110.80	119.93	1
CA-CB-CG	113.80	109.65	1
C-N-CA	121.70	129.16	1
C-N-CA	121.70	129.14	1
C-N-CA	121.70	129.13	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CG1-CB-CG2	110.80	119.88	1
N-CA-C	111.00	99.44	1
CA-C-O	120.80	127.81	1
O-C-N	123.00	116.40	1
C-N-CA	121.70	129.12	2
CA-CB-CG	113.80	109.68	1
CA-CB-CG	112.60	116.72	1
CA-C-N	116.90	123.08	1
C-CA-CB	111.40	119.23	1
C-CA-CB	111.40	119.22	1
NE-CZ-NH2	119.20	115.49	1
CA-C-O	120.80	127.80	1
C-N-CA	121.70	129.10	2
CA-CB-CG	113.80	109.69	1
O-C-N	123.00	116.42	3
CG1-CB-CG2	110.80	119.84	1
CA-C-N	116.90	123.06	1
NH1-CZ-NH2	119.30	113.96	1
C-N-CA	121.70	129.08	2
CA-C-O	120.80	127.77	1
O-C-N	123.00	116.45	1
C-N-CA	121.70	129.07	1
CA-CB-CG	112.60	116.69	5

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O-C-N	123.00	116.46	2
CA-CB-CG	112.60	116.68	1
CA-CB-CG	113.80	109.72	1
CA-CB-CG	112.60	108.52	2
C-CA-CB	111.40	119.15	1
CG1-CB-CG2	110.80	119.76	1
C-N-CA	121.70	129.03	1
CA-CB-CG	112.60	116.67	1
CA-CB-CG	113.80	109.73	1
CG1-CB-CG2	110.80	119.75	1
SG-C7-C8	109.23	97.03	1
C-N-CA	121.70	129.02	1
CA-C-N	116.90	123.00	1
C-CA-CB	111.40	119.13	1
SG-C7-C8	109.23	97.04	1
CA-CB-CG	112.60	116.66	4
CA-CB-CG	113.80	109.74	2
O-C-N	123.00	116.50	2
C-N-CA	121.70	129.01	1
C-CA-CB	111.40	119.11	1
CG1-CB-CG2	110.80	119.73	1
CA-C-N	116.90	122.99	1
C-N-CA	121.70	129.00	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
NE-CZ-NH1	121.50	125.55	1
C-CA-CB	111.40	119.10	1
O-C-N	123.00	116.51	1
CG1-CB-CG2	110.80	119.71	1
O-C-N	123.00	116.52	1
CA-C-N	116.90	122.97	2
SG-C7-C8	109.23	97.09	1
C-N-CA	121.70	128.98	1
CA-CB-CG	113.80	109.76	1
CA-C-N	116.90	122.96	1
C-N-CA	121.70	128.96	2
CA-CB-CG	112.60	116.63	4
O-C-N	123.00	116.55	1
CA-CB-CG	112.60	108.57	1
NH1-CZ-NH2	119.30	114.06	1
C-N-CA	121.70	128.95	1
C-CA-CB	111.40	119.05	1
C-N-CA	121.70	128.94	3
CA-CB-CG	112.60	116.62	2
SG-C7-C8	109.23	97.16	1
O-C-N	123.00	116.56	1
CA-C-O	120.80	127.63	3
C-N-CA	121.70	128.93	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
SG-C7-C8	109.23	97.18	1
CA-CB-CG	113.80	109.78	1
CA-CB-CG	112.60	116.61	2
C-N-CA	121.70	128.92	1
C-N-CA	121.70	114.49	1
CA-CB-CG	112.60	116.60	2
O-C-N	123.00	116.60	1
CZ-NH2-HH21	107.90	120.00	1
HH21-NH2-HH22	107.83	120.00	1
HZ1-NZ-HZ2	96.71	109.00	1
HE21-NE2-HE22	107.69	120.00	1
CZ-NH2-HH21	107.58	120.00	1
CZ-NH2-HH21	107.39	120.00	1
HH11-NH1-HH12	106.80	120.00	1
HH21-NH2-HH22	106.66	120.00	1
HH21-NH2-HH22	106.26	120.00	1
HH21-NH2-HH22	106.02	120.00	1
HH21-NH2-HH22	105.43	120.00	1
HH21-NH2-HH22	105.28	120.00	1
HH21-NH2-HH22	105.25	120.00	1
HN1-N-HN2	118.32	103.16	1
HH21-NH2-HH22	104.80	120.00	1
HH21-NH2-HH22	104.40	120.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
HN1-N-HN2	118.81	103.16	1
HN1-N-HN2	119.09	103.16	1
HN1-N-HN2	119.30	103.16	1
HN1-N-HN2	119.33	103.16	1
HH11-NH1-HH12	103.79	120.00	1
HN1-N-HN2	119.69	103.16	1
HH21-NH2-HH22	103.41	120.00	1
HN1-N-HN2	119.78	103.16	1
HN1-N-HN2	119.97	103.16	1
HN1-N-HN2	120.06	103.16	1
HN1-N-HN2	120.14	103.16	1
HN1-N-HN2	120.23	103.16	1
HN1-N-HN2	120.30	103.16	1
HN1-N-HN2	120.35	103.16	1
HN1-N-HN2	120.37	103.16	1
HN1-N-HN2	120.43	103.16	1
HN1-N-HN2	120.49	103.16	1
HN1-N-HN2	120.59	103.16	1
HN1-N-HN2	120.63	103.16	1
HH21-NH2-HH22	102.48	120.00	1
HN1-N-HN2	120.89	103.16	1
HH21-NH2-HH22	102.24	120.00	1
HN1-N-HN2	121.07	103.16	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
HN1-N-HN2	121.10	103.16	1
HN1-N-HN2	121.30	103.16	1
HN1-N-HN2	121.34	103.16	1
HN1-N-HN2	121.37	103.16	1
HN1-N-HN2	121.54	103.16	1
HN1-N-HN2	121.55	103.16	2
HN1-N-HN2	121.67	103.16	1
HN1-N-HN2	121.69	103.16	1
HN1-N-HN2	121.70	103.16	1
HN1-N-HN2	121.74	103.16	1
HN1-N-HN2	121.90	103.16	1
HN1-N-HN2	121.93	103.16	1
HN1-N-HN2	121.94	103.16	1
HN1-N-HN2	122.13	103.16	1
HN1-N-HN2	122.17	103.16	1
HN1-N-HN2	122.33	103.16	1
HN1-N-HN2	122.39	103.16	1
HN1-N-HN2	122.45	103.16	1
HN1-N-HN2	122.56	103.16	1
HN1-N-HN2	122.58	103.16	1
HN1-N-HN2	122.59	103.16	1
HN1-N-HN2	122.65	103.16	1
HN1-N-HN2	122.77	103.16	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
HN1-N-HN2	122.78	103.16	2
HN1-N-HN2	122.92	103.16	1
HN1-N-HN2	122.94	103.16	1
HN1-N-HN2	123.03	103.16	1
HN1-N-HN2	123.06	103.16	2
HN1-N-HN2	123.78	103.16	1
HH21-NH2-HH22	94.23	120.00	1
HH21-NH2-HH22	90.49	120.00	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	2.61	480

All 480 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	SA:86:LEU:HD23	TA:186:VAL:HG12	0.663
1	YA:89:VAL:HG21	ZA:185:LYS:HG2	0.555
1	XA:89:VAL:HG21	YA:185:LYS:HG2	0.534
1	SA:86:LEU:HD12	TA:186:VAL:CG1	0.529
1	JA:89:VAL:HG21	KA:185:LYS:HG2	0.522
1	SA:86:LEU:HD12	TA:186:VAL:HG11	0.516
1	SA:86:LEU:CD2	TA:186:VAL:HG12	0.514
1	E:89:VAL:HG21	F:185:LYS:HG2	0.513

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	QA:89:VAL:HG21	RA:185:LYS:HG2	0.512
1	U:89:VAL:HG21	V:185:LYS:HG2	0.510
1	S:89:VAL:HG21	T:185:LYS:HG2	0.507
1	F:229:LEU:HB2	G:141:VAL:HG13	0.503
1	Z:229:LEU:HB2	AA:141:VAL:HG13	0.502
1	TA:89:VAL:HG21	UA:185:LYS:HG2	0.500
1	NA:229:LEU:HB2	OA:141:VAL:HG13	0.497
1	UA:229:LEU:HB2	VA:141:VAL:HG13	0.496
1	H:89:VAL:HG21	I:185:LYS:HG2	0.495
1	O:89:VAL:HG21	P:185:LYS:HG2	0.495
1	B:229:LEU:HB2	C:141:VAL:HG13	0.494
1	QA:229:LEU:HB2	RA:141:VAL:HG13	0.494
1	L:229:LEU:HB2	M:141:VAL:HG13	0.493
1	DA:229:LEU:HB2	EA:141:VAL:HG13	0.493
1	Y:229:LEU:HB2	Z:141:VAL:HG13	0.492
1	A:141:VAL:HG13	ZA:229:LEU:HB2	0.490
1	EA:229:LEU:HB2	FA:141:VAL:HG13	0.490
1	PA:229:LEU:HB2	QA:141:VAL:HG13	0.490
1	KA:89:VAL:HG21	LA:185:LYS:HG2	0.489
1	I:229:LEU:HB2	J:141:VAL:HG13	0.488
1	BA:229:LEU:HB2	CA:141:VAL:HG13	0.488
1	K:24:ARG:HH21	K:27:ILE:CD	0.487
1	K:229:LEU:HB2	L:141:VAL:HG13	0.487

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	HA:229:LEU:HB2	IA:141:VAL:HG13	0.487
1	KA:229:LEU:HB2	LA:141:VAL:HG13	0.487
1	NA:24:ARG:HH21	NA:27:ILE:CD	0.487
1	SA:229:LEU:HB2	TA:141:VAL:HG13	0.487
1	JA:229:LEU:HB2	KA:141:VAL:HG13	0.486
1	E:229:LEU:HB2	F:141:VAL:HG13	0.485
1	J:229:LEU:HB2	K:141:VAL:HG13	0.485
1	O:229:LEU:HB2	P:141:VAL:HG13	0.485
1	Y:89:VAL:HG21	Z:185:LYS:HG2	0.485
1	MA:229:LEU:HB2	NA:141:VAL:HG13	0.485
1	FA:229:LEU:HB2	GA:141:VAL:HG13	0.484
1	A:229:LEU:HB2	B:141:VAL:HG13	0.482
1	G:229:LEU:HB2	H:141:VAL:HG13	0.482
1	H:229:LEU:HB2	I:141:VAL:HG13	0.482
1	P:229:LEU:HB2	Q:141:VAL:HG13	0.482
1	Q:229:LEU:HB2	R:141:VAL:HG13	0.482
1	AA:229:LEU:HB2	BA:141:VAL:HG13	0.482
1	IA:229:LEU:HB2	JA:141:VAL:HG13	0.482
1	OA:229:LEU:HB2	PA:141:VAL:HG13	0.482
1	WA:229:LEU:HB2	XA:141:VAL:HG13	0.482
1	R:229:LEU:HB2	S:141:VAL:HG13	0.481
1	C:229:LEU:HB2	D:141:VAL:HG13	0.480
1	M:229:LEU:HB2	N:141:VAL:HG13	0.480

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	GA:229:LEU:HB2	HA:141:VAL:HG13	0.480
1	TA:229:LEU:HB2	UA:141:VAL:HG13	0.480
1	N:89:VAL:HG21	O:185:LYS:HG2	0.479
1	V:229:LEU:HB2	W:141:VAL:HG13	0.479
1	X:229:LEU:HB2	Y:141:VAL:HG13	0.479
1	LA:229:LEU:HB2	MA:141:VAL:HG13	0.479
1	D:229:LEU:HB2	E:141:VAL:HG13	0.478
1	T:229:LEU:HB2	U:141:VAL:HG13	0.478
1	CA:229:LEU:HB2	DA:141:VAL:HG13	0.478
1	RA:229:LEU:HB2	SA:141:VAL:HG13	0.478
1	D:89:VAL:HG21	E:185:LYS:HG2	0.477
1	G:89:VAL:HG21	H:185:LYS:HG2	0.477
1	S:229:LEU:HB2	T:141:VAL:HG13	0.476
1	Y:24:ARG:HH21	Y:27:ILE:CD	0.476
1	VA:229:LEU:HB2	WA:141:VAL:HG13	0.476
1	W:229:LEU:HB2	X:141:VAL:HG13	0.475
1	HA:24:ARG:HH21	HA:27:ILE:CD	0.475
1	XA:229:LEU:HB2	YA:141:VAL:HG13	0.475
1	P:89:VAL:HG21	Q:185:LYS:HG2	0.474
1	U:229:LEU:HB2	V:141:VAL:HG13	0.474
1	FA:89:VAL:HG21	GA:185:LYS:HG2	0.474
1	L:24:ARG:HH21	L:27:ILE:CD	0.473
1	X:89:VAL:HG21	Y:185:LYS:HG2	0.472

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	I:89:VAL:HG21	J:185:LYS:HG2	0.471
1	MA:89:VAL:HG21	NA:185:LYS:HG2	0.471
1	YA:229:LEU:HB2	ZA:141:VAL:HG13	0.470
1	N:229:LEU:HB2	O:141:VAL:HG13	0.464
1	U:24:ARG:HH21	U:27:ILE:CD	0.464
1	P:24:ARG:HH21	P:27:ILE:CD	0.463
1	F:89:VAL:HG21	G:185:LYS:HG2	0.462
1	LA:89:VAL:HG21	MA:185:LYS:HG2	0.460
1	SA:24:ARG:HH21	SA:27:ILE:CD	0.460
1	Z:89:VAL:HG21	AA:185:LYS:HG2	0.459
1	GA:24:ARG:HH21	GA:27:ILE:CD	0.459
1	FA:24:ARG:HH21	FA:27:ILE:CD	0.453
1	OA:24:ARG:HH21	OA:27:ILE:CD	0.452
1	L:89:VAL:HG21	M:185:LYS:HG2	0.451
1	MA:24:ARG:HH21	MA:27:ILE:CD	0.451
1	SA:89:VAL:HG21	TA:185:LYS:HG2	0.451
1	LA:24:ARG:HH21	LA:27:ILE:CD	0.450
1	M:15:LEU:HD22	N:22:LEU:HD13	0.449
1	E:84:ASN:O	F:187:VAL:HA	0.446
1	M:24:ARG:HH21	M:27:ILE:CD	0.446
1	RA:89:VAL:HG21	SA:185:LYS:HG2	0.445
1	XA:84:ASN:O	YA:187:VAL:HA	0.445
1	T:24:ARG:HH21	T:27:ILE:CD	0.444

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	NA:3:LEU:H	NA:3:LEU:HD13	0.444
1	A:24:ARG:HH21	A:27:ILE:CD	0.443
1	X:24:ARG:HH21	X:27:ILE:CD	0.443
1	QA:84:ASN:O	RA:187:VAL:HA	0.442
1	R:89:VAL:HG21	S:185:LYS:HG2	0.441
1	PA:84:ASN:O	QA:187:VAL:HA	0.441
1	RA:15:LEU:HD22	SA:22:LEU:HD13	0.441
1	A:185:LYS:HG2	ZA:89:VAL:HG21	0.440
1	N:24:ARG:HH21	N:27:ILE:CD	0.440
1	N:67:ALA:HA	O:205:TYR:CD1	0.440
1	R:84:ASN:O	S:187:VAL:HA	0.440
1	J:84:ASN:O	K:187:VAL:HA	0.439
1	O:24:ARG:HH21	O:27:ILE:CD	0.439
1	UA:15:LEU:HD22	VA:22:LEU:HD13	0.439
1	V:15:LEU:HD22	W:22:LEU:HD13	0.438
1	RA:24:ARG:HH21	RA:27:ILE:CD	0.438
1	C:15:LEU:HD22	D:22:LEU:HD13	0.437
1	F:24:ARG:HH21	F:27:ILE:CD	0.437
1	N:15:LEU:HD22	O:22:LEU:HD13	0.437
1	B:15:LEU:HD22	C:22:LEU:HD13	0.436
1	CA:89:VAL:HG21	DA:185:LYS:HG2	0.436
1	VA:89:VAL:HG21	WA:185:LYS:HG2	0.436
1	P:84:ASN:O	Q:187:VAL:HA	0.435

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	F:84:ASN:O	G:187:VAL:HA	0.434
1	DA:15:LEU:HD22	EA:22:LEU:HD13	0.434
1	JA:67:ALA:HA	KA:205:TYR:CD1	0.434
1	K:89:VAL:HG21	L:185:LYS:HG2	0.433
1	L:27:ILE:HB	L:212:VAL:HG21	0.433
1	M:89:VAL:HG21	N:185:LYS:HG2	0.433
1	O:15:LEU:HD22	P:22:LEU:HD13	0.433
1	W:15:LEU:HD22	X:22:LEU:HD13	0.433
1	Z:67:ALA:HA	AA:205:TYR:CD1	0.433
1	JA:24:ARG:HH21	JA:27:ILE:CD	0.433
1	QA:15:LEU:HD22	RA:22:LEU:HD13	0.433
1	UA:84:ASN:O	VA:187:VAL:HA	0.433
1	L:3:LEU:H	L:3:LEU:HD13	0.432
1	K:84:ASN:O	L:187:VAL:HA	0.432
1	T:67:ALA:HA	U:205:TYR:CD1	0.432
1	T:208:GLU:CD	T:208:GLU:H	0.432
1	AA:15:LEU:HD22	BA:22:LEU:HD13	0.432
1	IA:24:ARG:HH21	IA:27:ILE:CD	0.432
1	JA:84:ASN:O	KA:187:VAL:HA	0.432
1	QA:67:ALA:HA	RA:205:TYR:CD1	0.432
1	WA:15:LEU:HD22	XA:22:LEU:HD13	0.432
1	C:24:ARG:HH21	C:27:ILE:CD	0.431
1	HA:67:ALA:HA	IA:205:TYR:CD1	0.431

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	E:3:LEU:H	E:3:LEU:HD13	0.430
1	F:15:LEU:HD22	G:22:LEU:HD13	0.430
1	H:3:LEU:H	H:3:LEU:HD13	0.430
1	J:67:ALA:HA	K:205:TYR:CD1	0.430
1	L:84:ASN:O	M:187:VAL:HA	0.430
1	W:67:ALA:HA	X:205:TYR:CD1	0.430
1	X:15:LEU:HD22	Y:22:LEU:HD13	0.430
1	CA:84:ASN:O	DA:187:VAL:HA	0.430
1	FA:3:LEU:H	FA:3:LEU:HD13	0.430
1	GA:84:ASN:O	HA:187:VAL:HA	0.430
1	S:24:ARG:HH21	S:27:ILE:CD	0.429
1	GA:89:VAL:HG21	HA:185:LYS:HG2	0.429
1	OA:89:VAL:HG21	PA:185:LYS:HG2	0.429
1	G:67:ALA:HA	H:205:TYR:CD1	0.428
1	I:84:ASN:O	J:187:VAL:HA	0.428
1	P:3:LEU:H	P:3:LEU:HD13	0.428
1	Q:89:VAL:HG21	R:185:LYS:HG2	0.428
1	S:67:ALA:HA	T:205:TYR:CD1	0.428
1	X:84:ASN:O	Y:187:VAL:HA	0.428
1	BA:84:ASN:O	CA:187:VAL:HA	0.428
1	HA:24:ARG:O	HA:212:VAL:HG22	0.428
1	KA:84:ASN:O	LA:187:VAL:HA	0.428
1	A:3:LEU:H	A:3:LEU:HD13	0.427

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	D:27:ILE:HB	D:212:VAL:HG21	0.427
1	K:67:ALA:HA	L:205:TYR:CD1	0.427
1	L:15:LEU:HD22	M:22:LEU:HD13	0.427
1	M:27:ILE:HB	M:212:VAL:HG21	0.427
1	W:24:ARG:HH21	W:27:ILE:CD	0.427
1	LA:67:ALA:HA	MA:205:TYR:CD1	0.427
1	QA:24:ARG:HH21	QA:27:ILE:CD	0.427
1	TA:84:ASN:O	UA:187:VAL:HA	0.427
1	D:67:ALA:HA	E:205:TYR:CD1	0.426
1	U:27:ILE:HB	U:212:VAL:HG21	0.426
1	V:84:ASN:O	W:187:VAL:HA	0.426
1	CA:67:ALA:HA	DA:205:TYR:CD1	0.426
1	DA:67:ALA:HA	EA:205:TYR:CD1	0.426
1	KA:67:ALA:HA	LA:205:TYR:CD1	0.426
1	LA:27:ILE:HB	LA:212:VAL:HG21	0.426
1	SA:15:LEU:HD22	TA:22:LEU:HD13	0.426
1	UA:24:ARG:HH21	UA:27:ILE:CD	0.426
1	YA:84:ASN:O	ZA:187:VAL:HA	0.426
1	K:15:LEU:HD22	L:22:LEU:HD13	0.425
1	O:27:ILE:HB	O:212:VAL:HG21	0.425
1	P:27:ILE:HB	P:212:VAL:HG21	0.425
1	U:15:LEU:HD22	V:22:LEU:HD13	0.425
1	CA:3:LEU:H	CA:3:LEU:HD13	0.425

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	DA:27:ILE:HB	DA:212:VAL:HG21	0.425
1	FA:67:ALA:HA	GA:205:TYR:CD1	0.425
1	HA:89:VAL:HG21	IA:185:LYS:HG2	0.425
1	MA:84:ASN:O	NA:187:VAL:HA	0.425
1	OA:67:ALA:HA	PA:205:TYR:CD1	0.425
1	SA:67:ALA:HA	TA:205:TYR:CD1	0.425
1	VA:15:LEU:HD22	WA:22:LEU:HD13	0.425
1	A:22:LEU:HD13	ZA:15:LEU:HD22	0.424
1	C:84:ASN:O	D:187:VAL:HA	0.424
1	P:24:ARG:O	P:212:VAL:HG22	0.424
1	U:24:ARG:O	U:212:VAL:HG22	0.424
1	Y:67:ALA:HA	Z:205:TYR:CD1	0.424
1	Y:84:ASN:O	Z:187:VAL:HA	0.424
1	FA:27:ILE:HB	FA:212:VAL:HG21	0.424
1	IA:24:ARG:O	IA:212:VAL:HG22	0.424
1	IA:84:ASN:O	JA:187:VAL:HA	0.424
1	NA:67:ALA:HA	OA:205:TYR:CD1	0.424
1	OA:84:ASN:O	PA:187:VAL:HA	0.424
1	UA:67:ALA:HA	VA:205:TYR:CD1	0.424
1	A:15:LEU:HD22	B:22:LEU:HD13	0.423
1	A:67:ALA:HA	B:205:TYR:CD1	0.423
1	B:27:ILE:HB	B:212:VAL:HG21	0.423
1	E:67:ALA:HA	F:205:TYR:CD1	0.423

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	F:27:ILE:HB	F:212:VAL:HG21	0.423
1	I:67:ALA:HA	J:205:TYR:CD1	0.423
1	H:84:ASN:O	I:187:VAL:HA	0.423
1	M:84:ASN:O	N:187:VAL:HA	0.423
1	V:89:VAL:HG21	W:185:LYS:HG2	0.423
1	Z:24:ARG:O	Z:212:VAL:HG22	0.423
1	JA:27:ILE:HB	JA:212:VAL:HG21	0.423
1	PA:15:LEU:HD22	QA:22:LEU:HD13	0.423
1	C:27:ILE:HB	C:212:VAL:HG21	0.422
1	F:67:ALA:HA	G:205:TYR:CD1	0.422
1	J:15:LEU:HD22	K:22:LEU:HD13	0.422
1	M:229:LEU:CB	N:141:VAL:HG13	0.422
1	Y:15:LEU:HD22	Z:22:LEU:HD13	0.422
1	EA:15:LEU:HD22	FA:22:LEU:HD13	0.422
1	DA:84:ASN:O	EA:187:VAL:HA	0.422
1	IA:27:ILE:HB	IA:212:VAL:HG21	0.422
1	IA:89:VAL:HG21	JA:185:LYS:HG2	0.422
1	KA:24:ARG:O	KA:212:VAL:HG22	0.422
1	NA:24:ARG:O	NA:212:VAL:HG22	0.422
1	PA:27:ILE:HB	PA:212:VAL:HG21	0.422
1	PA:67:ALA:HA	QA:205:TYR:CD1	0.422
1	C:89:VAL:HG21	D:185:LYS:HG2	0.421
1	X:67:ALA:HA	Y:205:TYR:CD1	0.421

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	JA:15:LEU:HD22	KA:22:LEU:HD13	0.421
1	LA:84:ASN:O	MA:187:VAL:HA	0.421
1	PA:3:LEU:H	PA:3:LEU:HD13	0.421
1	TA:15:LEU:HD22	UA:22:LEU:HD13	0.421
1	XA:15:LEU:HD22	YA:22:LEU:HD13	0.421
1	D:15:LEU:HD22	E:22:LEU:HD13	0.420
1	D:84:ASN:O	E:187:VAL:HA	0.420
1	E:24:ARG:O	E:212:VAL:HG22	0.420
1	H:24:ARG:HH21	H:27:ILE:CD	0.420
1	K:3:LEU:H	K:3:LEU:HD13	0.420
1	Q:15:LEU:HD22	R:22:LEU:HD13	0.420
1	Q:67:ALA:HA	R:205:TYR:CD1	0.420
1	T:15:LEU:HD22	U:22:LEU:HD13	0.420
1	CA:15:LEU:HD22	DA:22:LEU:HD13	0.420
1	DA:89:VAL:HG21	EA:185:LYS:HG2	0.420
1	LA:24:ARG:O	LA:212:VAL:HG22	0.420
1	VA:24:ARG:O	VA:212:VAL:HG22	0.420
1	WA:84:ASN:O	XA:187:VAL:HA	0.420
1	B:84:ASN:O	C:187:VAL:HA	0.419
1	E:15:LEU:HD22	F:22:LEU:HD13	0.419
1	H:67:ALA:HA	I:205:TYR:CD1	0.419
1	G:84:ASN:O	H:187:VAL:HA	0.419
1	S:15:LEU:HD22	T:22:LEU:HD13	0.419

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	V:67:ALA:HA	W:205:TYR:CD1	0.419
1	Z:15:LEU:HD22	AA:22:LEU:HD13	0.419
1	Z:229:LEU:CB	AA:141:VAL:HG13	0.419
1	AA:24:ARG:O	AA:212:VAL:HG22	0.419
1	BA:24:ARG:HH21	BA:27:ILE:CD	0.419
1	KA:15:LEU:HD22	LA:22:LEU:HD13	0.419
1	MA:24:ARG:O	MA:212:VAL:HG22	0.419
1	NA:27:ILE:HB	NA:212:VAL:HG21	0.419
1	NA:84:ASN:O	OA:187:VAL:HA	0.419
1	WA:67:ALA:HA	XA:205:TYR:CD1	0.419
1	XA:67:ALA:HA	YA:205:TYR:CD1	0.419
1	YA:15:LEU:HD22	ZA:22:LEU:HD13	0.419
1	A:24:ARG:O	A:212:VAL:HG22	0.418
1	A:84:ASN:O	B:187:VAL:HA	0.418
1	C:67:ALA:HA	D:205:TYR:CD1	0.418
1	I:24:ARG:O	I:212:VAL:HG22	0.418
1	L:24:ARG:O	L:212:VAL:HG22	0.418
1	P:15:LEU:HD22	Q:22:LEU:HD13	0.418
1	T:84:ASN:O	U:187:VAL:HA	0.418
1	FA:15:LEU:HD22	GA:22:LEU:HD13	0.418
1	EA:84:ASN:O	FA:187:VAL:HA	0.418
1	FA:84:ASN:O	GA:187:VAL:HA	0.418
1	GA:24:ARG:O	GA:212:VAL:HG22	0.418

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	KA:27:ILE:HB	KA:212:VAL:HG21	0.418
1	QA:27:ILE:HB	QA:212:VAL:HG21	0.418
1	B:24:ARG:HH21	B:27:ILE:CD	0.418
1	P:229:LEU:CB	Q:141:VAL:HG13	0.417
1	Y:24:ARG:O	Y:212:VAL:HG22	0.417
1	AA:24:ARG:HH21	AA:27:ILE:CD	0.417
1	BA:67:ALA:HA	CA:205:TYR:CD1	0.417
1	EA:24:ARG:O	EA:212:VAL:HG22	0.417
1	UA:3:LEU:H	UA:3:LEU:HD13	0.417
1	VA:67:ALA:HA	WA:205:TYR:CD1	0.417
1	B:67:ALA:HA	C:205:TYR:CD1	0.416
1	F:229:LEU:CB	G:141:VAL:HG13	0.416
1	H:27:ILE:HB	H:212:VAL:HG21	0.416
1	M:24:ARG:O	M:212:VAL:HG22	0.416
1	N:27:ILE:HB	N:212:VAL:HG21	0.416
1	P:67:ALA:HA	Q:205:TYR:CD1	0.416
1	S:27:ILE:HB	S:212:VAL:HG21	0.416
1	HA:27:ILE:HB	HA:212:VAL:HG21	0.416
1	TA:3:LEU:H	TA:3:LEU:HD13	0.416
1	TA:24:ARG:HH21	TA:27:ILE:CD	0.416
1	WA:24:ARG:O	WA:212:VAL:HG22	0.416
1	V:24:ARG:O	V:212:VAL:HG22	0.415
1	FA:24:ARG:O	FA:212:VAL:HG22	0.415

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	HA:84:ASN:O	IA:187:VAL:HA	0.415
1	JA:24:ARG:O	JA:212:VAL:HG22	0.415
1	MA:67:ALA:HA	NA:205:TYR:CD1	0.415
1	NA:15:LEU:HD22	OA:22:LEU:HD13	0.415
1	VA:84:ASN:O	WA:187:VAL:HA	0.415
1	YA:67:ALA:HA	ZA:205:TYR:CD1	0.415
1	A:187:VAL:HA	ZA:84:ASN:O	0.414
1	J:27:ILE:HB	J:212:VAL:HG21	0.414
1	J:24:ARG:O	J:212:VAL:HG22	0.414
1	M:67:ALA:HA	N:205:TYR:CD1	0.414
1	S:24:ARG:O	S:212:VAL:HG22	0.414
1	AA:67:ALA:HA	BA:205:TYR:CD1	0.414
1	CA:27:ILE:HB	CA:212:VAL:HG21	0.414
1	IA:15:LEU:HD22	JA:22:LEU:HD13	0.414
1	UA:27:ILE:HB	UA:212:VAL:HG21	0.414
1	A:141:VAL:HG13	ZA:229:LEU:CB	0.413
1	D:229:LEU:CB	E:141:VAL:HG13	0.413
1	H:229:LEU:CB	I:141:VAL:HG13	0.413
1	J:229:LEU:CB	K:141:VAL:HG13	0.413
1	N:84:ASN:O	O:187:VAL:HA	0.413
1	O:24:ARG:O	O:212:VAL:HG22	0.413
1	Q:229:LEU:CB	R:141:VAL:HG13	0.413
1	R:15:LEU:HD22	S:22:LEU:HD13	0.413

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	Z:24:ARG:HH21	Z:27:ILE:CD	0.413
1	CA:24:ARG:O	CA:212:VAL:HG22	0.413
1	EA:67:ALA:HA	FA:205:TYR:CD1	0.413
1	GA:67:ALA:HA	HA:205:TYR:CD1	0.413
1	LA:15:LEU:HD22	MA:22:LEU:HD13	0.413
1	RA:24:ARG:O	RA:212:VAL:HG22	0.413
1	RA:84:ASN:O	SA:187:VAL:HA	0.413
1	CA:24:ARG:HH21	CA:27:ILE:CD	0.413
1	AA:84:ASN:O	BA:187:VAL:HA	0.413
1	F:24:ARG:O	F:212:VAL:HG22	0.412
1	G:24:ARG:O	G:212:VAL:HG22	0.412
1	L:67:ALA:HA	M:205:TYR:CD1	0.412
1	O:67:ALA:HA	P:205:TYR:CD1	0.412
1	R:229:LEU:CB	S:141:VAL:HG13	0.412
1	U:67:ALA:HA	V:205:TYR:CD1	0.412
1	X:24:ARG:O	X:212:VAL:HG22	0.412
1	Y:229:LEU:CB	Z:141:VAL:HG13	0.412
1	EA:229:LEU:CB	FA:141:VAL:HG13	0.412
1	GA:27:ILE:HB	GA:212:VAL:HG21	0.412
1	HA:15:LEU:HD22	IA:22:LEU:HD13	0.412
1	RA:67:ALA:HA	SA:205:TYR:CD1	0.412
1	TA:67:ALA:HA	UA:205:TYR:CD1	0.412
1	YA:27:ILE:HB	YA:212:VAL:HG21	0.412

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	S:86:LEU:N	T:186:VAL:O	0.412
1	BA:86:LEU:N	CA:186:VAL:O	0.412
1	T:86:LEU:N	U:186:VAL:O	0.412
1	A:205:TYR:CD1	ZA:67:ALA:HA	0.411
1	G:27:ILE:HB	G:212:VAL:HG21	0.411
1	H:24:ARG:O	H:212:VAL:HG22	0.411
1	I:15:LEU:HD22	J:22:LEU:HD13	0.411
1	K:27:ILE:HB	K:212:VAL:HG21	0.411
1	N:24:ARG:O	N:212:VAL:HG22	0.411
1	R:67:ALA:HA	S:205:TYR:CD1	0.411
1	S:84:ASN:O	T:187:VAL:HA	0.411
1	AA:27:ILE:HB	AA:212:VAL:HG21	0.411
1	BA:15:LEU:HD22	CA:22:LEU:HD13	0.411
1	BA:24:ARG:O	BA:212:VAL:HG22	0.411
1	QA:229:LEU:CB	RA:141:VAL:HG13	0.411
1	WA:27:ILE:HB	WA:212:VAL:HG21	0.411
1	XA:27:ILE:HB	XA:212:VAL:HG21	0.411
1	YA:24:ARG:HH21	YA:27:ILE:CD	0.411
1	Z:86:LEU:N	AA:186:VAL:O	0.411
1	EA:24:ARG:HH21	EA:27:ILE:CD	0.411
1	EA:86:LEU:N	FA:186:VAL:O	0.411
1	KA:86:LEU:N	LA:186:VAL:O	0.411
1	QA:86:LEU:N	RA:186:VAL:O	0.411

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	G:15:LEU:HD22	H:22:LEU:HD13	0.410
1	I:24:ARG:HH21	I:27:ILE:CD	0.410
1	J:24:ARG:HH21	J:27:ILE:CD	0.410
1	K:24:ARG:O	K:212:VAL:HG22	0.410
1	L:229:LEU:CB	M:141:VAL:HG13	0.410
1	O:229:LEU:CB	P:141:VAL:HG13	0.410
1	Q:84:ASN:O	R:187:VAL:HA	0.410
1	X:229:LEU:CB	Y:141:VAL:HG13	0.410
1	DA:24:ARG:O	DA:212:VAL:HG22	0.410
1	IA:67:ALA:HA	JA:205:TYR:CD1	0.410
1	IA:229:LEU:CB	JA:141:VAL:HG13	0.410
1	SA:84:ASN:O	TA:187:VAL:HA	0.410
1	TA:24:ARG:O	TA:212:VAL:HG22	0.410
1	ZA:27:ILE:HB	ZA:212:VAL:HG21	0.410
1	U:3:LEU:H	U:3:LEU:HD13	0.410
1	W:86:LEU:N	X:186:VAL:O	0.410
1	X:86:LEU:N	Y:186:VAL:O	0.410
1	I:27:ILE:HB	I:212:VAL:HG21	0.409
1	Q:27:ILE:HB	Q:212:VAL:HG21	0.409
1	X:27:ILE:HB	X:212:VAL:HG21	0.409
1	AA:229:LEU:CB	BA:141:VAL:HG13	0.409
1	DA:229:LEU:CB	EA:141:VAL:HG13	0.409
1	HA:229:LEU:CB	IA:141:VAL:HG13	0.409

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	Q:24:ARG:O	Q:212:VAL:HG22	0.408
1	R:24:ARG:O	R:212:VAL:HG22	0.408
1	T:27:ILE:HB	T:212:VAL:HG21	0.408
1	T:24:ARG:O	T:212:VAL:HG22	0.408
1	U:84:ASN:O	V:187:VAL:HA	0.408
1	W:24:ARG:O	W:212:VAL:HG22	0.408
1	Y:3:LEU:H	Y:3:LEU:HD13	0.408
1	Y:27:ILE:HB	Y:212:VAL:HG21	0.408
1	GA:15:LEU:HD22	HA:22:LEU:HD13	0.408
1	MA:15:LEU:HD22	NA:22:LEU:HD13	0.408
1	PA:229:LEU:CB	QA:141:VAL:HG13	0.408
1	QA:24:ARG:O	QA:212:VAL:HG22	0.408
1	WA:89:VAL:HG21	XA:185:LYS:HG2	0.408
1	H:15:LEU:HD22	I:22:LEU:HD13	0.407
1	J:89:VAL:HG21	K:185:LYS:HG2	0.407
1	K:229:LEU:CB	L:141:VAL:HG13	0.407
1	R:27:ILE:HB	R:212:VAL:HG21	0.407
1	GA:229:LEU:CB	HA:141:VAL:HG13	0.407
1	OA:27:ILE:HB	OA:212:VAL:HG21	0.407
1	PA:24:ARG:O	PA:212:VAL:HG22	0.407
1	SA:229:LEU:CB	TA:141:VAL:HG13	0.407
1	TA:27:ILE:HB	TA:212:VAL:HG21	0.407
1	UA:24:ARG:O	UA:212:VAL:HG22	0.407

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	DA:86:LEU:N	EA:186:VAL:O	0.407
1	T:229:LEU:CB	U:141:VAL:HG13	0.406
1	Z:84:ASN:O	AA:187:VAL:HA	0.406
1	BA:229:LEU:CB	CA:141:VAL:HG13	0.406
1	SA:27:ILE:HB	SA:212:VAL:HG21	0.406
1	L:86:LEU:N	M:186:VAL:O	0.406
1	R:86:LEU:N	S:186:VAL:O	0.406
1	GA:3:LEU:H	GA:3:LEU:HD13	0.406
1	B:229:LEU:CB	C:141:VAL:HG13	0.405
1	C:24:ARG:O	C:212:VAL:HG22	0.405
1	V:229:LEU:CB	W:141:VAL:HG13	0.405
1	KA:229:LEU:CB	LA:141:VAL:HG13	0.405
1	MA:229:LEU:CB	NA:141:VAL:HG13	0.405
1	OA:15:LEU:HD22	PA:22:LEU:HD13	0.405
1	WA:229:LEU:CB	XA:141:VAL:HG13	0.405
1	D:86:LEU:N	E:186:VAL:O	0.405
1	IA:86:LEU:N	JA:186:VAL:O	0.405
1	NA:86:LEU:N	OA:186:VAL:O	0.405
1	I:229:LEU:CB	J:141:VAL:HG13	0.404
1	P:131:LYS:NZ	Q:138:ASP:HB2	0.404
1	V:27:ILE:HB	V:212:VAL:HG21	0.404
1	Z:3:LEU:H	Z:3:LEU:HD13	0.404
1	CA:229:LEU:CB	DA:141:VAL:HG13	0.404

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	FA:229:LEU:CB	GA:141:VAL:HG13	0.404
1	UA:229:LEU:CB	VA:141:VAL:HG13	0.404
1	XA:86:LEU:N	YA:186:VAL:O	0.404
1	D:24:ARG:O	D:212:VAL:HG22	0.403
1	O:84:ASN:O	P:187:VAL:HA	0.403
1	Z:131:LYS:NZ	AA:138:ASP:HB2	0.403
1	OA:24:ARG:O	OA:212:VAL:HG22	0.403
1	O:86:LEU:N	P:186:VAL:O	0.403
1	G:86:LEU:N	H:186:VAL:O	0.403
1	U:86:LEU:N	V:186:VAL:O	0.403
1	GA:86:LEU:N	HA:186:VAL:O	0.403
1	N:229:LEU:CB	O:141:VAL:HG13	0.402
1	S:229:LEU:CB	T:141:VAL:HG13	0.402
1	AA:89:VAL:HG21	BA:185:LYS:HG2	0.402
1	DA:24:ARG:HH21	DA:27:ILE:CD	0.402
1	EA:27:ILE:HB	EA:212:VAL:HG21	0.402
1	OA:229:LEU:CB	PA:141:VAL:HG13	0.402
1	RA:27:ILE:HB	RA:212:VAL:HG21	0.402
1	VA:27:ILE:HB	VA:212:VAL:HG21	0.402
1	YA:24:ARG:O	YA:212:VAL:HG22	0.402
1	AA:3:LEU:H	AA:3:LEU:HD13	0.402
1	MA:86:LEU:N	NA:186:VAL:O	0.402
1	WA:86:LEU:N	XA:186:VAL:O	0.402

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	M:86:LEU:N	N:186:VAL:O	0.402
1	AA:86:LEU:N	BA:186:VAL:O	0.402
1	PA:86:LEU:N	QA:186:VAL:O	0.402
1	B:24:ARG:O	B:212:VAL:HG22	0.401
1	JA:86:LEU:N	KA:186:VAL:O	0.401
1	C:86:LEU:N	D:186:VAL:O	0.401
1	J:86:LEU:N	K:186:VAL:O	0.401
1	P:86:LEU:N	Q:186:VAL:O	0.401
1	A:229:LEU:CB	B:141:VAL:HG13	0.400
1	G:229:LEU:CB	H:141:VAL:HG13	0.400
1	W:27:ILE:HB	W:212:VAL:HG21	0.400
1	YA:3:LEU:H	YA:3:LEU:HD13	0.400

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	Analyzed	Favored	Allowed	Outliers
1	11856	10687	989	180

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	9100	7627	910	563

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	3	LEU

Model ID	Chain	Residue ID	Residue type
1	A	35	GLN
1	A	47	GLU
1	A	76	ASN
1	A	86	LEU
1	A	87	LYS
1	A	88	SER
1	A	90	LEU
1	A	104	ASN
1	A	115	ASN
1	A	119	ASP
1	A	124	LEU
1	B	3	LEU
1	B	35	GLN
1	B	87	LYS
1	B	88	SER
1	B	104	ASN
1	B	119	ASP
1	B	122	GLU
1	B	124	LEU
1	B	141	VAL
1	C	3	LEU
1	C	35	GLN
1	C	47	GLU

Model ID	Chain	Residue ID	Residue type
1	C	86	LEU
1	C	87	LYS
1	C	88	SER
1	C	104	ASN
1	C	119	ASP
1	C	124	LEU
1	D	3	LEU
1	D	35	GLN
1	D	47	GLU
1	D	76	ASN
1	D	86	LEU
1	D	87	LYS
1	D	88	SER
1	D	90	LEU
1	D	104	ASN
1	D	115	ASN
1	D	119	ASP
1	D	122	GLU
1	D	124	LEU
1	D	177	GLN
1	E	3	LEU
1	E	35	GLN
1	E	47	GLU

Model ID	Chain	Residue ID	Residue type
1	E	86	LEU
1	E	87	LYS
1	E	88	SER
1	E	104	ASN
1	E	119	ASP
1	E	122	GLU
1	E	124	LEU
1	F	3	LEU
1	F	35	GLN
1	F	86	LEU
1	F	87	LYS
1	F	88	SER
1	F	104	ASN
1	F	115	ASN
1	F	119	ASP
1	F	122	GLU
1	F	124	LEU
1	G	3	LEU
1	G	35	GLN
1	G	86	LEU
1	G	87	LYS
1	G	88	SER
1	G	90	LEU

Model ID	Chain	Residue ID	Residue type
1	G	104	ASN
1	G	119	ASP
1	G	122	GLU
1	G	124	LEU
1	H	3	LEU
1	H	35	GLN
1	H	47	GLU
1	H	86	LEU
1	H	87	LYS
1	H	88	SER
1	H	90	LEU
1	H	104	ASN
1	H	119	ASP
1	H	122	GLU
1	H	124	LEU
1	H	138	ASP
1	H	141	VAL
1	I	3	LEU
1	I	35	GLN
1	I	47	GLU
1	I	86	LEU
1	I	87	LYS
1	I	104	ASN

Model ID	Chain	Residue ID	Residue type
1	I	119	ASP
1	I	122	GLU
1	I	124	LEU
1	I	141	VAL
1	J	3	LEU
1	J	35	GLN
1	J	47	GLU
1	J	87	LYS
1	J	88	SER
1	J	104	ASN
1	J	115	ASN
1	J	119	ASP
1	J	122	GLU
1	J	124	LEU
1	J	138	ASP
1	J	141	VAL
1	K	3	LEU
1	K	35	GLN
1	K	86	LEU
1	K	87	LYS
1	K	88	SER
1	K	104	ASN
1	K	119	ASP

Model ID	Chain	Residue ID	Residue type
1	K	122	GLU
1	K	124	LEU
1	L	3	LEU
1	L	35	GLN
1	L	86	LEU
1	L	87	LYS
1	L	88	SER
1	L	90	LEU
1	L	104	ASN
1	L	115	ASN
1	L	119	ASP
1	L	122	GLU
1	L	124	LEU
1	M	3	LEU
1	M	35	GLN
1	M	47	GLU
1	M	86	LEU
1	M	87	LYS
1	M	88	SER
1	M	90	LEU
1	M	104	ASN
1	M	119	ASP
1	M	124	LEU

Model ID	Chain	Residue ID	Residue type
1	M	138	ASP
1	M	228	THR
1	N	3	LEU
1	N	35	GLN
1	N	47	GLU
1	N	86	LEU
1	N	87	LYS
1	N	88	SER
1	N	104	ASN
1	N	115	ASN
1	N	119	ASP
1	N	122	GLU
1	N	124	LEU
1	O	3	LEU
1	O	35	GLN
1	O	47	GLU
1	O	86	LEU
1	O	87	LYS
1	O	88	SER
1	O	104	ASN
1	O	115	ASN
1	O	119	ASP
1	O	122	GLU

Model ID	Chain	Residue ID	Residue type
1	O	124	LEU
1	O	138	ASP
1	P	3	LEU
1	P	35	GLN
1	P	47	GLU
1	P	86	LEU
1	P	87	LYS
1	P	88	SER
1	P	104	ASN
1	P	115	ASN
1	P	119	ASP
1	P	122	GLU
1	P	124	LEU
1	P	138	ASP
1	P	141	VAL
1	Q	3	LEU
1	Q	35	GLN
1	Q	47	GLU
1	Q	86	LEU
1	Q	87	LYS
1	Q	88	SER
1	Q	104	ASN
1	Q	119	ASP

Model ID	Chain	Residue ID	Residue type
1	Q	122	GLU
1	Q	124	LEU
1	R	3	LEU
1	R	35	GLN
1	R	47	GLU
1	R	86	LEU
1	R	88	SER
1	R	90	LEU
1	R	104	ASN
1	R	115	ASN
1	R	119	ASP
1	R	122	GLU
1	R	124	LEU
1	R	141	VAL
1	S	3	LEU
1	S	35	GLN
1	S	47	GLU
1	S	87	LYS
1	S	88	SER
1	S	104	ASN
1	S	115	ASN
1	S	119	ASP
1	S	122	GLU

Model ID	Chain	Residue ID	Residue type
1	S	124	LEU
1	S	141	VAL
1	T	3	LEU
1	T	35	GLN
1	T	86	LEU
1	T	87	LYS
1	T	88	SER
1	T	90	LEU
1	T	104	ASN
1	T	115	ASN
1	T	119	ASP
1	T	122	GLU
1	T	124	LEU
1	T	141	VAL
1	U	3	LEU
1	U	35	GLN
1	U	86	LEU
1	U	87	LYS
1	U	88	SER
1	U	104	ASN
1	U	115	ASN
1	U	119	ASP
1	U	122	GLU

Model ID	Chain	Residue ID	Residue type
1	U	124	LEU
1	U	138	ASP
1	U	141	VAL
1	V	3	LEU
1	V	35	GLN
1	V	86	LEU
1	V	88	SER
1	V	90	LEU
1	V	104	ASN
1	V	119	ASP
1	V	122	GLU
1	V	124	LEU
1	V	141	VAL
1	W	3	LEU
1	W	35	GLN
1	W	86	LEU
1	W	87	LYS
1	W	88	SER
1	W	90	LEU
1	W	104	ASN
1	W	115	ASN
1	W	119	ASP
1	W	122	GLU

Model ID	Chain	Residue ID	Residue type
1	W	124	LEU
1	W	138	ASP
1	W	141	VAL
1	W	228	THR
1	X	3	LEU
1	X	35	GLN
1	X	86	LEU
1	X	87	LYS
1	X	104	ASN
1	X	119	ASP
1	X	122	GLU
1	X	124	LEU
1	Y	3	LEU
1	Y	35	GLN
1	Y	47	GLU
1	Y	86	LEU
1	Y	87	LYS
1	Y	88	SER
1	Y	90	LEU
1	Y	104	ASN
1	Y	119	ASP
1	Y	122	GLU
1	Y	124	LEU

Model ID	Chain	Residue ID	Residue type
1	Z	3	LEU
1	Z	35	GLN
1	Z	76	ASN
1	Z	86	LEU
1	Z	87	LYS
1	Z	88	SER
1	Z	90	LEU
1	Z	104	ASN
1	Z	115	ASN
1	Z	119	ASP
1	Z	124	LEU
1	AA	3	LEU
1	AA	35	GLN
1	AA	76	ASN
1	AA	86	LEU
1	AA	87	LYS
1	AA	88	SER
1	AA	104	ASN
1	AA	119	ASP
1	AA	122	GLU
1	AA	124	LEU
1	BA	3	LEU
1	BA	35	GLN

Model ID	Chain	Residue ID	Residue type
1	BA	47	GLU
1	BA	86	LEU
1	BA	87	LYS
1	BA	88	SER
1	BA	104	ASN
1	BA	119	ASP
1	BA	124	LEU
1	BA	138	ASP
1	BA	141	VAL
1	CA	3	LEU
1	CA	35	GLN
1	CA	47	GLU
1	CA	86	LEU
1	CA	87	LYS
1	CA	88	SER
1	CA	104	ASN
1	CA	119	ASP
1	CA	122	GLU
1	CA	124	LEU
1	DA	3	LEU
1	DA	35	GLN
1	DA	47	GLU
1	DA	76	ASN

Model ID	Chain	Residue ID	Residue type
1	DA	87	LYS
1	DA	88	SER
1	DA	104	ASN
1	DA	119	ASP
1	DA	122	GLU
1	DA	124	LEU
1	EA	3	LEU
1	EA	35	GLN
1	EA	47	GLU
1	EA	87	LYS
1	EA	88	SER
1	EA	104	ASN
1	EA	119	ASP
1	EA	122	GLU
1	EA	124	LEU
1	FA	3	LEU
1	FA	35	GLN
1	FA	47	GLU
1	FA	86	LEU
1	FA	87	LYS
1	FA	88	SER
1	FA	104	ASN
1	FA	119	ASP

Model ID	Chain	Residue ID	Residue type
1	FA	122	GLU
1	FA	124	LEU
1	FA	138	ASP
1	GA	3	LEU
1	GA	35	GLN
1	GA	47	GLU
1	GA	87	LYS
1	GA	88	SER
1	GA	104	ASN
1	GA	119	ASP
1	GA	122	GLU
1	GA	124	LEU
1	GA	138	ASP
1	HA	3	LEU
1	HA	35	GLN
1	HA	47	GLU
1	HA	76	ASN
1	HA	86	LEU
1	HA	87	LYS
1	HA	88	SER
1	HA	104	ASN
1	HA	119	ASP
1	HA	122	GLU

Model ID	Chain	Residue ID	Residue type
1	HA	124	LEU
1	HA	138	ASP
1	IA	3	LEU
1	IA	35	GLN
1	IA	47	GLU
1	IA	86	LEU
1	IA	87	LYS
1	IA	88	SER
1	IA	90	LEU
1	IA	104	ASN
1	IA	115	ASN
1	IA	119	ASP
1	IA	122	GLU
1	IA	124	LEU
1	IA	138	ASP
1	JA	3	LEU
1	JA	35	GLN
1	JA	47	GLU
1	JA	87	LYS
1	JA	88	SER
1	JA	90	LEU
1	JA	104	ASN
1	JA	119	ASP

Model ID	Chain	Residue ID	Residue type
1	JA	122	GLU
1	JA	124	LEU
1	JA	138	ASP
1	JA	141	VAL
1	KA	3	LEU
1	KA	35	GLN
1	KA	47	GLU
1	KA	86	LEU
1	KA	87	LYS
1	KA	88	SER
1	KA	104	ASN
1	KA	119	ASP
1	KA	122	GLU
1	KA	124	LEU
1	KA	141	VAL
1	LA	3	LEU
1	LA	35	GLN
1	LA	86	LEU
1	LA	87	LYS
1	LA	88	SER
1	LA	90	LEU
1	LA	104	ASN
1	LA	119	ASP

Model ID	Chain	Residue ID	Residue type
1	LA	122	GLU
1	LA	124	LEU
1	MA	3	LEU
1	MA	35	GLN
1	MA	86	LEU
1	MA	87	LYS
1	MA	88	SER
1	MA	90	LEU
1	MA	104	ASN
1	MA	119	ASP
1	MA	122	GLU
1	MA	124	LEU
1	MA	138	ASP
1	NA	3	LEU
1	NA	35	GLN
1	NA	47	GLU
1	NA	86	LEU
1	NA	88	SER
1	NA	104	ASN
1	NA	119	ASP
1	NA	122	GLU
1	NA	124	LEU
1	OA	3	LEU

Model ID	Chain	Residue ID	Residue type
1	OA	35	GLN
1	OA	47	GLU
1	OA	86	LEU
1	OA	87	LYS
1	OA	88	SER
1	OA	90	LEU
1	OA	104	ASN
1	OA	115	ASN
1	OA	119	ASP
1	OA	122	GLU
1	OA	124	LEU
1	OA	226	GLU
1	PA	3	LEU
1	PA	35	GLN
1	PA	76	ASN
1	PA	86	LEU
1	PA	87	LYS
1	PA	88	SER
1	PA	90	LEU
1	PA	104	ASN
1	PA	119	ASP
1	PA	122	GLU
1	PA	124	LEU

Model ID	Chain	Residue ID	Residue type
1	PA	138	ASP
1	QA	3	LEU
1	QA	35	GLN
1	QA	47	GLU
1	QA	86	LEU
1	QA	88	SER
1	QA	104	ASN
1	QA	115	ASN
1	QA	119	ASP
1	QA	124	LEU
1	RA	3	LEU
1	RA	35	GLN
1	RA	47	GLU
1	RA	86	LEU
1	RA	87	LYS
1	RA	104	ASN
1	RA	119	ASP
1	RA	124	LEU
1	RA	141	VAL
1	SA	3	LEU
1	SA	35	GLN
1	SA	86	LEU
1	SA	87	LYS

Model ID	Chain	Residue ID	Residue type
1	SA	88	SER
1	SA	104	ASN
1	SA	119	ASP
1	SA	122	GLU
1	SA	124	LEU
1	SA	141	VAL
1	TA	3	LEU
1	TA	35	GLN
1	TA	47	GLU
1	TA	86	LEU
1	TA	87	LYS
1	TA	90	LEU
1	TA	104	ASN
1	TA	115	ASN
1	TA	119	ASP
1	TA	122	GLU
1	TA	124	LEU
1	TA	138	ASP
1	TA	141	VAL
1	TA	228	THR
1	UA	3	LEU
1	UA	35	GLN
1	UA	47	GLU

Model ID	Chain	Residue ID	Residue type
1	UA	88	SER
1	UA	90	LEU
1	UA	92	GLN
1	UA	104	ASN
1	UA	119	ASP
1	UA	122	GLU
1	UA	124	LEU
1	VA	3	LEU
1	VA	35	GLN
1	VA	47	GLU
1	VA	76	ASN
1	VA	87	LYS
1	VA	88	SER
1	VA	90	LEU
1	VA	104	ASN
1	VA	115	ASN
1	VA	119	ASP
1	VA	124	LEU
1	VA	138	ASP
1	WA	3	LEU
1	WA	35	GLN
1	WA	47	GLU
1	WA	86	LEU

Model ID	Chain	Residue ID	Residue type
1	WA	87	LYS
1	WA	88	SER
1	WA	104	ASN
1	WA	119	ASP
1	WA	124	LEU
1	XA	3	LEU
1	XA	35	GLN
1	XA	87	LYS
1	XA	88	SER
1	XA	104	ASN
1	XA	119	ASP
1	XA	122	GLU
1	XA	124	LEU
1	XA	138	ASP
1	XA	228	THR
1	YA	3	LEU
1	YA	35	GLN
1	YA	47	GLU
1	YA	86	LEU
1	YA	87	LYS
1	YA	104	ASN
1	YA	115	ASN
1	YA	119	ASP

Model ID	Chain	Residue ID	Residue type
1	YA	124	LEU
1	ZA	3	LEU
1	ZA	35	GLN
1	ZA	47	GLU
1	ZA	86	LEU
1	ZA	87	LYS
1	ZA	104	ASN
1	ZA	119	ASP
1	ZA	122	GLU
1	ZA	124	LEU

Fit of model to data used for modeling ?

2DEM class average

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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