



wwPDB EM Map/Model Validation Report ⓘ

Oct 6, 2016 – 05:32 PM EDT

PDB ID : 5GAI
EMDB ID: : EMD-8005
Title : Probabilistic Structural Models of Mature P22 Bacteriophage Portal, Hub, and Tailspike proteins
Authors : Pintilie, G.; Chen, D.H.; Haase-Pettingell, C.A.; King, J.A.; Chiu, W.
Deposited on : 2015-12-01
Resolution : 10.50 Å(reported)

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) : rb-20027939

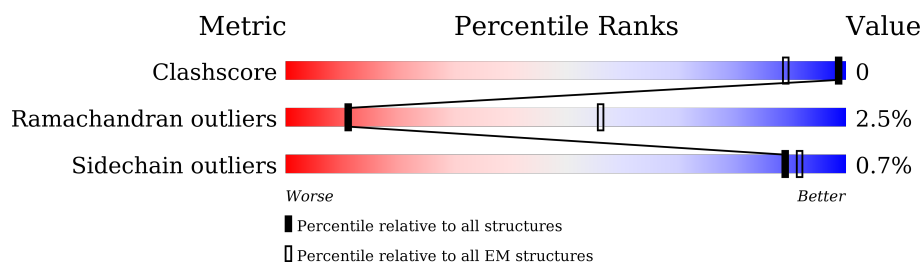
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 10.50 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.



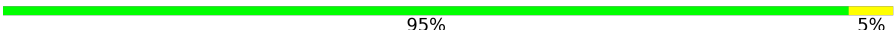
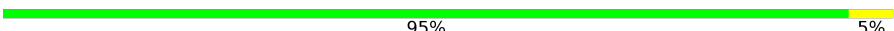
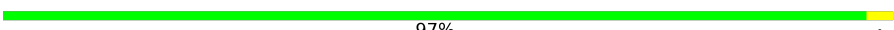
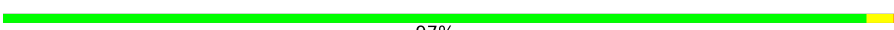






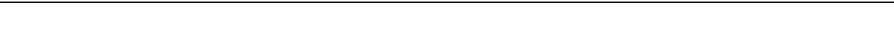

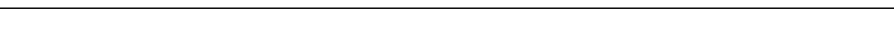
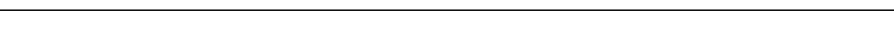
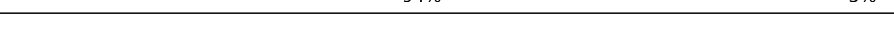
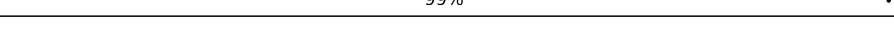
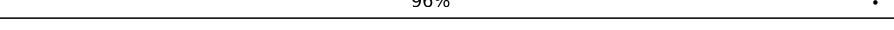
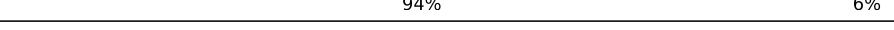
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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	721	96% . .
1	B	721	96% .
1	C	721	94% 6%
1	D	721	95% 5%
1	E	721	95% .
1	F	721	96% .
1	G	721	95% 5%
1	H	721	96% . .
1	I	721	97% . .

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Mol	Chain	Length	Quality of chain
1	J	721	 95% 5%
1	W	721	 95% 5%
1	X	721	 97% .
2	K	146	 97% ..
2	L	146	 97% .
2	M	146	 97% ..
2	N	146	 99% ..
2	O	146	 98% ..
2	P	146	 97% .
2	Q	146	 99% .
2	R	146	 95% 5%
2	S	146	 99% .
2	T	146	 97% ..
2	U	146	 94% 5% ..
2	V	146	 99% ..
3	0	662	 96% .
3	Y	662	 94% 6%
3	Z	662	 97% .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 98043 atoms, of which 0 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 Portal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	721	Total	C	N	O	S	0	0
			5792	3622	1005	1141	24		
1	B	721	Total	C	N	O	S	0	0
			5792	3622	1005	1141	24		
1	C	721	Total	C	N	O	S	0	0
			5792	3622	1005	1141	24		
1	D	721	Total	C	N	O	S	0	0
			5792	3622	1005	1141	24		
1	E	721	Total	C	N	O	S	0	0
			5792	3622	1005	1141	24		
1	F	721	Total	C	N	O	S	0	0
			5792	3622	1005	1141	24		
1	G	721	Total	C	N	O	S	0	0
			5792	3622	1005	1141	24		
1	H	721	Total	C	N	O	S	0	0
			5792	3622	1005	1141	24		
1	I	721	Total	C	N	O	S	0	0
			5792	3622	1005	1141	24		
1	J	721	Total	C	N	O	S	0	0
			5792	3622	1005	1141	24		
1	W	721	Total	C	N	O	S	0	0
			5792	3622	1005	1141	24		
1	X	721	Total	C	N	O	S	0	0
			5792	3622	1005	1141	24		

- Molecule 2 is a protein called Peptidoglycan hydrolase gp4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	K	146	Total	C	N	O	S	0	0
			1122	704	192	221	5		
2	L	146	Total	C	N	O	S	0	0
			1122	704	192	221	5		
2	M	146	Total	C	N	O	S	0	0
			1122	704	192	221	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	146	Total	C	N	O	S	0	0
			1122	704	192	221	5		
2	O	146	Total	C	N	O	S	0	0
			1122	704	192	221	5		
2	P	146	Total	C	N	O	S	0	0
			1122	704	192	221	5		
2	Q	146	Total	C	N	O	S	0	0
			1122	704	192	221	5		
2	R	146	Total	C	N	O	S	0	0
			1122	704	192	221	5		
2	S	146	Total	C	N	O	S	0	0
			1122	704	192	221	5		
2	T	146	Total	C	N	O	S	0	0
			1122	704	192	221	5		
2	U	146	Total	C	N	O	S	0	0
			1122	704	192	221	5		
2	V	146	Total	C	N	O	S	0	0
			1122	704	192	221	5		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	150	PRO	ALA	engineered mutation	UNP P26746
L	150	PRO	ALA	engineered mutation	UNP P26746
M	150	PRO	ALA	engineered mutation	UNP P26746
N	150	PRO	ALA	engineered mutation	UNP P26746
O	150	PRO	ALA	engineered mutation	UNP P26746
P	150	PRO	ALA	engineered mutation	UNP P26746
Q	150	PRO	ALA	engineered mutation	UNP P26746
R	150	PRO	ALA	engineered mutation	UNP P26746
S	150	PRO	ALA	engineered mutation	UNP P26746
T	150	PRO	ALA	engineered mutation	UNP P26746
U	150	PRO	ALA	engineered mutation	UNP P26746
V	150	PRO	ALA	engineered mutation	UNP P26746

- Molecule 3 is a protein called Tail fiber protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Y	662	Total	C	N	O	S	0	0
			5025	3169	855	985	16		
3	Z	662	Total	C	N	O	S	0	0
			5025	3169	855	985	16		

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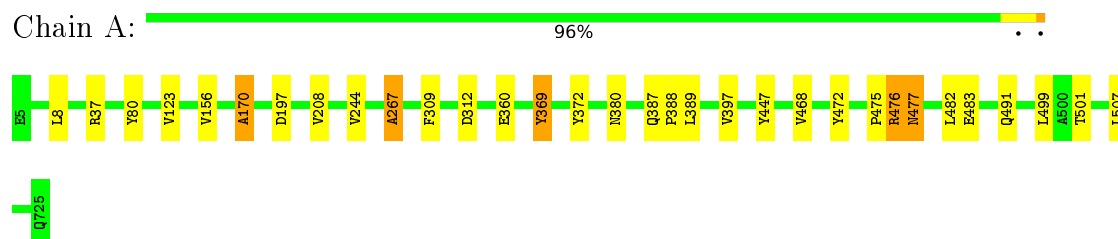
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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	0	662	5025	3169	855	985	16	0	0

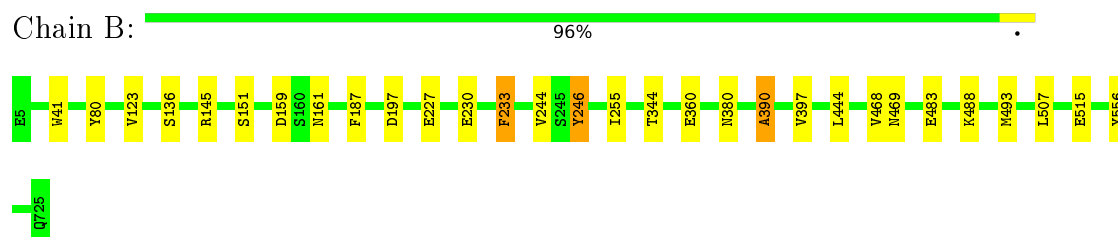
3 Residue-property plots [i](#)

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.

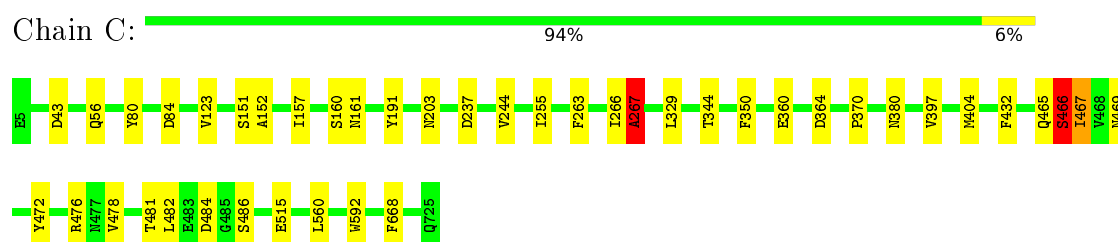
- Molecule 1: Portal protein



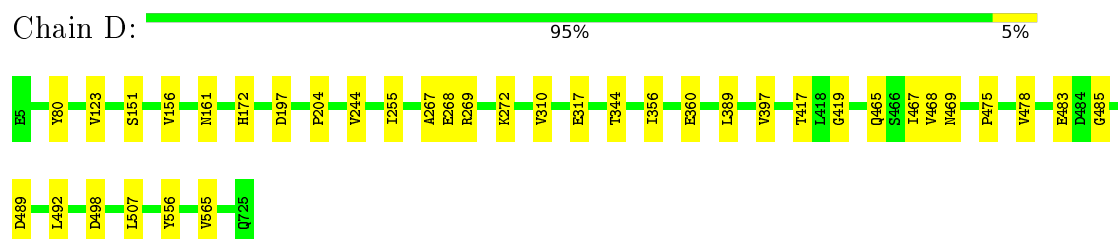
- Molecule 1: Portal protein



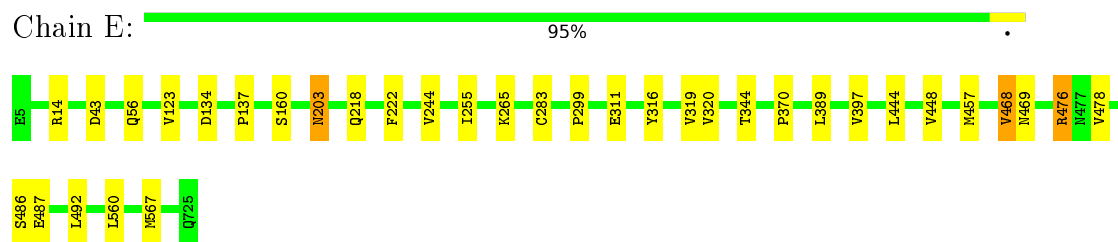
- Molecule 1: Portal protein



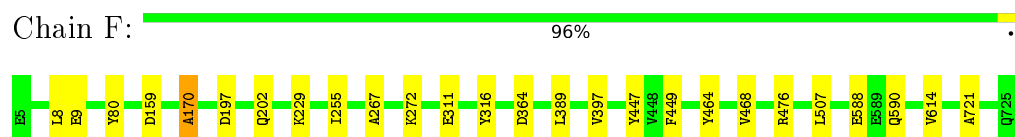
- Molecule 1: Portal protein



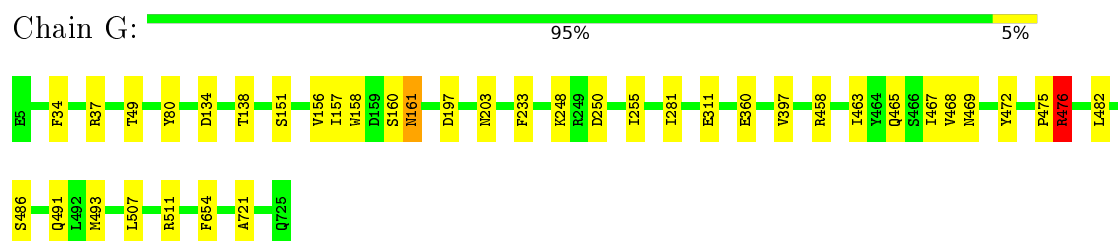
- Molecule 1: Portal protein



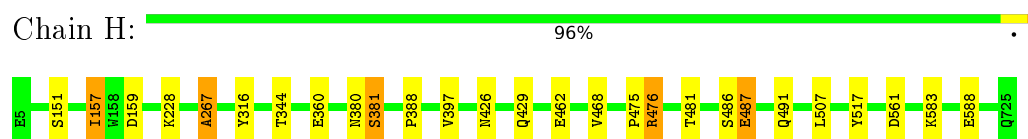
- Molecule 1: Portal protein



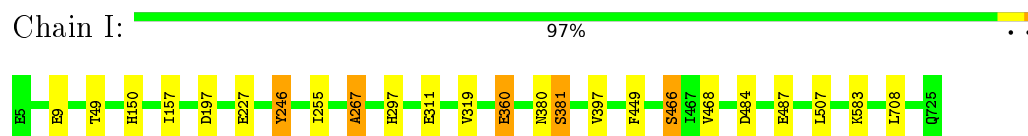
- Molecule 1: Portal protein



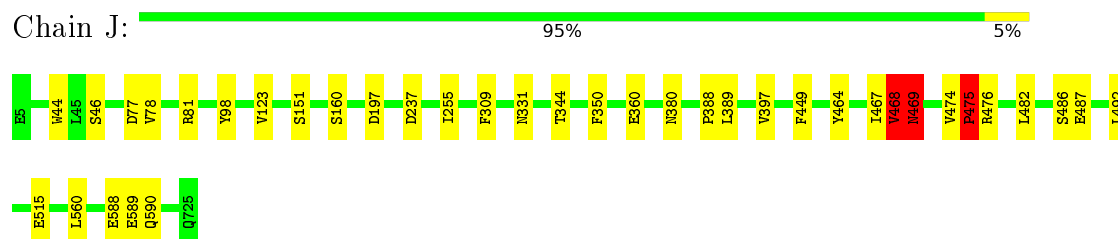
- Molecule 1: Portal protein



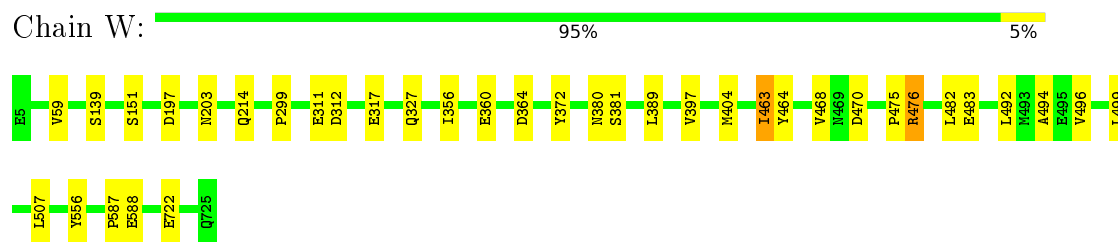
- Molecule 1: Portal protein



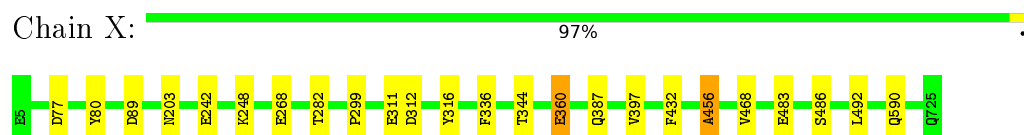
- Molecule 1: Portal protein



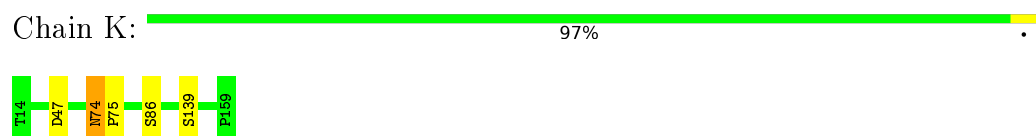
- Molecule 1: Portal protein



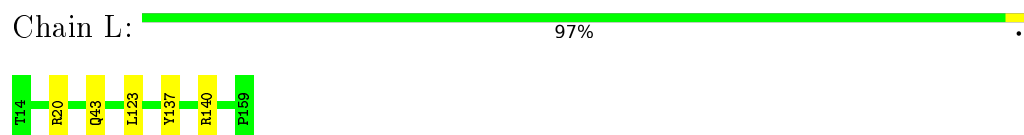
- Molecule 1: Portal protein



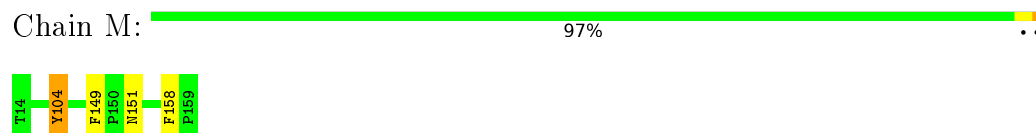
- Molecule 2: Peptidoglycan hydrolase gp4



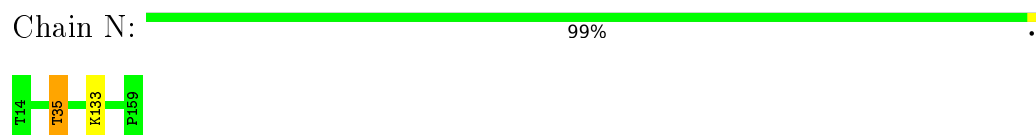
- Molecule 2: Peptidoglycan hydrolase gp4



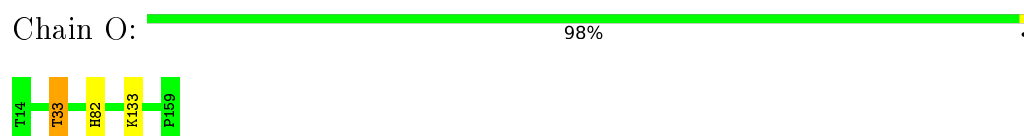
- Molecule 2: Peptidoglycan hydrolase gp4



- Molecule 2: Peptidoglycan hydrolase gp4



- Molecule 2: Peptidoglycan hydrolase gp4



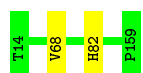
- Molecule 2: Peptidoglycan hydrolase gp4

Chain P:  97% .



- Molecule 2: Peptidoglycan hydrolase gp4

Chain Q:  99% .



- Molecule 2: Peptidoglycan hydrolase gp4

Chain R:  95% 5%



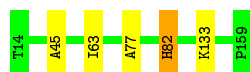
- Molecule 2: Peptidoglycan hydrolase gp4

Chain S:  99% .



- Molecule 2: Peptidoglycan hydrolase gp4

Chain T:  97% ..



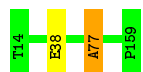
- Molecule 2: Peptidoglycan hydrolase gp4

Chain U:  94% 5% ..



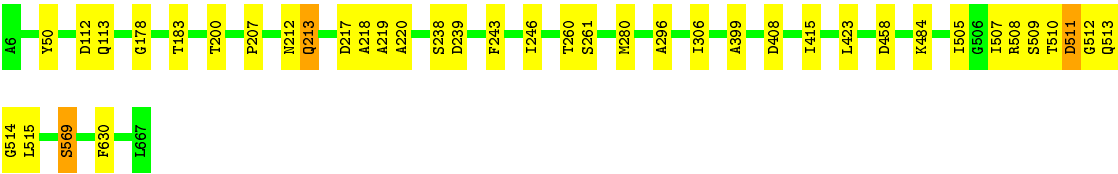
- Molecule 2: Peptidoglycan hydrolase gp4

Chain V:  99% ..



- Molecule 3: Tail fiber protein

Chain Y:  94% 6%



• Molecule 3: Tail fiber protein



• Molecule 3: Tail fiber protein



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	79731	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	40000	Depositor
Image detector	Not provided	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	0.94	0/5902	0.96	4/7997 (0.1%)
1	B	0.94	0/5902	0.96	9/7997 (0.1%)
1	C	0.94	0/5902	0.97	9/7997 (0.1%)
1	D	0.94	0/5902	0.94	2/7997 (0.0%)
1	E	0.94	0/5902	0.94	2/7997 (0.0%)
1	F	0.94	0/5902	0.95	3/7997 (0.0%)
1	G	0.94	0/5902	0.94	6/7997 (0.1%)
1	H	0.94	0/5902	0.94	2/7997 (0.0%)
1	I	0.94	0/5902	0.95	7/7997 (0.1%)
1	J	0.94	0/5902	0.95	6/7997 (0.1%)
1	W	0.94	0/5902	0.95	5/7997 (0.1%)
1	X	0.94	0/5902	0.95	5/7997 (0.1%)
2	K	0.92	0/1148	0.92	0/1558
2	L	0.92	0/1148	0.99	2/1558 (0.1%)
2	M	0.91	0/1148	0.97	4/1558 (0.3%)
2	N	0.92	0/1148	0.99	0/1558
2	O	0.91	0/1148	0.95	0/1558
2	P	0.92	0/1148	0.99	2/1558 (0.1%)
2	Q	0.91	0/1148	0.95	0/1558
2	R	0.92	0/1148	0.96	0/1558
2	S	0.92	0/1148	0.98	2/1558 (0.1%)
2	T	0.92	0/1148	0.98	0/1558
2	U	0.92	0/1148	1.01	0/1558
2	V	0.92	0/1148	0.99	1/1558 (0.1%)
3	O	0.92	0/5128	1.02	6/6966 (0.1%)
3	Y	0.93	0/5128	1.02	5/6966 (0.1%)
3	Z	0.92	0/5128	0.98	6/6966 (0.1%)
All	All	0.93	0/99984	0.96	88/135558 (0.1%)

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	6
1	B	0	1
1	C	0	5
1	D	0	5
1	E	0	5
1	F	0	3
1	G	0	4
1	H	0	5
1	J	0	8
1	W	0	4
1	X	0	2
2	K	0	1
2	U	0	1
2	V	0	1
3	O	0	9
3	Y	0	17
3	Z	0	1
All	All	0	78

There are no bond length outliers.

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	404	MET	CG-SD-CE	-7.64	87.97	100.20
1	W	556	TYR	CB-CG-CD2	-7.22	116.67	121.00
1	C	432	PHE	CB-CG-CD2	6.80	125.56	120.80
1	I	246	TYR	CB-CG-CD2	-6.80	116.92	121.00
1	I	246	TYR	CB-CG-CD1	6.71	125.03	121.00
1	X	456	ALA	N-CA-CB	6.57	119.30	110.10
1	J	449	PHE	CB-CG-CD1	6.55	125.39	120.80
1	C	191	TYR	CB-CG-CD1	6.47	124.88	121.00
1	C	191	TYR	CB-CG-CD2	-6.43	117.14	121.00
1	G	233	PHE	CB-CG-CD1	6.43	125.30	120.80
2	P	149	PHE	CB-CG-CD1	6.38	125.26	120.80
3	O	240	TYR	CB-CG-CD2	-6.35	117.19	121.00
1	A	267	ALA	N-CA-CB	6.27	118.88	110.10
2	S	124	TYR	CB-CG-CD2	-6.26	117.25	121.00
3	Y	50	TYR	CB-CG-CD2	-6.24	117.25	121.00
2	M	104	TYR	CB-CG-CD2	-6.24	117.26	121.00
1	W	556	TYR	CB-CG-CD1	6.16	124.69	121.00
3	O	161	PHE	CB-CG-CD1	6.14	125.10	120.80
1	B	187	PHE	CB-CG-CD1	6.13	125.09	120.80
3	O	240	TYR	CB-CG-CD1	6.12	124.67	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	432	PHE	CB-CG-CD1	-6.11	116.52	120.80
1	B	246	TYR	CB-CG-CD2	6.11	124.67	121.00
1	I	449	PHE	CB-CG-CD1	6.08	125.06	120.80
3	Y	50	TYR	CB-CG-CD1	6.04	124.62	121.00
1	X	432	PHE	CB-CG-CD1	6.03	125.02	120.80
1	H	381	SER	N-CA-CB	6.02	119.52	110.50
1	B	556	TYR	CB-CG-CD2	-5.99	117.40	121.00
2	P	149	PHE	CB-CG-CD2	-5.99	116.61	120.80
1	G	233	PHE	CB-CG-CD2	-5.98	116.61	120.80
1	W	372	TYR	CB-CG-CD2	-5.98	117.41	121.00
2	M	104	TYR	CB-CG-CD1	5.97	124.58	121.00
3	Z	182	PHE	CB-CG-CD1	5.95	124.97	120.80
1	F	170	ALA	N-CA-CB	5.94	118.42	110.10
1	W	372	TYR	CB-CG-CD1	5.94	124.56	121.00
1	B	246	TYR	CB-CG-CD1	-5.92	117.45	121.00
1	A	170	ALA	N-CA-CB	5.90	118.36	110.10
1	X	336	PHE	CB-CG-CD1	5.89	124.93	120.80
2	V	77	ALA	N-CA-CB	5.88	118.34	110.10
1	I	267	ALA	N-CA-CB	5.88	118.33	110.10
1	E	222	PHE	CB-CG-CD1	5.83	124.88	120.80
1	C	668	PHE	CB-CG-CD1	5.74	124.81	120.80
1	X	432	PHE	CB-CG-CD2	-5.72	116.80	120.80
1	J	309	PHE	CB-CG-CD1	5.71	124.80	120.80
3	O	161	PHE	CB-CG-CD2	-5.71	116.80	120.80
3	O	630	PHE	CB-CG-CD1	5.70	124.79	120.80
3	Z	285	PHE	CB-CG-CD1	5.70	124.79	120.80
1	D	556	TYR	CB-CG-CD2	-5.69	117.59	121.00
2	M	149	PHE	CB-CG-CD1	5.69	124.78	120.80
2	S	124	TYR	CB-CG-CD1	5.69	124.41	121.00
1	J	449	PHE	CB-CG-CD2	-5.62	116.86	120.80
1	X	336	PHE	CB-CG-CD2	-5.62	116.87	120.80
3	Y	569	SER	N-CA-CB	5.61	118.91	110.50
3	Y	630	PHE	CB-CG-CD1	5.61	124.72	120.80
3	Y	630	PHE	CB-CG-CD2	-5.59	116.89	120.80
1	C	350	PHE	CB-CG-CD2	-5.58	116.89	120.80
1	C	350	PHE	CB-CG-CD1	5.53	124.67	120.80
2	L	137	TYR	CB-CG-CD2	-5.50	117.70	121.00
1	B	187	PHE	CB-CG-CD2	-5.48	116.97	120.80
1	F	449	PHE	CB-CG-CD1	5.45	124.62	120.80
1	I	449	PHE	CB-CG-CD2	-5.45	116.99	120.80
3	Z	182	PHE	CB-CG-CD2	-5.45	116.98	120.80
3	O	630	PHE	CB-CG-CD2	-5.44	116.99	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	654	PHE	CB-CG-CD2	-5.43	117.00	120.80
1	C	668	PHE	CB-CG-CD2	-5.42	117.00	120.80
3	Z	285	PHE	CB-CG-CD2	-5.34	117.06	120.80
1	J	309	PHE	CB-CG-CD2	-5.32	117.08	120.80
1	E	567	MET	CG-SD-CE	-5.28	91.75	100.20
1	A	477	ASN	N-CA-CB	5.26	120.07	110.60
1	C	267	ALA	N-CA-CB	5.18	117.35	110.10
1	I	381	SER	N-CA-CB	5.18	118.27	110.50
1	G	161	ASN	N-CA-CB	5.16	119.88	110.60
1	H	267	ALA	N-CA-CB	5.15	117.31	110.10
2	L	137	TYR	CB-CG-CD1	5.15	124.09	121.00
1	J	151	SER	N-CA-CB	5.14	118.21	110.50
1	F	449	PHE	CB-CG-CD2	-5.13	117.20	120.80
1	G	476	ARG	N-CA-CB	5.13	119.84	110.60
1	J	350	PHE	CB-CG-CD1	5.13	124.39	120.80
1	B	556	TYR	CB-CG-CD1	5.13	124.08	121.00
1	G	654	PHE	CB-CG-CD1	5.12	124.39	120.80
1	B	233	PHE	CB-CG-CD1	5.11	124.37	120.80
1	A	309	PHE	CB-CG-CD1	5.10	124.37	120.80
1	B	390	ALA	N-CA-CB	5.09	117.23	110.10
1	I	466	SER	N-CA-CB	5.08	118.12	110.50
1	D	556	TYR	CB-CG-CD1	5.08	124.05	121.00
3	Z	630	PHE	CB-CG-CD1	5.06	124.34	120.80
2	M	149	PHE	CB-CG-CD2	-5.04	117.27	120.80
3	Z	630	PHE	CB-CG-CD2	-5.02	117.29	120.80
1	B	233	PHE	CB-CG-CD2	-5.01	117.29	120.80

There are no chirality outliers.

All (78) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	0	113	GLN	Peptide
3	0	312	LEU	Peptide
3	0	401	THR	Peptide
3	0	402	ASP	Peptide
3	0	406	GLU	Peptide
3	0	412	ASP	Peptide
3	0	419	PRO	Peptide
3	0	445	ASP	Peptide
3	0	450	TYR	Sidechain
1	A	369	TYR	Sidechain
1	A	372	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	A	447	TYR	Sidechain
1	A	475	PRO	Peptide
1	A	476	ARG	Peptide
1	A	483	GLU	Peptide
1	B	483	GLU	Peptide
1	C	152	ALA	Peptide
1	C	465	GLN	Peptide
1	C	466	SER	Peptide
1	C	469	ASN	Peptide
1	C	486	SER	Peptide
1	D	465	GLN	Peptide
1	D	469	ASN	Peptide
1	D	475	PRO	Peptide
1	D	483	GLU	Peptide
1	D	485	GLY	Peptide
1	E	14	ARG	Sidechain
1	E	319	VAL	Peptide
1	E	468	VAL	Peptide
1	E	476	ARG	Peptide
1	E	486	SER	Peptide
1	F	447	TYR	Sidechain
1	F	476	ARG	Peptide
1	F	8	LEU	Peptide
1	G	158	TRP	Peptide
1	G	37	ARG	Sidechain
1	G	475	PRO	Peptide
1	G	486	SER	Peptide
1	H	468	VAL	Peptide
1	H	475	PRO	Peptide
1	H	476	ARG	Peptide
1	H	486	SER	Peptide
1	H	487	GLU	Peptide
1	J	464	TYR	Sidechain
1	J	468	VAL	Peptide
1	J	474	VAL	Peptide
1	J	475	PRO	Peptide
1	J	482	LEU	Peptide
1	J	486	SER	Peptide
1	J	487	GLU	Peptide
1	J	589	GLU	Peptide
2	K	139	SER	Peptide
2	U	73	GLU	Peptide

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Mol	Chain	Res	Type	Group
2	V	38	GLU	Peptide
1	W	476	ARG	Peptide
1	W	482	LEU	Peptide
1	W	492	LEU	Peptide
1	W	587	PRO	Peptide
1	X	486	SER	Peptide
1	X	492	LEU	Peptide
3	Y	112	ASP	Peptide
3	Y	178	GLY	Peptide
3	Y	213	GLN	Peptide
3	Y	217	ASP	Peptide
3	Y	218	ALA	Peptide
3	Y	219	ALA	Peptide
3	Y	238	SER	Peptide
3	Y	239	ASP	Peptide
3	Y	243	PHE	Peptide
3	Y	280	MET	Peptide
3	Y	458	ASP	Peptide
3	Y	484	LYS	Peptide
3	Y	507	ILE	Peptide
3	Y	509	SER	Peptide
3	Y	511	ASP	Peptide
3	Y	512	GLY	Peptide
3	Y	513	GLN	Peptide
3	Z	109	TYR	Peptide

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	5792	0	5623	1	0
1	B	5792	0	5623	1	0
1	C	5792	0	5623	5	0
1	D	5792	0	5623	4	0
1	E	5792	0	5623	4	0
1	F	5792	0	5623	2	0
1	G	5792	0	5623	3	0
1	H	5792	0	5623	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	5792	0	5623	1	0
1	J	5792	0	5623	3	0
1	W	5792	0	5623	3	0
1	X	5792	0	5623	0	0
2	K	1122	0	1082	1	0
2	L	1122	0	1082	1	0
2	M	1122	0	1082	0	0
2	N	1122	0	1082	0	0
2	O	1122	0	1082	0	0
2	P	1122	0	1082	0	0
2	Q	1122	0	1082	0	0
2	R	1122	0	1082	1	0
2	S	1122	0	1082	0	0
2	T	1122	0	1082	2	0
2	U	1122	0	1082	2	0
2	V	1122	0	1082	0	0
3	O	5025	0	4930	2	0
3	Y	5025	0	4930	2	0
3	Z	5025	0	4930	3	0
All	All	98043	0	95250	39	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 0.

All (39) 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)
2:L:20:ARG:HH22	3:Z:25:ALA:H	1.55	0.54
2:R:24:ARG:HH12	2:R:82:HIS:CE1	2.28	0.52
2:T:82:HIS:H	2:T:82:HIS:CD2	2.28	0.52
1:W:59:VAL:HG12	1:W:327:GLN:HE21	1.74	0.50
3:Y:260:THR:HG22	3:Y:261:SER:H	1.76	0.50
2:U:82:HIS:CG	2:U:83:GLY:H	2.31	0.49
3:Z:203:TRP:H	3:Z:257:GLN:HE22	1.61	0.49
1:C:266:ILE:HG13	1:C:267:ALA:H	1.78	0.48
3:Y:408:ASP:H	3:Y:415:ILE:HG22	1.80	0.47
1:F:255:ILE:HD12	1:F:255:ILE:H	1.79	0.47
1:D:161:ASN:HD22	1:D:172:HIS:CD2	2.33	0.47
1:C:466:SER:H	1:C:467:ILE:HG22	1.79	0.47
1:F:272:LYS:H	1:G:134:ASP:HB2	1.78	0.47
1:D:272:LYS:H	1:E:134:ASP:HB2	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:255:ILE:HD12	1:G:255:ILE:H	1.79	0.47
1:J:44:TRP:HE1	1:J:331:ASN:HD22	1.61	0.46
1:J:468:VAL:HA	1:J:469:ASN:HD22	1.79	0.46
1:C:255:ILE:HD12	1:C:255:ILE:H	1.81	0.46
1:D:255:ILE:H	1:D:255:ILE:HD12	1.81	0.46
3:O:407:LEU:HD23	3:O:407:LEU:H	1.80	0.46
1:I:255:ILE:H	1:I:255:ILE:HD12	1.81	0.45
2:U:74:ASN:H	2:U:75:PRO:HD2	1.82	0.45
1:C:43:ASP:H	1:C:56:GLN:HE22	1.65	0.45
1:C:329:LEU:HD21	1:C:404:MET:HE3	1.98	0.44
1:D:417:THR:HG22	1:D:419:GLY:H	1.82	0.44
1:E:255:ILE:HD12	1:E:255:ILE:H	1.82	0.44
1:H:426:ASN:H	1:H:429:GLN:HE21	1.67	0.43
2:K:74:ASN:H	2:K:75:PRO:HD2	1.83	0.43
1:W:463:ILE:HG12	1:W:464:TYR:H	1.83	0.43
1:A:37:ARG:HH22	1:A:208:VAL:HB	1.84	0.43
3:Z:340:ASN:H	3:Z:377:ASN:HD22	1.67	0.42
1:E:43:ASP:H	1:E:56:GLN:HE22	1.67	0.42
2:T:63:ILE:HD12	2:T:63:ILE:H	1.85	0.41
1:G:248:LYS:HA	1:G:511:ARG:HE	1.85	0.41
1:E:203:ASN:HA	1:E:218:GLN:HE22	1.85	0.41
1:W:496:VAL:HG13	1:W:499:LEU:HB2	2.03	0.41
1:J:255:ILE:HD12	1:J:255:ILE:H	1.86	0.40
1:B:136:SER:HB2	1:B:145:ARG:HH22	1.86	0.40
3:O:440:VAL:HG12	3:O:441:GLY:H	1.86	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	719/721 (100%)	646 (90%)	53 (7%)	20 (3%)	6 44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	719/721 (100%)	639 (89%)	60 (8%)	20 (3%)	6	44
1	C	719/721 (100%)	630 (88%)	67 (9%)	22 (3%)	5	42
1	D	719/721 (100%)	633 (88%)	67 (9%)	19 (3%)	7	45
1	E	719/721 (100%)	648 (90%)	51 (7%)	20 (3%)	6	44
1	F	719/721 (100%)	643 (89%)	59 (8%)	17 (2%)	7	47
1	G	719/721 (100%)	642 (89%)	54 (8%)	23 (3%)	5	41
1	H	719/721 (100%)	645 (90%)	56 (8%)	18 (2%)	7	46
1	I	719/721 (100%)	641 (89%)	60 (8%)	18 (2%)	7	46
1	J	719/721 (100%)	637 (89%)	62 (9%)	20 (3%)	6	44
1	W	719/721 (100%)	644 (90%)	52 (7%)	23 (3%)	5	41
1	X	719/721 (100%)	646 (90%)	56 (8%)	17 (2%)	7	47
2	K	144/146 (99%)	126 (88%)	16 (11%)	2 (1%)	14	58
2	L	144/146 (99%)	122 (85%)	20 (14%)	2 (1%)	14	58
2	M	144/146 (99%)	125 (87%)	17 (12%)	2 (1%)	14	58
2	N	144/146 (99%)	125 (87%)	17 (12%)	2 (1%)	14	58
2	O	144/146 (99%)	123 (85%)	19 (13%)	2 (1%)	14	58
2	P	144/146 (99%)	123 (85%)	17 (12%)	4 (3%)	6	44
2	Q	144/146 (99%)	131 (91%)	12 (8%)	1 (1%)	26	71
2	R	144/146 (99%)	129 (90%)	11 (8%)	4 (3%)	6	44
2	S	144/146 (99%)	130 (90%)	14 (10%)	0	100	100
2	T	144/146 (99%)	130 (90%)	11 (8%)	3 (2%)	9	50
2	U	144/146 (99%)	124 (86%)	14 (10%)	6 (4%)	3	34
2	V	144/146 (99%)	127 (88%)	16 (11%)	1 (1%)	26	71
3	O	660/662 (100%)	603 (91%)	44 (7%)	13 (2%)	9	51
3	Y	660/662 (100%)	606 (92%)	36 (6%)	18 (3%)	6	45
3	Z	660/662 (100%)	621 (94%)	32 (5%)	7 (1%)	17	63
All	All	12336/12390 (100%)	11039 (90%)	993 (8%)	304 (2%)	11	46

All (304) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	170	ALA
1	A	267	ALA

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Mol	Chain	Res	Type
1	A	476	ARG
1	A	477	ASN
1	A	501	THR
1	B	41	TRP
1	B	233	PHE
1	B	344	THR
1	B	469	ASN
1	C	151	SER
1	C	466	SER
1	C	467	ILE
1	C	484	ASP
1	E	203	ASN
1	E	469	ASN
1	F	9	GLU
1	F	170	ALA
1	F	507	LEU
1	G	161	ASN
1	H	159	ASP
1	H	267	ALA
1	H	491	GLN
1	H	588	GLU
1	I	267	ALA
1	I	468	VAL
1	I	507	LEU
1	J	467	ILE
1	J	560	LEU
1	J	590	GLN
2	U	44	ASP
2	V	77	ALA
1	W	483	GLU
1	W	588	GLU
3	Y	113	GLN
3	Y	508	ARG
1	A	8	LEU
1	A	380	ASN
1	A	507	LEU
1	B	197	ASP
1	B	230	GLU
1	B	488	LYS
1	B	507	LEU
1	C	160	SER
1	C	481	THR

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Mol	Chain	Res	Type
1	C	560	LEU
1	D	80	TYR
1	D	151	SER
1	D	197	ASP
1	D	468	VAL
1	D	489	ASP
1	D	507	LEU
1	E	311	GLU
1	F	80	TYR
1	G	458	ARG
1	G	467	ILE
1	G	469	ASN
1	G	476	ARG
1	G	493	MET
1	G	507	LEU
1	H	476	ARG
1	H	487	GLU
1	I	319	VAL
1	I	381	SER
1	I	466	SER
1	J	77	ASP
1	J	81	ARG
1	J	380	ASN
1	J	468	VAL
1	J	475	PRO
2	L	43	GLN
2	M	151	ASN
2	T	45	ALA
2	T	77	ALA
2	T	133	LYS
2	U	133	LYS
2	U	151	ASN
1	W	139	SER
1	W	214	GLN
1	W	312	ASP
1	W	507	LEU
1	X	268	GLU
1	X	456	ALA
1	X	468	VAL
1	X	590	GLN
3	Y	212	ASN
3	Y	213	GLN

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Mol	Chain	Res	Type
3	Y	220	ALA
3	Y	423	LEU
3	Y	505	ILE
3	Y	510	THR
3	Y	569	SER
3	0	70	ALA
3	0	507	ILE
1	A	197	ASP
1	A	312	ASP
1	A	499	LEU
1	B	151	SER
1	B	380	ASN
1	B	390	ALA
1	C	237	ASP
1	C	344	THR
1	C	515	GLU
1	C	592	TRP
1	E	160	SER
1	E	283	CYS
1	E	299	PRO
1	E	457	MET
1	F	159	ASP
1	F	197	ASP
1	F	588	GLU
1	G	197	ASP
1	G	463	ILE
1	G	468	VAL
1	H	228	LYS
1	H	380	ASN
1	H	381	SER
1	H	462	GLU
1	H	481	THR
1	I	197	ASP
1	I	360	GLU
1	J	197	ASP
2	K	86	SER
2	M	158	PHE
2	R	78	GLU
2	R	156	HIS
2	U	82	HIS
1	W	197	ASP
1	W	311	GLU

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Mol	Chain	Res	Type
1	W	381	SER
1	W	463	ILE
1	W	470	ASP
1	W	722	GLU
1	X	77	ASP
1	X	282	THR
1	X	311	GLU
1	X	312	ASP
1	X	483	GLU
3	Y	207	PRO
3	Y	514	GLY
3	Y	515	LEU
3	Z	569	SER
3	0	107	LEU
3	0	401	THR
1	A	397	VAL
1	B	161	ASN
1	B	227	GLU
1	B	397	VAL
1	C	267	ALA
1	C	370	PRO
1	C	380	ASN
1	C	397	VAL
1	C	482	LEU
1	D	267	ALA
1	D	268	GLU
1	D	269	ARG
1	D	344	THR
1	D	397	VAL
1	D	467	ILE
1	D	478	VAL
1	D	498	ASP
1	E	137	PRO
1	E	265	LYS
1	E	344	THR
1	E	397	VAL
1	E	478	VAL
1	E	492	LEU
1	E	560	LEU
1	F	202	GLN
1	F	364	ASP
1	F	397	VAL

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Mol	Chain	Res	Type
1	F	721	ALA
1	G	160	SER
1	G	203	ASN
1	G	397	VAL
1	G	472	TYR
1	G	482	LEU
1	G	721	ALA
1	H	388	PRO
1	H	397	VAL
1	H	507	LEU
1	I	157	ILE
1	I	227	GLU
1	I	397	VAL
1	I	484	ASP
1	J	46	SER
1	J	237	ASP
1	J	388	PRO
1	J	397	VAL
1	J	469	ASN
1	J	476	ARG
2	L	140	ARG
2	N	133	LYS
2	O	133	LYS
2	R	42	MET
2	U	74	ASN
1	W	299	PRO
1	W	364	ASP
1	W	468	VAL
1	W	475	PRO
1	W	476	ARG
1	W	494	ALA
1	X	203	ASN
1	X	344	THR
1	X	387	GLN
1	X	397	VAL
3	Y	200	THR
3	Y	296	ALA
3	Y	511	ASP
3	Z	7	ASN
3	Z	108	LYS
3	Z	207	PRO
3	0	318	LYS

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Mol	Chain	Res	Type
3	0	399	ALA
3	0	423	LEU
3	0	426	ASN
3	0	505	ILE
1	A	80	TYR
1	A	388	PRO
1	B	80	TYR
1	B	159	ASP
1	B	244	VAL
1	B	468	VAL
1	B	515	GLU
1	C	203	ASN
1	C	263	PHE
1	C	364	ASP
1	D	204	PRO
1	D	310	VAL
1	D	492	LEU
1	E	370	PRO
1	E	476	ARG
1	E	487	GLU
1	F	229	LYS
1	F	267	ALA
1	F	464	TYR
1	F	468	VAL
1	F	590	GLN
1	G	49	THR
1	G	80	TYR
1	G	151	SER
1	G	465	GLN
1	G	491	GLN
1	H	151	SER
1	I	49	THR
1	I	380	ASN
1	J	78	VAL
1	J	160	SER
1	J	344	THR
1	J	515	GLU
1	J	588	GLU
2	N	35	THR
2	O	33	THR
2	P	76	PRO
2	R	43	GLN

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Mol	Chain	Res	Type
2	U	138	PRO
1	W	151	SER
1	W	203	ASN
1	W	380	ASN
1	W	397	VAL
1	X	80	TYR
1	X	242	GLU
1	X	360	GLU
3	Y	399	ALA
3	Z	424	PRO
3	Z	505	ILE
3	0	207	PRO
3	0	515	LEU
3	0	569	SER
1	A	468	VAL
1	A	472	TYR
1	A	482	LEU
1	A	491	GLN
1	B	493	MET
1	D	244	VAL
1	D	356	ILE
1	E	123	VAL
1	F	311	GLU
1	G	311	GLU
1	I	9	GLU
1	I	311	GLU
1	I	487	GLU
2	P	57	TYR
2	P	139	SER
3	0	402	ASP
1	A	387	GLN
1	C	244	VAL
1	I	583	LYS
2	K	74	ASN
2	P	141	MET
2	Q	68	VAL
1	X	299	PRO
1	C	157	ILE
1	C	478	VAL
1	E	244	VAL
3	Y	246	ILE
1	A	244	VAL

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Mol	Chain	Res	Type
1	E	468	VAL
1	G	157	ILE
1	H	344	THR
1	W	356	ILE
3	Y	306	ILE
1	H	157	ILE
1	H	583	LYS
3	Z	110	ASP

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain 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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	627/627 (100%)	622 (99%)	5 (1%)	86	94
1	B	627/627 (100%)	622 (99%)	5 (1%)	86	94
1	C	627/627 (100%)	620 (99%)	7 (1%)	80	91
1	D	627/627 (100%)	621 (99%)	6 (1%)	82	92
1	E	627/627 (100%)	622 (99%)	5 (1%)	86	94
1	F	627/627 (100%)	624 (100%)	3 (0%)	92	96
1	G	627/627 (100%)	620 (99%)	7 (1%)	80	91
1	H	627/627 (100%)	622 (99%)	5 (1%)	86	94
1	I	627/627 (100%)	622 (99%)	5 (1%)	86	94
1	J	627/627 (100%)	620 (99%)	7 (1%)	80	91
1	W	627/627 (100%)	624 (100%)	3 (0%)	92	96
1	X	627/627 (100%)	623 (99%)	4 (1%)	90	95
2	K	116/116 (100%)	115 (99%)	1 (1%)	84	93
2	L	116/116 (100%)	115 (99%)	1 (1%)	84	93
2	M	116/116 (100%)	115 (99%)	1 (1%)	84	93
2	N	116/116 (100%)	115 (99%)	1 (1%)	84	93
2	O	116/116 (100%)	114 (98%)	2 (2%)	68	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	116/116 (100%)	116 (100%)	0	100	100
2	Q	116/116 (100%)	115 (99%)	1 (1%)	84	93
2	R	116/116 (100%)	115 (99%)	1 (1%)	84	93
2	S	116/116 (100%)	115 (99%)	1 (1%)	84	93
2	T	116/116 (100%)	115 (99%)	1 (1%)	84	93
2	U	116/116 (100%)	115 (99%)	1 (1%)	84	93
2	V	116/116 (100%)	116 (100%)	0	100	100
3	O	543/543 (100%)	540 (99%)	3 (1%)	90	95
3	Y	543/543 (100%)	542 (100%)	1 (0%)	95	97
3	Z	543/543 (100%)	542 (100%)	1 (0%)	95	97
All	All	10545/10545 (100%)	10467 (99%)	78 (1%)	89	94

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	VAL
1	A	156	VAL
1	A	360	GLU
1	A	369	TYR
1	A	389	LEU
1	B	123	VAL
1	B	246	TYR
1	B	255	ILE
1	B	360	GLU
1	B	444	LEU
1	C	80	TYR
1	C	84	ASP
1	C	123	VAL
1	C	161	ASN
1	C	360	GLU
1	C	472	TYR
1	C	476	ARG
1	D	123	VAL
1	D	156	VAL
1	D	317	GLU
1	D	360	GLU
1	D	389	LEU
1	D	565	VAL

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Mol	Chain	Res	Type
1	E	316	TYR
1	E	320	VAL
1	E	389	LEU
1	E	444	LEU
1	E	448	VAL
1	F	316	TYR
1	F	389	LEU
1	F	614	VAL
1	G	34	PHE
1	G	138	THR
1	G	156	VAL
1	G	250	ASP
1	G	281	ILE
1	G	360	GLU
1	G	476	ARG
1	H	157	ILE
1	H	316	TYR
1	H	360	GLU
1	H	517	TYR
1	H	561	ASP
1	I	150	HIS
1	I	246	TYR
1	I	297	HIS
1	I	360	GLU
1	I	708	LEU
1	J	98	TYR
1	J	123	VAL
1	J	360	GLU
1	J	389	LEU
1	J	469	ASN
1	J	475	PRO
1	J	492	LEU
2	K	47	ASP
2	L	123	LEU
2	M	104	TYR
2	N	35	THR
2	O	33	THR
2	O	82	HIS
2	Q	82	HIS
2	R	123	LEU
2	S	124	TYR
2	T	82	HIS

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Mol	Chain	Res	Type
2	U	82	HIS
1	W	317	GLU
1	W	360	GLU
1	W	389	LEU
1	X	89	ASP
1	X	248	LYS
1	X	316	TYR
1	X	360	GLU
3	Y	183	THR
3	Z	457	GLU
3	0	284	LEU
3	0	430	ASP
3	0	489	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
1	A	439	ASN
1	A	590	GLN
1	B	172	HIS
1	B	218	GLN
1	B	297	HIS
1	B	327	GLN
1	B	380	ASN
1	B	711	GLN
1	C	56	GLN
1	C	112	ASN
1	C	337	ASN
1	C	426	ASN
1	D	6	ASN
1	D	150	HIS
1	D	155	HIS
1	D	172	HIS
1	D	218	GLN
1	D	337	ASN
1	D	452	ASN
1	E	56	GLN
1	E	218	GLN
1	E	355	GLN
1	F	177	HIS
1	F	205	ASN

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Mol	Chain	Res	Type
1	F	355	GLN
1	F	530	GLN
1	F	610	GLN
1	G	6	ASN
1	G	56	GLN
1	G	104	HIS
1	G	150	HIS
1	G	172	HIS
1	G	182	ASN
1	G	337	ASN
1	H	135	GLN
1	H	327	GLN
1	H	337	ASN
1	H	619	GLN
1	I	105	ASN
1	J	172	HIS
1	J	297	HIS
1	J	469	ASN
2	M	82	HIS
2	M	153	ASN
2	N	147	ASN
2	O	82	HIS
2	O	95	ASN
2	P	94	HIS
2	R	82	HIS
2	R	94	HIS
2	S	94	HIS
2	T	82	HIS
2	T	153	ASN
2	U	82	HIS
1	W	150	HIS
1	W	161	ASN
1	W	172	HIS
1	W	297	HIS
1	W	327	GLN
1	X	104	HIS
1	X	172	HIS
1	X	205	ASN
3	Z	135	GLN
3	Z	212	ASN
3	Z	257	GLN
3	Z	548	ASN

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Mol	Chain	Res	Type
3	Z	611	HIS
3	0	274	HIS
3	0	582	ASN

5.3.3 RNA [i](#)

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.