Integrative Structure Validation Report July 22, 2024 - 04:44 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	9A1T
PDB-Dev ID	PDBDEV_00000119
Structure Title	SARS-CoV-2 nsp7-8 polyprotein
Structure Authors	Ruchi Yadav; Valentine V. Courouble; Sanjay K. Dey; Francesc X. Ruiz; Patrick R. Griffin; Eddy Arnold

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 5 datasets or restraints were used to build this entry. Each model is represented by 0 rigid bodies and 3 flexible or non-rigid units.

Entry composition?

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

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	SARS-CoV-2 nsp7-8 polyprotein	A	А	283
2	1	1	SARS-CoV-2 nsp7-8 polyprotein	А	A	283
3	1	1	SARS-CoV-2 nsp7-8 polyprotein	A	A	283
4	1	1	SARS-CoV-2 nsp7-8 polyprotein	A	A	283
5	1	1	SARS-CoV-2 nsp7-8 polyprotein	A	А	283
6	1	1	SARS-CoV-2 nsp7-8 polyprotein	A	A	283
7	1	1	SARS-CoV-2 nsp7-8 polyprotein	A	А	283
8	1	1	SARS-CoV-2 nsp7-8 polyprotein	А	A	283
9	1	1	SARS-CoV-2 nsp7-8 polyprotein	A	A	283

Mode	l Subunit	Subunit	Subunit name	Chain	Chain ID	Total
ID	number	ID		ID	[auth]	residues
10	1	1	SARS-CoV-2 nsp7-8 polyprotein	A	А	283

Datasets used for modeling

There are 5 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Crosslinking-MS data	PRIDE	PXD033748
2	H/D exchange data	PRIDE	PXD033698
3	SAS data	SASBDB	SASDPY2
4	Experimental model	PDB	6YHU
5	De Novo model	Not available	Not available

Representation ?

This entry has only one representation and includes 0 rigid bodies and 3 flexible units

Chain ID	Rigid bodies Non-rigid segments	
А	-	3-82, 161-277, 83-160

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	None	Integrative modeling	None	None	False	False

There is 1 software package reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	I-TASSER	Not available	Integrative modeling	https://zhanggroup.org/I-TASSER/

Data quality ?

SAS:Scattering profile

SAS data used in this integrative model could not be validated as the sascif file is currently unavailable.

Crosslinking-MS

Validation for this section is under development.

H/D exchange

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 22294 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)	ldeal distance (Å)	Number of outliers
CBHB	1.05	0.97	1
CBHB3	1.05	0.97	1
CAHA	1.05	0.97	2
CAHA2	1.05	0.97	1
CAHA	1.06	0.97	13
CBHB3	1.06	0.97	4
CDHD2	1.06	0.97	1
CG1HG11	1.06	0.97	1
CGHG3	1.06	0.97	4

Bond type	Observed distance (Å)	ldeal distance (Å)	Number of outliers
CBHB2	1.06	0.97	2
CBHB	1.06	0.97	1
CD1HD12	1.06	0.97	1
CD2HD21	1.06	0.97	1
CG2HG22	1.06	0.97	1
CG2HG22	1.07	0.97	6
CBHB3	1.07	0.97	18
CBHB2	1.07	0.97	28
CAHA	1.07	0.97	34
CG1HG12	1.07	0.97	5
CD1HD13	1.07	0.97	1
CBHB	1.07	0.97	8
CGHG3	1.07	0.97	4
CG2HG23	1.07	0.97	7
CGHG	1.07	0.97	2
CD1HD11	1.07	0.97	2
CG2HG21	1.07	0.97	3
CD2HD22	1.07	0.97	2
CGHG2	1.07	0.97	8
CG1HG13	1.07	0.97	4
CDHD3	1.07	0.97	2
CD2HD21	1.07	0.97	1
CBHB1	1.07	0.97	2

Bond type	Observed distance (Å)	ldeal distance (Å)	Number of outliers
CD1HD12	1.07	0.97	2
CEHE2	1.07	0.97	1
CD2HD23	1.07	0.97	1
CAHA	1.08	0.97	243
CD2HD21	1.08	0.97	27
CBHB3	1.08	0.97	181
CBHB2	1.08	0.97	181
CGHG	1.08	0.97	47
CBHB	1.08	0.97	69
CDHD2	1.08	0.97	19
CEHE1	1.08	0.97	5
CD1HD13	1.08	0.97	50
CG2HG22	1.08	0.97	42
CG1HG12	1.08	0.97	35
CG1HG13	1.08	0.97	35
CGHG3	1.08	0.97	50
CG2HG21	1.08	0.97	50
CD2HD22	1.08	0.97	28
CD1HD12	1.08	0.97	39
CG1HG11	1.08	0.97	20
CBHB1	1.08	0.97	22
CGHG2	1.08	0.97	58
CEHE3	1.08	0.97	5

Bond type	Observed distance (Å)	ldeal distance (Å)	Number of outliers
CEHE2	1.08	0.97	3
CD1HD11	1.08	0.97	33
CAHA2	1.08	0.97	3
CG2HG23	1.08	0.97	41
CAHA3	1.08	0.97	4
CDHD3	1.08	0.97	21
CD2HD23	1.08	0.97	25
NZHZ1	1.00	0.89	18
NZHZ2	1.00	0.89	10
NZHZ3	1.00	0.89	12
CDHD2	1.09	0.97	350
CD1HD12	1.09	0.97	408
CBHB3	1.09	0.97	2064
CAHA	1.09	0.97	2460
CDHD3	1.09	0.97	347
CD1HD11	1.09	0.97	415
CG2HG23	1.09	0.97	462
CG2HG21	1.09	0.97	456
CG1HG11	1.09	0.97	199
CGHG3	1.09	0.97	751
CD2HD22	1.09	0.97	300
CG1HG12	1.09	0.97	300
CD1HD13	1.09	0.97	399

Bond type	Observed distance (Å)	ldeal distance (Å)	Number of outliers
NZHZ2	1.01	0.89	96
CD2HD23	1.09	0.97	304
CGHG2	1.09	0.97	743
CBHB2	1.09	0.97	2057
CBHB	1.09	0.97	429
NZHZ1	1.01	0.89	95
CG2HG22	1.09	0.97	460
CG1HG13	1.09	0.97	301
CGHG	1.09	0.97	281
CD2HD21	1.09	0.97	301
NZHZ3	1.01	0.89	105
CBHB1	1.09	0.97	308
CEHE2	1.09	0.97	313
CEHE1	1.09	0.97	125
CEHE3	1.09	0.97	321
OHHH	0.96	0.84	49
CAHA2	1.09	0.97	46
OG1HG1	0.96	0.84	52
CAHA3	1.09	0.97	46
NH	0.98	0.86	2
CE1HE1	1.05	0.93	1
OGHG	0.96	0.84	81
CEHE2	1.10	0.97	23

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CEHE3	1.10	0.97	14
OGHG	0.97	0.84	121
CAHA	1.10	0.97	19
NZHZ1	1.02	0.89	80
OG1HG1	0.97	0.84	97
NZHZ3	1.02	0.89	81
NZHZ2	1.02	0.89	90
OHHH	0.97	0.84	7
CBHB	1.10	0.97	2
CG2HG22	1.10	0.97	1
NH	0.99	0.86	8
CG2HG21	1.10	0.97	1
CD1HD1	1.06	0.93	1
SGHG	1.33	1.20	2
ND2HD22	0.99	0.86	1
NH2HH22	0.99	0.86	3
NH1HH11	0.99	0.86	3
NH1HH12	0.99	0.86	2
NE2HE22	1.00	0.86	119
NZHZ2	1.03	0.89	14
NZHZ3	1.03	0.89	12
NH1HH12	1.00	0.86	39
OGHG	0.98	0.84	40

Bond type	Observed distance (Å)	ldeal distance (Å)	Number of outliers
NZHZ1	1.03	0.89	17
NH1HH11	1.00	0.86	47
CE1HE1	1.07	0.93	2
NH2HH21	1.00	0.86	30
OG1HG1	0.98	0.84	18
CZHZ	1.07	0.93	2
OHHH	0.98	0.84	3
NH2HH22	1.00	0.86	35
NH	1.00	0.86	148
ND2HD22	1.00	0.86	127
CAHA	1.11	0.97	2
SGHG	1.34	1.20	41
ND2HD21	1.00	0.86	43
CE2HE2	1.07	0.93	5
NE2HE21	1.00	0.86	51
NEHE	1.00	0.86	22
CD1HD1	1.07	0.93	5
CGHG3	1.11	0.97	1
CGHG2	1.11	0.97	1
CD2HD2	1.07	0.93	5
CZ2HZ2	1.07	0.93	1
CE3HE3	1.07	0.93	5
CH2HH2	1.07	0.93	1

Bond type	Observed distance (Å)	ldeal distance (Å)	Number of outliers
NH	1.01	0.86	1900
ND2HD22	1.01	0.86	19
NE2HE22	1.01	0.86	37
NH1HH11	1.01	0.86	17
NH2HH22	1.01	0.86	26
NEHE	1.01	0.86	41
NH1HH12	1.01	0.86	23
ND2HD21	1.01	0.86	68
CD2HD2	1.08	0.93	121
NH2HH21	1.01	0.86	31
CD1HD1	1.08	0.93	137
NE2HE21	1.01	0.86	51
CE1HE1	1.08	0.93	127
CZHZ	1.08	0.93	57
SGHG	1.35	1.20	6
CZ2HZ2	1.08	0.93	29
CE2HE2	1.08	0.93	114
CZ3HZ3	1.08	0.93	30
CE3HE3	1.08	0.93	25
CH2HH2	1.08	0.93	29
NE1HE1	1.01	0.86	19
OG1HG1	0.99	0.84	3
OGHG	0.99	0.84	6

Bond type	Observed distance (Å)	ldeal distance (Å)	Number of outliers
NE2HE2	1.01	0.86	10
OHHH	0.99	0.84	1
CAHA	1.12	0.97	1
NH	1.02	0.86	689
ND2HD21	1.02	0.86	34
NEHE	1.02	0.86	24
NE2HE21	1.02	0.86	44
NH1HH11	1.02	0.86	15
CD1HD1	1.09	0.93	7
CD2HD2	1.09	0.93	4
OGHG	1.00	0.84	2
NH2HH21	1.02	0.86	21
NH2HH22	1.02	0.86	18
NH1HH12	1.02	0.86	16
NE1HE1	1.02	0.86	8
NE2HE22	1.02	0.86	10
ND2HD22	1.02	0.86	7
CZHZ	1.09	0.93	1
CE2HE2	1.09	0.93	1
CAHA	1.13	0.97	1
SGHG	1.36	1.20	1
NEHE	1.03	0.86	3
NE1HE1	1.03	0.86	3

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Bond type	Observed distance (Å)	ldeal distance (Å)	Number of outliers
ND2HD21	1.03	0.86	15
NH1HH12	1.03	0.86	10
NH2HH22	1.03	0.86	7
ND2HD22	1.03	0.86	6
NH2HH21	1.03	0.86	8
NE2HE21	1.03	0.86	23
NH	1.03	0.86	3
NH1HH11	1.03	0.86	8
NE2HE22	1.03	0.86	4
NH2HH22	1.04	0.86	1
CAHA	1.15	0.97	1
NE2HE21	1.04	0.86	1

Standard geometry: angle outliers?

There are 594 angle outliers in this entry. A summary is provided below, and a detailed list of outliers can be found here.

Angle type	Observed angle (°)	ldeal angle (°)	Number of outliers
CB-CG-CD1	120.80	101.69	1
C-CA-CB	110.10	132.69	1
C-N-CA	121.70	141.78	1
C-N-CA	121.70	141.34	1
CA-CB-CG	112.60	123.13	1
CA-CB-CG	112.60	122.76	1
CA-C-N	116.90	132.07	1
C-N-CA	121.70	138.92	1

Angle type	Observed angle (°)	ldeal angle (°)	Number of outliers
C-N-CA	121.70	138.89	1
CB-CG-CD1	120.70	104.97	1
CA-CB-CG	113.80	123.00	1
CA-CB-CG	113.80	122.96	1
CA-C-N	116.90	130.36	1
C-CA-CB	110.10	126.98	1
CA-CB-CG	113.80	122.68	1
C-N-CA	121.70	137.36	1
C-CA-CB	110.10	126.20	1
C-CA-CB	110.50	123.18	1
C-CA-CB	111.60	128.11	1
CA-C-N	116.20	132.61	1
CA-C-N	116.20	132.56	1
N-CA-CB	110.50	124.30	1
C-N-CA	121.70	136.22	1
C-CA-CB	110.10	125.17	1
CA-CB-CG	112.60	120.45	1
C-CA-CB	110.10	124.83	1
CA-CB-CG	114.10	129.56	1
C-CA-CB	110.10	124.54	1
CA-CB-CG	112.60	120.16	1
CA-C-N	116.20	131.23	1
CA-CB-CG	112.60	120.04	1

Angle type	Observed angle (°)	ldeal angle (°)	Number of outliers
C-N-CA	121.70	135.06	1
CA-C-N	116.20	130.93	1
C-N-CA	121.70	134.94	1
CA-C-N	116.90	127.86	1
CA-CB-CG	112.60	119.82	1
CA-CB-CG2	110.50	122.75	1
OE1-CD-NE2	122.60	115.40	1
C-N-CA	121.70	134.45	1
CA-CB-CG2	110.40	122.38	1
C-CA-CB	110.50	100.03	1
CA-CB-CG	113.80	120.73	1
C-N-CA	121.70	134.15	1
N-CA-CB	110.50	122.18	1
CA-CB-CG	112.60	105.76	1
C-N-CA	121.70	133.97	1
C-N-CA	121.70	133.95	2
C-N-CA	121.70	133.94	1
OE1-CD-NE2	122.60	115.81	1
CA-CB-CG	112.60	119.38	1
CA-CB-CG	112.60	105.83	1
CA-N-CD	112.00	102.55	1
CA-CB-CG	113.80	120.55	1
C-N-CA	121.70	133.75	1

Angle type	Observed angle (°)	ldeal angle (°)	Number of outliers
O-C-N	123.00	112.30	1
CA-CB-CG	112.60	119.27	1
CA-CB-CG	113.80	120.45	1
C-N-CA	121.70	133.64	1
O-C-N	123.00	112.50	1
CD1-CG-CD2	118.10	127.93	1
N-CA-C	112.10	128.34	1
N-CA-CB	110.50	121.39	1
CA-CB-CG	112.60	119.01	1
C-N-CA	121.70	133.15	1
C-CA-CB	111.60	124.31	1
C-CA-CB	111.40	123.44	1
N-CA-CB	110.50	121.27	1
CA-CB-CG	112.60	118.92	1
CA-CB-CG2	110.50	121.22	1
C-CA-CB	110.10	122.08	1
CA-CB-CG	113.80	120.05	1
C-CA-CB	110.10	121.92	1
OE1-CD-NE2	122.60	116.40	1
C-N-CA	121.70	132.85	1
C-CA-CB	110.10	121.86	1
CA-N-CD	112.00	103.34	1
CA-N-CD	112.00	103.35	1

Angle type	Observed angle (°)	ldeal angle (°)	Number of outliers
O-C-N	123.00	113.12	1
CA-CB-CG	112.60	118.76	1
CA-CB-CG	112.60	118.75	1
C-CA-CB	110.10	121.74	1
N-CA-CB	110.50	120.91	1
C-N-CA	121.70	132.72	1
C-CA-CB	111.60	123.79	1
C-N-CA	121.70	132.64	1
CA-CB-CG1	110.40	120.73	1
C-CA-CB	111.40	99.89	1
CB-CG-CD	112.60	122.82	1
C-CA-CB	110.10	121.51	1
CA-CB-CG	113.80	119.78	1
N-CA-C	112.10	127.03	1
C-N-CA	121.70	132.42	1
C-CA-CB	110.10	121.40	1
O-C-N	123.00	113.49	1
CA-CB-CG	114.10	125.95	1
CE1-CZ-OH	119.90	137.62	1
C-N-CA	121.70	132.31	1
C-CA-CB	110.10	121.29	1
CA-CB-CG2	110.50	120.48	1
C-CA-CB	110.10	121.22	1

Angle type	Observed angle (°)	ldeal angle (°)	Number of outliers
CD-NE-CZ	124.40	132.56	1
N-CA-C	111.00	127.29	1
O-C-N	123.00	113.71	1
N-CA-C	112.10	126.61	1
N-CA-CB	110.50	100.64	1
N-CA-C	111.00	94.77	1
CG1-CB-CG2	110.70	127.98	1
OE1-CD-NE2	122.60	116.84	1
CA-CB-CG2	110.40	120.17	1
CA-C-N	116.20	127.69	1
C-CA-CB	110.10	121.01	1
C-CA-CB	110.10	120.97	1
CA-CB-CG	112.60	118.32	1
OE1-CD-NE2	122.60	116.89	1
CA-CB-CG	112.60	118.31	1
CA-CB-CG	112.60	118.29	3
N-CA-CB	111.50	101.82	1
C-N-CA	121.70	131.92	1
CD2-CE2-CZ	120.00	109.79	1
O-C-N	123.00	113.93	1
CE1-CZ-CE2	120.30	108.97	1
C-N-CA	121.70	131.89	1
N-CA-CB	111.50	121.10	1

Angle type	Observed angle (°)	ldeal angle (°)	Number of outliers
C-N-CA	121.70	131.86	1
O-C-N	123.00	113.98	1
C-CA-CB	110.10	120.80	1
N-CA-CB	111.50	101.93	1
N-CA-CB	103.00	109.19	1
CA-CB-CG	114.10	125.35	1
CA-CB-CG2	110.50	120.02	1
N-CA-CB	110.50	120.00	1
C-CA-CB	110.50	102.14	1
C-N-CA	121.70	131.70	1
C-CA-CB	110.10	120.65	1
CA-CB-CG	112.60	107.05	1
CD1-CG-CD2	118.60	126.91	1
C-CA-CB	111.40	121.91	1
C-N-CA	121.70	131.58	1
CA-CB-CG	112.60	118.09	1
CA-N-CD	112.00	104.33	1
C-N-CA	121.70	131.53	2
C-CA-CB	110.10	120.46	1
CA-CB-CG	113.80	119.25	1
N-CA-CB	110.50	119.76	1
OE1-CD-NE2	122.60	117.16	1
C-N-CA	121.70	131.49	1

Angle type	Observed angle (°)	ldeal angle (°)	Number of outliers
N-CA-CB	111.50	120.74	1
C-N-CA	121.70	131.45	1
N-CA-C	111.00	126.17	1
C-CA-CB	110.10	120.37	1
CA-CB-CG	113.80	119.18	1
C-N-CA	121.70	131.38	1
N-CA-CB	110.50	101.38	1
C-CA-CB	110.10	120.29	1
C-N-CA	121.70	131.35	1
C-CA-CB	111.60	122.32	1
C-N-CA	121.70	131.34	1
OE1-CD-NE2	122.60	117.24	1
CA-CB-CG	112.60	107.25	1
CA-N-CD	112.00	104.54	1
CA-C-N	116.20	126.85	1
C-CA-CB	110.50	118.49	1
CA-CB-CG1	110.40	119.41	1
C-N-CA	121.70	131.23	1
N-CA-CB	110.50	119.47	1
CA-CB-CG	112.60	117.86	1
C-CA-CB	110.10	100.13	1
C-CA-CB	111.60	101.11	1
N-CA-CB	110.50	119.39	1

Angle type	Observed angle (°)	ldeal angle (°)	Number of outliers
OE1-CD-NE2	122.60	117.37	1
C-CA-CB	109.10	97.61	1
C-N-CA	121.70	131.10	1
C-N-CA	121.70	131.09	1
CA-CB-CG	112.60	117.81	1
CA-CB-CG	113.80	119.00	1
C-N-CA	121.70	131.03	2
N-CA-C	112.10	99.14	1
NE-CZ-NH2	119.20	123.87	1
C-N-CA	121.70	131.00	2
CB-CG-CD	111.30	123.16	1
CA-C-N	116.90	124.63	1
CA-C-N	116.20	126.51	1
C-N-CA	121.70	130.98	1
C-CA-CB	110.10	119.89	1
OE1-CD-NE2	122.60	117.45	1
C-N-CA	121.70	130.96	1
CA-C-N	116.90	124.61	1
CD-NE-CZ	124.40	131.58	1
CA-CB-CG	112.60	117.73	1
C-N-CA	121.70	130.91	1
C-N-CA	121.70	130.90	1
C-N-CA	121.70	130.87	1

Angle type	Observed angle (°)	ldeal angle (°)	Number of outliers
CA-CB-CG	112.60	117.68	1
N-CA-C	111.00	125.22	1
CA-CB-CG	113.80	118.88	1
C-CA-CB	110.10	119.74	1
OE1-CD-NE2	122.60	117.53	1
C-N-CA	121.70	130.83	1
C-N-CA	121.70	130.81	2
CA-CB-CG1	110.40	118.99	1
N-CA-C	111.00	96.85	1
OD1-CG-ND2	122.60	117.55	1
C-CA-CB	110.10	119.69	1
CA-CB-CG	113.80	118.84	1
C-CA-CB	110.10	119.68	1
OD1-CG-ND2	122.60	117.56	1
C-CA-CB	110.10	119.67	1
C-N-CA	121.70	130.76	1
C-CA-CB	110.10	119.65	1
CB-CG-CD2	126.80	133.83	1
O-C-N	123.00	114.99	1
CA-CB-CG	113.60	123.10	1
OE1-CD-NE2	122.60	117.61	1
C-N-CA	121.70	130.65	1
N-CA-CB	111.50	119.94	1

Angle type	Observed angle (°)	ldeal angle (°)	Number of outliers
C-N-CA	121.70	130.64	1
OE1-CD-NE2	122.60	117.64	1
C-CA-CB	110.10	119.53	1
N-CA-CB	110.50	118.92	1
N-CA-CB	110.50	118.90	1
CA-CB-CG2	110.40	118.80	1
CB-CG-CD2	131.20	124.78	1
N-CA-CB	110.50	102.12	1
CB-CG-CD2	131.20	124.79	1
C-CA-CB	110.10	119.46	1
CA-CB-CG	112.60	117.50	2
N-CA-CB	110.50	102.18	1
N-CA-CB	110.50	118.82	1
CA-CB-CG	113.80	118.69	1
C-N-CA	121.70	130.51	2
C-N-CA	121.70	130.49	1
N-CA-CB	110.50	118.80	1
C-N-CA	121.70	130.48	2
N-CA-CB	110.50	102.23	1
CA-CB-CG	113.90	122.65	1
C-N-CA	121.70	130.45	1
C-N-CA	121.70	130.43	2
NE-CZ-NH2	119.20	123.56	1

Angle type	Observed angle (°)	ldeal angle (°)	Number of outliers
C-N-CA	121.70	130.40	1
CA-CB-CG	112.60	117.43	1
N-CA-CB	110.50	118.70	1
N-CA-CB	110.50	118.69	1
CA-C-O	120.80	112.61	1
C-CA-CB	109.10	119.69	1
OE1-CD-NE2	122.60	117.79	1
C-N-CA	121.70	130.36	1
CA-CB-CG	112.60	117.41	1
C-N-CA	121.70	130.35	1
CA-CB-CG2	110.40	118.52	1
C-CA-CB	110.10	101.03	1
CD-NE-CZ	124.40	131.08	1
OE1-CD-NE2	122.60	117.83	2
CA-CB-CG	112.60	117.37	1
C-N-CA	121.70	130.28	1
CA-CB-CG2	110.40	118.50	1
CA-CB-CG	112.60	117.36	1
C-N-CA	121.70	130.26	1
CA-C-N	116.20	125.69	1
OE1-CD-NE2	122.60	117.86	1
CA-CB-CG	112.60	117.33	1
CA-CB-CG	112.60	117.32	1

Angle type	Observed angle (°)	ldeal angle (°)	Number of outliers
C-N-CA	121.70	130.18	1
CA-CB-CG	114.10	123.51	1
CA-CB-CG1	110.40	118.38	1
OE1-CD-NE2	122.60	117.91	1
CA-C-O	120.80	112.83	1
C-CA-CB	110.10	119.00	1
CA-CB-CG	112.60	117.28	1
N-CA-CB	110.50	102.55	1
N-CA-CB	111.50	103.55	1
C-N-CA	121.70	130.11	1
CA-CB-CG	112.60	117.27	1
C-CA-CB	111.60	102.27	1
C-CA-CB	110.10	118.96	1
N-CA-C	111.00	124.04	1
CG-CD1-CE1	120.70	128.60	1
CA-N-CD	112.00	105.49	1
C-N-CA	121.70	130.07	1
N-CA-CB	110.50	102.61	1
C-N-CA	121.70	130.04	1
CA-CB-CG	112.60	117.22	1
OE1-CD-NE2	122.60	117.98	1
C-N-CA	121.70	130.00	2
OE1-CD-NE2	122.60	117.99	1

Angle type	Observed angle (°)	ldeal angle (°)	Number of outliers
CA-CB-CG	114.10	123.30	1
C-N-CA	121.70	129.98	1
CA-CB-CG	113.90	105.62	1
O-C-N	123.00	115.64	1
CA-CB-CG	114.10	123.29	1
C-N-CA	121.70	129.96	1
CA-CB-CG1	110.40	118.20	1
C-CA-CB	110.10	118.80	1
C-N-CA	121.70	129.95	1
CA-CB-CG2	110.40	118.19	1
C-N-CA	121.70	129.94	2
CA-CB-CG	112.60	117.18	1
C-CA-CB	110.10	118.79	1
C-N-CA	121.70	129.93	1
C-CA-CB	110.10	118.78	1
N-CA-CB	111.50	103.76	1
CA-C-N	116.90	123.73	1
CA-C-N	116.20	125.30	1
OE1-CD-NE2	122.60	118.06	2
NH1-CZ-NH2	119.30	113.40	1
OE1-CD-NE2	122.60	118.07	2
C-CA-CB	110.10	118.70	1
C-N-CA	121.70	129.84	1

Angle type	Observed angle (°)	ldeal angle (°)	Number of outliers
CA-CB-CG	112.60	117.12	1
C-N-CA	121.70	129.83	1
CA-C-N	116.90	123.67	1
C-N-CA	121.70	113.58	1
C-CA-CB	111.60	120.61	1
OE1-CD-NE2	122.60	118.10	1
C-N-CA	121.70	129.79	2
CE1-CZ-CE2	120.00	111.92	1
CA-CB-CG1	110.40	118.03	1
OE1-CD-NE2	122.60	118.12	1
CA-C-N	116.20	125.15	1
OE1-CD-NE2	122.60	118.13	1
N-CA-C	111.00	123.52	1
CA-CB-CG	112.60	117.07	1
C-CA-CB	110.10	118.58	1
C-N-CA	121.70	129.73	1
OE1-CD-NE2	122.60	118.14	1
CA-CB-CG	112.60	108.15	1
CA-C-N	116.90	123.58	1
N-CA-CB	110.50	102.94	1
CB-CG-CD	112.60	105.04	1
CB-CG-CD2	131.20	125.42	1
CA-CB-CG	112.60	117.04	1

Angle type	Observed angle (°)	ldeal angle (°)	Number of outliers
N-CA-CB	103.00	107.89	1
C-N-CA	121.70	113.71	1
C-N-CA	121.70	129.69	1
C-CA-CB	111.60	120.46	1
CA-CB-CG	112.60	117.03	1
C-N-CA	121.70	129.68	1
CA-C-O	120.80	113.28	1
OE1-CD-NE2	122.60	118.18	1
CA-C-N	116.20	125.02	1
CA-CB-CG	113.80	118.21	1
C-N-CA	121.70	129.63	1
C-CA-CB	110.10	118.47	2
OE1-CD-NE2	122.60	118.21	2
CA-C-N	116.90	123.48	1
C-CA-CB	110.10	118.43	1
OD1-CG-ND2	122.60	118.22	2
CA-CB-CG2	110.50	117.95	1
N-CD-CG	103.20	109.77	1
C-CA-CB	110.10	118.41	1
CA-CB-CG	113.80	118.17	1
C-N-CA	121.70	129.57	2
CA-CB-CG	114.10	122.84	1
OE1-CD-NE2	122.60	118.23	1

Angle type	Observed angle (°)	ldeal angle (°)	Number of outliers
C-CA-CB	110.10	118.40	1
CA-CB-CG2	110.50	117.92	1
C-CA-CB	110.10	118.39	1
CB-CG-CD	111.30	121.34	1
C-N-CA	121.70	129.55	1
CA-C-O	120.80	128.21	1
C-N-CA	121.70	129.54	1
CA-CB-CG	112.60	116.95	1
C-N-CA	121.70	129.53	1
CA-CB-CG	112.60	116.94	1
OE1-CD-NE2	122.60	118.26	2
C-N-CA	121.70	129.51	2
C-CA-CB	110.10	118.34	1
CB-CG-CD	111.30	121.26	1
C-N-CA	121.70	129.50	1
N-CA-CB	110.50	117.86	1
CA-C-N	116.90	123.40	1
CA-CB-CG	113.90	121.69	1
OE1-CD-NE2	122.60	118.27	1
CA-CB-CG1	110.40	117.75	1
N-CA-CB	110.50	103.15	1
CD-NE-CZ	124.40	130.45	1
CA-CB-CG	113.80	118.12	1

Angle type	Observed angle (°)	ldeal angle (°)	Number of outliers
CA-CB-CG	112.60	116.91	1
N-CA-CB	110.50	103.17	1
C-CA-CB	110.10	118.29	1
CB-CG-CD2	131.20	125.60	1
C-CA-CB	110.10	118.28	1
C-N-CA	121.70	129.45	2
CA-CB-CG1	110.40	117.70	1
N-CA-C	111.00	123.02	1
CA-CB-CG	113.90	121.61	1
C-CA-CB	110.10	118.24	1
OE1-CD-NE2	122.60	118.32	1
N-CA-C	112.10	122.80	1
OD1-CG-ND2	122.60	118.32	1
OE1-CD-NE2	122.60	118.33	1
CB-CG-CD	112.60	119.86	1
N-CA-CB	110.50	117.75	1
CA-CB-CG1	110.40	117.64	1
C-N-CA	121.70	129.36	1
CA-CB-CG	112.60	116.85	1
CB-CG-CD	111.30	121.08	1
CA-C-N	116.20	124.70	1
C-CA-CB	110.10	118.18	1
CD-NE-CZ	124.40	130.35	1

Angle type	Observed angle (°)	ldeal angle (°)	Number of outliers
C-N-CA	121.70	129.34	1
C-CA-CB	110.10	118.16	1
C-N-CA	121.70	129.33	1
OE1-CD-NE2	122.60	118.37	2
C-CA-CB	110.10	118.14	1
CA-CB-CG1	110.40	117.59	1
N-CA-CB	110.50	117.69	1
CA-CB-CG2	110.50	103.32	1
N-CA-C	111.00	122.83	1
C-CA-CB	109.10	118.39	1
O-C-N	123.00	116.25	1
OD1-CG-ND2	122.60	118.38	1
C-N-CA	121.70	129.29	1
CA-C-N	116.90	123.22	1
CG-CD-CE	111.30	121.00	1
CA-CB-CG	112.60	116.81	1
OE1-CD-NE2	122.60	118.39	3
CD-NE-CZ	124.40	130.30	1
C-CA-CB	110.10	118.10	1
CA-CB-CG2	110.50	117.66	1
N-CA-CB	110.50	103.34	1
CA-C-N	116.20	124.61	1
CA-CB-CG	112.60	116.80	1

Angle type	Observed angle (°)	ldeal angle (°)	Number of outliers
CA-CB-CG	113.80	118.00	1
N-CA-CB	110.40	116.69	1
CA-C-O	120.80	113.67	1
C-CA-CB	110.50	116.79	2
CB-CG-CD2	131.20	125.75	1
C-CA-CB	110.10	118.06	1
N-CA-CB	110.40	104.12	1
CD-NE-CZ	124.40	130.26	1
CG-CD-NE2	116.40	122.67	1
N-CA-CB	110.50	103.39	1
C-N-CA	121.70	129.22	1
OD1-CG-ND2	122.60	118.42	1
CB-CG-CD	111.30	120.91	1
N-CA-CB	110.50	103.40	1
C-N-CA	121.70	129.21	2
C-CA-CB	110.10	118.02	1
CA-CB-CG1	110.40	117.48	1
CA-CB-CG	112.60	116.76	2
C-CA-CB	110.10	118.00	1
C-N-CA	121.70	129.18	1
C-N-CA	121.70	129.17	1
CA-CB-CG	114.10	122.40	1
C-CA-CB	110.10	117.97	2

Angle type	Observed angle (°)	ldeal angle (°)	Number of outliers
N-CA-CB	110.40	104.19	1
CA-CB-CG	112.60	116.74	1
C-CA-CB	110.50	116.71	1
OE1-CD-NE2	122.60	118.46	1
CA-CB-CG	114.10	105.83	1
OG1-CB-CG2	109.30	101.03	1
CA-CB-CG2	110.50	117.52	1
CB-CG-CD	111.30	120.80	1
OE1-CD-NE2	122.60	118.47	2
OD1-CG-ND2	122.60	118.47	1
CA-CB-CG	114.10	122.35	1
CA-CB-CG	113.80	117.92	2
N-CA-CB	110.50	103.50	1
C-N-CA	121.70	129.11	1
OE1-CD-NE2	122.60	118.48	1
N-CA-CB	110.50	117.48	1
CA-CB-CG	112.60	116.70	1
CA-CB-OG1	109.60	115.76	1
C-CA-CB	111.60	119.81	1
CD-NE-CZ	124.40	130.14	1
CA-C-N	116.20	124.39	2
OE1-CD-NE2	122.60	118.50	1
C-CA-CB	110.10	117.88	1

Angle type	Observed angle (°)	ldeal angle (°)	Number of outliers
C-N-CA	121.70	129.07	1
CA-CB-CG2	110.50	117.46	1
C-N-CA	121.70	114.34	1
C-CA-CB	110.10	117.87	1
C-N-CA	121.70	129.06	1
NH1-CZ-NH2	119.30	113.99	1
N-CA-CB	110.50	103.56	1
N-CA-CB	110.40	116.52	1
CA-C-N	116.20	124.36	1
C-N-CA	121.70	129.04	2
CA-CB-CG	114.10	122.25	1
OE1-CD-NE2	122.60	118.53	1
C-N-CA	121.70	129.03	1
CA-CB-CG2	110.40	117.32	1
C-CA-CB	110.10	117.83	1
CA-CB-CG	112.60	108.53	1
C-CA-CB	111.40	119.12	1
CA-CB-CG1	110.40	117.30	1
C-CA-CB	110.10	117.81	1
OD1-CG-ND2	122.60	118.55	1
N-CA-C	112.10	101.97	1
OE1-CD-NE2	122.60	118.55	2
C-N-CA	121.70	128.98	2

Angle type	Observed angle (°)	ldeal angle (°)	Number of outliers
CA-C-O	120.80	113.92	1
CA-C-N	116.20	124.29	1
C-CA-CB	110.10	117.78	1
CA-CB-CG	112.60	116.64	1
CA-C-O	120.80	113.93	1
OD1-CG-ND2	122.60	118.56	1
C-N-CA	121.70	128.96	1
OE1-CD-NE2	122.60	118.56	1
CD-NE-CZ	124.40	130.05	1
NH1-CZ-NH2	119.30	114.06	1
CB-CG-CD	111.30	120.57	1
OE1-CD-NE2	122.60	118.57	2
CA-CB-CG	112.60	116.63	1
C-CA-CB	110.10	117.75	1
C-N-CA	121.70	128.94	1
OD1-CG-ND2	122.60	118.58	1
CA-CB-CG	112.60	108.58	1
OE1-CD-NE2	122.60	118.58	4
N-CA-C	111.00	122.26	1
CB-CG-CD2	120.70	113.87	1
CG1-CB-CG2	110.80	101.96	1
C-CA-CB	110.10	117.73	1
CD-NE-CZ	124.40	130.02	1
Angle type	Observed angle (°)	ldeal angle (°)	Number of outliers
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CA-CB-CG2	110.40	117.22	1
N-CA-C	111.00	122.22	1
OE1-CD-NE2	122.60	118.59	1
CA-CB-CG2	110.40	117.21	1
CA-C-O	120.80	127.60	1
N-CA-HA	97.96	110.00	1
C-CA-HA	96.93	109.00	1
HZ1-NZ-HZ2	96.91	109.00	1
C-N-H	112.16	124.30	1
C-N-H	112.12	124.30	1
C-N-H	112.07	124.30	1
CB-CA-HA	96.76	109.00	1
C-N-H	112.06	124.30	1
C-N-H	111.94	124.30	1
C-CA-HA	96.53	109.00	1
N-CA-HA	97.53	110.00	1
HZ2-NZ-HZ3	96.44	109.00	1
C-CA-HA	96.38	109.00	1
C-CA-HA	96.30	109.00	1
C-N-H	111.59	124.30	1
C-CA-HA	96.07	109.00	1
C-N-H	111.24	124.30	1
C-CA-HA	95.86	109.00	1

Angle type	Observed angle (°)	ldeal angle (°)	Number of outliers
CZ-CE1-HE1	133.37	120.20	1
C-N-H	110.95	124.30	1
HB2-CB-HB3	96.51	110.00	1
C-N-H	110.81	124.30	1
C-CA-HA	95.49	109.00	1
C-CA-HA	95.01	109.00	1
CB-CA-HA	93.93	109.00	1
C-N-H	108.98	124.30	1
C-N-H	108.89	124.30	1
C-N-H	107.97	124.30	1
C-N-H	107.69	124.30	1
C-N-H	107.53	124.30	1
CB-CA-HA	91.56	109.00	1
C-N-H	106.62	124.30	1
C-CA-HA	92.14	110.00	1
C-CA-HA	89.44	109.00	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	11.56	51
2	3.40	15
3	3.63	16

Model ID	Clash score	Number of clashes
4	5.44	24
5	1.81	8
6	2.72	12
7	19.71	87
8	24.47	108
9	5.67	25
10	12.46	55

All 401 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	A:234:TYR:CE2	A:234:TYR:CZ	1.655
1	A:232:PHE:CE2	A:234:TYR:CE1	1.373
1	A:232:PHE:CZ	A:234:TYR:CE1	1.363
1	A:232:PHE:CZ	A:234:TYR:CZ	1.362
1	A:232:PHE:CE2	A:234:TYR:CZ	1.361
1	A:232:PHE:CZ	A:234:TYR:CE2	1.191
1	A:232:PHE:CD2	A:234:TYR:CE1	1.189
1	A:232:PHE:CG	A:234:TYR:CE1	1.188
1	A:232:PHE:CE2	A:234:TYR:CD1	1.185
1	A:232:PHE:CE2	A:234:TYR:CE2	1.176
1	A:232:PHE:CD2	A:234:TYR:CZ	1.173
1	A:232:PHE:CE1	A:234:TYR:CZ	1.162
1	A:232:PHE:CZ	A:234:TYR:CD2	1.155
1	A:232:PHE:CE1	A:234:TYR:CE1	1.154

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:232:PHE:CZ	A:234:TYR:CG	1.146
1	A:232:PHE:CZ	A:234:TYR:CD1	1.139
1	A:232:PHE:CD1	A:234:TYR:CE1	1.135
1	A:232:PHE:CD1	A:234:TYR:CZ	1.124
1	A:232:PHE:CE2	A:234:TYR:CD2	1.120
1	A:232:PHE:CE2	A:234:TYR:CG	1.105
1	A:232:PHE:CG	A:234:TYR:CZ	1.063
1	A:232:PHE:CE2	A:232:PHE:CZ	0.948
1	A:234:TYR:CE1	A:234:TYR:CZ	0.939
1	A:252:VAL:H	A:270:ILE:HA	0.897
1	A:58:LEU:HG	A:84:LEU:HD12	0.759
1	A:239:TRP:O	A:273:ALA:HB3	0.677
1	A:59:SER:HA	A:87:ILE:HG23	0.672
1	A:234:TYR:CD1	A:234:TYR:N	0.625
1	A:59:SER:HB2	A:87:ILE:HD12	0.618
1	A:77:MET:O	A:84:LEU:HD13	0.617
1	A:232:PHE:CG	A:234:TYR:HE1	0.570
1	A:252:VAL:N	A:270:ILE:HA	0.555
1	A:260:ASP:CG	A:261:ASN:H	0.516
1	A:233:THR:N	A:234:TYR:CE1	0.508
1	A:250:LYS:HA	A:250:LYS:HE3	0.504
1	A:223:TYR:C	A:223:TYR:CD1	0.492
1	A:232:PHE:CD1	A:234:TYR:OH	0.488

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:232:PHE:CG	A:234:TYR:OH	0.484
1	A:47:THR:HG23	A:213:LEU:HD23	0.483
1	A:232:PHE:CD1	A:234:TYR:HE1	0.454
1	A:92:SER:CB	A:159:ALA:H	0.440
1	A:55:VAL:HG13	A:87:ILE:HD11	0.439
1	A:5:MET:SD	A:9:LYS:HE3	0.435
1	A:244:VAL:HA	A:252:VAL:HA	0.429
1	A:58:LEU:HD21	A:77:MET:HB3	0.422
1	A:9:LYS:HE2	A:41:ILE:O	0.421
1	A:55:VAL:CG1	A:87:ILE:HD11	0.419
1	A:232:PHE:HZ	A:234:TYR:CD2	0.413
1	A:59:SER:CB	A:87:ILE:HD12	0.412
1	A:120:LEU:O	A:124:LYS:CB	0.404
1	A:72:LYS:HA	A:72:LYS:HE3	0.402
2	A:212:LYS:HA	A:212:LYS:HE2	0.550
2	A:74:CYS:SG	A:102:THR:HG21	0.541
2	A:6:SER:HA	A:9:LYS:HE3	0.532
2	A:73:LEU:HB3	A:102:THR:HG22	0.523
2	A:87:ILE:HG13	A:281:LYS:HA	0.495
2	A:220:TYR:C	A:220:TYR:CD1	0.483
2	A:247:ALA:HA	A:252:VAL:HA	0.480
2	A:252:VAL:HG22	A:254:LEU:H	0.465
2	A:138:ALA:HA	A:141:GLN:HE21	0.452

Model ID	Atom-1	Atom-2	Clash overlap (Å)
2	A:37:LEU:O	A:41:ILE:HG22	0.448
2	A:1:GLY:O	A:5:MET:HB2	0.447
2	A:41:ILE:HD13	A:41:ILE:HG21	0.412
2	A:205:ILE:HG23	A:206:PRO:HD2	0.410
2	A:151:ALA:O	A:155:MET:CB	0.406
2	A:38:HIS:HA	A:41:ILE:HG22	0.403
3	A:184:ASP:HA	A:187:ALA:HB3	0.570
3	A:157:LYS:HA	A:157:LYS:HE3	0.531
3	A:162:GLU:HA	A:165:ARG:HG3	0.510
3	A:200:VAL:HG11	A:207:LEU:HD13	0.502
3	A:220:TYR:CD2	A:237:ALA:HB2	0.498
3	A:8:VAL:HG21	A:50:ALA:HB1	0.482
3	A:206:PRO:HD3	A:215:VAL:HB	0.480
3	A:205:ILE:HB	A:238:LEU:HA	0.476
3	A:142:ARG:HB3	A:147:MET:HB2	0.469
3	A:15:LEU:HB3	A:57:LEU:HD22	0.449
3	A:51:PHE:CD1	A:84:LEU:HD13	0.445
3	A:137:ASP:C	A:143:LYS:HA	0.443
3	A:9:LYS:HA	A:9:LYS:HE3	0.422
3	A:160:ARG:CD	A:160:ARG:H	0.422
3	A:160:ARG:H	A:160:ARG:HD3	0.416
3	A:51:PHE:CG	A:84:LEU:HD13	0.407
4	A:54:MET:HA	A:54:MET:HE2	0.777

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	A:9:LYS:HA	A:41:ILE:HG22	0.651
4	A:58:LEU:HD13	A:77:MET:HB2	0.578
4	A:215:VAL:CG1	A:233:THR:H	0.545
4	A:58:LEU:HD22	A:77:MET:HB2	0.542
4	A:54:MET:CE	A:54:MET:HA	0.529
4	A:146:LYS:HA	A:146:LYS:HE2	0.525
4	A:193:ASN:O	A:195:ALA:HB2	0.503
4	A:192:ILE:O	A:195:ALA:HA	0.488
4	A:205:ILE:H	A:205:ILE:HD13	0.479
4	A:91:PHE:CE1	A:164:LYS:HE3	0.452
4	A:220:TYR:CG	A:224:LYS:HE3	0.447
4	A:58:LEU:HD13	A:77:MET:CB	0.442
4	A:172:MET:HG3	A:270:ILE:H	0.441
4	A:12:SER:HB3	A:41:ILE:HG21	0.422
4	A:91:PHE:CZ	A:164:LYS:HE3	0.419
4	A:170:SER:HA	A:232:PHE:CE1	0.418
4	A:213:LEU:HD12	A:232:PHE:CZ	0.418
4	A:177:PHE:HA	A:234:TYR:CZ	0.413
4	A:243:GLN:HE21	A:244:VAL:H	0.410
4	A:176:LEU:HB3	A:234:TYR:HB3	0.404
4	A:8:VAL:HG11	A:50:ALA:HB1	0.403
4	A:173:GLN:HB3	A:232:PHE:CG	0.401
4	A:191:ILE:HG21	A:200:VAL:H	0.401

Model ID	Atom-1	Atom-2	Clash overlap (Å)
5	A:254:LEU:H	A:254:LEU:HD13	0.697
5	A:19:LEU:HD13	A:34:CYS:SG	0.646
5	A:264:ASN:C	A:265:LEU:HD12	0.522
5	A:248:ASP:C	A:250:LYS:H	0.513
5	A:55:VAL:HG13	A:173:GLN:HA	0.469
5	A:254:LEU:CD1	A:254:LEU:H	0.429
5	A:252:VAL:HG13	A:257:ILE:HB	0.427
5	A:2:PRO:HA	A:5:MET:HE3	0.414
6	A:178:THR:HA	A:183:LEU:HD22	0.499
6	A:262:SER:C	A:264:ASN:H	0.467
6	A:25:GLU:HA	A:31:TRP:CG	0.464
6	A:107:TYR:HB3	A:167:LYS:HE2	0.461
6	A:112:ALA:HB3	A:119:VAL:CG2	0.450
6	A:205:ILE:H	A:206:PRO:CD	0.441
6	A:143:LYS:HA	A:143:LYS:HE2	0.425
6	A:12:SER:HB2	A:41:ILE:HG21	0.423
6	A:119:VAL:HA	A:122:LYS:CE	0.422
6	A:252:VAL:HG12	A:255:SER:H	0.413
6	A:4:LYS:HE2	A:47:THR:HG21	0.401
6	A:119:VAL:HA	A:122:LYS:HE2	0.401
7	A:200:VAL:HA	A:216:VAL:HG21	0.863
7	A:257:ILE:HG21	A:269:LEU:C	0.782
7	A:148:ALA:HA	A:276:ALA:HB2	0.739

Model ID	Atom-1	Atom-2	Clash overlap (Å)
7	A:207:LEU:HD13	A:211:ALA:HB2	0.736
7	A:152:MET:HA	A:155:MET:HG3	0.645
7	A:92:SER:HB3	A:98:ALA:HB2	0.628
7	A:149:ASP:HB2	A:273:ALA:HB1	0.628
7	A:183:LEU:HB2	A:191:ILE:HG21	0.624
7	A:215:VAL:C	A:216:VAL:HG22	0.620
7	A:257:ILE:HG22	A:258:SER:N	0.608
7	A:202:LEU:N	A:216:VAL:HG23	0.602
7	A:251:ILE:HA	A:257:ILE:HD11	0.578
7	A:171:ALA:HB2	A:234:TYR:H	0.576
7	A:241:ILE:H	A:282:LEU:HA	0.575
7	A:151:ALA:HB3	A:276:ALA:CB	0.572
7	A:167:LYS:C	A:233:THR:HB	0.557
7	A:244:VAL:CG2	A:273:ALA:HB2	0.556
7	A:171:ALA:HB2	A:233:THR:HA	0.549
7	A:257:ILE:HG21	A:269:LEU:CA	0.546
7	A:250:LYS:HG3	A:252:VAL:HG22	0.534
7	A:152:MET:HG2	A:273:ALA:CA	0.533
7	A:152:MET:HG3	A:153:THR:N	0.521
7	A:215:VAL:O	A:216:VAL:HG22	0.520
7	A:152:MET:HG2	A:273:ALA:HA	0.508
7	A:244:VAL:HG23	A:273:ALA:HB2	0.508
7	A:152:MET:CA	A:155:MET:HG3	0.501

Model ID	Atom-1	Atom-2	Clash overlap (Å)
7	A:88:ALA:HA	A:183:LEU:HD21	0.495
7	A:171:ALA:HB3	A:215:VAL:HG12	0.487
7	A:244:VAL:N	A:271:VAL:HG12	0.485
7	A:151:ALA:HB3	A:276:ALA:HA	0.481
7	A:245:VAL:HG12	A:250:LYS:HA	0.479
7	A:152:MET:SD	A:273:ALA:HA	0.479
7	A:88:ALA:HB2	A:188:LEU:HB2	0.478
7	A:152:MET:SD	A:282:LEU:HD13	0.475
7	A:200:VAL:CA	A:216:VAL:HG21	0.473
7	A:171:ALA:HB2	A:234:TYR:N	0.472
7	A:74:CYS:SG	A:213:LEU:HD12	0.470
7	A:148:ALA:HA	A:276:ALA:CB	0.469
7	A:5:MET:HE2	A:47:THR:HA	0.468
7	A:172:MET:HG3	A:202:LEU:HD22	0.464
7	A:251:ILE:HA	A:257:ILE:CG1	0.464
7	A:58:LEU:HG	A:207:LEU:HD21	0.462
7	A:151:ALA:HB3	A:276:ALA:HB1	0.461
7	A:7:ASP:HB3	A:82:ALA:H	0.458
7	A:156:TYR:N	A:282:LEU:H	0.458
7	A:243:GLN:C	A:271:VAL:HG12	0.452
7	A:151:ALA:HB1	A:278:SER:HA	0.450
7	A:251:ILE:HA	A:257:ILE:CD1	0.449
7	A:155:MET:HB2	A:280:VAL:C	0.448

Model ID	Atom-1	Atom-2 Clash overlap (Å)	
7	A:244:VAL:HA	A:271:VAL:C	0.446
7	A:62:LEU:HB3	A:208:THR:HG23 0.443	
7	A:172:MET:HA	A:202:LEU:CB	0.441
7	A:215:VAL:HG11	A:233:THR:HG22	0.438
7	A:251:ILE:N	A:251:ILE:HD13	0.438
7	A:92:SER:HB3	A:98:ALA:CB	0.436
7	A:202:LEU:HA	A:215:VAL:N	0.436
7	A:202:LEU:HD12	A:215:VAL:HG13	0.436
7	A:202:LEU:HB2	A:215:VAL:HA	0.435
7	A:51:PHE:O	A:55:VAL:HG13	0.434
7	A:51:PHE:HB2	A:83:THR:HG21	0.432
7	A:58:LEU:CD2	A:207:LEU:HD11	0.432
7	A:171:ALA:HB2	A:233:THR:CA 0.431	
7	A:163:ASP:C	A:165:ARG:H	0.430
7	A:170:SER:HB3	A:234:TYR:CD2	0.430
7	A:171:ALA:CB	A:234:TYR:H	0.430
7	A:172:MET:HB2	A:202:LEU:HD13	0.428
7	A:256:GLU:O	A:257:ILE:HD13	0.428
7	A:281:LYS:C	A:283:GLN:H	0.428
7	A:217:ILE:HG23	A:232:PHE:HB3	0.427
7	A:108:GLU:HA	A:111:VAL:O	0.425
7	A:267:TRP:HB3	A:268:PRO:CD	0.420
7	A:244:VAL:HG21	A:273:ALA:HB2	0.419

Model ID	Atom-1	Atom-2 Clash overlap (Å)	
7	A:244:VAL:HG22	A:245:VAL:HG22	0.419
7	A:257:ILE:HD12	A:268:PRO:N	0.418
7	A:253:GLN:H	A:256:GLU:HB2	0.417
7	A:167:LYS:HA	A:233:THR:C	0.416
7	A:152:MET:CG	A:153:THR:N	0.415
7	A:151:ALA:O	A:152:MET:C	0.414
7	A:168:VAL:HG13	A:169:THR:HG23	0.414
7	A:9:LYS:HG2	A:42:LEU:HA	0.413
7	A:151:ALA:HB3	A:276:ALA:CA	0.410
7	A:32:ALA:HA	A:35:VAL:HG12	0.408
7	A:204:ILE:H	A:213:LEU:C	0.408
7	A:155:MET:HB2	A:282:LEU:N	0.406
7	A:58:LEU:HD23	A:207:LEU:HD11 0.405	
7	A:152:MET:HG2	A:273:ALA:C 0.404	
7	A:92:SER:HB3	A:98:ALA:CA	0.403
8	A:199:CYS:HA	A:273:ALA:HB3	0.879
8	A:54:MET:SD	A:77:MET:HE2	0.757
8	A:262:SER:HA	A:265:LEU:HB3	0.712
8	A:244:VAL:HG21	A:249:SER:C	0.709
8	A:120:LEU:HA	A:124:LYS:H	0.707
8	A:254:LEU:HA	A:257:ILE:HB	0.707
8	A:205:ILE:HA	A:208:THR:HB	0.700
8	A:252:VAL:HG13	A:253:GLN:HA	0.673

Model ID	Atom-1	Atom-2 Clash overlap (Å)	
8	A:143:LYS:HE2	A:180:LEU:HB3	0.666
8	A:142:ARG:HA	A:177:PHE:CD1	0.653
8	A:174:THR:O	A:178:THR:HG23	0.648
8	A:244:VAL:HG22	A:245:VAL:N	0.648
8	A:110:ALA:HA	A:113:ASN:HB3	0.638
8	A:201:PRO:HB3	A:273:ALA:HA	0.634
8	A:199:CYS:HA	A:273:ALA:CB	0.627
8	A:240:GLU:C	A:257:ILE:HG23	0.625
8	A:92:SER:HA	A:95:PRO:CD	0.617
8	A:82:ALA:HA	A:96:SER:HB3	0.613
8	A:122:LYS:HA	A:126:SER:HB3	0.607
8	A:121:LYS:HA	A:125:LYS:HB2	0.605
8	A:93:SER:HB2	A:178:THR:HB 0.602	
8	A:174:THR:HA	A:177:PHE:CD1	0.601
8	A:252:VAL:HB	A:257:ILE:HD11	0.598
8	A:241:ILE:H	A:257:ILE:HA	0.592
8	A:152:MET:HA	A:155:MET:HB3	0.587
8	A:243:GLN:C	A:252:VAL:HG11	0.580
8	A:243:GLN:HA	A:252:VAL:HG11	0.580
8	A:58:LEU:HB2	A:77:MET:HE1	0.579
8	A:95:PRO:CA	A:99:ALA:HB3	0.578
8	A:142:ARG:HB3	A:148:ALA:HA	0.577
8	A:8:VAL:HG22	A:41:ILE:HD11	0.573

Model ID	Atom-1	Atom-2 Clash overlap (Å)	
8	A:119:VAL:HA	A:123:LEU:H	0.564
8	A:85:GLN:HB3	A:95:PRO:HG2	0.563
8	A:90:GLU:HA	A:93:SER:HB2	0.555
8	A:254:LEU:HA	A:257:ILE:CB	0.546
8	A:201:PRO:HB3	A:273:ALA:CA	0.542
8	A:121:LYS:O	A:136:ARG:HB2	0.540
8	A:243:GLN:O	A:252:VAL:HG11	0.535
8	A:201:PRO:HA	A:273:ALA:HB1	0.520
8	A:41:ILE:HD12	A:50:ALA:O	0.518
8	A:138:ALA:HA	A:142:ARG:HH21	0.515
8	A:161:SER:H	A:165:ARG:HB3	0.515
8	A:142:ARG:CB	A:148:ALA:HA	0.508
8	A:241:ILE:N	A:257:ILE:HG23 0.507	
8	A:250:LYS:O	A:252:VAL:HG12 0.505	
8	A:252:VAL:HG23	A:274:LEU:HA	0.505
8	A:98:ALA:HA	A:101:ALA:HB3	0.502
8	A:254:LEU:HA	A:257:ILE:HD12	0.499
8	A:104:GLN:C	A:108:GLU:H	0.497
8	A:254:LEU:CA	A:257:ILE:HD12	0.494
8	A:151:ALA:HA	A:154:GLN:HB3	0.487
8	A:158:GLN:HA	A:280:VAL:HB	0.487
8	A:205:ILE:O	A:208:THR:HB	0.485
8	A:250:LYS:HE3	A:251:ILE:HG23	0.478

Model ID	Atom-1	Atom-2 Clash overlap (Å)	
8	A:62:LEU:HB2	A:70:ILE:HD13 0.477	
8	A:92:SER:HA	A:95:PRO:HD3 0.475	
8	A:218:PRO:HG3	A:269:LEU:H	0.475
8	A:90:GLU:C	A:93:SER:H	0.473
8	A:93:SER:CB	A:178:THR:HB	0.473
8	A:259:MET:C	A:261:ASN:H	0.473
8	A:201:PRO:HD2	A:202:LEU:HA	0.469
8	A:95:PRO:C	A:99:ALA:HB3	0.466
8	A:126:SER:H	A:128:ASN:H	0.466
8	A:201:PRO:HB3	A:273:ALA:CB	0.465
8	A:82:ALA:HA	A:96:SER:CB	0.459
8	A:208:THR:HA	A:213:LEU:H	0.458
8	A:244:VAL:HG21	A:249:SER:O 0.457	
8	A:95:PRO:C	A:99:ALA:H 0.456	
8	A:173:GLN:HB3	A:177:PHE:CZ	0.455
8	A:125:LYS:HE3	A:135:ASP:OD1	0.453
8	A:54:MET:HG2	A:84:LEU:HD11	0.450
8	A:89:SER:O	A:178:THR:HG22	0.448
8	A:208:THR:HA	A:213:LEU:HB2 0.447	
8	A:280:VAL:O	A:283:GLN:O	0.445
8	A:85:GLN:CB	A:95:PRO:HG2	0.439
8	A:143:LYS:HB2	A:177:PHE:HB3	0.439
8	A:239:TRP:HB3	A:241:ILE:CD1	0.435

Model ID	Atom-1	Atom-2	Clash overlap (Å)
8	A:273:ALA:O	A:274:LEU:C	0.433
8	A:251:ILE:C	A:273:ALA:O	0.432
8	A:95:PRO:O	A:97:TYR:N	0.432
8	A:58:LEU:CD1	A:70:ILE:HD11	0.431
8	A:85:GLN:CB	A:96:SER:HB3	0.430
8	A:85:GLN:HB3	A:96:SER:HB3	0.430
8	A:244:VAL:HG22	A:245:VAL:H	0.430
8	A:200:VAL:C	A:273:ALA:HB2	0.427
8	A:126:SER:N	A:128:ASN:H	0.427
8	A:154:GLN:HA	A:282:LEU:H	0.424
8	A:142:ARG:HB2	A:148:ALA:CB	0.422
8	A:223:TYR:CG	A:234:TYR:CE1	0.422
8	A:257:ILE:HG22	A:258:SER:OG	0.422
8	A:58:LEU:O	A:60:VAL:N 0.419	
8	A:89:SER:HB3	A:92:SER:HB2	0.416
8	A:125:LYS:CB	A:132:SER:HB2	0.415
8	A:252:VAL:H	A:274:LEU:HA	0.414
8	A:125:LYS:HB3	A:132:SER:HB2	0.413
8	A:143:LYS:HB2	A:177:PHE:CB	0.413
8	A:194:ASN:HB3	A:199:CYS:HB2	0.412
8	A:257:ILE:HG22	A:258:SER:N	0.412
8	A:255:SER:HA	A:258:SER:H	0.410
8	A:89:SER:CB	A:92:SER:HB2	0.408

Model ID	Atom-1	Atom-2	Clash overlap (Å)
8	A:95:PRO:HA	A:99:ALA:CB	0.407
8	A:218:PRO:HB2	A:220:TYR:CA	0.407
8	A:143:LYS:HD3	A:144:LEU:CB	0.406
8	A:208:THR:HA	A:213:LEU:N	0.405
8	A:239:TRP:CH2	A:271:VAL:HG22	0.405
8	A:77:MET:HB3	A:84:LEU:HD13	0.404
8	A:92:SER:HA	A:95:PRO:CG	0.404
8	A:73:LEU:HD11	A:77:MET:HE3	0.402
9	A:91:PHE:CD1	A:147:MET:HB2	0.593
9	A:87:ILE:HD11	A:152:MET:H	0.589
9	A:203:ASN:O	A:204:ILE:HG23	0.572
9	A:204:ILE:H	A:272:THR:HG21	0.542
9	A:126:SER:HB2	A:212:LYS:HB3	0.538
9	A:204:ILE:HG22	A:213:LEU:HA	0.512
9	A:91:PHE:CG	A:92:SER:N	0.502
9	A:99:ALA:HB1	A:202:LEU:CD2	0.500
9	A:41:ILE:HD12	A:50:ALA:O	0.480
9	A:99:ALA:HB1	A:202:LEU:HD23	0.480
9	A:133:GLU:CD	A:133:GLU:H	0.473
9	A:5:MET:HE2	A:44:ALA:O	0.470
9	A:91:PHE:CE1	A:94:LEU:HA	0.469
9	A:241:ILE:O	A:252:VAL:HG21	0.460
9	A:122:LYS:HA	A:122:LYS:HE3	0.447

Model ID	Atom-1	Atom-2 Clash overlap (
9	A:282:LEU:HD23	A:283:GLN:O	0.447
9	A:91:PHE:CG	A:147:MET:HB2	0.446
9	A:87:ILE:HG22	A:91:PHE:CD2	0.444
9	A:160:ARG:HG2	A:161:SER:H	0.437
9	A:91:PHE:CZ	A:94:LEU:HA	0.433
9	A:122:LYS:HG3	A:210:ALA:HB3	0.423
9	A:206:PRO:HB3	A:210:ALA:HA	0.413
9	A:260:ASP:CG	A:261:ASN:H	0.409
9	A:88:ALA:HA	A:91:PHE:HB3	0.407
9	A:200:VAL:N	A:201:PRO:CD	0.402
10	A:239:TRP:H	A:271:VAL:HG12	0.857
10	A:213:LEU:HD22	A:241:ILE:HG23 0.783	
10	A:217:ILE:HD12	A:218:PRO:HD2 0.774	
10	A:213:LEU:HD21	A:272:THR:HA	0.701
10	A:213:LEU:HD13	A:241:ILE:HG12	0.686
10	A:207:LEU:H	A:274:LEU:HD23	0.653
10	A:213:LEU:HD13	A:241:ILE:CG1	0.650
10	A:168:VAL:H	A:217:ILE:HB	0.627
10	A:213:LEU:HD21	A:272:THR:CA	0.618
10	A:13:VAL:HG22	A:38:HIS:HE2	0.617
10	A:191:ILE:O	A:195:ALA:HB3	0.596
10	A:204:ILE:O	A:274:LEU:HD21	0.586
10	A:244:VAL:HG23	A:252:VAL:HG23	0.575

Model ID	Atom-1	Atom-2 Clash overlap (
10	A:214:MET:HA	A:271:VAL:CG1 0.570	
10	A:213:LEU:C	A:213:LEU:HD23 0.564	
10	A:214:MET:HB3	A:238:LEU:HA	0.557
10	A:144:LEU:O	A:148:ALA:HB3	0.545
10	A:167:LYS:C	A:217:ILE:HD13	0.543
10	A:17:SER:HB2	A:177:PHE:CD1	0.538
10	A:180:LEU:HA	A:183:LEU:HB3	0.531
10	A:213:LEU:HD21	A:271:VAL:C	0.524
10	A:213:LEU:CD2	A:241:ILE:HG23	0.505
10	A:214:MET:HA	A:271:VAL:HG11	0.488
10	A:207:LEU:N	A:274:LEU:HD23	0.487
10	A:126:SER:O	A:130:ALA:HB3	0.484
10	A:214:MET:CB	A:238:LEU:HA 0.480	
10	A:213:LEU:HD13	A:241:ILE:CD1	0.470
10	A:213:LEU:HD12	A:273:ALA:HB2	0.467
10	A:244:VAL:CG2	A:252:VAL:HG23	0.467
10	A:277:ASN:C	A:279:ALA:H	0.463
10	A:264:ASN:HA	A:268:PRO:HD3	0.462
10	A:207:LEU:HB3	A:214:MET:HG3	0.460
10	A:188:LEU:O	A:192:ILE:HB	0.457
10	A:241:ILE:HG21	A:252:VAL:HG22	0.456
10	A:213:LEU:HD11	A:272:THR:HA	0.454
10	A:264:ASN:HA	A:268:PRO:CD	0.452

Model ID	Atom-1	Atom-2	Clash overlap (Å)
10	A:213:LEU:HD21	A:272:THR:N 0.451	
10	A:213:LEU:HD13	A:241:ILE:HD13	0.450
10	A:192:ILE:HA	A:195:ALA:C	0.438
10	A:264:ASN:HA	A:268:PRO:CG	0.437
10	A:192:ILE:HG23	A:275:ARG:HH11	0.431
10	A:271:VAL:HG13	A:272:THR:H	0.430
10	A:176:LEU:HA	A:179:MET:CG	0.424
10	A:112:ALA:O	A:113:ASN:C	0.417
10	A:180:LEU:HA	A:183:LEU:CB 0.417	
10	A:205:ILE:N	A:206:PRO:CD	0.416
10	A:215:VAL:HB	A:274:LEU:HD22 0.416	
10	A:167:LYS:HE3	A:234:TYR:CG 0.413	
10	A:267:TRP:H	A:268:PRO:CD	0.412
10	A:245:VAL:H	A:251:ILE:HG22	0.404
10	A:168:VAL:HB	A:217:ILE:HB	0.403
10	A:192:ILE:O	A:192:ILE:HG22 0.403	
10	A:213:LEU:HB3	A:241:ILE:H	0.403
10	A:168:VAL:CG1	A:169:THR:N	0.403
10	A:214:MET:HB3	A:238:LEU:CA	0.401

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	281	217	45	19

Model ID	Analyzed	Favored	Allowed	Outliers
2	281	204	39	38
3	281	205	50	26
4	281	208	55	18
5	281	223	33	25
6	281	232	34	15
7	281	218	44	19
8	281	183	51	47
9	281	188	45	48
10	281	213	47	21

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	245	191	17	37
2	245	182	39	24
3	245	187	22	36
4	245	192	26	27
5	245	200	19	26
6	245	197	28	20
7	245	170	39	36
8	245	189	21	35
9	245	189	23	33
10	245	188	26	31

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	А	45	LYS
1	А	46	ASP
1	А	47	THR
1	А	59	SER
1	А	69	ASP
1	А	71	ASN
1	А	72	LYS
1	А	73	LEU
1	А	78	LEU
1	А	83	THR
1	А	87	ILE
1	А	89	SER
1	А	90	GLU
1	А	94	LEU
1	А	124	LYS
1	А	146	LYS
1	А	163	ASP
1	A	164	LYS
1	A	189	ASN
1	A	193	ASN
1	A	196	ARG
1	A	197	ASP
1	А	213	LEU

Model ID	Chain	Residue ID	Residue type
1	A	216	VAL
1	А	218	PRO
1	А	223	TYR
1	А	226	THR
1	A	230	THR
1	A	231	THR
1	А	234	TYR
1	А	244	VAL
1	А	250	LYS
1	А	251	ILE
1	А	252	VAL
1	А	256	GLU
1	А	270	ILE
1	A	275	ARG
2	A	42	LEU
2	A	43	LEU
2	A	56	SER
2	А	62	LEU
2	А	85	GLN
2	А	117	GLU
2	А	125	LYS
2	А	137	ASP
2	А	156	TYR

Model ID	Chain	Residue ID	Residue type
2	A	158	GLN
2	А	168	VAL
2	A	189	ASN
2	А	205	ILE
2	A	207	LEU
2	A	209	THR
2	A	212	LYS
2	А	220	TYR
2	A	223	TYR
2	А	240	GLU
2	A	249	SER
2	А	250	LYS
2	A	251	ILE
2	A	256	GLU
2	A	281	LYS
3	A	3	SER
3	A	4	LYS
3	A	6	SER
3	A	8	VAL
3	A	9	LYS
3	A	24	VAL
3	A	38	HIS
3	А	42	LEU

Model ID	Chain	Residue ID	Residue type
3	A	48	THR
3	A	55	VAL
3	A	65	GLN
3	A	71	ASN
3	A	84	LEU
3	A	87	ILE
3	A	89	SER
3	А	100	PHE
3	A	146	LYS
3	A	155	MET
3	A	157	LYS
3	A	160	ARG
3	A	162	GLU
3	А	180	LEU
3	A	185	ASN
3	А	186	ASP
3	A	205	ILE
3	A	208	THR
3	A	215	VAL
3	А	224	LYS
3	А	239	TRP
3	A	241	ILE
3	А	245	VAL

Model ID	Chain	Residue ID	Residue type
3	A	246	ASP
3	A	252	VAL
3	A	262	SER
3	A	271	VAL
3	A	280	VAL
4	A	3	SER
4	A	13	VAL
4	A	40	ASP
4	A	51	PHE
4	A	54	МЕТ
4	A	77	МЕТ
4	A	81	ARG
4	A	113	ASN
4	A	119	VAL
4	A	128	ASN
4	A	169	THR
4	A	173	GLN
4	A	175	MET
4	A	196	ARG
4	A	199	CYS
4	A	205	ILE
4	A	209	THR
4	А	213	LEU

Model ID	Chain	Residue ID	Residue type
4	А	214	MET
4	А	224	LYS
4	А	232	PHE
4	А	233	THR
4	A	245	VAL
4	A	252	VAL
4	A	254	LEU
4	А	259	MET
4	A	270	ILE
5	A	5	МЕТ
5	A	7	ASP
5	A	9	LYS
5	А	24	VAL
5	А	45	LYS
5	А	46	ASP
5	А	52	GLU
5	А	65	GLN
5	А	68	VAL
5	А	79	ASP
5	А	83	THR
5	А	115	ASP
5	А	120	LEU
5	А	133	GLU

Model ID	Chain	Residue ID	Residue type
5	A	137	ASP
5	А	142	ARG
5	A	180	LEU
5	A	192	ILE
5	A	196	ARG
5	A	212	LYS
5	A	215	VAL
5	A	230	THR
5	A	250	LYS
5	A	254	LEU
5	A	267	TRP
5	А	281	LYS
6	A	23	ARG
6	A	57	LEU
6	A	70	ILE
6	A	72	LYS
6	A	73	LEU
6	A	81	ARG
6	A	105	GLU
6	A	108	GLU
6	A	119	VAL
6	A	123	LEU
6	А	137	ASP

Model ID	Chain	Residue ID	Residue type
6	A	152	МЕТ
6	A	153	THR
6	A	203	ASN
6	A	226	THR
6	A	252	VAL
6	A	254	LEU
6	A	260	ASP
6	A	261	ASN
6	A	277	ASN
7	A	6	SER
7	A	11	THR
7	A	46	ASP
7	A	55	VAL
7	A	70	ILE
7	A	80	ASN
7	A	89	SER
7	A	116	SER
7	A	119	VAL
7	A	123	LEU
7	A	128	ASN
7	A	141	GLN
7	A	145	GLU
7	А	146	LYS

Model ID	Chain	Residue ID	Residue type
7	A	152	MET
7	A	155	MET
7	A	162	GLU
7	A	167	LYS
7	A	188	LEU
7	A	191	ILE
7	A	192	ILE
7	A	205	ILE
7	A	215	VAL
7	A	217	ILE
7	A	219	ASP
7	A	222	THR
7	A	238	LEU
7	A	245	VAL
7	A	249	SER
7	A	251	ILE
7	A	255	SER
7	A	261	ASN
7	A	262	SER
7	A	263	PRO
7	A	271	VAL
7	A	277	ASN
8	А	7	ASP

Model ID	Chain	Residue ID	Residue type
8	A	24	VAL
8	А	38	HIS
8	А	72	LYS
8	A	78	LEU
8	A	81	ARG
8	А	84	LEU
8	А	87	ILE
8	А	90	GLU
8	А	105	GLU
8	А	107	TYR
8	А	108	GLU
8	A	115	ASP
8	A	135	ASP
8	А	137	ASP
8	А	142	ARG
8	А	164	LYS
8	А	168	VAL
8	A	178	THR
8	A	185	ASN
8	A	191	ILE
8	А	192	ILE
8	A	193	ASN
8	A	199	CYS

Model ID	Chain	Residue ID	Residue type
8	A	205	ILE
8	А	208	THR
8	А	212	LYS
8	А	230	THR
8	А	231	THR
8	А	234	TYR
8	А	238	LEU
8	А	250	LYS
8	А	251	ILE
8	А	265	LEU
8	А	269	LEU
9	А	8	VAL
9	А	40	ASP
9	А	47	THR
9	А	54	MET
9	A	64	MET
9	A	81	ARG
9	A	95	PRO
9	A	105	GLU
9	A	122	LYS
9	A	125	LYS
9	A	129	VAL
9	А	144	LEU

Model ID	Chain	Residue ID	Residue type
9	A	152	МЕТ
9	A	155	МЕТ
9	A	156	TYR
9	А	179	МЕТ
9	A	184	ASP
9	А	193	ASN
9	A	196	ARG
9	А	202	LEU
9	А	203	ASN
9	А	212	LYS
9	А	213	LEU
9	A	217	ILE
9	А	223	TYR
9	А	224	LYS
9	A	230	THR
9	A	232	PHE
9	A	240	GLU
9	A	245	VAL
9	A	261	ASN
9	A	264	ASN
9	A	281	LYS
10	A	14	VAL
10	A	29	LYS

Model ID	Chain	Residue ID	Residue type
10	A	35	VAL
10	A	45	LYS
10	A	79	ASP
10	A	89	SER
10	A	93	SER
10	A	95	PRO
10	A	109	GLN
10	A	124	LYS
10	A	137	ASP
10	A	146	LYS
10	A	150	GLN
10	A	165	ARG
10	A	170	SER
10	A	175	МЕТ
10	A	179	MET
10	A	180	LEU
10	A	193	ASN
10	A	194	ASN
10	A	203	ASN
10	A	215	VAL
10	A	231	THR
10	A	233	THR
10	А	234	TYR

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Model ID	Chain	Residue ID	Residue type
10	А	242	GLN
10	А	253	GLN
10	А	265	LEU
10	A	270	ILE
10	А	271	VAL
10	А	277	ASN

Fit of model to data used for modeling

SAS data used in this integrative model could not be validated as the sascif file is currently unavailable.

Crosslinking-MS

Validation for this section is under development.

H/D exchange

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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