



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:08 PM BST

PDB ID : 4USN
EMDB ID: : EMD-2706
Title : The structure of the immature HIV-1 capsid in intact virus particles at sub-nm resolution
Authors : Schur, F.K.M.; Hagen, W.J.H.; Rumlova, M.; Ruml, T.; Mueller, B.; Kraeusslich, H.-G.; Briggs, J.A.G.
Deposited on : 2014-07-11
Resolution : 8.80 Å(reported)
Based on PDB ID : 1L6N,3DS2

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

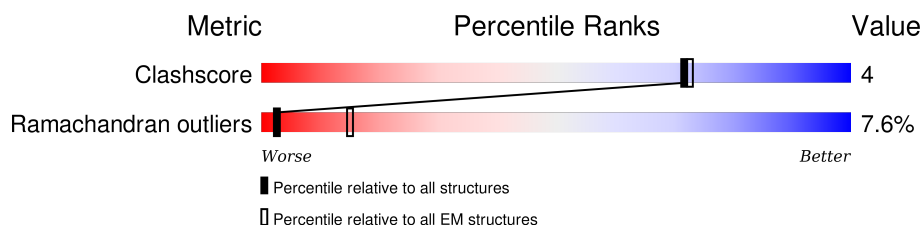
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY




The reported resolution of this entry is 8.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	210	 75% 22% •
1	B	210	 81% 18% •
1	C	210	 86% 13% •
1	D	210	 76% 23% •
1	E	210	 78% 21% •
1	F	210	 84% 14% •
1	G	210	 85% 14%
1	H	210	 79% 19% •
1	I	210	 85% 14% •
1	J	210	 82% 14% •
1	K	210	 80% 18% •

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Mol	Chain	Length	Quality of chain
1	L	210	<div><div></div><div>85%</div><div>12%</div><div></div></div>
1	M	210	<div><div></div><div>81%</div><div>17%</div><div></div></div>
1	N	210	<div><div></div><div>89%</div><div>9%</div><div></div></div>
1	O	210	<div><div></div><div>88%</div><div>10%</div><div></div></div>
1	P	210	<div><div></div><div>84%</div><div>13%</div><div></div></div>
1	Q	210	<div><div></div><div>84%</div><div>15%</div><div></div></div>
1	R	210	<div><div></div><div>82%</div><div>15%</div><div></div></div>

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 22662 atoms, of which 7542 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called P24.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	210	Total	C	H	N	O	0	0
			1259	420	419	210	210		
1	B	210	Total	C	H	N	O	0	0
			1259	420	419	210	210		
1	C	210	Total	C	H	N	O	0	0
			1259	420	419	210	210		
1	D	210	Total	C	H	N	O	0	0
			1259	420	419	210	210		
1	E	210	Total	C	H	N	O	0	0
			1259	420	419	210	210		
1	F	210	Total	C	H	N	O	0	0
			1259	420	419	210	210		
1	G	210	Total	C	H	N	O	0	0
			1259	420	419	210	210		
1	H	210	Total	C	H	N	O	0	0
			1259	420	419	210	210		
1	I	210	Total	C	H	N	O	0	0
			1259	420	419	210	210		
1	J	210	Total	C	H	N	O	0	0
			1259	420	419	210	210		
1	K	210	Total	C	H	N	O	0	0
			1259	420	419	210	210		
1	L	210	Total	C	H	N	O	0	0
			1259	420	419	210	210		
1	M	210	Total	C	H	N	O	0	0
			1259	420	419	210	210		
1	N	210	Total	C	H	N	O	0	0
			1259	420	419	210	210		
1	O	210	Total	C	H	N	O	0	0
			1259	420	419	210	210		
1	P	210	Total	C	H	N	O	0	0
			1259	420	419	210	210		
1	Q	210	Total	C	H	N	O	0	0
			1259	420	419	210	210		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	210	Total	C	H	N	O	0	0
			1259	420	419	210	210		

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	207	GLU	ASP	CONFLICT	UNP Q9IVM8
A	301	ALA	TYR	CONFLICT	UNP Q9IVM8
A	340	GLY	ALA	CONFLICT	UNP Q9IVM8
B	207	GLU	ASP	CONFLICT	UNP Q9IVM8
B	301	ALA	TYR	CONFLICT	UNP Q9IVM8
B	340	GLY	ALA	CONFLICT	UNP Q9IVM8
C	207	GLU	ASP	CONFLICT	UNP Q9IVM8
C	301	ALA	TYR	CONFLICT	UNP Q9IVM8
C	340	GLY	ALA	CONFLICT	UNP Q9IVM8
D	207	GLU	ASP	CONFLICT	UNP Q9IVM8
D	301	ALA	TYR	CONFLICT	UNP Q9IVM8
D	340	GLY	ALA	CONFLICT	UNP Q9IVM8
E	207	GLU	ASP	CONFLICT	UNP Q9IVM8
E	301	ALA	TYR	CONFLICT	UNP Q9IVM8
E	340	GLY	ALA	CONFLICT	UNP Q9IVM8
F	207	GLU	ASP	CONFLICT	UNP Q9IVM8
F	301	ALA	TYR	CONFLICT	UNP Q9IVM8
F	340	GLY	ALA	CONFLICT	UNP Q9IVM8
G	207	GLU	ASP	CONFLICT	UNP Q9IVM8
G	301	ALA	TYR	CONFLICT	UNP Q9IVM8
G	340	GLY	ALA	CONFLICT	UNP Q9IVM8
H	207	GLU	ASP	CONFLICT	UNP Q9IVM8
H	301	ALA	TYR	CONFLICT	UNP Q9IVM8
H	340	GLY	ALA	CONFLICT	UNP Q9IVM8
I	207	GLU	ASP	CONFLICT	UNP Q9IVM8
I	301	ALA	TYR	CONFLICT	UNP Q9IVM8
I	340	GLY	ALA	CONFLICT	UNP Q9IVM8
J	207	GLU	ASP	CONFLICT	UNP Q9IVM8
J	301	ALA	TYR	CONFLICT	UNP Q9IVM8
J	340	GLY	ALA	CONFLICT	UNP Q9IVM8
K	207	GLU	ASP	CONFLICT	UNP Q9IVM8
K	301	ALA	TYR	CONFLICT	UNP Q9IVM8
K	340	GLY	ALA	CONFLICT	UNP Q9IVM8
L	207	GLU	ASP	CONFLICT	UNP Q9IVM8
L	301	ALA	TYR	CONFLICT	UNP Q9IVM8
L	340	GLY	ALA	CONFLICT	UNP Q9IVM8

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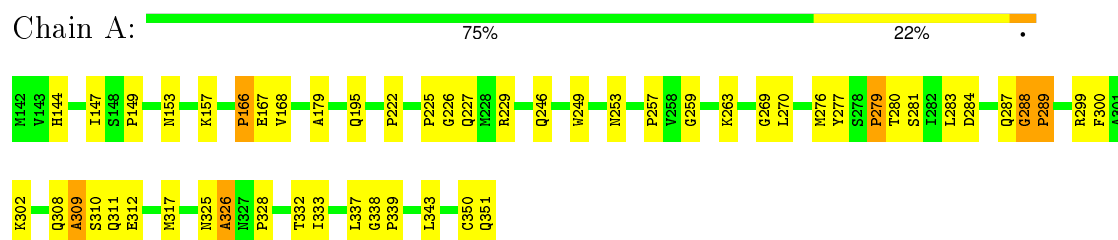
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Chain	Residue	Modelled	Actual	Comment	Reference
M	207	GLU	ASP	CONFLICT	UNP Q9IVM8
M	301	ALA	TYR	CONFLICT	UNP Q9IVM8
M	340	GLY	ALA	CONFLICT	UNP Q9IVM8
N	207	GLU	ASP	CONFLICT	UNP Q9IVM8
N	301	ALA	TYR	CONFLICT	UNP Q9IVM8
N	340	GLY	ALA	CONFLICT	UNP Q9IVM8
O	207	GLU	ASP	CONFLICT	UNP Q9IVM8
O	301	ALA	TYR	CONFLICT	UNP Q9IVM8
O	340	GLY	ALA	CONFLICT	UNP Q9IVM8
P	207	GLU	ASP	CONFLICT	UNP Q9IVM8
P	301	ALA	TYR	CONFLICT	UNP Q9IVM8
P	340	GLY	ALA	CONFLICT	UNP Q9IVM8
Q	207	GLU	ASP	CONFLICT	UNP Q9IVM8
Q	301	ALA	TYR	CONFLICT	UNP Q9IVM8
Q	340	GLY	ALA	CONFLICT	UNP Q9IVM8
R	207	GLU	ASP	CONFLICT	UNP Q9IVM8
R	301	ALA	TYR	CONFLICT	UNP Q9IVM8
R	340	GLY	ALA	CONFLICT	UNP Q9IVM8

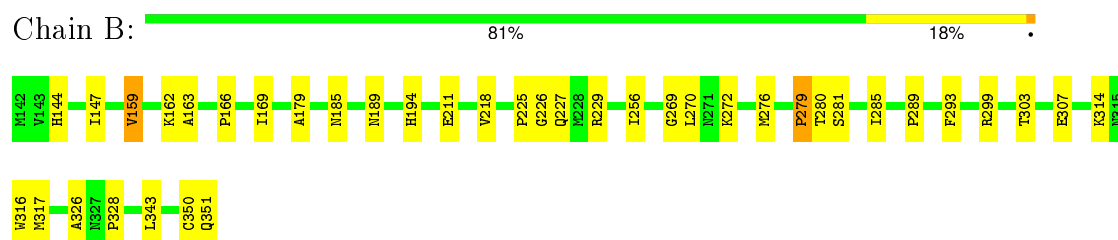
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

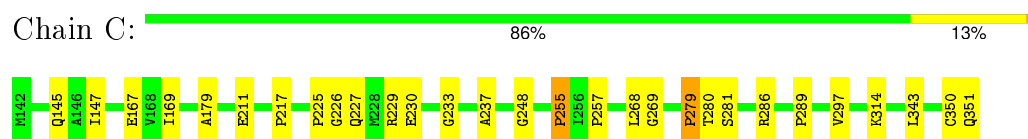
• Molecule 1: P24



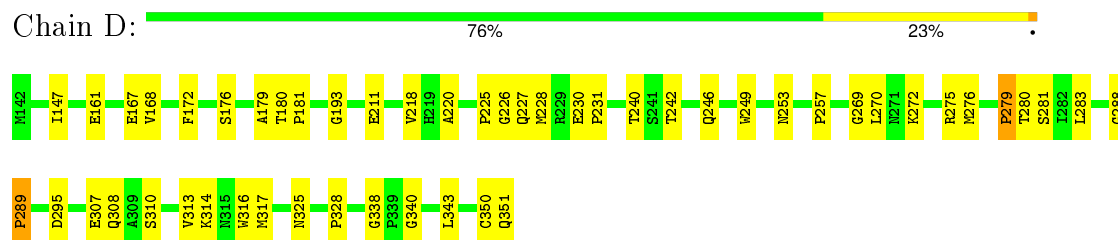
• Molecule 1: P24



• Molecule 1: P24



• Molecule 1: P24



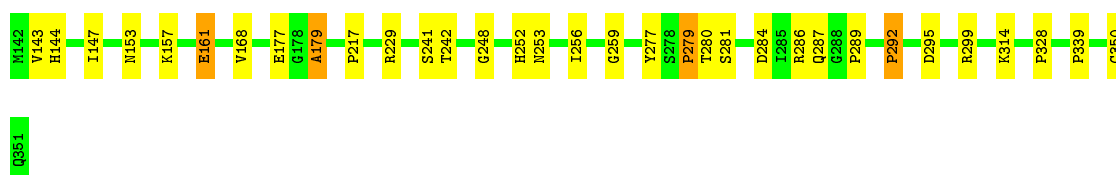
• Molecule 1: P24





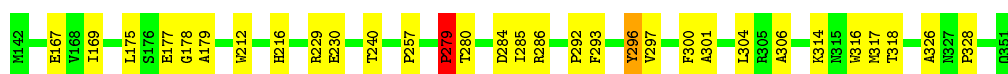
- Molecule 1: P24

Chain F: 84% 14%



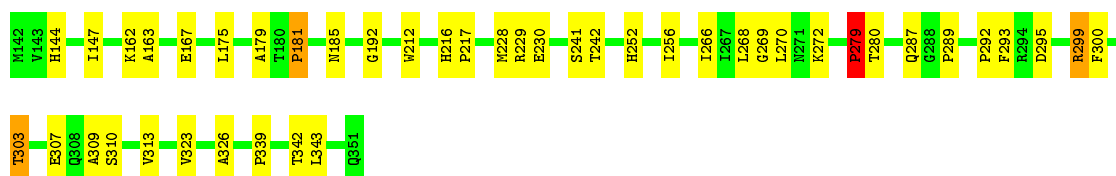
- Molecule 1: P24

Chain G: 85% 14%



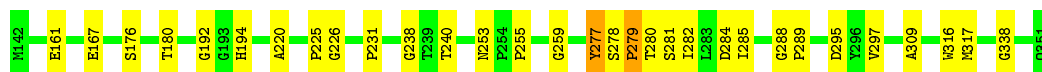
- Molecule 1: P24

Chain H: 79% 19%



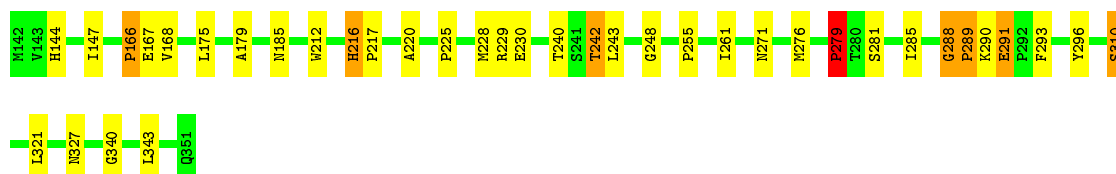
- Molecule 1: P24

Chain I: 85% 14%

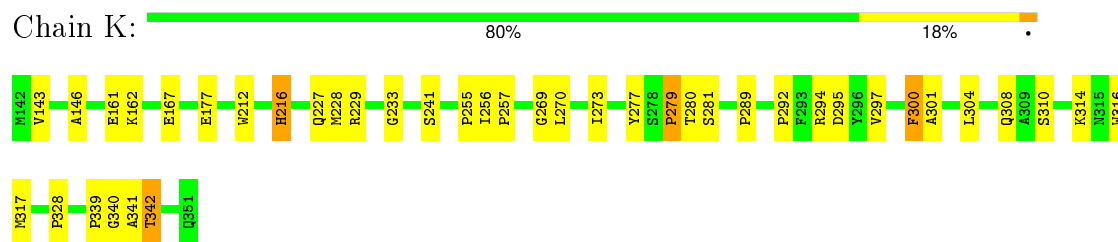


- Molecule 1: P24

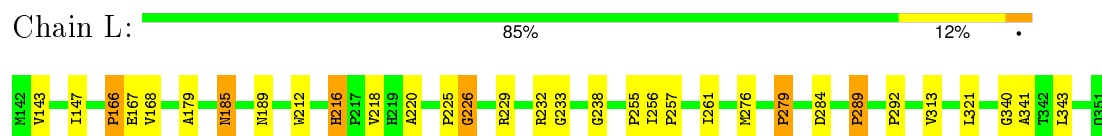
Chain J: 82% 14%



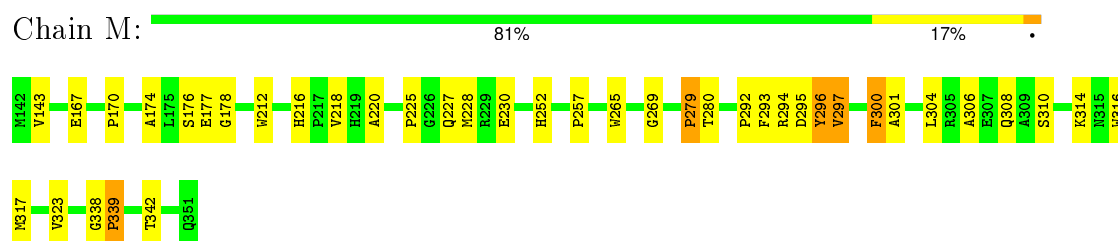
- Molecule 1: P24



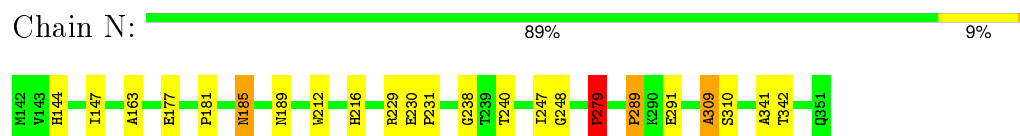
- Molecule 1: P24



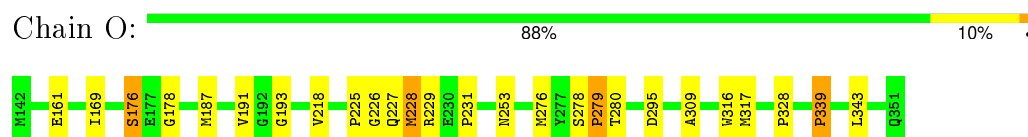
- Molecule 1: P24



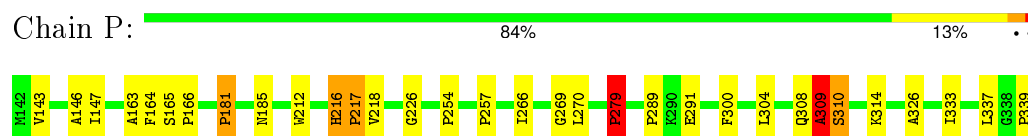
- Molecule 1: P24



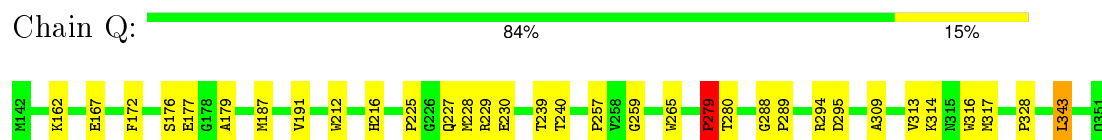
- Molecule 1: P24



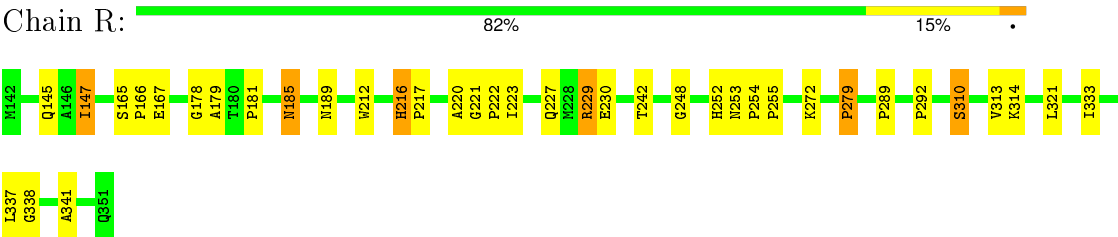
- Molecule 1: P24



- Molecule 1: P24



● Molecule 1: P24



4 Experimental information

Property	Value	Source
Reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	PHASE FLIPPING OF INDIVIDUAL TILTS	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	42000	Depositor
Image detector	GATAN MULTISCAN	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z > 2	RMSZ	# Z > 2
1	A	1.98	7/839 (0.8%)	1.74	9/1047 (0.9%)
1	B	1.96	3/839 (0.4%)	1.73	9/1047 (0.9%)
1	C	1.95	3/839 (0.4%)	1.67	4/1047 (0.4%)
1	D	1.95	4/839 (0.5%)	1.67	11/1047 (1.1%)
1	E	1.98	11/839 (1.3%)	1.66	8/1047 (0.8%)
1	F	1.98	6/839 (0.7%)	1.64	6/1047 (0.6%)
1	G	1.91	5/839 (0.6%)	1.63	4/1047 (0.4%)
1	H	1.91	6/839 (0.7%)	1.71	9/1047 (0.9%)
1	I	1.89	2/839 (0.2%)	1.67	7/1047 (0.7%)
1	J	1.84	4/839 (0.5%)	1.71	11/1047 (1.1%)
1	K	1.84	5/839 (0.6%)	1.66	5/1047 (0.5%)
1	L	1.83	4/839 (0.5%)	1.68	10/1047 (1.0%)
1	M	1.94	7/839 (0.8%)	1.65	8/1047 (0.8%)
1	N	1.91	3/839 (0.4%)	1.71	8/1047 (0.8%)
1	O	1.91	2/839 (0.2%)	1.66	5/1047 (0.5%)
1	P	1.90	2/839 (0.2%)	1.68	8/1047 (0.8%)
1	Q	1.91	6/839 (0.7%)	1.61	4/1047 (0.4%)
1	R	1.94	5/839 (0.6%)	1.69	5/1047 (0.5%)
All	All	1.92	85/15102 (0.6%)	1.68	131/18846 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9
1	B	0	6
1	C	0	6
1	D	0	12
1	E	0	2
1	F	0	9
1	G	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	14
1	I	0	5
1	J	0	12
1	K	0	5
1	L	0	6
1	M	0	5
1	N	0	5
1	O	0	6
1	P	0	5
1	Q	0	2
1	R	0	6
All	All	0	118

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	185	ASN	CA-C	-6.31	1.36	1.52
1	F	295	ASP	CA-C	-6.24	1.36	1.52
1	D	328	PRO	CA-C	-6.23	1.40	1.52
1	L	238	GLY	CA-C	-6.18	1.42	1.51
1	A	328	PRO	CA-C	-6.15	1.40	1.52
1	J	248	GLY	CA-C	-6.11	1.42	1.51
1	Q	295	ASP	CA-C	-6.09	1.37	1.52
1	Q	314	LYS	CA-C	-6.05	1.37	1.52
1	K	300	PHE	N-CA	-6.01	1.34	1.46
1	K	328	PRO	CA-C	-5.97	1.41	1.52
1	C	297	VAL	CA-C	-5.96	1.37	1.52
1	G	318	THR	CA-C	-5.89	1.37	1.52
1	B	299	ARG	CA-C	-5.88	1.37	1.52
1	L	289	PRO	CA-C	-5.80	1.41	1.52
1	Q	314	LYS	N-CA	-5.80	1.34	1.46
1	H	300	PHE	N-CA	-5.71	1.34	1.46
1	E	211	GLU	CA-C	-5.69	1.38	1.52
1	M	295	ASP	N-CA	-5.58	1.35	1.46
1	C	248	GLY	CA-C	-5.58	1.43	1.51
1	K	295	ASP	N-CA	-5.56	1.35	1.46
1	A	299	ARG	CA-C	-5.55	1.38	1.52
1	C	211	GLU	CA-C	-5.55	1.38	1.52
1	A	302	LYS	CA-C	-5.50	1.38	1.52
1	R	248	GLY	CA-C	-5.49	1.43	1.51
1	F	299	ARG	CA-C	-5.48	1.38	1.52
1	J	185	ASN	CA-C	-5.48	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	248	GLY	CA-C	-5.47	1.43	1.51
1	M	295	ASP	CA-C	-5.47	1.38	1.52
1	F	328	PRO	CA-C	-5.46	1.42	1.52
1	N	185	ASN	CA-C	-5.42	1.38	1.52
1	N	248	GLY	CA-C	-5.42	1.43	1.51
1	E	238	GLY	CA-C	-5.40	1.43	1.51
1	D	295	ASP	CA-C	-5.40	1.39	1.52
1	N	289	PRO	CA-C	-5.38	1.42	1.52
1	E	332	THR	CA-C	-5.36	1.39	1.52
1	E	300	PHE	N-CA	-5.35	1.35	1.46
1	O	328	PRO	CA-C	-5.35	1.42	1.52
1	M	300	PHE	N-CA	-5.34	1.35	1.46
1	R	185	ASN	CA-C	-5.34	1.39	1.52
1	H	287	GLN	N-CA	-5.33	1.35	1.46
1	A	317	MET	CA-C	-5.32	1.39	1.52
1	E	299	ARG	CA-C	-5.30	1.39	1.52
1	H	303	THR	CA-C	-5.28	1.39	1.52
1	A	276	MET	CA-C	-5.28	1.39	1.52
1	J	217	PRO	CA-C	-5.28	1.42	1.52
1	R	313	VAL	N-CA	-5.25	1.35	1.46
1	K	233	GLY	CA-C	-5.25	1.43	1.51
1	A	332	THR	CA-C	-5.24	1.39	1.52
1	D	313	VAL	CA-C	-5.24	1.39	1.52
1	R	272	LYS	CA-C	-5.23	1.39	1.52
1	L	313	VAL	N-CA	-5.22	1.35	1.46
1	O	295	ASP	CA-C	-5.22	1.39	1.52
1	B	211	GLU	CA-C	-5.20	1.39	1.52
1	P	181	PRO	CA-C	-5.17	1.42	1.52
1	E	296	TYR	CA-C	-5.17	1.39	1.52
1	H	299	ARG	CA-C	-5.17	1.39	1.52
1	H	313	VAL	N-CA	-5.17	1.36	1.46
1	F	287	GLN	N-CA	-5.17	1.36	1.46
1	H	272	LYS	N-CA	-5.15	1.36	1.46
1	J	271	ASN	CA-C	-5.15	1.39	1.52
1	Q	343	LEU	N-CA	-5.14	1.36	1.46
1	E	314	LYS	CA-C	-5.13	1.39	1.52
1	P	314	LYS	CA-C	-5.12	1.39	1.52
1	F	295	ASP	N-CA	-5.12	1.36	1.46
1	D	211	GLU	CA-C	-5.11	1.39	1.52
1	M	314	LYS	N-CA	-5.11	1.36	1.46
1	I	295	ASP	CA-C	-5.11	1.39	1.52
1	K	314	LYS	CA-C	-5.10	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	294	ARG	N-CA	-5.10	1.36	1.46
1	G	316	TRP	CA-C	-5.10	1.39	1.52
1	I	297	VAL	CA-C	-5.10	1.39	1.52
1	M	296	TYR	CA-C	-5.09	1.39	1.52
1	E	267	ILE	CA-C	-5.09	1.39	1.52
1	F	248	GLY	CA-C	-5.08	1.43	1.51
1	A	300	PHE	N-CA	-5.08	1.36	1.46
1	R	314	LYS	CA-C	-5.08	1.39	1.52
1	G	314	LYS	N-CA	-5.07	1.36	1.46
1	E	295	ASP	CA-C	-5.07	1.39	1.52
1	Q	328	PRO	CA-C	-5.07	1.42	1.52
1	G	328	PRO	CA-C	-5.04	1.42	1.52
1	M	269	GLY	CA-C	-5.04	1.43	1.51
1	B	328	PRO	CA-C	-5.03	1.42	1.52
1	E	314	LYS	N-CA	-5.02	1.36	1.46
1	M	297	VAL	N-CA	-5.01	1.36	1.46
1	G	296	TYR	N-CA	-5.00	1.36	1.46

All (131) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	242	THR	CA-C-N	-8.27	99.01	117.20
1	A	289	PRO	N-CA-C	-7.78	91.86	112.10
1	J	166	PRO	N-CA-C	7.57	131.77	112.10
1	L	166	PRO	N-CA-C	7.45	131.46	112.10
1	D	351	GLN	N-CA-C	-7.17	91.64	111.00
1	Q	313	VAL	CA-C-N	-7.13	101.51	117.20
1	H	163	ALA	N-CA-C	6.98	129.84	111.00
1	I	278	SER	N-CA-C	-6.97	92.17	111.00
1	I	277	TYR	N-CA-C	-6.93	92.29	111.00
1	R	253	ASN	N-CA-C	-6.66	93.01	111.00
1	I	277	TYR	CA-C-N	-6.64	102.60	117.20
1	P	309	ALA	N-CA-C	6.63	128.91	111.00
1	P	270	LEU	C-N-CA	6.46	137.85	121.70
1	A	351	GLN	N-CA-C	-6.45	93.58	111.00
1	J	288	GLY	N-CA-C	-6.43	97.02	113.10
1	N	177	GLU	N-CA-C	-6.42	93.66	111.00
1	J	279	PRO	CA-C-N	6.38	131.23	117.20
1	M	294	ARG	C-N-CA	6.36	137.59	121.70
1	B	169	ILE	CA-C-N	6.34	134.84	117.10
1	P	217	PRO	N-CA-C	-6.29	95.73	112.10
1	P	351	GLN	N-CA-C	6.18	127.68	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	343	LEU	N-CA-C	6.17	127.66	111.00
1	A	309	ALA	N-CA-C	6.12	127.53	111.00
1	J	279	PRO	C-N-CA	6.12	136.99	121.70
1	B	162	LYS	C-N-CA	6.06	136.84	121.70
1	E	287	GLN	C-N-CA	6.06	135.02	122.30
1	O	228	MET	C-N-CA	6.02	136.75	121.70
1	H	162	LYS	C-N-CA	5.99	136.68	121.70
1	F	286	ARG	N-CA-C	-5.96	94.92	111.00
1	A	338	GLY	N-CA-C	-5.95	98.23	113.10
1	H	270	LEU	CA-C-O	5.92	132.54	120.10
1	K	294	ARG	C-N-CA	5.92	136.51	121.70
1	J	343	LEU	N-CA-C	5.89	126.90	111.00
1	R	341	ALA	C-N-CA	5.88	136.39	121.70
1	D	314	LYS	C-N-CA	-5.86	107.04	121.70
1	E	144	HIS	N-CA-C	-5.86	95.19	111.00
1	E	166	PRO	N-CA-C	5.82	127.23	112.10
1	C	351	GLN	N-CA-C	-5.81	95.30	111.00
1	G	279	PRO	C-N-CA	5.76	136.09	121.70
1	M	177	GLU	C-N-CA	5.75	134.36	122.30
1	A	166	PRO	C-N-CA	5.74	136.04	121.70
1	E	313	VAL	CA-C-N	-5.73	104.59	117.20
1	N	163	ALA	N-CA-C	5.72	126.44	111.00
1	D	270	LEU	N-CA-C	5.66	126.27	111.00
1	N	238	GLY	CA-C-N	-5.64	104.78	117.20
1	N	144	HIS	C-N-CA	5.62	135.74	121.70
1	L	166	PRO	CA-C-N	5.61	129.54	117.20
1	K	167	GLU	C-N-CA	5.60	135.70	121.70
1	L	233	GLY	N-CA-C	5.60	127.10	113.10
1	D	307	GLU	C-N-CA	5.58	135.65	121.70
1	F	242	THR	N-CA-C	-5.58	95.95	111.00
1	L	261	ILE	CA-C-N	-5.57	104.96	117.20
1	A	270	LEU	C-N-CA	5.56	135.61	121.70
1	O	278	SER	N-CA-C	-5.56	96.00	111.00
1	D	227	GLN	C-N-CA	5.55	135.57	121.70
1	B	314	LYS	C-N-CA	-5.54	107.85	121.70
1	G	178	GLY	C-N-CA	5.54	135.56	121.70
1	Q	279	PRO	C-N-CA	5.53	135.53	121.70
1	B	256	ILE	N-CA-C	-5.53	96.07	111.00
1	M	265	TRP	CA-C-O	5.53	131.70	120.10
1	C	169	ILE	CA-C-N	5.51	132.54	117.10
1	O	169	ILE	CA-C-N	5.51	132.53	117.10
1	C	268	LEU	C-N-CA	-5.49	110.77	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	238	GLY	C-N-CA	5.47	135.38	121.70
1	G	306	ALA	N-CA-C	5.46	125.76	111.00
1	D	283	LEU	C-N-CA	5.46	135.35	121.70
1	J	327	ASN	CA-C-N	5.44	132.33	117.10
1	H	270	LEU	C-N-CA	5.44	135.29	121.70
1	G	169	ILE	CA-C-N	5.42	132.28	117.10
1	M	308	GLN	N-CA-C	5.42	125.62	111.00
1	D	253	ASN	N-CA-C	-5.38	96.48	111.00
1	E	313	VAL	O-C-N	5.36	131.28	122.70
1	A	195	GLN	CA-C-N	-5.36	105.41	117.20
1	L	218	VAL	C-N-CA	5.35	135.07	121.70
1	M	227	GLN	CA-C-N	-5.35	105.44	117.20
1	L	256	ILE	N-CA-C	-5.34	96.58	111.00
1	D	338	GLY	N-CA-C	-5.33	99.78	113.10
1	F	252	HIS	N-CA-C	-5.32	96.64	111.00
1	B	169	ILE	N-CA-C	5.31	125.34	111.00
1	H	241	SER	N-CA-C	-5.31	96.67	111.00
1	M	339	PRO	N-CA-C	5.31	125.91	112.10
1	B	159	VAL	O-C-N	-5.30	114.22	122.70
1	K	270	LEU	N-CA-C	5.30	125.31	111.00
1	R	252	HIS	N-CA-C	-5.30	96.69	111.00
1	C	314	LYS	C-N-CA	-5.29	108.47	121.70
1	P	146	ALA	C-N-CA	5.28	134.91	121.70
1	M	306	ALA	N-CA-C	5.28	125.25	111.00
1	F	314	LYS	C-N-CA	-5.28	108.51	121.70
1	D	289	PRO	N-CA-C	-5.27	98.39	112.10
1	I	194	HIS	C-N-CA	5.27	134.89	121.70
1	Q	162	LYS	CA-C-N	-5.25	105.65	117.20
1	L	292	PRO	CA-C-N	-5.25	105.65	117.20
1	D	340	GLY	N-CA-C	-5.25	99.98	113.10
1	L	226	GLY	N-CA-C	-5.24	100.00	113.10
1	B	194	HIS	C-N-CA	5.23	134.77	121.70
1	I	238	GLY	C-N-CA	5.21	134.74	121.70
1	L	343	LEU	N-CA-C	5.21	125.08	111.00
1	B	270	LEU	N-CA-C	5.21	125.08	111.00
1	N	309	ALA	N-CA-C	5.19	125.01	111.00
1	A	253	ASN	N-CA-C	-5.18	97.00	111.00
1	F	256	ILE	N-CA-C	-5.17	97.05	111.00
1	J	261	ILE	CA-C-N	-5.16	105.86	117.20
1	P	163	ALA	N-CA-C	5.15	124.92	111.00
1	J	285	ILE	N-CA-C	-5.15	97.09	111.00
1	P	279	PRO	O-C-N	-5.15	114.46	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	253	ASN	N-CA-C	-5.14	97.12	111.00
1	A	283	LEU	C-N-CA	5.14	134.54	121.70
1	I	338	GLY	N-CA-C	-5.13	100.26	113.10
1	L	167	GLU	N-CA-C	5.13	124.85	111.00
1	F	253	ASN	N-CA-C	-5.12	97.16	111.00
1	R	338	GLY	N-CA-C	-5.12	100.30	113.10
1	K	341	ALA	C-N-CA	5.12	134.49	121.70
1	H	279	PRO	CA-C-N	5.11	128.44	117.20
1	D	275	ARG	O-C-N	-5.09	114.56	122.70
1	H	268	LEU	CA-C-N	5.09	126.38	116.20
1	J	243	LEU	N-CA-C	5.09	124.73	111.00
1	N	247	ILE	C-N-CA	5.08	132.98	122.30
1	M	338	GLY	N-CA-C	-5.08	100.40	113.10
1	H	266	ILE	CA-C-N	-5.07	106.06	117.20
1	E	169	ILE	CA-C-N	5.05	131.25	117.10
1	Q	265	TRP	CA-C-O	5.05	130.70	120.10
1	B	351	GLN	N-CA-C	-5.04	97.38	111.00
1	N	279	PRO	CA-C-N	5.04	128.29	117.20
1	J	167	GLU	N-CA-C	5.04	124.61	111.00
1	O	253	ASN	N-CA-C	-5.03	97.42	111.00
1	P	266	ILE	CA-C-N	-5.03	106.14	117.20
1	O	339	PRO	N-CA-C	5.02	125.16	112.10
1	R	147	ILE	N-CA-C	5.02	124.55	111.00
1	E	270	LEU	C-N-CA	5.00	134.21	121.70
1	E	338	GLY	N-CA-C	-5.00	100.59	113.10
1	K	308	GLN	N-CA-C	5.00	124.50	111.00

There are no chirality outliers.

All (118) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	269	GLY	Mainchain
1	A	277	TYR	Mainchain
1	A	279	PRO	Peptide
1	A	284	ASP	Mainchain
1	A	288	GLY	Mainchain
1	A	325	ASN	Mainchain
1	A	343	LEU	Mainchain,Peptide
1	A	350	CYS	Mainchain
1	B	269	GLY	Mainchain
1	B	279	PRO	Peptide
1	B	293	PHE	Mainchain

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Mol	Chain	Res	Type	Group
1	B	343	LEU	Mainchain,Peptide
1	B	350	CYS	Mainchain
1	C	255	PRO	Mainchain
1	C	269	GLY	Mainchain
1	C	279	PRO	Peptide
1	C	343	LEU	Mainchain,Peptide
1	C	350	CYS	Mainchain
1	D	161	GLU	Mainchain,Peptide
1	D	167	GLU	Mainchain
1	D	168	VAL	Mainchain
1	D	181	PRO	Mainchain
1	D	242	THR	Mainchain
1	D	269	GLY	Mainchain
1	D	279	PRO	Peptide
1	D	325	ASN	Mainchain
1	D	343	LEU	Mainchain,Peptide
1	D	350	CYS	Mainchain
1	E	279	PRO	Peptide
1	E	343	LEU	Mainchain
1	F	143	VAL	Mainchain
1	F	161	GLU	Mainchain,Peptide
1	F	168	VAL	Mainchain
1	F	277	TYR	Mainchain
1	F	279	PRO	Peptide
1	F	284	ASP	Mainchain
1	F	292	PRO	Mainchain
1	F	350	CYS	Mainchain
1	G	279	PRO	Peptide
1	G	317	MET	Mainchain,Peptide
1	H	175	LEU	Mainchain
1	H	181	PRO	Mainchain
1	H	228	MET	Mainchain,Peptide
1	H	242	THR	Mainchain,Peptide
1	H	269	GLY	Mainchain
1	H	279	PRO	Peptide
1	H	293	PHE	Mainchain
1	H	310	SER	Mainchain,Peptide
1	H	326	ALA	Mainchain
1	H	342	THR	Mainchain,Peptide
1	I	161	GLU	Mainchain
1	I	176	SER	Mainchain
1	I	277	TYR	Mainchain,Peptide

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Mol	Chain	Res	Type	Group
1	I	279	PRO	Peptide
1	J	168	VAL	Mainchain,Peptide
1	J	175	LEU	Mainchain
1	J	240	THR	Mainchain
1	J	242	THR	Mainchain,Peptide
1	J	279	PRO	Peptide
1	J	290	LYS	Mainchain
1	J	291	GLU	Mainchain
1	J	310	SER	Mainchain,Peptide
1	J	321	LEU	Mainchain
1	K	161	GLU	Mainchain,Peptide
1	K	162	LYS	Mainchain
1	K	269	GLY	Mainchain
1	K	279	PRO	Peptide
1	L	168	VAL	Mainchain
1	L	216	HIS	Mainchain
1	L	226	GLY	Mainchain
1	L	279	PRO	Peptide
1	L	284	ASP	Mainchain
1	L	321	LEU	Mainchain
1	M	167	GLU	Mainchain
1	M	176	SER	Mainchain,Peptide
1	M	279	PRO	Peptide
1	M	342	THR	Mainchain
1	N	240	THR	Mainchain,Peptide
1	N	279	PRO	Peptide
1	N	291	GLU	Mainchain
1	N	342	THR	Mainchain
1	O	161	GLU	Mainchain
1	O	176	SER	Mainchain
1	O	227	GLN	Mainchain
1	O	279	PRO	Peptide
1	O	343	LEU	Mainchain,Peptide
1	P	269	GLY	Mainchain
1	P	279	PRO	Peptide
1	P	309	ALA	Peptide
1	P	310	SER	Mainchain
1	P	326	ALA	Mainchain
1	Q	279	PRO	Peptide
1	Q	343	LEU	Mainchain
1	R	227	GLN	Mainchain
1	R	242	THR	Mainchain

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Mol	Chain	Res	Type	Group
1	R	279	PRO	Peptide
1	R	310	SER	Mainchain,Peptide
1	R	321	LEU	Mainchain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	840	419	218	8	0
1	B	840	419	218	5	0
1	C	840	419	219	1	0
1	D	840	419	217	4	0
1	E	840	419	218	7	0
1	F	840	419	219	3	0
1	G	840	419	219	6	0
1	H	840	419	218	4	0
1	I	840	419	219	4	0
1	J	840	419	219	3	0
1	K	840	419	217	6	0
1	L	840	419	219	2	0
1	M	840	419	218	6	0
1	N	840	419	219	3	0
1	O	840	419	219	3	0
1	P	840	419	218	5	0
1	Q	840	419	219	6	0
1	R	840	419	219	5	0
All	All	15120	7542	3932	81	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (81) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:179:ALA:O	1:F:259:GLY:HA3	2.08	0.54
1:Q:179:ALA:O	1:Q:259:GLY:HA2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:181:PRO:O	1:R:185:ASN:N	2.45	0.50
1:G:175:LEU:C	1:G:177:GLU:H	2.17	0.48
1:H:303:THR:O	1:H:307:GLU:N	2.46	0.48
1:P:181:PRO:O	1:P:185:ASN:N	2.43	0.48
1:R:185:ASN:O	1:R:189:ASN:N	2.46	0.47
1:L:185:ASN:O	1:L:189:ASN:N	2.48	0.47
1:P:212:TRP:O	1:P:216:HIS:N	2.48	0.47
1:O:187:MET:O	1:O:191:VAL:N	2.48	0.46
1:Q:179:ALA:C	1:Q:259:GLY:HA2	2.36	0.46
1:A:166:PRO:C	1:A:168:VAL:H	2.17	0.45
1:I:180:THR:CA	1:I:259:GLY:HA3	2.47	0.45
1:M:293:PHE:C	1:M:296:TYR:H	2.20	0.45
1:K:273:ILE:O	1:K:277:TYR:N	2.49	0.45
1:F:157:LYS:O	1:F:161:GLU:N	2.49	0.45
1:B:272:LYS:O	1:B:276:MET:N	2.50	0.45
1:G:297:VAL:O	1:G:301:ALA:N	2.49	0.45
1:R:212:TRP:O	1:R:216:HIS:N	2.50	0.45
1:D:272:LYS:O	1:D:276:MET:N	2.50	0.44
1:O:176:SER:C	1:O:178:GLY:H	2.19	0.44
1:A:311:GLN:O	1:A:312:GLU:C	2.55	0.44
1:M:297:VAL:O	1:M:301:ALA:N	2.51	0.44
1:K:316:TRP:O	1:K:317:MET:C	2.54	0.44
1:K:340:GLY:C	1:K:342:THR:H	2.20	0.43
1:K:300:PHE:O	1:K:304:LEU:N	2.46	0.43
1:I:282:ILE:C	1:I:284:ASP:H	2.19	0.43
1:B:185:ASN:O	1:B:189:ASN:N	2.51	0.43
1:L:212:TRP:O	1:L:216:HIS:N	2.51	0.43
1:H:212:TRP:O	1:H:216:HIS:N	2.51	0.43
1:G:293:PHE:C	1:G:296:TYR:H	2.22	0.43
1:Q:316:TRP:O	1:Q:317:MET:C	2.54	0.43
1:H:295:ASP:O	1:H:299:ARG:N	2.50	0.43
1:N:212:TRP:O	1:N:216:HIS:N	2.52	0.43
1:I:316:TRP:O	1:I:317:MET:C	2.55	0.43
1:P:300:PHE:O	1:P:304:LEU:N	2.48	0.43
1:K:212:TRP:O	1:K:216:HIS:N	2.52	0.43
1:P:347:MET:O	1:P:351:GLN:N	2.52	0.42
1:A:333:ILE:O	1:A:337:LEU:N	2.53	0.42
1:K:297:VAL:O	1:K:301:ALA:N	2.49	0.42
1:M:316:TRP:O	1:M:317:MET:C	2.55	0.42
1:E:284:ASP:C	1:E:286:ARG:H	2.22	0.42
1:Q:172:PHE:O	1:Q:176:SER:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:293:PHE:O	1:J:296:TYR:N	2.52	0.42
1:Q:187:MET:O	1:Q:191:VAL:N	2.53	0.42
1:E:153:ASN:O	1:E:157:LYS:N	2.53	0.42
1:A:149:PRO:O	1:A:153:ASN:N	2.52	0.42
1:M:170:PRO:O	1:M:174:ALA:N	2.51	0.42
1:D:316:TRP:O	1:D:317:MET:C	2.56	0.42
1:G:212:TRP:O	1:G:216:HIS:N	2.53	0.42
1:F:153:ASN:O	1:F:157:LYS:N	2.53	0.42
1:B:303:THR:O	1:B:307:GLU:N	2.53	0.42
1:N:181:PRO:O	1:N:185:ASN:N	2.45	0.42
1:N:185:ASN:O	1:N:189:ASN:N	2.52	0.42
1:J:288:GLY:O	1:J:289:PRO:O	2.38	0.41
1:A:287:GLN:H	1:A:326:ALA:CA	2.33	0.41
1:H:181:PRO:O	1:H:185:ASN:N	2.45	0.41
1:D:246:GLN:O	1:D:249:TRP:N	2.53	0.41
1:C:233:GLY:O	1:C:237:ALA:N	2.53	0.41
1:A:246:GLN:O	1:A:249:TRP:N	2.53	0.41
1:E:159:VAL:O	1:E:163:ALA:N	2.53	0.41
1:E:295:ASP:O	1:E:299:ARG:N	2.53	0.41
1:G:300:PHE:O	1:G:304:LEU:N	2.48	0.41
1:J:212:TRP:O	1:J:216:HIS:N	2.54	0.41
1:B:159:VAL:O	1:B:163:ALA:N	2.53	0.41
1:M:300:PHE:O	1:M:304:LEU:N	2.48	0.41
1:G:284:ASP:C	1:G:286:ARG:H	2.24	0.41
1:I:180:THR:C	1:I:259:GLY:HA3	2.41	0.41
1:A:153:ASN:O	1:A:157:LYS:N	2.54	0.41
1:E:185:ASN:O	1:E:189:ASN:N	2.54	0.41
1:O:316:TRP:O	1:O:317:MET:C	2.56	0.40
1:A:259:GLY:O	1:A:263:LYS:N	2.54	0.40
1:Q:212:TRP:O	1:Q:216:HIS:N	2.53	0.40
1:R:333:ILE:O	1:R:337:LEU:N	2.54	0.40
1:M:212:TRP:O	1:M:216:HIS:N	2.54	0.40
1:B:316:TRP:O	1:B:317:MET:C	2.57	0.40
1:P:333:ILE:O	1:P:337:LEU:N	2.53	0.40
1:E:149:PRO:O	1:E:153:ASN:N	2.52	0.40
1:D:172:PHE:O	1:D:176:SER:N	2.55	0.40
1:E:333:ILE:O	1:E:337:LEU:N	2.54	0.40
1:R:229:ARG:O	1:R:230:GLU:C	2.60	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	208/210 (99%)	168 (81%)	20 (10%)	20 (10%)	1	15
1	B	208/210 (99%)	170 (82%)	23 (11%)	15 (7%)	1	22
1	C	208/210 (99%)	167 (80%)	24 (12%)	17 (8%)	1	18
1	D	208/210 (99%)	169 (81%)	19 (9%)	20 (10%)	1	15
1	E	208/210 (99%)	169 (81%)	22 (11%)	17 (8%)	1	18
1	F	208/210 (99%)	170 (82%)	25 (12%)	13 (6%)	2	25
1	G	208/210 (99%)	176 (85%)	21 (10%)	11 (5%)	2	29
1	H	208/210 (99%)	174 (84%)	17 (8%)	17 (8%)	1	18
1	I	208/210 (99%)	169 (81%)	24 (12%)	15 (7%)	1	22
1	J	208/210 (99%)	173 (83%)	17 (8%)	18 (9%)	1	17
1	K	208/210 (99%)	171 (82%)	18 (9%)	19 (9%)	1	17
1	L	208/210 (99%)	173 (83%)	20 (10%)	15 (7%)	1	22
1	M	208/210 (99%)	176 (85%)	17 (8%)	15 (7%)	1	22
1	N	208/210 (99%)	179 (86%)	20 (10%)	9 (4%)	3	34
1	O	208/210 (99%)	168 (81%)	28 (14%)	12 (6%)	2	27
1	P	208/210 (99%)	177 (85%)	13 (6%)	18 (9%)	1	17
1	Q	208/210 (99%)	178 (86%)	15 (7%)	15 (7%)	1	22
1	R	208/210 (99%)	177 (85%)	11 (5%)	20 (10%)	1	15
All	All	3744/3780 (99%)	3104 (83%)	354 (10%)	286 (8%)	2	20

All (286) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	HIS
1	A	147	ILE
1	A	167	GLU
1	A	179	ALA

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Mol	Chain	Res	Type
1	A	225	PRO
1	A	227	GLN
1	A	279	PRO
1	A	280	THR
1	A	288	GLY
1	A	289	PRO
1	A	308	GLN
1	A	309	ALA
1	B	144	HIS
1	B	179	ALA
1	B	218	VAL
1	B	225	PRO
1	B	279	PRO
1	B	280	THR
1	B	281	SER
1	C	147	ILE
1	C	225	PRO
1	C	226	GLY
1	C	229	ARG
1	C	255	PRO
1	C	279	PRO
1	C	280	THR
1	C	281	SER
1	C	286	ARG
1	D	147	ILE
1	D	225	PRO
1	D	228	MET
1	D	240	THR
1	D	279	PRO
1	D	280	THR
1	D	308	GLN
1	E	167	GLU
1	E	216	HIS
1	E	218	VAL
1	E	225	PRO
1	E	239	THR
1	E	280	THR
1	E	289	PRO
1	F	279	PRO
1	F	280	THR
1	F	289	PRO
1	G	179	ALA

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Mol	Chain	Res	Type
1	G	257	PRO
1	G	279	PRO
1	G	280	THR
1	G	326	ALA
1	H	147	ILE
1	H	217	PRO
1	H	229	ARG
1	H	289	PRO
1	H	309	ALA
1	H	323	VAL
1	H	339	PRO
1	I	225	PRO
1	I	226	GLY
1	I	279	PRO
1	I	280	THR
1	I	281	SER
1	I	309	ALA
1	J	144	HIS
1	J	179	ALA
1	J	216	HIS
1	J	279	PRO
1	J	289	PRO
1	K	146	ALA
1	K	216	HIS
1	K	279	PRO
1	K	280	THR
1	K	281	SER
1	K	289	PRO
1	K	292	PRO
1	L	147	ILE
1	L	166	PRO
1	L	179	ALA
1	L	220	ALA
1	L	229	ARG
1	L	289	PRO
1	M	225	PRO
1	M	279	PRO
1	M	280	THR
1	M	292	PRO
1	N	147	ILE
1	N	229	ARG
1	N	231	PRO

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Mol	Chain	Res	Type
1	N	279	PRO
1	N	289	PRO
1	N	309	ALA
1	O	225	PRO
1	O	228	MET
1	O	229	ARG
1	O	276	MET
1	O	279	PRO
1	O	280	THR
1	O	309	ALA
1	P	147	ILE
1	P	164	PHE
1	P	165	SER
1	P	166	PRO
1	P	217	PRO
1	P	279	PRO
1	P	289	PRO
1	P	308	GLN
1	P	309	ALA
1	Q	225	PRO
1	Q	228	MET
1	Q	279	PRO
1	Q	280	THR
1	Q	309	ALA
1	R	145	GLN
1	R	147	ILE
1	R	165	SER
1	R	166	PRO
1	R	179	ALA
1	R	217	PRO
1	R	220	ALA
1	R	222	PRO
1	R	289	PRO
1	A	226	GLY
1	A	281	SER
1	A	326	ALA
1	B	226	GLY
1	B	227	GLN
1	B	289	PRO
1	B	326	ALA
1	C	145	GLN
1	C	167	GLU

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Mol	Chain	Res	Type
1	C	217	PRO
1	D	220	ALA
1	D	226	GLY
1	D	281	SER
1	D	288	GLY
1	D	289	PRO
1	E	147	ILE
1	E	230	GLU
1	E	288	GLY
1	F	144	HIS
1	F	179	ALA
1	F	241	SER
1	G	229	ARG
1	G	285	ILE
1	H	144	HIS
1	H	179	ALA
1	H	252	HIS
1	H	279	PRO
1	H	280	THR
1	I	288	GLY
1	J	147	ILE
1	J	220	ALA
1	J	228	MET
1	J	229	ARG
1	K	177	GLU
1	K	228	MET
1	K	310	SER
1	K	342	THR
1	L	225	PRO
1	L	341	ALA
1	M	257	PRO
1	N	310	SER
1	O	193	GLY
1	O	226	GLY
1	P	218	VAL
1	P	226	GLY
1	Q	177	GLU
1	Q	229	ARG
1	Q	288	GLY
1	Q	289	PRO
1	R	178	GLY
1	R	221	GLY

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Mol	Chain	Res	Type
1	R	229	ARG
1	R	279	PRO
1	A	222	PRO
1	A	310	SER
1	B	166	PRO
1	C	227	GLN
1	C	289	PRO
1	D	179	ALA
1	D	231	PRO
1	D	310	SER
1	E	229	ARG
1	F	177	GLU
1	F	229	ARG
1	F	281	SER
1	F	292	PRO
1	F	339	PRO
1	G	240	THR
1	G	292	PRO
1	H	292	PRO
1	I	220	ALA
1	I	231	PRO
1	I	255	PRO
1	J	225	PRO
1	J	255	PRO
1	J	340	GLY
1	K	229	ARG
1	L	279	PRO
1	L	340	GLY
1	M	143	VAL
1	M	228	MET
1	M	252	HIS
1	O	231	PRO
1	O	339	PRO
1	P	143	VAL
1	P	257	PRO
1	P	291	GLU
1	Q	167	GLU
1	Q	239	THR
1	R	167	GLU
1	R	255	PRO
1	R	310	SER
1	A	229	ARG

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Mol	Chain	Res	Type
1	B	147	ILE
1	B	229	ARG
1	C	179	ALA
1	C	230	GLU
1	C	257	PRO
1	E	341	ALA
1	G	230	GLU
1	H	192	GLY
1	H	256	ILE
1	I	192	GLY
1	I	240	THR
1	J	166	PRO
1	J	276	MET
1	K	241	SER
1	K	257	PRO
1	L	276	MET
1	M	178	GLY
1	M	310	SER
1	M	339	PRO
1	P	254	PRO
1	Q	257	PRO
1	R	254	PRO
1	R	292	PRO
1	A	257	PRO
1	D	180	THR
1	E	231	PRO
1	F	217	PRO
1	G	167	GLU
1	H	167	GLU
1	I	167	GLU
1	I	285	ILE
1	J	281	SER
1	J	310	SER
1	K	227	GLN
1	K	255	PRO
1	L	255	PRO
1	L	257	PRO
1	M	230	GLU
1	M	323	VAL
1	N	341	ALA
1	P	216	HIS
1	P	310	SER

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Mol	Chain	Res	Type
1	P	339	PRO
1	Q	227	GLN
1	Q	240	THR
1	A	339	PRO
1	E	193	GLY
1	E	217	PRO
1	E	257	PRO
1	J	291	GLU
1	K	143	VAL
1	K	256	ILE
1	L	143	VAL
1	L	232	ARG
1	M	218	VAL
1	M	220	ALA
1	O	218	VAL
1	B	285	ILE
1	D	230	GLU
1	D	257	PRO
1	E	285	ILE
1	D	193	GLY
1	F	147	ILE
1	I	289	PRO
1	J	230	GLU
1	K	339	PRO
1	R	223	ILE
1	H	230	GLU
1	N	230	GLU
1	Q	230	GLU
1	R	216	HIS
1	D	218	VAL

5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.