Full wwPDB EM Validation Report ⓘ

Mar 29, 2022 – 04:10 pm BST

PDB ID	:	7QGQ
EMDB ID	:	EMD-13957
Title	:	Extended H/L (SLPH/SLPL) complex from C. difficile (CD630 strain) fit into R20291 S-layer negative stain map
Authors	:	Banerji, O.; Wilson, J.S.; Bullough, P.A.
Deposited on	:	2021-12-09
Resolution	:	Not provided

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

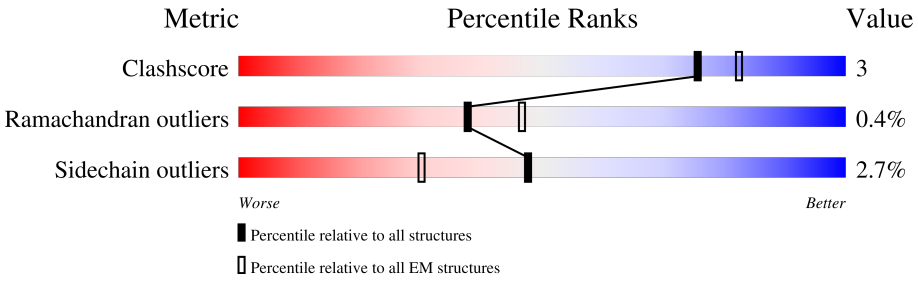
EMDB validation analysis	:	0.0.0.dev97
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON CRYSTALLOGRAPHY

The reported resolution of this entry is unknown.

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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=5%

Mol	Chain	Length	Quality of chain
1	B	373	93% 6% •
1	D	373	92% 7%
1	J	373	94% 5% •
1	K	373	93% 6% •
1	L	373	93% 6% •
1	M	373	94% 5% •
1	N	373	94% 5% •
1	T	373	92% 7%
1	U	373	91% 8% •

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Mol	Chain	Length	Quality of chain
1	V	373	91% 8%
1	W	373	92% 8%
1	X	373	90% 9%
2	A	318	88% 10%
2	C	318	90% 9%
2	E	318	84% 13%
2	F	318	88% 10%
2	G	318	85% 13%
2	H	318	88% 10%
2	I	318	89% 10%
2	O	318	93% 6%
2	P	318	88% 10%
2	Q	318	89% 8%
2	R	318	84% 14%
2	S	318	84% 14%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 124044 atoms, of which 62208 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 Precursor of the S-layer proteins.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	B	373	Total	C	H	N	O	S	0	0
			5562	1711	2795	457	594	5		
1	J	373	Total	C	H	N	O	S	0	0
			5562	1711	2795	457	594	5		
1	D	373	Total	C	H	N	O	S	0	0
			5562	1711	2795	457	594	5		
1	T	373	Total	C	H	N	O	S	0	0
			5562	1711	2795	457	594	5		
1	K	373	Total	C	H	N	O	S	0	0
			5562	1711	2795	457	594	5		
1	L	373	Total	C	H	N	O	S	0	0
			5562	1711	2795	457	594	5		
1	U	373	Total	C	H	N	O	S	0	0
			5562	1711	2795	457	594	5		
1	V	373	Total	C	H	N	O	S	0	0
			5562	1711	2795	457	594	5		
1	M	373	Total	C	H	N	O	S	0	0
			5562	1711	2795	457	594	5		
1	N	373	Total	C	H	N	O	S	0	0
			5562	1711	2795	457	594	5		
1	W	373	Total	C	H	N	O	S	0	0
			5562	1711	2795	457	594	5		
1	X	373	Total	C	H	N	O	S	0	0
			5562	1711	2795	457	594	5		

- Molecule 2 is a protein called Precursor of the S-layer proteins.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	318	Total	C	H	N	O	S	0	0
			4775	1490	2389	394	500	2		
2	O	318	Total	C	H	N	O	S	0	0
			4775	1490	2389	394	500	2		
2	A	318	Total	C	H	N	O	S	0	0
			4775	1490	2389	394	500	2		

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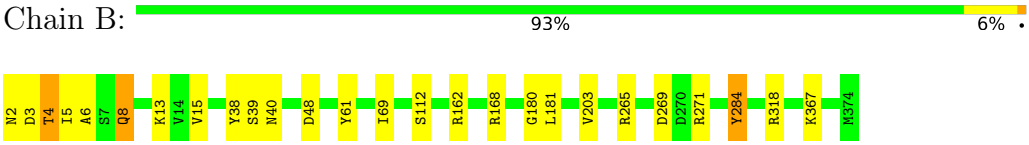
Mol	Chain	Residues	Atoms						AltConf	Trace
2	P	318	Total	C	H	N	O	S	0	0
			4775	1490	2389	394	500	2		
2	Q	318	Total	C	H	N	O	S	0	0
			4775	1490	2389	394	500	2		
2	E	318	Total	C	H	N	O	S	0	0
			4775	1490	2389	394	500	2		
2	F	318	Total	C	H	N	O	S	0	0
			4775	1490	2389	394	500	2		
2	R	318	Total	C	H	N	O	S	0	0
			4775	1490	2389	394	500	2		
2	S	318	Total	C	H	N	O	S	0	0
			4775	1490	2389	394	500	2		
2	G	318	Total	C	H	N	O	S	0	0
			4775	1490	2389	394	500	2		
2	H	318	Total	C	H	N	O	S	0	0
			4775	1490	2389	394	500	2		
2	I	318	Total	C	H	N	O	S	0	0
			4775	1490	2389	394	500	2		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

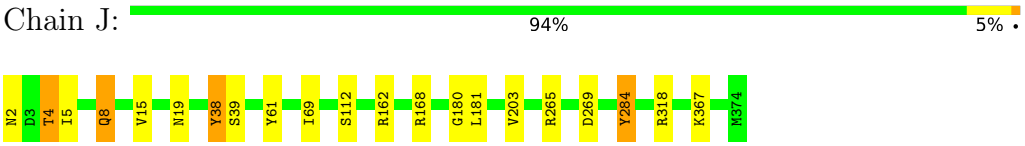
• Molecule 1: Precursor of the S-layer proteins

Chain B:



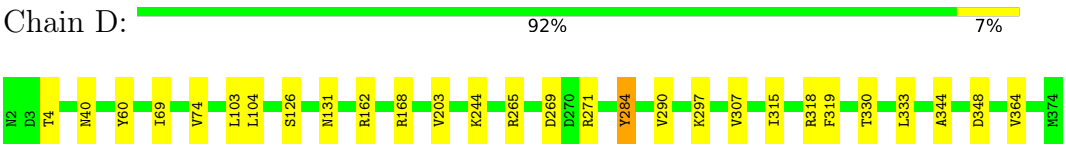
• Molecule 1: Precursor of the S-layer proteins

Chain J:



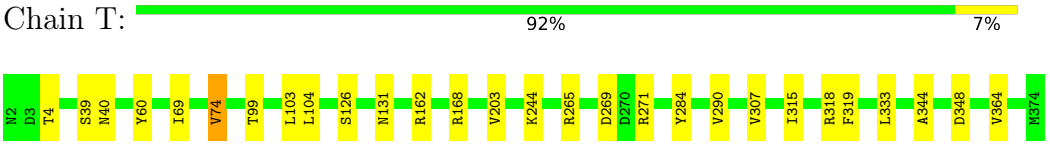
• Molecule 1: Precursor of the S-layer proteins

Chain D:



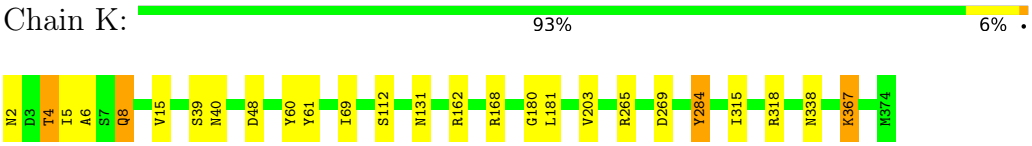
• Molecule 1: Precursor of the S-layer proteins

Chain T:



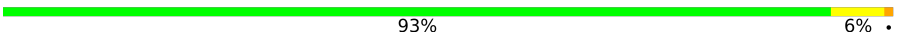
• Molecule 1: Precursor of the S-layer proteins

Chain K:



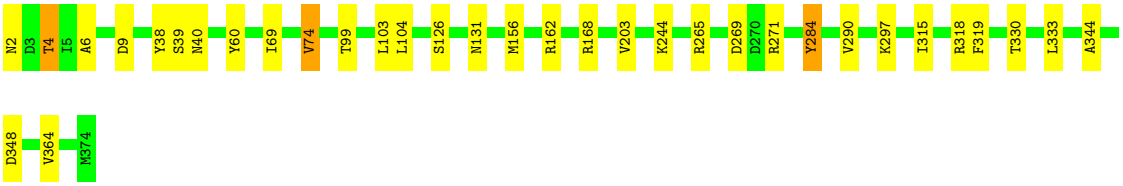
• Molecule 1: Precursor of the S-layer proteins

Chain L:



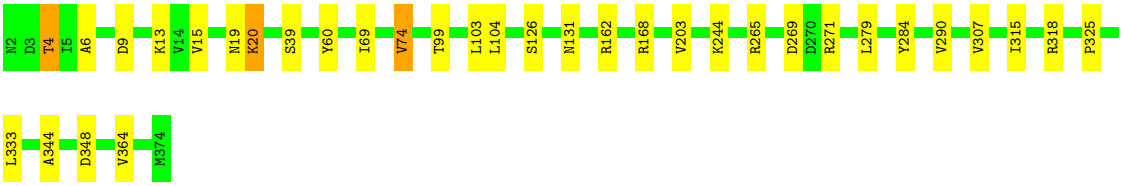
• Molecule 1: Precursor of the S-layer proteins

Chain U:



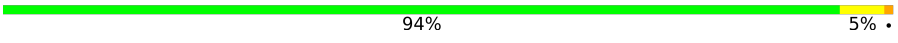
• Molecule 1: Precursor of the S-layer proteins

Chain V:



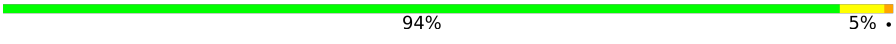
• Molecule 1: Precursor of the S-layer proteins

Chain M:



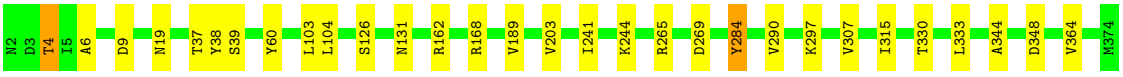
• Molecule 1: Precursor of the S-layer proteins

Chain N:



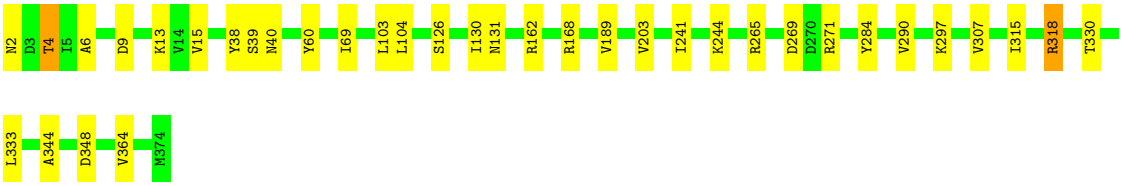
• Molecule 1: Precursor of the S-layer proteins

Chain W:



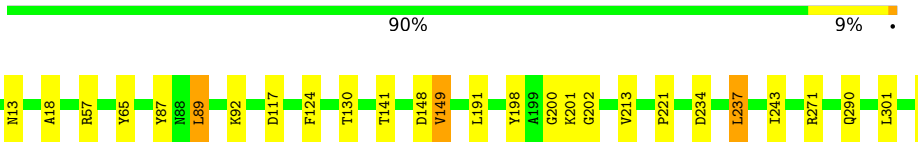
• Molecule 1: Precursor of the S-layer proteins

Chain X:



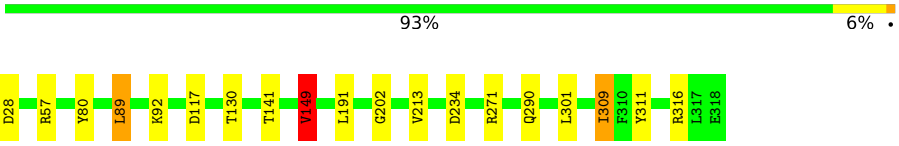
• Molecule 2: Precursor of the S-layer proteins

Chain C:



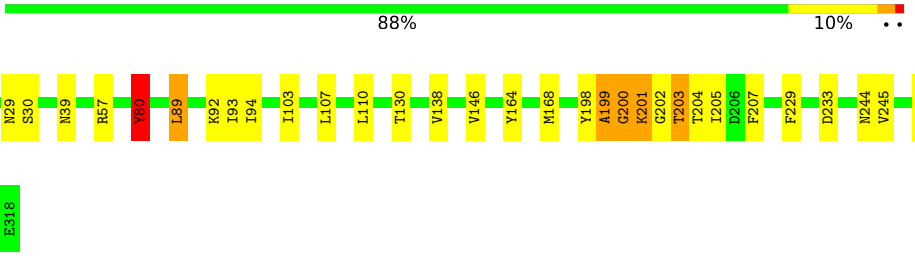
• Molecule 2: Precursor of the S-layer proteins

Chain O:



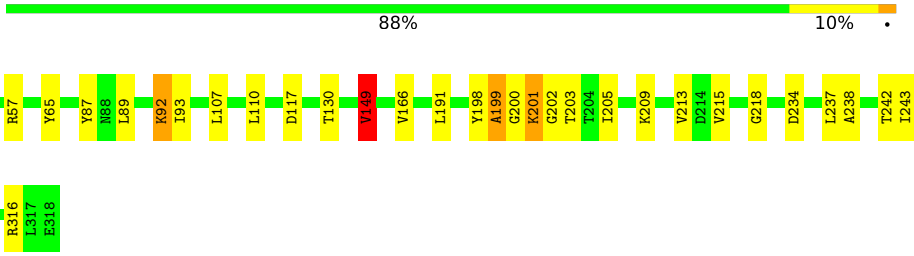
• Molecule 2: Precursor of the S-layer proteins

Chain A:



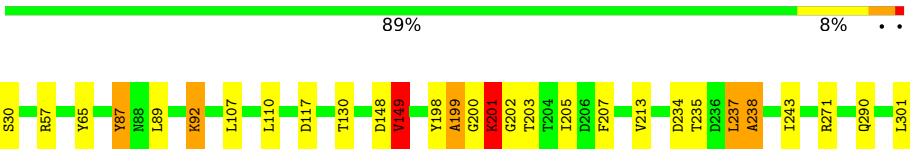
• Molecule 2: Precursor of the S-layer proteins

Chain P:



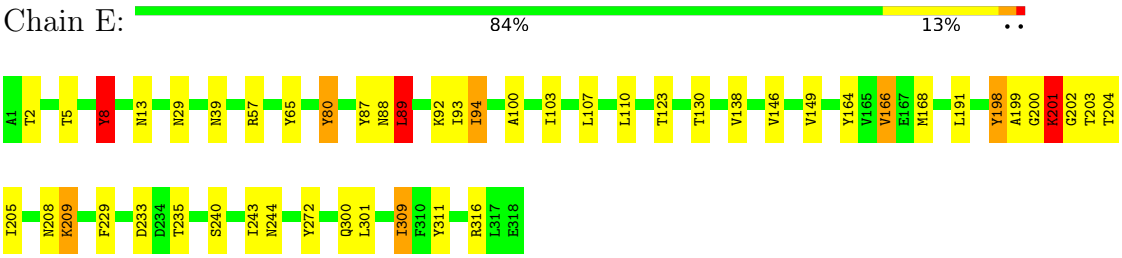
• Molecule 2: Precursor of the S-layer proteins

Chain Q:



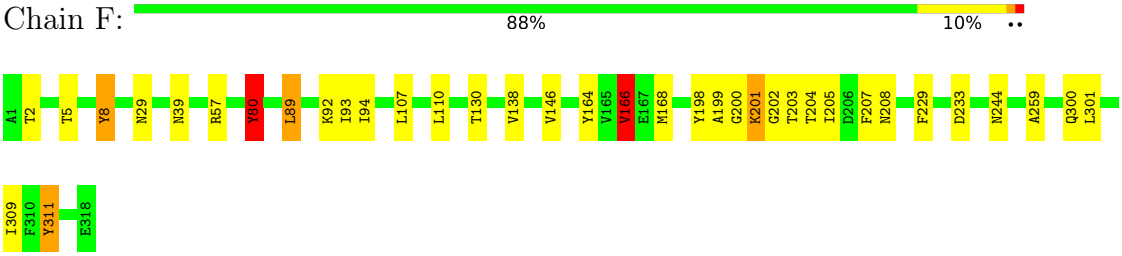
• Molecule 2: Precursor of the S-layer proteins

Chain E:



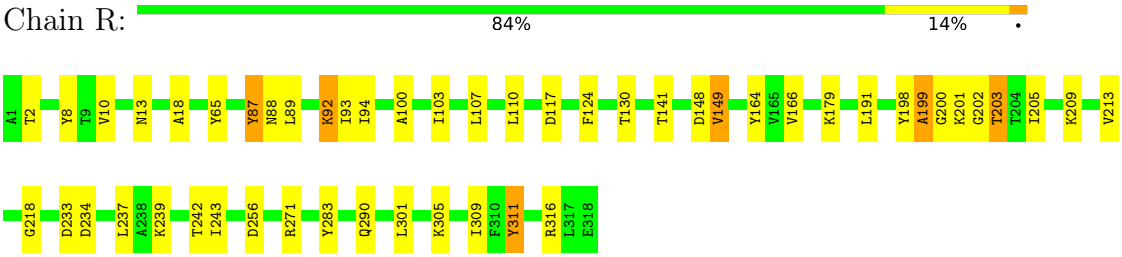
• Molecule 2: Precursor of the S-layer proteins

Chain F:



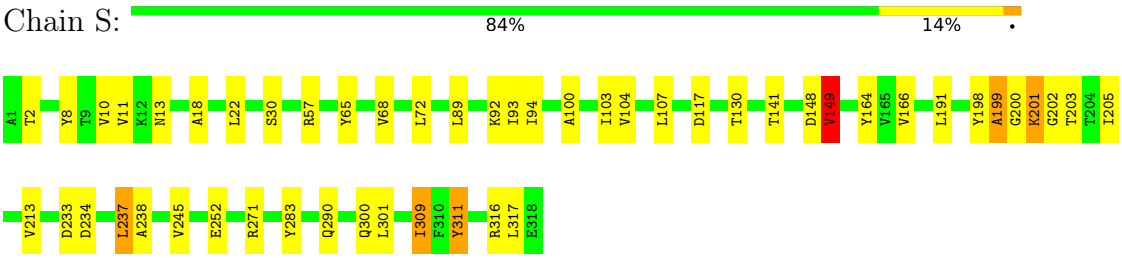
• Molecule 2: Precursor of the S-layer proteins

Chain R:



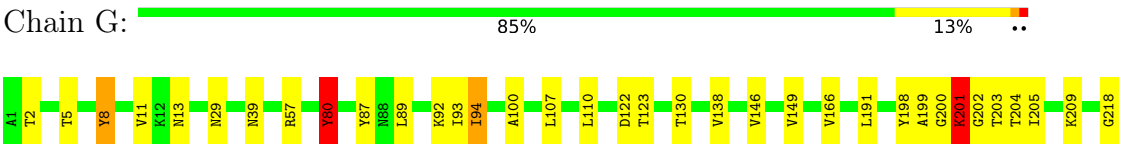
• Molecule 2: Precursor of the S-layer proteins

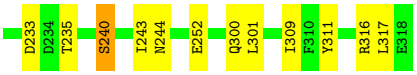
Chain S:



• Molecule 2: Precursor of the S-layer proteins

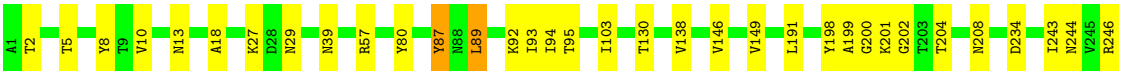
Chain G:

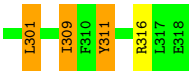




• Molecule 2: Precursor of the S-layer proteins

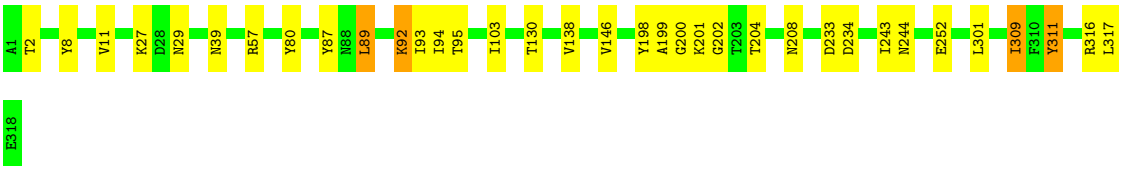
Chain H:





• Molecule 2: Precursor of the S-layer proteins

Chain I:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	CRYSTALLOGRAPHY	Depositor
Imposed symmetry	3D CRYSTAL, a=80 Å, b=80 Å, c=160 Å, α=90°, β=90°, γ=100°, space group=P 1 1 2	Depositor
Number of images used	Not provided	
Resolution determination method	DIFFRACTION PATTERN/LAYERLINES	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI/PHILIPS CM200FEG	Depositor
Voltage (kV)	200	Depositor
Electron dose (e^-/Å^2)	0.1	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	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	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	B	0.62	0/2790	1.10	13/3774 (0.3%)
1	D	0.61	0/2790	1.04	10/3774 (0.3%)
1	J	0.61	0/2790	1.06	9/3774 (0.2%)
1	K	0.61	0/2790	1.08	13/3774 (0.3%)
1	L	0.61	0/2790	1.05	10/3774 (0.3%)
1	M	0.62	0/2790	1.08	13/3774 (0.3%)
1	N	0.63	0/2790	1.08	12/3774 (0.3%)
1	T	0.60	0/2790	1.01	8/3774 (0.2%)
1	U	0.60	0/2790	1.04	12/3774 (0.3%)
1	V	0.60	0/2790	1.03	10/3774 (0.3%)
1	W	0.61	0/2790	1.05	10/3774 (0.3%)
1	X	0.61	0/2790	1.07	12/3774 (0.3%)
2	A	0.65	0/2412	1.15	11/3261 (0.3%)
2	C	0.63	0/2412	1.03	7/3261 (0.2%)
2	E	0.65	0/2412	1.18	20/3261 (0.6%)
2	F	0.63	0/2412	1.12	9/3261 (0.3%)
2	G	0.65	0/2412	1.15	11/3261 (0.3%)
2	H	0.64	0/2412	1.06	8/3261 (0.2%)
2	I	0.64	0/2412	1.05	7/3261 (0.2%)
2	O	0.63	0/2412	1.03	6/3261 (0.2%)
2	P	0.66	0/2412	1.14	11/3261 (0.3%)
2	Q	0.64	0/2412	1.11	11/3261 (0.3%)
2	R	0.66	0/2412	1.17	13/3261 (0.4%)
2	S	0.65	0/2412	1.14	11/3261 (0.3%)
All	All	0.63	0/62424	1.08	257/84420 (0.3%)

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	B	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	J	0	2
1	K	0	1
1	L	0	1
1	M	0	1
1	T	0	1
1	U	0	1
2	A	0	4
2	C	0	4
2	E	0	3
2	F	0	3
2	G	0	2
2	H	0	3
2	I	0	2
2	O	0	2
2	P	0	1
2	Q	0	2
2	R	0	2
2	S	0	2
All	All	0	39

There are no bond length outliers.

All (257) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	R	199	ALA	CB-CA-C	12.01	128.11	110.10
1	N	265	ARG	NE-CZ-NH2	-11.42	114.59	120.30
1	N	265	ARG	NE-CZ-NH1	10.94	125.77	120.30
2	S	199	ALA	CB-CA-C	10.84	126.37	110.10
1	L	265	ARG	NE-CZ-NH1	10.83	125.71	120.30
1	J	265	ARG	NE-CZ-NH1	10.31	125.46	120.30
1	M	40	ASN	N-CA-C	10.12	138.31	111.00
1	M	265	ARG	NE-CZ-NH1	9.98	125.29	120.30
1	L	265	ARG	NE-CZ-NH2	-9.77	115.41	120.30
1	K	265	ARG	NE-CZ-NH1	9.76	125.18	120.30
1	K	265	ARG	NE-CZ-NH2	-9.45	115.57	120.30
1	K	40	ASN	N-CA-C	9.21	135.85	111.00
2	I	57	ARG	NE-CZ-NH1	9.18	124.89	120.30
1	N	40	ASN	N-CA-C	9.16	135.75	111.00
2	A	199	ALA	CB-CA-C	9.14	123.81	110.10
1	U	265	ARG	NE-CZ-NH1	9.01	124.81	120.30
2	P	199	ALA	CB-CA-C	8.87	123.40	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	265	ARG	NE-CZ-NH2	-8.81	115.90	120.30
1	D	40	ASN	N-CA-C	8.78	134.71	111.00
1	B	265	ARG	NE-CZ-NH1	8.75	124.68	120.30
1	V	265	ARG	NE-CZ-NH1	8.63	124.62	120.30
2	Q	199	ALA	CB-CA-C	8.59	122.99	110.10
2	P	8	TYR	CB-CG-CD2	-8.58	115.85	121.00
2	A	199	ALA	N-CA-CB	-8.53	98.16	110.10
2	A	8	TYR	CB-CG-CD2	-8.50	115.90	121.00
1	X	265	ARG	NE-CZ-NH1	8.46	124.53	120.30
2	S	271	ARG	NE-CZ-NH1	8.37	124.48	120.30
1	U	39	SER	N-CA-C	8.34	133.52	111.00
1	X	40	ASN	N-CA-C	8.27	133.32	111.00
1	B	40	ASN	N-CA-C	8.21	133.16	111.00
1	T	265	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	M	265	ARG	NE-CZ-NH2	-8.17	116.21	120.30
1	W	39	SER	N-CA-C	8.17	133.06	111.00
1	D	265	ARG	NE-CZ-NH1	8.10	124.35	120.30
2	S	316	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	X	39	SER	N-CA-C	8.09	132.83	111.00
1	B	4	THR	OG1-CB-CG2	-8.03	91.52	110.00
1	J	265	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	B	39	SER	N-CA-C	8.01	132.63	111.00
1	M	168	ARG	NE-CZ-NH1	7.98	124.29	120.30
1	T	39	SER	N-CA-C	7.96	132.48	111.00
2	Q	316	ARG	NE-CZ-NH1	7.89	124.25	120.30
2	A	57	ARG	NE-CZ-NH1	7.86	124.23	120.30
2	E	316	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	K	168	ARG	NE-CZ-NH1	7.73	124.17	120.30
2	E	198	TYR	CB-CG-CD1	-7.67	116.40	121.00
2	S	199	ALA	N-CA-CB	-7.64	99.40	110.10
2	F	233	ASP	CB-CA-C	7.64	125.68	110.40
1	B	162	ARG	NE-CZ-NH1	7.63	124.11	120.30
1	L	168	ARG	NE-CZ-NH1	7.61	124.11	120.30
2	P	316	ARG	NE-CZ-NH1	7.56	124.08	120.30
2	C	316	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	V	39	SER	N-CA-C	7.49	131.23	111.00
1	X	162	ARG	NE-CZ-NH1	7.48	124.04	120.30
2	R	199	ALA	N-CA-CB	-7.47	99.64	110.10
1	W	265	ARG	NE-CZ-NH1	7.47	124.04	120.30
2	F	57	ARG	NE-CZ-NH1	7.44	124.02	120.30
2	R	271	ARG	NE-CZ-NH1	7.42	124.01	120.30
2	P	271	ARG	NE-CZ-NH1	7.41	124.00	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	4	THR	OG1-CB-CG2	-7.40	92.98	110.00
2	H	57	ARG	NE-CZ-NH1	7.39	124.00	120.30
2	O	316	ARG	NE-CZ-NH1	7.33	123.96	120.30
1	V	162	ARG	NE-CZ-NH1	7.32	123.96	120.30
2	G	80	TYR	CB-CG-CD2	-7.31	116.61	121.00
1	J	168	ARG	NE-CZ-NH1	7.29	123.94	120.30
2	O	271	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	M	39	SER	N-CA-C	7.25	130.57	111.00
2	A	233	ASP	CB-CA-C	7.24	124.88	110.40
1	M	40	ASN	CA-C-N	7.20	133.05	117.20
2	G	233	ASP	CB-CA-C	7.13	124.66	110.40
1	J	39	SER	N-CA-C	7.12	130.21	111.00
1	M	162	ARG	NE-CZ-NH1	7.08	123.84	120.30
2	G	316	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	X	168	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	D	162	ARG	NE-CZ-NH1	6.98	123.79	120.30
2	E	80	TYR	CB-CG-CD2	-6.98	116.81	121.00
2	P	203	THR	CA-CB-CG2	6.98	122.17	112.40
1	V	271	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	T	162	ARG	NE-CZ-NH1	6.90	123.75	120.30
2	Q	203	THR	CA-CB-CG2	6.89	122.05	112.40
1	W	39	SER	N-CA-CB	-6.88	100.18	110.50
1	W	168	ARG	NE-CZ-NH1	6.84	123.72	120.30
2	F	94	ILE	CB-CA-C	6.83	125.26	111.60
1	N	40	ASN	CA-C-N	6.81	132.19	117.20
2	S	65	TYR	CB-CG-CD1	-6.81	116.91	121.00
1	M	39	SER	N-CA-CB	-6.77	100.35	110.50
1	X	39	SER	N-CA-CB	-6.73	100.41	110.50
2	C	65	TYR	CB-CG-CD1	-6.72	116.97	121.00
1	K	162	ARG	NE-CZ-NH1	6.71	123.65	120.30
1	U	265	ARG	NE-CZ-NH2	-6.71	116.95	120.30
1	V	168	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	X	4	THR	OG1-CB-CG2	-6.68	94.63	110.00
1	B	39	SER	N-CA-CB	-6.67	100.50	110.50
1	K	39	SER	N-CA-CB	-6.65	100.52	110.50
1	U	168	ARG	NE-CZ-NH1	6.65	123.63	120.30
2	O	57	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	T	39	SER	N-CA-CB	-6.65	100.52	110.50
1	U	39	SER	N-CA-CB	-6.65	100.53	110.50
1	N	39	SER	N-CA-CB	-6.64	100.53	110.50
2	Q	271	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	B	271	ARG	NE-CZ-NH1	6.61	123.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	40	ASN	CA-C-N	6.61	131.74	117.20
1	W	4	THR	OG1-CB-CG2	-6.58	94.85	110.00
2	E	8	TYR	CB-CG-CD1	-6.58	117.05	121.00
2	F	80	TYR	CB-CG-CD2	-6.58	117.05	121.00
1	K	39	SER	N-CA-C	6.57	128.74	111.00
1	V	39	SER	N-CA-CB	-6.57	100.65	110.50
1	X	271	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	U	4	THR	OG1-CB-CG2	-6.51	95.02	110.00
1	N	162	ARG	NE-CZ-NH1	6.50	123.55	120.30
2	Q	65	TYR	CB-CG-CD1	-6.46	117.13	121.00
1	J	162	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	L	40	ASN	N-CA-C	6.43	128.36	111.00
2	P	65	TYR	CB-CG-CD1	-6.42	117.15	121.00
2	G	94	ILE	CB-CA-C	6.42	124.44	111.60
1	J	4	THR	OG1-CB-CG2	-6.41	95.25	110.00
2	E	57	ARG	NE-CZ-NH1	6.41	123.50	120.30
2	R	316	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	N	39	SER	N-CA-C	6.34	128.13	111.00
1	U	162	ARG	NE-CZ-NH1	6.32	123.46	120.30
2	E	233	ASP	CB-CA-C	6.31	123.02	110.40
1	T	40	ASN	N-CA-C	6.30	128.01	111.00
2	Q	8	TYR	CB-CG-CD1	-6.29	117.23	121.00
1	M	40	ASN	N-CA-CB	-6.29	99.29	110.60
1	X	265	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	J	39	SER	N-CA-CB	-6.25	101.13	110.50
2	H	89	LEU	CB-CG-CD2	6.23	121.59	111.00
1	L	39	SER	N-CA-C	6.22	127.80	111.00
1	M	40	ASN	O-C-N	-6.20	112.77	122.70
1	L	162	ARG	NE-CZ-NH1	6.20	123.40	120.30
2	P	57	ARG	NE-CZ-NH1	6.18	123.39	120.30
2	E	272	TYR	CB-CG-CD2	-6.17	117.30	121.00
1	X	39	SER	CA-C-N	6.17	130.76	117.20
2	E	65	TYR	CB-CG-CD1	-6.16	117.31	121.00
2	I	89	LEU	CB-CG-CD2	6.14	121.44	111.00
1	N	168	ARG	NE-CZ-NH1	6.13	123.37	120.30
2	S	149	VAL	CG1-CB-CG2	-6.12	101.11	110.90
2	A	80	TYR	CB-CG-CD2	-6.12	117.33	121.00
2	S	203	THR	CA-CB-CG2	6.12	120.96	112.40
2	E	94	ILE	CB-CA-C	6.11	123.81	111.60
1	K	40	ASN	N-CA-CB	-6.06	99.69	110.60
2	E	209	LYS	CA-CB-CG	-6.06	100.06	113.40
1	U	271	ARG	NE-CZ-NH1	6.06	123.33	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	S	283	TYR	CB-CG-CD1	-6.05	117.37	121.00
1	D	271	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	M	39	SER	CA-C-N	6.05	130.50	117.20
1	K	40	ASN	CA-C-N	6.03	130.46	117.20
1	W	162	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	B	39	SER	CA-C-N	5.99	130.38	117.20
2	R	283	TYR	CB-CG-CD1	-5.98	117.41	121.00
2	G	316	ARG	CD-NE-CZ	5.98	131.97	123.60
1	T	271	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	L	39	SER	N-CA-CB	-5.93	101.60	110.50
2	Q	149	VAL	CG1-CB-CG2	-5.92	101.43	110.90
1	D	284	TYR	CB-CG-CD2	-5.88	117.47	121.00
1	B	284	TYR	CB-CG-CD2	-5.87	117.48	121.00
2	R	110	LEU	CB-CG-CD2	-5.87	101.03	111.00
2	R	65	TYR	CB-CG-CD1	-5.86	117.49	121.00
2	R	203	THR	CA-CB-CG2	5.85	120.60	112.40
1	B	168	ARG	NE-CZ-NH1	5.85	123.22	120.30
2	C	271	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	U	39	SER	CA-C-N	5.84	130.05	117.20
2	G	201	LYS	C-N-CA	5.80	134.48	122.30
1	N	40	ASN	O-C-N	-5.79	113.44	122.70
2	C	57	ARG	NE-CZ-NH1	5.75	123.17	120.30
2	E	201	LYS	C-N-CA	5.73	134.33	122.30
1	N	39	SER	CA-C-N	5.72	129.78	117.20
1	W	265	ARG	NE-CZ-NH2	-5.70	117.45	120.30
2	G	240	SER	CB-CA-C	5.69	120.92	110.10
1	V	4	THR	OG1-CB-CG2	-5.69	96.91	110.00
1	U	40	ASN	N-CA-C	5.68	126.35	111.00
2	S	233	ASP	CB-CA-C	5.68	121.76	110.40
2	F	57	ARG	CD-NE-CZ	5.67	131.54	123.60
2	O	80	TYR	CB-CG-CD2	-5.67	117.60	121.00
1	D	168	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	L	4	THR	OG1-CB-CG2	-5.65	97.00	110.00
1	V	265	ARG	NE-CZ-NH2	-5.65	117.48	120.30
2	I	92	LYS	CB-CG-CD	5.63	126.24	111.60
2	H	94	ILE	CB-CA-C	5.63	122.86	111.60
1	T	168	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	K	284	TYR	CB-CG-CD2	-5.59	117.65	121.00
1	U	284	TYR	CB-CG-CD2	-5.58	117.65	121.00
1	N	40	ASN	N-CA-CB	-5.58	100.56	110.60
2	G	57	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	T	39	SER	CA-C-N	5.57	129.45	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	149	VAL	CG1-CB-CG2	-5.56	102.00	110.90
2	A	89	LEU	CB-CG-CD2	5.56	120.45	111.00
2	O	149	VAL	CG1-CB-CG2	-5.55	102.01	110.90
2	A	164	TYR	N-CA-C	-5.55	96.00	111.00
2	A	316	ARG	NE-CZ-NH1	5.55	123.08	120.30
2	R	164	TYR	N-CA-C	-5.55	96.02	111.00
1	D	40	ASN	O-C-N	-5.54	113.83	122.70
2	H	316	ARG	NE-CZ-NH1	5.53	123.06	120.30
2	R	8	TYR	CB-CG-CD2	-5.51	117.69	121.00
2	S	164	TYR	N-CA-C	-5.51	96.12	111.00
2	R	92	LYS	CB-CG-CD	5.49	125.88	111.60
2	E	110	LEU	CB-CG-CD2	-5.49	101.67	111.00
2	I	94	ILE	CB-CA-C	5.47	122.53	111.60
2	F	8	TYR	CB-CG-CD1	-5.46	117.72	121.00
2	G	316	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	D	265	ARG	NE-CZ-NH2	-5.45	117.58	120.30
2	E	164	TYR	N-CA-C	-5.45	96.29	111.00
1	K	39	SER	CA-C-N	5.45	129.18	117.20
2	I	57	ARG	CD-NE-CZ	5.44	131.22	123.60
2	E	166	VAL	CA-CB-CG2	5.42	119.03	110.90
2	E	316	ARG	CD-NE-CZ	5.42	131.18	123.60
2	H	316	ARG	CD-NE-CZ	5.39	131.15	123.60
1	W	284	TYR	CB-CG-CD2	-5.38	117.77	121.00
1	B	40	ASN	CA-C-N	5.38	129.03	117.20
2	Q	57	ARG	CD-NE-CZ	5.38	131.13	123.60
2	H	57	ARG	CD-NE-CZ	5.37	131.12	123.60
2	H	92	LYS	CB-CG-CD	5.37	125.55	111.60
2	E	203	THR	N-CA-CB	-5.36	100.11	110.30
2	R	256	ASP	CB-CG-OD2	5.35	123.12	118.30
2	F	89	LEU	CB-CG-CD2	5.35	120.10	111.00
2	C	237	LEU	CB-CA-C	5.35	120.36	110.20
2	A	271	ARG	NE-CZ-NH2	5.34	122.97	120.30
2	A	203	THR	N-CA-CB	-5.34	100.16	110.30
2	E	89	LEU	CB-CG-CD2	5.34	120.07	111.00
2	C	89	LEU	CB-CG-CD2	5.33	120.05	111.00
1	U	104	LEU	CB-CG-CD2	-5.31	101.97	111.00
2	G	110	LEU	CB-CA-C	-5.27	100.19	110.20
1	X	318	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	D	40	ASN	N-CA-CB	-5.25	101.15	110.60
2	Q	92	LYS	CB-CG-CD	5.25	125.26	111.60
2	E	233	ASP	N-CA-CB	-5.24	101.17	110.60
2	Q	87	TYR	CB-CG-CD1	-5.23	117.86	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	W	39	SER	CA-C-N	5.23	128.71	117.20
2	E	87	TYR	CB-CG-CD2	-5.22	117.86	121.00
1	V	20	LYS	CA-CB-CG	5.22	124.88	113.40
1	X	40	ASN	CA-C-N	5.19	128.62	117.20
2	I	233	ASP	CB-CA-C	5.18	120.76	110.40
2	P	110	LEU	CB-CG-CD2	-5.18	102.20	111.00
1	B	4	THR	CA-CB-CG2	5.14	119.59	112.40
1	V	39	SER	CA-C-N	5.13	128.49	117.20
1	K	40	ASN	O-C-N	-5.13	114.49	122.70
2	H	87	TYR	CB-CG-CD2	-5.13	117.92	121.00
2	P	92	LYS	CB-CG-CD	5.12	124.92	111.60
2	F	164	TYR	N-CA-C	-5.12	97.19	111.00
1	N	284	TYR	CB-CG-CD2	-5.11	117.93	121.00
1	L	20	LYS	CA-CB-CG	5.10	124.62	113.40
2	C	92	LYS	CB-CG-CD	5.09	124.84	111.60
2	P	316	ARG	CD-NE-CZ	5.09	130.73	123.60
2	F	166	VAL	CG1-CB-CG2	5.09	119.04	110.90
2	S	57	ARG	CD-NE-CZ	5.09	130.73	123.60
1	M	60	TYR	CB-CG-CD1	-5.08	117.95	121.00
1	J	39	SER	CA-C-N	5.08	128.37	117.20
2	G	110	LEU	CB-CG-CD2	-5.07	102.38	111.00
1	M	284	TYR	CB-CG-CD2	-5.06	117.97	121.00
2	Q	201	LYS	C-N-CA	5.05	132.90	122.30
1	L	284	TYR	CB-CG-CD2	-5.04	117.97	121.00
2	I	316	ARG	NE-CZ-NH1	5.04	122.82	120.30
2	R	233	ASP	CB-CA-C	5.02	120.44	110.40
1	W	37	THR	N-CA-C	5.02	124.56	111.00
2	O	89	LEU	CB-CG-CD2	5.01	119.52	111.00
2	E	89	LEU	CB-CA-C	5.01	119.71	110.20
1	J	284	TYR	CB-CG-CD2	-5.01	118.00	121.00

There are no chirality outliers.

All (39) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	200	GLY	Mainchain
2	A	311	TYR	Sidechain
2	A	8	TYR	Sidechain
2	A	80	TYR	Sidechain
1	B	61	TYR	Sidechain
2	C	311	TYR	Sidechain
2	C	316	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	C	8	TYR	Sidechain
2	C	87	TYR	Sidechain
1	D	319	PHE	Sidechain
2	E	311	TYR	Sidechain
2	E	8	TYR	Sidechain
2	E	89	LEU	Mainchain
2	F	311	TYR	Sidechain
2	F	8	TYR	Sidechain
2	F	80	TYR	Sidechain
2	G	8	TYR	Sidechain
2	G	80	TYR	Sidechain
2	H	246	ARG	Sidechain
2	H	311	TYR	Sidechain
2	H	8	TYR	Sidechain
2	I	311	TYR	Sidechain
2	I	8	TYR	Sidechain
1	J	38	TYR	Sidechain
1	J	61	TYR	Sidechain
1	K	61	TYR	Sidechain
1	L	61	TYR	Sidechain
1	M	61	TYR	Sidechain
2	O	311	TYR	Sidechain
2	O	8	TYR	Sidechain
2	P	8	TYR	Sidechain
2	Q	311	TYR	Sidechain
2	Q	8	TYR	Sidechain
2	R	311	TYR	Sidechain
2	R	87	TYR	Sidechain
2	S	311	TYR	Sidechain
2	S	8	TYR	Sidechain
1	T	319	PHE	Sidechain
1	U	319	PHE	Sidechain

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	B	2767	2795	2792	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2767	2795	2792	9	0
1	J	2767	2795	2792	17	0
1	K	2767	2795	2792	17	0
1	L	2767	2795	2792	16	0
1	M	2767	2795	2792	11	0
1	N	2767	2795	2792	12	0
1	T	2767	2795	2792	10	0
1	U	2767	2795	2792	17	0
1	V	2767	2795	2792	22	0
1	W	2767	2795	2792	13	0
1	X	2767	2795	2792	19	0
2	A	2386	2389	2389	36	0
2	C	2386	2389	2389	11	0
2	E	2386	2389	2389	41	0
2	F	2386	2389	2389	28	0
2	G	2386	2389	2389	37	0
2	H	2386	2389	2389	22	0
2	I	2386	2389	2389	17	0
2	O	2386	2389	2389	4	0
2	P	2386	2389	2389	24	0
2	Q	2386	2389	2389	25	0
2	R	2386	2389	2389	36	0
2	S	2386	2389	2389	31	0
All	All	61836	62208	62172	384	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 3.

All (384) 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:P:237:LEU:HD13	2:P:243:ILE:HG22	1.51	0.89
2:S:309:ILE:HD13	1:X:4:THR:H	1.45	0.80
1:B:4:THR:H	2:A:309:ILE:HD13	1.47	0.79
1:K:4:THR:H	2:F:309:ILE:HD13	1.49	0.78
2:Q:309:ILE:HD13	1:U:4:THR:H	1.49	0.77
2:R:218:GLY:HA3	2:G:240:SER:HB3	1.67	0.75
2:R:237:LEU:HD13	2:R:243:ILE:HG22	1.70	0.72
1:J:4:THR:H	2:E:309:ILE:HD13	1.55	0.71
2:E:92:LYS:HD3	2:E:202:GLY:H	1.53	0.71
1:L:4:THR:H	2:G:309:ILE:HD13	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:92:LYS:HD3	2:G:202:GLY:H	1.59	0.67
2:A:107:LEU:HD21	2:A:205:ILE:HD13	1.76	0.67
2:G:198:TYR:CZ	2:G:200:GLY:HA2	2.30	0.67
1:B:8:GLN:HG2	2:A:80:TYR:CE1	2.31	0.66
2:A:89:LEU:HD22	2:A:202:GLY:HA3	1.77	0.65
1:T:290:VAL:CG1	1:T:344:ALA:HB1	2.27	0.65
1:J:19:ASN:HB3	1:V:19:ASN:CB	2.25	0.65
1:X:290:VAL:CG1	1:X:344:ALA:HB1	2.25	0.65
1:D:290:VAL:CG1	1:D:344:ALA:HB1	2.27	0.65
1:V:290:VAL:CG1	1:V:344:ALA:HB1	2.26	0.64
2:P:198:TYR:CZ	2:P:200:GLY:HA2	2.32	0.64
2:E:107:LEU:HD21	2:E:205:ILE:HD13	1.79	0.64
2:F:198:TYR:CZ	2:F:200:GLY:HA2	2.32	0.64
2:P:309:ILE:HD13	1:V:4:THR:H	1.61	0.64
2:F:92:LYS:HD3	2:F:202:GLY:H	1.61	0.64
1:L:4:THR:HG22	2:G:309:ILE:CD1	2.28	0.64
2:A:110:LEU:HD11	2:A:207:PHE:CD1	2.33	0.64
2:R:107:LEU:HD21	2:R:205:ILE:HD13	1.80	0.63
2:R:198:TYR:CZ	2:R:200:GLY:HA2	2.33	0.63
2:A:8:TYR:CD2	2:A:245:VAL:HG22	2.33	0.63
1:L:8:GLN:HG2	2:G:80:TYR:CE1	2.34	0.63
1:U:290:VAL:CG1	1:U:344:ALA:HB1	2.29	0.62
2:S:198:TYR:CZ	2:S:200:GLY:HA2	2.34	0.62
2:A:198:TYR:CZ	2:A:200:GLY:HA2	2.34	0.62
2:H:89:LEU:HD22	2:H:202:GLY:HA3	1.82	0.61
2:P:87:TYR:CE1	2:P:243:ILE:HG23	2.34	0.61
2:C:237:LEU:HD13	2:C:243:ILE:HG22	1.82	0.61
2:Q:311:TYR:CG	1:U:6:ALA:HB2	2.34	0.61
1:K:8:GLN:HG2	2:F:80:TYR:CE1	2.36	0.61
2:P:309:ILE:CD1	1:V:4:THR:HG22	2.31	0.61
2:E:93:ILE:C	2:E:199:ALA:HB1	2.20	0.61
2:R:218:GLY:HA3	2:G:240:SER:CB	2.31	0.61
2:Q:198:TYR:CZ	2:Q:200:GLY:HA2	2.35	0.60
2:G:89:LEU:HD22	2:G:202:GLY:HA3	1.84	0.60
1:B:8:GLN:HG2	2:A:80:TYR:CD1	2.37	0.60
2:E:198:TYR:CZ	2:E:200:GLY:HA2	2.36	0.60
2:Q:237:LEU:HD13	2:Q:243:ILE:HG22	1.83	0.60
1:K:8:GLN:HG2	2:F:80:TYR:CD1	2.36	0.60
1:L:8:GLN:HG2	2:G:80:TYR:CD1	2.36	0.60
2:S:10:VAL:HG21	2:S:18:ALA:HB1	1.83	0.60
2:S:309:ILE:HD13	1:X:4:THR:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:89:LEU:HD22	2:F:202:GLY:HA3	1.84	0.59
1:N:69:ILE:HD12	1:N:318:ARG:HB2	1.84	0.59
1:J:8:GLN:HG2	2:E:80:TYR:CE1	2.38	0.59
1:M:5:ILE:HD11	2:H:244:ASN:HB2	1.84	0.59
1:J:8:GLN:HG2	2:E:80:TYR:CD1	2.38	0.58
2:F:39:ASN:HA	2:F:80:TYR:CE1	2.38	0.58
2:I:89:LEU:HD22	2:I:202:GLY:HA3	1.84	0.58
2:R:309:ILE:HD13	1:W:4:THR:H	1.68	0.58
1:J:19:ASN:HB3	1:V:19:ASN:HB3	1.85	0.58
1:W:290:VAL:CG1	1:W:344:ALA:HB1	2.33	0.58
2:S:311:TYR:CG	1:X:6:ALA:HB2	2.38	0.58
2:A:94:ILE:CD1	2:A:103:ILE:HD12	2.34	0.58
2:I:198:TYR:CZ	2:I:200:GLY:HA2	2.40	0.57
2:S:237:LEU:HD23	2:S:238:ALA:H	1.68	0.57
1:W:333:LEU:CD1	1:W:364:VAL:HG13	2.35	0.57
1:X:333:LEU:CD1	1:X:364:VAL:HG13	2.34	0.57
2:A:110:LEU:HD11	2:A:207:PHE:HD1	1.69	0.57
2:G:107:LEU:HD21	2:G:205:ILE:HD13	1.87	0.57
1:T:333:LEU:CD1	1:T:364:VAL:HG13	2.35	0.57
2:G:166:VAL:HG22	2:G:198:TYR:O	2.03	0.56
2:H:198:TYR:CZ	2:H:200:GLY:HA2	2.40	0.56
2:A:93:ILE:HA	2:A:199:ALA:HB1	1.86	0.56
2:P:107:LEU:HD21	2:P:205:ILE:HD13	1.86	0.56
2:E:166:VAL:HG22	2:E:198:TYR:O	2.05	0.56
1:J:4:THR:HG22	2:E:309:ILE:CD1	2.36	0.56
1:D:333:LEU:CD1	1:D:364:VAL:HG13	2.35	0.56
1:T:203:VAL:HG11	1:T:284:TYR:CD1	2.40	0.56
2:R:93:ILE:HA	2:R:199:ALA:HB1	1.88	0.56
2:A:39:ASN:HA	2:A:80:TYR:CE1	2.41	0.55
1:N:4:THR:H	2:I:309:ILE:HD13	1.71	0.55
2:G:39:ASN:HA	2:G:80:TYR:CE1	2.41	0.55
1:M:8:GLN:HG2	2:H:80:TYR:CD1	2.42	0.55
2:H:93:ILE:HA	2:H:199:ALA:HB1	1.89	0.55
1:B:6:ALA:HB2	2:A:311:TYR:CG	2.41	0.55
1:T:69:ILE:HG13	1:T:318:ARG:HB2	1.88	0.55
1:V:333:LEU:CD1	1:V:364:VAL:HG13	2.37	0.55
2:P:89:LEU:HD13	2:P:202:GLY:O	2.07	0.54
1:B:2:ASN:HA	2:A:300:GLN:NE2	2.22	0.54
1:V:290:VAL:HG11	1:V:344:ALA:HB1	1.89	0.54
1:X:290:VAL:HG11	1:X:344:ALA:HB1	1.89	0.54
2:E:39:ASN:HA	2:E:80:TYR:CE1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:93:ILE:HA	2:I:199:ALA:HB1	1.90	0.53
2:E:198:TYR:CZ	2:E:205:ILE:HG13	2.44	0.53
2:S:107:LEU:HD21	2:S:205:ILE:HD13	1.89	0.53
1:W:60:TYR:CD2	1:W:315:ILE:HD13	2.44	0.53
1:U:69:ILE:HG13	1:U:318:ARG:HB2	1.91	0.53
1:X:104:LEU:HD21	1:X:307:VAL:HB	1.90	0.53
1:B:4:THR:H	2:A:309:ILE:CD1	2.21	0.53
2:Q:235:THR:HG1	1:U:2:ASN:N	2.07	0.53
2:S:92:LYS:HB3	2:S:202:GLY:H	1.73	0.53
2:E:198:TYR:CE2	2:E:200:GLY:HA2	2.43	0.53
1:D:290:VAL:HG11	1:D:344:ALA:HB1	1.90	0.52
2:Q:235:THR:HG21	2:Q:243:ILE:HG21	1.92	0.52
2:P:92:LYS:HB3	2:P:202:GLY:N	2.25	0.52
2:P:311:TYR:CG	1:V:6:ALA:HB2	2.45	0.52
1:V:104:LEU:HD21	1:V:307:VAL:HB	1.91	0.52
1:T:290:VAL:HG11	1:T:344:ALA:HB1	1.90	0.52
2:Q:107:LEU:HD21	2:Q:205:ILE:HD13	1.92	0.52
2:E:198:TYR:CE2	2:E:205:ILE:HG13	2.45	0.52
1:N:8:GLN:HG2	2:I:80:TYR:CE1	2.45	0.52
2:R:149:VAL:HG23	2:R:191:LEU:HD22	1.91	0.52
1:M:5:ILE:HD12	2:H:5:THR:HB	1.92	0.52
1:J:19:ASN:CB	1:V:19:ASN:HB3	2.39	0.52
2:F:107:LEU:HD21	2:F:205:ILE:HD13	1.92	0.51
2:S:93:ILE:HA	2:S:199:ALA:HB1	1.92	0.51
2:G:201:LYS:O	2:G:203:THR:HG22	2.09	0.51
1:J:19:ASN:HD21	1:V:20:LYS:HG3	1.75	0.51
2:I:39:ASN:HA	2:I:80:TYR:CE1	2.45	0.51
1:J:5:ILE:HD11	2:E:244:ASN:HB2	1.92	0.51
1:X:60:TYR:CD2	1:X:315:ILE:HD13	2.46	0.51
2:C:89:LEU:HD22	2:C:202:GLY:HA3	1.93	0.51
1:W:297:LYS:HE3	1:W:330:THR:HG23	1.93	0.51
1:D:60:TYR:CD2	1:D:315:ILE:HD13	2.46	0.51
1:K:6:ALA:HB2	2:F:311:TYR:CG	2.46	0.51
2:P:149:VAL:HG23	2:P:191:LEU:HD22	1.92	0.51
2:F:110:LEU:HD11	2:F:207:PHE:CD1	2.46	0.50
1:X:69:ILE:HG13	1:X:318:ARG:HB2	1.92	0.50
1:W:104:LEU:HD21	1:W:307:VAL:HB	1.92	0.50
1:U:333:LEU:CD1	1:U:364:VAL:HG13	2.41	0.50
2:P:92:LYS:HB3	2:P:202:GLY:H	1.76	0.50
2:R:107:LEU:HD12	2:R:166:VAL:HG21	1.94	0.50
2:G:149:VAL:HG23	2:G:191:LEU:HD22	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:209:LYS:HD3	2:G:209:LYS:HE3	1.93	0.50
2:G:198:TYR:CZ	2:G:205:ILE:HG13	2.47	0.50
1:D:104:LEU:HD21	1:D:307:VAL:HB	1.93	0.50
2:A:103:ILE:HD13	2:A:198:TYR:HE2	1.76	0.50
1:M:8:GLN:HG2	2:H:80:TYR:CE1	2.47	0.50
2:R:87:TYR:CE1	2:R:243:ILE:HG23	2.47	0.49
2:I:198:TYR:CE1	2:I:200:GLY:HA2	2.47	0.49
1:U:290:VAL:HG11	1:U:344:ALA:HB1	1.93	0.49
1:V:60:TYR:CD2	1:V:315:ILE:HD13	2.47	0.49
1:D:297:LYS:HE3	1:D:330:THR:HG23	1.94	0.49
2:E:94:ILE:CD1	2:E:103:ILE:HD12	2.42	0.49
1:L:69:ILE:HD12	1:L:318:ARG:HB2	1.95	0.49
2:E:93:ILE:HA	2:E:199:ALA:CB	2.43	0.49
1:M:5:ILE:HD11	2:H:244:ASN:CB	2.42	0.49
1:N:8:GLN:HG2	2:I:80:TYR:CD1	2.47	0.49
2:G:92:LYS:HD3	2:G:200:GLY:O	2.12	0.49
1:L:60:TYR:CD2	1:L:315:ILE:HD13	2.48	0.49
2:S:92:LYS:HB3	2:S:202:GLY:N	2.27	0.49
1:V:69:ILE:HG13	1:V:318:ARG:HB2	1.95	0.49
2:I:103:ILE:HD13	2:I:198:TYR:HE2	1.77	0.49
2:P:209:LYS:HE2	2:E:209:LYS:HE2	1.94	0.49
1:N:60:TYR:CD2	1:N:315:ILE:HD13	2.48	0.49
2:H:89:LEU:HD13	2:H:202:GLY:O	2.12	0.49
2:R:311:TYR:CG	1:W:6:ALA:HB2	2.48	0.48
1:N:203:VAL:HG11	1:N:284:TYR:CD1	2.47	0.48
1:B:6:ALA:CB	2:A:311:TYR:CG	2.97	0.48
1:X:297:LYS:HE3	1:X:330:THR:HG23	1.95	0.48
1:U:297:LYS:HE3	1:U:330:THR:HG23	1.96	0.48
2:S:317:LEU:HD12	1:N:156:MET:O	2.12	0.48
1:B:15:VAL:HG12	2:A:309:ILE:HG22	1.95	0.48
2:S:89:LEU:HD22	2:S:202:GLY:HA3	1.94	0.48
2:S:104:VAL:HG22	2:S:166:VAL:HG23	1.94	0.48
2:O:309:ILE:HD13	1:T:4:THR:H	1.79	0.48
2:Q:92:LYS:HB3	2:Q:202:GLY:N	2.28	0.48
1:N:6:ALA:HB2	2:I:311:TYR:CG	2.48	0.48
1:N:69:ILE:HD12	1:N:318:ARG:CB	2.43	0.48
1:W:203:VAL:HG11	1:W:284:TYR:CD1	2.49	0.48
2:F:92:LYS:HD3	2:F:200:GLY:O	2.14	0.47
2:R:88:ASN:CG	2:G:218:GLY:CA	2.83	0.47
1:K:2:ASN:HA	2:F:300:GLN:NE2	2.28	0.47
2:R:88:ASN:CG	2:G:218:GLY:HA3	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:10:VAL:HG21	2:C:18:ALA:HB1	1.95	0.47
1:J:5:ILE:HD12	2:E:5:THR:HB	1.97	0.47
1:K:4:THR:HG22	2:F:309:ILE:CD1	2.44	0.47
2:E:92:LYS:HD3	2:E:200:GLY:O	2.14	0.47
2:F:93:ILE:C	2:F:199:ALA:HB1	2.35	0.47
2:R:242:THR:HB	2:G:123:THR:HA	1.96	0.47
2:Q:92:LYS:HB3	2:Q:202:GLY:H	1.79	0.47
2:S:300:GLN:HG3	1:X:2:ASN:HA	1.97	0.47
2:H:39:ASN:HA	2:H:80:TYR:CE1	2.50	0.47
1:B:5:ILE:HD12	2:A:5:THR:HB	1.97	0.47
1:T:60:TYR:CD2	1:T:315:ILE:HD13	2.49	0.47
2:A:92:LYS:HE2	2:A:200:GLY:HA3	1.97	0.47
2:E:92:LYS:HB3	2:E:201:LYS:HA	1.97	0.47
2:F:168:MET:HG3	2:F:229:PHE:CZ	2.49	0.47
2:R:92:LYS:HB3	2:R:202:GLY:N	2.29	0.47
2:H:208:ASN:HD21	2:H:301:LEU:CD1	2.27	0.47
2:O:89:LEU:HB3	2:O:202:GLY:HA3	1.95	0.47
1:K:15:VAL:HG12	2:F:309:ILE:HG22	1.96	0.47
2:P:242:THR:O	2:E:123:THR:HG22	2.15	0.47
1:N:131:ASN:HB2	1:X:9:ASP:HB3	1.96	0.47
2:H:198:TYR:CE1	2:H:200:GLY:HA2	2.50	0.47
2:S:10:VAL:HG21	2:S:18:ALA:CB	2.45	0.46
1:V:203:VAL:HG11	1:V:284:TYR:CD1	2.50	0.46
2:R:103:ILE:HG22	2:R:166:VAL:HG11	1.97	0.46
2:S:148:ASP:O	2:S:149:VAL:HB	2.15	0.46
2:P:218:GLY:CA	2:E:88:ASN:HB2	2.46	0.46
2:S:149:VAL:HG23	2:S:191:LEU:HD22	1.97	0.46
2:P:93:ILE:HA	2:P:199:ALA:HB1	1.98	0.46
2:Q:87:TYR:CE1	2:Q:243:ILE:HG23	2.51	0.46
1:M:6:ALA:HB2	2:H:311:TYR:CG	2.50	0.46
2:C:198:TYR:CZ	2:C:200:GLY:HA2	2.50	0.46
2:A:198:TYR:CE1	2:A:200:GLY:HA2	2.50	0.46
2:E:92:LYS:O	2:E:199:ALA:HB3	2.15	0.46
2:R:89:LEU:HD12	2:R:239:LYS:HA	1.97	0.46
2:P:218:GLY:HA3	2:E:88:ASN:CG	2.37	0.46
2:Q:309:ILE:HD13	1:U:4:THR:N	2.24	0.46
2:G:89:LEU:HB3	2:G:201:LYS:O	2.15	0.46
2:P:89:LEU:HD22	2:P:202:GLY:HA3	1.97	0.46
2:I:11:VAL:HG21	2:I:252:GLU:HB2	1.98	0.46
1:B:5:ILE:HD11	2:A:244:ASN:HB2	1.97	0.45
1:M:4:THR:H	2:H:309:ILE:HD13	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:309:ILE:HD13	1:D:4:THR:H	1.81	0.45
1:B:2:ASN:HA	2:A:300:GLN:HE22	1.81	0.45
2:P:87:TYR:HE1	2:P:243:ILE:HG23	1.81	0.45
2:Q:110:LEU:HD11	2:Q:207:PHE:HD1	1.81	0.45
1:L:6:ALA:HB2	2:G:311:TYR:CG	2.51	0.45
2:S:22:LEU:HD21	2:S:245:VAL:HG21	1.98	0.45
2:S:92:LYS:HD3	2:S:200:GLY:O	2.16	0.45
1:D:203:VAL:HG11	1:D:284:TYR:CD1	2.51	0.45
2:Q:148:ASP:O	2:Q:149:VAL:HB	2.17	0.45
2:F:92:LYS:HB3	2:F:201:LYS:HA	1.98	0.45
1:W:290:VAL:HG11	1:W:344:ALA:HB1	1.98	0.45
2:P:215:VAL:CG1	2:E:240:SER:HB3	2.46	0.45
2:E:198:TYR:HB2	2:E:229:PHE:CD2	2.51	0.45
2:F:259:ALA:HB1	1:M:253:GLU:OE2	2.16	0.45
2:R:10:VAL:HG21	2:R:18:ALA:CB	2.46	0.45
2:H:10:VAL:HG21	2:H:18:ALA:HB1	1.97	0.45
1:B:5:ILE:HD11	2:A:244:ASN:CB	2.47	0.45
2:E:168:MET:HG3	2:E:229:PHE:CZ	2.52	0.45
1:K:69:ILE:HD12	1:K:318:ARG:HB2	1.99	0.45
1:U:60:TYR:CD2	1:U:315:ILE:HD13	2.52	0.45
1:U:74:VAL:CG2	1:U:99:THR:O	2.65	0.45
1:D:69:ILE:HG13	1:D:318:ARG:HB2	1.98	0.45
1:L:2:ASN:HA	2:G:300:GLN:NE2	2.32	0.45
1:L:8:GLN:CD	1:L:8:GLN:H	2.20	0.45
2:G:94:ILE:HG23	2:G:100:ALA:HB2	1.98	0.45
2:I:87:TYR:CD2	2:I:243:ILE:HG13	2.52	0.45
2:C:149:VAL:HG23	2:C:191:LEU:HD22	1.99	0.45
1:J:2:ASN:HA	2:E:300:GLN:NE2	2.32	0.45
1:J:4:THR:H	2:E:309:ILE:CD1	2.25	0.45
2:Q:311:TYR:CG	1:U:6:ALA:CB	3.00	0.45
2:E:94:ILE:N	2:E:199:ALA:HB1	2.31	0.45
2:S:68:VAL:HG23	2:S:72:LEU:HD12	1.99	0.45
2:C:124:PHE:CE2	2:C:221:PRO:HD2	2.52	0.44
1:J:5:ILE:HD11	2:E:244:ASN:CB	2.47	0.44
1:K:5:ILE:HD12	2:F:5:THR:HB	2.00	0.44
1:K:60:TYR:CD2	1:K:315:ILE:HD13	2.51	0.44
2:F:110:LEU:HD11	2:F:207:PHE:HD1	1.83	0.44
2:P:218:GLY:CA	2:E:88:ASN:CG	2.86	0.44
2:Q:89:LEU:HD22	2:Q:202:GLY:HA3	1.98	0.44
1:K:338:ASN:HD21	1:K:367:LYS:HD2	1.83	0.44
2:S:311:TYR:CG	1:X:6:ALA:CB	3.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:89:LEU:HD22	2:H:202:GLY:CA	2.48	0.44
2:A:30:SER:OG	2:A:92:LYS:HD2	2.18	0.44
2:E:94:ILE:HG23	2:E:100:ALA:HB2	1.99	0.44
1:U:203:VAL:HG11	1:U:284:TYR:CD1	2.52	0.44
2:F:198:TYR:CZ	2:F:205:ILE:HG13	2.51	0.44
2:R:94:ILE:HD13	2:R:100:ALA:HA	2.00	0.44
2:G:89:LEU:HD13	2:G:202:GLY:O	2.17	0.44
2:Q:237:LEU:HD23	2:Q:238:ALA:H	1.83	0.44
2:G:8:TYR:CE2	2:G:235:THR:HG22	2.52	0.44
2:G:11:VAL:HG21	2:G:252:GLU:HB2	2.00	0.44
1:J:19:ASN:HB3	1:V:19:ASN:CG	2.38	0.44
1:T:203:VAL:HG11	1:T:284:TYR:CG	2.52	0.44
2:Q:309:ILE:H	2:Q:309:ILE:HG13	1.60	0.44
2:E:8:TYR:HE2	2:E:235:THR:HG22	1.83	0.44
2:Q:199:ALA:H	2:Q:201:LYS:HG3	1.83	0.44
2:E:235:THR:HG21	2:E:243:ILE:HD13	2.00	0.44
1:K:203:VAL:HG11	1:K:284:TYR:CD1	2.53	0.44
1:N:5:ILE:HD11	2:I:244:ASN:HB2	2.00	0.44
2:P:199:ALA:H	2:P:201:LYS:HG3	1.81	0.44
2:Q:92:LYS:HD3	2:Q:200:GLY:O	2.18	0.44
2:O:28:ASP:OD2	2:O:92:LYS:HE3	2.18	0.43
1:T:74:VAL:CG2	1:T:99:THR:O	2.66	0.43
1:L:203:VAL:HG11	1:L:284:TYR:CD1	2.52	0.43
2:A:198:TYR:CE2	2:A:200:GLY:HA2	2.53	0.43
1:K:5:ILE:HD11	2:F:244:ASN:CB	2.48	0.43
1:B:13:LYS:HE2	1:B:15:VAL:CG1	2.48	0.43
2:E:92:LYS:HE2	2:E:199:ALA:O	2.18	0.43
2:R:198:TYR:CE2	2:R:200:GLY:HA2	2.53	0.43
2:H:87:TYR:CD2	2:H:243:ILE:HG13	2.52	0.43
2:Q:148:ASP:O	2:Q:149:VAL:CB	2.67	0.43
2:R:89:LEU:HB3	2:R:203:THR:HG23	2.00	0.43
1:V:13:LYS:HE2	1:V:15:VAL:CG2	2.48	0.43
1:M:131:ASN:HB2	1:W:9:ASP:HB3	1.99	0.43
2:Q:311:TYR:CD2	1:U:6:ALA:HB2	2.54	0.43
2:I:92:LYS:HD3	2:I:200:GLY:O	2.17	0.43
1:X:203:VAL:HG11	1:X:284:TYR:CD1	2.54	0.43
1:B:69:ILE:HD12	1:B:318:ARG:HB2	2.00	0.43
2:E:89:LEU:HB3	2:E:201:LYS:O	2.19	0.43
1:L:5:ILE:HD11	2:G:244:ASN:CB	2.49	0.43
1:L:131:ASN:HB2	1:U:9:ASP:HB3	2.00	0.43
2:R:242:THR:HG21	2:G:122:ASP:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:ALA:HB2	2:A:311:TYR:CD1	2.54	0.43
2:A:92:LYS:HB3	2:A:202:GLY:H	1.84	0.43
1:L:20:LYS:HE2	2:R:305:LYS:CE	2.49	0.43
2:R:92:LYS:O	2:R:199:ALA:CB	2.66	0.43
2:R:148:ASP:O	2:R:149:VAL:HG12	2.18	0.43
2:S:103:ILE:HG22	2:S:166:VAL:HG11	2.00	0.43
2:P:166:VAL:HG12	2:P:198:TYR:O	2.19	0.43
2:E:93:ILE:CA	2:E:199:ALA:HB1	2.48	0.43
2:S:148:ASP:O	2:S:149:VAL:CB	2.67	0.43
1:B:8:GLN:H	1:B:8:GLN:CD	2.22	0.43
2:O:149:VAL:HG23	2:O:191:LEU:HD22	2.01	0.43
2:P:309:ILE:HD12	1:V:4:THR:HG22	1.99	0.43
2:I:27:LYS:HB3	2:I:95:THR:HG21	2.01	0.43
2:A:198:TYR:CE1	2:A:205:ILE:HG13	2.54	0.42
2:A:89:LEU:HB3	2:A:201:LYS:O	2.19	0.42
2:Q:89:LEU:HD13	2:Q:202:GLY:O	2.19	0.42
2:A:92:LYS:HD3	2:A:200:GLY:O	2.19	0.42
2:R:124:PHE:CE2	2:R:179:LYS:HD2	2.54	0.42
2:C:237:LEU:HD13	2:C:243:ILE:CG2	2.48	0.42
1:U:156:MET:O	2:G:317:LEU:HD12	2.18	0.42
2:H:89:LEU:CD2	2:H:202:GLY:HA3	2.49	0.42
2:Q:110:LEU:HD11	2:Q:207:PHE:CD1	2.54	0.42
2:E:149:VAL:HG23	2:E:191:LEU:HD22	2.01	0.42
1:K:6:ALA:CB	2:F:311:TYR:CG	3.02	0.42
2:H:103:ILE:HD13	2:H:198:TYR:HE2	1.84	0.42
2:A:168:MET:HG3	2:A:229:PHE:CZ	2.54	0.42
2:H:27:LYS:C	2:H:95:THR:HG21	2.40	0.42
1:K:6:ALA:HB2	2:F:311:TYR:CD2	2.55	0.42
2:R:311:TYR:CD2	1:W:6:ALA:HB2	2.55	0.42
2:G:93:ILE:C	2:G:199:ALA:HB1	2.39	0.42
1:X:13:LYS:HE2	1:X:15:VAL:CG2	2.50	0.42
1:J:69:ILE:HD12	1:J:318:ARG:HB2	2.02	0.42
2:F:89:LEU:HD13	2:F:202:GLY:O	2.19	0.42
1:M:203:VAL:HG11	1:M:284:TYR:CD1	2.54	0.42
2:R:94:ILE:HG21	2:R:100:ALA:N	2.35	0.41
2:G:87:TYR:CD2	2:G:243:ILE:HG13	2.55	0.41
1:X:203:VAL:HG11	1:X:284:TYR:CG	2.55	0.41
2:C:148:ASP:O	2:C:149:VAL:CB	2.67	0.41
2:F:201:LYS:O	2:F:203:THR:HG22	2.20	0.41
2:S:309:ILE:H	2:S:309:ILE:HG13	1.60	0.41
1:B:3:ASP:HB3	2:A:8:TYR:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:104:LEU:HD21	1:T:307:VAL:HB	2.01	0.41
1:L:5:ILE:HD12	2:G:5:THR:HB	2.03	0.41
2:S:92:LYS:HB3	2:S:201:LYS:HA	2.01	0.41
2:H:10:VAL:HG11	2:H:18:ALA:CB	2.50	0.41
2:C:89:LEU:HB3	2:C:202:GLY:HA3	2.03	0.41
2:Q:87:TYR:HE1	2:Q:243:ILE:HG23	1.85	0.41
2:R:92:LYS:HD3	2:R:202:GLY:H	1.85	0.41
2:S:92:LYS:O	2:S:199:ALA:CB	2.68	0.41
1:V:203:VAL:HG11	1:V:284:TYR:CG	2.56	0.41
1:N:69:ILE:HG23	1:N:318:ARG:HD3	2.02	0.41
2:E:89:LEU:HD22	2:E:202:GLY:HA3	2.02	0.41
1:V:74:VAL:CG2	1:V:99:THR:O	2.68	0.41
2:G:92:LYS:HB3	2:G:201:LYS:HA	2.02	0.41
1:M:60:TYR:CD2	1:M:315:ILE:HD13	2.55	0.41
2:H:149:VAL:HG23	2:H:191:LEU:HD22	2.01	0.41
1:B:203:VAL:HG11	1:B:284:TYR:CD1	2.55	0.41
1:L:19:ASN:HB2	1:W:19:ASN:HB3	2.03	0.41
1:K:131:ASN:HB2	1:V:9:ASP:HB3	2.01	0.41
1:U:203:VAL:HG11	1:U:284:TYR:CG	2.56	0.41
2:R:148:ASP:O	2:R:149:VAL:CB	2.69	0.41
2:R:242:THR:CB	2:G:123:THR:HA	2.51	0.41
2:I:317:LEU:HD12	1:X:130:ILE:HD11	2.03	0.41
1:X:189:VAL:HG12	1:X:241:ILE:HB	2.01	0.41
1:J:15:VAL:HG12	2:E:309:ILE:HG22	2.03	0.41
2:R:89:LEU:HD22	2:R:202:GLY:HA3	2.02	0.41
2:R:107:LEU:CD2	2:R:205:ILE:HD13	2.47	0.41
2:S:10:VAL:HG11	2:S:18:ALA:CB	2.50	0.41
1:W:189:VAL:HG12	1:W:241:ILE:HB	2.01	0.41
1:J:203:VAL:HG11	1:J:284:TYR:CD1	2.56	0.41
1:V:279:LEU:HD13	1:V:325:PRO:HG3	2.03	0.41
2:A:201:LYS:C	2:A:203:THR:HG22	2.41	0.40
2:S:30:SER:OG	2:S:92:LYS:HD2	2.21	0.40
2:A:8:TYR:CE2	2:A:245:VAL:HG22	2.56	0.40
1:B:4:THR:HG22	2:A:309:ILE:CD1	2.51	0.40
2:C:148:ASP:O	2:C:149:VAL:HB	2.21	0.40
2:P:311:TYR:CG	1:V:6:ALA:CB	3.04	0.40
2:F:166:VAL:HG22	2:F:198:TYR:O	2.22	0.40
2:R:88:ASN:HB2	2:G:218:GLY:CA	2.52	0.40
2:S:311:TYR:CD1	1:X:6:ALA:HB2	2.56	0.40
2:Q:30:SER:OG	2:Q:92:LYS:HD2	2.21	0.40
1:K:4:THR:H	2:F:309:ILE:CD1	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:20:LYS:HE2	2:R:305:LYS:HE3	2.03	0.40
2:G:93:ILE:HA	2:G:199:ALA:CB	2.51	0.40
2:I:89:LEU:HD13	2:I:202:GLY:O	2.22	0.40
2:S:11:VAL:HG21	2:S:252:GLU:HB2	2.04	0.40
2:S:94:ILE:HD13	2:S:100:ALA:HA	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	B	371/373 (100%)	363 (98%)	6 (2%)	2 (0%)	29	29
1	D	371/373 (100%)	365 (98%)	6 (2%)	0	100	100
1	J	371/373 (100%)	361 (97%)	8 (2%)	2 (0%)	29	29
1	K	371/373 (100%)	364 (98%)	6 (2%)	1 (0%)	41	41
1	L	371/373 (100%)	364 (98%)	6 (2%)	1 (0%)	41	41
1	M	371/373 (100%)	363 (98%)	7 (2%)	1 (0%)	41	41
1	N	371/373 (100%)	364 (98%)	6 (2%)	1 (0%)	41	41
1	T	371/373 (100%)	363 (98%)	8 (2%)	0	100	100
1	U	371/373 (100%)	363 (98%)	7 (2%)	1 (0%)	41	41
1	V	371/373 (100%)	361 (97%)	10 (3%)	0	100	100
1	W	371/373 (100%)	361 (97%)	9 (2%)	1 (0%)	41	41
1	X	371/373 (100%)	363 (98%)	7 (2%)	1 (0%)	41	41
2	A	316/318 (99%)	308 (98%)	7 (2%)	1 (0%)	41	41
2	C	316/318 (99%)	309 (98%)	5 (2%)	2 (1%)	25	25
2	E	316/318 (99%)	308 (98%)	7 (2%)	1 (0%)	41	41
2	F	316/318 (99%)	308 (98%)	7 (2%)	1 (0%)	41	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	G	316/318 (99%)	309 (98%)	6 (2%)	1 (0%)	41	41
2	H	316/318 (99%)	309 (98%)	6 (2%)	1 (0%)	41	41
2	I	316/318 (99%)	308 (98%)	7 (2%)	1 (0%)	41	41
2	O	316/318 (99%)	309 (98%)	6 (2%)	1 (0%)	41	41
2	P	316/318 (99%)	309 (98%)	4 (1%)	3 (1%)	17	17
2	Q	316/318 (99%)	309 (98%)	4 (1%)	3 (1%)	17	17
2	R	316/318 (99%)	308 (98%)	6 (2%)	2 (1%)	25	25
2	S	316/318 (99%)	309 (98%)	5 (2%)	2 (1%)	25	25
All	All	8244/8292 (99%)	8058 (98%)	156 (2%)	30 (0%)	38	34

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	149	VAL
2	O	149	VAL
2	A	201	LYS
2	P	149	VAL
2	P	201	LYS
2	Q	149	VAL
2	Q	201	LYS
2	E	201	LYS
2	F	201	LYS
2	R	149	VAL
2	R	201	LYS
2	S	149	VAL
2	S	201	LYS
2	G	201	LYS
2	H	201	LYS
2	I	201	LYS
1	B	180	GLY
1	J	180	GLY
2	P	238	ALA
1	K	180	GLY
1	L	180	GLY
1	M	180	GLY
1	N	180	GLY
1	B	38	TYR
1	J	38	TYR
2	C	201	LYS

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Mol	Chain	Res	Type
2	Q	238	ALA
1	U	38	TYR
1	X	38	TYR
1	W	38	TYR

5.3.2 Protein sidechains (i)

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	B	312/312 (100%)	306 (98%)	6 (2%)	57	57
1	D	312/312 (100%)	305 (98%)	7 (2%)	52	52
1	J	312/312 (100%)	307 (98%)	5 (2%)	62	62
1	K	312/312 (100%)	306 (98%)	6 (2%)	57	57
1	L	312/312 (100%)	306 (98%)	6 (2%)	57	57
1	M	312/312 (100%)	306 (98%)	6 (2%)	57	57
1	N	312/312 (100%)	307 (98%)	5 (2%)	62	62
1	T	312/312 (100%)	305 (98%)	7 (2%)	52	52
1	U	312/312 (100%)	305 (98%)	7 (2%)	52	52
1	V	312/312 (100%)	305 (98%)	7 (2%)	52	52
1	W	312/312 (100%)	306 (98%)	6 (2%)	57	57
1	X	312/312 (100%)	306 (98%)	6 (2%)	57	57
2	A	259/259 (100%)	252 (97%)	7 (3%)	44	44
2	C	259/259 (100%)	250 (96%)	9 (4%)	36	36
2	E	259/259 (100%)	249 (96%)	10 (4%)	32	32
2	F	259/259 (100%)	250 (96%)	9 (4%)	36	36
2	G	259/259 (100%)	251 (97%)	8 (3%)	40	40
2	H	259/259 (100%)	249 (96%)	10 (4%)	32	32
2	I	259/259 (100%)	249 (96%)	10 (4%)	32	32
2	O	259/259 (100%)	249 (96%)	10 (4%)	32	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	259/259 (100%)	250 (96%)	9 (4%)	36	36
2	Q	259/259 (100%)	249 (96%)	10 (4%)	32	32
2	R	259/259 (100%)	250 (96%)	9 (4%)	36	36
2	S	259/259 (100%)	248 (96%)	11 (4%)	30	30
All	All	6852/6852 (100%)	6666 (97%)	186 (3%)	48	44

All (186) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	8	GLN
1	B	48	ASP
1	B	112	SER
1	B	181	LEU
1	B	269	ASP
1	B	367	LYS
2	C	2	THR
2	C	13	ASN
2	C	117	ASP
2	C	130	THR
2	C	141	THR
2	C	213	VAL
2	C	234	ASP
2	C	290	GLN
2	C	301	LEU
1	J	8	GLN
1	J	112	SER
1	J	181	LEU
1	J	269	ASP
1	J	367	LYS
2	O	2	THR
2	O	13	ASN
2	O	117	ASP
2	O	130	THR
2	O	141	THR
2	O	213	VAL
2	O	234	ASP
2	O	290	GLN
2	O	301	LEU
2	O	309	ILE
1	D	74	VAL
1	D	103	LEU

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Mol	Chain	Res	Type
1	D	126	SER
1	D	131	ASN
1	D	244	LYS
1	D	269	ASP
1	D	348	ASP
1	T	74	VAL
1	T	103	LEU
1	T	126	SER
1	T	131	ASN
1	T	244	LYS
1	T	269	ASP
1	T	348	ASP
2	A	2	THR
2	A	29	ASN
2	A	130	THR
2	A	138	VAL
2	A	146	VAL
2	A	204	THR
2	A	301	LEU
2	P	2	THR
2	P	13	ASN
2	P	117	ASP
2	P	130	THR
2	P	213	VAL
2	P	234	ASP
2	P	290	GLN
2	P	301	LEU
2	P	309	ILE
2	Q	2	THR
2	Q	13	ASN
2	Q	117	ASP
2	Q	130	THR
2	Q	213	VAL
2	Q	234	ASP
2	Q	237	LEU
2	Q	290	GLN
2	Q	301	LEU
2	Q	309	ILE
2	E	2	THR
2	E	13	ASN
2	E	29	ASN
2	E	130	THR

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Mol	Chain	Res	Type
2	E	138	VAL
2	E	146	VAL
2	E	204	THR
2	E	208	ASN
2	E	301	LEU
2	E	309	ILE
1	K	8	GLN
1	K	48	ASP
1	K	112	SER
1	K	181	LEU
1	K	269	ASP
1	K	367	LYS
1	L	8	GLN
1	L	48	ASP
1	L	112	SER
1	L	181	LEU
1	L	269	ASP
1	L	367	LYS
1	U	74	VAL
1	U	103	LEU
1	U	126	SER
1	U	131	ASN
1	U	244	LYS
1	U	269	ASP
1	U	348	ASP
1	V	74	VAL
1	V	103	LEU
1	V	126	SER
1	V	131	ASN
1	V	244	LYS
1	V	269	ASP
1	V	348	ASP
2	F	2	THR
2	F	29	ASN
2	F	130	THR
2	F	138	VAL
2	F	146	VAL
2	F	166	VAL
2	F	204	THR
2	F	208	ASN
2	F	301	LEU
2	R	2	THR

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Mol	Chain	Res	Type
2	R	13	ASN
2	R	117	ASP
2	R	130	THR
2	R	141	THR
2	R	213	VAL
2	R	234	ASP
2	R	290	GLN
2	R	301	LEU
2	S	2	THR
2	S	13	ASN
2	S	117	ASP
2	S	130	THR
2	S	141	THR
2	S	213	VAL
2	S	234	ASP
2	S	237	LEU
2	S	290	GLN
2	S	301	LEU
2	S	309	ILE
2	G	2	THR
2	G	13	ASN
2	G	29	ASN
2	G	130	THR
2	G	138	VAL
2	G	146	VAL
2	G	204	THR
2	G	301	LEU
1	M	8	GLN
1	M	48	ASP
1	M	112	SER
1	M	181	LEU
1	M	269	ASP
1	M	367	LYS
1	N	8	GLN
1	N	112	SER
1	N	181	LEU
1	N	269	ASP
1	N	367	LYS
1	W	103	LEU
1	W	126	SER
1	W	131	ASN
1	W	244	LYS

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Mol	Chain	Res	Type
1	W	269	ASP
1	W	348	ASP
2	H	2	THR
2	H	13	ASN
2	H	29	ASN
2	H	130	THR
2	H	138	VAL
2	H	146	VAL
2	H	204	THR
2	H	234	ASP
2	H	301	LEU
2	H	309	ILE
2	I	2	THR
2	I	29	ASN
2	I	130	THR
2	I	138	VAL
2	I	146	VAL
2	I	204	THR
2	I	208	ASN
2	I	234	ASP
2	I	301	LEU
2	I	309	ILE
1	X	103	LEU
1	X	126	SER
1	X	131	ASN
1	X	244	LYS
1	X	269	ASP
1	X	348	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	338	ASN
1	J	2	ASN
1	J	19	ASN
1	J	338	ASN
2	O	297	ASN
1	D	2	ASN
1	D	131	ASN
1	T	67	ASN
1	T	131	ASN
2	A	23	GLN

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Mol	Chain	Res	Type
2	Q	71	GLN
2	E	13	ASN
2	E	88	ASN
2	E	91	ASN
2	E	290	GLN
1	K	67	ASN
1	K	272	GLN
1	K	338	ASN
1	L	2	ASN
1	L	338	ASN
1	U	19	ASN
1	U	67	ASN
1	U	131	ASN
1	V	2	ASN
1	V	131	ASN
2	F	300	GLN
2	R	71	GLN
2	R	88	ASN
2	R	91	ASN
2	G	13	ASN
2	G	23	GLN
1	M	338	ASN
1	N	19	ASN
1	N	338	ASN
1	W	19	ASN
1	W	131	ASN
2	H	108	ASN
2	H	111	ASN
2	I	6	GLN
2	I	297	ASN
2	I	300	GLN
1	X	19	ASN
1	X	131	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates (i)

There are no monosaccharides 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.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13957. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal surface views

This section was not generated.

6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.