Full wwPDB EM Validation Report (i)

Mar 11, 2024 – 04:08 AM EDT

PDB ID	:	6TZ4
EMDB ID	:	EMD-20588
Title	:	CryoEM reconstruction of membrane-bound ESCRT-III filament composed of CHMP1B+IST1 (right-handed)
Authors	:	Nguyen, H.C.; Frost, A.
Deposited on	:	2019-08-10
Resolution	:	3.20 Å(reported)

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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

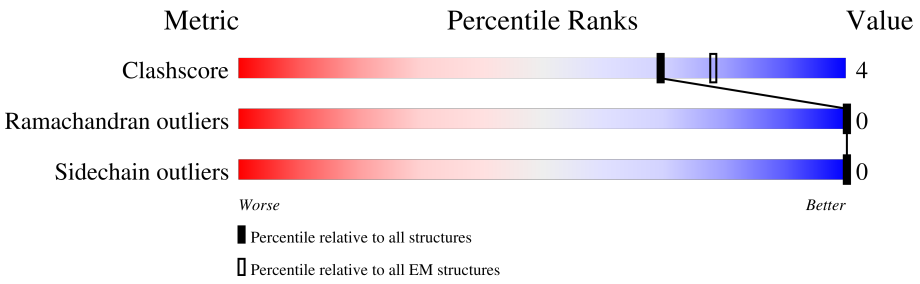
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.20 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	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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	02	199	42% 80% 8% 12%
1	A	199	30% 80% 8% 12%
1	BA	199	27% 81% 8% 12%
1	BB	199	35% 83% 6% 12%
1	C	199	38% 81% 8% 12%
1	DA	199	29% 78% 11% 12%
1	DB	199	33% 79% 10% 12%
1	E	199	27% 76% 12% 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	FA	199	24% 79% 10% 12%
1	FB	199	17% 81% 8% 12%
1	G	199	30% 81% 8% 12%
1	HA	199	24% 81% 7% 12%
1	HB	199	35% 82% 7% 12%
1	I	199	39% 82% 7% 12%
1	JA	199	32% 81% 7% 12%
1	JB	199	15% 79% 9% 12%
1	K	199	20% 79% 10% 12%
1	LA	199	31% 80% 8% 12%
1	LB	199	37% 81% 8% 12%
1	M	199	25% 80% 8% 12%
1	NA	199	22% 81% 8% 12%
1	NB	199	33% 81% 8% 12%
1	O	199	32% 81% 8% 12%
1	PA	199	39% 80% 8% 12%
1	PB	199	40% 80% 8% 12%
1	Q	199	27% 79% 9% 12%
1	RA	199	28% 81% 8% 12%
1	RB	199	31% 81% 7% 12%
1	S	199	23% 81% 8% 12%
1	TA	199	20% 81% 8% 12%
1	V	199	32% 81% 7% 12%
1	VA	199	34% 81% 8% 12%
1	X	199	29% 79% 10% 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	XA	199	37% 78% 10% 12%
1	Z	199	26% 78% 10% 12%
1	ZA	199	19% 80% 9% 12%
2	01	189	24% 86% 10% •
2	AA	189	36% 85% 11% •
2	AB	189	32% 87% 9% •
2	B	189	50% 86% 10% •
2	CA	189	42% 85% 11% •
2	CB	189	26% 87% 9% •
2	D	189	30% 85% 11% •
2	EA	189	10% 86% 10% •
2	EB	189	18% 86% 10% •
2	F	189	17% 86% 10% •
2	GA	189	34% 85% 11% •
2	GB	189	26% 86% 10% •
2	H	189	44% 85% 11% •
2	IA	189	39% 85% 11% •
2	IB	189	46% 87% 8% •
2	J	189	30% 86% 10% •
2	KA	189	15% 86% 10% •
2	KB	189	21% 86% 10% •
2	L	189	17% 86% 10% •
2	MA	189	26% 85% 11% •
2	MB	189	21% 85% 11% •
2	N	189	44% 85% 11% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	OA	189	35% 85% 11%
2	OB	189	49% 85% 11%
2	P	189	35% 87% 9%
2	QA	189	15% 87% 8%
2	QB	189	20% 86% 10%
2	R	189	12% 85% 11%
2	SA	189	22% 86% 10%
2	SB	189	48% 85% 11%
2	T	189	42% 86% 10%
2	UA	189	35% 85% 11%
2	W	189	40% 85% 11%
2	WA	189	25% 86% 10%
2	Y	189	15% 85% 11%
2	YA	189	20% 86% 10%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 99216 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 Charged multivesicular body protein 1b.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	JB	176	1366	839	247	267	13	0	0
1	A	176	1366	839	247	267	13	0	0
1	C	176	1366	839	247	267	13	0	0
1	E	176	1366	839	247	267	13	0	0
1	G	176	1366	839	247	267	13	0	0
1	I	176	1366	839	247	267	13	0	0
1	K	176	1366	839	247	267	13	0	0
1	M	176	1366	839	247	267	13	0	0
1	O	176	1366	839	247	267	13	0	0
1	Q	176	1366	839	247	267	13	0	0
1	S	176	1366	839	247	267	13	0	0
1	V	176	1366	839	247	267	13	0	0
1	X	176	1366	839	247	267	13	0	0
1	Z	176	1366	839	247	267	13	0	0
1	BA	176	1366	839	247	267	13	0	0
1	DA	176	1366	839	247	267	13	0	0
1	FA	176	1366	839	247	267	13	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	HA	176	1366	839	247	267	13	0	0
1	JA	176	1366	839	247	267	13	0	0
1	LA	176	1366	839	247	267	13	0	0
1	NA	176	1366	839	247	267	13	0	0
1	PA	176	1366	839	247	267	13	0	0
1	RA	176	1366	839	247	267	13	0	0
1	TA	176	1366	839	247	267	13	0	0
1	VA	176	1366	839	247	267	13	0	0
1	XA	176	1366	839	247	267	13	0	0
1	ZA	176	1366	839	247	267	13	0	0
1	BB	176	1366	839	247	267	13	0	0
1	DB	176	1366	839	247	267	13	0	0
1	FB	176	1366	839	247	267	13	0	0
1	HB	176	1366	839	247	267	13	0	0
1	LB	176	1366	839	247	267	13	0	0
1	NB	176	1366	839	247	267	13	0	0
1	PB	176	1366	839	247	267	13	0	0
1	RB	176	1366	839	247	267	13	0	0
1	02	176	1366	839	247	267	13	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
JB	37	GLU	LYS	engineered mutation	UNP Q7LBR1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	GLU	LYS	engineered mutation	UNP Q7LBR1
C	37	GLU	LYS	engineered mutation	UNP Q7LBR1
E	37	GLU	LYS	engineered mutation	UNP Q7LBR1
G	37	GLU	LYS	engineered mutation	UNP Q7LBR1
I	37	GLU	LYS	engineered mutation	UNP Q7LBR1
K	37	GLU	LYS	engineered mutation	UNP Q7LBR1
M	37	GLU	LYS	engineered mutation	UNP Q7LBR1
O	37	GLU	LYS	engineered mutation	UNP Q7LBR1
Q	37	GLU	LYS	engineered mutation	UNP Q7LBR1
S	37	GLU	LYS	engineered mutation	UNP Q7LBR1
V	37	GLU	LYS	engineered mutation	UNP Q7LBR1
X	37	GLU	LYS	engineered mutation	UNP Q7LBR1
Z	37	GLU	LYS	engineered mutation	UNP Q7LBR1
BA	37	GLU	LYS	engineered mutation	UNP Q7LBR1
DA	37	GLU	LYS	engineered mutation	UNP Q7LBR1
FA	37	GLU	LYS	engineered mutation	UNP Q7LBR1
HA	37	GLU	LYS	engineered mutation	UNP Q7LBR1
JA	37	GLU	LYS	engineered mutation	UNP Q7LBR1
LA	37	GLU	LYS	engineered mutation	UNP Q7LBR1
NA	37	GLU	LYS	engineered mutation	UNP Q7LBR1
PA	37	GLU	LYS	engineered mutation	UNP Q7LBR1
RA	37	GLU	LYS	engineered mutation	UNP Q7LBR1
TA	37	GLU	LYS	engineered mutation	UNP Q7LBR1
VA	37	GLU	LYS	engineered mutation	UNP Q7LBR1
XA	37	GLU	LYS	engineered mutation	UNP Q7LBR1
ZA	37	GLU	LYS	engineered mutation	UNP Q7LBR1
BB	37	GLU	LYS	engineered mutation	UNP Q7LBR1
DB	37	GLU	LYS	engineered mutation	UNP Q7LBR1
FB	37	GLU	LYS	engineered mutation	UNP Q7LBR1
HB	37	GLU	LYS	engineered mutation	UNP Q7LBR1
LB	37	GLU	LYS	engineered mutation	UNP Q7LBR1
NB	37	GLU	LYS	engineered mutation	UNP Q7LBR1
PB	37	GLU	LYS	engineered mutation	UNP Q7LBR1
RB	37	GLU	LYS	engineered mutation	UNP Q7LBR1
02	37	GLU	LYS	engineered mutation	UNP Q7LBR1

- Molecule 2 is a protein called IST1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	MB	181	1390	885	246	254	5	0	0
			Total	C	N	O	S		
2	B	181	1390	885	246	254	5	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	181	1390	885	246	254	5	0	0
2	F	181	1390	885	246	254	5	0	0
2	H	181	1390	885	246	254	5	0	0
2	J	181	1390	885	246	254	5	0	0
2	L	181	1390	885	246	254	5	0	0
2	N	181	1390	885	246	254	5	0	0
2	P	181	1390	885	246	254	5	0	0
2	R	181	1390	885	246	254	5	0	0
2	T	181	1390	885	246	254	5	0	0
2	W	181	1390	885	246	254	5	0	0
2	Y	181	1390	885	246	254	5	0	0
2	AA	181	1390	885	246	254	5	0	0
2	CA	181	1390	885	246	254	5	0	0
2	EA	181	1390	885	246	254	5	0	0
2	GA	181	1390	885	246	254	5	0	0
2	IA	181	1390	885	246	254	5	0	0
2	KA	181	1390	885	246	254	5	0	0
2	MA	181	1390	885	246	254	5	0	0
2	OA	181	1390	885	246	254	5	0	0
2	QA	181	1390	885	246	254	5	0	0
2	SA	181	1390	885	246	254	5	0	0

Continued on next page...

Continued from previous page...

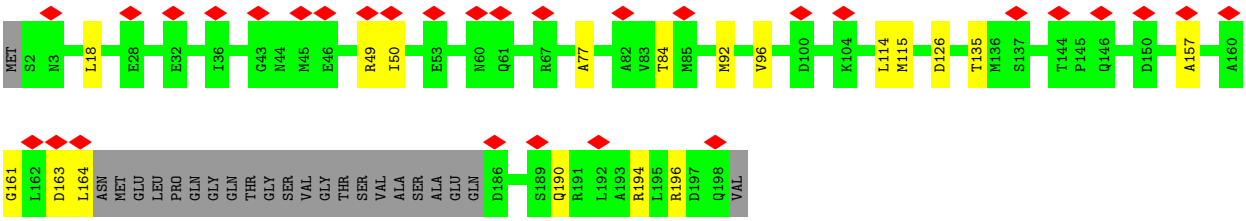
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	UA	181	1390	885	246	254	5	0	0
2	WA	181	1390	885	246	254	5	0	0
2	YA	181	1390	885	246	254	5	0	0
2	AB	181	1390	885	246	254	5	0	0
2	CB	181	1390	885	246	254	5	0	0
2	EB	181	1390	885	246	254	5	0	0
2	GB	181	1390	885	246	254	5	0	0
2	IB	181	1390	885	246	254	5	0	0
2	KB	181	1390	885	246	254	5	0	0
2	OB	181	1390	885	246	254	5	0	0
2	QB	181	1390	885	246	254	5	0	0
2	SB	181	1390	885	246	254	5	0	0
2	01	181	1390	885	246	254	5	0	0

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 and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

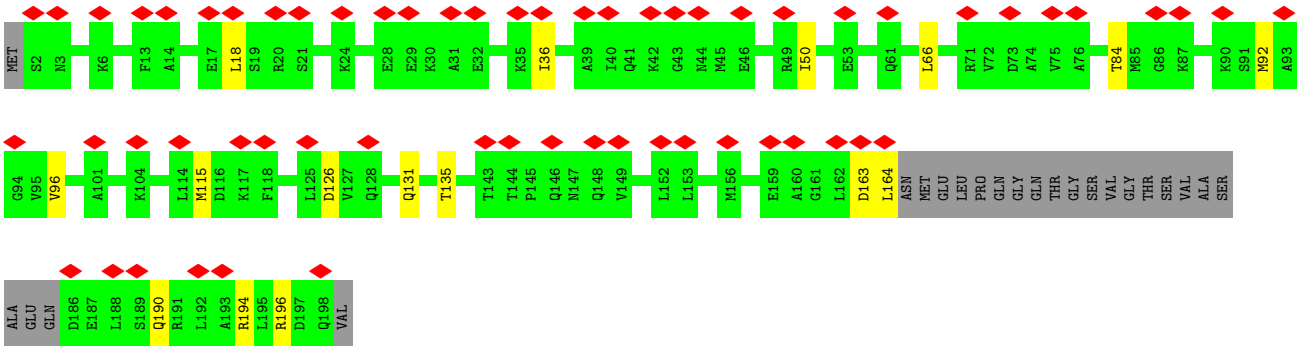
• Molecule 1: Charged multivesicular body protein 1b

Chain JB:



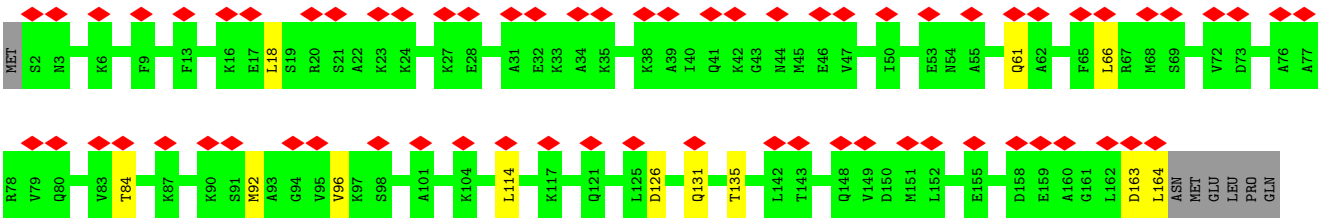
• Molecule 1: Charged multivesicular body protein 1b

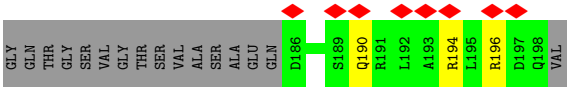
Chain A:



• Molecule 1: Charged multivesicular body protein 1b

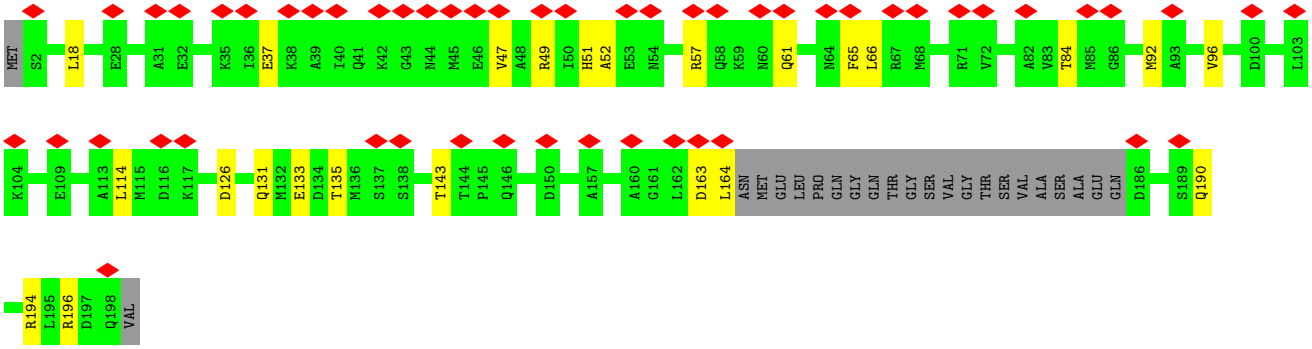
Chain C:





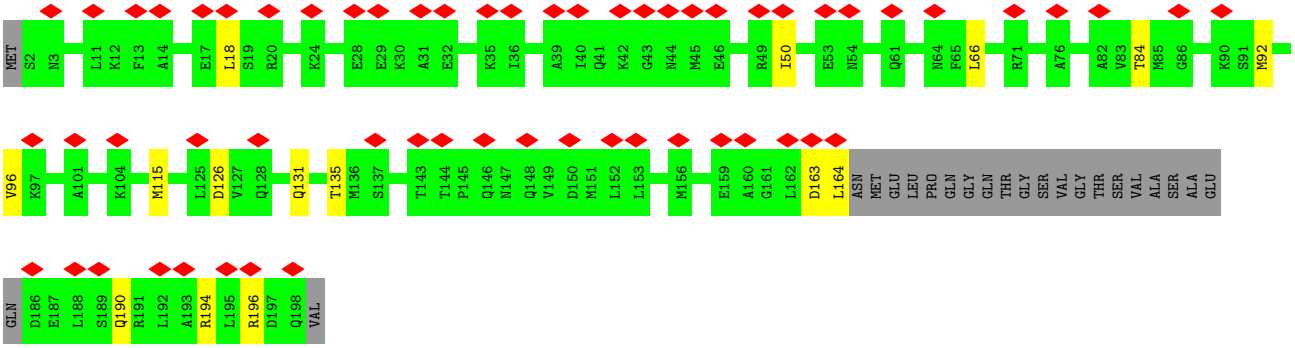
• Molecule 1: Charged multivesicular body protein 1b

Chain E:



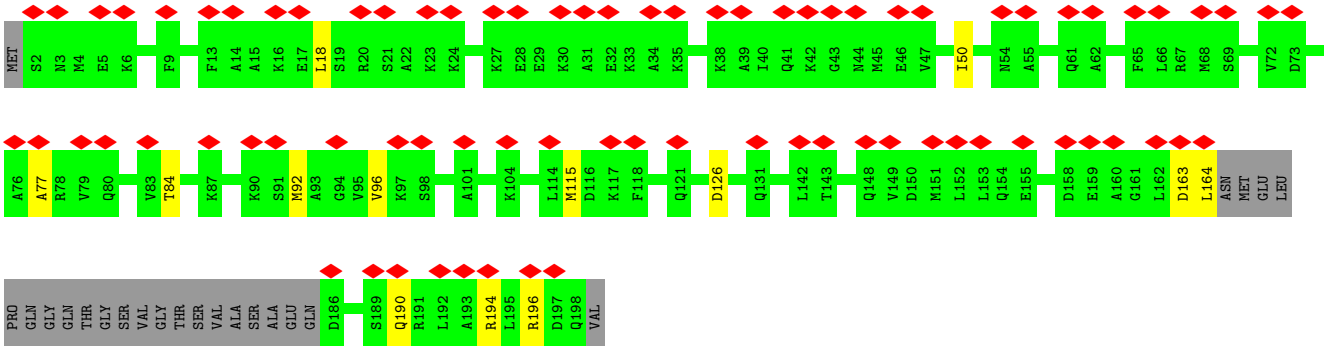
• Molecule 1: Charged multivesicular body protein 1b

Chain G:



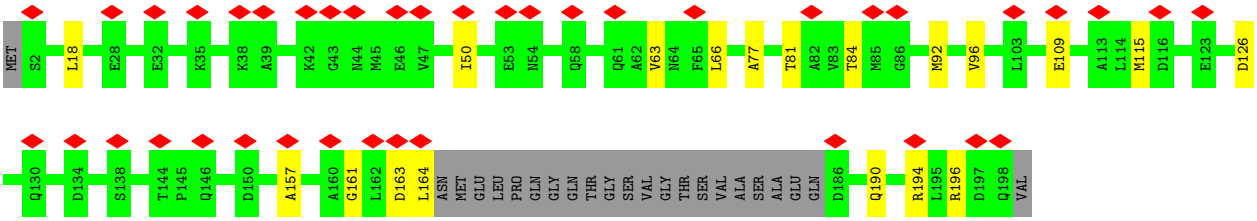
• Molecule 1: Charged multivesicular body protein 1b

Chain I:



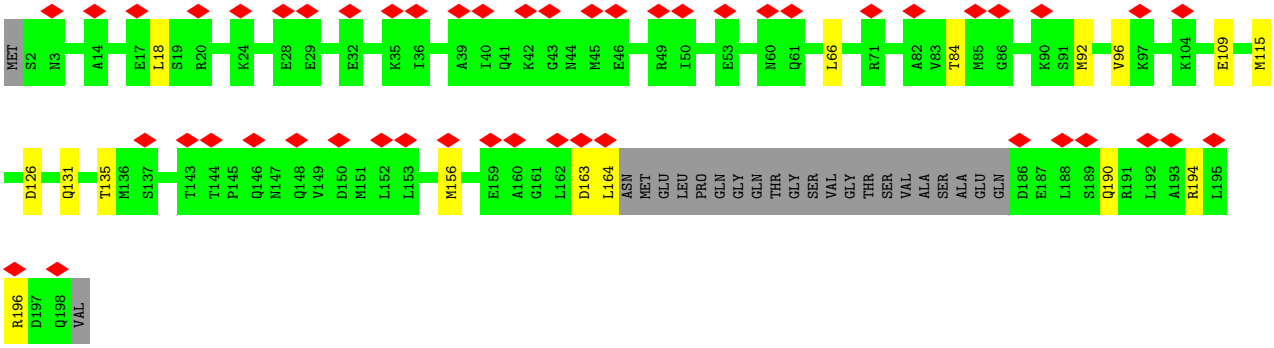
• Molecule 1: Charged multivesicular body protein 1b

Chain K:



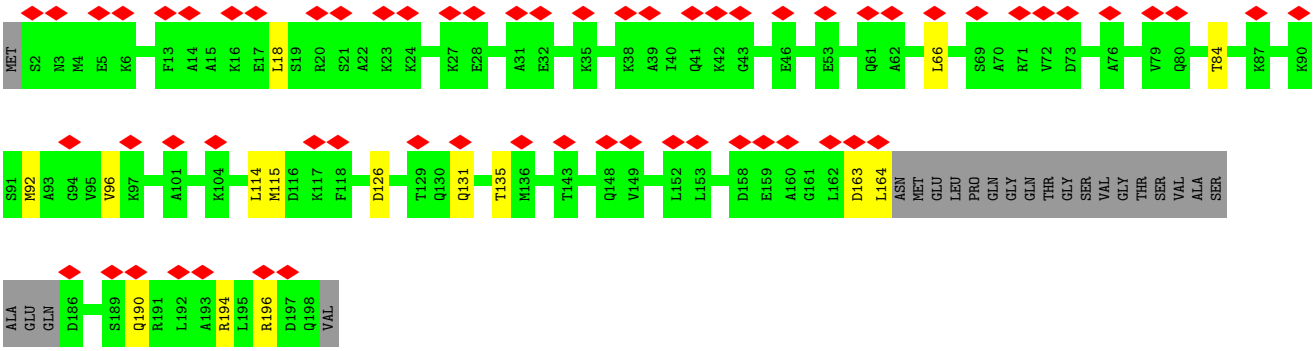
- Molecule 1: Charged multivesicular body protein 1b

Chain M:



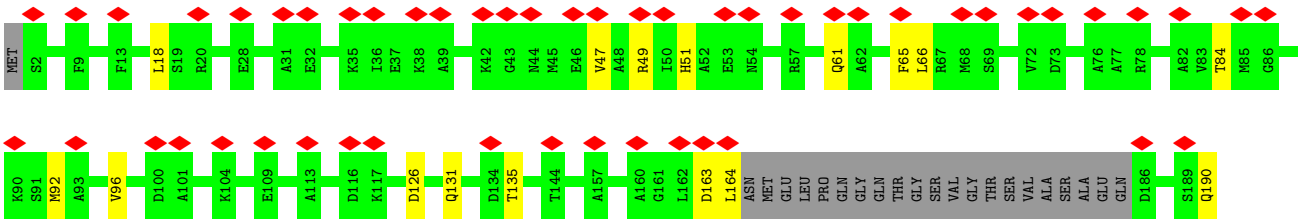
- Molecule 1: Charged multivesicular body protein 1b

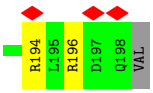
Chain O:



- Molecule 1: Charged multivesicular body protein 1b

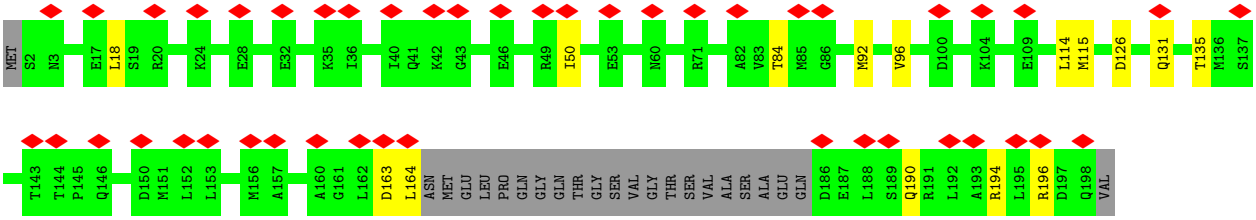
Chain Q:





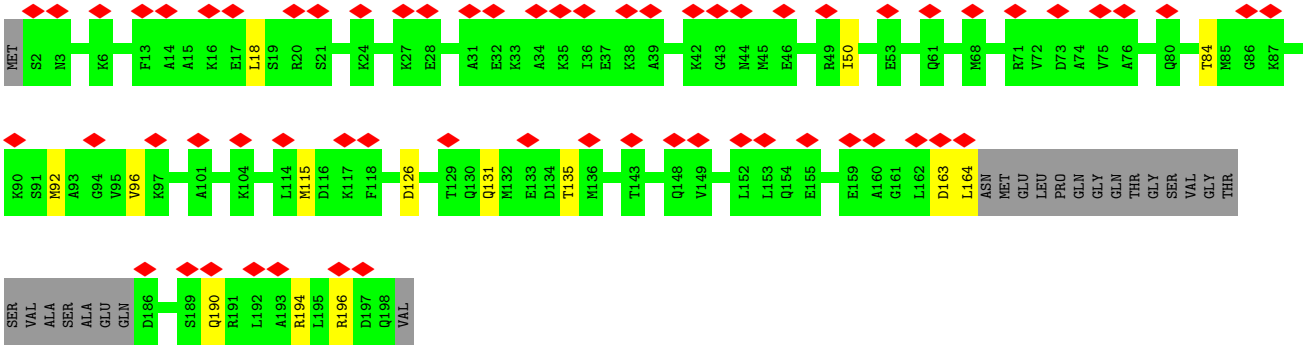
• Molecule 1: Charged multivesicular body protein 1b

Chain S:



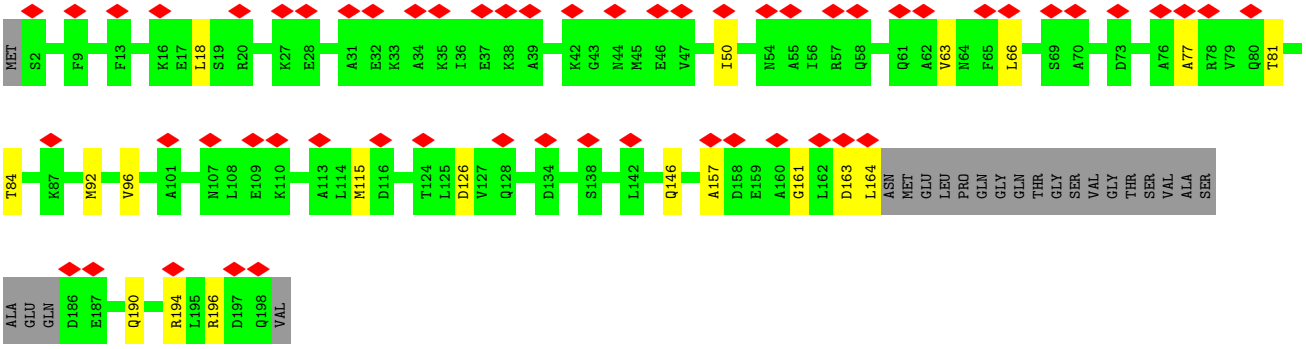
• Molecule 1: Charged multivesicular body protein 1b

Chain V:



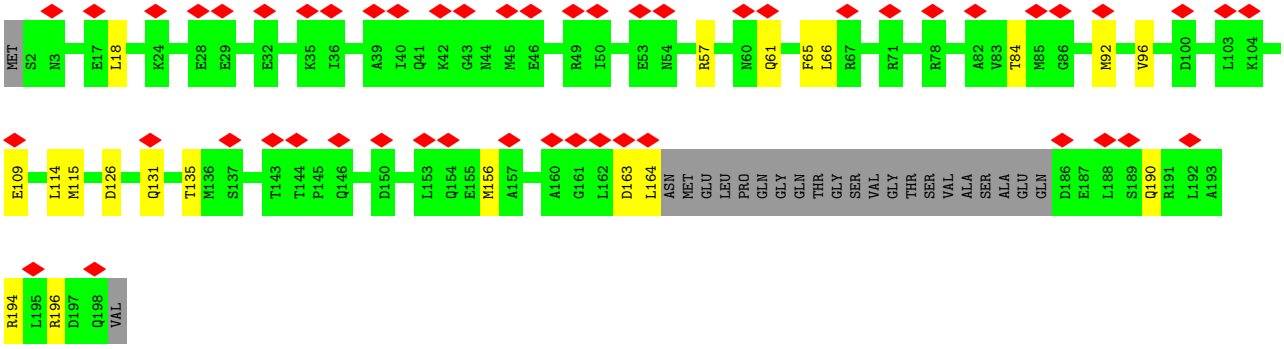
• Molecule 1: Charged multivesicular body protein 1b

Chain X:



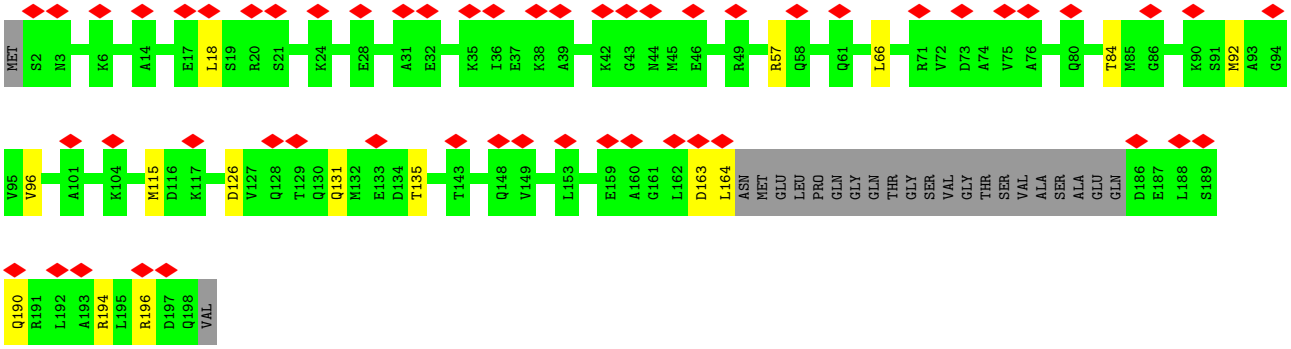
• Molecule 1: Charged multivesicular body protein 1b

Chain Z:



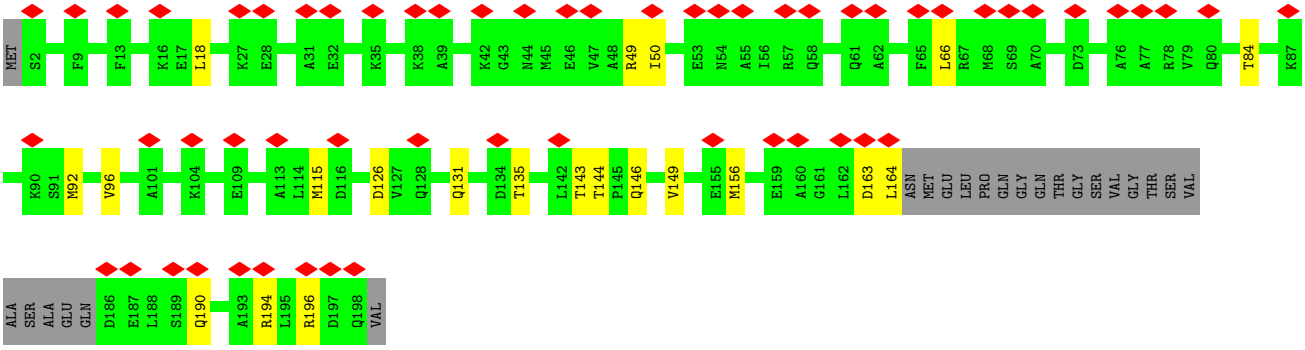
• Molecule 1: Charged multivesicular body protein 1b

Chain BA:



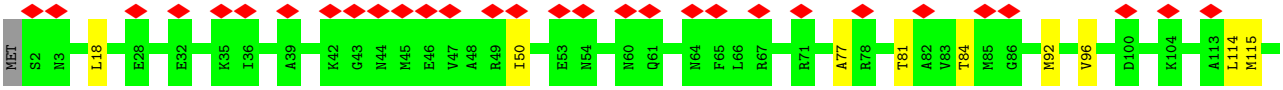
• Molecule 1: Charged multivesicular body protein 1b

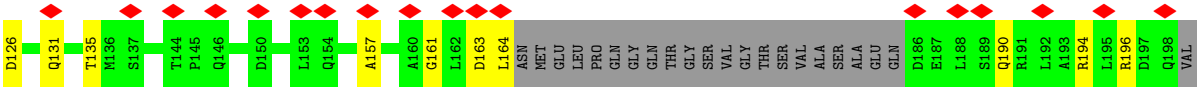
Chain DA:



• Molecule 1: Charged multivesicular body protein 1b

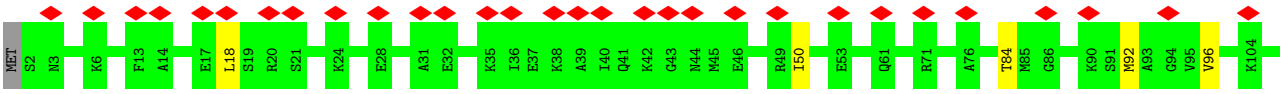
Chain FA:

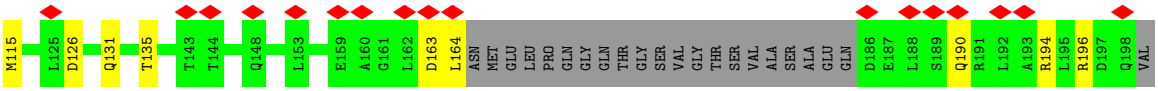




• Molecule 1: Charged multivesicular body protein 1b

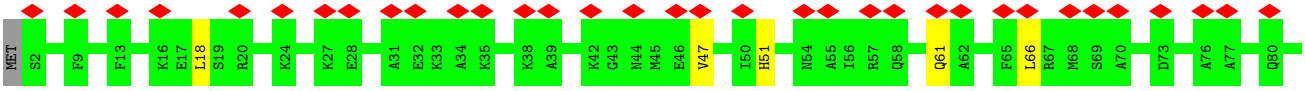
Chain HA:

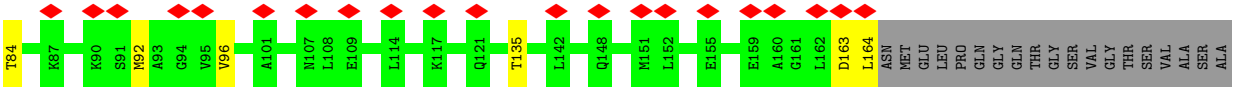


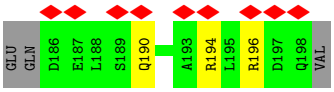


• Molecule 1: Charged multivesicular body protein 1b

Chain JA:

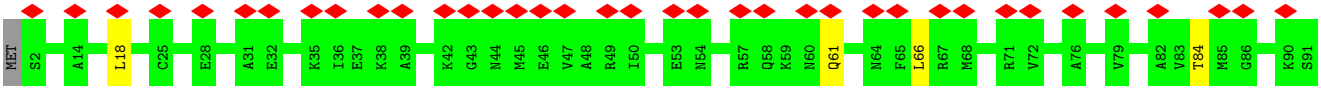


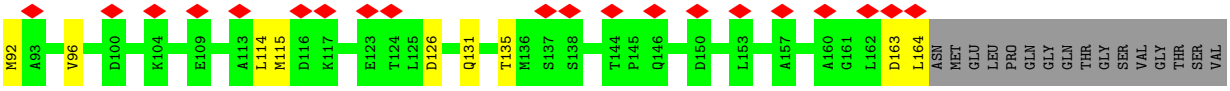


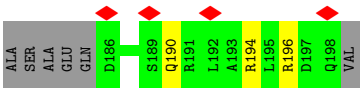


• Molecule 1: Charged multivesicular body protein 1b

Chain LA:

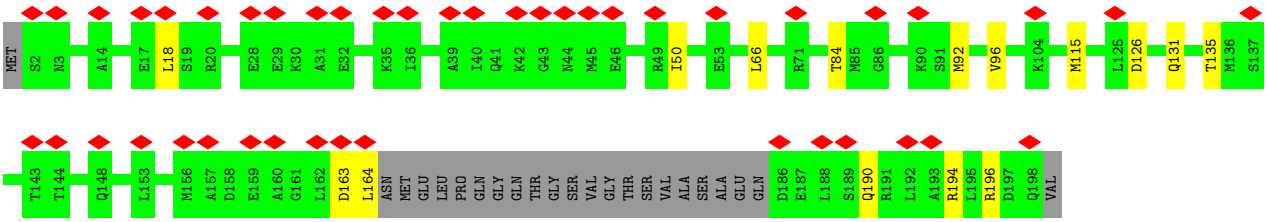






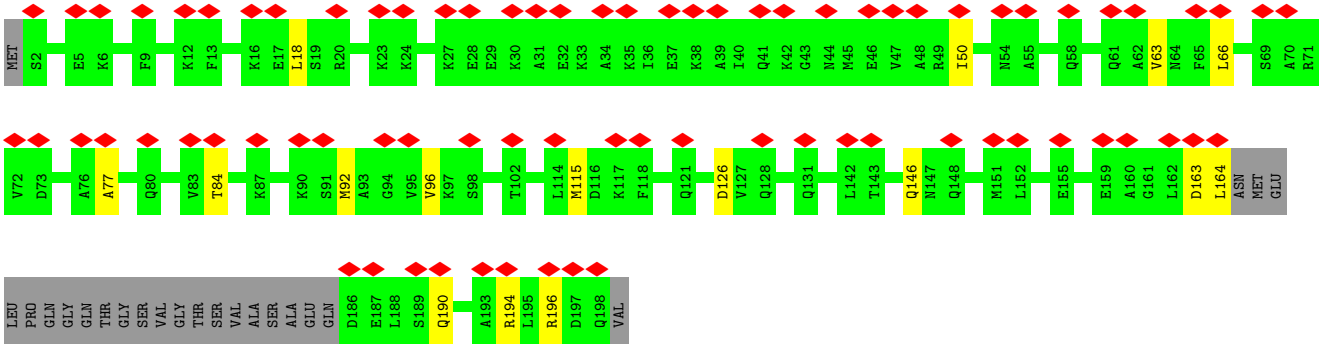
• Molecule 1: Charged multivesicular body protein 1b

Chain NA:



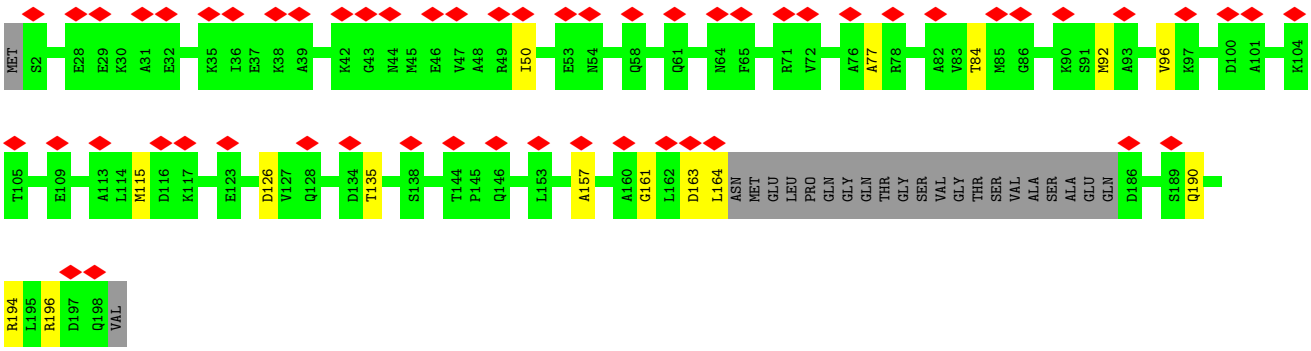
• Molecule 1: Charged multivesicular body protein 1b

Chain PA:



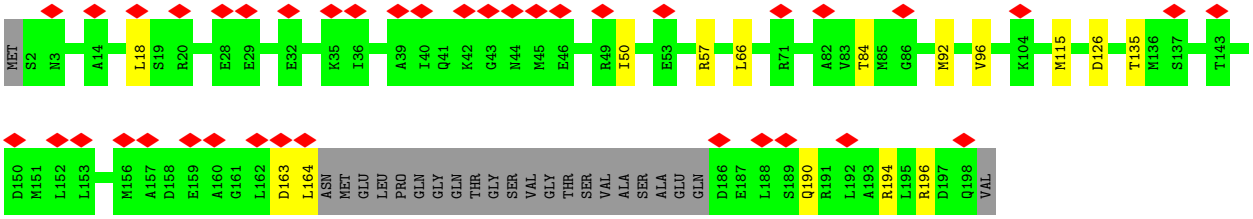
• Molecule 1: Charged multivesicular body protein 1b

Chain RA:



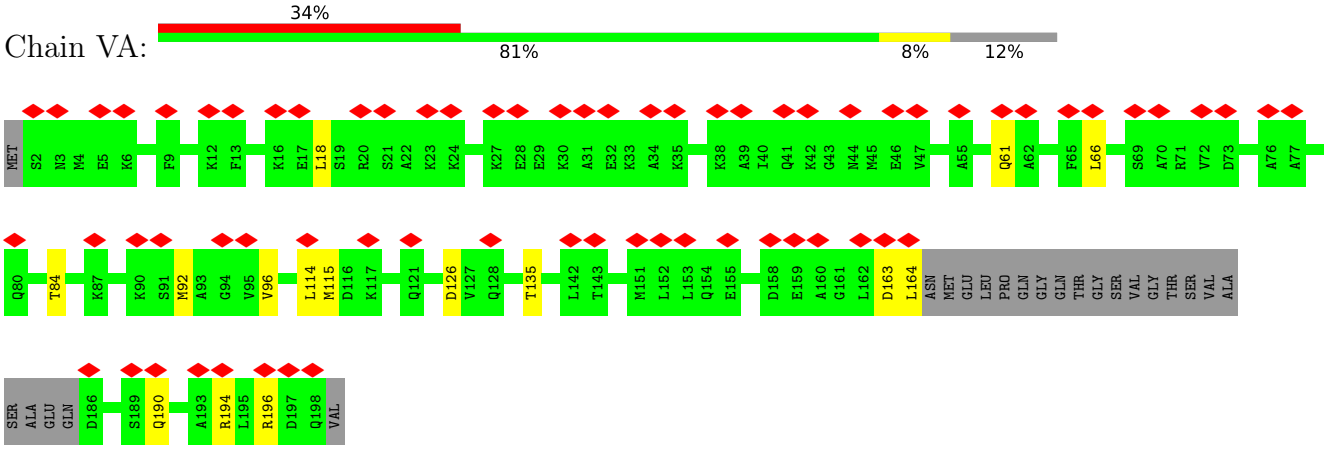
• Molecule 1: Charged multivesicular body protein 1b

Chain TA:



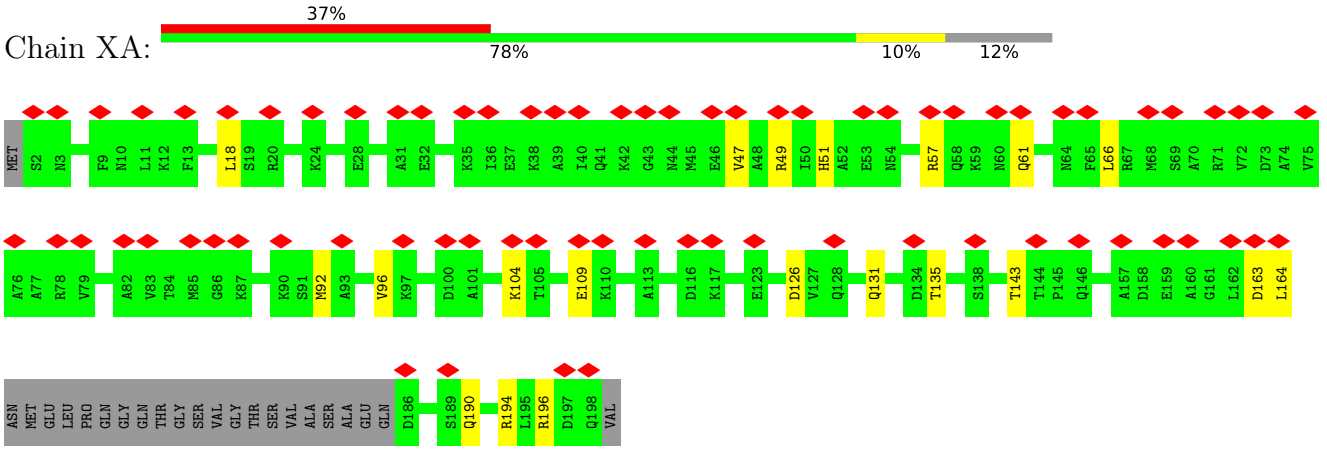
• Molecule 1: Charged multivesicular body protein 1b

Chain VA:



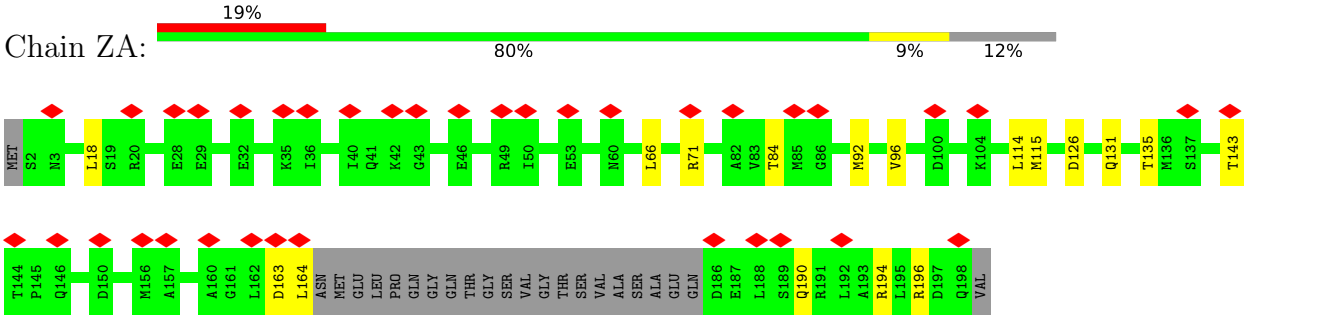
• Molecule 1: Charged multivesicular body protein 1b

Chain XA:



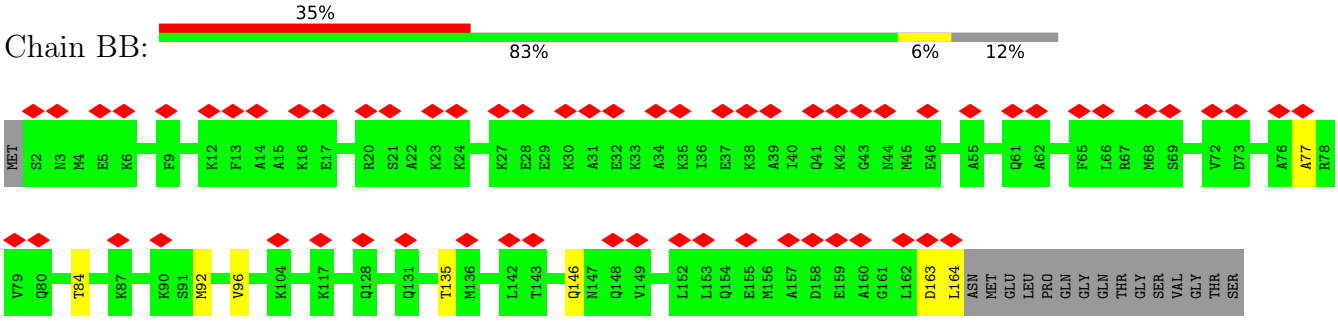
• Molecule 1: Charged multivesicular body protein 1b

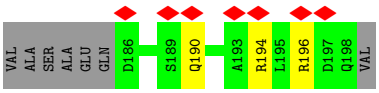
Chain ZA:



• Molecule 1: Charged multivesicular body protein 1b

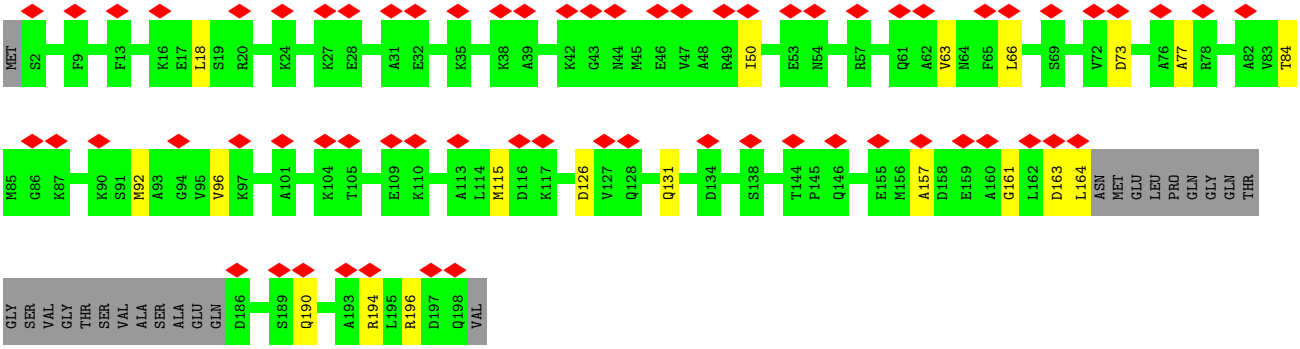
Chain BB:





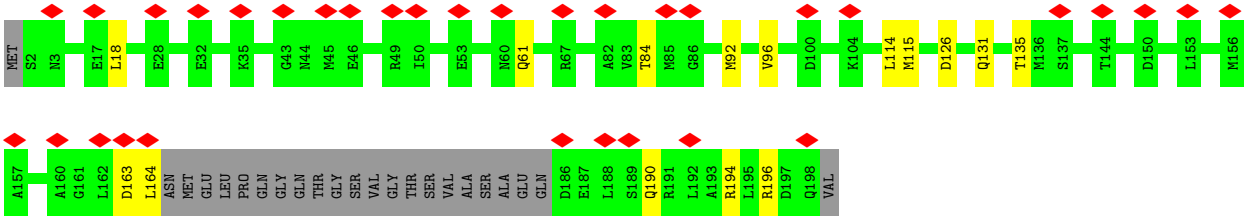
- Molecule 1: Charged multivesicular body protein 1b

Chain DB:



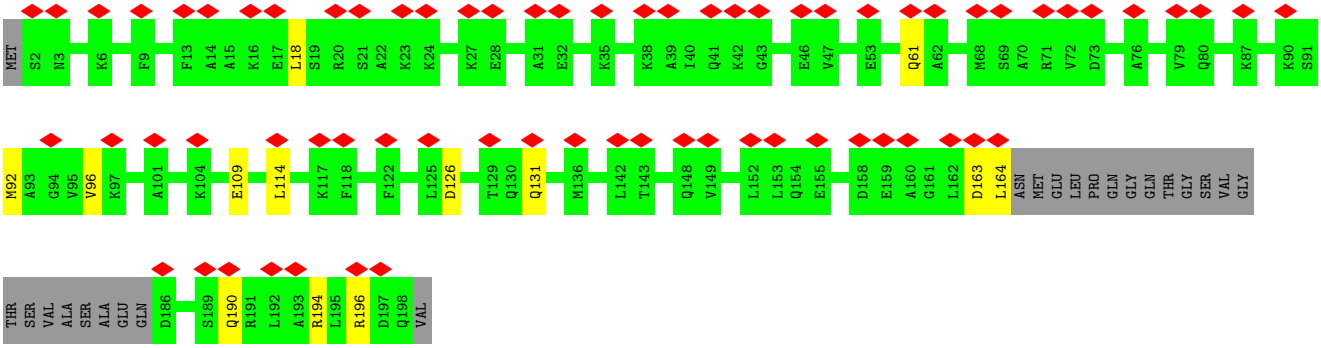
- Molecule 1: Charged multivesicular body protein 1b

Chain FB:



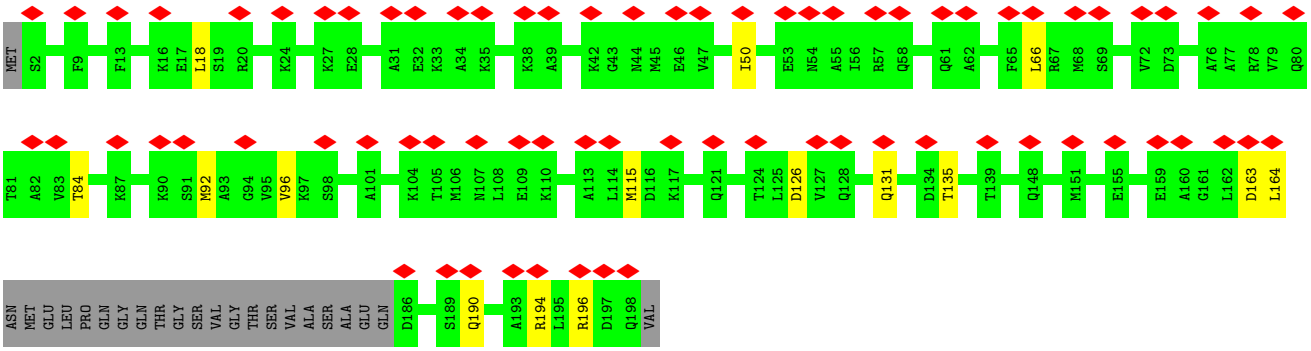
- Molecule 1: Charged multivesicular body protein 1b

Chain HB:



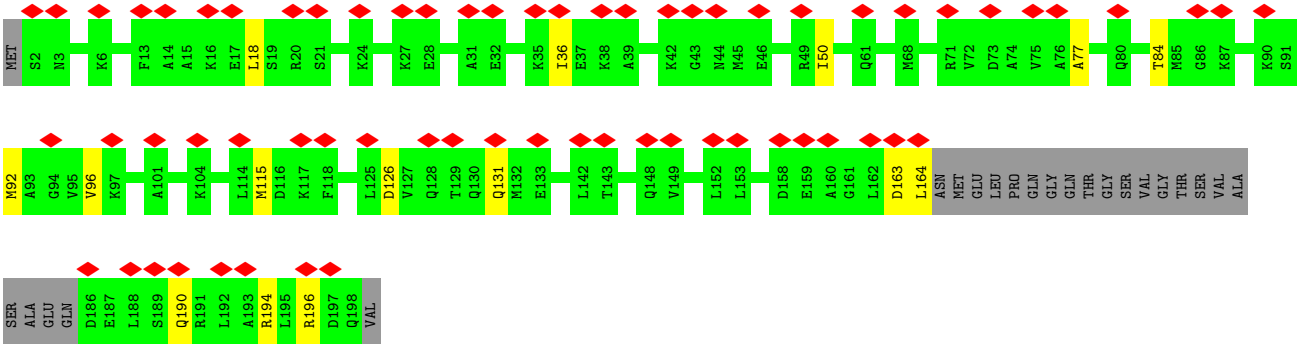
- Molecule 1: Charged multivesicular body protein 1b

Chain LB:



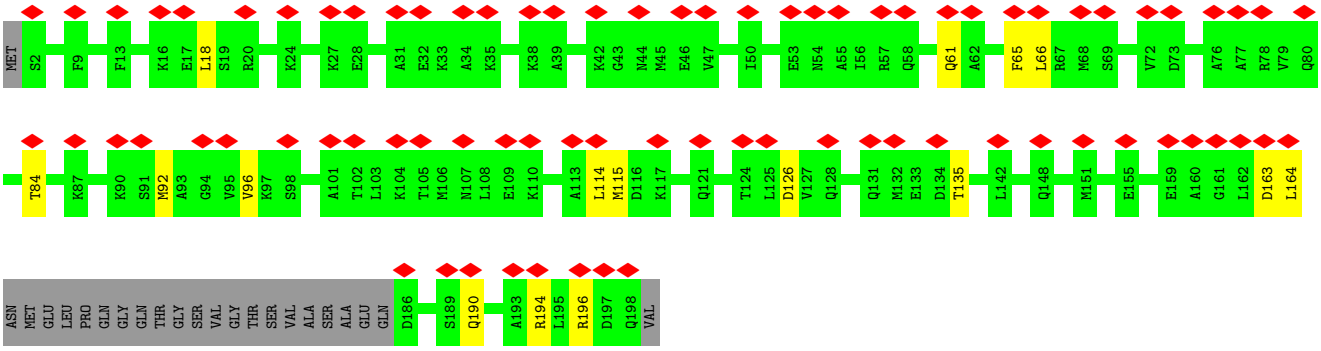
- Molecule 1: Charged multivesicular body protein 1b

Chain NB:



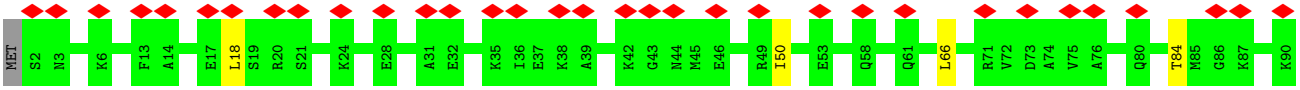
- Molecule 1: Charged multivesicular body protein 1b

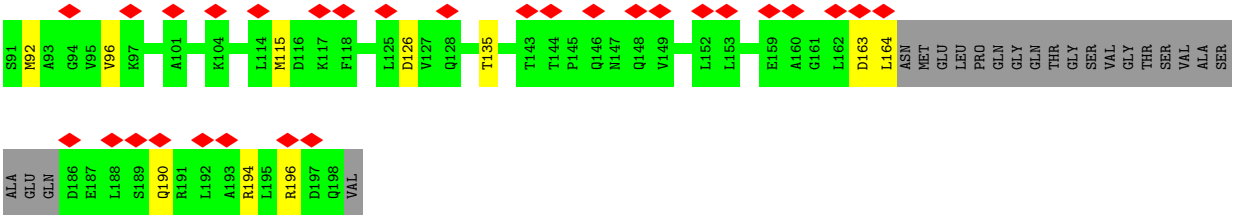
Chain PB:



- Molecule 1: Charged multivesicular body protein 1b

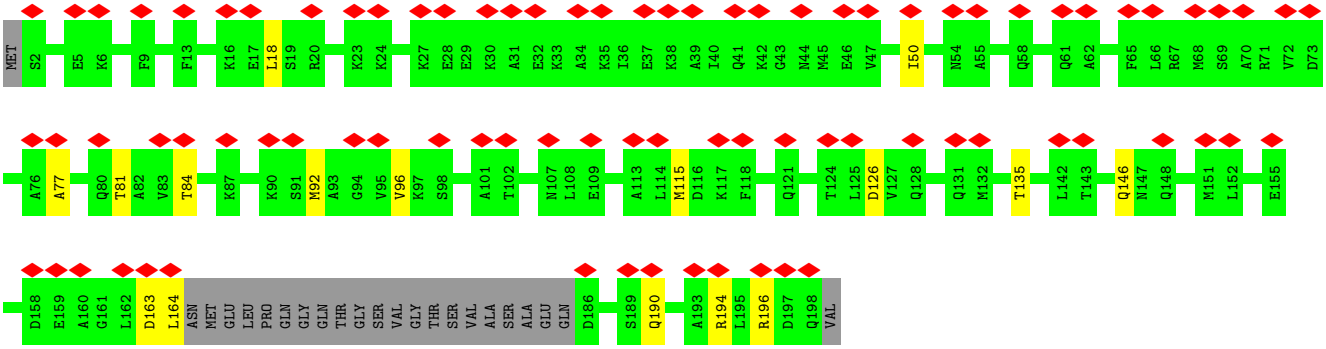
Chain RB:





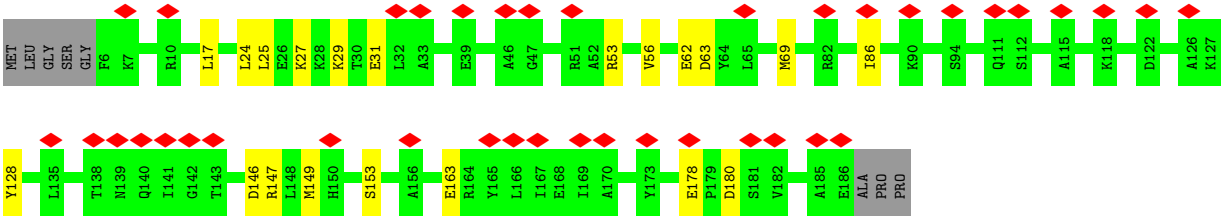
• Molecule 1: Charged multivesicular body protein 1b

Chain 02:



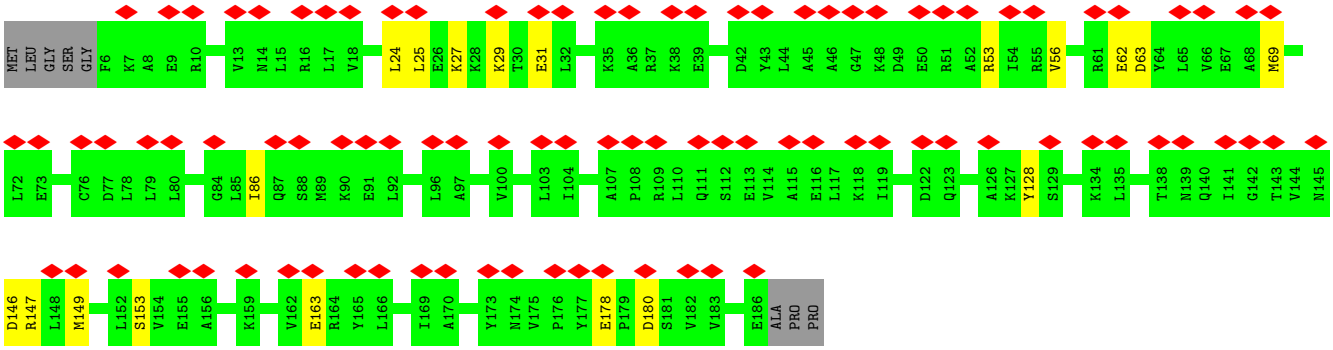
• Molecule 2: IST1 homolog

Chain MB:



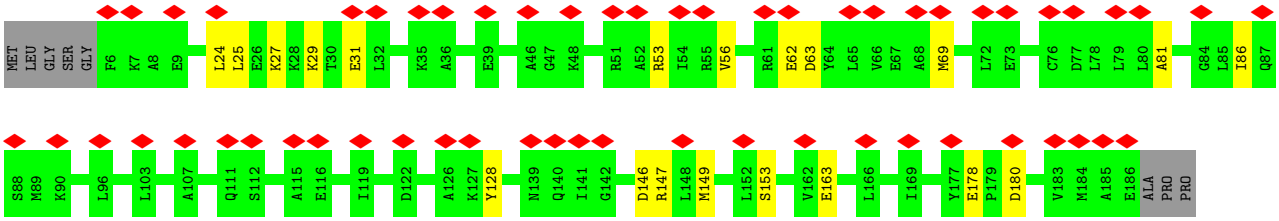
• Molecule 2: IST1 homolog

Chain B:



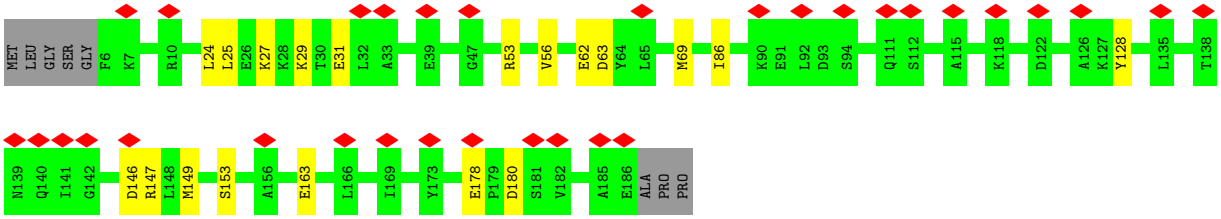
• Molecule 2: IST1 homolog

Chain D: 30% 85% 11%



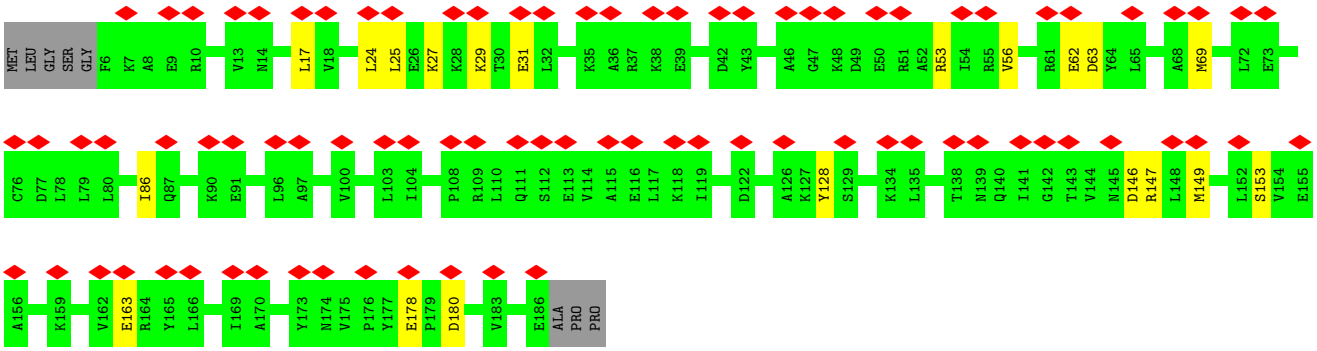
- Molecule 2: IST1 homolog

Chain F: 17% 86% 10%



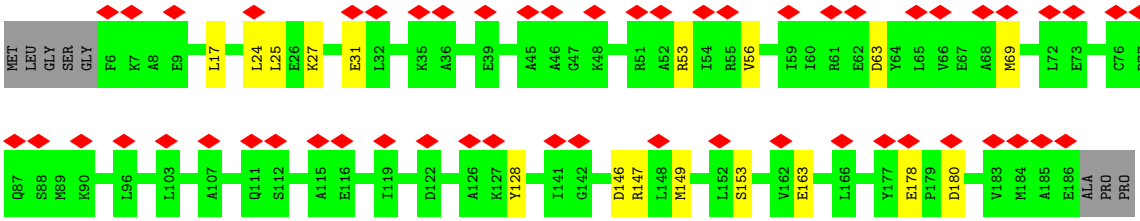
- Molecule 2: IST1 homolog

Chain H: 44% 85% 11%



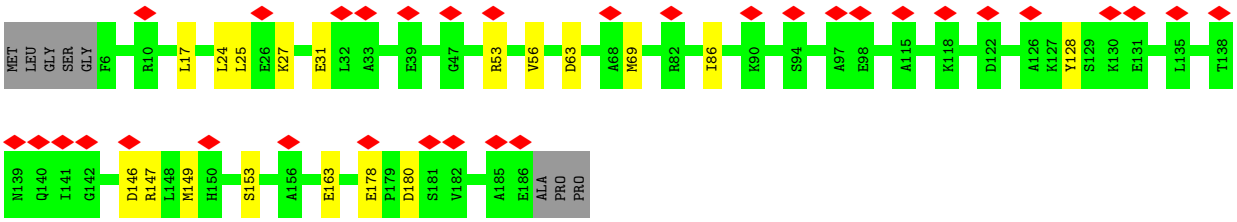
- Molecule 2: IST1 homolog

Chain J: 30% 86% 10%



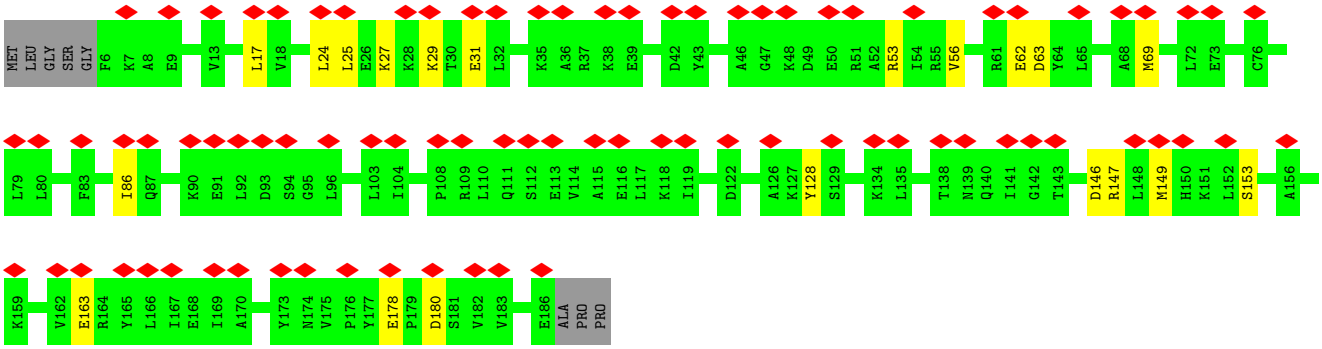
- Molecule 2: IST1 homolog

Chain L: 17% 86% 10%



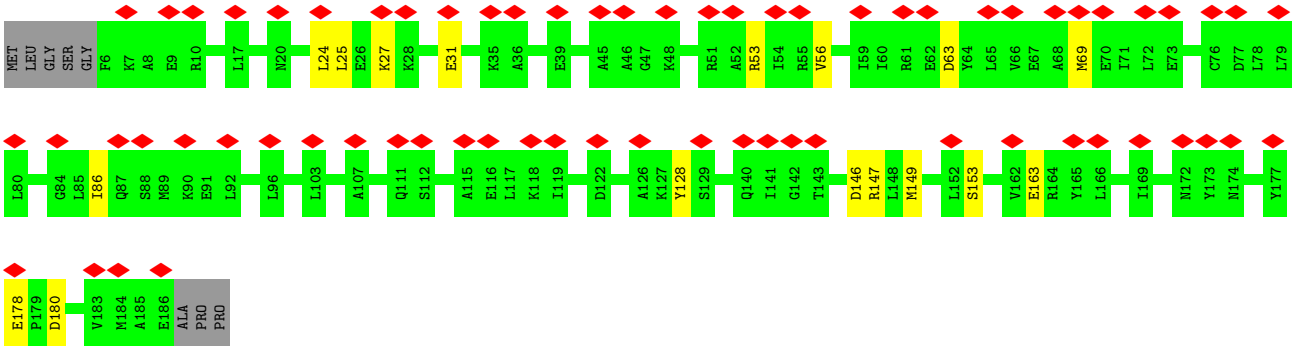
• Molecule 2: IST1 homolog

Chain N:



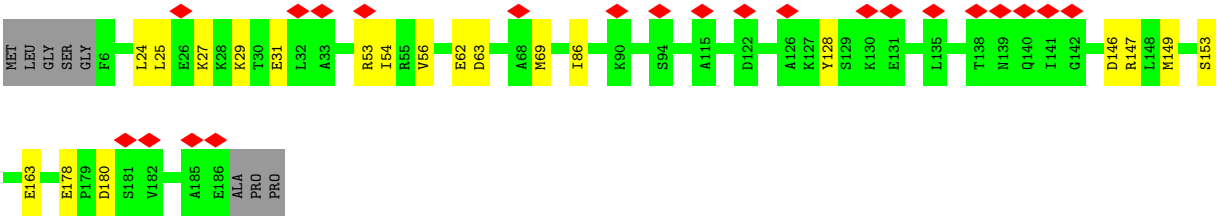
• Molecule 2: IST1 homolog

Chain P:



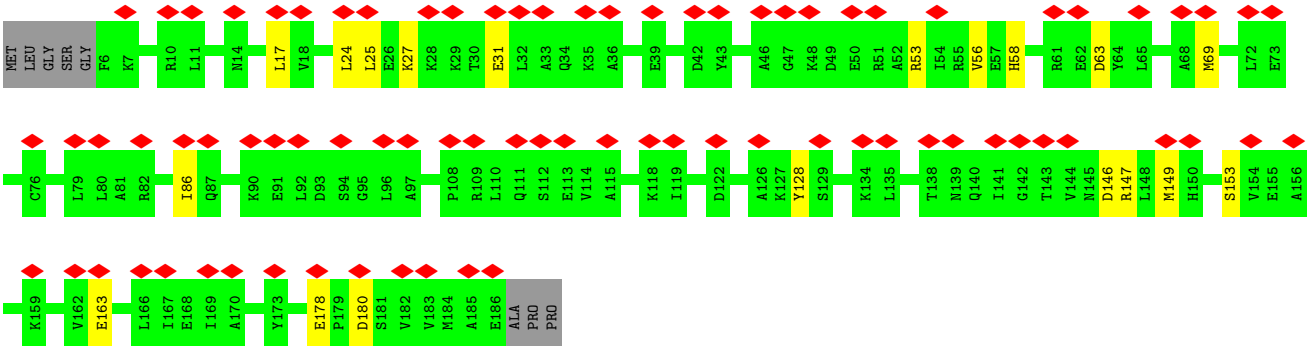
• Molecule 2: IST1 homolog

Chain R:



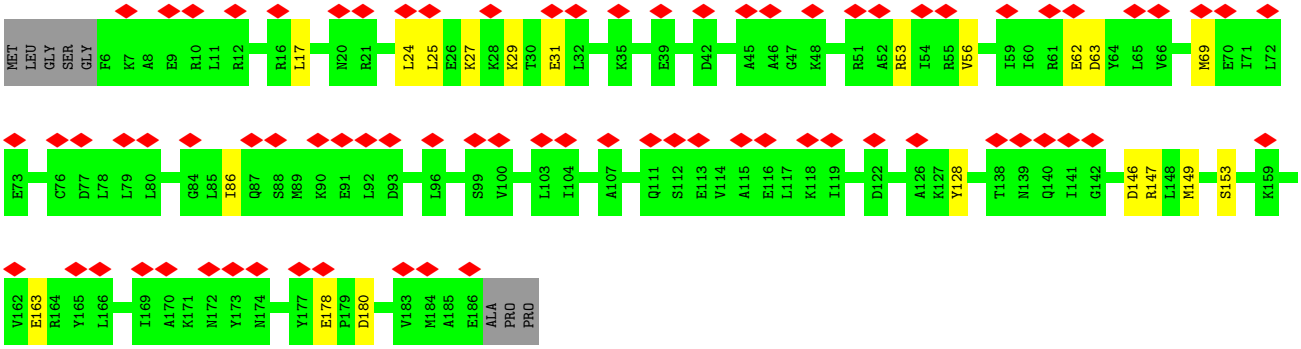
• Molecule 2: IST1 homolog

Chain T:



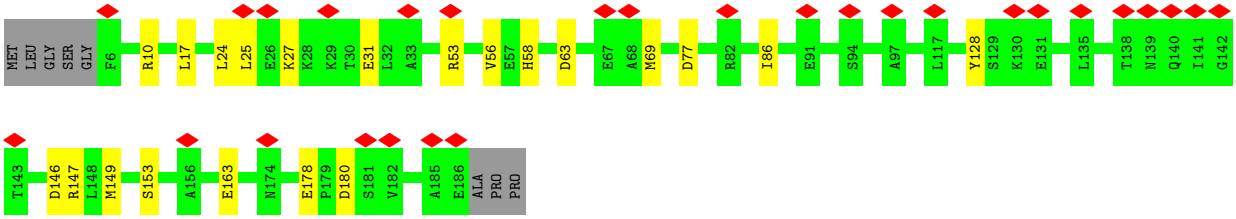
- Molecule 2: IST1 homolog

Chain W:



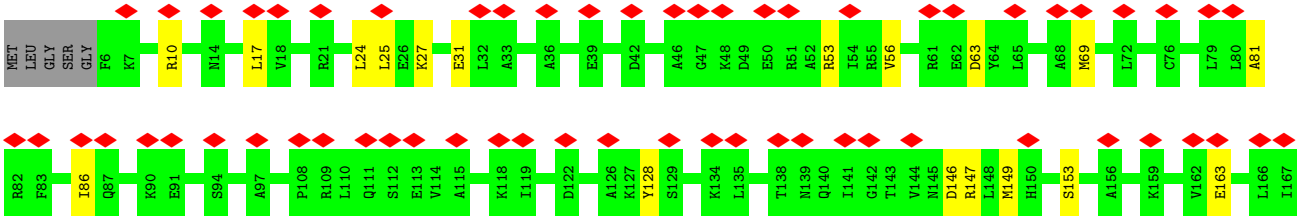
- Molecule 2: IST1 homolog

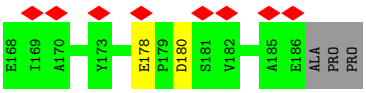
Chain Y:



- Molecule 2: IST1 homolog

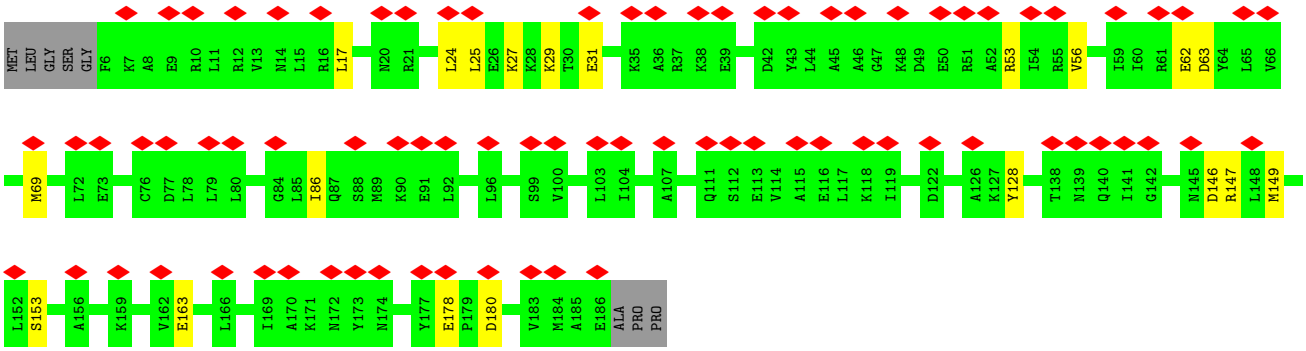
Chain AA:





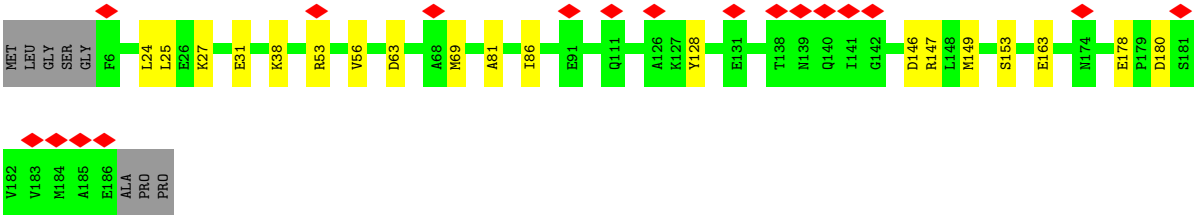
• Molecule 2: IST1 homolog

Chain CA:



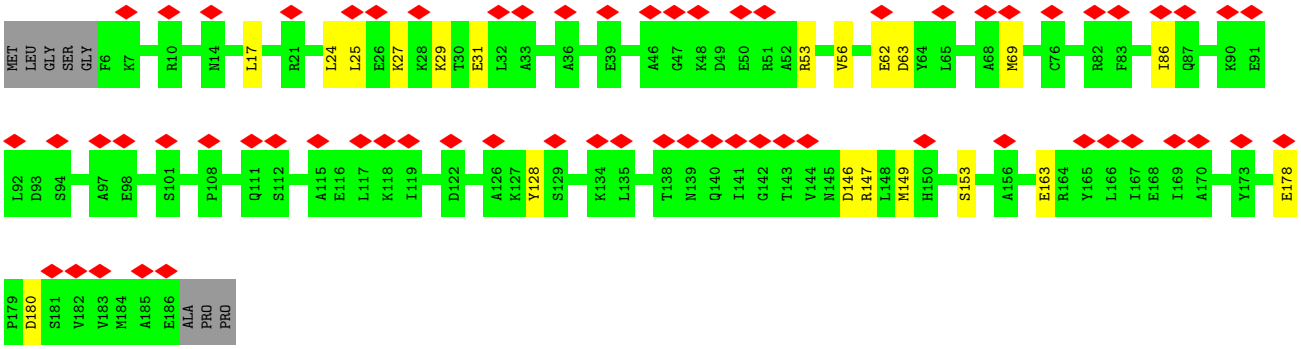
• Molecule 2: IST1 homolog

Chain EA:



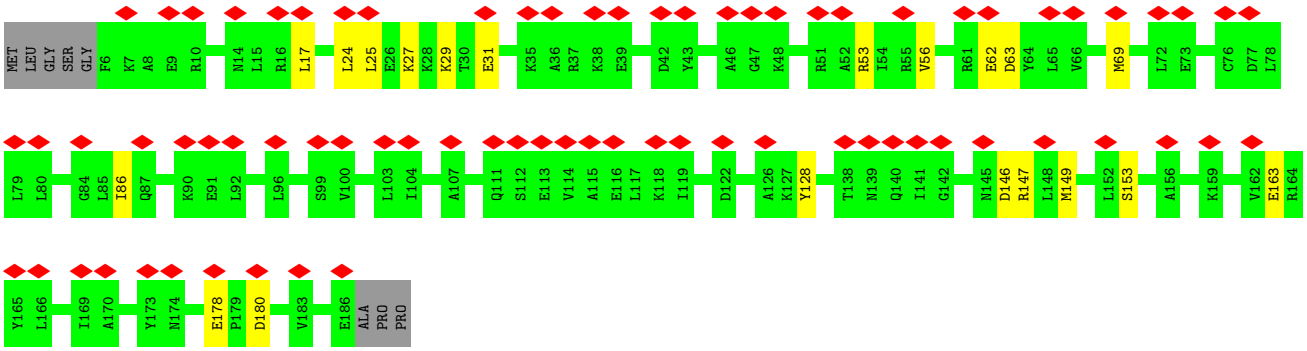
• Molecule 2: IST1 homolog

Chain GA:



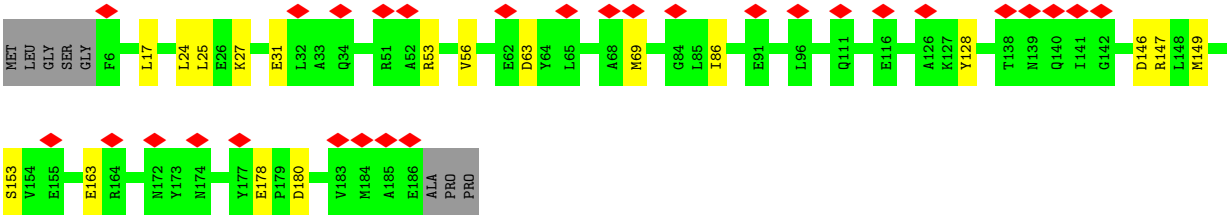
• Molecule 2: IST1 homolog

Chain IA:



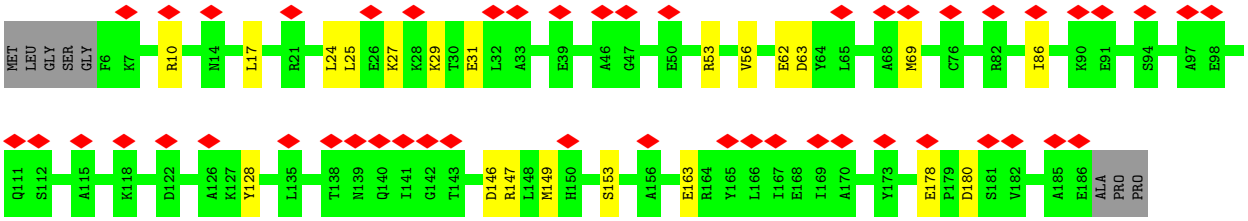
• Molecule 2: IST1 homolog

Chain KA:



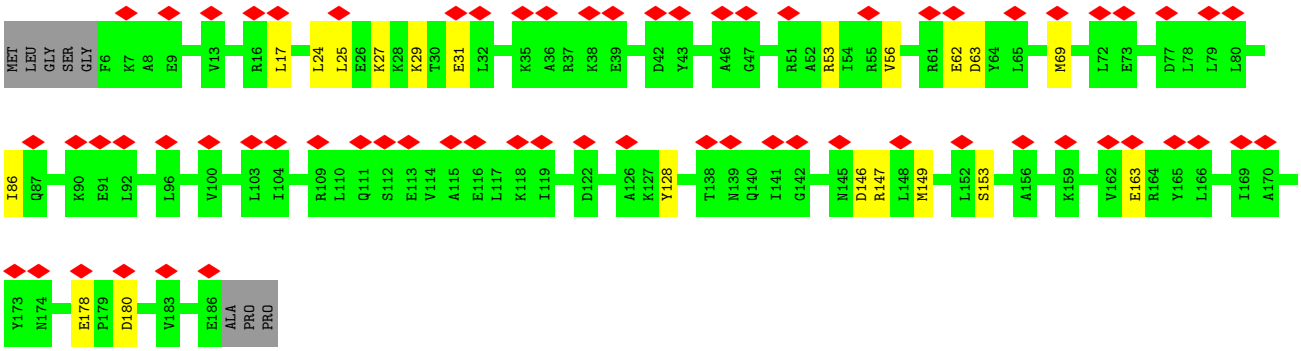
• Molecule 2: IST1 homolog

Chain MA:



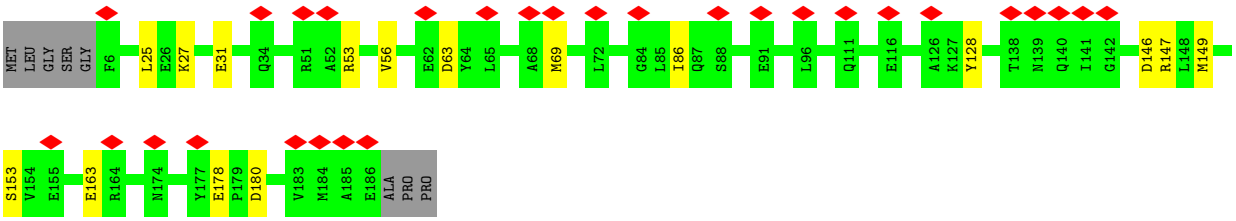
• Molecule 2: IST1 homolog

Chain OA:



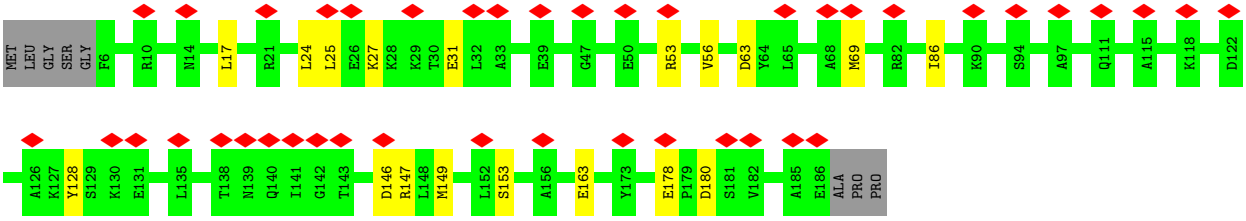
• Molecule 2: IST1 homolog

Chain QA:



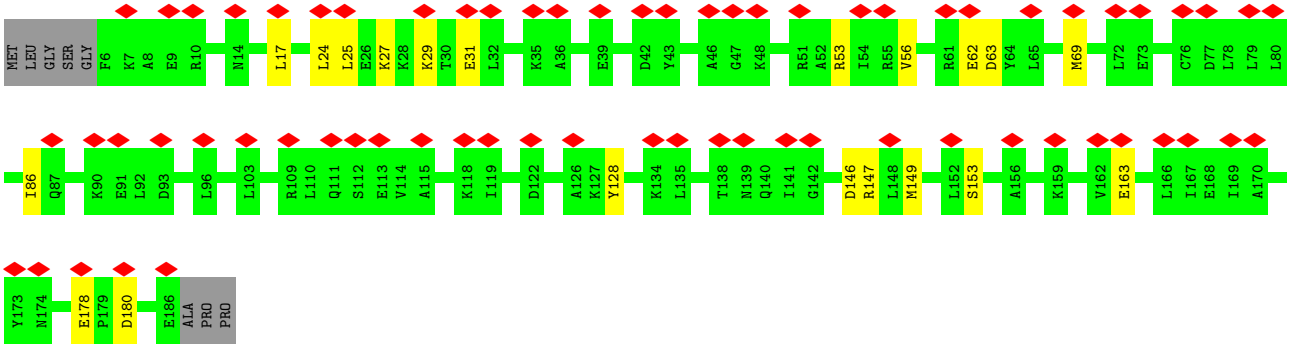
- Molecule 2: IST1 homolog

Chain SA:



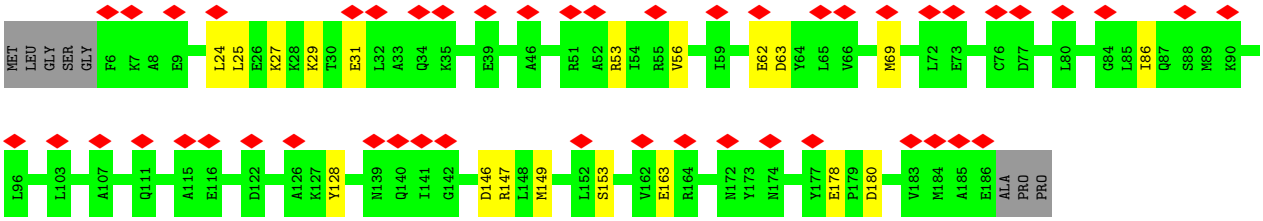
- Molecule 2: IST1 homolog

Chain UA:



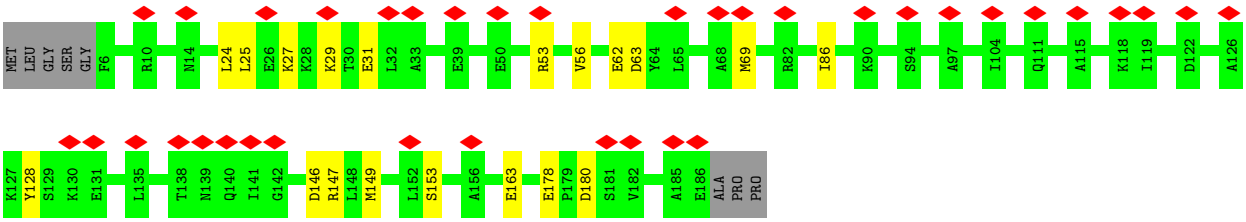
- Molecule 2: IST1 homolog

Chain WA:



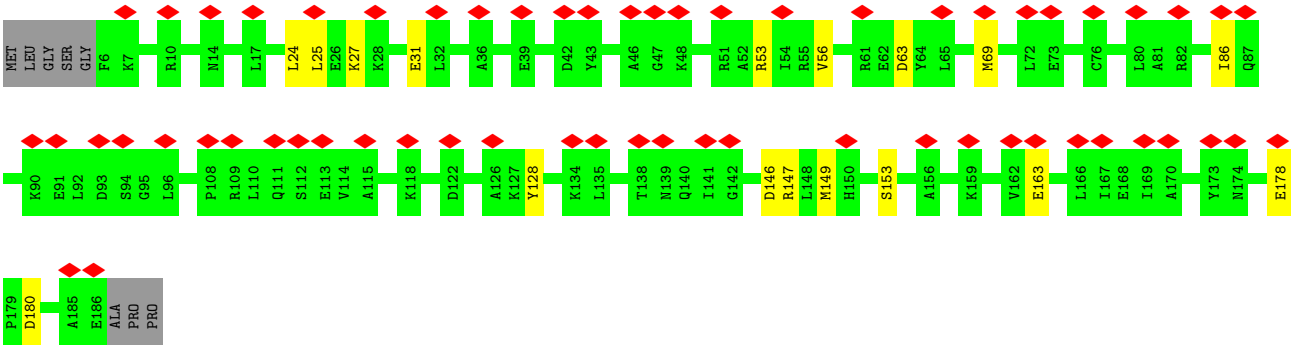
- Molecule 2: IST1 homolog

Chain YA:



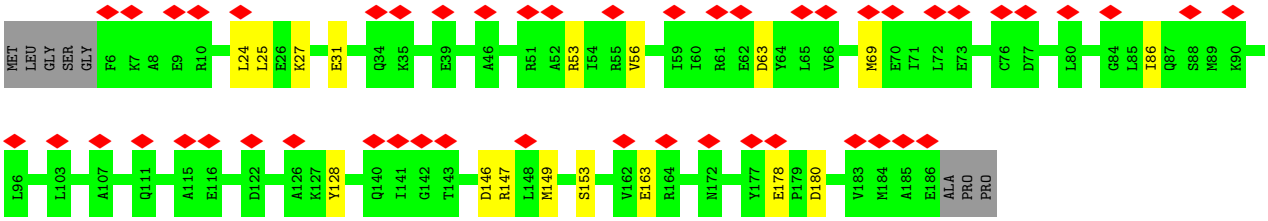
• Molecule 2: IST1 homolog

Chain AB:



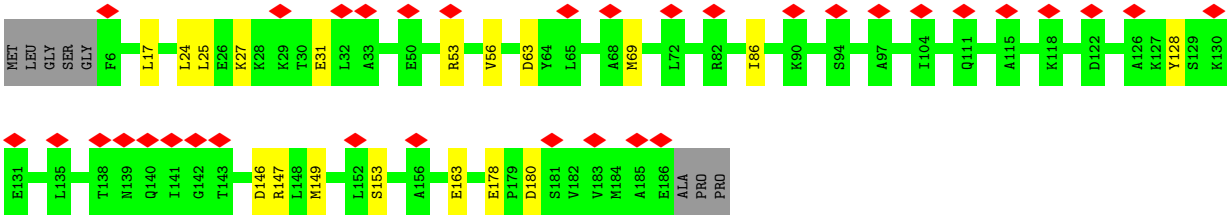
• Molecule 2: IST1 homolog

Chain CB:



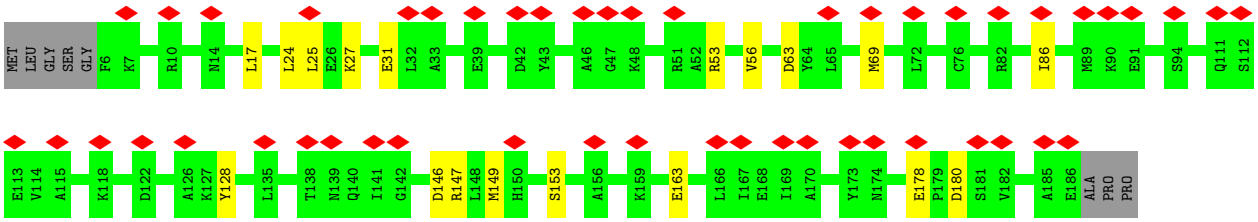
• Molecule 2: IST1 homolog

Chain EB:



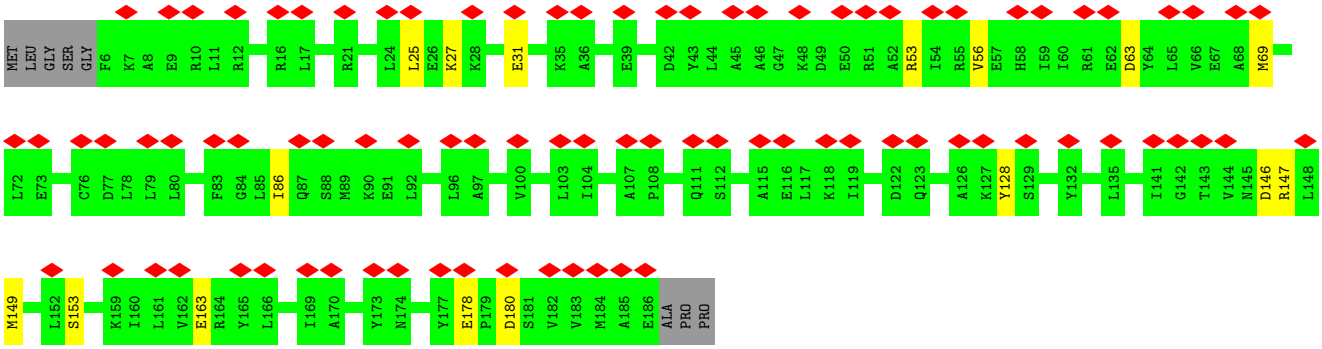
• Molecule 2: IST1 homolog

Chain GB:



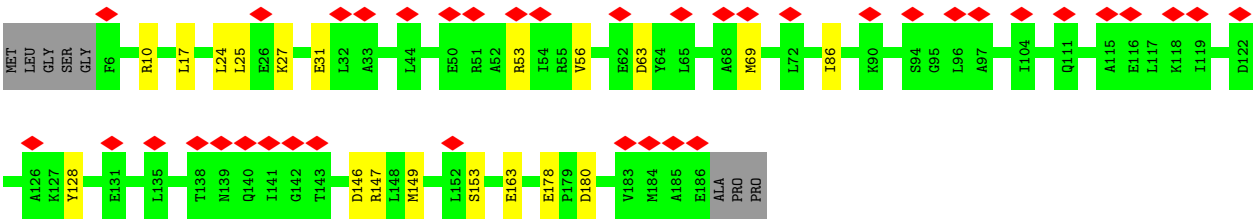
- Molecule 2: IST1 homolog

Chain IB:



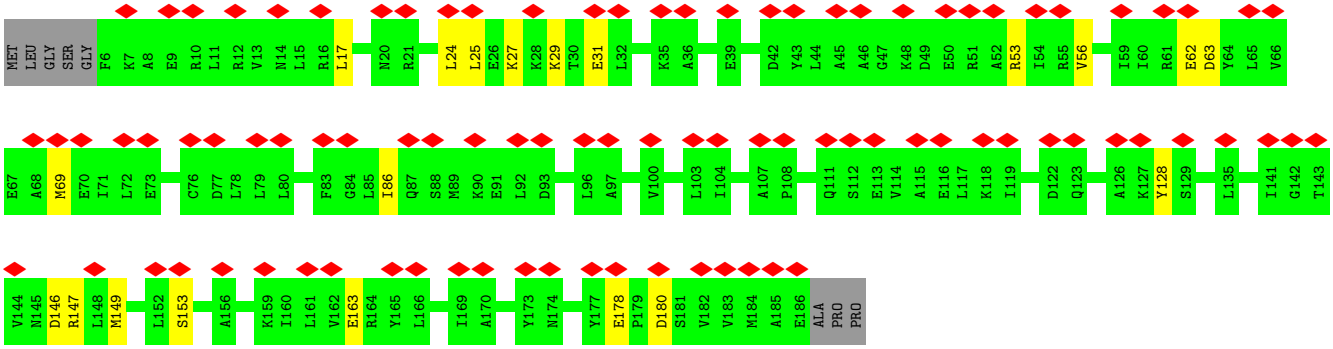
- Molecule 2: IST1 homolog

Chain KB:



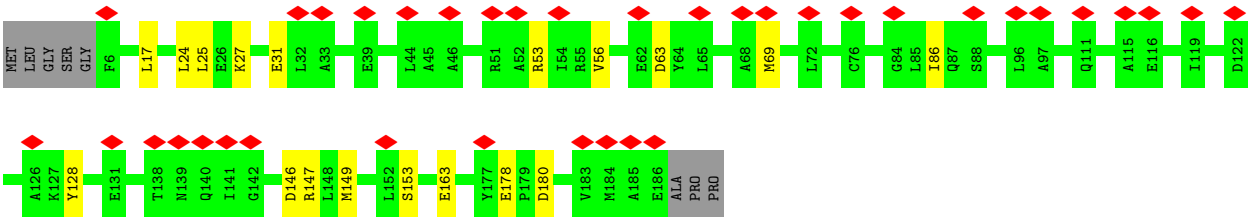
- Molecule 2: IST1 homolog

Chain OB:



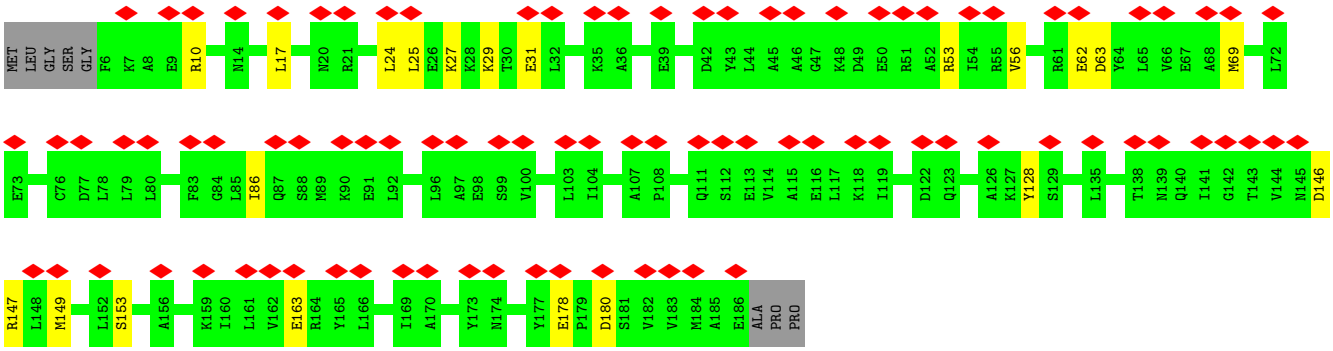
- Molecule 2: IST1 homolog

Chain QB:



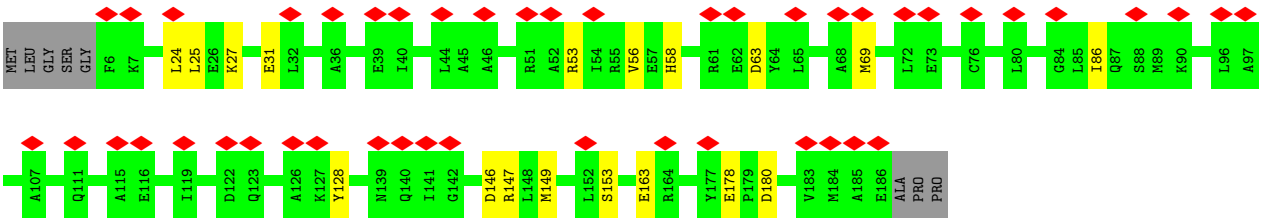
- Molecule 2: IST1 homolog

Chain SB:



- Molecule 2: IST1 homolog

Chain 01:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=20.02°, rise=2.96 Å, axial sym=C1	Depositor
Number of segments used	61974	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	44	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.048	Depositor
Minimum map value	-0.020	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	429.44, 429.44, 429.44	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.22, 1.22, 1.22	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	02	0.51	0/1373	0.40	0/1833
1	A	0.51	0/1373	0.40	0/1833
1	BA	0.51	0/1373	0.40	0/1833
1	BB	0.51	0/1373	0.40	0/1833
1	C	0.51	0/1373	0.40	0/1833
1	DA	0.51	0/1373	0.40	0/1833
1	DB	0.51	0/1373	0.40	0/1833
1	E	0.51	0/1373	0.40	0/1833
1	FA	0.51	0/1373	0.40	0/1833
1	FB	0.51	0/1373	0.40	0/1833
1	G	0.51	0/1373	0.40	0/1833
1	HA	0.51	0/1373	0.40	0/1833
1	HB	0.51	0/1373	0.40	0/1833
1	I	0.51	0/1373	0.40	0/1833
1	JA	0.51	0/1373	0.40	0/1833
1	JB	0.51	0/1373	0.40	0/1833
1	K	0.51	0/1373	0.40	0/1833
1	LA	0.51	0/1373	0.40	0/1833
1	LB	0.51	0/1373	0.40	0/1833
1	M	0.51	0/1373	0.40	0/1833
1	NA	0.51	0/1373	0.40	0/1833
1	NB	0.51	0/1373	0.40	0/1833
1	O	0.51	0/1373	0.40	0/1833
1	PA	0.51	0/1373	0.40	0/1833
1	PB	0.51	0/1373	0.40	0/1833
1	Q	0.51	0/1373	0.40	0/1833
1	RA	0.51	0/1373	0.40	0/1833
1	RB	0.51	0/1373	0.40	0/1833
1	S	0.51	0/1373	0.40	0/1833
1	TA	0.51	0/1373	0.40	0/1833
1	V	0.51	0/1373	0.40	0/1833
1	VA	0.51	0/1373	0.40	0/1833
1	X	0.51	0/1373	0.40	0/1833
1	XA	0.51	0/1373	0.40	0/1833

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	Z	0.51	0/1373	0.40	0/1833
1	ZA	0.51	0/1373	0.40	0/1833
2	01	0.45	0/1407	0.39	0/1901
2	AA	0.45	0/1407	0.39	0/1901
2	AB	0.45	0/1407	0.39	0/1901
2	B	0.45	0/1407	0.39	0/1901
2	CA	0.45	0/1407	0.39	0/1901
2	CB	0.45	0/1407	0.39	0/1901
2	D	0.45	0/1407	0.39	0/1901
2	EA	0.45	0/1407	0.39	0/1901
2	EB	0.45	0/1407	0.39	0/1901
2	F	0.45	0/1407	0.39	0/1901
2	GA	0.45	0/1407	0.39	0/1901
2	GB	0.45	0/1407	0.39	0/1901
2	H	0.45	0/1407	0.39	0/1901
2	IA	0.45	0/1407	0.39	0/1901
2	IB	0.45	0/1407	0.39	0/1901
2	J	0.45	0/1407	0.39	0/1901
2	KA	0.45	0/1407	0.39	0/1901
2	KB	0.45	0/1407	0.39	0/1901
2	L	0.45	0/1407	0.39	0/1901
2	MA	0.45	0/1407	0.39	0/1901
2	MB	0.45	0/1407	0.39	0/1901
2	N	0.45	0/1407	0.39	0/1901
2	OA	0.45	0/1407	0.39	0/1901
2	OB	0.45	0/1407	0.39	0/1901
2	P	0.45	0/1407	0.39	0/1901
2	QA	0.45	0/1407	0.39	0/1901
2	QB	0.45	0/1407	0.39	0/1901
2	R	0.45	0/1407	0.39	0/1901
2	SA	0.45	0/1407	0.39	0/1901
2	SB	0.45	0/1407	0.39	0/1901
2	T	0.45	0/1407	0.39	0/1901
2	UA	0.45	0/1407	0.39	0/1901
2	W	0.45	0/1407	0.39	0/1901
2	WA	0.45	0/1407	0.39	0/1901
2	Y	0.45	0/1407	0.39	0/1901
2	YA	0.45	0/1407	0.39	0/1901
All	All	0.48	0/100080	0.40	0/134424

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	02	1366	0	1399	17	0
1	A	1366	0	1399	16	0
1	BA	1366	0	1399	16	0
1	BB	1366	0	1399	9	0
1	C	1366	0	1399	15	0
1	DA	1366	0	1399	23	0
1	DB	1366	0	1399	22	0
1	E	1366	0	1399	30	0
1	FA	1366	0	1399	18	0
1	FB	1366	0	1399	15	0
1	G	1366	0	1399	15	0
1	HA	1366	0	1399	14	0
1	HB	1366	0	1399	12	0
1	I	1366	0	1399	13	0
1	JA	1366	0	1399	14	0
1	JB	1366	0	1399	17	0
1	K	1366	0	1399	20	0
1	LA	1366	0	1399	16	0
1	LB	1366	0	1399	15	0
1	M	1366	0	1399	16	0
1	NA	1366	0	1399	16	0
1	NB	1366	0	1399	15	0
1	O	1366	0	1399	15	0
1	PA	1366	0	1399	17	0
1	PB	1366	0	1399	17	0
1	Q	1366	0	1399	23	0
1	RA	1366	0	1399	13	0
1	RB	1366	0	1399	14	0
1	S	1366	0	1399	15	0
1	TA	1366	0	1399	17	0
1	V	1366	0	1399	15	0
1	VA	1366	0	1399	15	0
1	X	1366	0	1399	27	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	XA	1366	0	1399	23	0
1	Z	1366	0	1399	20	0
1	ZA	1366	0	1399	19	0
2	01	1390	0	1390	12	0
2	AA	1390	0	1390	14	0
2	AB	1390	0	1390	11	0
2	B	1390	0	1390	12	0
2	CA	1390	0	1390	13	0
2	CB	1390	0	1390	11	0
2	D	1390	0	1390	13	0
2	EA	1390	0	1390	15	0
2	EB	1390	0	1390	12	0
2	F	1390	0	1390	12	0
2	GA	1390	0	1390	13	0
2	GB	1390	0	1390	12	0
2	H	1390	0	1390	13	0
2	IA	1390	0	1390	13	0
2	IB	1390	0	1390	9	0
2	J	1390	0	1390	12	0
2	KA	1390	0	1390	12	0
2	KB	1390	0	1390	13	0
2	L	1390	0	1390	11	0
2	MA	1390	0	1390	14	0
2	MB	1390	0	1390	13	0
2	N	1390	0	1390	13	0
2	OA	1390	0	1390	13	0
2	OB	1390	0	1390	13	0
2	P	1390	0	1390	11	0
2	QA	1390	0	1390	9	0
2	QB	1390	0	1390	12	0
2	R	1390	0	1390	13	0
2	SA	1390	0	1390	12	0
2	SB	1390	0	1390	14	0
2	T	1390	0	1390	13	0
2	UA	1390	0	1390	13	0
2	W	1390	0	1390	13	0
2	WA	1390	0	1390	12	0
2	Y	1390	0	1390	14	0
2	YA	1390	0	1390	12	0
All	All	99216	0	100404	747	0

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

All (747) 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:X:50:ILE:HD12	1:DA:66:LEU:HD22	1.41	0.99
1:X:50:ILE:CD1	1:DA:66:LEU:HD22	1.98	0.94
1:XA:18:LEU:HD21	1:DB:84:THR:HG21	1.56	0.84
1:C:66:LEU:HD22	1:02:50:ILE:HD12	1.64	0.78
1:XA:18:LEU:CD2	1:DB:84:THR:HG21	2.17	0.73
2:T:178:GLU:OE1	2:T:178:GLU:N	2.23	0.72
2:B:178:GLU:N	2:B:178:GLU:OE1	2.23	0.72
2:AA:178:GLU:N	2:AA:178:GLU:OE1	2.23	0.72
2:AB:178:GLU:N	2:AB:178:GLU:OE1	2.23	0.72
2:N:178:GLU:N	2:N:178:GLU:OE1	2.23	0.71
2:IA:178:GLU:N	2:IA:178:GLU:OE1	2.23	0.71
2:WA:178:GLU:N	2:WA:178:GLU:OE1	2.23	0.71
2:GB:178:GLU:OE1	2:GB:178:GLU:N	2.23	0.71
2:D:178:GLU:N	2:D:178:GLU:OE1	2.23	0.71
1:X:18:LEU:HD21	1:DA:84:THR:HG21	1.72	0.71
2:QA:178:GLU:OE1	2:QA:178:GLU:N	2.23	0.71
2:UA:178:GLU:N	2:UA:178:GLU:OE1	2.23	0.71
2:CB:178:GLU:N	2:CB:178:GLU:OE1	2.23	0.71
2:01:178:GLU:N	2:01:178:GLU:OE1	2.23	0.71
2:MB:178:GLU:N	2:MB:178:GLU:OE1	2.23	0.71
2:H:178:GLU:N	2:H:178:GLU:OE1	2.23	0.71
2:J:178:GLU:OE1	2:J:178:GLU:N	2.23	0.71
2:GA:178:GLU:OE1	2:GA:178:GLU:N	2.23	0.71
2:OA:178:GLU:OE1	2:OA:178:GLU:N	2.23	0.71
2:P:178:GLU:N	2:P:178:GLU:OE1	2.23	0.71
2:IB:178:GLU:OE1	2:IB:178:GLU:N	2.23	0.71
2:SB:178:GLU:OE1	2:SB:178:GLU:N	2.23	0.71
2:CA:178:GLU:N	2:CA:178:GLU:OE1	2.23	0.71
2:EA:178:GLU:OE1	2:EA:178:GLU:N	2.23	0.71
2:Y:178:GLU:N	2:Y:178:GLU:OE1	2.23	0.71
2:EB:178:GLU:N	2:EB:178:GLU:OE1	2.23	0.71
2:KB:178:GLU:N	2:KB:178:GLU:OE1	2.23	0.71
2:QB:178:GLU:N	2:QB:178:GLU:OE1	2.23	0.71
2:KA:178:GLU:N	2:KA:178:GLU:OE1	2.23	0.71
2:F:178:GLU:N	2:F:178:GLU:OE1	2.23	0.71
2:MA:178:GLU:N	2:MA:178:GLU:OE1	2.23	0.71
2:YA:178:GLU:N	2:YA:178:GLU:OE1	2.23	0.71
2:R:178:GLU:N	2:R:178:GLU:OE1	2.23	0.70
2:W:178:GLU:N	2:W:178:GLU:OE1	2.23	0.70
1:I:18:LEU:HD21	1:O:84:THR:HG21	1.74	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:OB:178:GLU:N	2:OB:178:GLU:OE1	2.23	0.70
2:L:178:GLU:OE1	2:L:178:GLU:N	2.23	0.70
1:I:50:ILE:HD12	1:O:66:LEU:HD22	1.74	0.70
2:SA:178:GLU:N	2:SA:178:GLU:OE1	2.23	0.70
1:E:18:LEU:HD21	1:K:84:THR:HG21	1.73	0.69
1:X:50:ILE:HD12	1:DA:66:LEU:CD2	2.20	0.69
1:DA:18:LEU:HD21	1:JA:84:THR:HG21	1.74	0.69
1:X:126:ASP:CG	2:EA:24:LEU:HD13	2.12	0.69
1:TA:18:LEU:HD21	1:ZA:84:THR:HG21	1.74	0.68
1:PB:18:LEU:HD21	1:02:84:THR:HG21	1.75	0.68
1:LA:18:LEU:HD21	1:RA:84:THR:HG21	1.76	0.68
1:V:18:LEU:HD21	1:BA:84:THR:HG21	1.76	0.68
1:I:50:ILE:CD1	1:O:66:LEU:HD22	2.24	0.67
1:JB:84:THR:HG21	1:FB:18:LEU:HD21	1.75	0.67
1:JA:18:LEU:HD21	1:PA:84:THR:HG21	1.76	0.66
1:NA:18:LEU:HD21	1:TA:84:THR:HG21	1.77	0.66
1:PA:18:LEU:HD21	1:VA:84:THR:HG21	1.77	0.66
1:S:50:ILE:HD12	1:Z:66:LEU:HD22	1.78	0.66
1:Z:18:LEU:HD21	1:FA:84:THR:HG21	1.76	0.66
1:JB:126:ASP:CG	2:F:24:LEU:HD13	2.17	0.65
1:DA:126:ASP:CG	2:KA:24:LEU:HD13	2.17	0.65
1:K:163:ASP:OD1	1:K:164:LEU:N	2.30	0.65
1:S:126:ASP:CG	2:AA:24:LEU:HD13	2.17	0.65
1:HB:18:LEU:HD21	1:NB:84:THR:HG21	1.77	0.65
1:JB:163:ASP:OD1	1:JB:164:LEU:N	2.30	0.65
1:K:126:ASP:CG	2:R:24:LEU:HD13	2.17	0.65
1:PA:126:ASP:CG	2:WA:24:LEU:HD13	2.17	0.65
1:RA:163:ASP:OD1	1:RA:164:LEU:N	2.30	0.65
1:DB:163:ASP:OD1	1:DB:164:LEU:N	2.30	0.65
1:NB:163:ASP:OD1	1:NB:164:LEU:N	2.30	0.65
1:I:163:ASP:OD1	1:I:164:LEU:N	2.30	0.65
1:K:50:ILE:HD12	1:Q:66:LEU:HD22	1.77	0.65
1:V:163:ASP:OD1	1:V:164:LEU:N	2.30	0.65
1:FA:163:ASP:OD1	1:FA:164:LEU:N	2.30	0.65
1:BB:163:ASP:OD1	1:BB:164:LEU:N	2.30	0.65
1:S:163:ASP:OD1	1:S:164:LEU:N	2.30	0.65
1:ZA:163:ASP:OD1	1:ZA:164:LEU:N	2.30	0.65
1:A:163:ASP:OD1	1:A:164:LEU:N	2.30	0.65
1:X:163:ASP:OD1	1:X:164:LEU:N	2.30	0.65
1:HA:163:ASP:OD1	1:HA:164:LEU:N	2.30	0.65
1:JA:163:ASP:OD1	1:JA:164:LEU:N	2.30	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:18:LEU:HD21	1:HA:84:THR:HG21	1.78	0.65
1:PA:163:ASP:OD1	1:PA:164:LEU:N	2.30	0.65
1:PB:163:ASP:OD1	1:PB:164:LEU:N	2.30	0.65
1:02:163:ASP:OD1	1:02:164:LEU:N	2.30	0.65
1:NA:163:ASP:OD1	1:NA:164:LEU:N	2.30	0.64
1:G:163:ASP:OD1	1:G:164:LEU:N	2.30	0.64
1:M:18:LEU:HD21	1:S:84:THR:HG21	1.78	0.64
1:M:163:ASP:OD1	1:M:164:LEU:N	2.30	0.64
1:E:163:ASP:OD1	1:E:164:LEU:N	2.30	0.64
1:Q:131:GLN:OE1	2:Y:17:LEU:HD23	1.97	0.64
1:TA:163:ASP:OD1	1:TA:164:LEU:N	2.30	0.64
1:LA:163:ASP:OD1	1:LA:164:LEU:N	2.30	0.64
1:VA:163:ASP:OD1	1:VA:164:LEU:N	2.30	0.64
1:C:163:ASP:OD1	1:C:164:LEU:N	2.30	0.64
1:DA:163:ASP:OD1	1:DA:164:LEU:N	2.30	0.64
1:LB:163:ASP:OD1	1:LB:164:LEU:N	2.30	0.64
1:BA:163:ASP:OD1	1:BA:164:LEU:N	2.30	0.64
1:RB:163:ASP:OD1	1:RB:164:LEU:N	2.30	0.64
1:O:18:LEU:HD21	1:V:84:THR:HG21	1.78	0.64
1:Q:18:LEU:HD21	1:X:84:THR:HG21	1.80	0.64
1:Q:163:ASP:OD1	1:Q:164:LEU:N	2.30	0.64
1:VA:18:LEU:HD21	1:BB:84:THR:HG21	1.79	0.64
1:O:163:ASP:OD1	1:O:164:LEU:N	2.30	0.64
1:XA:163:ASP:OD1	1:XA:164:LEU:N	2.30	0.64
1:C:66:LEU:HD22	1:02:50:ILE:CD1	2.27	0.64
1:HB:163:ASP:OD1	1:HB:164:LEU:N	2.30	0.64
1:Q:61:GLN:NE2	1:X:77:ALA:HB1	2.12	0.63
1:Z:163:ASP:OD1	1:Z:164:LEU:N	2.30	0.63
1:FB:163:ASP:OD1	1:FB:164:LEU:N	2.30	0.63
2:D:24:LEU:HD13	1:02:126:ASP:CG	2.18	0.63
1:E:18:LEU:CD2	1:K:84:THR:HG21	2.28	0.63
1:HA:18:LEU:HD21	1:NA:84:THR:HG21	1.80	0.63
1:TA:126:ASP:CG	2:AB:24:LEU:HD13	2.19	0.63
1:A:84:THR:HG21	1:RB:18:LEU:HD21	1.81	0.62
1:DB:18:LEU:HD21	1:LB:84:THR:HG21	1.80	0.62
1:E:57:ARG:HA	1:DA:143:THR:O	1.99	0.62
1:Q:18:LEU:CD2	1:X:84:THR:HG21	2.31	0.61
1:S:126:ASP:OD2	2:AA:24:LEU:HD13	2.00	0.61
1:JB:50:ILE:HD12	1:E:66:LEU:HD22	1.80	0.61
1:A:126:ASP:CG	2:H:24:LEU:HD13	2.20	0.61
1:NA:126:ASP:CG	2:UA:24:LEU:HD13	2.21	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:MB:146:ASP:OD1	2:MB:147:ARG:N	2.34	0.61
2:F:146:ASP:OD1	2:F:147:ARG:N	2.34	0.61
2:GA:146:ASP:OD1	2:GA:147:ARG:N	2.34	0.61
1:G:126:ASP:CG	2:N:24:LEU:HD13	2.21	0.61
2:L:146:ASP:OD1	2:L:147:ARG:N	2.34	0.61
2:AA:146:ASP:OD1	2:AA:147:ARG:N	2.34	0.61
2:MA:146:ASP:OD1	2:MA:147:ARG:N	2.34	0.61
2:QA:146:ASP:OD1	2:QA:147:ARG:N	2.34	0.61
2:GB:146:ASP:OD1	2:GB:147:ARG:N	2.34	0.61
2:KA:146:ASP:OD1	2:KA:147:ARG:N	2.34	0.61
2:SA:146:ASP:OD1	2:SA:147:ARG:N	2.34	0.61
2:01:146:ASP:OD1	2:01:147:ARG:N	2.34	0.61
2:D:146:ASP:OD1	2:D:147:ARG:N	2.34	0.61
2:WA:146:ASP:OD1	2:WA:147:ARG:N	2.34	0.61
2:QB:146:ASP:OD1	2:QB:147:ARG:N	2.34	0.61
2:J:146:ASP:OD1	2:J:147:ARG:N	2.34	0.61
2:N:146:ASP:OD1	2:N:147:ARG:N	2.34	0.61
2:R:146:ASP:OD1	2:R:147:ARG:N	2.34	0.61
1:FA:126:ASP:CG	2:MA:24:LEU:HD13	2.21	0.61
2:CB:146:ASP:OD1	2:CB:147:ARG:N	2.34	0.61
1:LB:126:ASP:CG	2:QB:24:LEU:HD13	2.22	0.61
2:H:146:ASP:OD1	2:H:147:ARG:N	2.34	0.60
2:T:146:ASP:OD1	2:T:147:ARG:N	2.34	0.60
2:EA:146:ASP:OD1	2:EA:147:ARG:N	2.34	0.60
2:YA:146:ASP:OD1	2:YA:147:ARG:N	2.34	0.60
1:ZA:18:LEU:HD21	1:FB:84:THR:HG21	1.81	0.60
2:AB:146:ASP:OD1	2:AB:147:ARG:N	2.34	0.60
2:KB:146:ASP:OD1	2:KB:147:ARG:N	2.34	0.60
2:Y:146:ASP:OD1	2:Y:147:ARG:N	2.34	0.60
2:OA:146:ASP:OD1	2:OA:147:ARG:N	2.34	0.60
2:UA:146:ASP:OD1	2:UA:147:ARG:N	2.34	0.60
2:B:146:ASP:OD1	2:B:147:ARG:N	2.34	0.60
2:P:146:ASP:OD1	2:P:147:ARG:N	2.34	0.60
2:W:146:ASP:OD1	2:W:147:ARG:N	2.34	0.60
2:IA:146:ASP:OD1	2:IA:147:ARG:N	2.34	0.60
2:EB:146:ASP:OD1	2:EB:147:ARG:N	2.34	0.60
2:IB:146:ASP:OD1	2:IB:147:ARG:N	2.34	0.60
2:CA:146:ASP:OD1	2:CA:147:ARG:N	2.34	0.60
2:OB:146:ASP:OD1	2:OB:147:ARG:N	2.34	0.60
2:SB:146:ASP:OD1	2:SB:147:ARG:N	2.34	0.60
1:LB:18:LEU:HD21	1:PB:84:THR:HG21	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:126:ASP:CG	2:P:24:LEU:HD13	2.22	0.60
1:Q:47:VAL:HG22	1:X:63:VAL:HG23	1.83	0.59
1:PA:50:ILE:HD12	1:VA:66:LEU:HD22	1.84	0.59
1:V:126:ASP:CG	2:CA:24:LEU:HD13	2.22	0.59
1:JA:61:GLN:NE2	1:PA:77:ALA:HB1	2.18	0.59
1:O:126:ASP:CG	2:W:24:LEU:HD13	2.23	0.59
1:JA:18:LEU:CD2	1:PA:84:THR:HG21	2.33	0.59
2:D:24:LEU:HD13	1:02:126:ASP:OD2	2.03	0.58
2:B:24:LEU:HD13	1:RB:126:ASP:CG	2.24	0.58
1:NA:126:ASP:OD2	2:UA:24:LEU:HD13	2.04	0.58
1:C:18:LEU:HD21	1:I:84:THR:HG21	1.86	0.58
1:E:47:VAL:HG22	1:K:63:VAL:HG23	1.86	0.58
1:PA:50:ILE:CD1	1:VA:66:LEU:HD22	2.33	0.58
1:G:18:LEU:HD21	1:M:84:THR:HG21	1.86	0.58
1:BA:126:ASP:CG	2:IA:24:LEU:HD13	2.25	0.58
1:FA:126:ASP:OD2	2:MA:24:LEU:HD13	2.04	0.58
1:RA:126:ASP:CG	2:YA:24:LEU:HD13	2.25	0.58
1:X:126:ASP:OD2	2:EA:24:LEU:HD13	2.04	0.57
1:HB:126:ASP:CG	2:OB:24:LEU:HD13	2.25	0.57
1:X:115:MET:HB3	1:DA:135:THR:HG21	1.86	0.57
1:PA:126:ASP:OD2	2:WA:24:LEU:HD13	2.04	0.57
1:ZA:126:ASP:CG	2:GB:24:LEU:HD13	2.24	0.57
1:C:190:GLN:OE1	1:C:194:ARG:NE	2.38	0.57
1:I:190:GLN:OE1	1:I:194:ARG:NE	2.38	0.57
1:O:190:GLN:OE1	1:O:194:ARG:NE	2.38	0.57
1:V:190:GLN:OE1	1:V:194:ARG:NE	2.38	0.57
1:VA:190:GLN:OE1	1:VA:194:ARG:NE	2.38	0.57
1:HB:190:GLN:OE1	1:HB:194:ARG:NE	2.38	0.57
1:NB:190:GLN:OE1	1:NB:194:ARG:NE	2.38	0.57
1:A:190:GLN:OE1	1:A:194:ARG:NE	2.38	0.57
1:G:190:GLN:OE1	1:G:194:ARG:NE	2.38	0.57
1:X:190:GLN:OE1	1:X:194:ARG:NE	2.38	0.57
1:BA:190:GLN:OE1	1:BA:194:ARG:NE	2.38	0.57
1:NA:190:GLN:OE1	1:NA:194:ARG:NE	2.38	0.57
1:BB:190:GLN:OE1	1:BB:194:ARG:NE	2.38	0.57
1:LB:126:ASP:OD2	2:QB:24:LEU:HD13	2.05	0.57
1:RB:190:GLN:OE1	1:RB:194:ARG:NE	2.38	0.57
1:HA:190:GLN:OE1	1:HA:194:ARG:NE	2.38	0.57
1:02:190:GLN:OE1	1:02:194:ARG:NE	2.38	0.57
1:Q:190:GLN:OE1	1:Q:194:ARG:NE	2.38	0.57
1:XA:190:GLN:OE1	1:XA:194:ARG:NE	2.38	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DB:190:GLN:OE1	1:DB:194:ARG:NE	2.38	0.57
1:PB:190:GLN:OE1	1:PB:194:ARG:NE	2.38	0.57
1:PA:190:GLN:OE1	1:PA:194:ARG:NE	2.38	0.57
1:RA:190:GLN:OE1	1:RA:194:ARG:NE	2.38	0.57
1:TA:190:GLN:OE1	1:TA:194:ARG:NE	2.38	0.57
1:K:190:GLN:OE1	1:K:194:ARG:NE	2.38	0.56
1:M:190:GLN:OE1	1:M:194:ARG:NE	2.38	0.56
1:FA:18:LEU:HD21	1:LA:84:THR:HG21	1.87	0.56
1:JA:190:GLN:OE1	1:JA:194:ARG:NE	2.38	0.56
1:LB:190:GLN:OE1	1:LB:194:ARG:NE	2.38	0.56
2:MB:24:LEU:HD13	1:FB:126:ASP:CG	2.25	0.56
2:J:149:MET:O	2:J:153:SER:OG	2.21	0.56
1:DA:190:GLN:OE1	1:DA:194:ARG:NE	2.38	0.56
1:HA:126:ASP:CG	2:OA:24:LEU:HD13	2.25	0.56
1:LA:126:ASP:CG	2:SA:24:LEU:HD13	2.25	0.56
1:LA:190:GLN:OE1	1:LA:194:ARG:NE	2.38	0.56
1:DB:126:ASP:CG	2:KB:24:LEU:HD13	2.25	0.56
1:K:50:ILE:CD1	1:Q:66:LEU:HD22	2.36	0.56
2:N:149:MET:O	2:N:153:SER:OG	2.21	0.56
2:B:24:LEU:HD13	1:RB:126:ASP:OD2	2.05	0.56
1:E:190:GLN:OE1	1:E:194:ARG:NE	2.38	0.56
1:K:115:MET:HB3	1:Q:135:THR:HG21	1.87	0.56
1:S:190:GLN:OE1	1:S:194:ARG:NE	2.38	0.56
2:SA:149:MET:O	2:SA:153:SER:OG	2.21	0.56
1:ZA:190:GLN:OE1	1:ZA:194:ARG:NE	2.38	0.56
2:L:25:LEU:HD23	2:L:69:MET:SD	2.46	0.56
1:DA:126:ASP:OD2	2:KA:24:LEU:HD13	2.06	0.56
2:CB:149:MET:O	2:CB:153:SER:OG	2.21	0.56
2:SA:25:LEU:HD23	2:SA:69:MET:SD	2.46	0.56
2:UA:149:MET:O	2:UA:153:SER:OG	2.21	0.56
1:FA:190:GLN:OE1	1:FA:194:ARG:NE	2.38	0.56
1:JB:190:GLN:OE1	1:JB:194:ARG:NE	2.38	0.56
2:L:149:MET:O	2:L:153:SER:OG	2.21	0.56
2:GA:25:LEU:HD23	2:GA:69:MET:SD	2.46	0.56
2:MB:25:LEU:HD23	2:MB:69:MET:SD	2.46	0.56
1:E:52:ALA:HB1	1:DA:149:VAL:HG23	1.88	0.56
2:Y:25:LEU:HD23	2:Y:69:MET:SD	2.46	0.56
1:XA:126:ASP:CG	2:EB:24:LEU:HD13	2.26	0.55
2:AB:25:LEU:HD23	2:AB:69:MET:SD	2.46	0.55
1:FB:190:GLN:OE1	1:FB:194:ARG:NE	2.38	0.55
1:Z:190:GLN:OE1	1:Z:194:ARG:NE	2.38	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:EA:25:LEU:HD23	2:EA:69:MET:SD	2.46	0.55
2:EB:25:LEU:HD23	2:EB:69:MET:SD	2.46	0.55
2:GB:25:LEU:HD23	2:GB:69:MET:SD	2.46	0.55
2:R:25:LEU:HD23	2:R:69:MET:SD	2.46	0.55
2:T:25:LEU:HD23	2:T:69:MET:SD	2.46	0.55
2:YA:25:LEU:HD23	2:YA:69:MET:SD	2.46	0.55
2:D:149:MET:O	2:D:153:SER:OG	2.21	0.55
2:AA:25:LEU:HD23	2:AA:69:MET:SD	2.46	0.55
2:UA:25:LEU:HD23	2:UA:69:MET:SD	2.46	0.55
2:KB:25:LEU:HD23	2:KB:69:MET:SD	2.46	0.55
2:OB:25:LEU:HD23	2:OB:69:MET:SD	2.46	0.55
1:G:126:ASP:OD2	2:N:24:LEU:HD13	2.07	0.55
2:J:25:LEU:HD23	2:J:69:MET:SD	2.46	0.55
2:N:25:LEU:HD23	2:N:69:MET:SD	2.46	0.55
2:W:25:LEU:HD23	2:W:69:MET:SD	2.46	0.55
2:CB:25:LEU:HD23	2:CB:69:MET:SD	2.46	0.55
2:SB:25:LEU:HD23	2:SB:69:MET:SD	2.46	0.55
2:MA:25:LEU:HD23	2:MA:69:MET:SD	2.46	0.55
2:QA:25:LEU:HD23	2:QA:69:MET:SD	2.46	0.55
1:E:49:ARG:HH12	2:EA:38:LYS:NZ	2.03	0.55
2:F:25:LEU:HD23	2:F:69:MET:SD	2.46	0.55
2:WA:149:MET:O	2:WA:153:SER:OG	2.21	0.55
2:IB:25:LEU:HD23	2:IB:69:MET:SD	2.46	0.55
2:B:25:LEU:HD23	2:B:69:MET:SD	2.46	0.55
2:H:149:MET:O	2:H:153:SER:OG	2.21	0.55
1:I:126:ASP:OD2	2:P:24:LEU:HD13	2.07	0.55
2:CA:25:LEU:HD23	2:CA:69:MET:SD	2.46	0.55
2:IA:25:LEU:HD23	2:IA:69:MET:SD	2.46	0.55
2:WA:25:LEU:HD23	2:WA:69:MET:SD	2.46	0.55
2:01:25:LEU:HD23	2:01:69:MET:SD	2.46	0.55
2:D:25:LEU:HD23	2:D:69:MET:SD	2.46	0.55
2:H:25:LEU:HD23	2:H:69:MET:SD	2.46	0.55
2:OA:25:LEU:HD23	2:OA:69:MET:SD	2.46	0.55
1:PB:18:LEU:CD2	1:02:84:THR:HG21	2.36	0.55
2:P:25:LEU:HD23	2:P:69:MET:SD	2.46	0.54
1:TA:126:ASP:OD2	2:AB:24:LEU:HD13	2.07	0.54
1:BA:126:ASP:OD2	2:IA:24:LEU:HD13	2.07	0.54
2:MA:149:MET:O	2:MA:153:SER:OG	2.21	0.54
2:OA:149:MET:O	2:OA:153:SER:OG	2.21	0.54
1:A:126:ASP:OD2	2:H:24:LEU:HD13	2.07	0.54
2:MB:149:MET:O	2:MB:153:SER:OG	2.21	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:149:MET:O	2:F:153:SER:OG	2.21	0.54
2:KA:25:LEU:HD23	2:KA:69:MET:SD	2.46	0.54
2:QB:25:LEU:HD23	2:QB:69:MET:SD	2.46	0.54
1:JB:115:MET:HB3	1:E:135:THR:HG21	1.90	0.54
1:Z:126:ASP:CG	2:GA:24:LEU:HD13	2.27	0.54
1:XA:126:ASP:OD2	2:EB:24:LEU:HD13	2.08	0.54
1:S:50:ILE:CD1	1:Z:66:LEU:HD22	2.36	0.54
1:XA:61:GLN:CD	1:DB:77:ALA:HB1	2.27	0.54
1:JB:50:ILE:CD1	1:E:66:LEU:HD22	2.38	0.54
1:A:50:ILE:HD12	1:G:66:LEU:HD22	1.89	0.54
1:K:126:ASP:OD2	2:R:24:LEU:HD13	2.08	0.54
1:V:126:ASP:OD2	2:CA:24:LEU:HD13	2.07	0.54
1:E:61:GLN:NE2	1:K:77:ALA:HB1	2.23	0.53
1:JA:47:VAL:HG22	1:PA:63:VAL:HG23	1.90	0.53
2:01:149:MET:O	2:01:153:SER:OG	2.21	0.53
1:JB:126:ASP:OD2	2:F:24:LEU:HD13	2.08	0.53
1:M:126:ASP:CG	2:T:24:LEU:HD13	2.28	0.53
1:Q:61:GLN:CD	1:X:77:ALA:HB1	2.28	0.53
2:B:149:MET:O	2:B:153:SER:OG	2.21	0.53
1:E:57:ARG:HB2	1:DA:144:THR:OG1	2.09	0.53
2:QA:149:MET:O	2:QA:153:SER:OG	2.21	0.53
1:XA:51:HIS:CD2	1:DB:66:LEU:HD21	2.43	0.53
1:ZA:126:ASP:OD2	2:GB:24:LEU:HD13	2.09	0.53
1:JB:18:LEU:HD21	1:E:84:THR:HG21	1.91	0.53
2:IA:149:MET:O	2:IA:153:SER:OG	2.21	0.53
1:NB:126:ASP:CG	2:SB:24:LEU:HD13	2.29	0.53
1:NB:18:LEU:HD21	1:RB:84:THR:HG21	1.92	0.52
2:GA:149:MET:O	2:GA:153:SER:OG	2.21	0.52
1:DB:126:ASP:OD2	2:KB:24:LEU:HD13	2.09	0.52
1:O:126:ASP:OD2	2:W:24:LEU:HD13	2.10	0.52
1:S:18:LEU:HD21	1:Z:84:THR:HG21	1.91	0.52
1:NB:126:ASP:OD2	2:SB:24:LEU:HD13	2.08	0.52
1:HB:126:ASP:OD2	2:OB:24:LEU:HD13	2.09	0.52
2:QB:149:MET:O	2:QB:153:SER:OG	2.21	0.52
1:A:18:LEU:HD21	1:G:84:THR:HG21	1.92	0.52
1:XA:61:GLN:NE2	1:DB:77:ALA:HB1	2.25	0.52
2:YA:149:MET:O	2:YA:153:SER:OG	2.21	0.52
2:KA:149:MET:O	2:KA:153:SER:OG	2.21	0.52
1:A:66:LEU:HD22	1:RB:50:ILE:HD12	1.91	0.52
1:E:49:ARG:NH1	1:DA:146:GLN:OE1	2.33	0.52
2:R:149:MET:O	2:R:153:SER:OG	2.21	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:18:LEU:CD2	1:FA:84:THR:HG21	2.40	0.52
1:M:126:ASP:OD2	2:T:24:LEU:HD13	2.09	0.51
1:DB:50:ILE:HD12	1:LB:66:LEU:HD22	1.92	0.51
1:LA:126:ASP:OD2	2:SA:24:LEU:HD13	2.10	0.51
2:SB:149:MET:O	2:SB:153:SER:OG	2.21	0.51
1:K:18:LEU:HD21	1:Q:84:THR:HG21	1.93	0.51
1:FA:50:ILE:HD12	1:LA:66:LEU:HD22	1.91	0.51
1:XA:18:LEU:HD21	1:DB:84:THR:CG2	2.34	0.51
2:CA:149:MET:O	2:CA:153:SER:OG	2.21	0.51
1:HA:126:ASP:OD2	2:OA:24:LEU:HD13	2.11	0.50
1:JB:84:THR:HG21	1:FB:18:LEU:CD2	2.41	0.50
1:DA:18:LEU:CD2	1:JA:84:THR:HG21	2.42	0.50
1:RA:126:ASP:OD2	2:YA:24:LEU:HD13	2.11	0.50
2:IB:149:MET:O	2:IB:153:SER:OG	2.21	0.50
1:C:135:THR:HG21	1:02:115:MET:HB3	1.93	0.50
2:KB:149:MET:O	2:KB:153:SER:OG	2.21	0.50
1:A:66:LEU:HD22	1:RB:50:ILE:CD1	2.42	0.50
2:P:149:MET:O	2:P:153:SER:OG	2.21	0.50
1:RA:115:MET:HB3	1:XA:135:THR:HG21	1.93	0.50
2:AA:149:MET:O	2:AA:153:SER:OG	2.21	0.50
1:JA:61:GLN:CD	1:PA:77:ALA:HB1	2.32	0.50
2:OA:29:LYS:NZ	2:OA:62:GLU:OE2	2.31	0.50
1:XA:57:ARG:HH22	1:DB:73:ASP:HB3	1.76	0.50
1:E:52:ALA:CB	1:DA:149:VAL:HG23	2.41	0.50
2:EA:149:MET:O	2:EA:153:SER:OG	2.21	0.50
1:NB:50:ILE:HD12	1:RB:66:LEU:HD22	1.92	0.50
2:R:29:LYS:NZ	2:R:62:GLU:OE2	2.31	0.50
2:MB:24:LEU:HD13	1:FB:126:ASP:OD2	2.12	0.49
1:RA:50:ILE:HD12	1:XA:66:LEU:HD22	1.94	0.49
2:GB:149:MET:O	2:GB:153:SER:OG	2.21	0.49
2:H:29:LYS:NZ	2:H:62:GLU:OE2	2.31	0.49
2:YA:29:LYS:NZ	2:YA:62:GLU:OE2	2.31	0.49
2:B:163:GLU:OE2	2:B:180:ASP:N	2.46	0.49
1:VA:126:ASP:CG	2:CB:24:LEU:HD13	2.33	0.49
2:H:163:GLU:OE2	2:H:180:ASP:N	2.46	0.49
2:IA:163:GLU:OE2	2:IA:180:ASP:N	2.46	0.49
2:OA:163:GLU:OE2	2:OA:180:ASP:N	2.46	0.49
1:XA:49:ARG:NH1	1:02:146:GLN:OE1	2.40	0.49
1:DB:50:ILE:CD1	1:LB:66:LEU:HD22	2.41	0.49
1:PB:61:GLN:NE2	1:02:77:ALA:HB1	2.28	0.49
1:S:115:MET:HB3	1:Z:135:THR:HG21	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:IA:29:LYS:NZ	2:IA:62:GLU:OE2	2.31	0.49
2:OB:149:MET:O	2:OB:153:SER:OG	2.21	0.49
2:SB:163:GLU:OE2	2:SB:180:ASP:N	2.46	0.49
2:CA:163:GLU:OE2	2:CA:180:ASP:N	2.46	0.49
1:PA:115:MET:HB3	1:VA:135:THR:HG21	1.94	0.49
2:AB:163:GLU:OE2	2:AB:180:ASP:N	2.46	0.49
2:T:163:GLU:OE2	2:T:180:ASP:N	2.46	0.49
2:AA:163:GLU:OE2	2:AA:180:ASP:N	2.46	0.49
2:UA:163:GLU:OE2	2:UA:180:ASP:N	2.46	0.49
2:GB:163:GLU:OE2	2:GB:180:ASP:N	2.46	0.49
1:HB:18:LEU:CD2	1:NB:84:THR:HG21	2.43	0.49
2:MB:163:GLU:OE2	2:MB:180:ASP:N	2.46	0.49
2:N:163:GLU:OE2	2:N:180:ASP:N	2.46	0.49
2:W:149:MET:O	2:W:153:SER:OG	2.21	0.48
2:GA:163:GLU:OE2	2:GA:180:ASP:N	2.46	0.48
1:C:84:THR:HG21	1:02:18:LEU:HD21	1.95	0.48
2:F:163:GLU:OE2	2:F:180:ASP:N	2.46	0.48
2:P:163:GLU:OE2	2:P:180:ASP:N	2.46	0.48
2:W:163:GLU:OE2	2:W:180:ASP:N	2.46	0.48
2:OB:163:GLU:OE2	2:OB:180:ASP:N	2.46	0.48
1:XA:47:VAL:HG22	1:DB:63:VAL:HG23	1.95	0.48
2:CB:163:GLU:OE2	2:CB:180:ASP:N	2.46	0.48
2:B:29:LYS:NZ	2:B:62:GLU:OE2	2.31	0.48
1:C:126:ASP:CG	2:J:24:LEU:HD13	2.33	0.48
2:L:163:GLU:OE2	2:L:180:ASP:N	2.46	0.48
2:CA:29:LYS:NZ	2:CA:62:GLU:OE2	2.31	0.48
2:MA:163:GLU:OE2	2:MA:180:ASP:N	2.46	0.48
1:A:36:ILE:HG23	1:Z:156:MET:SD	2.53	0.48
2:J:163:GLU:OE2	2:J:180:ASP:N	2.46	0.48
2:WA:163:GLU:OE2	2:WA:180:ASP:N	2.46	0.48
1:HB:131:GLN:OE1	2:OB:17:LEU:HD23	2.14	0.48
1:PB:126:ASP:CG	2:01:24:LEU:HD13	2.33	0.48
2:D:163:GLU:OE2	2:D:180:ASP:N	2.46	0.48
1:M:156:MET:SD	1:NB:36:ILE:HG23	2.52	0.48
2:KA:163:GLU:OE2	2:KA:180:ASP:N	2.46	0.48
2:IB:163:GLU:OE2	2:IB:180:ASP:N	2.46	0.48
2:KB:163:GLU:OE2	2:KB:180:ASP:N	2.46	0.48
2:QB:163:GLU:OE2	2:QB:180:ASP:N	2.46	0.48
2:SA:163:GLU:OE2	2:SA:180:ASP:N	2.46	0.48
2:EB:149:MET:O	2:EB:153:SER:OG	2.21	0.48
2:01:163:GLU:OE2	2:01:180:ASP:N	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:49:ARG:NH1	1:PA:146:GLN:OE1	2.40	0.48
1:Q:51:HIS:CD2	1:X:66:LEU:HD21	2.49	0.48
2:R:163:GLU:OE2	2:R:180:ASP:N	2.46	0.48
1:Z:126:ASP:OD2	2:GA:24:LEU:HD13	2.13	0.48
2:EA:163:GLU:OE2	2:EA:180:ASP:N	2.46	0.48
2:QA:163:GLU:OE2	2:QA:180:ASP:N	2.46	0.48
2:Y:163:GLU:OE2	2:Y:180:ASP:N	2.46	0.48
2:YA:163:GLU:OE2	2:YA:180:ASP:N	2.46	0.48
1:FA:50:ILE:CD1	1:LA:66:LEU:HD22	2.44	0.48
1:LA:18:LEU:CD2	1:RA:84:THR:HG21	2.43	0.48
2:EB:163:GLU:OE2	2:EB:180:ASP:N	2.46	0.48
2:WA:29:LYS:NZ	2:WA:62:GLU:OE2	2.31	0.47
1:M:18:LEU:CD2	1:S:84:THR:HG21	2.44	0.47
2:T:149:MET:O	2:T:153:SER:OG	2.21	0.47
2:SB:29:LYS:NZ	2:SB:62:GLU:OE2	2.31	0.47
1:DB:115:MET:HB3	1:LB:135:THR:HG21	1.96	0.47
1:Z:65:PHE:HE1	1:FA:81:THR:HG1	1.60	0.47
2:AB:149:MET:O	2:AB:153:SER:OG	2.21	0.47
1:DA:196:ARG:NH2	2:EA:63:ASP:OD2	2.48	0.47
1:NA:50:ILE:CD1	1:TA:66:LEU:HD22	2.45	0.47
1:VA:18:LEU:CD2	1:BB:84:THR:HG21	2.45	0.47
1:DB:196:ARG:NH2	2:EB:63:ASP:OD2	2.48	0.47
1:LB:196:ARG:NH2	2:KB:63:ASP:OD2	2.48	0.47
2:D:29:LYS:NZ	2:D:62:GLU:OE2	2.31	0.47
1:M:196:ARG:NH2	2:N:63:ASP:OD2	2.48	0.47
1:O:196:ARG:NH2	2:P:63:ASP:OD2	2.48	0.47
1:S:196:ARG:NH2	2:T:63:ASP:OD2	2.48	0.47
1:X:196:ARG:NH2	2:Y:63:ASP:OD2	2.48	0.47
2:Y:149:MET:O	2:Y:153:SER:OG	2.21	0.47
1:TA:196:ARG:NH2	2:UA:63:ASP:OD2	2.48	0.47
1:ZA:196:ARG:NH2	2:AB:63:ASP:OD2	2.48	0.47
1:E:61:GLN:CD	1:K:77:ALA:HB1	2.35	0.47
1:V:196:ARG:NH2	2:W:63:ASP:OD2	2.48	0.47
1:XA:196:ARG:NH2	2:YA:63:ASP:OD2	2.48	0.47
1:HB:196:ARG:NH2	2:IB:63:ASP:OD2	2.48	0.47
1:G:196:ARG:NH2	2:H:63:ASP:OD2	2.48	0.47
1:Q:196:ARG:NH2	2:R:63:ASP:OD2	2.48	0.47
1:Z:196:ARG:NH2	2:AA:63:ASP:OD2	2.48	0.47
1:JA:196:ARG:NH2	2:KA:63:ASP:OD2	2.48	0.47
1:NA:196:ARG:NH2	2:OA:63:ASP:OD2	2.48	0.47
1:FB:196:ARG:NH2	2:GB:63:ASP:OD2	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:MET:HB3	1:G:135:THR:HG21	1.96	0.47
1:I:196:ARG:NH2	2:J:63:ASP:OD2	2.48	0.47
1:BB:196:ARG:NH2	2:CB:63:ASP:OD2	2.48	0.47
1:NB:196:ARG:NH2	2:OB:63:ASP:OD2	2.48	0.47
1:PB:196:ARG:NH2	2:QB:63:ASP:OD2	2.48	0.47
1:V:50:ILE:CD1	1:BA:66:LEU:HD22	2.45	0.46
1:BA:196:ARG:NH2	2:CA:63:ASP:OD2	2.48	0.46
1:FA:196:ARG:NH2	2:GA:63:ASP:OD2	2.48	0.46
1:NB:131:GLN:OE1	2:SB:17:LEU:HD23	2.15	0.46
1:JB:196:ARG:NH2	2:MB:63:ASP:OD2	2.48	0.46
1:A:50:ILE:CD1	1:G:66:LEU:HD22	2.45	0.46
1:RA:196:ARG:NH2	2:SA:63:ASP:OD2	2.48	0.46
1:A:196:ARG:NH2	2:B:63:ASP:OD2	2.48	0.46
1:RB:196:ARG:NH2	2:SB:63:ASP:OD2	2.48	0.46
1:C:196:ARG:NH2	2:D:63:ASP:OD2	2.48	0.46
1:K:196:ARG:NH2	2:L:63:ASP:OD2	2.48	0.46
1:HA:196:ARG:NH2	2:IA:63:ASP:OD2	2.48	0.46
1:C:131:GLN:OE1	2:J:17:LEU:HD23	2.16	0.46
1:DA:115:MET:HB3	1:JA:135:THR:HG21	1.97	0.46
1:PA:196:ARG:NH2	2:QA:63:ASP:OD2	2.48	0.46
1:TA:50:ILE:CD1	1:ZA:66:LEU:HD22	2.45	0.46
1:TA:115:MET:HB3	1:ZA:135:THR:HG21	1.97	0.46
1:VA:196:ARG:NH2	2:WA:63:ASP:OD2	2.48	0.46
2:MB:29:LYS:NZ	2:MB:62:GLU:OE2	2.31	0.46
1:E:133:GLU:HA	1:ZA:71:ARG:HH11	1.81	0.46
2:F:29:LYS:NZ	2:F:62:GLU:OE2	2.31	0.46
1:FA:115:MET:HB3	1:LA:135:THR:HG21	1.98	0.46
1:LA:196:ARG:NH2	2:MA:63:ASP:OD2	2.48	0.46
2:MA:29:LYS:NZ	2:MA:62:GLU:OE2	2.31	0.46
1:02:196:ARG:NH2	2:01:63:ASP:OD2	2.48	0.46
1:E:196:ARG:NH2	2:F:63:ASP:OD2	2.48	0.46
1:NA:50:ILE:HD12	1:TA:66:LEU:HD22	1.98	0.46
1:X:161:GLY:HA3	1:XA:104:LYS:O	2.16	0.45
1:VA:126:ASP:OD2	2:CB:24:LEU:HD13	2.16	0.45
1:A:135:THR:HG21	1:RB:115:MET:HB3	1.96	0.45
1:XA:109:GLU:OE1	2:KB:10:ARG:NH1	2.49	0.45
1:LB:50:ILE:HD12	1:PB:66:LEU:HD22	1.98	0.45
1:C:126:ASP:OD2	2:J:24:LEU:HD13	2.16	0.45
1:I:115:MET:HB3	1:O:135:THR:HG21	1.96	0.45
2:GA:29:LYS:NZ	2:GA:62:GLU:OE2	2.31	0.45
1:M:131:GLN:OE1	2:T:17:LEU:HD23	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LB:131:GLN:OE1	2:QB:17:LEU:HD23	2.16	0.45
1:Q:65:PHE:HE1	1:X:81:THR:HG23	1.82	0.45
1:Q:18:LEU:HG	1:X:84:THR:HG21	1.99	0.45
1:V:115:MET:HB3	1:BA:135:THR:HG21	1.97	0.45
1:Z:61:GLN:NE2	1:FA:77:ALA:HB1	2.32	0.45
1:XA:131:GLN:OE1	2:EB:17:LEU:HD23	2.17	0.45
1:HB:109:GLU:OE1	2:SB:10:ARG:NH1	2.50	0.45
1:C:61:GLN:NE2	1:I:77:ALA:HB1	2.32	0.45
1:V:50:ILE:HD12	1:BA:66:LEU:HD22	1.99	0.45
2:N:27:LYS:NZ	2:N:31:GLU:OE2	2.51	0.44
2:UA:27:LYS:NZ	2:UA:31:GLU:OE2	2.51	0.44
2:AB:27:LYS:NZ	2:AB:31:GLU:OE2	2.51	0.44
1:Q:51:HIS:NE2	1:X:66:LEU:HD21	2.32	0.44
2:T:27:LYS:NZ	2:T:31:GLU:OE2	2.51	0.44
1:V:18:LEU:CD2	1:BA:84:THR:HG21	2.45	0.44
2:H:27:LYS:NZ	2:H:31:GLU:OE2	2.50	0.44
2:P:27:LYS:NZ	2:P:31:GLU:OE2	2.51	0.44
2:GB:27:LYS:NZ	2:GB:31:GLU:OE2	2.51	0.44
2:IB:27:LYS:NZ	2:IB:31:GLU:OE2	2.50	0.44
1:E:51:HIS:CD2	1:K:66:LEU:HD21	2.53	0.44
1:E:143:THR:O	1:TA:57:ARG:HA	2.17	0.44
1:G:131:GLN:OE1	2:N:17:LEU:HD23	2.17	0.44
2:J:27:LYS:NZ	2:J:31:GLU:OE2	2.51	0.44
2:AA:27:LYS:NZ	2:AA:31:GLU:OE2	2.51	0.44
2:OA:27:LYS:NZ	2:OA:31:GLU:OE2	2.51	0.44
2:CB:27:LYS:NZ	2:CB:31:GLU:OE2	2.51	0.44
1:A:131:GLN:OE1	2:H:17:LEU:HD23	2.18	0.44
1:G:115:MET:HB3	1:M:135:THR:HG21	1.98	0.44
2:W:27:LYS:NZ	2:W:31:GLU:OE2	2.51	0.44
1:ZA:115:MET:HB3	1:FB:135:THR:HG21	1.99	0.44
1:XA:18:LEU:CG	1:DB:84:THR:HG21	2.46	0.44
1:JA:51:HIS:CD2	1:PA:66:LEU:HD21	2.53	0.44
1:TA:18:LEU:CD2	1:ZA:84:THR:HG21	2.43	0.44
1:XA:51:HIS:NE2	1:DB:66:LEU:HD11	2.31	0.44
2:OB:27:LYS:NZ	2:OB:31:GLU:OE2	2.51	0.44
2:MB:27:LYS:NZ	2:MB:31:GLU:OE2	2.50	0.44
2:B:27:LYS:NZ	2:B:31:GLU:OE2	2.50	0.44
1:O:115:MET:HB3	1:V:135:THR:HG21	1.99	0.44
1:HA:131:GLN:OE1	2:OA:17:LEU:HD23	2.18	0.44
2:D:27:LYS:NZ	2:D:31:GLU:OE2	2.51	0.44
2:F:27:LYS:NZ	2:F:31:GLU:OE2	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:18:LEU:CD2	1:V:84:THR:HG21	2.44	0.43
2:CA:27:LYS:NZ	2:CA:31:GLU:OE2	2.51	0.43
2:GA:27:LYS:NZ	2:GA:31:GLU:OE2	2.51	0.43
2:IA:27:LYS:NZ	2:IA:31:GLU:OE2	2.51	0.43
1:LA:131:GLN:OE1	2:SA:17:LEU:HD23	2.18	0.43
1:TA:50:ILE:HD12	1:ZA:66:LEU:HD22	2.00	0.43
2:WA:27:LYS:NZ	2:WA:31:GLU:OE2	2.51	0.43
1:NB:50:ILE:CD1	1:RB:66:LEU:HD22	2.48	0.43
1:PB:126:ASP:OD2	2:01:24:LEU:HD13	2.18	0.43
1:E:49:ARG:NH1	2:EA:38:LYS:NZ	2.66	0.43
1:E:65:PHE:HE1	1:K:81:THR:HG23	1.83	0.43
2:L:27:LYS:NZ	2:L:31:GLU:OE2	2.51	0.43
1:Q:18:LEU:CG	1:X:84:THR:HG21	2.48	0.43
2:R:27:LYS:NZ	2:R:31:GLU:OE2	2.50	0.43
1:BA:131:GLN:OE1	2:IA:17:LEU:HD23	2.18	0.43
2:MA:27:LYS:NZ	2:MA:31:GLU:OE2	2.51	0.43
1:LB:115:MET:HB3	1:PB:135:THR:HG21	2.00	0.43
2:YA:27:LYS:NZ	2:YA:31:GLU:OE2	2.51	0.43
2:SB:27:LYS:NZ	2:SB:31:GLU:OE2	2.50	0.43
1:JB:135:THR:HG21	1:FB:115:MET:HB3	1.99	0.43
2:Y:27:LYS:NZ	2:Y:31:GLU:OE2	2.51	0.43
1:LA:115:MET:HB3	1:RA:135:THR:HG21	2.01	0.43
2:SA:27:LYS:NZ	2:SA:31:GLU:OE2	2.51	0.43
1:VA:115:MET:HB3	1:BB:135:THR:HG21	1.99	0.43
2:EB:27:LYS:NZ	2:EB:31:GLU:OE2	2.51	0.43
2:EA:27:LYS:NZ	2:EA:31:GLU:OE2	2.51	0.43
1:NA:115:MET:HB3	1:TA:135:THR:HG21	1.99	0.43
2:T:58:HIS:CE1	2:AA:81:ALA:HB2	2.54	0.43
2:QA:27:LYS:NZ	2:QA:31:GLU:OE2	2.51	0.43
1:LB:50:ILE:CD1	1:PB:66:LEU:HD22	2.47	0.43
2:KB:27:LYS:NZ	2:KB:31:GLU:OE2	2.50	0.43
1:K:109:GLU:OE1	2:Y:10:ARG:NH1	2.52	0.43
1:FA:131:GLN:OE1	2:MA:17:LEU:HD23	2.18	0.43
2:KA:27:LYS:NZ	2:KA:31:GLU:OE2	2.50	0.43
1:C:18:LEU:CD2	1:I:84:THR:HG21	2.48	0.43
1:E:37:GLU:HG3	1:DA:156:MET:SD	2.59	0.43
1:Z:131:GLN:OE1	2:GA:17:LEU:HD23	2.18	0.43
2:QB:27:LYS:NZ	2:QB:31:GLU:OE2	2.51	0.43
1:HA:115:MET:HB3	1:NA:135:THR:HG21	2.00	0.43
2:01:27:LYS:NZ	2:01:31:GLU:OE2	2.51	0.43
1:E:133:GLU:HA	1:ZA:71:ARG:NH1	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HB:61:GLN:NE2	1:NB:77:ALA:HB1	2.34	0.43
1:G:50:ILE:HD12	1:M:66:LEU:HD22	2.00	0.42
1:M:92:MET:O	1:M:96:VAL:HG23	2.19	0.42
1:FA:92:MET:O	1:FA:96:VAL:HG23	2.19	0.42
1:NA:131:GLN:OE1	2:UA:17:LEU:HD23	2.19	0.42
1:ZA:92:MET:O	1:ZA:96:VAL:HG23	2.19	0.42
1:FB:92:MET:O	1:FB:96:VAL:HG23	2.19	0.42
1:JB:92:MET:O	1:JB:96:VAL:HG23	2.20	0.42
1:S:92:MET:O	1:S:96:VAL:HG23	2.19	0.42
1:TA:92:MET:O	1:TA:96:VAL:HG23	2.19	0.42
2:H:53:ARG:O	2:H:56:VAL:HG12	2.20	0.42
1:Z:92:MET:O	1:Z:96:VAL:HG23	2.19	0.42
2:AA:86:ILE:HD11	2:AA:128:TYR:OH	2.20	0.42
1:HA:18:LEU:CD2	1:NA:84:THR:HG21	2.48	0.42
2:MA:53:ARG:O	2:MA:56:VAL:HG12	2.20	0.42
1:RA:92:MET:O	1:RA:96:VAL:HG23	2.19	0.42
2:SB:86:ILE:HD11	2:SB:128:TYR:OH	2.20	0.42
2:D:81:ALA:HB2	2:01:58:HIS:CE1	2.54	0.42
2:F:53:ARG:O	2:F:56:VAL:HG12	2.20	0.42
1:G:92:MET:O	1:G:96:VAL:HG23	2.19	0.42
1:K:92:MET:O	1:K:96:VAL:HG23	2.19	0.42
1:Q:92:MET:O	1:Q:96:VAL:HG23	2.19	0.42
2:W:53:ARG:O	2:W:56:VAL:HG12	2.20	0.42
1:Z:57:ARG:HA	1:XA:143:THR:O	2.20	0.42
2:CA:86:ILE:HD11	2:CA:128:TYR:OH	2.20	0.42
1:NA:18:LEU:CD2	1:TA:84:THR:HG21	2.47	0.42
2:OA:53:ARG:O	2:OA:56:VAL:HG12	2.20	0.42
2:UA:86:ILE:HD11	2:UA:128:TYR:OH	2.20	0.42
2:AB:53:ARG:O	2:AB:56:VAL:HG12	2.20	0.42
2:GB:86:ILE:HD11	2:GB:128:TYR:OH	2.20	0.42
1:NB:115:MET:HB3	1:RB:135:THR:HG21	2.00	0.42
2:QB:86:ILE:HD11	2:QB:128:TYR:OH	2.20	0.42
2:N:86:ILE:HD11	2:N:128:TYR:OH	2.20	0.42
1:Q:47:VAL:HG22	1:X:63:VAL:CG2	2.50	0.42
2:T:53:ARG:O	2:T:56:VAL:HG12	2.20	0.42
1:BA:57:ARG:HA	1:ZA:143:THR:O	2.19	0.42
2:KA:86:ILE:HD11	2:KA:128:TYR:OH	2.20	0.42
1:NA:92:MET:O	1:NA:96:VAL:HG23	2.20	0.42
2:J:86:ILE:HD11	2:J:128:TYR:OH	2.20	0.42
2:Y:86:ILE:HD11	2:Y:128:TYR:OH	2.20	0.42
1:BA:18:LEU:CD2	1:HA:84:THR:HG21	2.46	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DA:50:ILE:CD1	1:JA:66:LEU:HD22	2.49	0.42
1:DA:92:MET:O	1:DA:96:VAL:HG23	2.20	0.42
1:HA:92:MET:O	1:HA:96:VAL:HG23	2.19	0.42
1:VA:61:GLN:NE2	1:BB:77:ALA:HB1	2.34	0.42
1:XA:92:MET:O	1:XA:96:VAL:HG23	2.20	0.42
2:CB:86:ILE:HD11	2:CB:128:TYR:OH	2.20	0.42
1:LB:92:MET:O	1:LB:96:VAL:HG23	2.19	0.42
2:OB:53:ARG:O	2:OB:56:VAL:HG12	2.20	0.42
1:A:92:MET:O	1:A:96:VAL:HG23	2.19	0.42
2:F:86:ILE:HD11	2:F:128:TYR:OH	2.20	0.42
2:L:86:ILE:HD11	2:L:128:TYR:OH	2.20	0.42
1:Q:126:ASP:OD2	2:Y:24:LEU:HD13	2.20	0.42
2:MA:86:ILE:HD11	2:MA:128:TYR:OH	2.20	0.42
2:SA:86:ILE:HD11	2:SA:128:TYR:OH	2.20	0.42
1:DB:92:MET:O	1:DB:96:VAL:HG23	2.19	0.42
2:EB:53:ARG:O	2:EB:56:VAL:HG12	2.20	0.42
2:EB:86:ILE:HD11	2:EB:128:TYR:OH	2.20	0.42
2:H:86:ILE:HD11	2:H:128:TYR:OH	2.20	0.42
1:Q:65:PHE:CE1	1:X:81:THR:OG1	2.73	0.42
2:R:53:ARG:O	2:R:56:VAL:HG12	2.20	0.42
2:W:86:ILE:HD11	2:W:128:TYR:OH	2.20	0.42
2:Y:53:ARG:O	2:Y:56:VAL:HG12	2.20	0.42
2:AA:53:ARG:O	2:AA:56:VAL:HG12	2.20	0.42
1:JA:92:MET:O	1:JA:96:VAL:HG23	2.19	0.42
2:OA:86:ILE:HD11	2:OA:128:TYR:OH	2.20	0.42
2:UA:29:LYS:NZ	2:UA:62:GLU:OE2	2.31	0.42
2:WA:53:ARG:O	2:WA:56:VAL:HG12	2.20	0.42
2:OB:86:ILE:HD11	2:OB:128:TYR:OH	2.20	0.42
2:D:86:ILE:HD11	2:D:128:TYR:OH	2.20	0.42
1:E:51:HIS:NE2	1:K:66:LEU:HD21	2.35	0.42
1:E:92:MET:O	1:E:96:VAL:HG23	2.19	0.42
2:CA:53:ARG:O	2:CA:56:VAL:HG12	2.20	0.42
2:WA:86:ILE:HD11	2:WA:128:TYR:OH	2.20	0.42
2:GB:53:ARG:O	2:GB:56:VAL:HG12	2.20	0.42
1:PB:92:MET:O	1:PB:96:VAL:HG23	2.19	0.42
1:JB:77:ALA:HB1	1:FB:61:GLN:NE2	2.35	0.42
2:D:53:ARG:O	2:D:56:VAL:HG12	2.20	0.42
1:E:126:ASP:CG	2:L:24:LEU:HD13	2.40	0.42
2:Y:58:HIS:CE1	2:EA:81:ALA:HB2	2.54	0.42
2:YA:53:ARG:O	2:YA:56:VAL:HG12	2.20	0.42
2:SB:53:ARG:O	2:SB:56:VAL:HG12	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:01:86:ILE:HD11	2:01:128:TYR:OH	2.20	0.42
1:G:50:ILE:CD1	1:M:66:LEU:HD22	2.50	0.41
2:IA:53:ARG:O	2:IA:56:VAL:HG12	2.20	0.41
1:PA:92:MET:O	1:PA:96:VAL:HG23	2.19	0.41
2:QA:86:ILE:HD11	2:QA:128:TYR:OH	2.20	0.41
2:AB:86:ILE:HD11	2:AB:128:TYR:OH	2.20	0.41
1:PB:115:MET:HB3	1:02:135:THR:HG21	2.00	0.41
2:MB:53:ARG:O	2:MB:56:VAL:HG12	2.20	0.41
2:B:53:ARG:O	2:B:56:VAL:HG12	2.20	0.41
1:O:92:MET:O	1:O:96:VAL:HG23	2.19	0.41
2:T:86:ILE:HD11	2:T:128:TYR:OH	2.20	0.41
1:V:131:GLN:OE1	2:CA:17:LEU:HD23	2.20	0.41
1:X:92:MET:O	1:X:96:VAL:HG23	2.19	0.41
2:GA:53:ARG:O	2:GA:56:VAL:HG12	2.20	0.41
2:GA:86:ILE:HD11	2:GA:128:TYR:OH	2.20	0.41
1:LA:92:MET:O	1:LA:96:VAL:HG23	2.20	0.41
2:QA:53:ARG:O	2:QA:56:VAL:HG12	2.20	0.41
1:02:92:MET:O	1:02:96:VAL:HG23	2.19	0.41
2:MB:86:ILE:HD11	2:MB:128:TYR:OH	2.20	0.41
1:O:131:GLN:OE1	2:W:17:LEU:HD23	2.20	0.41
2:R:86:ILE:HD11	2:R:128:TYR:OH	2.20	0.41
1:BA:92:MET:O	1:BA:96:VAL:HG23	2.19	0.41
1:VA:92:MET:O	1:VA:96:VAL:HG23	2.19	0.41
2:YA:86:ILE:HD11	2:YA:128:TYR:OH	2.20	0.41
1:ZA:18:LEU:CD2	1:FB:84:THR:HG21	2.49	0.41
2:CB:53:ARG:O	2:CB:56:VAL:HG12	2.20	0.41
1:RB:92:MET:O	1:RB:96:VAL:HG23	2.19	0.41
2:01:53:ARG:O	2:01:56:VAL:HG12	2.20	0.41
2:B:86:ILE:HD11	2:B:128:TYR:OH	2.20	0.41
1:C:92:MET:O	1:C:96:VAL:HG23	2.19	0.41
2:J:53:ARG:O	2:J:56:VAL:HG12	2.20	0.41
2:L:53:ARG:O	2:L:56:VAL:HG12	2.20	0.41
1:X:126:ASP:CG	2:EA:24:LEU:CD1	2.86	0.41
1:Z:109:GLU:OE1	2:MA:10:ARG:NH1	2.53	0.41
2:EA:53:ARG:O	2:EA:56:VAL:HG12	2.20	0.41
2:IA:86:ILE:HD11	2:IA:128:TYR:OH	2.20	0.41
2:SA:53:ARG:O	2:SA:56:VAL:HG12	2.20	0.41
1:HB:92:MET:O	1:HB:96:VAL:HG23	2.19	0.41
2:KB:53:ARG:O	2:KB:56:VAL:HG12	2.20	0.41
1:E:131:GLN:OE1	2:L:17:LEU:HD23	2.21	0.41
2:P:53:ARG:O	2:P:56:VAL:HG12	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:29:LYS:NZ	2:W:62:GLU:OE2	2.31	0.41
2:IB:53:ARG:O	2:IB:56:VAL:HG12	2.20	0.41
2:N:29:LYS:NZ	2:N:62:GLU:OE2	2.31	0.41
1:LA:61:GLN:NE2	1:RA:77:ALA:HB1	2.36	0.41
1:ZA:131:GLN:OE1	2:GB:17:LEU:HD23	2.19	0.41
1:JB:49:ARG:NH1	1:X:146:GLN:OE1	2.44	0.41
2:UA:53:ARG:O	2:UA:56:VAL:HG12	2.20	0.41
2:N:53:ARG:O	2:N:56:VAL:HG12	2.20	0.41
2:P:86:ILE:HD11	2:P:128:TYR:OH	2.20	0.41
1:V:92:MET:O	1:V:96:VAL:HG23	2.19	0.41
1:BB:92:MET:O	1:BB:96:VAL:HG23	2.19	0.41
1:JB:114:LEU:C	1:JB:114:LEU:HD23	2.42	0.41
1:I:92:MET:O	1:I:96:VAL:HG23	2.19	0.41
1:M:109:GLU:OE1	2:AA:10:ARG:NH1	2.53	0.41
1:M:115:MET:HB3	1:S:135:THR:HG21	2.02	0.41
1:Z:115:MET:HB3	1:FA:135:THR:HG21	2.01	0.41
2:EA:86:ILE:HD11	2:EA:128:TYR:OH	2.20	0.41
1:FA:114:LEU:C	1:FA:114:LEU:HD23	2.41	0.41
2:KA:53:ARG:O	2:KA:56:VAL:HG12	2.20	0.41
1:FB:114:LEU:C	1:FB:114:LEU:HD23	2.42	0.41
2:IB:86:ILE:HD11	2:IB:128:TYR:OH	2.20	0.41
2:KB:86:ILE:HD11	2:KB:128:TYR:OH	2.20	0.41
1:S:131:GLN:OE1	2:AA:17:LEU:HD23	2.20	0.41
1:BA:115:MET:HB3	1:HA:135:THR:HG21	2.01	0.41
1:NB:92:MET:O	1:NB:96:VAL:HG23	2.19	0.41
2:QB:53:ARG:O	2:QB:56:VAL:HG12	2.20	0.41
1:E:114:LEU:C	1:E:114:LEU:HD23	2.42	0.40
1:Z:114:LEU:C	1:Z:114:LEU:HD23	2.42	0.40
1:LA:114:LEU:C	1:LA:114:LEU:HD23	2.42	0.40
1:RA:157:ALA:O	1:RA:161:GLY:N	2.54	0.40
1:PB:61:GLN:CD	1:02:77:ALA:HB1	2.41	0.40
1:C:114:LEU:HD23	1:C:114:LEU:C	2.42	0.40
1:K:157:ALA:O	1:K:161:GLY:N	2.54	0.40
1:X:157:ALA:O	1:X:161:GLY:N	2.54	0.40
1:DA:49:ARG:NH1	1:BB:146:GLN:OE1	2.43	0.40
1:HA:50:ILE:CD1	1:NA:66:LEU:HD22	2.51	0.40
1:DB:157:ALA:O	1:DB:161:GLY:N	2.54	0.40
2:OB:29:LYS:NZ	2:OB:62:GLU:OE2	2.31	0.40
1:PB:65:PHE:HE1	1:02:81:THR:HG1	1.66	0.40
1:O:114:LEU:HD23	1:O:114:LEU:C	2.42	0.40
1:VA:114:LEU:HD23	1:VA:114:LEU:C	2.42	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:ZA:114:LEU:C	1:ZA:114:LEU:HD23	2.42	0.40
1:DB:131:GLN:OE1	2:KB:17:LEU:HD23	2.21	0.40
1:HB:114:LEU:HD23	1:HB:114:LEU:C	2.42	0.40
1:JB:157:ALA:O	1:JB:161:GLY:N	2.54	0.40
2:MB:17:LEU:HD23	1:FB:131:GLN:OE1	2.21	0.40
2:R:54:ILE:CG2	2:Y:77:ASP:OD2	2.69	0.40
1:S:114:LEU:C	1:S:114:LEU:HD23	2.42	0.40
1:DA:131:GLN:OE1	2:KA:17:LEU:HD23	2.22	0.40
1:FA:157:ALA:O	1:FA:161:GLY:N	2.54	0.40
1:PB:114:LEU:HD23	1:PB:114:LEU:C	2.42	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	02	172/199 (86%)	170 (99%)	2 (1%)	0	100	100
1	A	172/199 (86%)	170 (99%)	2 (1%)	0	100	100
1	BA	172/199 (86%)	170 (99%)	2 (1%)	0	100	100
1	BB	172/199 (86%)	170 (99%)	2 (1%)	0	100	100
1	C	172/199 (86%)	170 (99%)	2 (1%)	0	100	100
1	DA	172/199 (86%)	170 (99%)	2 (1%)	0	100	100
1	DB	172/199 (86%)	170 (99%)	2 (1%)	0	100	100
1	E	172/199 (86%)	170 (99%)	2 (1%)	0	100	100
1	FA	172/199 (86%)	170 (99%)	2 (1%)	0	100	100
1	FB	172/199 (86%)	170 (99%)	2 (1%)	0	100	100
1	G	172/199 (86%)	170 (99%)	2 (1%)	0	100	100
1	HA	172/199 (86%)	170 (99%)	2 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	HB	172/199 (86%)	170 (99%)	2 (1%)	0	100	100
1	I	172/199 (86%)	170 (99%)	2 (1%)	0	100	100
1	JA	172/199 (86%)	170 (99%)	2 (1%)	0	100	100
1	JB	172/199 (86%)	170 (99%)	2 (1%)	0	100	100
1	K	172/199 (86%)	170 (99%)	2 (1%)	0	100	100
1	LA	172/199 (86%)	170 (99%)	2 (1%)	0	100	100
1	LB	172/199 (86%)	170 (99%)	2 (1%)	0	100	100
1	M	172/199 (86%)	170 (99%)	2 (1%)	0	100	100
1	NA	172/199 (86%)	170 (99%)	2 (1%)	0	100	100
1	NB	172/199 (86%)	170 (99%)	2 (1%)	0	100	100
1	O	172/199 (86%)	170 (99%)	2 (1%)	0	100	100
1	PA	172/199 (86%)	170 (99%)	2 (1%)	0	100	100
1	PB	172/199 (86%)	170 (99%)	2 (1%)	0	100	100
1	Q	172/199 (86%)	170 (99%)	2 (1%)	0	100	100
1	RA	172/199 (86%)	170 (99%)	2 (1%)	0	100	100
1	RB	172/199 (86%)	170 (99%)	2 (1%)	0	100	100
1	S	172/199 (86%)	170 (99%)	2 (1%)	0	100	100
1	TA	172/199 (86%)	170 (99%)	2 (1%)	0	100	100
1	V	172/199 (86%)	170 (99%)	2 (1%)	0	100	100
1	VA	172/199 (86%)	170 (99%)	2 (1%)	0	100	100
1	X	172/199 (86%)	170 (99%)	2 (1%)	0	100	100
1	XA	172/199 (86%)	170 (99%)	2 (1%)	0	100	100
1	Z	172/199 (86%)	170 (99%)	2 (1%)	0	100	100
1	ZA	172/199 (86%)	170 (99%)	2 (1%)	0	100	100
2	01	179/189 (95%)	176 (98%)	3 (2%)	0	100	100
2	AA	179/189 (95%)	176 (98%)	3 (2%)	0	100	100
2	AB	179/189 (95%)	176 (98%)	3 (2%)	0	100	100
2	B	179/189 (95%)	176 (98%)	3 (2%)	0	100	100
2	CA	179/189 (95%)	176 (98%)	3 (2%)	0	100	100
2	CB	179/189 (95%)	176 (98%)	3 (2%)	0	100	100
2	D	179/189 (95%)	176 (98%)	3 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	EA	179/189 (95%)	176 (98%)	3 (2%)	0	100	100
2	EB	179/189 (95%)	176 (98%)	3 (2%)	0	100	100
2	F	179/189 (95%)	176 (98%)	3 (2%)	0	100	100
2	GA	179/189 (95%)	176 (98%)	3 (2%)	0	100	100
2	GB	179/189 (95%)	176 (98%)	3 (2%)	0	100	100
2	H	179/189 (95%)	176 (98%)	3 (2%)	0	100	100
2	IA	179/189 (95%)	176 (98%)	3 (2%)	0	100	100
2	IB	179/189 (95%)	176 (98%)	3 (2%)	0	100	100
2	J	179/189 (95%)	176 (98%)	3 (2%)	0	100	100
2	KA	179/189 (95%)	176 (98%)	3 (2%)	0	100	100
2	KB	179/189 (95%)	176 (98%)	3 (2%)	0	100	100
2	L	179/189 (95%)	176 (98%)	3 (2%)	0	100	100
2	MA	179/189 (95%)	176 (98%)	3 (2%)	0	100	100
2	MB	179/189 (95%)	176 (98%)	3 (2%)	0	100	100
2	N	179/189 (95%)	176 (98%)	3 (2%)	0	100	100
2	OA	179/189 (95%)	176 (98%)	3 (2%)	0	100	100
2	OB	179/189 (95%)	176 (98%)	3 (2%)	0	100	100
2	P	179/189 (95%)	176 (98%)	3 (2%)	0	100	100
2	QA	179/189 (95%)	176 (98%)	3 (2%)	0	100	100
2	QB	179/189 (95%)	176 (98%)	3 (2%)	0	100	100
2	R	179/189 (95%)	176 (98%)	3 (2%)	0	100	100
2	SA	179/189 (95%)	176 (98%)	3 (2%)	0	100	100
2	SB	179/189 (95%)	176 (98%)	3 (2%)	0	100	100
2	T	179/189 (95%)	176 (98%)	3 (2%)	0	100	100
2	UA	179/189 (95%)	176 (98%)	3 (2%)	0	100	100
2	W	179/189 (95%)	176 (98%)	3 (2%)	0	100	100
2	WA	179/189 (95%)	176 (98%)	3 (2%)	0	100	100
2	Y	179/189 (95%)	176 (98%)	3 (2%)	0	100	100
2	YA	179/189 (95%)	176 (98%)	3 (2%)	0	100	100
All	All	12636/13968 (90%)	12456 (99%)	180 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	02	148/169 (88%)	148 (100%)	0	100	100
1	A	148/169 (88%)	148 (100%)	0	100	100
1	BA	148/169 (88%)	148 (100%)	0	100	100
1	BB	148/169 (88%)	148 (100%)	0	100	100
1	C	148/169 (88%)	148 (100%)	0	100	100
1	DA	148/169 (88%)	148 (100%)	0	100	100
1	DB	148/169 (88%)	148 (100%)	0	100	100
1	E	148/169 (88%)	148 (100%)	0	100	100
1	FA	148/169 (88%)	148 (100%)	0	100	100
1	FB	148/169 (88%)	148 (100%)	0	100	100
1	G	148/169 (88%)	148 (100%)	0	100	100
1	HA	148/169 (88%)	148 (100%)	0	100	100
1	HB	148/169 (88%)	148 (100%)	0	100	100
1	I	148/169 (88%)	148 (100%)	0	100	100
1	JA	148/169 (88%)	148 (100%)	0	100	100
1	JB	148/169 (88%)	148 (100%)	0	100	100
1	K	148/169 (88%)	148 (100%)	0	100	100
1	LA	148/169 (88%)	148 (100%)	0	100	100
1	LB	148/169 (88%)	148 (100%)	0	100	100
1	M	148/169 (88%)	148 (100%)	0	100	100
1	NA	148/169 (88%)	148 (100%)	0	100	100
1	NB	148/169 (88%)	148 (100%)	0	100	100
1	O	148/169 (88%)	148 (100%)	0	100	100
1	PA	148/169 (88%)	148 (100%)	0	100	100
1	PB	148/169 (88%)	148 (100%)	0	100	100
1	Q	148/169 (88%)	148 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	RA	148/169 (88%)	148 (100%)	0	100	100
1	RB	148/169 (88%)	148 (100%)	0	100	100
1	S	148/169 (88%)	148 (100%)	0	100	100
1	TA	148/169 (88%)	148 (100%)	0	100	100
1	V	148/169 (88%)	148 (100%)	0	100	100
1	VA	148/169 (88%)	148 (100%)	0	100	100
1	X	148/169 (88%)	148 (100%)	0	100	100
1	XA	148/169 (88%)	148 (100%)	0	100	100
1	Z	148/169 (88%)	148 (100%)	0	100	100
1	ZA	148/169 (88%)	148 (100%)	0	100	100
2	01	136/163 (83%)	136 (100%)	0	100	100
2	AA	136/163 (83%)	136 (100%)	0	100	100
2	AB	136/163 (83%)	136 (100%)	0	100	100
2	B	136/163 (83%)	136 (100%)	0	100	100
2	CA	136/163 (83%)	136 (100%)	0	100	100
2	CB	136/163 (83%)	136 (100%)	0	100	100
2	D	136/163 (83%)	136 (100%)	0	100	100
2	EA	136/163 (83%)	136 (100%)	0	100	100
2	EB	136/163 (83%)	136 (100%)	0	100	100
2	F	136/163 (83%)	136 (100%)	0	100	100
2	GA	136/163 (83%)	136 (100%)	0	100	100
2	GB	136/163 (83%)	136 (100%)	0	100	100
2	H	136/163 (83%)	136 (100%)	0	100	100
2	IA	136/163 (83%)	136 (100%)	0	100	100
2	IB	136/163 (83%)	136 (100%)	0	100	100
2	J	136/163 (83%)	136 (100%)	0	100	100
2	KA	136/163 (83%)	136 (100%)	0	100	100
2	KB	136/163 (83%)	136 (100%)	0	100	100
2	L	136/163 (83%)	136 (100%)	0	100	100
2	MA	136/163 (83%)	136 (100%)	0	100	100
2	MB	136/163 (83%)	136 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	N	136/163 (83%)	136 (100%)	0	100	100
2	OA	136/163 (83%)	136 (100%)	0	100	100
2	OB	136/163 (83%)	136 (100%)	0	100	100
2	P	136/163 (83%)	136 (100%)	0	100	100
2	QA	136/163 (83%)	136 (100%)	0	100	100
2	QB	136/163 (83%)	136 (100%)	0	100	100
2	R	136/163 (83%)	136 (100%)	0	100	100
2	SA	136/163 (83%)	136 (100%)	0	100	100
2	SB	136/163 (83%)	136 (100%)	0	100	100
2	T	136/163 (83%)	136 (100%)	0	100	100
2	UA	136/163 (83%)	136 (100%)	0	100	100
2	W	136/163 (83%)	136 (100%)	0	100	100
2	WA	136/163 (83%)	136 (100%)	0	100	100
2	Y	136/163 (83%)	136 (100%)	0	100	100
2	YA	136/163 (83%)	136 (100%)	0	100	100
All	All	10224/11952 (86%)	10224 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (105) such sidechains are listed below:

Mol	Chain	Res	Type
1	JB	154	GLN
2	MB	123	GLN
2	MB	172	ASN
1	A	154	GLN
2	B	123	GLN
2	B	172	ASN
1	C	154	GLN
2	D	123	GLN
2	D	172	ASN
1	E	154	GLN
2	F	123	GLN
2	F	172	ASN
1	G	154	GLN
2	H	123	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	172	ASN
1	I	154	GLN
2	J	123	GLN
2	J	172	ASN
1	K	154	GLN
2	L	123	GLN
2	L	172	ASN
1	M	154	GLN
2	N	123	GLN
2	N	172	ASN
1	O	154	GLN
2	P	123	GLN
2	P	172	ASN
1	Q	154	GLN
2	R	123	GLN
2	R	172	ASN
1	S	154	GLN
2	T	123	GLN
2	T	172	ASN
1	V	154	GLN
2	W	123	GLN
2	W	172	ASN
2	Y	123	GLN
2	Y	172	ASN
1	Z	154	GLN
2	AA	123	GLN
2	AA	172	ASN
1	BA	154	GLN
2	CA	123	GLN
2	CA	172	ASN
1	DA	154	GLN
2	EA	123	GLN
2	EA	172	ASN
1	FA	154	GLN
2	GA	123	GLN
2	GA	172	ASN
1	HA	154	GLN
2	IA	123	GLN
2	IA	172	ASN
1	JA	154	GLN
2	KA	123	GLN
2	KA	172	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	LA	154	GLN
2	MA	123	GLN
2	MA	172	ASN
1	NA	154	GLN
2	OA	123	GLN
2	OA	172	ASN
1	PA	154	GLN
2	QA	123	GLN
2	QA	172	ASN
1	RA	154	GLN
2	SA	123	GLN
2	SA	172	ASN
1	TA	154	GLN
2	UA	123	GLN
2	UA	172	ASN
1	VA	154	GLN
2	WA	123	GLN
2	WA	172	ASN
1	XA	154	GLN
2	YA	123	GLN
2	YA	172	ASN
1	ZA	154	GLN
2	AB	123	GLN
2	AB	172	ASN
1	BB	131	GLN
1	BB	154	GLN
2	CB	123	GLN
2	CB	172	ASN
2	EB	123	GLN
2	EB	172	ASN
1	FB	154	GLN
2	GB	123	GLN
2	GB	172	ASN
2	IB	123	GLN
2	IB	172	ASN
1	LB	154	GLN
2	KB	123	GLN
2	KB	172	ASN
1	NB	154	GLN
2	OB	123	GLN
2	OB	172	ASN
2	QB	123	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	QB	172	ASN
1	RB	154	GLN
2	SB	123	GLN
2	SB	172	ASN
1	02	154	GLN
2	01	123	GLN
2	01	172	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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.

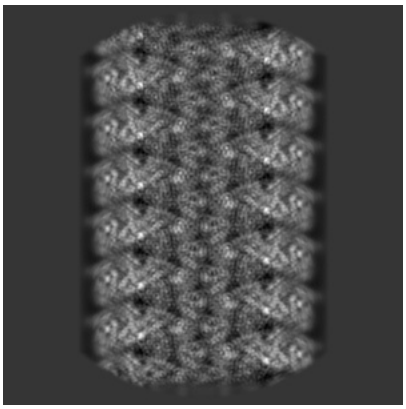
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-20588. These allow visual inspection of the internal detail of the map and identification of artifacts.

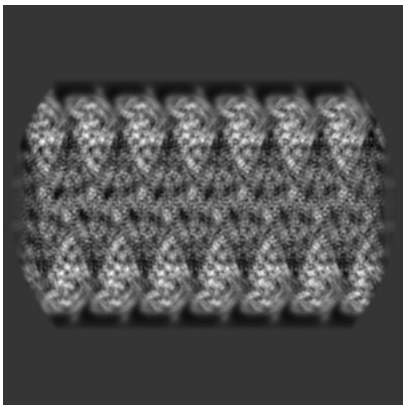
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

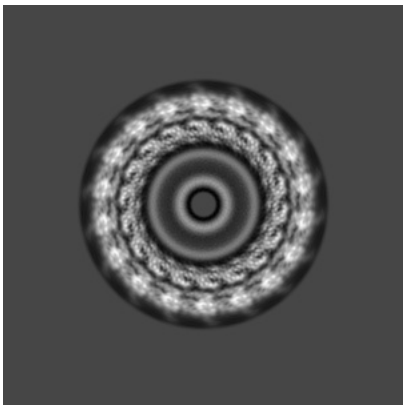
6.1.1 Primary map



X

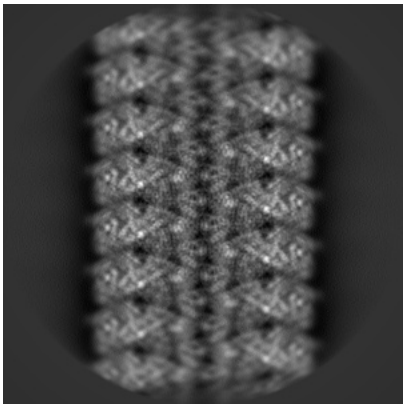


Y

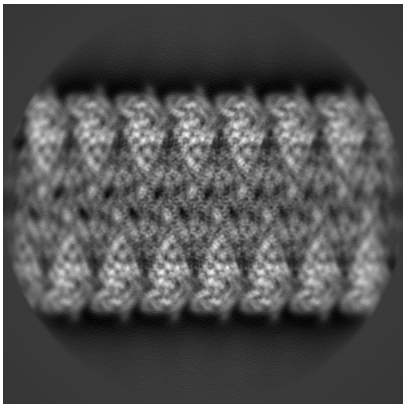


Z

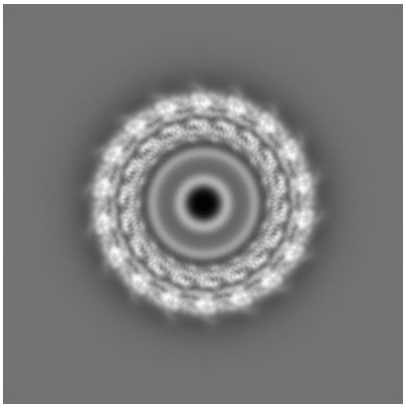
6.1.2 Raw map



X



Y

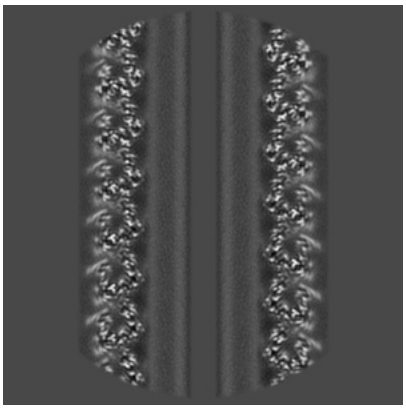


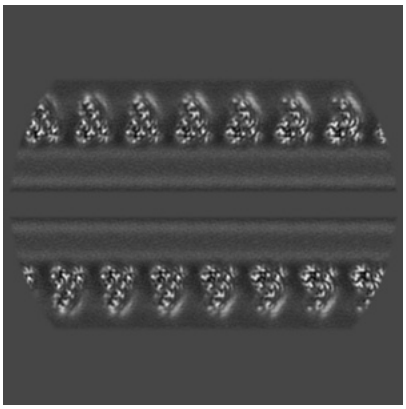
Z

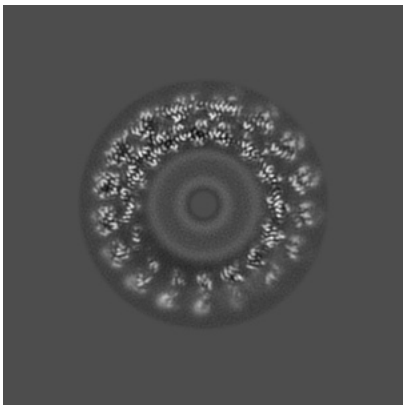
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

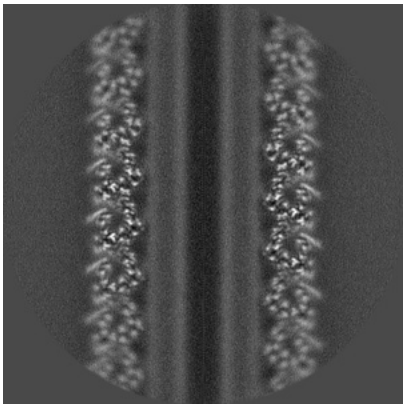
6.2.1 Primary map

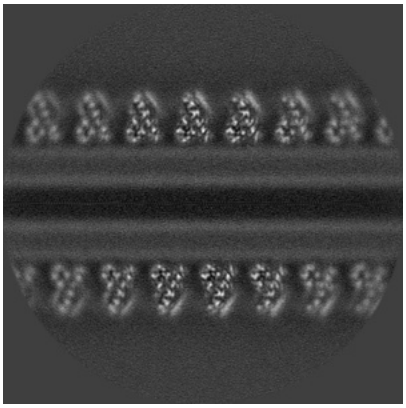

X Index: 176

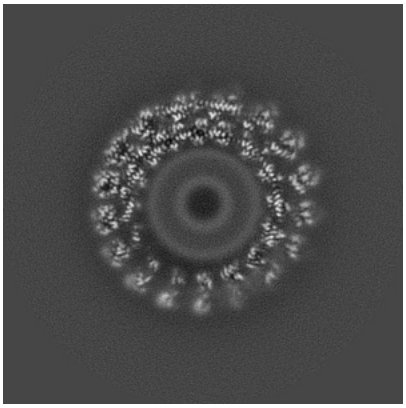

Y Index: 176


Z Index: 176

6.2.2 Raw map


X Index: 176

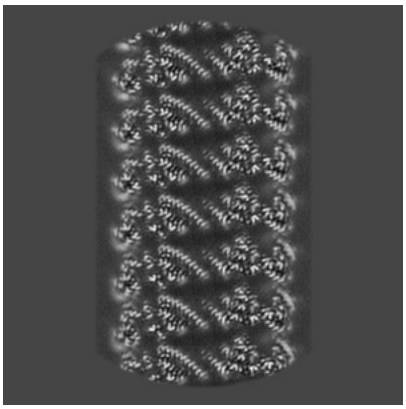

Y Index: 176

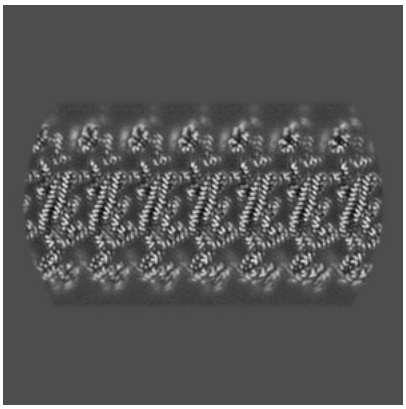

Z Index: 176

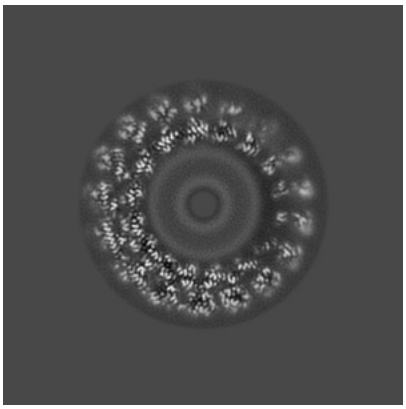
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

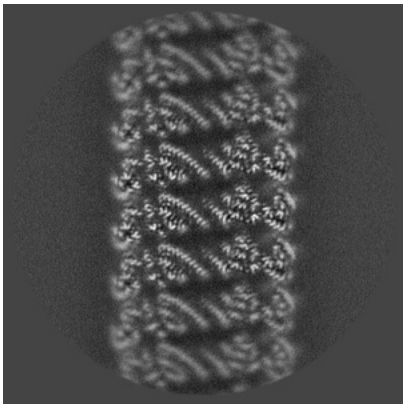
6.3.1 Primary map

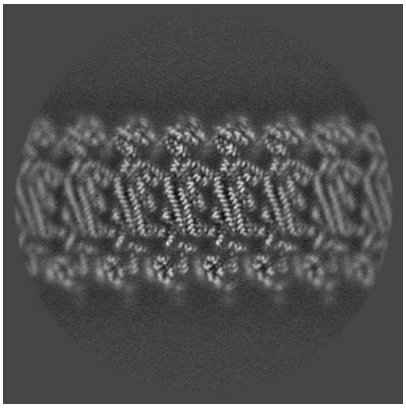

X Index: 231

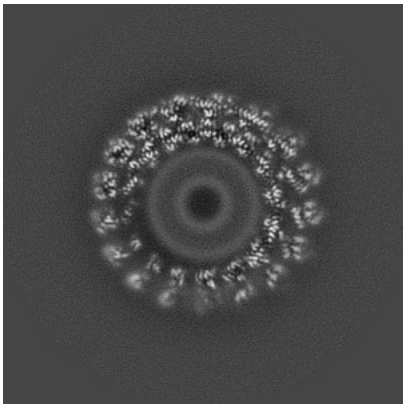

Y Index: 239


Z Index: 146

6.3.2 Raw map


X Index: 231

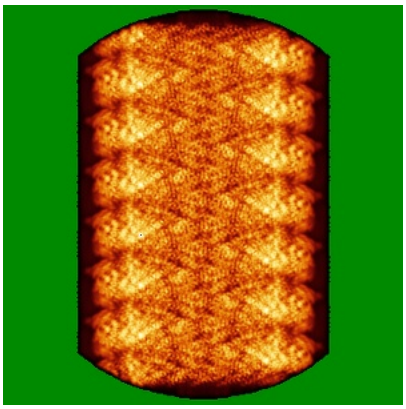

Y Index: 113

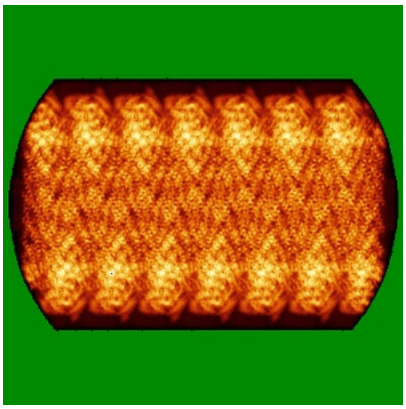

Z Index: 173

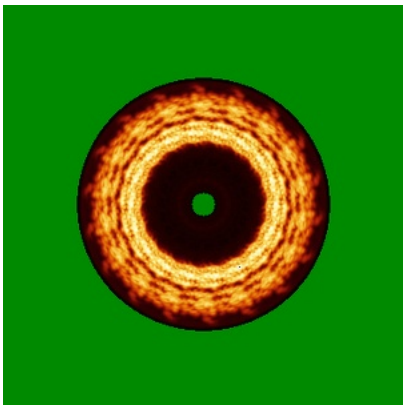
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

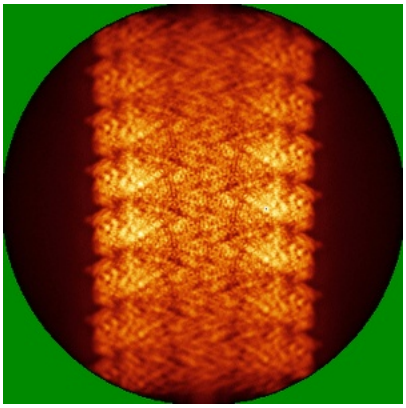
6.4.1 Primary map

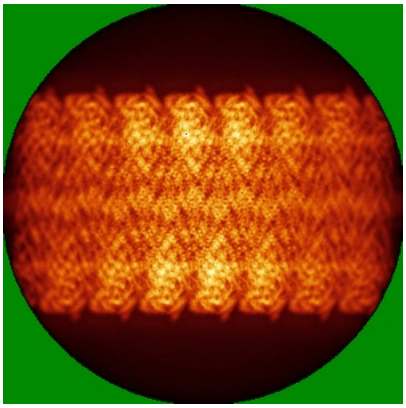

X

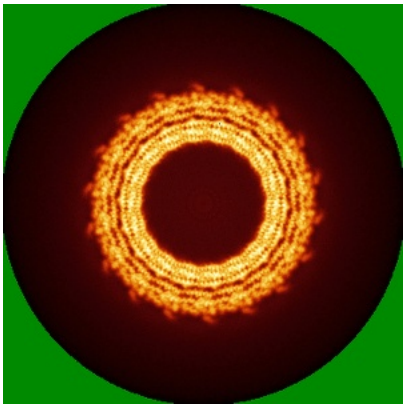

Y


Z

6.4.2 Raw map


X

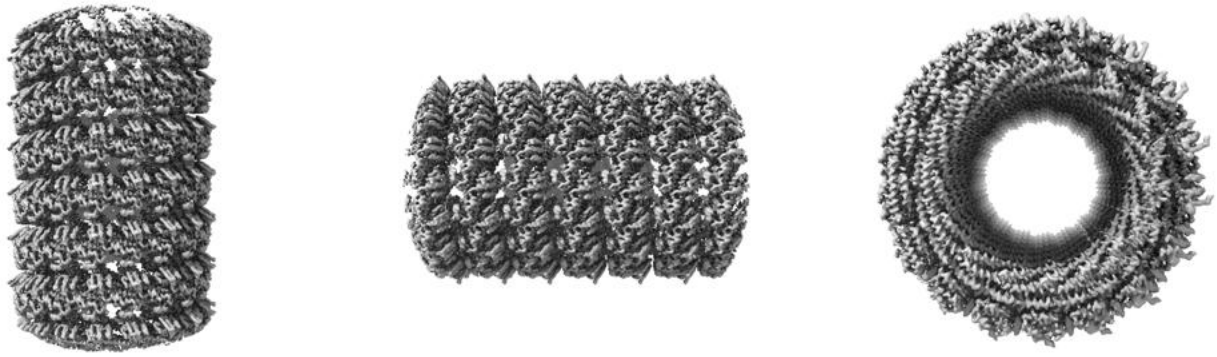

Y


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

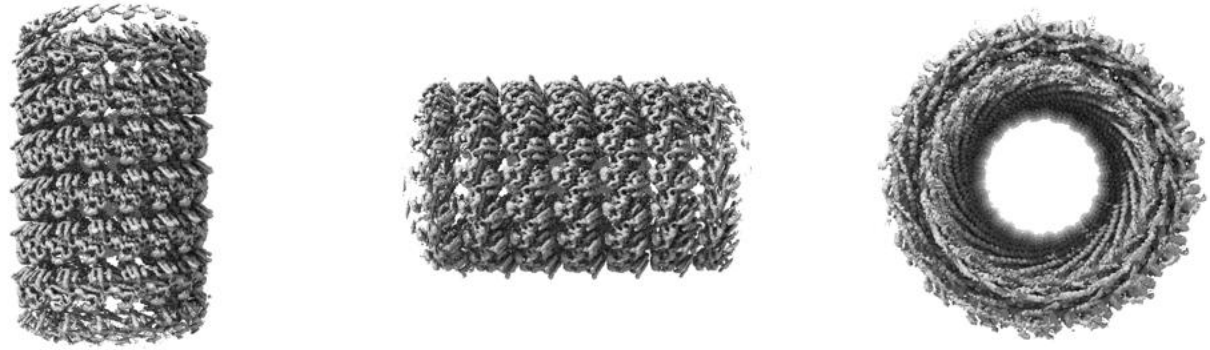
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

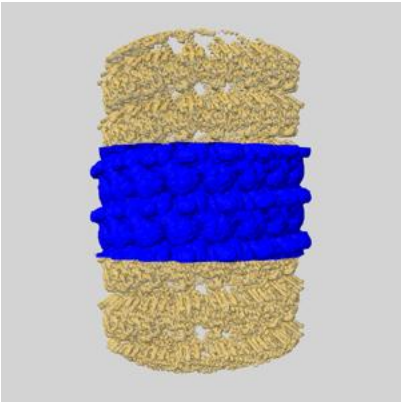
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

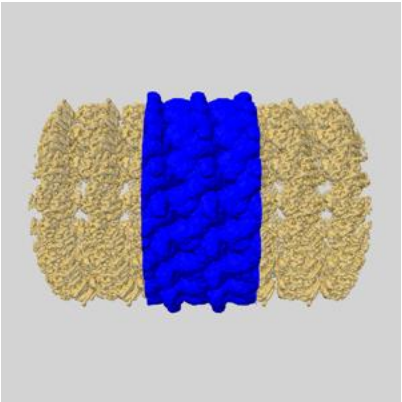
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

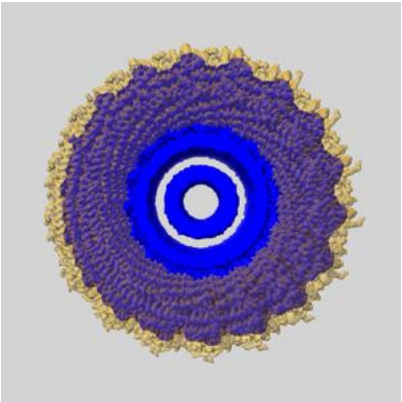
6.6.1 emd_20588_msk_1.map (i)



X



Y

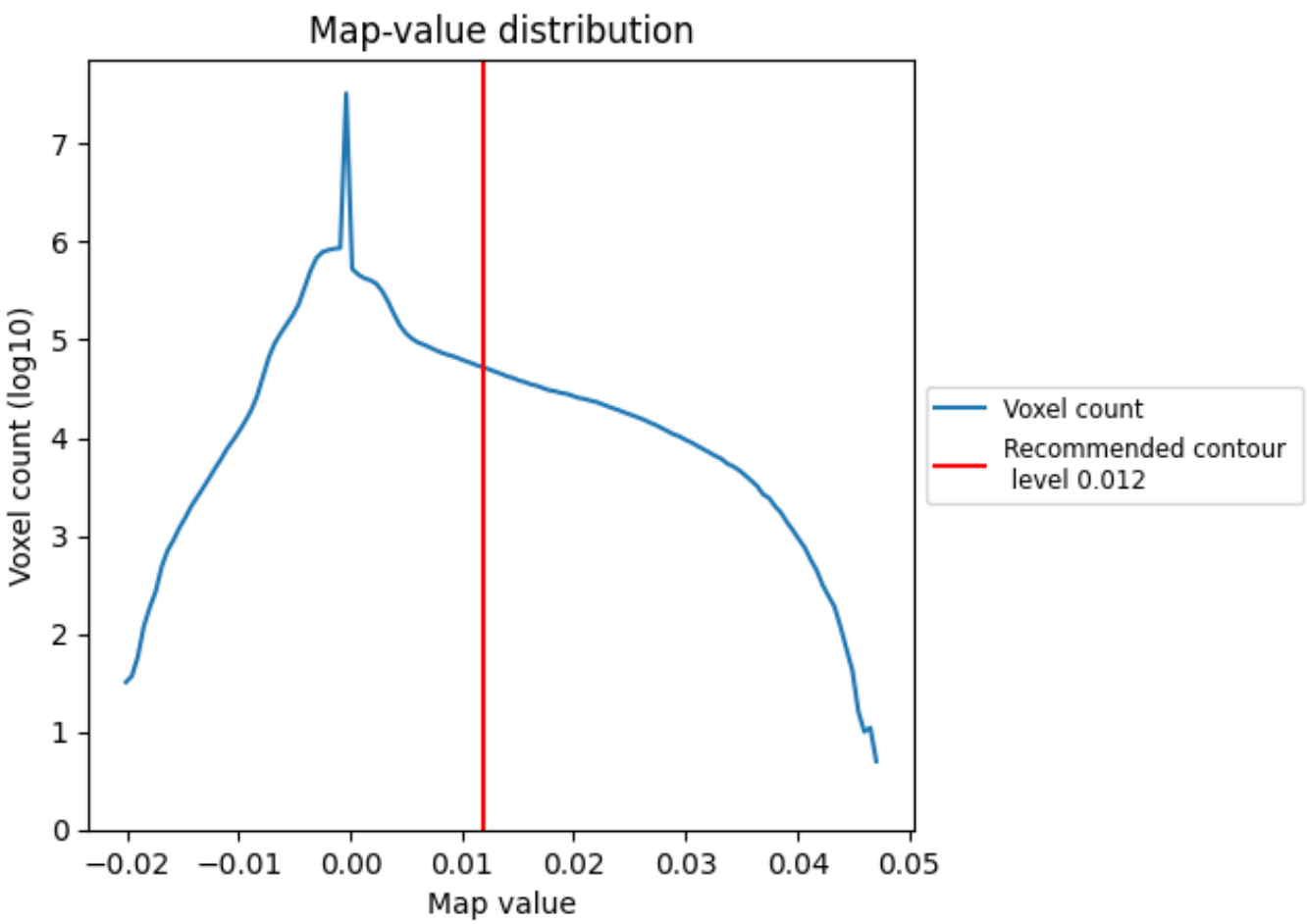


Z

7 Map analysis (i)

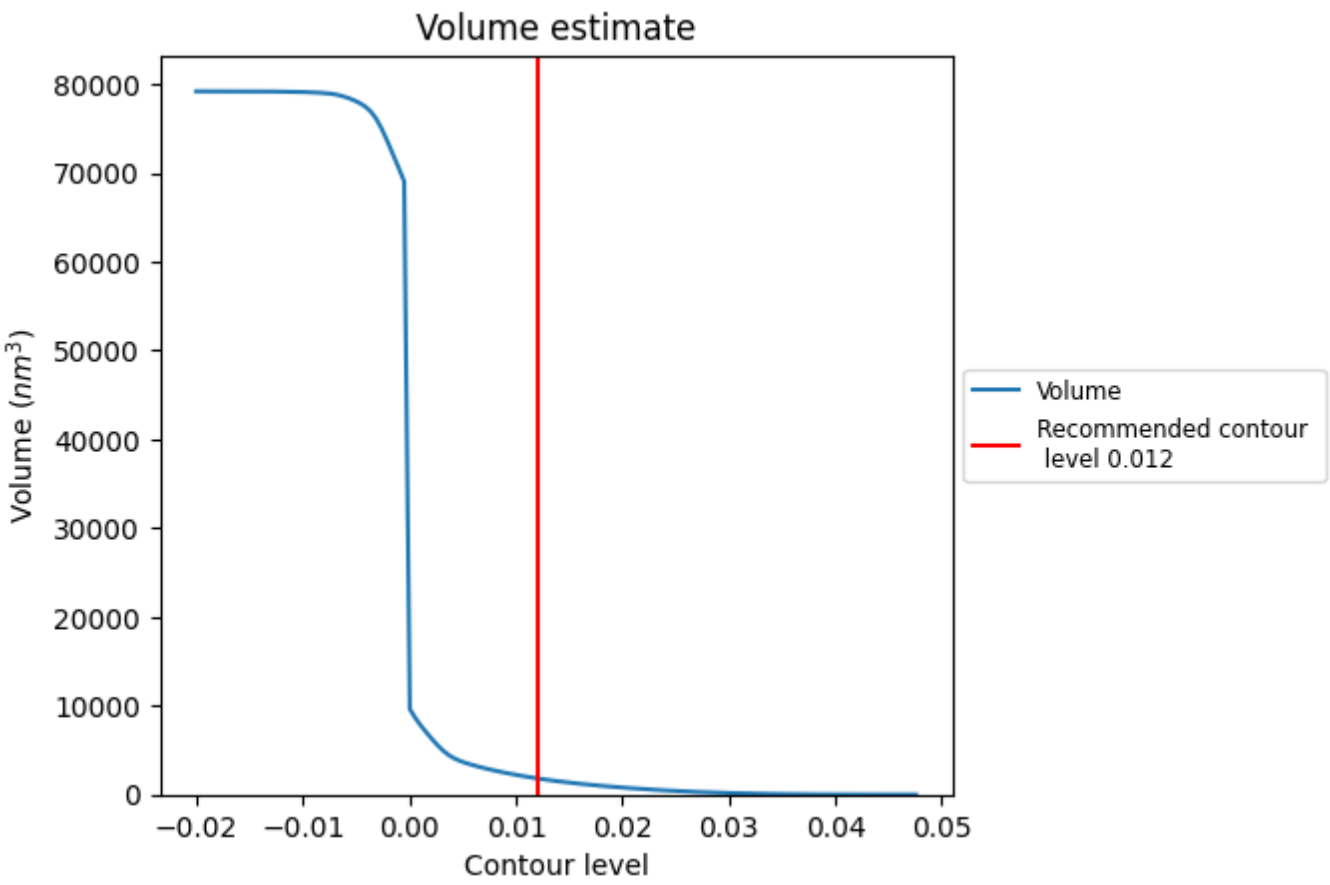
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

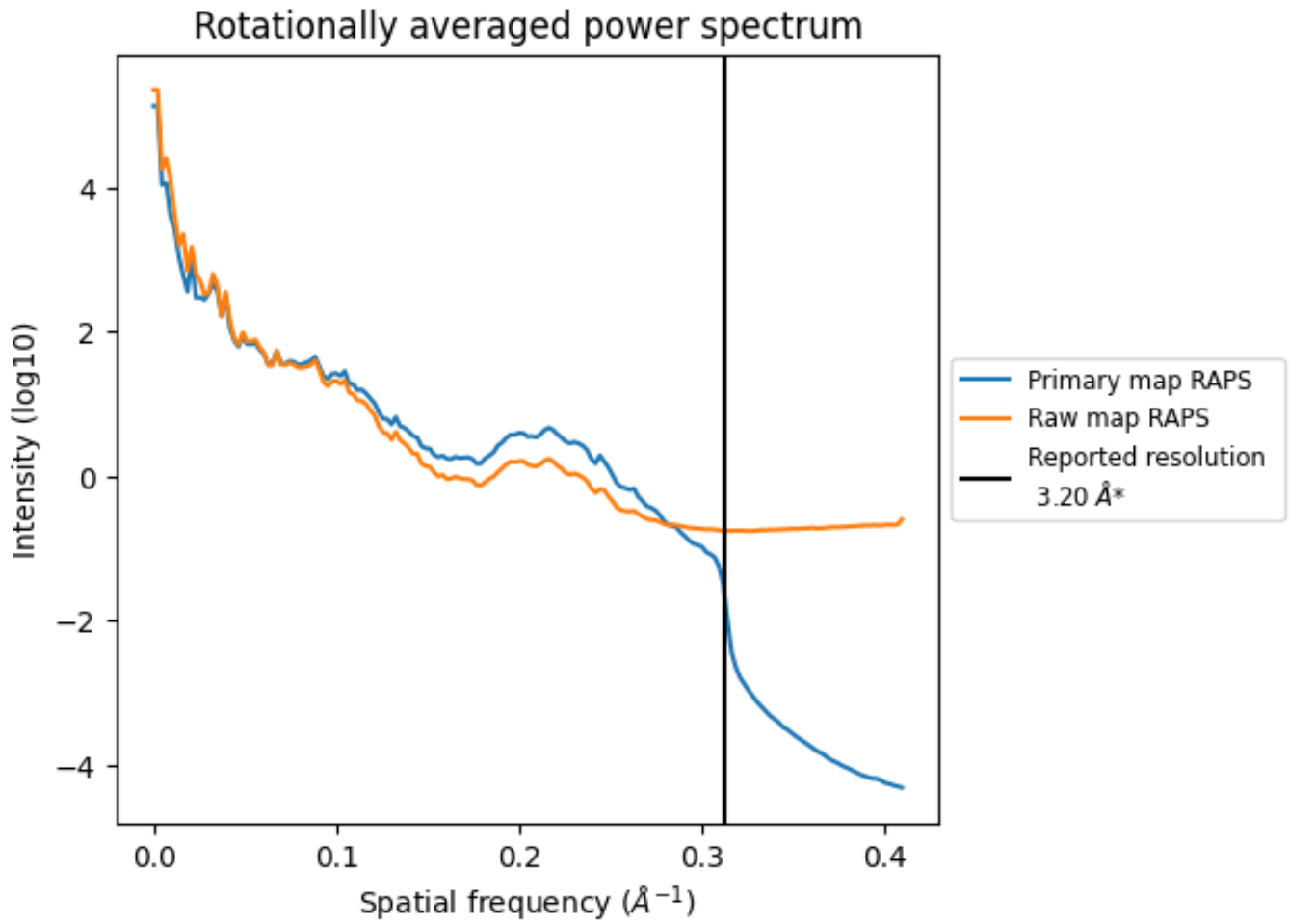
7.2 Volume estimate (i)



The volume at the recommended contour level is 1820 nm^3; this corresponds to an approximate mass of 1644 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

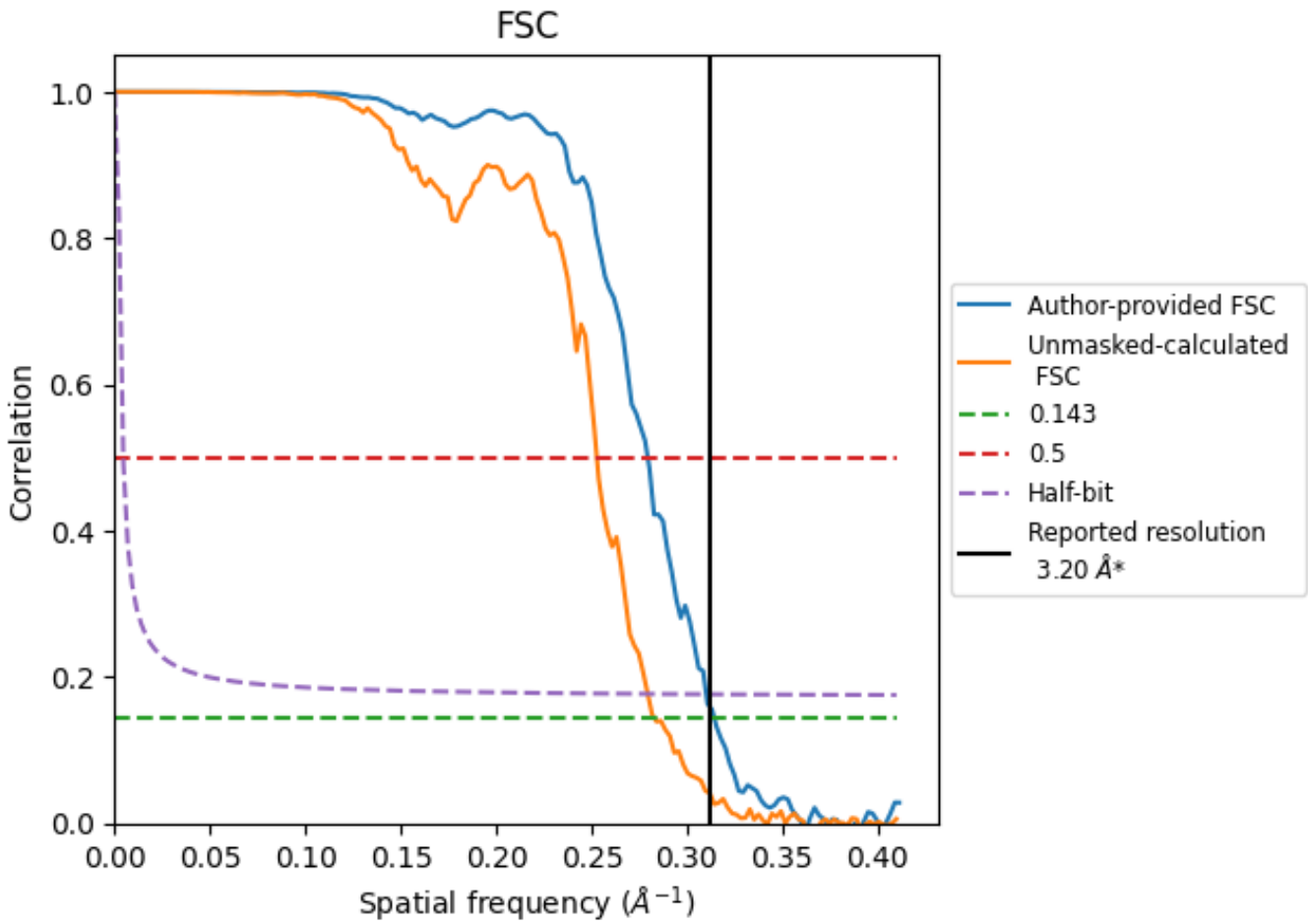


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2 Resolution estimates (i)

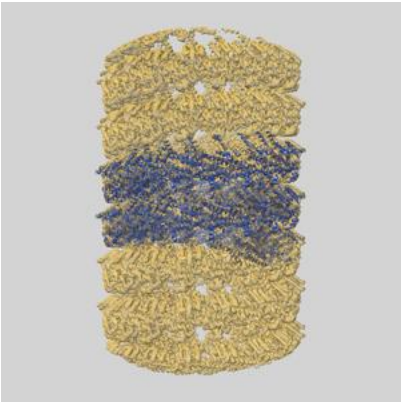
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.18	3.58	3.22
Unmasked-calculated*	3.53	3.96	3.58

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.53 differs from the reported value 3.2 by more than 10 %

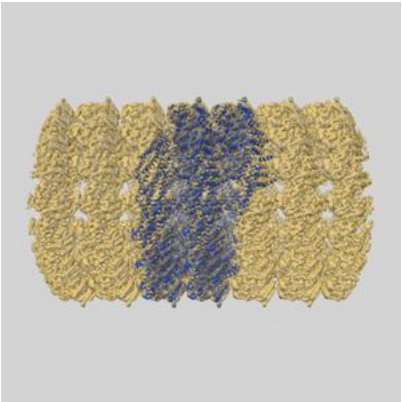
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-20588 and PDB model 6TZ4. Per-residue inclusion information can be found in section 3 on page 11.

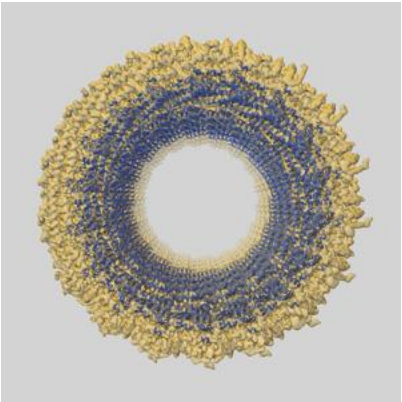
9.1 Map-model overlay (i)



X



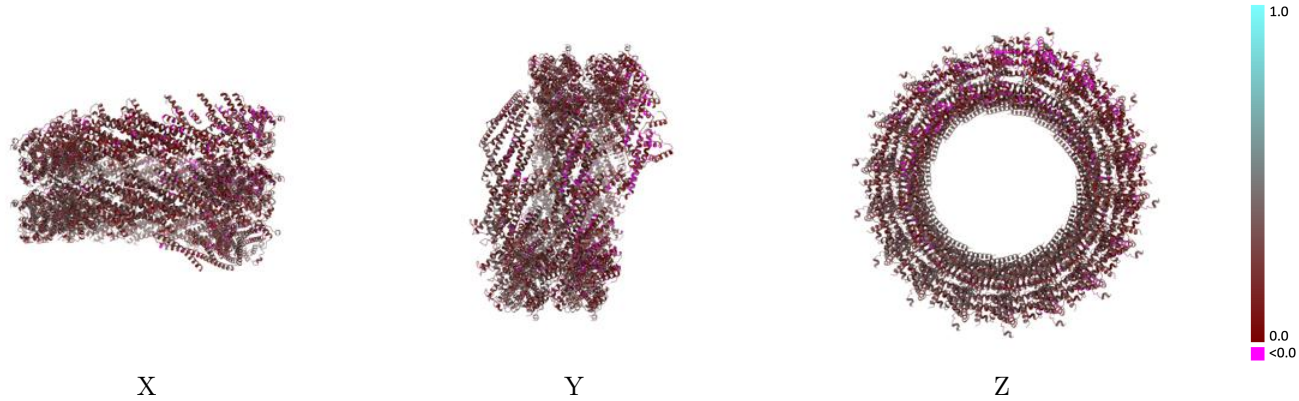
Y



Z

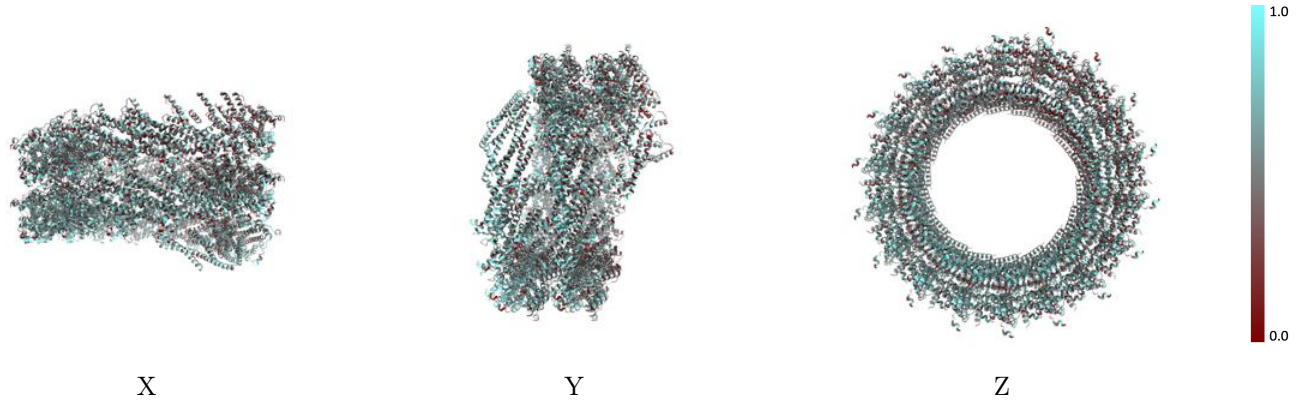
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



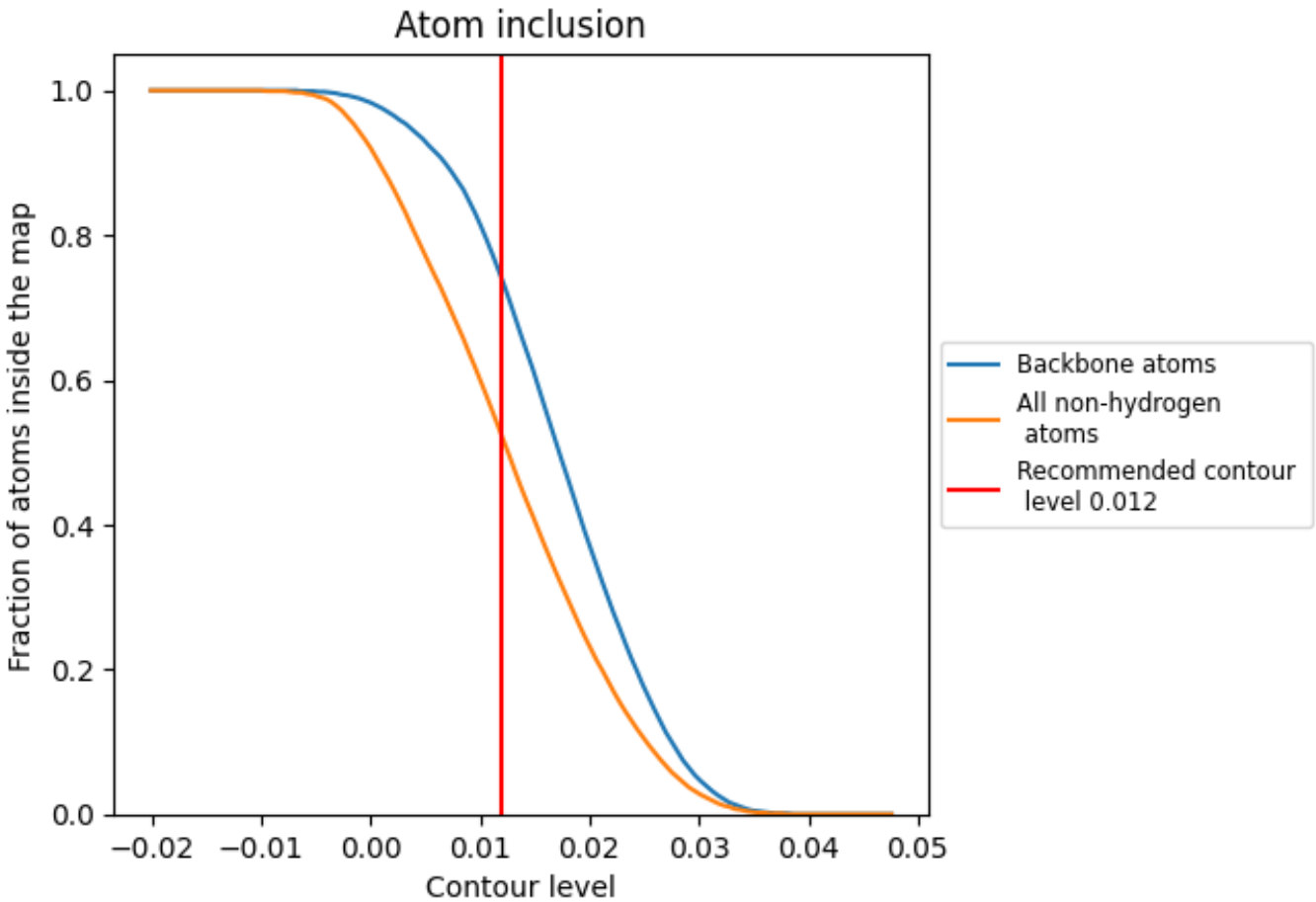
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.012).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 52% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5220	0.2530
01	0.5380	0.2140
02	0.4570	0.2190
A	0.5050	0.2650
AA	0.5150	0.2230
AB	0.5410	0.2450
B	0.4600	0.1620
BA	0.5130	0.2900
BB	0.4920	0.2620
C	0.4750	0.2370
CA	0.4900	0.2070
CB	0.5680	0.2620
D	0.5320	0.2120
DA	0.4970	0.2460
DB	0.4850	0.2090
E	0.5260	0.2760
EA	0.6140	0.3100
EB	0.5800	0.2770
F	0.6180	0.3440
FA	0.5230	0.2760
FB	0.5630	0.3310
G	0.4920	0.2600
GA	0.5380	0.2500
GB	0.5660	0.2730
H	0.4700	0.1660
HA	0.5240	0.2990
HB	0.4750	0.2240
I	0.4670	0.2300
IA	0.5030	0.2140
IB	0.4690	0.1590
J	0.5410	0.2220
JA	0.4920	0.2530
JB	0.5710	0.3390
K	0.5440	0.3030
KA	0.5940	0.2880

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
KB	0.5660	0.2560
L	0.6020	0.3350
LA	0.4940	0.2490
LB	0.4670	0.2010
M	0.5030	0.2560
MA	0.5750	0.2820
MB	0.5840	0.3060
N	0.4830	0.1800
NA	0.5380	0.3120
NB	0.4860	0.2470
O	0.5020	0.2670
OA	0.5170	0.2240
OB	0.4510	0.1570
P	0.5220	0.2100
PA	0.4670	0.2440
PB	0.4600	0.2120
Q	0.5180	0.2520
QA	0.5910	0.2720
QB	0.5580	0.2430
R	0.6160	0.3500
RA	0.5040	0.2440
RB	0.4950	0.2620
S	0.5310	0.2850
SA	0.5750	0.2960
SB	0.4520	0.1700
T	0.4980	0.1960
TA	0.5330	0.3100
UA	0.5300	0.2280
V	0.5040	0.2760
VA	0.4930	0.2630
W	0.5030	0.2130
WA	0.5630	0.2550
X	0.5000	0.2520
XA	0.4490	0.1780
Y	0.5990	0.3200
YA	0.5730	0.2960
Z	0.5060	0.2460
ZA	0.5430	0.3200