wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 02:34 PM BST

PDB ID	:	3J9R
EMDB ID:	:	EMD-6271
Title	:	Atomic structures of a bactericidal contractile nanotube in its pre- and post-contraction states
Authors	:	Ge, P.; Scholl, D.; Leiman, P.G.; Yu, X.; Miller, J.F.; Zhou, Z.H.
Deposited on	:	2015-02-17
Resolution	:	3.90 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

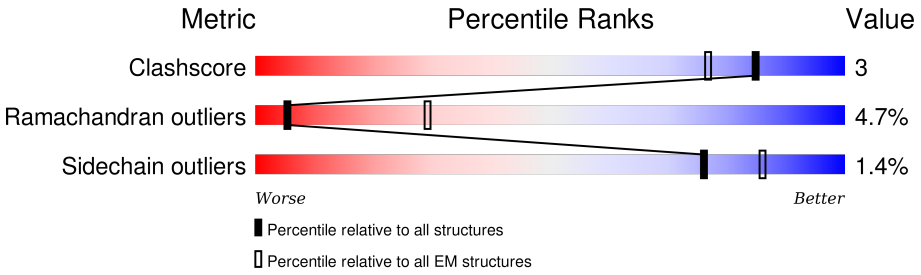
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.90 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 <=5%

Mol	Chain	Length	Quality of chain
1	0	386	85% 13% ••
1	1	386	84% 13% ••
1	2	386	85% 12% ••
1	3	386	85% 13% ••
1	4	386	85% 12% ••
1	5	386	85% 12% ••
1	A	386	84% 13% ••
1	B	386	83% 14% ••
1	C	386	84% 13% ••

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Mol	Chain	Length	Quality of chain
1	D	386	84% 13%
1	E	386	85% 13%
1	F	386	84% 13%
1	G	386	84% 13%
1	H	386	84% 13%
1	I	386	84% 13%
1	J	386	85% 13%
1	K	386	84% 13%
1	L	386	84% 13%
1	M	386	84% 14%
1	N	386	85% 13%
1	O	386	84% 14%
1	P	386	84% 13%
1	Q	386	84% 13%
1	R	386	84% 14%
1	a	386	94% 6%
1	b	386	94% 6%
1	c	386	93% 6%
1	d	386	93% 6%
1	e	386	94% 6%
1	f	386	94% 6%
1	g	386	93% 6%
1	h	386	94% 6%
1	i	386	94% 6%
1	j	386	94% 6%

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Mol	Chain	Length	Quality of chain
1	k	386	94% 6%
1	l	386	94% 6%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 103824 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 sheath.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	B	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	F	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	E	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	D	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	C	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	0	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	1	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	5	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	4	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	3	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	2	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	G	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	H	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	L	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	K	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	J	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		

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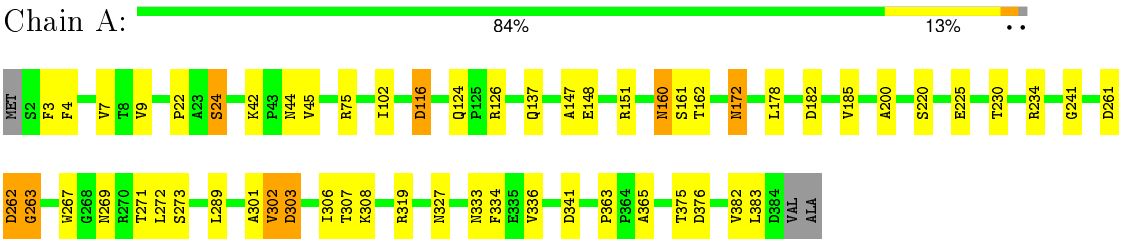
Mol	Chain	Residues	Atoms					AltConf	Trace
1	I	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	M	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	N	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	R	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	Q	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	P	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	O	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	a	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	b	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	f	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	e	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	d	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	c	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	g	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	h	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	l	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	k	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	j	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	i	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		

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.

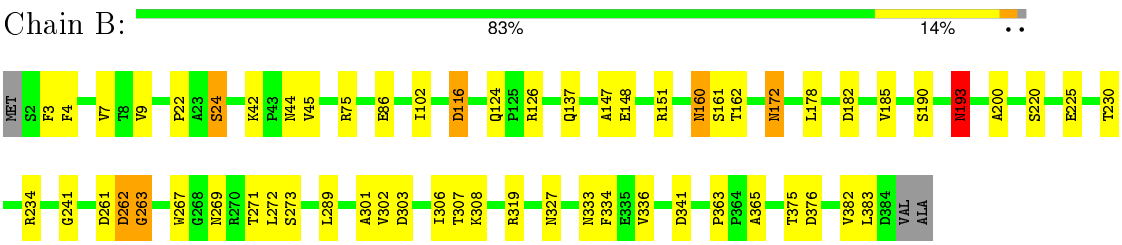
- Molecule 1: sheath

Chain A:



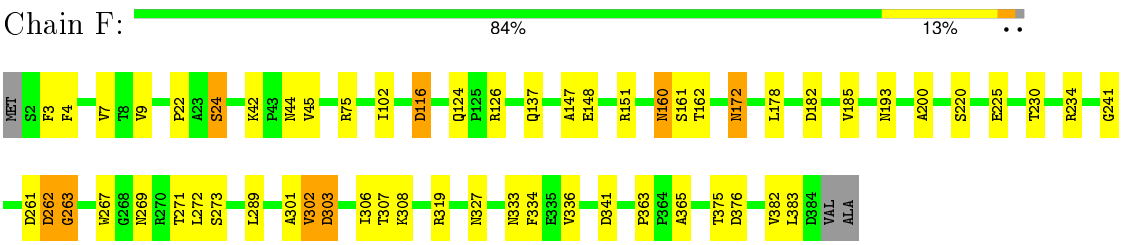
- Molecule 1: sheath

Chain B:



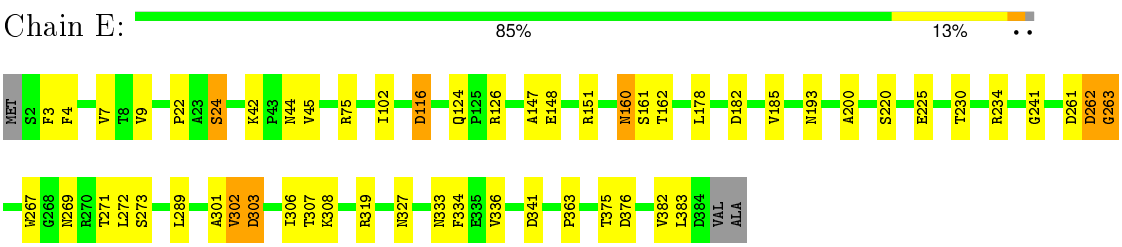
- Molecule 1: sheath

Chain F:



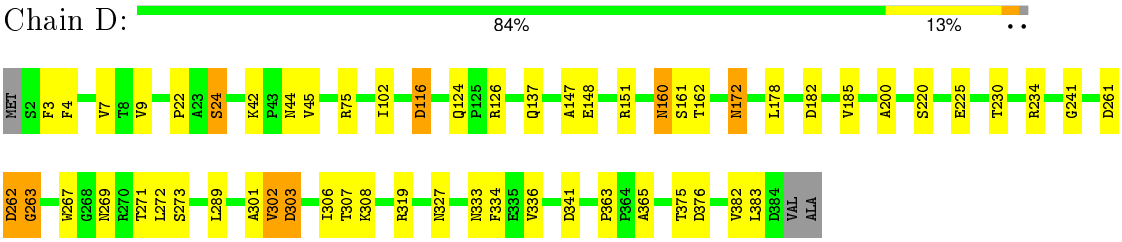
- Molecule 1: sheath

Chain E:



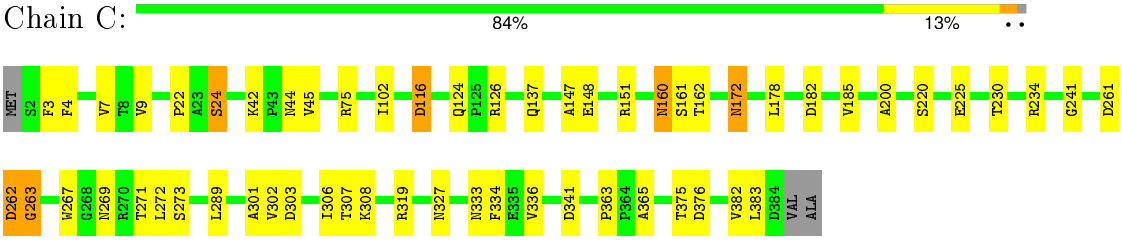
- Molecule 1: sheath

Chain D:



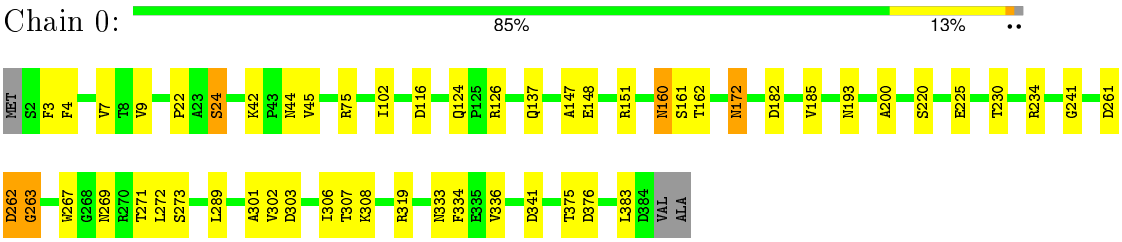
- Molecule 1: sheath

Chain C:



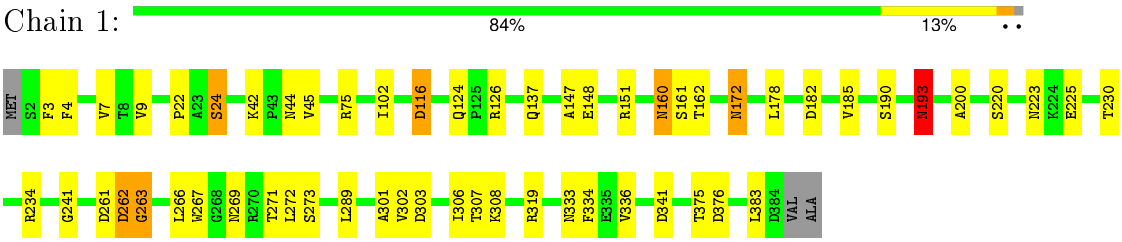
- Molecule 1: sheath

Chain 0:



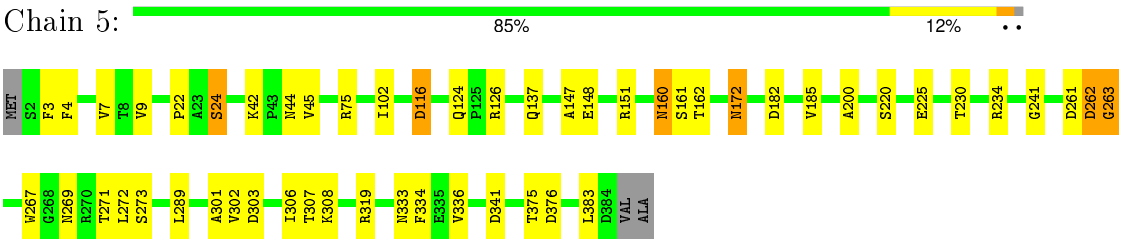
- Molecule 1: sheath

Chain 1:



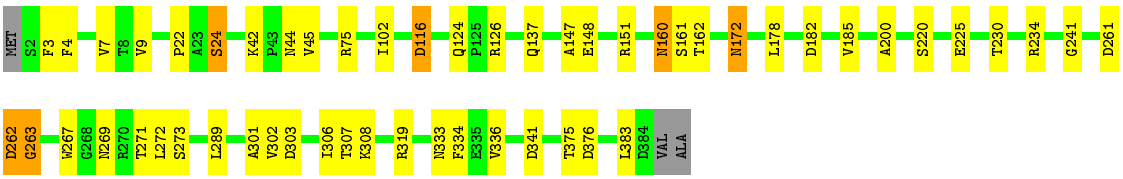
- Molecule 1: sheath

Chain 5:



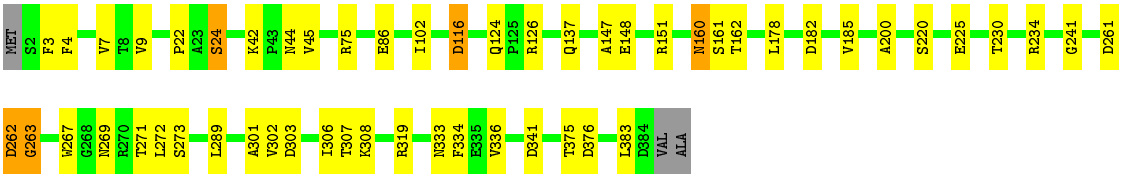
- Molecule 1: sheath

Chain 4:



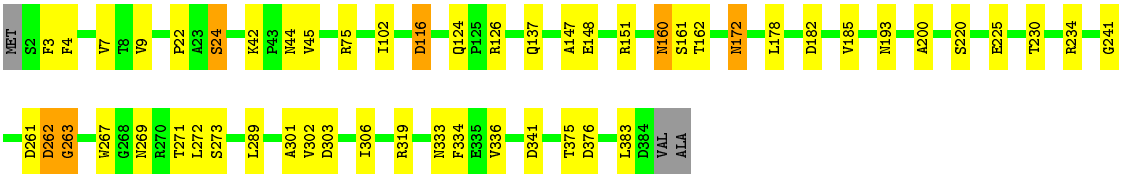
- Molecule 1: sheath

Chain 3:



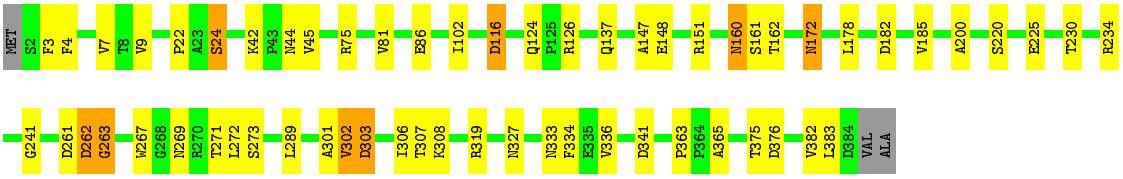
- Molecule 1: sheath

Chain 2:



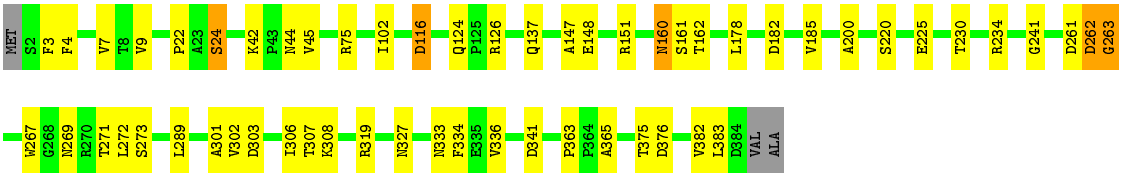
- Molecule 1: sheath

Chain G:



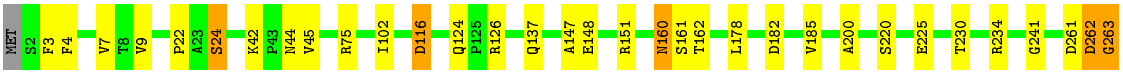
- Molecule 1: sheath

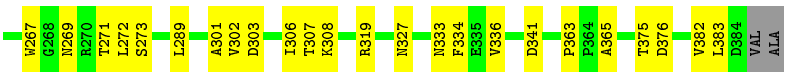
Chain H:



- Molecule 1: sheath

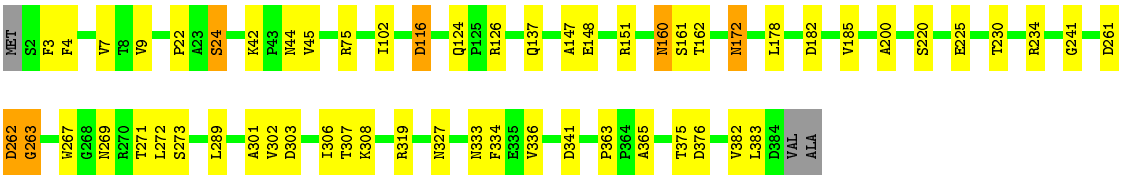
Chain L:





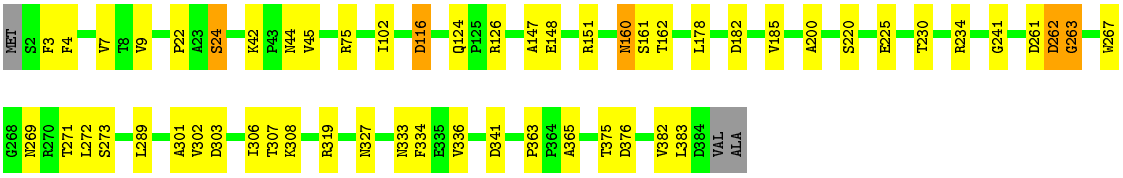
- Molecule 1: sheath

Chain K:



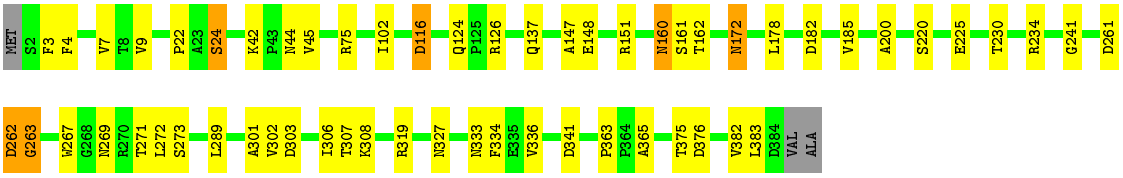
- Molecule 1: sheath

Chain J:



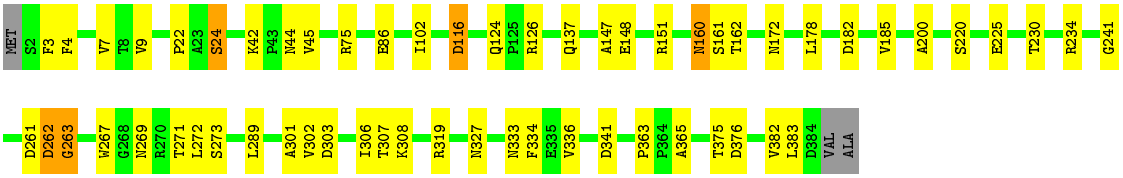
- Molecule 1: sheath

Chain I:



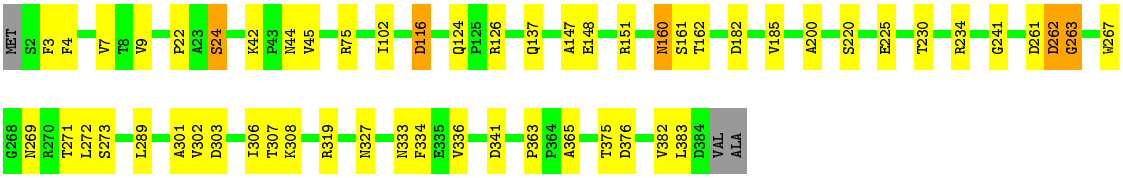
- Molecule 1: sheath

Chain M:



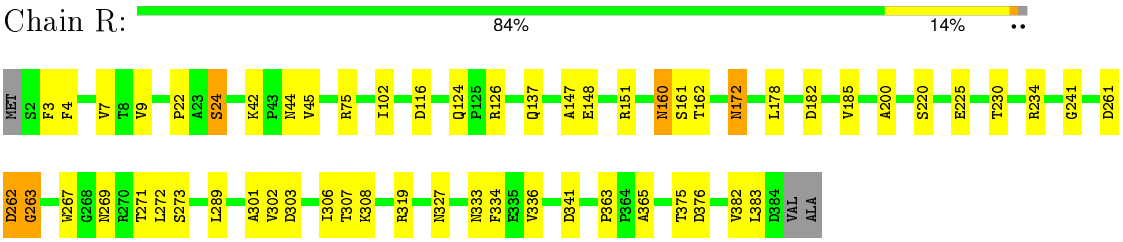
- Molecule 1: sheath

Chain N:



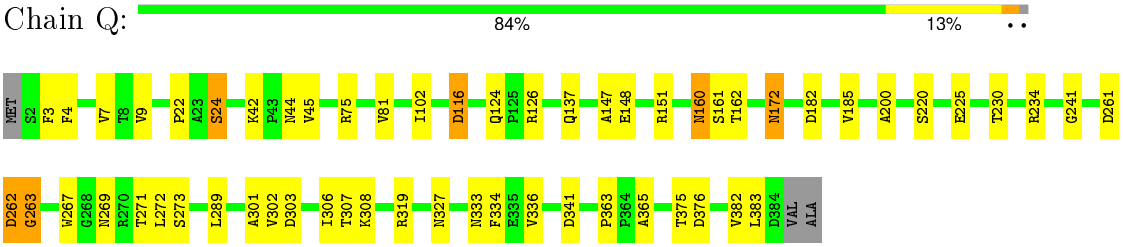
- Molecule 1: sheath

Chain R:



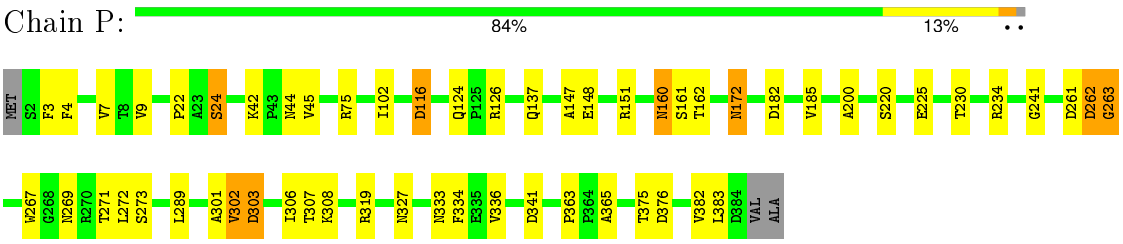
- Molecule 1: sheath

Chain Q:



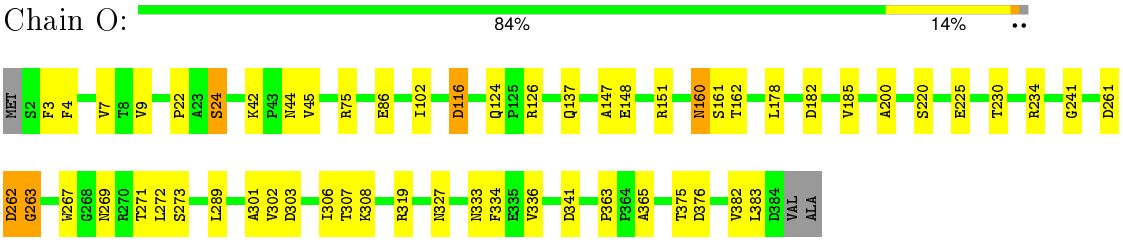
- Molecule 1: sheath

Chain P:



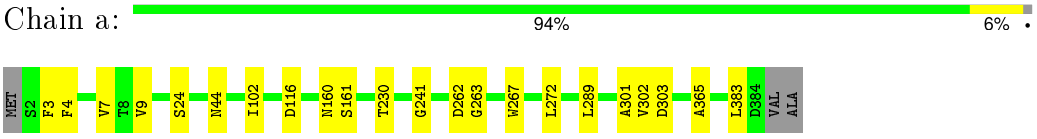
- Molecule 1: sheath

Chain O:



- Molecule 1: sheath

Chain a:



- Molecule 1: sheath

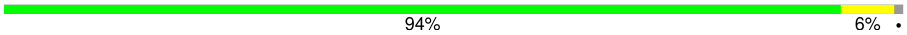
Chain b:

• Molecule 1: sheath

Chain f:

• Molecule 1: sheath

Chain e:

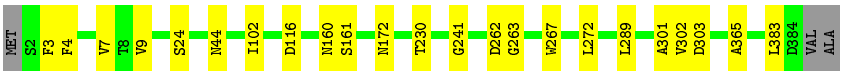


• Molecule 1: sheath

Chain d:

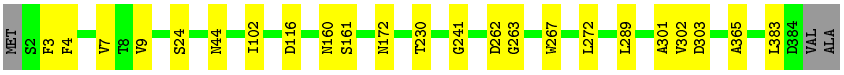
• Molecule 1: sheath

Chain c:



• Molecule 1: sheath

Chain g:



• Molecule 1: sheath

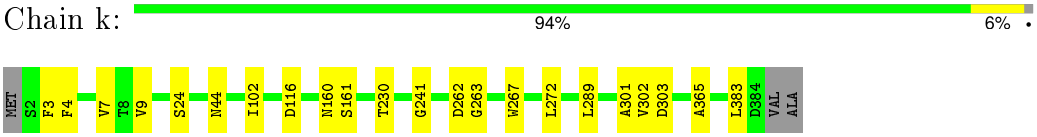
Chain h:

• Molecule 1: sheath

Chain l:

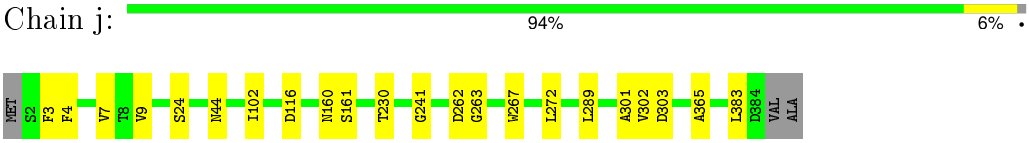
- Molecule 1: sheath

Chain k:



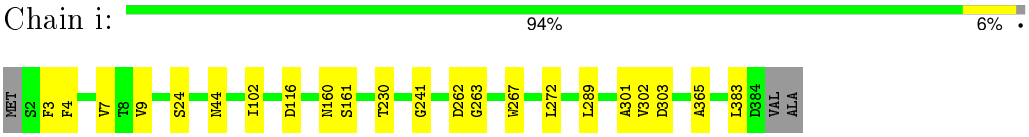
- Molecule 1: sheath

Chain j:



- Molecule 1: sheath

Chain i:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	59000	Depositor
Image detector	KODAK SO-163 FILM	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	0	0.35	3/2942 (0.1%)	0.37	0/4010
1	1	0.32	3/2942 (0.1%)	0.37	0/4010
1	2	0.36	4/2942 (0.1%)	0.37	0/4010
1	3	0.31	1/2942 (0.0%)	0.37	0/4010
1	4	0.29	1/2942 (0.0%)	0.37	0/4010
1	5	0.29	1/2942 (0.0%)	0.37	0/4010
1	A	0.28	1/2942 (0.0%)	0.37	0/4010
1	B	0.31	3/2942 (0.1%)	0.37	0/4010
1	C	0.29	1/2942 (0.0%)	0.37	0/4010
1	D	0.29	1/2942 (0.0%)	0.37	0/4010
1	E	0.36	2/2942 (0.1%)	0.37	0/4010
1	F	0.35	3/2942 (0.1%)	0.37	0/4010
1	G	0.29	1/2942 (0.0%)	0.37	0/4010
1	H	0.30	1/2942 (0.0%)	0.37	0/4010
1	I	0.29	2/2942 (0.1%)	0.37	0/4010
1	J	0.29	0/2942	0.37	0/4010
1	K	0.29	1/2942 (0.0%)	0.37	0/4010
1	L	0.30	1/2942 (0.0%)	0.37	0/4010
1	M	0.31	2/2942 (0.1%)	0.36	0/4010
1	N	0.30	1/2942 (0.0%)	0.37	0/4010
1	O	0.30	1/2942 (0.0%)	0.36	0/4010
1	P	0.29	1/2942 (0.0%)	0.37	0/4010
1	Q	0.29	1/2942 (0.0%)	0.37	0/4010
1	R	0.29	2/2942 (0.1%)	0.37	0/4010
1	a	0.28	0/2942	0.37	0/4010
1	b	0.28	0/2942	0.37	0/4010
1	c	0.29	1/2942 (0.0%)	0.37	0/4010
1	d	0.28	1/2942 (0.0%)	0.37	0/4010
1	e	0.27	0/2942	0.37	0/4010
1	f	0.27	0/2942	0.37	0/4010
1	g	0.28	1/2942 (0.0%)	0.37	0/4010
1	h	0.27	0/2942	0.37	0/4010
1	i	0.28	0/2942	0.37	0/4010
1	j	0.27	0/2942	0.37	0/4010

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >2	RMSZ	#|Z| >2
1	k	0.28	0/2942	0.37	0/4010
1	l	0.28	0/2942	0.36	0/4010
All	All	0.30	41/105912 (0.0%)	0.37	0/144360

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	1	0	1
1	B	0	1
All	All	0	2

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	193	ASN	CG-ND2	-9.37	1.09	1.32
1	E	193	ASN	CG-ND2	-9.23	1.09	1.32
1	F	193	ASN	CG-ND2	-8.72	1.11	1.32
1	0	193	ASN	CG-ND2	-8.42	1.11	1.32
1	2	193	ASN	CG-OD1	-8.29	1.05	1.24
1	E	193	ASN	CG-OD1	-8.17	1.05	1.24
1	0	193	ASN	CG-OD1	-6.96	1.08	1.24
1	1	193	ASN	CG-ND2	-6.67	1.16	1.32
1	F	193	ASN	CG-OD1	-6.54	1.09	1.24
1	3	137	GLN	CD-NE2	-6.31	1.17	1.32
1	M	137	GLN	CD-NE2	-6.00	1.17	1.32
1	H	137	GLN	CD-NE2	-5.84	1.18	1.32
1	I	172	ASN	CG-ND2	-5.82	1.18	1.32
1	1	172	ASN	CG-ND2	-5.81	1.18	1.32
1	B	172	ASN	CG-ND2	-5.79	1.18	1.32
1	N	137	GLN	CD-NE2	-5.79	1.18	1.32
1	O	137	GLN	CD-NE2	-5.75	1.18	1.32
1	B	193	ASN	CG-ND2	-5.75	1.18	1.32
1	R	172	ASN	CG-ND2	-5.74	1.18	1.32
1	F	172	ASN	CG-ND2	-5.73	1.18	1.32
1	K	172	ASN	CG-ND2	-5.70	1.18	1.32
1	0	172	ASN	CG-ND2	-5.69	1.18	1.32
1	G	172	ASN	CG-ND2	-5.69	1.18	1.32
1	C	172	ASN	CG-ND2	-5.69	1.18	1.32
1	D	172	ASN	CG-ND2	-5.67	1.18	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	172	ASN	CG-ND2	-5.67	1.18	1.32
1	5	172	ASN	CG-ND2	-5.67	1.18	1.32
1	2	172	ASN	CG-ND2	-5.63	1.18	1.32
1	Q	172	ASN	CG-ND2	-5.62	1.18	1.32
1	A	172	ASN	CG-ND2	-5.60	1.18	1.32
1	4	172	ASN	CG-ND2	-5.60	1.18	1.32
1	c	172	ASN	CG-ND2	-5.54	1.19	1.32
1	B	172	ASN	CG-OD1	-5.14	1.12	1.24
1	L	137	GLN	CD-NE2	-5.08	1.20	1.32
1	1	172	ASN	CG-OD1	-5.08	1.12	1.24
1	I	172	ASN	CG-OD1	-5.08	1.12	1.24
1	g	172	ASN	CG-OD1	-5.02	1.12	1.24
1	M	172	ASN	CG-OD1	-5.01	1.12	1.24
1	R	172	ASN	CG-OD1	-5.00	1.12	1.24
1	2	172	ASN	CG-OD1	-5.00	1.12	1.24
1	d	172	ASN	CG-OD1	-5.00	1.12	1.24

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	193	ASN	Sidechain
1	B	193	ASN	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	0	2884	0	2841	22	0
1	1	2884	0	2841	26	0
1	2	2884	0	2841	23	0
1	3	2884	0	2841	24	0
1	4	2884	0	2841	24	0
1	5	2884	0	2841	23	0
1	A	2884	0	2841	30	0
1	B	2884	0	2841	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2884	0	2841	30	0
1	D	2884	0	2841	31	0
1	E	2884	0	2841	29	0
1	F	2884	0	2841	30	0
1	G	2884	0	2841	33	0
1	H	2884	0	2841	30	0
1	I	2884	0	2841	31	0
1	J	2884	0	2841	30	0
1	K	2884	0	2841	31	0
1	L	2884	0	2841	30	0
1	M	2884	0	2841	27	0
1	N	2884	0	2841	26	0
1	O	2884	0	2841	29	0
1	P	2884	0	2841	29	0
1	Q	2884	0	2841	28	0
1	R	2884	0	2841	27	0
1	a	2884	0	2841	0	0
1	b	2884	0	2841	0	0
1	c	2884	0	2841	0	0
1	d	2884	0	2841	0	0
1	e	2884	0	2841	0	0
1	f	2884	0	2841	0	0
1	g	2884	0	2841	0	0
1	h	2884	0	2841	0	0
1	i	2884	0	2841	0	0
1	j	2884	0	2841	0	0
1	k	2884	0	2841	0	0
1	l	2884	0	2841	0	0
All	All	103824	0	102276	577	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 (577) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:220:SER:OG	1:L:269:ASN:OD1	2.11	0.69
1:4:220:SER:OG	1:4:269:ASN:OD1	2.11	0.69
1:5:220:SER:OG	1:5:269:ASN:OD1	2.11	0.68
1:D:148:GLU:OE2	1:O:75:ARG:NH2	2.27	0.68
1:O:220:SER:OG	1:O:269:ASN:OD1	2.12	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:220:SER:OG	1:N:269:ASN:OD1	2.12	0.68
1:R:220:SER:OG	1:R:269:ASN:OD1	2.12	0.68
1:1:220:SER:OG	1:1:269:ASN:OD1	2.11	0.68
1:E:220:SER:OG	1:E:269:ASN:OD1	2.12	0.68
1:F:220:SER:OG	1:F:269:ASN:OD1	2.12	0.68
1:I:220:SER:OG	1:I:269:ASN:OD1	2.12	0.68
1:G:220:SER:OG	1:G:269:ASN:OD1	2.12	0.68
1:B:220:SER:OG	1:B:269:ASN:OD1	2.12	0.67
1:H:220:SER:OG	1:H:269:ASN:OD1	2.12	0.67
1:J:220:SER:OG	1:J:269:ASN:OD1	2.12	0.67
1:K:220:SER:OG	1:K:269:ASN:OD1	2.12	0.67
1:C:220:SER:OG	1:C:269:ASN:OD1	2.12	0.67
1:A:220:SER:OG	1:A:269:ASN:OD1	2.12	0.67
1:3:220:SER:OG	1:3:269:ASN:OD1	2.12	0.67
1:Q:220:SER:OG	1:Q:269:ASN:OD1	2.12	0.67
1:M:220:SER:OG	1:M:269:ASN:OD1	2.12	0.67
1:2:220:SER:OG	1:2:269:ASN:OD1	2.12	0.67
1:4:148:GLU:OE2	1:J:75:ARG:NH2	2.28	0.67
1:0:220:SER:OG	1:0:269:ASN:OD1	2.12	0.67
1:D:220:SER:OG	1:D:269:ASN:OD1	2.12	0.67
1:E:75:ARG:NH2	1:L:148:GLU:OE2	132.74	0.67
1:P:220:SER:OG	1:P:269:ASN:OD1	2.12	0.67
1:K:75:ARG:NH2	1:R:148:GLU:OE2	132.74	0.66
1:G:75:ARG:NH2	1:N:148:GLU:OE2	132.76	0.66
1:C:148:GLU:OE2	1:N:75:ARG:NH2	2.28	0.66
1:E:148:GLU:OE2	1:P:75:ARG:NH2	2.29	0.66
1:A:148:GLU:OE2	1:R:75:ARG:NH2	2.28	0.66
1:L:75:ARG:NH2	1:M:148:GLU:OE2	132.72	0.66
1:F:148:GLU:OE2	1:Q:75:ARG:NH2	2.28	0.66
1:O:124:GLN:OE1	1:O:126:ARG:NH2	2.29	0.66
1:J:75:ARG:NH2	1:Q:148:GLU:OE2	132.72	0.65
1:H:75:ARG:NH2	1:O:148:GLU:OE2	132.73	0.65
1:D:124:GLN:OE1	1:D:126:ARG:NH2	2.29	0.65
1:F:75:ARG:NH2	1:G:148:GLU:OE2	132.73	0.65
1:A:75:ARG:NH2	1:H:148:GLU:OE2	132.73	0.65
1:J:124:GLN:OE1	1:J:126:ARG:NH2	2.29	0.65
1:M:124:GLN:OE1	1:M:126:ARG:NH2	2.30	0.65
1:5:148:GLU:OE2	1:K:75:ARG:NH2	2.29	0.65
1:1:148:GLU:OE2	1:G:75:ARG:NH2	2.29	0.65
1:C:75:ARG:NH2	1:J:148:GLU:OE2	132.73	0.65
1:2:124:GLN:OE1	1:2:126:ARG:NH2	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:124:GLN:OE1	1:L:126:ARG:NH2	2.30	0.65
1:E:124:GLN:OE1	1:E:126:ARG:NH2	2.30	0.65
1:A:124:GLN:OE1	1:A:126:ARG:NH2	2.30	0.65
1:I:124:GLN:OE1	1:I:126:ARG:NH2	2.30	0.65
1:R:124:GLN:OE1	1:R:126:ARG:NH2	2.30	0.65
1:F:124:GLN:OE1	1:F:126:ARG:NH2	2.30	0.65
1:B:148:GLU:OE2	1:M:75:ARG:NH2	2.29	0.65
1:C:124:GLN:OE1	1:C:126:ARG:NH2	2.30	0.65
1:K:124:GLN:OE1	1:K:126:ARG:NH2	2.30	0.65
1:G:124:GLN:OE1	1:G:126:ARG:NH2	2.30	0.65
1:D:75:ARG:NH2	1:K:148:GLU:OE2	132.70	0.65
1:3:148:GLU:OE2	1:I:75:ARG:NH2	2.30	0.65
1:5:124:GLN:OE1	1:5:126:ARG:NH2	2.30	0.65
1:B:124:GLN:OE1	1:B:126:ARG:NH2	2.29	0.65
1:2:148:GLU:OE2	1:H:75:ARG:NH2	2.29	0.65
1:P:124:GLN:OE1	1:P:126:ARG:NH2	2.29	0.65
1:B:75:ARG:NH2	1:I:148:GLU:OE2	132.74	0.65
1:1:124:GLN:OE1	1:1:126:ARG:NH2	2.30	0.64
1:4:124:GLN:OE1	1:4:126:ARG:NH2	2.30	0.64
1:N:124:GLN:OE1	1:N:126:ARG:NH2	2.30	0.64
1:0:124:GLN:OE1	1:0:126:ARG:NH2	2.30	0.64
1:Q:124:GLN:OE1	1:Q:126:ARG:NH2	2.30	0.64
1:H:124:GLN:OE1	1:H:126:ARG:NH2	2.30	0.64
1:I:75:ARG:NH2	1:P:148:GLU:OE2	132.69	0.64
1:3:124:GLN:OE1	1:3:126:ARG:NH2	2.30	0.64
1:0:148:GLU:OE2	1:L:75:ARG:NH2	2.30	0.63
1:E:182:ASP:OD2	1:E:234:ARG:NH1	2.34	0.61
1:J:182:ASP:OD2	1:J:234:ARG:NH1	2.34	0.61
1:Q:182:ASP:OD2	1:Q:234:ARG:NH1	2.34	0.61
1:L:182:ASP:OD2	1:L:234:ARG:NH1	2.34	0.61
1:F:182:ASP:OD2	1:F:234:ARG:NH1	2.34	0.61
1:4:182:ASP:OD2	1:4:234:ARG:NH1	2.34	0.61
1:I:182:ASP:OD2	1:I:234:ARG:NH1	2.34	0.61
1:D:182:ASP:OD2	1:D:234:ARG:NH1	2.34	0.60
1:R:182:ASP:OD2	1:R:234:ARG:NH1	2.34	0.60
1:P:182:ASP:OD2	1:P:234:ARG:NH1	2.34	0.60
1:C:182:ASP:OD2	1:C:234:ARG:NH1	2.34	0.60
1:K:182:ASP:OD2	1:K:234:ARG:NH1	2.34	0.60
1:O:182:ASP:OD2	1:O:234:ARG:NH1	2.34	0.60
1:0:182:ASP:OD2	1:0:234:ARG:NH1	2.34	0.60
1:5:182:ASP:OD2	1:5:234:ARG:NH1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:182:ASP:OD2	1:G:234:ARG:NH1	2.34	0.60
1:1:182:ASP:OD2	1:1:234:ARG:NH1	2.34	0.60
1:B:182:ASP:OD2	1:B:234:ARG:NH1	2.34	0.60
1:H:182:ASP:OD2	1:H:234:ARG:NH1	2.34	0.60
1:A:182:ASP:OD2	1:A:234:ARG:NH1	2.34	0.59
1:H:160:ASN:O	1:H:162:THR:N	2.36	0.59
1:M:182:ASP:OD2	1:M:234:ARG:NH1	2.34	0.59
1:3:182:ASP:OD2	1:3:234:ARG:NH1	2.34	0.59
1:G:160:ASN:O	1:G:162:THR:N	2.36	0.59
1:L:160:ASN:O	1:L:162:THR:N	2.36	0.59
1:I:160:ASN:O	1:I:162:THR:N	2.36	0.59
1:2:182:ASP:OD2	1:2:234:ARG:NH1	2.34	0.59
1:N:160:ASN:O	1:N:162:THR:N	2.36	0.58
1:C:160:ASN:O	1:C:162:THR:N	2.36	0.58
1:N:182:ASP:OD2	1:N:234:ARG:NH1	2.34	0.58
1:3:160:ASN:O	1:3:162:THR:N	2.36	0.58
1:L:75:ARG:NH1	1:L:225:GLU:O	2.36	0.58
1:I:75:ARG:NH1	1:I:225:GLU:O	2.37	0.58
1:M:160:ASN:O	1:M:162:THR:N	2.36	0.58
1:A:160:ASN:O	1:A:162:THR:N	2.37	0.58
1:B:160:ASN:O	1:B:162:THR:N	2.36	0.58
1:D:160:ASN:O	1:D:162:THR:N	2.36	0.58
1:2:75:ARG:NH1	1:2:225:GLU:O	2.37	0.58
1:F:160:ASN:O	1:F:162:THR:N	2.36	0.58
1:O:75:ARG:NH1	1:O:225:GLU:O	2.37	0.58
1:K:75:ARG:NH1	1:K:225:GLU:O	2.37	0.58
1:G:75:ARG:NH1	1:G:225:GLU:O	2.37	0.58
1:5:160:ASN:O	1:5:162:THR:N	2.36	0.58
1:F:75:ARG:NH1	1:F:225:GLU:O	2.37	0.58
1:A:75:ARG:NH1	1:A:225:GLU:O	2.37	0.58
1:C:75:ARG:NH1	1:C:225:GLU:O	2.37	0.58
1:B:75:ARG:NH1	1:B:225:GLU:O	2.37	0.58
1:J:160:ASN:O	1:J:162:THR:N	2.36	0.58
1:J:75:ARG:NH1	1:J:225:GLU:O	2.37	0.58
1:M:75:ARG:NH1	1:M:225:GLU:O	2.37	0.58
1:P:160:ASN:O	1:P:162:THR:N	2.36	0.58
1:E:75:ARG:NH1	1:E:225:GLU:O	2.37	0.58
1:C:137:GLN:OE1	1:C:172:ASN:ND2	2.41	0.58
1:G:261:ASP:OD2	1:G:262:ASP:N	2.38	0.58
1:O:160:ASN:O	1:O:162:THR:N	2.36	0.58
1:E:160:ASN:O	1:E:162:THR:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:160:ASN:O	1:2:162:THR:N	2.36	0.58
1:H:75:ARG:NH1	1:H:225:GLU:O	2.37	0.57
1:D:75:ARG:NH1	1:D:225:GLU:O	2.37	0.57
1:K:160:ASN:O	1:K:162:THR:N	2.36	0.57
1:0:160:ASN:O	1:0:162:THR:N	2.36	0.57
1:R:160:ASN:O	1:R:162:THR:N	2.36	0.57
1:0:75:ARG:NH1	1:0:225:GLU:O	2.37	0.57
1:Q:160:ASN:O	1:Q:162:THR:N	2.37	0.57
1:H:261:ASP:OD2	1:H:262:ASP:N	2.38	0.57
1:5:75:ARG:NH1	1:5:225:GLU:O	2.37	0.57
1:N:75:ARG:NH1	1:N:225:GLU:O	2.37	0.57
1:P:75:ARG:NH1	1:P:225:GLU:O	2.37	0.57
1:R:75:ARG:NH1	1:R:225:GLU:O	2.37	0.57
1:Q:75:ARG:NH1	1:Q:225:GLU:O	2.37	0.57
1:A:137:GLN:OE1	1:A:172:ASN:ND2	2.37	0.57
1:1:75:ARG:NH1	1:1:225:GLU:O	2.37	0.57
1:I:261:ASP:OD2	1:I:262:ASP:N	2.38	0.57
1:3:261:ASP:OD2	1:3:262:ASP:N	2.38	0.57
1:R:261:ASP:OD2	1:R:262:ASP:N	2.38	0.57
1:1:261:ASP:OD2	1:1:262:ASP:N	2.38	0.57
1:Q:261:ASP:OD2	1:Q:262:ASP:N	2.38	0.57
1:E:261:ASP:OD2	1:E:262:ASP:N	2.38	0.57
1:L:261:ASP:OD2	1:L:262:ASP:N	2.38	0.57
1:1:160:ASN:O	1:1:162:THR:N	2.37	0.57
1:B:261:ASP:OD2	1:B:262:ASP:N	2.38	0.57
1:3:75:ARG:NH1	1:3:225:GLU:O	2.37	0.57
1:N:261:ASP:OD2	1:N:262:ASP:N	2.38	0.57
1:F:261:ASP:OD2	1:F:262:ASP:N	2.38	0.57
1:4:261:ASP:OD2	1:4:262:ASP:N	2.38	0.57
1:M:261:ASP:OD2	1:M:262:ASP:N	2.38	0.57
1:A:261:ASP:OD2	1:A:262:ASP:N	2.38	0.57
1:C:261:ASP:OD2	1:C:262:ASP:N	2.38	0.57
1:Q:137:GLN:OE1	1:Q:172:ASN:ND2	2.38	0.57
1:4:75:ARG:NH1	1:4:225:GLU:O	2.37	0.57
1:J:261:ASP:OD2	1:J:262:ASP:N	2.38	0.57
1:4:160:ASN:O	1:4:162:THR:N	2.36	0.56
1:D:261:ASP:OD2	1:D:262:ASP:N	2.38	0.56
1:K:261:ASP:OD2	1:K:262:ASP:N	2.38	0.56
1:O:261:ASP:OD2	1:O:262:ASP:N	2.38	0.56
1:5:261:ASP:OD2	1:5:262:ASP:N	2.38	0.56
1:2:261:ASP:OD2	1:2:262:ASP:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:261:ASP:OD2	1:P:262:ASP:N	2.38	0.56
1:0:261:ASP:OD2	1:0:262:ASP:N	2.38	0.56
1:B:190:SER:O	1:B:193:ASN:OD1	2.24	0.56
1:H:327:ASN:ND2	1:O:341:ASP:O	100.45	0.56
1:G:327:ASN:ND2	1:N:341:ASP:O	100.48	0.56
1:A:341:ASP:O	1:R:327:ASN:ND2	2.39	0.55
1:C:327:ASN:ND2	1:J:341:ASP:O	100.47	0.55
1:0:137:GLN:OE1	1:0:172:ASN:ND2	2.39	0.55
1:K:137:GLN:OE1	1:K:172:ASN:ND2	2.40	0.55
1:1:190:SER:O	1:1:193:ASN:OD1	2.23	0.55
1:E:341:ASP:O	1:P:327:ASN:ND2	2.40	0.55
1:E:327:ASN:ND2	1:L:341:ASP:O	100.48	0.55
1:K:327:ASN:ND2	1:R:341:ASP:O	100.49	0.55
1:5:137:GLN:OE1	1:5:172:ASN:ND2	2.38	0.55
1:A:185:VAL:HG12	1:A:200:ALA:HB2	1.89	0.55
1:R:185:VAL:HG12	1:R:200:ALA:HB2	1.89	0.55
1:N:185:VAL:HG12	1:N:200:ALA:HB2	1.89	0.54
1:K:185:VAL:HG12	1:K:200:ALA:HB2	1.91	0.54
1:G:137:GLN:OE1	1:G:172:ASN:ND2	2.40	0.54
1:L:185:VAL:HG12	1:L:200:ALA:HB2	1.96	0.54
1:C:341:ASP:O	1:N:327:ASN:ND2	2.40	0.54
1:H:185:VAL:HG12	1:H:200:ALA:HB2	1.89	0.54
1:E:185:VAL:HG12	1:E:200:ALA:HB2	1.94	0.54
1:3:185:VAL:HG12	1:3:200:ALA:HB2	1.89	0.54
1:J:327:ASN:ND2	1:Q:341:ASP:O	100.45	0.54
1:0:185:VAL:HG12	1:0:200:ALA:HB2	1.89	0.54
1:H:261:ASP:O	1:H:263:GLY:N	2.41	0.54
1:1:185:VAL:HG12	1:1:200:ALA:HB2	1.89	0.54
1:B:327:ASN:ND2	1:I:341:ASP:O	100.48	0.54
1:5:185:VAL:HG12	1:5:200:ALA:HB2	1.89	0.54
1:B:261:ASP:O	1:B:263:GLY:N	2.42	0.53
1:N:261:ASP:O	1:N:263:GLY:N	2.41	0.53
1:2:341:ASP:O	1:H:327:ASN:ND2	2.40	0.53
1:5:341:ASP:O	1:K:327:ASN:ND2	2.41	0.53
1:L:261:ASP:O	1:L:263:GLY:N	2.42	0.53
1:D:341:ASP:O	1:O:327:ASN:ND2	2.41	0.53
1:P:137:GLN:OE1	1:P:172:ASN:ND2	2.41	0.53
1:J:261:ASP:O	1:J:263:GLY:N	2.41	0.53
1:D:261:ASP:O	1:D:263:GLY:N	2.42	0.53
1:I:185:VAL:HG12	1:I:200:ALA:HB2	1.90	0.53
1:3:261:ASP:O	1:3:263:GLY:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261:ASP:O	1:C:263:GLY:N	2.42	0.53
1:F:261:ASP:O	1:F:263:GLY:N	2.42	0.53
1:O:261:ASP:O	1:O:263:GLY:N	2.41	0.53
1:4:341:ASP:O	1:J:327:ASN:ND2	2.41	0.53
1:I:261:ASP:O	1:I:263:GLY:N	2.42	0.53
1:A:327:ASN:ND2	1:H:341:ASP:O	100.46	0.53
1:4:185:VAL:HG12	1:4:200:ALA:HB2	1.90	0.53
1:G:261:ASP:O	1:G:263:GLY:N	2.41	0.53
1:F:341:ASP:O	1:Q:327:ASN:ND2	2.41	0.53
1:1:341:ASP:O	1:G:327:ASN:ND2	2.42	0.52
1:F:185:VAL:HG12	1:F:200:ALA:HB2	1.91	0.52
1:B:341:ASP:O	1:M:327:ASN:ND2	2.41	0.52
1:G:185:VAL:HG12	1:G:200:ALA:HB2	1.90	0.52
1:J:185:VAL:HG12	1:J:200:ALA:HB2	1.89	0.52
1:R:261:ASP:O	1:R:263:GLY:N	2.41	0.52
1:A:261:ASP:O	1:A:263:GLY:N	2.42	0.52
1:F:327:ASN:ND2	1:G:341:ASP:O	100.46	0.52
1:L:327:ASN:ND2	1:M:341:ASP:O	100.44	0.52
1:Q:261:ASP:O	1:Q:263:GLY:N	2.41	0.52
1:M:261:ASP:O	1:M:263:GLY:N	2.41	0.52
1:K:261:ASP:O	1:K:263:GLY:N	2.41	0.52
1:0:261:ASP:O	1:0:263:GLY:N	2.42	0.52
1:0:341:ASP:O	1:L:327:ASN:ND2	2.42	0.52
1:F:137:GLN:OE1	1:F:172:ASN:ND2	2.41	0.52
1:C:306:ILE:O	1:C:306:ILE:HG23	2.10	0.52
1:2:261:ASP:O	1:2:263:GLY:N	2.42	0.52
1:R:137:GLN:OE1	1:R:172:ASN:ND2	2.42	0.52
1:4:137:GLN:OE1	1:4:172:ASN:ND2	2.38	0.52
1:D:306:ILE:O	1:P:382:VAL:HG11	2.10	0.52
1:E:261:ASP:O	1:E:263:GLY:N	2.42	0.52
1:P:261:ASP:O	1:P:263:GLY:N	2.42	0.52
1:H:306:ILE:HG23	1:H:306:ILE:O	2.10	0.52
1:3:341:ASP:O	1:I:327:ASN:ND2	2.43	0.51
1:1:261:ASP:O	1:1:263:GLY:N	2.42	0.51
1:5:261:ASP:O	1:5:263:GLY:N	2.42	0.51
1:1:306:ILE:O	1:1:306:ILE:HG23	2.10	0.51
1:K:306:ILE:HG23	1:K:306:ILE:O	2.11	0.51
1:C:185:VAL:HG12	1:C:200:ALA:HB2	1.92	0.51
1:2:185:VAL:HG12	1:2:200:ALA:HB2	1.92	0.51
1:I:327:ASN:ND2	1:P:341:ASP:O	100.42	0.51
1:D:137:GLN:OE1	1:D:172:ASN:ND2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:327:ASN:ND2	1:K:341:ASP:O	100.42	0.51
1:4:306:ILE:O	1:4:306:ILE:HG23	2.11	0.51
1:P:306:ILE:HG23	1:P:306:ILE:O	2.11	0.51
1:4:261:ASP:O	1:4:263:GLY:N	2.42	0.51
1:D:185:VAL:HG12	1:D:200:ALA:HB2	1.93	0.50
1:2:137:GLN:OE1	1:2:172:ASN:ND2	2.39	0.50
1:M:306:ILE:O	1:M:306:ILE:HG23	2.11	0.50
1:C:382:VAL:HG11	1:I:306:ILE:O	104.34	0.50
1:O:185:VAL:HG12	1:O:200:ALA:HB2	1.93	0.50
1:B:306:ILE:O	1:N:382:VAL:HG11	2.12	0.50
1:O:306:ILE:HG23	1:O:306:ILE:O	2.11	0.50
1:Q:306:ILE:O	1:Q:306:ILE:HG23	2.11	0.50
1:A:382:VAL:HG11	1:G:306:ILE:O	104.29	0.50
1:I:137:GLN:OE1	1:I:172:ASN:ND2	2.45	0.49
1:M:185:VAL:HG12	1:M:200:ALA:HB2	1.95	0.49
1:Q:185:VAL:HG12	1:Q:200:ALA:HB2	1.94	0.49
1:5:306:ILE:O	1:L:382:VAL:HG11	2.12	0.49
1:A:22:PRO:O	1:A:24:SER:N	2.45	0.49
1:F:22:PRO:O	1:F:24:SER:N	2.45	0.49
1:B:137:GLN:OE1	1:B:172:ASN:ND2	2.46	0.49
1:B:185:VAL:HG12	1:B:200:ALA:HB2	1.95	0.49
1:1:22:PRO:O	1:1:24:SER:N	2.46	0.49
1:2:22:PRO:O	1:2:24:SER:N	2.46	0.49
1:E:306:ILE:O	1:Q:382:VAL:HG11	2.13	0.48
1:F:382:VAL:HG11	1:L:306:ILE:O	104.35	0.48
1:0:306:ILE:O	1:G:382:VAL:HG11	2.12	0.48
1:P:185:VAL:HG12	1:P:200:ALA:HB2	1.95	0.48
1:C:22:PRO:O	1:C:24:SER:N	2.45	0.48
1:3:306:ILE:O	1:J:382:VAL:HG11	2.14	0.48
1:E:22:PRO:O	1:E:24:SER:N	2.45	0.48
1:B:22:PRO:O	1:B:24:SER:N	2.45	0.48
1:K:178:LEU:O	1:K:271:THR:OG1	2.27	0.48
1:0:22:PRO:O	1:0:24:SER:N	2.45	0.48
1:1:137:GLN:OE1	1:1:172:ASN:ND2	2.46	0.48
1:G:22:PRO:O	1:G:24:SER:N	2.45	0.48
1:2:375:THR:OG1	1:2:376:ASP:N	2.47	0.48
1:L:22:PRO:O	1:L:24:SER:N	2.46	0.48
1:3:375:THR:OG1	1:3:376:ASP:N	2.47	0.48
1:M:375:THR:OG1	1:M:376:ASP:N	2.47	0.48
1:J:375:THR:OG1	1:J:376:ASP:N	2.47	0.48
1:D:375:THR:OG1	1:D:376:ASP:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:382:VAL:HG11	1:J:306:ILE:O	104.32	0.48
1:G:375:THR:OG1	1:G:376:ASP:N	2.47	0.48
1:K:271:THR:O	1:K:273:SER:N	2.48	0.47
1:C:375:THR:OG1	1:C:376:ASP:N	2.47	0.47
1:2:271:THR:O	1:2:273:SER:N	2.47	0.47
1:M:271:THR:O	1:M:273:SER:N	2.48	0.47
1:5:271:THR:O	1:5:273:SER:N	2.47	0.47
1:H:271:THR:O	1:H:273:SER:N	2.47	0.47
1:N:271:THR:O	1:N:273:SER:N	2.47	0.47
1:B:271:THR:O	1:B:273:SER:N	2.48	0.47
1:I:271:THR:O	1:I:273:SER:N	2.47	0.47
1:L:306:ILE:HG22	1:R:363:PRO:O	2.14	0.47
1:A:271:THR:O	1:A:273:SER:N	2.47	0.47
1:K:22:PRO:O	1:K:24:SER:N	2.46	0.47
1:1:271:THR:O	1:1:273:SER:N	2.47	0.47
1:Q:271:THR:O	1:Q:273:SER:N	2.47	0.47
1:G:271:THR:O	1:G:273:SER:N	2.48	0.47
1:E:271:THR:O	1:E:273:SER:N	2.47	0.47
1:R:271:THR:O	1:R:273:SER:N	2.48	0.47
1:J:271:THR:O	1:J:273:SER:N	2.47	0.47
1:C:271:THR:O	1:C:273:SER:N	2.47	0.47
1:2:306:ILE:O	1:I:382:VAL:HG11	2.15	0.47
1:2:178:LEU:O	1:2:271:THR:OG1	2.26	0.47
1:A:306:ILE:O	1:M:382:VAL:HG11	2.13	0.47
1:I:319:ARG:NH1	1:I:336:VAL:O	2.48	0.47
1:P:22:PRO:O	1:P:24:SER:N	2.46	0.47
1:A:363:PRO:O	1:0:306:ILE:HG22	2.15	0.47
1:A:306:ILE:HG22	1:G:363:PRO:O	2.17	0.47
1:L:271:THR:O	1:L:273:SER:N	2.48	0.47
1:J:319:ARG:NH1	1:J:336:VAL:O	2.48	0.47
1:A:375:THR:OG1	1:A:376:ASP:N	2.47	0.47
1:D:271:THR:O	1:D:273:SER:N	2.47	0.47
1:G:319:ARG:NH1	1:G:336:VAL:O	2.48	0.47
1:E:375:THR:OG1	1:E:376:ASP:N	2.47	0.47
1:F:271:THR:O	1:F:273:SER:N	2.47	0.47
1:N:319:ARG:NH1	1:N:336:VAL:O	2.48	0.47
1:O:319:ARG:NH1	1:O:336:VAL:O	2.48	0.47
1:O:271:THR:O	1:O:273:SER:N	2.48	0.47
1:K:319:ARG:NH1	1:K:336:VAL:O	2.48	0.47
1:L:382:VAL:HG11	1:R:306:ILE:O	104.33	0.47
1:I:178:LEU:O	1:I:271:THR:OG1	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:319:ARG:NH1	1:M:336:VAL:O	2.48	0.47
1:0:319:ARG:NH1	1:0:336:VAL:O	2.48	0.47
1:F:375:THR:OG1	1:F:376:ASP:N	2.47	0.47
1:F:306:ILE:O	1:R:382:VAL:HG11	2.14	0.47
1:5:22:PRO:O	1:5:24:SER:N	2.45	0.47
1:G:42:LYS:HB2	1:G:45:VAL:HG22	1.99	0.47
1:H:375:THR:OG1	1:H:376:ASP:N	2.47	0.47
1:B:375:THR:OG1	1:B:376:ASP:N	2.47	0.47
1:E:306:ILE:HG22	1:K:363:PRO:O	2.15	0.47
1:K:42:LYS:HB2	1:K:45:VAL:HG22	1.97	0.47
1:E:42:LYS:HB2	1:E:45:VAL:HG22	1.98	0.47
1:H:319:ARG:NH1	1:H:336:VAL:O	2.48	0.47
1:C:319:ARG:NH1	1:C:336:VAL:O	2.49	0.47
1:R:42:LYS:HB2	1:R:45:VAL:HG22	1.97	0.47
1:4:375:THR:OG1	1:4:376:ASP:N	2.47	0.47
1:P:271:THR:O	1:P:273:SER:N	2.48	0.47
1:I:22:PRO:O	1:I:24:SER:N	2.46	0.47
1:F:363:PRO:O	1:R:306:ILE:HG22	110.29	0.47
1:D:22:PRO:O	1:D:24:SER:N	2.45	0.47
1:B:319:ARG:NH1	1:B:336:VAL:O	2.48	0.47
1:C:42:LYS:HB2	1:C:45:VAL:HG22	1.99	0.47
1:F:319:ARG:NH1	1:F:336:VAL:O	2.48	0.47
1:J:22:PRO:O	1:J:24:SER:N	2.46	0.46
1:P:319:ARG:NH1	1:P:336:VAL:O	2.49	0.46
1:I:375:THR:OG1	1:I:376:ASP:N	2.48	0.46
1:Q:22:PRO:O	1:Q:24:SER:N	2.45	0.46
1:A:319:ARG:NH1	1:A:336:VAL:O	2.49	0.46
1:L:375:THR:OG1	1:L:376:ASP:N	2.48	0.46
1:A:42:LYS:HB2	1:A:45:VAL:HG22	1.97	0.46
1:2:42:LYS:HB2	1:2:45:VAL:HG22	1.98	0.46
1:4:271:THR:O	1:4:273:SER:N	2.48	0.46
1:5:42:LYS:HB2	1:5:45:VAL:HG22	1.98	0.46
1:N:375:THR:OG1	1:N:376:ASP:N	2.47	0.46
1:N:42:LYS:HB2	1:N:45:VAL:HG22	1.98	0.46
1:Q:319:ARG:NH1	1:Q:336:VAL:O	2.48	0.46
1:0:375:THR:OG1	1:0:376:ASP:N	2.47	0.46
1:R:319:ARG:NH1	1:R:336:VAL:O	2.49	0.46
1:E:319:ARG:NH1	1:E:336:VAL:O	2.47	0.46
1:M:178:LEU:O	1:M:271:THR:OG1	2.27	0.46
1:H:178:LEU:O	1:H:271:THR:OG1	2.27	0.46
1:Q:42:LYS:HB2	1:Q:45:VAL:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:271:THR:O	1:3:273:SER:N	2.48	0.46
1:0:271:THR:O	1:0:273:SER:N	2.48	0.46
1:J:42:LYS:HB2	1:J:45:VAL:HG22	1.99	0.46
1:G:178:LEU:O	1:G:271:THR:OG1	2.28	0.46
1:K:375:THR:OG1	1:K:376:ASP:N	2.48	0.46
1:H:42:LYS:HB2	1:H:45:VAL:HG22	1.98	0.46
1:L:319:ARG:NH1	1:L:336:VAL:O	2.49	0.46
1:B:363:PRO:O	1:N:306:ILE:HG22	110.28	0.46
1:4:319:ARG:NH1	1:4:336:VAL:O	2.49	0.46
1:L:42:LYS:HB2	1:L:45:VAL:HG22	1.98	0.46
1:O:22:PRO:O	1:O:24:SER:N	2.45	0.46
1:D:319:ARG:NH1	1:D:336:VAL:O	2.49	0.46
1:3:319:ARG:NH1	1:3:336:VAL:O	2.48	0.46
1:B:42:LYS:HB2	1:B:45:VAL:HG22	1.98	0.46
1:D:42:LYS:HB2	1:D:45:VAL:HG22	1.98	0.46
1:F:42:LYS:HB2	1:F:45:VAL:HG22	1.98	0.46
1:H:22:PRO:O	1:H:24:SER:N	2.46	0.46
1:O:42:LYS:HB2	1:O:45:VAL:HG22	1.98	0.46
1:D:178:LEU:O	1:D:271:THR:OG1	2.26	0.46
1:1:375:THR:OG1	1:1:376:ASP:N	2.47	0.46
1:P:42:LYS:HB2	1:P:45:VAL:HG22	1.98	0.46
1:B:363:PRO:O	1:1:306:ILE:HG22	2.17	0.45
1:H:382:VAL:HG11	1:N:306:ILE:O	104.35	0.45
1:C:178:LEU:O	1:C:271:THR:OG1	2.27	0.45
1:I:42:LYS:HB2	1:I:45:VAL:HG22	1.98	0.45
1:1:319:ARG:NH1	1:1:336:VAL:O	2.48	0.45
1:5:375:THR:OG1	1:5:376:ASP:N	2.47	0.45
1:E:363:PRO:O	1:4:306:ILE:HG22	2.16	0.45
1:5:319:ARG:NH1	1:5:336:VAL:O	2.49	0.45
1:2:319:ARG:NH1	1:2:336:VAL:O	2.49	0.45
1:M:42:LYS:HB2	1:M:45:VAL:HG22	1.98	0.45
1:D:306:ILE:O	1:D:306:ILE:HG23	2.17	0.45
1:5:306:ILE:O	1:5:306:ILE:HG23	2.17	0.45
1:1:42:LYS:HB2	1:1:45:VAL:HG22	1.98	0.45
1:I:306:ILE:HG22	1:O:363:PRO:O	2.16	0.45
1:3:42:LYS:HB2	1:3:45:VAL:HG22	1.99	0.45
1:4:42:LYS:HB2	1:4:45:VAL:HG22	1.99	0.45
1:G:306:ILE:HG23	1:G:306:ILE:O	2.17	0.45
1:N:22:PRO:O	1:N:24:SER:N	2.45	0.45
1:1:333:ASN:OD1	1:1:334:PHE:N	2.50	0.45
1:K:147:ALA:O	1:K:151:ARG:N	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:363:PRO:O	1:2:306:ILE:HG22	2.17	0.45
1:N:147:ALA:O	1:N:151:ARG:N	2.50	0.45
1:B:333:ASN:OD1	1:B:334:PHE:N	2.50	0.45
1:C:306:ILE:HG22	1:I:363:PRO:O	2.17	0.45
1:0:306:ILE:HG23	1:0:306:ILE:O	2.17	0.45
1:G:306:ILE:HG22	1:M:363:PRO:O	2.17	0.45
1:A:178:LEU:O	1:A:271:THR:OG1	2.28	0.45
1:A:306:ILE:HG23	1:A:306:ILE:O	2.17	0.45
1:L:178:LEU:O	1:L:271:THR:OG1	2.26	0.45
1:3:178:LEU:O	1:3:271:THR:OG1	2.27	0.45
1:0:333:ASN:OD1	1:0:334:PHE:N	2.50	0.45
1:G:147:ALA:O	1:G:151:ARG:N	2.50	0.45
1:E:306:ILE:O	1:E:306:ILE:HG23	2.17	0.45
1:L:306:ILE:O	1:L:306:ILE:HG23	2.17	0.45
1:Q:375:THR:OG1	1:Q:376:ASP:N	2.47	0.45
1:4:22:PRO:O	1:4:24:SER:N	2.46	0.45
1:L:147:ALA:O	1:L:151:ARG:N	2.50	0.45
1:M:147:ALA:O	1:M:151:ARG:N	2.51	0.45
1:I:306:ILE:O	1:I:306:ILE:HG23	2.17	0.44
1:2:306:ILE:HG23	1:2:306:ILE:O	2.17	0.44
1:R:306:ILE:HG23	1:R:306:ILE:O	2.17	0.44
1:F:147:ALA:O	1:F:151:ARG:N	2.50	0.44
1:E:333:ASN:OD1	1:E:334:PHE:N	2.50	0.44
1:D:363:PRO:O	1:P:306:ILE:HG22	110.23	0.44
1:B:306:ILE:HG23	1:B:306:ILE:O	2.17	0.44
1:F:178:LEU:O	1:F:271:THR:OG1	2.28	0.44
1:B:147:ALA:O	1:B:151:ARG:N	2.50	0.44
1:C:147:ALA:O	1:C:151:ARG:N	2.50	0.44
1:F:333:ASN:OD1	1:F:334:PHE:N	2.50	0.44
1:B:178:LEU:O	1:B:271:THR:OG1	2.27	0.44
1:A:147:ALA:O	1:A:151:ARG:N	2.51	0.44
1:H:147:ALA:O	1:H:151:ARG:N	2.51	0.44
1:J:147:ALA:O	1:J:151:ARG:N	2.51	0.44
1:D:147:ALA:O	1:D:151:ARG:N	2.51	0.44
1:2:147:ALA:O	1:2:151:ARG:N	2.51	0.44
1:0:42:LYS:HB2	1:0:45:VAL:HG22	1.99	0.44
1:4:333:ASN:OD1	1:4:334:PHE:N	2.50	0.44
1:J:306:ILE:HG22	1:P:363:PRO:O	2.16	0.44
1:4:178:LEU:O	1:4:271:THR:OG1	2.27	0.44
1:O:375:THR:OG1	1:O:376:ASP:N	2.48	0.44
1:L:333:ASN:OD1	1:L:334:PHE:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:333:ASN:OD1	1:I:334:PHE:N	2.50	0.44
1:C:333:ASN:OD1	1:C:334:PHE:N	2.50	0.44
1:R:333:ASN:OD1	1:R:334:PHE:N	2.50	0.44
1:E:363:PRO:O	1:Q:306:ILE:HG22	110.25	0.44
1:J:306:ILE:HG23	1:J:306:ILE:O	2.17	0.44
1:E:178:LEU:O	1:E:271:THR:OG1	2.27	0.44
1:H:333:ASN:OD1	1:H:334:PHE:N	2.50	0.44
1:O:333:ASN:OD1	1:O:334:PHE:N	2.50	0.44
1:I:147:ALA:O	1:I:151:ARG:N	2.51	0.44
1:3:147:ALA:O	1:3:151:ARG:N	2.51	0.44
1:J:178:LEU:O	1:J:271:THR:OG1	2.27	0.44
1:E:147:ALA:O	1:E:151:ARG:N	2.50	0.44
1:3:22:PRO:O	1:3:24:SER:N	2.45	0.44
1:R:147:ALA:O	1:R:151:ARG:N	2.51	0.44
1:C:363:PRO:O	1:O:306:ILE:HG22	110.24	0.44
1:5:147:ALA:O	1:5:151:ARG:N	2.51	0.44
1:1:147:ALA:O	1:1:151:ARG:N	2.51	0.44
1:3:306:ILE:O	1:3:306:ILE:HG23	2.17	0.43
1:B:306:ILE:HG22	1:H:363:PRO:O	2.20	0.43
1:G:333:ASN:OD1	1:G:334:PHE:N	2.50	0.43
1:M:22:PRO:O	1:M:24:SER:N	2.45	0.43
1:Q:333:ASN:OD1	1:Q:334:PHE:N	2.50	0.43
1:4:147:ALA:O	1:4:151:ARG:N	2.50	0.43
1:Q:147:ALA:O	1:Q:151:ARG:N	2.50	0.43
1:R:22:PRO:O	1:R:24:SER:N	2.46	0.43
1:O:147:ALA:O	1:O:151:ARG:N	2.50	0.43
1:2:333:ASN:OD1	1:2:334:PHE:N	2.50	0.43
1:F:306:ILE:HG23	1:F:306:ILE:O	2.17	0.43
1:F:306:ILE:HG22	1:L:363:PRO:O	2.21	0.43
1:H:306:ILE:HG22	1:N:363:PRO:O	2.18	0.43
1:K:306:ILE:HG22	1:Q:363:PRO:O	2.19	0.43
1:A:333:ASN:OD1	1:A:334:PHE:N	2.50	0.43
1:R:375:THR:OG1	1:R:376:ASP:N	2.48	0.43
1:D:306:ILE:HG22	1:J:363:PRO:O	2.18	0.43
1:N:306:ILE:O	1:N:306:ILE:HG23	2.18	0.43
1:O:178:LEU:O	1:O:271:THR:OG1	2.27	0.43
1:P:147:ALA:O	1:P:151:ARG:N	2.51	0.43
1:K:333:ASN:OD1	1:K:334:PHE:N	2.50	0.43
1:N:333:ASN:OD1	1:N:334:PHE:N	2.50	0.43
1:0:147:ALA:O	1:0:151:ARG:N	2.51	0.43
1:B:382:VAL:HG11	1:H:306:ILE:O	104.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:333:ASN:OD1	1:M:334:PHE:N	2.50	0.42
1:P:333:ASN:OD1	1:P:334:PHE:N	2.50	0.42
1:A:363:PRO:O	1:M:306:ILE:HG22	110.23	0.42
1:K:307:THR:HG22	1:K:308:LYS:N	2.35	0.42
1:J:333:ASN:OD1	1:J:334:PHE:N	2.50	0.42
1:D:363:PRO:O	1:3:306:ILE:HG22	2.18	0.42
1:P:375:THR:OG1	1:P:376:ASP:N	2.48	0.42
1:R:178:LEU:O	1:R:271:THR:OG1	2.27	0.42
1:D:333:ASN:OD1	1:D:334:PHE:N	2.50	0.42
1:C:306:ILE:O	1:O:382:VAL:HG11	2.20	0.42
1:5:333:ASN:OD1	1:5:334:PHE:N	2.50	0.42
1:1:116:ASP:N	1:1:116:ASP:OD2	2.53	0.42
1:F:363:PRO:O	1:5:306:ILE:HG22	2.19	0.42
1:M:116:ASP:OD2	1:M:116:ASP:N	2.53	0.42
1:3:333:ASN:OD1	1:3:334:PHE:N	2.50	0.42
1:4:307:THR:HG22	1:4:308:LYS:N	2.35	0.42
1:C:116:ASP:OD2	1:C:116:ASP:N	2.54	0.42
1:D:116:ASP:N	1:D:116:ASP:OD2	2.53	0.42
1:E:116:ASP:OD2	1:E:116:ASP:N	2.53	0.42
1:1:178:LEU:O	1:1:271:THR:OG1	2.28	0.41
1:G:307:THR:HG22	1:G:308:LYS:N	2.36	0.41
1:P:307:THR:HG22	1:P:308:LYS:N	2.35	0.41
1:J:307:THR:HG22	1:J:308:LYS:N	2.36	0.41
1:3:86:GLU:N	1:3:86:GLU:OE1	2.50	0.41
1:O:307:THR:HG22	1:O:308:LYS:N	2.35	0.41
1:2:116:ASP:OD2	1:2:116:ASP:N	2.53	0.41
1:3:116:ASP:N	1:3:116:ASP:OD2	2.53	0.41
1:L:116:ASP:N	1:L:116:ASP:OD2	2.54	0.41
1:4:116:ASP:N	1:4:116:ASP:OD2	2.53	0.41
1:H:307:THR:HG22	1:H:308:LYS:N	2.35	0.41
1:B:307:THR:HG22	1:B:308:LYS:N	2.35	0.41
1:I:307:THR:HG22	1:I:308:LYS:N	2.35	0.41
1:R:307:THR:HG22	1:R:308:LYS:N	2.36	0.41
1:F:307:THR:HG22	1:F:308:LYS:N	2.36	0.41
1:G:86:GLU:OE1	1:G:86:GLU:N	2.51	0.41
1:H:116:ASP:OD2	1:H:116:ASP:N	2.54	0.41
1:I:116:ASP:OD2	1:I:116:ASP:N	2.53	0.41
1:F:116:ASP:N	1:F:116:ASP:OD2	2.53	0.41
1:E:307:THR:HG22	1:E:308:LYS:N	2.36	0.41
1:J:116:ASP:OD2	1:J:116:ASP:N	2.54	0.41
1:G:116:ASP:N	1:G:116:ASP:OD2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:382:VAL:HG11	1:P:306:ILE:O	104.41	0.41
1:1:307:THR:HG22	1:1:308:LYS:N	2.35	0.41
1:P:302:VAL:HG12	1:P:303:ASP:H	1.85	0.41
1:E:382:VAL:HG11	1:K:306:ILE:O	104.40	0.41
1:0:307:THR:HG22	1:0:308:LYS:N	2.36	0.41
1:L:307:THR:HG22	1:L:308:LYS:N	2.36	0.41
1:Q:116:ASP:OD2	1:Q:116:ASP:N	2.54	0.41
1:K:116:ASP:OD2	1:K:116:ASP:N	2.54	0.41
1:C:307:THR:HG22	1:C:308:LYS:N	2.36	0.41
1:A:307:THR:HG22	1:A:308:LYS:N	2.36	0.41
1:A:116:ASP:OD2	1:A:116:ASP:N	2.54	0.41
1:D:307:THR:HG22	1:D:308:LYS:N	2.35	0.41
1:Q:307:THR:HG22	1:Q:308:LYS:N	2.35	0.41
1:5:116:ASP:N	1:5:116:ASP:OD2	2.54	0.41
1:D:308:LYS:N	1:P:382:VAL:HG13	2.36	0.41
1:3:307:THR:HG22	1:3:308:LYS:N	2.36	0.41
1:B:86:GLU:N	1:B:86:GLU:OE1	2.51	0.41
1:N:307:THR:HG22	1:N:308:LYS:N	2.36	0.41
1:A:302:VAL:HG12	1:A:303:ASP:H	1.86	0.41
1:E:302:VAL:HG12	1:E:303:ASP:H	1.85	0.41
1:G:302:VAL:HG12	1:G:303:ASP:H	1.86	0.41
1:1:306:ILE:O	1:H:382:VAL:HG11	2.20	0.41
1:M:307:THR:HG22	1:M:308:LYS:N	2.35	0.41
1:M:86:GLU:N	1:M:86:GLU:OE1	2.51	0.41
1:B:116:ASP:OD2	1:B:116:ASP:N	2.54	0.41
1:5:307:THR:HG22	1:5:308:LYS:N	2.36	0.41
1:P:116:ASP:OD2	1:P:116:ASP:N	2.53	0.41
1:C:308:LYS:N	1:O:382:VAL:HG13	2.36	0.40
1:D:302:VAL:HG12	1:D:303:ASP:H	1.85	0.40
1:N:116:ASP:OD2	1:N:116:ASP:N	2.54	0.40
1:Q:81:VAL:O	1:Q:81:VAL:HG13	2.21	0.40
1:I:382:VAL:HG11	1:O:306:ILE:O	104.39	0.40
1:F:302:VAL:HG12	1:F:303:ASP:H	1.86	0.40
1:O:86:GLU:N	1:O:86:GLU:OE1	2.50	0.40
1:K:382:VAL:HG11	1:Q:306:ILE:O	104.44	0.40
1:4:306:ILE:O	1:K:382:VAL:HG11	2.22	0.40
1:1:223:ASN:N	1:1:266:LEU:O	2.54	0.40
1:O:116:ASP:N	1:O:116:ASP:OD2	2.54	0.40
1:G:81:VAL:O	1:G:81:VAL:HG13	2.21	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	0	381/386 (99%)	307 (81%)	57 (15%)	17 (4%)	3	33
1	1	381/386 (99%)	307 (81%)	57 (15%)	17 (4%)	3	33
1	2	381/386 (99%)	307 (81%)	57 (15%)	17 (4%)	3	33
1	3	381/386 (99%)	307 (81%)	57 (15%)	17 (4%)	3	33
1	4	381/386 (99%)	308 (81%)	56 (15%)	17 (4%)	3	33
1	5	381/386 (99%)	309 (81%)	55 (14%)	17 (4%)	3	33
1	A	381/386 (99%)	309 (81%)	54 (14%)	18 (5%)	3	33
1	B	381/386 (99%)	307 (81%)	56 (15%)	18 (5%)	3	33
1	C	381/386 (99%)	307 (81%)	56 (15%)	18 (5%)	3	33
1	D	381/386 (99%)	308 (81%)	55 (14%)	18 (5%)	3	33
1	E	381/386 (99%)	308 (81%)	56 (15%)	17 (4%)	3	33
1	F	381/386 (99%)	306 (80%)	57 (15%)	18 (5%)	3	33
1	G	381/386 (99%)	308 (81%)	55 (14%)	18 (5%)	3	33
1	H	381/386 (99%)	309 (81%)	54 (14%)	18 (5%)	3	33
1	I	381/386 (99%)	307 (81%)	56 (15%)	18 (5%)	3	33
1	J	381/386 (99%)	308 (81%)	55 (14%)	18 (5%)	3	33
1	K	381/386 (99%)	309 (81%)	54 (14%)	18 (5%)	3	33
1	L	381/386 (99%)	308 (81%)	55 (14%)	18 (5%)	3	33
1	M	381/386 (99%)	309 (81%)	54 (14%)	18 (5%)	3	33
1	N	381/386 (99%)	307 (81%)	56 (15%)	18 (5%)	3	33
1	O	381/386 (99%)	309 (81%)	54 (14%)	18 (5%)	3	33
1	P	381/386 (99%)	309 (81%)	54 (14%)	18 (5%)	3	33
1	Q	381/386 (99%)	308 (81%)	55 (14%)	18 (5%)	3	33
1	R	381/386 (99%)	307 (81%)	56 (15%)	18 (5%)	3	33
1	a	381/386 (99%)	308 (81%)	55 (14%)	18 (5%)	3	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	b	381/386 (99%)	309 (81%)	54 (14%)	18 (5%)	3	33
1	c	381/386 (99%)	307 (81%)	56 (15%)	18 (5%)	3	33
1	d	381/386 (99%)	307 (81%)	56 (15%)	18 (5%)	3	33
1	e	381/386 (99%)	308 (81%)	55 (14%)	18 (5%)	3	33
1	f	381/386 (99%)	308 (81%)	55 (14%)	18 (5%)	3	33
1	g	381/386 (99%)	308 (81%)	55 (14%)	18 (5%)	3	33
1	h	381/386 (99%)	308 (81%)	55 (14%)	18 (5%)	3	33
1	i	381/386 (99%)	308 (81%)	55 (14%)	18 (5%)	3	33
1	j	381/386 (99%)	308 (81%)	55 (14%)	18 (5%)	3	33
1	k	381/386 (99%)	308 (81%)	55 (14%)	18 (5%)	3	33
1	l	381/386 (99%)	307 (81%)	56 (15%)	18 (5%)	3	33
All	All	13716/13896 (99%)	11082 (81%)	1993 (14%)	641 (5%)	5	33

All (641) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	VAL
1	B	9	VAL
1	F	9	VAL
1	E	9	VAL
1	D	9	VAL
1	C	9	VAL
1	0	9	VAL
1	1	9	VAL
1	5	9	VAL
1	4	9	VAL
1	3	9	VAL
1	2	9	VAL
1	G	9	VAL
1	H	9	VAL
1	L	9	VAL
1	K	9	VAL
1	J	9	VAL
1	I	9	VAL
1	M	9	VAL
1	N	9	VAL
1	R	9	VAL
1	Q	9	VAL

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Mol	Chain	Res	Type
1	P	9	VAL
1	O	9	VAL
1	a	9	VAL
1	b	9	VAL
1	f	9	VAL
1	e	9	VAL
1	d	9	VAL
1	c	9	VAL
1	g	9	VAL
1	h	9	VAL
1	l	9	VAL
1	k	9	VAL
1	j	9	VAL
1	i	9	VAL
1	A	7	VAL
1	A	102	ILE
1	A	160	ASN
1	A	161	SER
1	A	263	GLY
1	A	301	ALA
1	A	302	VAL
1	B	7	VAL
1	B	102	ILE
1	B	160	ASN
1	B	161	SER
1	B	263	GLY
1	B	301	ALA
1	B	302	VAL
1	F	7	VAL
1	F	102	ILE
1	F	160	ASN
1	F	161	SER
1	F	263	GLY
1	F	301	ALA
1	F	302	VAL
1	E	7	VAL
1	E	102	ILE
1	E	160	ASN
1	E	161	SER
1	E	263	GLY
1	E	301	ALA
1	E	302	VAL

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Mol	Chain	Res	Type
1	D	7	VAL
1	D	102	ILE
1	D	160	ASN
1	D	161	SER
1	D	263	GLY
1	D	301	ALA
1	D	302	VAL
1	C	7	VAL
1	C	102	ILE
1	C	160	ASN
1	C	161	SER
1	C	263	GLY
1	C	301	ALA
1	C	302	VAL
1	0	7	VAL
1	0	102	ILE
1	0	160	ASN
1	0	161	SER
1	0	263	GLY
1	0	301	ALA
1	0	302	VAL
1	1	7	VAL
1	1	102	ILE
1	1	160	ASN
1	1	161	SER
1	1	263	GLY
1	1	301	ALA
1	1	302	VAL
1	5	7	VAL
1	5	102	ILE
1	5	160	ASN
1	5	161	SER
1	5	263	GLY
1	5	301	ALA
1	5	302	VAL
1	4	7	VAL
1	4	102	ILE
1	4	160	ASN
1	4	161	SER
1	4	263	GLY
1	4	301	ALA
1	4	302	VAL

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Mol	Chain	Res	Type
1	3	7	VAL
1	3	102	ILE
1	3	160	ASN
1	3	161	SER
1	3	263	GLY
1	3	301	ALA
1	3	302	VAL
1	2	7	VAL
1	2	102	ILE
1	2	160	ASN
1	2	161	SER
1	2	263	GLY
1	2	301	ALA
1	2	302	VAL
1	G	7	VAL
1	G	102	ILE
1	G	160	ASN
1	G	161	SER
1	G	263	GLY
1	G	301	ALA
1	G	302	VAL
1	H	7	VAL
1	H	102	ILE
1	H	160	ASN
1	H	161	SER
1	H	263	GLY
1	H	301	ALA
1	H	302	VAL
1	L	7	VAL
1	L	102	ILE
1	L	160	ASN
1	L	161	SER
1	L	263	GLY
1	L	301	ALA
1	L	302	VAL
1	K	7	VAL
1	K	102	ILE
1	K	160	ASN
1	K	161	SER
1	K	230	THR
1	K	263	GLY
1	K	301	ALA

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Mol	Chain	Res	Type
1	K	302	VAL
1	J	7	VAL
1	J	102	ILE
1	J	160	ASN
1	J	161	SER
1	J	263	GLY
1	J	301	ALA
1	J	302	VAL
1	I	7	VAL
1	I	102	ILE
1	I	160	ASN
1	I	161	SER
1	I	263	GLY
1	I	301	ALA
1	I	302	VAL
1	M	7	VAL
1	M	102	ILE
1	M	160	ASN
1	M	161	SER
1	M	263	GLY
1	M	301	ALA
1	M	302	VAL
1	N	7	VAL
1	N	102	ILE
1	N	160	ASN
1	N	161	SER
1	N	263	GLY
1	N	301	ALA
1	N	302	VAL
1	R	7	VAL
1	R	102	ILE
1	R	160	ASN
1	R	161	SER
1	R	263	GLY
1	R	302	VAL
1	Q	7	VAL
1	Q	102	ILE
1	Q	160	ASN
1	Q	161	SER
1	Q	263	GLY
1	Q	301	ALA
1	Q	302	VAL

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Mol	Chain	Res	Type
1	P	7	VAL
1	P	102	ILE
1	P	160	ASN
1	P	161	SER
1	P	263	GLY
1	P	301	ALA
1	P	302	VAL
1	O	7	VAL
1	O	102	ILE
1	O	160	ASN
1	O	161	SER
1	O	263	GLY
1	O	301	ALA
1	O	302	VAL
1	a	7	VAL
1	a	102	ILE
1	a	160	ASN
1	a	161	SER
1	a	230	THR
1	a	263	GLY
1	a	301	ALA
1	a	302	VAL
1	b	7	VAL
1	b	102	ILE
1	b	160	ASN
1	b	161	SER
1	b	263	GLY
1	b	301	ALA
1	b	302	VAL
1	f	7	VAL
1	f	102	ILE
1	f	160	ASN
1	f	161	SER
1	f	263	GLY
1	f	301	ALA
1	f	302	VAL
1	e	7	VAL
1	e	102	ILE
1	e	160	ASN
1	e	161	SER
1	e	263	GLY
1	e	301	ALA

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Mol	Chain	Res	Type
1	e	302	VAL
1	d	7	VAL
1	d	102	ILE
1	d	160	ASN
1	d	161	SER
1	d	230	THR
1	d	263	GLY
1	d	301	ALA
1	d	302	VAL
1	c	7	VAL
1	c	102	ILE
1	c	160	ASN
1	c	161	SER
1	c	263	GLY
1	c	301	ALA
1	c	302	VAL
1	g	7	VAL
1	g	102	ILE
1	g	160	ASN
1	g	161	SER
1	g	263	GLY
1	g	301	ALA
1	g	302	VAL
1	h	7	VAL
1	h	102	ILE
1	h	160	ASN
1	h	161	SER
1	h	263	GLY
1	h	301	ALA
1	h	302	VAL
1	l	7	VAL
1	l	102	ILE
1	l	160	ASN
1	l	161	SER
1	l	263	GLY
1	l	301	ALA
1	l	302	VAL
1	k	7	VAL
1	k	102	ILE
1	k	160	ASN
1	k	161	SER
1	k	263	GLY

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Mol	Chain	Res	Type
1	k	301	ALA
1	k	302	VAL
1	j	7	VAL
1	j	102	ILE
1	j	160	ASN
1	j	161	SER
1	j	263	GLY
1	j	301	ALA
1	j	302	VAL
1	i	7	VAL
1	i	102	ILE
1	i	160	ASN
1	i	161	SER
1	i	263	GLY
1	i	301	ALA
1	i	302	VAL
1	A	230	THR
1	A	272	LEU
1	A	383	LEU
1	B	230	THR
1	B	262	ASP
1	B	272	LEU
1	B	383	LEU
1	F	230	THR
1	F	262	ASP
1	F	272	LEU
1	F	383	LEU
1	E	230	THR
1	E	262	ASP
1	E	272	LEU
1	E	383	LEU
1	D	230	THR
1	D	262	ASP
1	D	272	LEU
1	D	383	LEU
1	C	230	THR
1	C	262	ASP
1	C	272	LEU
1	C	383	LEU
1	0	230	THR
1	0	262	ASP
1	0	272	LEU

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Mol	Chain	Res	Type
1	0	383	LEU
1	1	230	THR
1	1	262	ASP
1	1	272	LEU
1	1	383	LEU
1	5	230	THR
1	5	262	ASP
1	5	272	LEU
1	5	383	LEU
1	4	230	THR
1	4	262	ASP
1	4	272	LEU
1	4	383	LEU
1	3	230	THR
1	3	262	ASP
1	3	272	LEU
1	3	383	LEU
1	2	230	THR
1	2	262	ASP
1	2	272	LEU
1	2	383	LEU
1	G	230	THR
1	G	262	ASP
1	G	272	LEU
1	G	383	LEU
1	H	230	THR
1	H	272	LEU
1	H	383	LEU
1	L	230	THR
1	L	262	ASP
1	L	272	LEU
1	L	383	LEU
1	K	262	ASP
1	K	272	LEU
1	K	383	LEU
1	J	230	THR
1	J	272	LEU
1	J	383	LEU
1	I	230	THR
1	I	272	LEU
1	I	383	LEU
1	M	230	THR

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Mol	Chain	Res	Type
1	M	272	LEU
1	M	383	LEU
1	N	230	THR
1	N	262	ASP
1	N	272	LEU
1	N	383	LEU
1	R	230	THR
1	R	262	ASP
1	R	272	LEU
1	R	301	ALA
1	R	383	LEU
1	Q	230	THR
1	Q	262	ASP
1	Q	272	LEU
1	Q	383	LEU
1	P	230	THR
1	P	272	LEU
1	P	383	LEU
1	O	230	THR
1	O	272	LEU
1	O	383	LEU
1	a	272	LEU
1	a	383	LEU
1	b	230	THR
1	b	272	LEU
1	b	383	LEU
1	f	230	THR
1	f	272	LEU
1	f	383	LEU
1	e	230	THR
1	e	272	LEU
1	e	383	LEU
1	d	272	LEU
1	d	383	LEU
1	c	230	THR
1	c	272	LEU
1	c	383	LEU
1	g	230	THR
1	g	272	LEU
1	g	383	LEU
1	h	230	THR
1	h	272	LEU

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Mol	Chain	Res	Type
1	h	383	LEU
1	l	230	THR
1	l	272	LEU
1	l	383	LEU
1	k	230	THR
1	k	272	LEU
1	k	383	LEU
1	j	230	THR
1	j	272	LEU
1	j	383	LEU
1	i	230	THR
1	i	262	ASP
1	i	272	LEU
1	i	383	LEU
1	A	262	ASP
1	H	262	ASP
1	J	262	ASP
1	I	262	ASP
1	M	262	ASP
1	P	262	ASP
1	O	262	ASP
1	a	262	ASP
1	b	262	ASP
1	f	262	ASP
1	e	262	ASP
1	d	262	ASP
1	c	262	ASP
1	g	262	ASP
1	h	262	ASP
1	l	262	ASP
1	k	262	ASP
1	j	262	ASP
1	A	4	PHE
1	A	365	ALA
1	B	4	PHE
1	F	4	PHE
1	E	4	PHE
1	D	4	PHE
1	D	24	SER
1	D	365	ALA
1	C	4	PHE
1	C	365	ALA

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Mol	Chain	Res	Type
1	0	4	PHE
1	1	4	PHE
1	5	4	PHE
1	4	4	PHE
1	3	4	PHE
1	2	4	PHE
1	G	4	PHE
1	G	365	ALA
1	H	4	PHE
1	H	365	ALA
1	L	4	PHE
1	K	4	PHE
1	K	365	ALA
1	J	4	PHE
1	J	365	ALA
1	I	4	PHE
1	I	365	ALA
1	M	4	PHE
1	M	365	ALA
1	N	4	PHE
1	R	3	PHE
1	R	4	PHE
1	R	365	ALA
1	Q	4	PHE
1	Q	365	ALA
1	P	4	PHE
1	P	365	ALA
1	O	4	PHE
1	O	365	ALA
1	a	4	PHE
1	a	365	ALA
1	b	4	PHE
1	f	4	PHE
1	e	4	PHE
1	e	365	ALA
1	d	4	PHE
1	d	365	ALA
1	c	4	PHE
1	g	4	PHE
1	h	4	PHE
1	h	365	ALA
1	l	4	PHE

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Mol	Chain	Res	Type
1	l	365	ALA
1	k	4	PHE
1	k	365	ALA
1	j	4	PHE
1	i	4	PHE
1	i	365	ALA
1	A	3	PHE
1	A	24	SER
1	A	44	ASN
1	B	3	PHE
1	B	24	SER
1	B	44	ASN
1	B	365	ALA
1	F	3	PHE
1	F	24	SER
1	F	44	ASN
1	F	365	ALA
1	E	3	PHE
1	E	24	SER
1	E	44	ASN
1	D	3	PHE
1	D	44	ASN
1	C	3	PHE
1	C	24	SER
1	C	44	ASN
1	0	3	PHE
1	0	24	SER
1	0	44	ASN
1	1	3	PHE
1	1	24	SER
1	1	44	ASN
1	5	3	PHE
1	5	24	SER
1	5	44	ASN
1	4	3	PHE
1	4	24	SER
1	4	44	ASN
1	3	3	PHE
1	3	24	SER
1	3	44	ASN
1	2	3	PHE
1	2	24	SER

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Mol	Chain	Res	Type
1	2	44	ASN
1	G	3	PHE
1	G	24	SER
1	G	44	ASN
1	H	3	PHE
1	H	24	SER
1	H	44	ASN
1	L	3	PHE
1	L	24	SER
1	L	44	ASN
1	L	365	ALA
1	K	3	PHE
1	K	24	SER
1	K	44	ASN
1	J	3	PHE
1	J	24	SER
1	J	44	ASN
1	I	3	PHE
1	I	24	SER
1	I	44	ASN
1	M	3	PHE
1	M	24	SER
1	M	44	ASN
1	N	3	PHE
1	N	24	SER
1	N	44	ASN
1	N	365	ALA
1	R	24	SER
1	R	44	ASN
1	Q	3	PHE
1	Q	24	SER
1	Q	44	ASN
1	P	3	PHE
1	P	24	SER
1	P	44	ASN
1	O	3	PHE
1	O	24	SER
1	O	44	ASN
1	a	3	PHE
1	a	24	SER
1	a	44	ASN
1	b	3	PHE

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Mol	Chain	Res	Type
1	b	24	SER
1	b	44	ASN
1	b	365	ALA
1	f	3	PHE
1	f	24	SER
1	f	44	ASN
1	f	365	ALA
1	e	3	PHE
1	e	24	SER
1	e	44	ASN
1	d	3	PHE
1	d	24	SER
1	d	44	ASN
1	c	3	PHE
1	c	24	SER
1	c	44	ASN
1	c	365	ALA
1	g	3	PHE
1	g	24	SER
1	g	44	ASN
1	g	365	ALA
1	h	3	PHE
1	h	24	SER
1	h	44	ASN
1	l	3	PHE
1	l	24	SER
1	l	44	ASN
1	k	3	PHE
1	k	24	SER
1	k	44	ASN
1	j	3	PHE
1	j	24	SER
1	j	44	ASN
1	j	365	ALA
1	i	3	PHE
1	i	24	SER
1	i	44	ASN
1	A	241	GLY
1	B	241	GLY
1	F	241	GLY
1	E	241	GLY
1	D	241	GLY

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Mol	Chain	Res	Type
1	C	241	GLY
1	0	241	GLY
1	1	241	GLY
1	5	241	GLY
1	4	241	GLY
1	3	241	GLY
1	2	241	GLY
1	G	241	GLY
1	H	241	GLY
1	L	241	GLY
1	K	241	GLY
1	J	241	GLY
1	I	241	GLY
1	M	241	GLY
1	N	241	GLY
1	R	241	GLY
1	Q	241	GLY
1	P	241	GLY
1	O	241	GLY
1	a	241	GLY
1	b	241	GLY
1	f	241	GLY
1	e	241	GLY
1	d	241	GLY
1	c	241	GLY
1	g	241	GLY
1	h	241	GLY
1	l	241	GLY
1	k	241	GLY
1	j	241	GLY
1	i	241	GLY

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	0	296/298 (99%)	292 (99%)	4 (1%)	74 89
1	1	296/298 (99%)	292 (99%)	4 (1%)	74 89
1	2	296/298 (99%)	292 (99%)	4 (1%)	74 89
1	3	296/298 (99%)	292 (99%)	4 (1%)	74 89
1	4	296/298 (99%)	292 (99%)	4 (1%)	74 89
1	5	296/298 (99%)	292 (99%)	4 (1%)	74 89
1	A	296/298 (99%)	292 (99%)	4 (1%)	74 89
1	B	296/298 (99%)	292 (99%)	4 (1%)	74 89
1	C	296/298 (99%)	292 (99%)	4 (1%)	74 89
1	D	296/298 (99%)	292 (99%)	4 (1%)	74 89
1	E	296/298 (99%)	292 (99%)	4 (1%)	74 89
1	F	296/298 (99%)	292 (99%)	4 (1%)	74 89
1	G	296/298 (99%)	292 (99%)	4 (1%)	74 89
1	H	296/298 (99%)	292 (99%)	4 (1%)	74 89
1	I	296/298 (99%)	292 (99%)	4 (1%)	74 89
1	J	296/298 (99%)	292 (99%)	4 (1%)	74 89
1	K	296/298 (99%)	292 (99%)	4 (1%)	74 89
1	L	296/298 (99%)	292 (99%)	4 (1%)	74 89
1	M	296/298 (99%)	292 (99%)	4 (1%)	74 89
1	N	296/298 (99%)	292 (99%)	4 (1%)	74 89
1	O	296/298 (99%)	292 (99%)	4 (1%)	74 89
1	P	296/298 (99%)	292 (99%)	4 (1%)	74 89
1	Q	296/298 (99%)	292 (99%)	4 (1%)	74 89
1	R	296/298 (99%)	292 (99%)	4 (1%)	74 89
1	a	296/298 (99%)	292 (99%)	4 (1%)	74 89
1	b	296/298 (99%)	292 (99%)	4 (1%)	74 89
1	c	296/298 (99%)	292 (99%)	4 (1%)	74 89
1	d	296/298 (99%)	292 (99%)	4 (1%)	74 89
1	e	296/298 (99%)	292 (99%)	4 (1%)	74 89
1	f	296/298 (99%)	292 (99%)	4 (1%)	74 89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	g	296/298 (99%)	292 (99%)	4 (1%)	74 89
1	h	296/298 (99%)	292 (99%)	4 (1%)	74 89
1	i	296/298 (99%)	292 (99%)	4 (1%)	74 89
1	j	296/298 (99%)	292 (99%)	4 (1%)	74 89
1	k	296/298 (99%)	292 (99%)	4 (1%)	74 89
1	l	296/298 (99%)	292 (99%)	4 (1%)	74 89
All	All	10656/10728 (99%)	10512 (99%)	144 (1%)	76 89

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	ASP
1	A	267	TRP
1	A	289	LEU
1	A	303	ASP
1	B	116	ASP
1	B	267	TRP
1	B	289	LEU
1	B	303	ASP
1	F	116	ASP
1	F	267	TRP
1	F	289	LEU
1	F	303	ASP
1	E	116	ASP
1	E	267	TRP
1	E	289	LEU
1	E	303	ASP
1	D	116	ASP
1	D	267	TRP
1	D	289	LEU
1	D	303	ASP
1	C	116	ASP
1	C	267	TRP
1	C	289	LEU
1	C	303	ASP
1	0	116	ASP
1	0	267	TRP
1	0	289	LEU
1	0	303	ASP
1	1	116	ASP

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Mol	Chain	Res	Type
1	1	267	TRP
1	1	289	LEU
1	1	303	ASP
1	5	116	ASP
1	5	267	TRP
1	5	289	LEU
1	5	303	ASP
1	4	116	ASP
1	4	267	TRP
1	4	289	LEU
1	4	303	ASP
1	3	116	ASP
1	3	267	TRP
1	3	289	LEU
1	3	303	ASP
1	2	116	ASP
1	2	267	TRP
1	2	289	LEU
1	2	303	ASP
1	G	116	ASP
1	G	267	TRP
1	G	289	LEU
1	G	303	ASP
1	H	116	ASP
1	H	267	TRP
1	H	289	LEU
1	H	303	ASP
1	L	116	ASP
1	L	267	TRP
1	L	289	LEU
1	L	303	ASP
1	K	116	ASP
1	K	267	TRP
1	K	289	LEU
1	K	303	ASP
1	J	116	ASP
1	J	267	TRP
1	J	289	LEU
1	J	303	ASP
1	I	116	ASP
1	I	267	TRP
1	I	289	LEU

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Mol	Chain	Res	Type
1	I	303	ASP
1	M	116	ASP
1	M	267	TRP
1	M	289	LEU
1	M	303	ASP
1	N	116	ASP
1	N	267	TRP
1	N	289	LEU
1	N	303	ASP
1	R	116	ASP
1	R	267	TRP
1	R	289	LEU
1	R	303	ASP
1	Q	116	ASP
1	Q	267	TRP
1	Q	289	LEU
1	Q	303	ASP
1	P	116	ASP
1	P	267	TRP
1	P	289	LEU
1	P	303	ASP
1	O	116	ASP
1	O	267	TRP
1	O	289	LEU
1	O	303	ASP
1	a	116	ASP
1	a	267	TRP
1	a	289	LEU
1	a	303	ASP
1	b	116	ASP
1	b	267	TRP
1	b	289	LEU
1	b	303	ASP
1	f	116	ASP
1	f	267	TRP
1	f	289	LEU
1	f	303	ASP
1	e	116	ASP
1	e	267	TRP
1	e	289	LEU
1	e	303	ASP
1	d	116	ASP

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Mol	Chain	Res	Type
1	d	267	TRP
1	d	289	LEU
1	d	303	ASP
1	c	116	ASP
1	c	267	TRP
1	c	289	LEU
1	c	303	ASP
1	g	116	ASP
1	g	267	TRP
1	g	289	LEU
1	g	303	ASP
1	h	116	ASP
1	h	267	TRP
1	h	289	LEU
1	h	303	ASP
1	l	116	ASP
1	l	267	TRP
1	l	289	LEU
1	l	303	ASP
1	k	116	ASP
1	k	267	TRP
1	k	289	LEU
1	k	303	ASP
1	j	116	ASP
1	j	267	TRP
1	j	289	LEU
1	j	303	ASP
1	i	116	ASP
1	i	267	TRP
1	i	289	LEU
1	i	303	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	347	GLN
1	E	172	ASN
1	C	347	GLN
1	0	193	ASN
1	1	347	GLN
1	3	137	GLN
1	2	347	GLN

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Mol	Chain	Res	Type
1	H	137	GLN
1	L	172	ASN
1	M	137	GLN
1	M	347	GLN
1	N	172	ASN
1	O	172	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.