



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Nov 14, 2019 – 09:34 AM EST

PDB ID : 6E8G
EMDB ID: : EMD-9005
Title : CryoEM reconstruction of IST1-CHMP1B copolymer filament bound to ss-DNA at 2.9 Angstrom resolution
Authors : Talledge, N.; Frost, A.; McCullough, J.
Deposited on : 2018-07-29
Resolution : 2.90 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

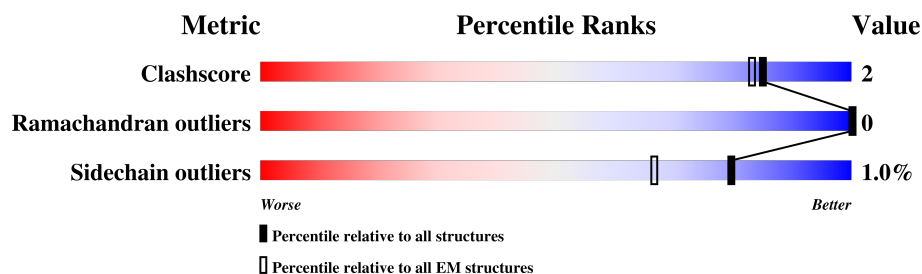
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 Å.

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




























Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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

Mol	Chain	Length	Quality of chain
1	A	366	43% . 54%
1	BA	366	43% . 54%
1	BB	366	43% . 54%
1	C	366	43% . 54%
1	DA	366	43% . 54%
1	DB	366	43% . 54%
1	E	366	43% . 54%
1	FA	366	43% . 54%
1	FB	366	43% . 54%


























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Mol	Chain	Length	Quality of chain	
1	G	366		
1	HA	366		
1	HB	366		
1	I	366		
1	JA	366		
1	JB	366		
1	K	366		
1	LA	366		
1	LB	366		
1	M	366		
1	NA	366		
1	NB	366		
1	O	366		
1	PA	366		
1	PB	366		
1	Q	366		
1	RA	366		
1	RB	366		
1	S	366		
1	TA	366		
1	TB	366		
1	V	366		
1	VA	366		
1	X	366		
1	XA	366		











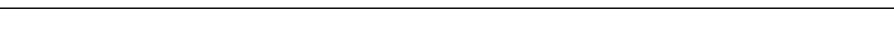
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Mol	Chain	Length	Quality of chain
1	Z	366	
1	ZA	366	
2	AA	199	
2	AB	199	
2	B	199	
2	CA	199	
2	CB	199	
2	D	199	
2	EA	199	
2	EB	199	
2	F	199	
2	GA	199	
2	GB	199	
2	H	199	
2	IA	199	
2	IB	199	
2	J	199	
2	KA	199	
2	KB	199	
2	L	199	
2	MA	199	
2	MB	199	
2	N	199	
2	OA	199	
2	OB	199	

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Mol	Chain	Length	Quality of chain
2	P	199	 80%7%13%
2	QA	199	 80%7%13%
2	QB	199	 80%7%13%
2	R	199	 81%7%13%
2	SA	199	 81%7%13%
2	SB	199	 80%7%13%
2	T	199	 80%7%13%
2	UA	199	 80%8%13%
2	UB	199	 79%8%13%
2	W	199	 79%9%13%
2	WA	199	 81%7%13%
2	Y	199	 81%7%13%
2	YA	199	 80%8%13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 97272 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 IST1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	S	167	Total	C	N	O	S	0	0
			1349	862	234	248	5		
1	A	167	Total	C	N	O	S	0	0
			1349	862	234	248	5		
1	C	167	Total	C	N	O	S	0	0
			1349	862	234	248	5		
1	E	167	Total	C	N	O	S	0	0
			1349	862	234	248	5		
1	G	167	Total	C	N	O	S	0	0
			1349	862	234	248	5		
1	I	167	Total	C	N	O	S	0	0
			1349	862	234	248	5		
1	K	167	Total	C	N	O	S	0	0
			1349	862	234	248	5		
1	M	167	Total	C	N	O	S	0	0
			1349	862	234	248	5		
1	O	167	Total	C	N	O	S	0	0
			1349	862	234	248	5		
1	Q	167	Total	C	N	O	S	0	0
			1349	862	234	248	5		
1	V	167	Total	C	N	O	S	0	0
			1349	862	234	248	5		
1	X	167	Total	C	N	O	S	0	0
			1349	862	234	248	5		
1	Z	167	Total	C	N	O	S	0	0
			1349	862	234	248	5		
1	BA	167	Total	C	N	O	S	0	0
			1349	862	234	248	5		
1	DA	167	Total	C	N	O	S	0	0
			1349	862	234	248	5		
1	FA	167	Total	C	N	O	S	0	0
			1349	862	234	248	5		
1	HA	167	Total	C	N	O	S	0	0
			1349	862	234	248	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	JA	167	Total	C	N	O	S	0	0
			1349	862	234	248	5		
1	LA	167	Total	C	N	O	S	0	0
			1349	862	234	248	5		
1	NA	167	Total	C	N	O	S	0	0
			1349	862	234	248	5		
1	PA	167	Total	C	N	O	S	0	0
			1349	862	234	248	5		
1	RA	167	Total	C	N	O	S	0	0
			1349	862	234	248	5		
1	TA	167	Total	C	N	O	S	0	0
			1349	862	234	248	5		
1	VA	167	Total	C	N	O	S	0	0
			1349	862	234	248	5		
1	XA	167	Total	C	N	O	S	0	0
			1349	862	234	248	5		
1	ZA	167	Total	C	N	O	S	0	0
			1349	862	234	248	5		
1	BB	167	Total	C	N	O	S	0	0
			1349	862	234	248	5		
1	DB	167	Total	C	N	O	S	0	0
			1349	862	234	248	5		
1	FB	167	Total	C	N	O	S	0	0
			1349	862	234	248	5		
1	HB	167	Total	C	N	O	S	0	0
			1349	862	234	248	5		
1	JB	167	Total	C	N	O	S	0	0
			1349	862	234	248	5		
1	LB	167	Total	C	N	O	S	0	0
			1349	862	234	248	5		
1	NB	167	Total	C	N	O	S	0	0
			1349	862	234	248	5		
1	PB	167	Total	C	N	O	S	0	0
			1349	862	234	248	5		
1	RB	167	Total	C	N	O	S	0	0
			1349	862	234	248	5		
1	TB	167	Total	C	N	O	S	0	0
			1349	862	234	248	5		

- Molecule 2 is a protein called Charged multivesicular body protein 1b.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	T	174	Total	C	N	O	S	0	0
			1353	831	245	264	13		
2	B	174	Total	C	N	O	S	0	0
			1353	831	245	264	13		
2	D	174	Total	C	N	O	S	0	0
			1353	831	245	264	13		
2	F	174	Total	C	N	O	S	0	0
			1353	831	245	264	13		
2	H	174	Total	C	N	O	S	0	0
			1353	831	245	264	13		
2	J	174	Total	C	N	O	S	0	0
			1353	831	245	264	13		
2	L	174	Total	C	N	O	S	0	0
			1353	831	245	264	13		
2	N	174	Total	C	N	O	S	0	0
			1353	831	245	264	13		
2	P	174	Total	C	N	O	S	0	0
			1353	831	245	264	13		
2	R	174	Total	C	N	O	S	0	0
			1353	831	245	264	13		
2	W	174	Total	C	N	O	S	0	0
			1353	831	245	264	13		
2	Y	174	Total	C	N	O	S	0	0
			1353	831	245	264	13		
2	AA	174	Total	C	N	O	S	0	0
			1353	831	245	264	13		
2	CA	174	Total	C	N	O	S	0	0
			1353	831	245	264	13		
2	EA	174	Total	C	N	O	S	0	0
			1353	831	245	264	13		
2	GA	174	Total	C	N	O	S	0	0
			1353	831	245	264	13		
2	IA	174	Total	C	N	O	S	0	0
			1353	831	245	264	13		
2	KA	174	Total	C	N	O	S	0	0
			1353	831	245	264	13		
2	MA	174	Total	C	N	O	S	0	0
			1353	831	245	264	13		
2	OA	174	Total	C	N	O	S	0	0
			1353	831	245	264	13		
2	QA	174	Total	C	N	O	S	0	0
			1353	831	245	264	13		
2	SA	174	Total	C	N	O	S	0	0
			1353	831	245	264	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	UA	174	Total	C	N	O	S	0	0
			1353	831	245	264	13		
2	WA	174	Total	C	N	O	S	0	0
			1353	831	245	264	13		
2	YA	174	Total	C	N	O	S	0	0
			1353	831	245	264	13		
2	AB	174	Total	C	N	O	S	0	0
			1353	831	245	264	13		
2	CB	174	Total	C	N	O	S	0	0
			1353	831	245	264	13		
2	EB	174	Total	C	N	O	S	0	0
			1353	831	245	264	13		
2	GB	174	Total	C	N	O	S	0	0
			1353	831	245	264	13		
2	IB	174	Total	C	N	O	S	0	0
			1353	831	245	264	13		
2	KB	174	Total	C	N	O	S	0	0
			1353	831	245	264	13		
2	MB	174	Total	C	N	O	S	0	0
			1353	831	245	264	13		
2	OB	174	Total	C	N	O	S	0	0
			1353	831	245	264	13		
2	QB	174	Total	C	N	O	S	0	0
			1353	831	245	264	13		
2	SB	174	Total	C	N	O	S	0	0
			1353	831	245	264	13		
2	UB	174	Total	C	N	O	S	0	0
			1353	831	245	264	13		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	37	GLU	LYS	engineered mutation	UNP Q7LBR1
B	37	GLU	LYS	engineered mutation	UNP Q7LBR1
D	37	GLU	LYS	engineered mutation	UNP Q7LBR1
F	37	GLU	LYS	engineered mutation	UNP Q7LBR1
H	37	GLU	LYS	engineered mutation	UNP Q7LBR1
J	37	GLU	LYS	engineered mutation	UNP Q7LBR1
L	37	GLU	LYS	engineered mutation	UNP Q7LBR1
N	37	GLU	LYS	engineered mutation	UNP Q7LBR1
P	37	GLU	LYS	engineered mutation	UNP Q7LBR1
R	37	GLU	LYS	engineered mutation	UNP Q7LBR1
W	37	GLU	LYS	engineered mutation	UNP Q7LBR1

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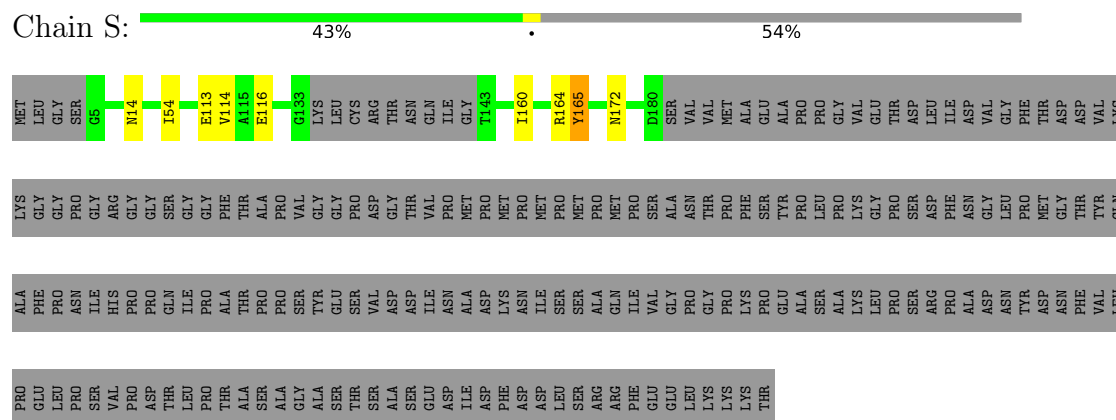
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Chain	Residue	Modelled	Actual	Comment	Reference
Y	37	GLU	LYS	engineered mutation	UNP Q7LBR1
AA	37	GLU	LYS	engineered mutation	UNP Q7LBR1
CA	37	GLU	LYS	engineered mutation	UNP Q7LBR1
EA	37	GLU	LYS	engineered mutation	UNP Q7LBR1
GA	37	GLU	LYS	engineered mutation	UNP Q7LBR1
IA	37	GLU	LYS	engineered mutation	UNP Q7LBR1
KA	37	GLU	LYS	engineered mutation	UNP Q7LBR1
MA	37	GLU	LYS	engineered mutation	UNP Q7LBR1
OA	37	GLU	LYS	engineered mutation	UNP Q7LBR1
QA	37	GLU	LYS	engineered mutation	UNP Q7LBR1
SA	37	GLU	LYS	engineered mutation	UNP Q7LBR1
UA	37	GLU	LYS	engineered mutation	UNP Q7LBR1
WA	37	GLU	LYS	engineered mutation	UNP Q7LBR1
YA	37	GLU	LYS	engineered mutation	UNP Q7LBR1
AB	37	GLU	LYS	engineered mutation	UNP Q7LBR1
CB	37	GLU	LYS	engineered mutation	UNP Q7LBR1
EB	37	GLU	LYS	engineered mutation	UNP Q7LBR1
GB	37	GLU	LYS	engineered mutation	UNP Q7LBR1
IB	37	GLU	LYS	engineered mutation	UNP Q7LBR1
KB	37	GLU	LYS	engineered mutation	UNP Q7LBR1
MB	37	GLU	LYS	engineered mutation	UNP Q7LBR1
OB	37	GLU	LYS	engineered mutation	UNP Q7LBR1
QB	37	GLU	LYS	engineered mutation	UNP Q7LBR1
SB	37	GLU	LYS	engineered mutation	UNP Q7LBR1
UB	37	GLU	LYS	engineered mutation	UNP Q7LBR1

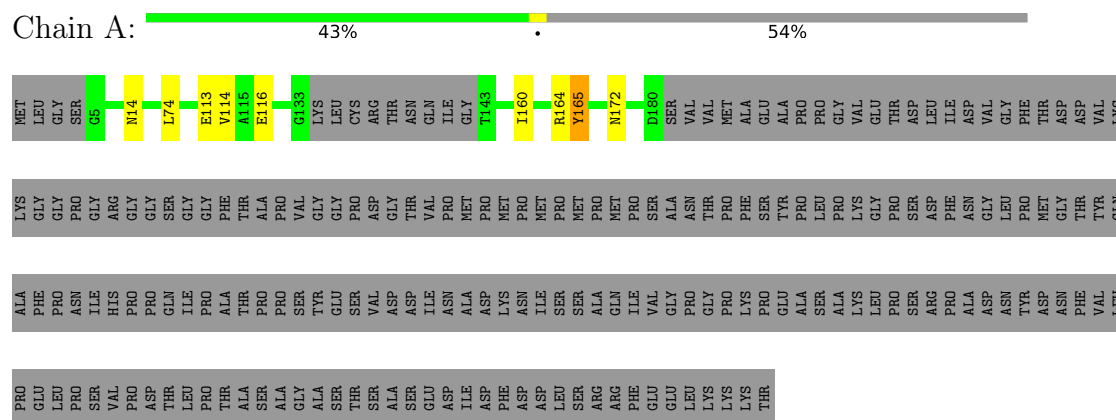
3 Residue-property plots [i](#)

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

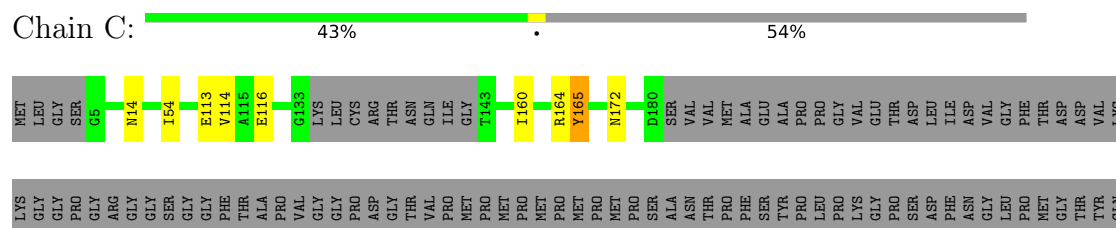
- Molecule 1: IST1 homolog



- Molecule 1: IST1 homolog



- Molecule 1: IST1 homolog



ALA	PHE	PRO	ASN	ILE	HIS	PRO	PRO	GLN	ILE	ALA	THR	PRO	PRO	SER	TYR	GLU	SER	VAL	ASP	ASP	ILE	ASN	ALA	ASN	LYS	ASN	ILE	SER	SER	ALA	GLN	ILE	VAL	GLY	PRO	GLY	PRO	PRO	LYS	LEU	PRO	SER	ARG	PRO	ALA	ASP	ASN	PHE	VAL	LEU
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PRO	GLU	LEU	PRO	PRO	VAL	ASP	THR	LEU	PRO	THR	ALA	SER	ALA	GLY	ALA	SER	THR	SER	ALA	SER	GLU	ASP	ILE	ASP	PHE	ASP	ASP	LEU	SER	ARG	ARG	PHE	GLU	GLU	LEU	LYS	LYS	LYS	THR
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- Molecule 1: IST1 homolog

Chain E: 43% . 54%

[illegible]

LYS GLY LYS GLY PRO ARG GLY SER PHE THR ALA VAL GLY ASP GLY THR VAL PRO MET PRO MET PRO MET PRO MET SER ASN THR PRO PHE SER TYR PRO LEU PRO LYS GLY PRO SER PHE ASN GLY LEU PRO MET GLY THR TYR

ALA	PHE	PRO	ASN	ILE	HIS	PRO	PRO	GLN	ILE	ALA	THR	PRO	PRO	SER	TYR	GLU	SER	VAL	ASP	ASN	ILE	ILE	ASN	ALA	ASN	ASP	LYS	ASN	ILE	SER	SER	ALA	ALA	GLN	ILE	ILE	VAL	GLY	PRO	GLY	PRO	PRO	LYS	LEU	PRO	SER	ARG	PRO	ALA	ALA	ASP	ASN	PHE	VAL	LEU
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PRO	GLU	LEU	PRO	PRO	SER	VAL	ASP	THR	LEU	PRO	PRO	THR	ALA	SER	ALA	GLY	ALA	SER	THR	SER	ALA	SER	GLU	ASP	ILE	ASP	PHE	ASP	ASP	LEU	SER	ARG	ARG	PHE	GLU	GLU	LEU	LYS	LYS	THR
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- Molecule 1: IST1 homolog

Chain G: 43% . 54%

MET LEU GLY SER G5 N14 E113 V114 A115 E116 G13 LYS LEU LEU CYS ARG THR ASN GLN ILE GLY T143 I160 R164 Y165 N172 D180 VAL VAL MET ALA GLU ALA PRO PRO GLY VAL GLU THR THR ASP ILE ASP VAL GLY PHE THR ASP VAL LYS LYS

GLY	PRO	GLY	ARG	GLY	GLY	GLY	PHE	THR	ALA	PRO	VAL	GLY	GLY	PRO	ASP	GLY	THR	VAL	PRO	MET	PRO	MET	MET	PRO	PRO	PRO	ASN	THR	PRO	PHE	TYR	PRO	LEU	PRO	LYS	GLY	PRO	PRO	ASP	ASP	PHE	ASN	GLY	LEU	GLY	PRO	MET	GLY	THR	GLN	ALA	PHE
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PRO	ASN	ILE	HIS	PRO	PRO	GLN	ILE	ALA	THR	PRO	PRO	SER	TYR	GLU	SER	VAL	ASP	ASP	ILE	ASN	ASN	ASP	LYS	ASN	ILE	SER	SER	ALA	GLN	ILE	VAL	GLY	PRO	GLY	PRO	LYS	PRO	PRO	GLU	ALA	SER	ALA	LYS	LEU	PRO	SER	ARG	PRO	ASP	ASN	PHE	VAL	LEU	PRO	TYR
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LEU	PRO	SER	VAL	PRO	ASP	THR	LEU	PRO	THR	ALA	SER	ALA	GLY	ALA	SER	THR	SER	THR	ALA	GLU	ASP	ILE	ASP	PHE	ASP	ASP	LEU	SER	ARG	ARG	PHE	GLU	GLU	LEU	LYS	LYS	LYS	THR
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- Molecule 1: IST1 homolog

Chain I: 43% . 54%

MET LEU GLY SER G5 N14 L78 E113 V114 A115 E116 G133 LYS LEU CYS ARG ASN GLN ILE GLY I143 I160 R164 Y165 N172 D180 SER VAL VAL MET MET ALA ALA ALA PRO PRO GLY VAL VAL GLU THR ASP LEU ASP VAL VAL PHE THR ASP ASP VAL VAL

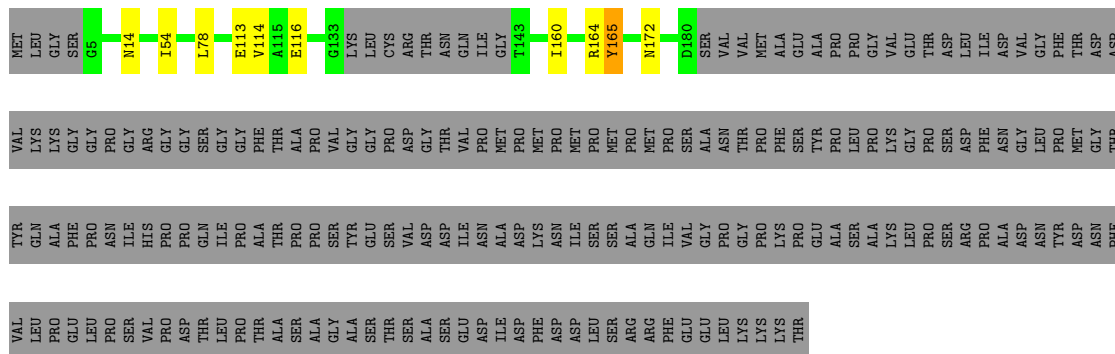
LYS	GLY	GLY	GLY	GLY	ARG	GLY	GLY	SER	GLY	GLY	PHE	THR	ALA	ALA	VAL	VAL	GLY	GLY	PRO	ASP	GLY	THR	THR	PRO	PRO	MET	MET	PRO	PRO	PRO	MET	MET	PRO	PRO	ASN	ALA	ALA	THR	THR	PRO	PRO	PHE	SER	SER	TYR	PRO	LEU	PRO	PRO	LYS	GLY	PRO	SER	SER	ASP	PHE	ASN	ASN	GLY	LEU	PRO	MET	GLY	THR	TYR	TIN
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ALA	PHE	PRO	ASN	ILE	HIS	PRO	PRO	GLN	PRO	ALA	ALA	THR	PRO	PRO	PRO	SER	SER	TYR	GLU	SER	VAL	ASP	ASP	ILE	ILE	ASN	ALA	ALA	ASP	LYS	ASN	ILE	ILE	SER	SER	ALA	GLN	VAL	GLY	PRO	GLY	PRO	PRO	LYS	PRO	PRO	GLU	SER	ALA	LEU	PRO	SER	ARG	PRO	PRO	ALA	ALA	ASP	ASN	PHE	VAL	LEU
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PRO	GLU	LEU	PRO	PRO	SER	VAL	ASP	THR	LEU	PRO	PRO	THR	ALA	SER	SER	GLY	ALA	SER	THR	SER	ALA	SER	GLU	ASP	ILE	ASP	PHE	ASP	ASP	LEU	SER	ARG	ARG	PHE	GLU	GLU	LEU	LYS	LYS	THR
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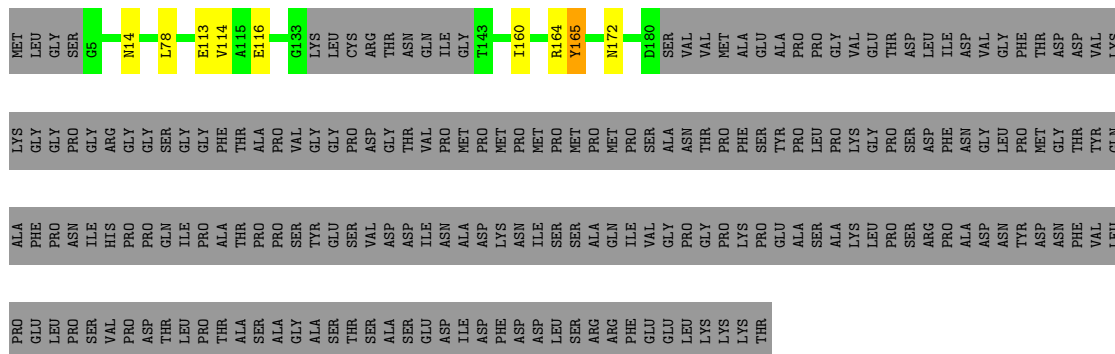
- Molecule 1: IST1 homolog

Chain K:  43% . 54%



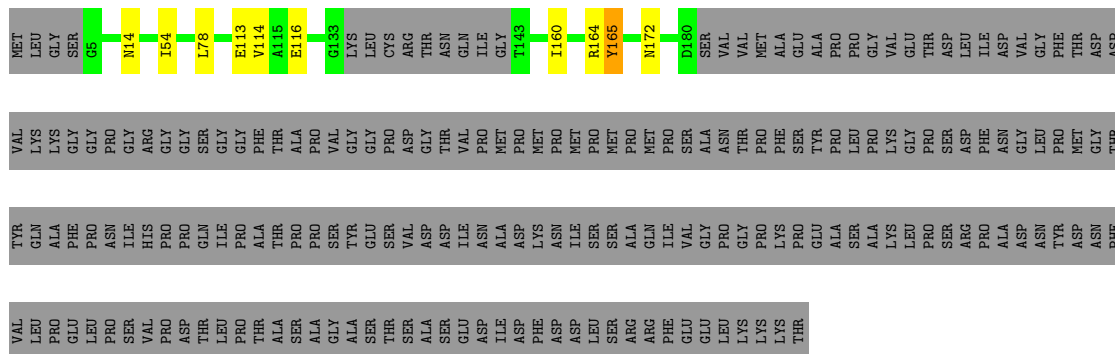
- Molecule 1: IST1 homolog

Chain M: 43% . 54%



- Molecule 1: IST1 homolog

Chain 0: 43% . 54%



- Molecule 1: IST1 homolog

Chain Q:  43% . 54%

TYR	GLN	ALA	ALA	ALA	PHE	PRO	ASN	ILE	HIS	PRO	PRO	GLN	ILE	PRO	THR	PRO	PRO	SER	TYR	GLU	SER	VAL	ASP	ASP	ILE	ASN	ALA	ASP	LYS	ASN	ILE	SER	SER	ALA	GLN	ILE	VAL	GLY	PRO	PRO	GLY	LYS	PRO	GLU	ALA	SER	LYS	LEU	PRO	SER	ARG	PRO	ALA	ASP	ASN	TYR	ASP	ASN	PHE
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VAL	LEU	PRO	GLU	LEU	PRO	SER	VAL	PRO	ASP	THR	LEU	PRO	THR	ALA	SER	SER	GLY	ALA	ALA	SER	THR	SER	ALA	SER	GLU	ASP	ILE	ASP	PHE	ASP	ASP	LEU	SER	SER	ARG	ARG	PHE	GLU	GLU	LEU	LYS	LYS	THR
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- Molecule 1: IST1 homolog

Chain BA:  43% . 54%

MET	LEU	GLY	SER	G5	M14	L78	E113	V114	A115	E116	G133	LVS	LEU	CYS	ARG	THR	ASN	GLN	ILE	GLY	T143	I160	R164	Y165	N172	D180	SER	VAL	VAL	MET	ALA	ALA	ALA	ALA	PRO	PRO	GLY	VAL	GLU	THR	ASP	ILE	LEU	ASP	VAL	GLY	PHE	THR	ASP	ASP	VAL	VAL	ASN
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LYS	GLY	GLY	PRO	GLY	ARG	GLY	GLY	SER	GLY	GLY	PHE	THR	ALA	ALA	VAL	VAL	GLY	GLY	PRO	ASP	ASP	GLY	THR	THR	VAL	PRO	MET	MET	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	SER	SER	ALA	ALA	ASN	THR	THR	PRO	PRO	PHE	SER	SER	TYR	PRO	LEU	PRO	LYS	GLY	PRO	PRO	SER	SER	ASP	PHE	ASN	GLY	LEU	GLY	THR	THR	TYR	THR
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ALA	PHE	PRO	ASN	ILE	HIS	PRO	PRO	GLN	ILE	PRO	ALA	ALA	THR	PRO	PRO	PRO	SER	SER	TYR	GLU	GLU	SER	VAL	ASP	ASP	ILE	ASN	ALA	ALA	ASP	LYS	ASN	ILE	ILE	SER	SER	SER	ALA	GLN	VAL	GLY	PRO	GLY	PRO	PRO	LYS	PRO	GLU	GLU	ALA	SER	SER	ALA	LYS	LEU	PRO	PRO	SER	ARG	PRO	ALA	ASP	ASN	PHE	VAL	LEU
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PRO	GLU	LEU	PRO	PRO	SER	VAL	PRO	ASP	THR	LEU	PRO	THR	ALA	SER	ALA	GLY	ALA	SER	THR	SER	ALA	SER	GLU	ASP	ILE	ASP	PHE	ASP	ASP	LEU	SER	ARG	ARG	PHE	GLU	GLU	LEU	LYS	LYS	LYS	THR
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- Molecule 1: IST1 homolog

Chain DA: 43% . 54%

MET	LEU	GLY	SER	G5	N14	I54	E113	V114	A115	E116	G133	LVS	LEU	CYS	ARG	THR	ASN	GLN	ILE	GLY	T143	I160	R164	Y165	N172	D180	SER	VAL	VAL	MET	ALA	ALA	ALA	ALA	PRO	PRO	GLY	VAL	GLU	THR	ASP	ILE	LEU	ASP	VAL	GLY	PHE	THR	ASP	ASP	VAL	VAL	ASN
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LYS	GLY	GLY	PRO	GLY	ARG	GLY	GLY	GLY	SER	SER	PHE	THR	ALA	ALA	VAL	VAL	GLY	GLY	PRO	ASP	GLY	THR	THR	VAL	VAL	PRO	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	ALA	ALA	ASN	THR	THR	PRO	PRO	PHE	SER	SER	TYR	PRO	LEU	PRO	LYS	PRO	GLY	PRO	SER	SER	ASP	PHE	ASN	ASN	GLY	LEU	TYR	THR	THR	GLY	MET	MET	PRO	PRO	TYR	TIN
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ALA	PHE	PRO	PRO	ASN	ILE	HIS	PRO	PRO	GLN	ILE	PRO	ALA	PRO	THR	PRO	PRO	SER	SER	TYR	GLU	SER	VAL	ASP	ASP	ILE	ASN	ALA	ALA	ASP	LYS	ILE	ILE	SER	SER	ALA	GLN	LYS	PRO	PRO	GLU	ALA	LYS	LEU	PRO	SER	ARG	PRO	ALA	ASP	ASN	PHE	VAL	LEU
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PRO	GLU	LEU	PRO	PRO	SER	VAL	PRO	ASP	THR	LEU	PRO	THR	ALA	SER	ALA	GLY	ALA	SER	THR	SER	ALA	SER	GLU	ASP	ILE	ASP	PHE	ASP	ASP	LEU	SER	ARG	ARG	PHE	GLU	GLU	LEU	LYS	LYS	LYS	THR
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- Molecule 1: IST1 homolog

Chain FA: 

MET	LEU	GLY	SER	G5	M14	L78	E113	V114	A115	E116	G133	LVS	LEU	CYS	ARG	THR	ASN	GLN	ILE	GLY	T143	I160	R164	Y165	M172	D180	SER	VAL	VAL	MET	MET	ALA	ALA	ALA	PRO	PRO	GLY	GLY	VAL	GLY	GLU	THR	ASP	LEU	ILE	ASP	VAL	VAL	GLY	PHE	THR	ASP	ASP	VAL	VAL	YS
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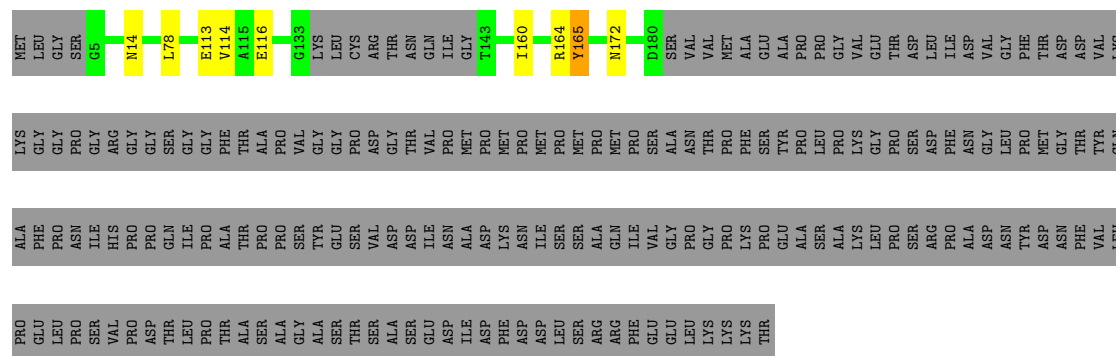
LYS	GLY	GLY	PRO	GLY	ARG	GLY	GLY	GLY	SER	GLY	GLY	PHE	THR	ALA	ALA	PRO	VAL	GLY	GLY	PRO	ASP	GLY	THR	THR	VAL	PRO	MET	PRO	MET	MET	PRO	PRO	MET	PRO	PRO	ASN	ALA	SER	THR	THR	PRO	PHE	SER	THR	TYR	PRO	LEU	PRO	LYS	PRO	GLY	PRO	SER	ASP	PHE	ASN	GLY	LEU	GLY	THR	THR	TYR	TIN
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ALA	PHE	PRO	PRO	ASN	ILE	HIS	PRO	PRO	GLN	ILE	PRO	ALA	PRO	THR	PRO	PRO	SER	SER	GLU	GLU	VAL	ASP	ASP	ASN	ILE	ASN	ALA	ASP	LYS	LYS	ILE	ILE	SER	SER	ALA	ALA	GLN	ILE	VAL	GLY	PRO	PRO	GLY	PRO	LYS	PRO	PRO	GLU	ALA	ALA	LYS	LEU	PRO	SER	ASN	ASP	ASN	PHE	VAL	LEU
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PRO	GLU	LEU	PRO	SER	VAL	PRO	ASP	THR	LEU	PRO	THR	ALA	SER	ALA	GLY	ALA	SER	THR	SER	ALA	SER	GLU	ASP	ILE	ASP	PHE	ASP	ASP	LEU	SER	ARG	ARG	PHE	GLU	GLU	LEU	LYS	LYS	THR
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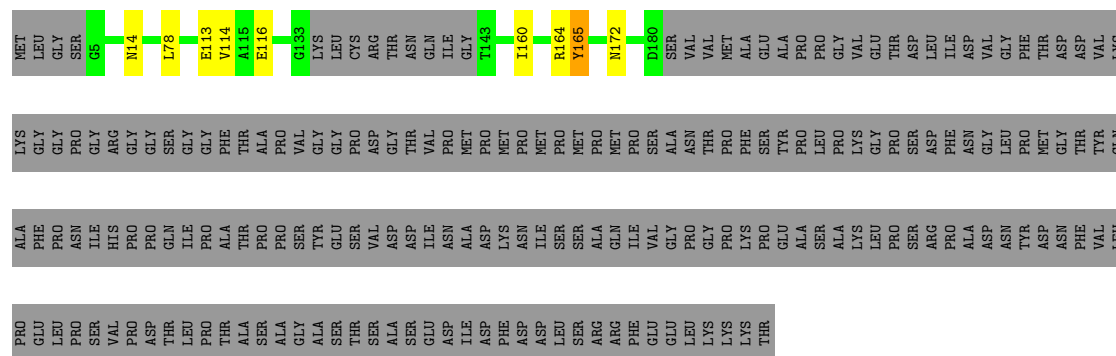
- Molecule 1: IST1 homolog

Chain HA:  43% 54%



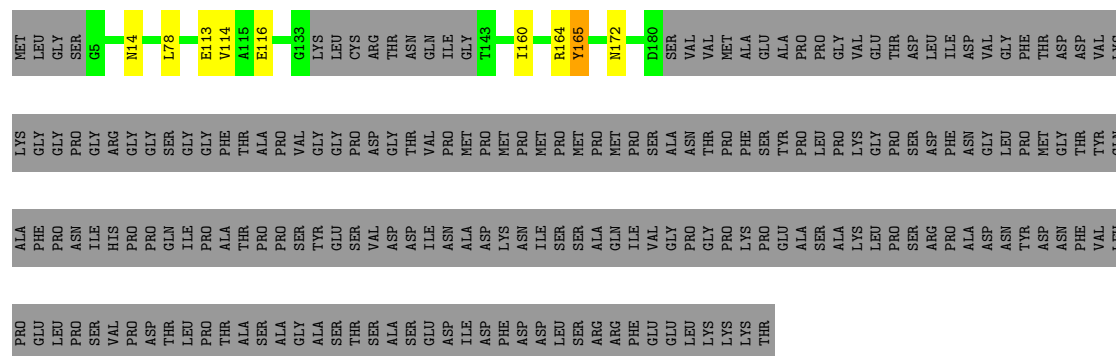
- Molecule 1: IST1 homolog

Chain JA:  43% 54%



- Molecule 1: IST1 homolog

Chain LA:  43% 54%



- Molecule 1: IST1 homolog

Chain NA:  43% 54%

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• Molecule 1: IST1 homolog

Chain VA:  43% 54%

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• Molecule 1: IST1 homolog

Chain XA:  43% 54%

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• Molecule 1: IST1 homolog

Chain ZA:  43% 54%

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V114
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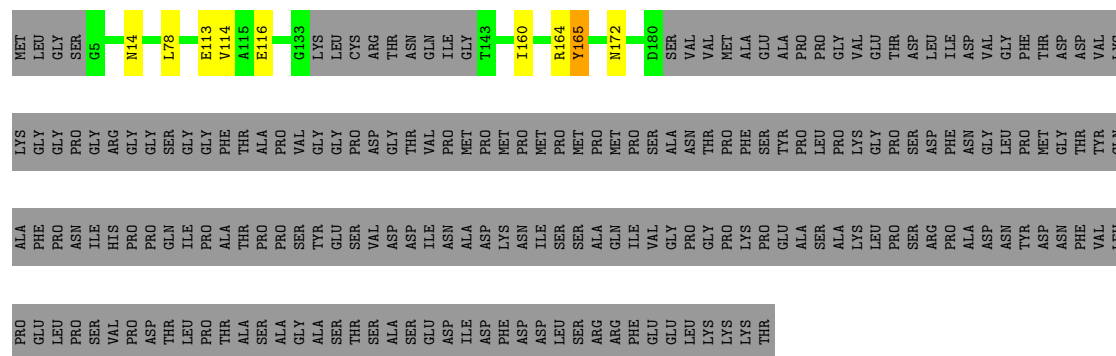
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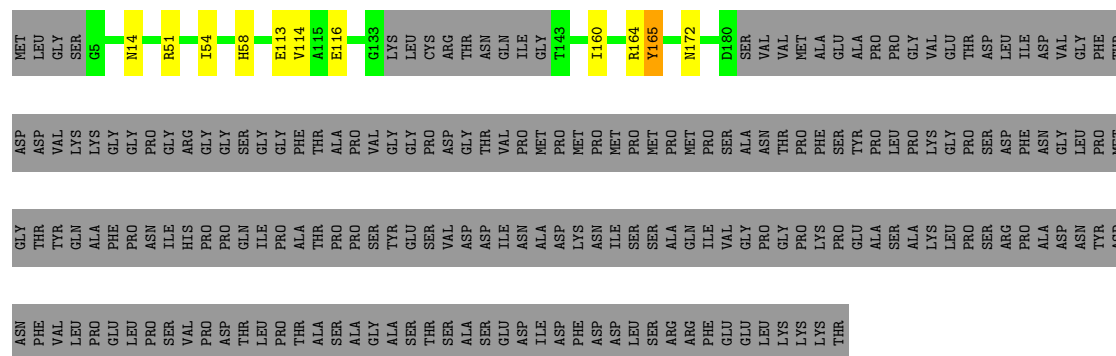
- Molecule 1: IST1 homolog

Chain BB:  43% 1% 54%



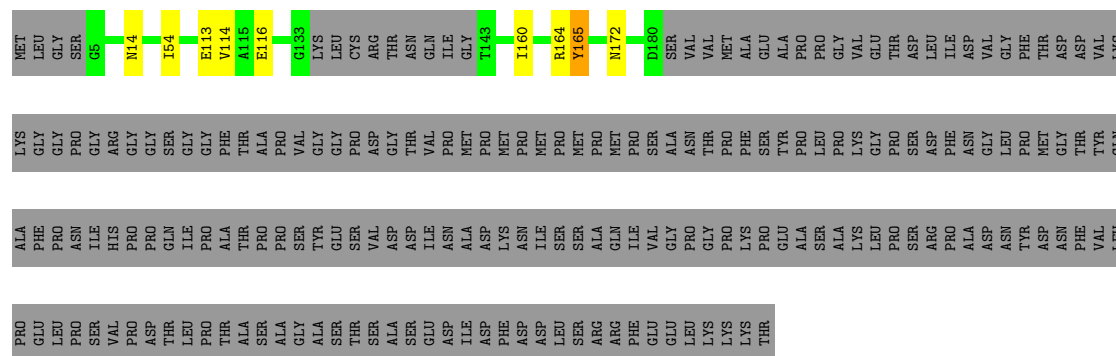
- Molecule 1: IST1 homolog

Chain DB:  43% 1% 54%



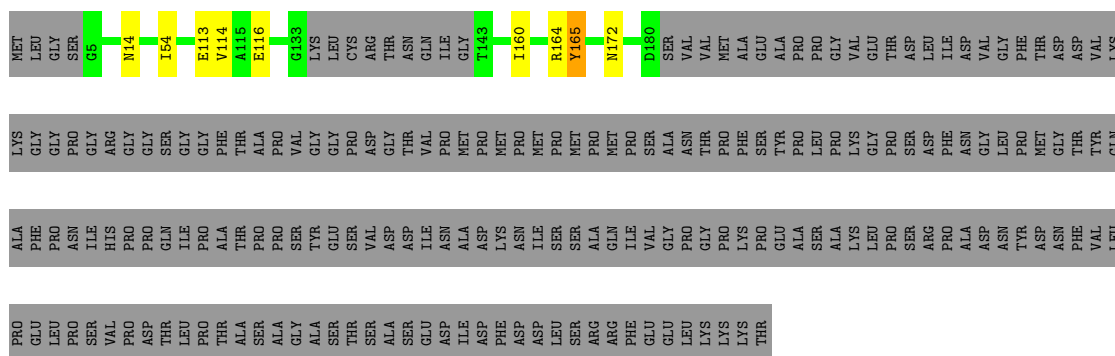
- Molecule 1: IST1 homolog

Chain FB:  43% 0% 54%



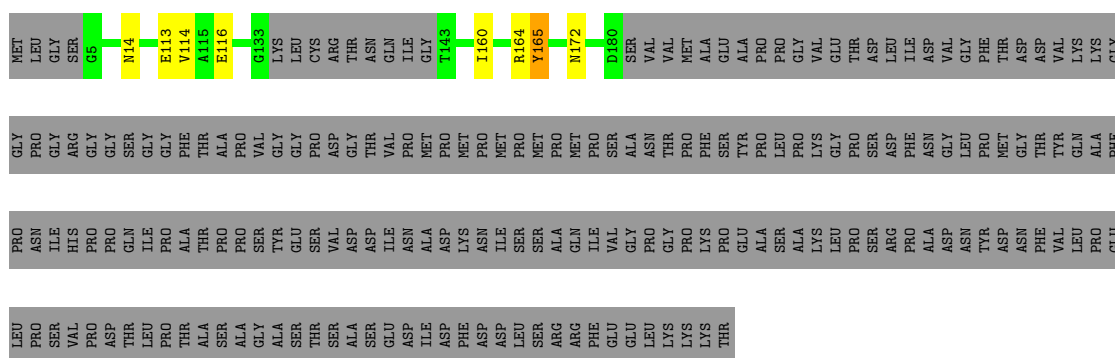
- Molecule 1: IST1 homolog

Chain HB:  43% . 54%



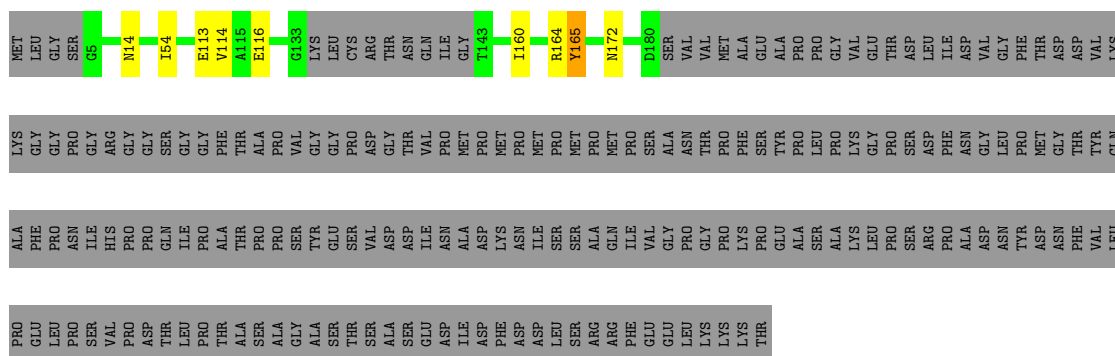
- Molecule 1: IST1 homolog

Chain JB:  43% . 54%



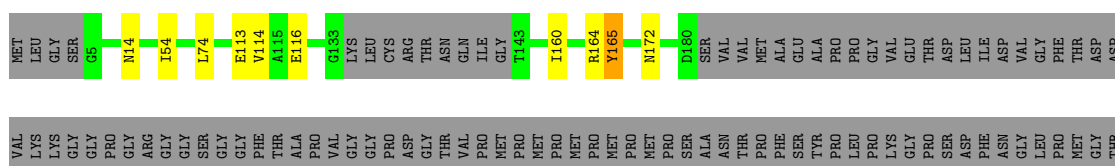
- Molecule 1: IST1 homolog

Chain LB:  43% . 54%



- Molecule 1: IST1 homolog

Chain NB: 43% 54%



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ALA
ASP
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ASN
ILE
GLY
ASP
ASP
ILE
ASP
PHE
ASP
ASP
LEU
SER
SER
ARG
PHE
GLY
GLU
GLY
LEU
LYS
LYS
THR

• Molecule 1: IST1 homolog

Chain PB: 43% 54%

MET
LEU
GLY
SER
G5
M14
L74
E113
V114
A115
E116
G133
LYS
LEU
CYS
ARG
THR
THR
GLN
ASN
ILE
GLY
T143
I160
R164
Y165
N172
D180
SER
VAL
VAL
MET
ALA
GLY
LEU
LYS
LYS
THR

LYS
GLY
GLY
PRO
ASN
SER
ARG
GLY
GLY
SER
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CYS
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GLY
LEU
LYS
LYS
THR

• Molecule 1: IST1 homolog

Chain RB: 43% 54%

MET
LEU
GLY
SER
G5
M14
I64
L78
E113
V114
A115
E116
G133
LYS
LEU
CYS
ARG
THR
THR
GLN
ASN
ILE
GLY
T143
I160
R164
Y165
N172
D180
SER
VAL
VAL
MET
ALA
GLY
LEU
LYS
LYS
THR

VAL
LYS
GLY
GLY
PRO
GLY
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GLY
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LEU
LYS
LYS
THR

• Molecule 1: IST1 homolog

Chain TB: 43% 54%

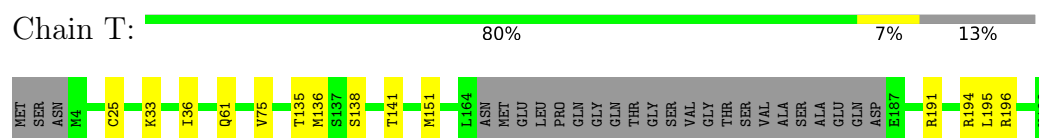
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GLY
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G5
M14
L78
E113
V114
A115
E116
G133
LYS
LEU
CYS
ARG
THR
THR
GLN
ASN
ILE
GLY
T143
I160
R164
Y165
N172
D180
SER
VAL
VAL
MET
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THR

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CYS
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MET
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MET
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SER
PRO
SER
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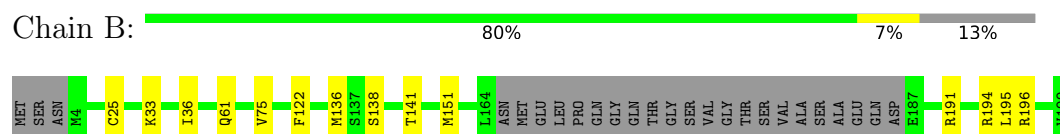
ALA
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GLY
GLY
SER
SER
VAL
ASP
PHE
LYS
ASN
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ASP
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LEU
SER
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LYS
THR

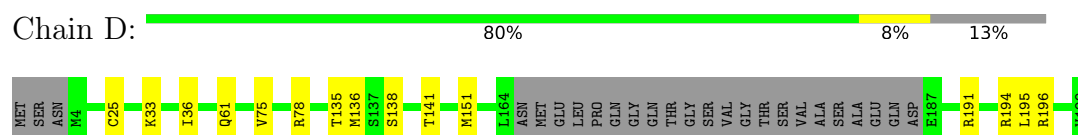
- Molecule 2: Charged multivesicular body protein 1b



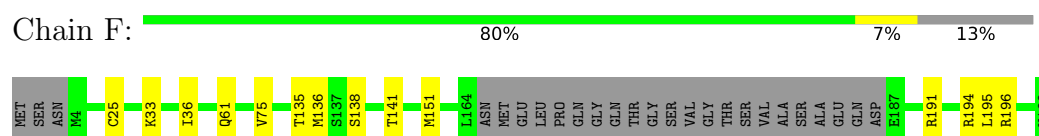
- Molecule 2: Charged multivesicular body protein 1b



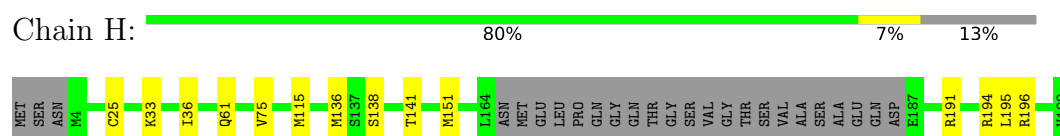
- Molecule 2: Charged multivesicular body protein 1b



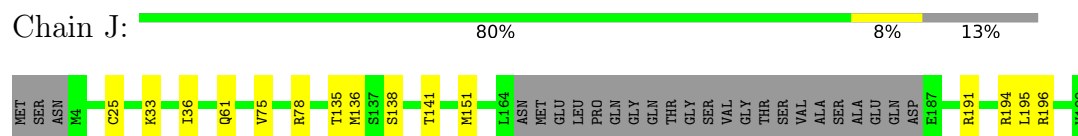
- Molecule 2: Charged multivesicular body protein 1b



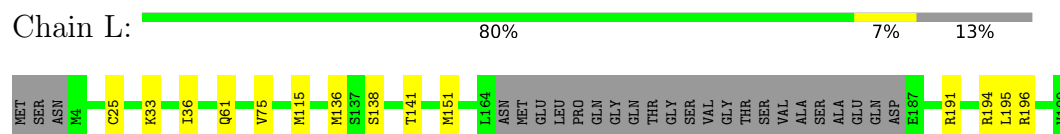
- Molecule 2: Charged multivesicular body protein 1b




- Molecule 2: Charged multivesicular body protein 1b

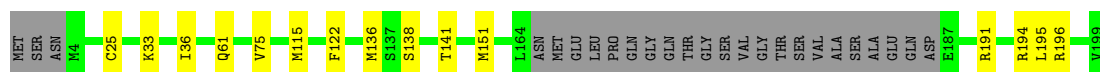


- Molecule 2: Charged multivesicular body protein 1b




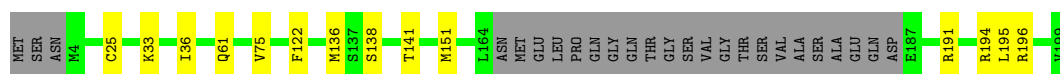
- Molecule 2: Charged multivesicular body protein 1b

Chain N: 




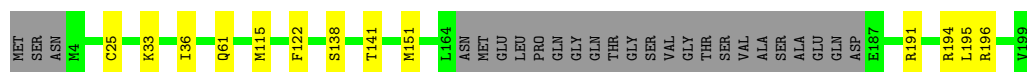
- Molecule 2: Charged multivesicular body protein 1b

Chain P: 




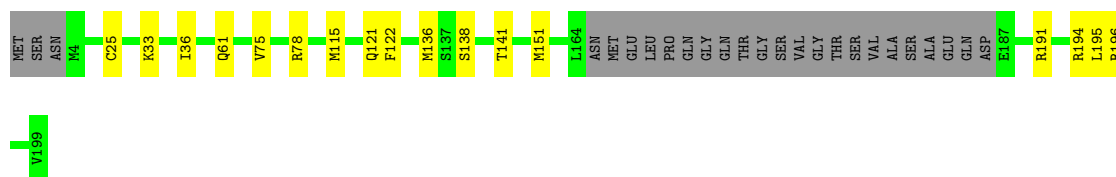
- Molecule 2: Charged multivesicular body protein 1b

Chain R: 




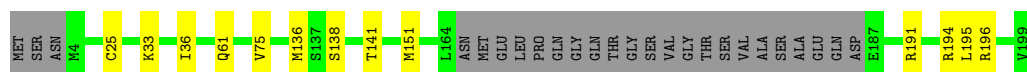
- Molecule 2: Charged multivesicular body protein 1b

Chain W: 




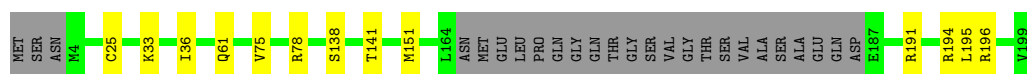
- Molecule 2: Charged multivesicular body protein 1b

Chain Y: 




- Molecule 2: Charged multivesicular body protein 1b

Chain AA: 

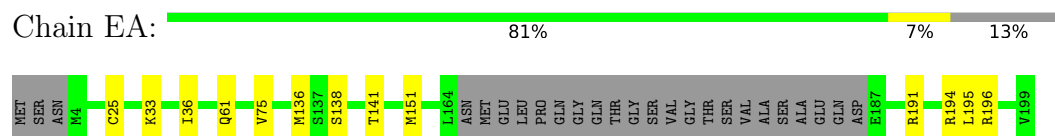


- Molecule 2: Charged multivesicular body protein 1b

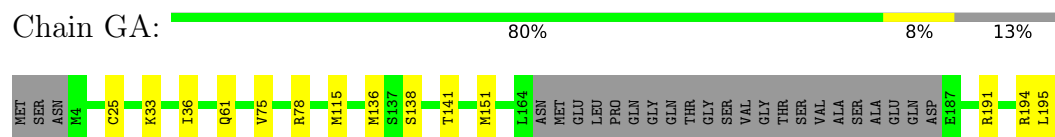
Chain CA: 



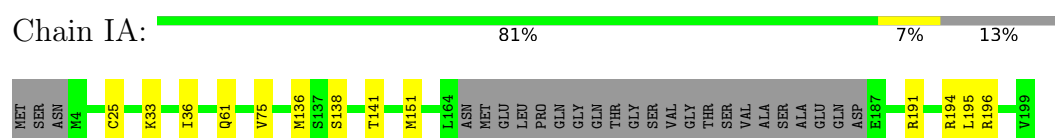
- Molecule 2: Charged multivesicular body protein 1b



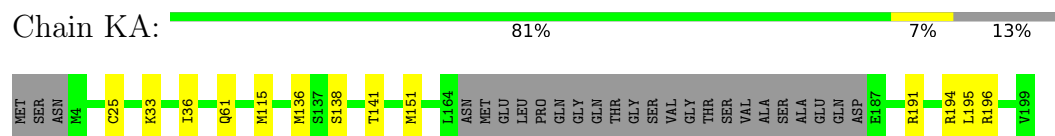
- Molecule 2: Charged multivesicular body protein 1b



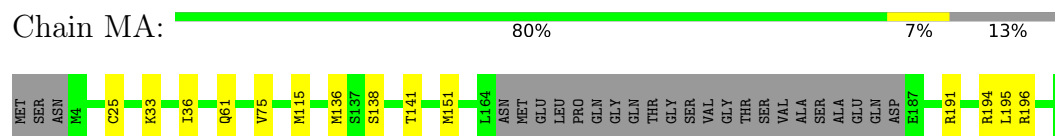
- Molecule 2: Charged multivesicular body protein 1b



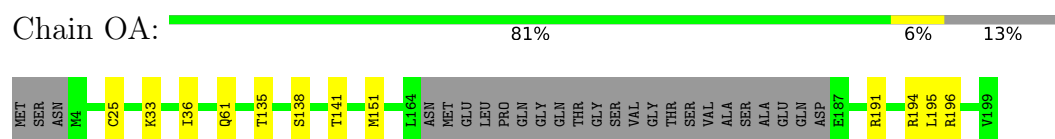
- Molecule 2: Charged multivesicular body protein 1b



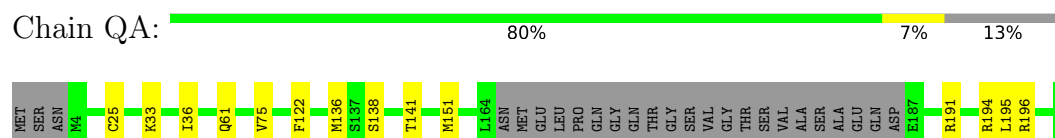
- Molecule 2: Charged multivesicular body protein 1b



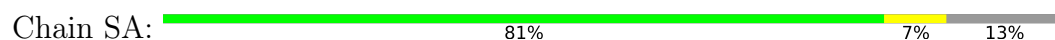
- Molecule 2: Charged multivesicular body protein 1b

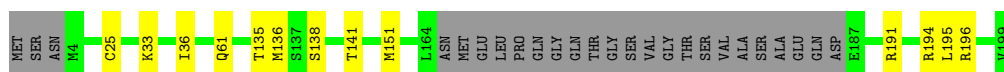


- Molecule 2: Charged multivesicular body protein 1b



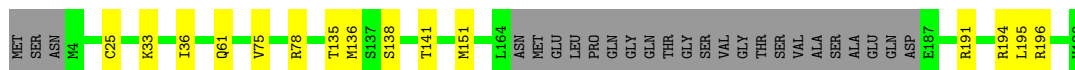
- Molecule 2: Charged multivesicular body protein 1b





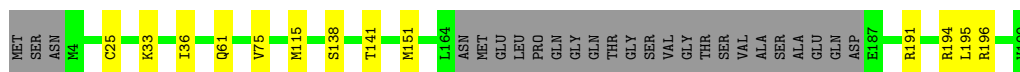
- Molecule 2: Charged multivesicular body protein 1b

Chain UA: 80% 8% 13%



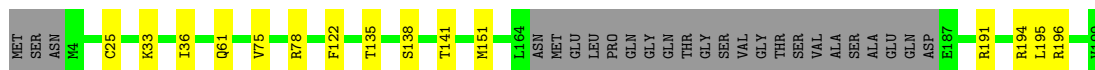
- Molecule 2: Charged multivesicular body protein 1b

Chain WA: 81% 7% 13%



- Molecule 2: Charged multivesicular body protein 1b

Chain YA: 80% 8% 13%



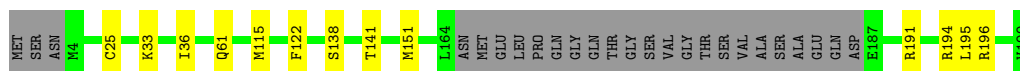
- Molecule 2: Charged multivesicular body protein 1b

Chain AB: 80% 7% 13%



- Molecule 2: Charged multivesicular body protein 1b

Chain CB: 81% 7% 13%



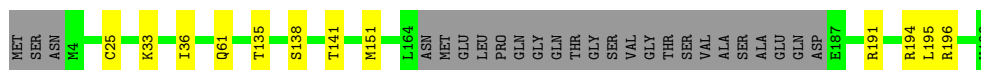
- Molecule 2: Charged multivesicular body protein 1b

Chain EB: 79% 8% 13%


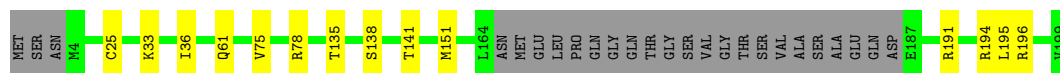


- Molecule 2: Charged multivesicular body protein 1b


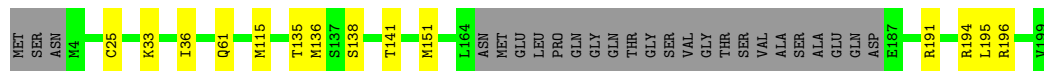
Chain GB: 81% 6% 13%




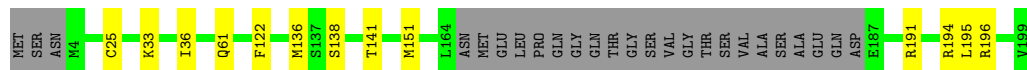
● Molecule 2: Charged multivesicular body protein 1b

Chain IB:  80% 7% 13%


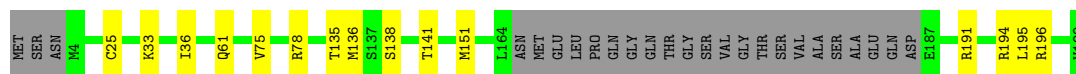
● Molecule 2: Charged multivesicular body protein 1b

Chain KB:  80% 7% 13%


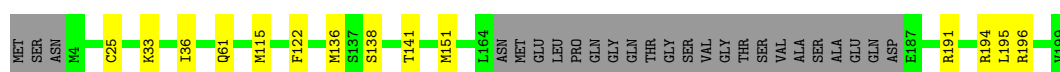
● Molecule 2: Charged multivesicular body protein 1b

Chain MB:  81% 7% 13%


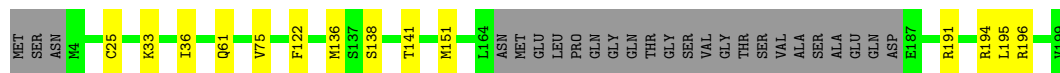
● Molecule 2: Charged multivesicular body protein 1b

Chain OB:  80% 8% 13%


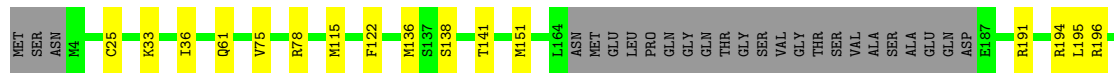
● Molecule 2: Charged multivesicular body protein 1b

Chain QB:  80% 7% 13%

● Molecule 2: Charged multivesicular body protein 1b

Chain SB:  80% 7% 13%

● Molecule 2: Charged multivesicular body protein 1b

Chain UB:  79% 8% 13%

V199

4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=21.16°, rise=3.17 Å, axial sym=C1	Depositor
Number of segments used	101990	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	62	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	29000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	A	0.32	0/1366	0.56	0/1838
1	BA	0.32	0/1366	0.56	0/1838
1	BB	0.32	0/1366	0.56	0/1838
1	C	0.32	0/1366	0.56	0/1838
1	DA	0.31	0/1366	0.56	0/1838
1	DB	0.32	0/1366	0.56	0/1838
1	E	0.31	0/1366	0.56	0/1838
1	FA	0.31	0/1366	0.56	0/1838
1	FB	0.32	0/1366	0.56	0/1838
1	G	0.32	0/1366	0.56	0/1838
1	HA	0.32	0/1366	0.56	0/1838
1	HB	0.32	0/1366	0.56	0/1838
1	I	0.32	0/1366	0.56	0/1838
1	JA	0.32	0/1366	0.56	0/1838
1	JB	0.32	0/1366	0.56	0/1838
1	K	0.32	0/1366	0.56	0/1838
1	LA	0.32	0/1366	0.56	0/1838
1	LB	0.32	0/1366	0.56	0/1838
1	M	0.32	0/1366	0.56	0/1838
1	NA	0.32	0/1366	0.56	0/1838
1	NB	0.32	0/1366	0.56	0/1838
1	O	0.32	0/1366	0.56	0/1838
1	PA	0.32	0/1366	0.56	0/1838
1	PB	0.32	0/1366	0.56	0/1838
1	Q	0.32	0/1366	0.56	0/1838
1	RA	0.32	0/1366	0.56	0/1838
1	RB	0.32	0/1366	0.56	0/1838
1	S	0.31	0/1366	0.56	0/1838
1	TA	0.32	0/1366	0.56	0/1838
1	TB	0.32	0/1366	0.56	0/1838
1	V	0.32	0/1366	0.56	0/1838
1	VA	0.32	0/1366	0.56	0/1838
1	X	0.32	0/1366	0.56	0/1838
1	XA	0.32	0/1366	0.56	0/1838

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	Z	0.32	0/1366	0.56	0/1838
1	ZA	0.32	0/1366	0.56	0/1838
2	AA	0.32	0/1360	0.51	0/1815
2	AB	0.32	0/1360	0.51	0/1815
2	B	0.32	0/1360	0.51	0/1815
2	CA	0.32	0/1360	0.51	0/1815
2	CB	0.32	0/1360	0.51	0/1815
2	D	0.32	0/1360	0.51	0/1815
2	EA	0.32	0/1360	0.51	0/1815
2	EB	0.32	0/1360	0.51	0/1815
2	F	0.32	0/1360	0.51	0/1815
2	GA	0.32	0/1360	0.51	0/1815
2	GB	0.32	0/1360	0.51	0/1815
2	H	0.32	0/1360	0.51	0/1815
2	IA	0.32	0/1360	0.51	0/1815
2	IB	0.32	0/1360	0.51	0/1815
2	J	0.32	0/1360	0.51	0/1815
2	KA	0.32	0/1360	0.51	0/1815
2	KB	0.32	0/1360	0.51	0/1815
2	L	0.32	0/1360	0.51	0/1815
2	MA	0.32	0/1360	0.51	0/1815
2	MB	0.32	0/1360	0.51	0/1815
2	N	0.32	0/1360	0.51	0/1815
2	OA	0.32	0/1360	0.51	0/1815
2	OB	0.32	0/1360	0.51	0/1815
2	P	0.32	0/1360	0.51	0/1815
2	QA	0.32	0/1360	0.51	0/1815
2	QB	0.32	0/1360	0.51	0/1815
2	R	0.32	0/1360	0.51	0/1815
2	SA	0.32	0/1360	0.51	0/1815
2	SB	0.32	0/1360	0.51	0/1815
2	T	0.32	0/1360	0.51	0/1815
2	UA	0.32	0/1360	0.51	0/1815
2	UB	0.32	0/1360	0.51	0/1815
2	W	0.32	0/1360	0.51	0/1815
2	WA	0.32	0/1360	0.51	0/1815
2	Y	0.32	0/1360	0.51	0/1815
2	YA	0.32	0/1360	0.51	0/1815
All	All	0.32	0/98136	0.53	0/131508

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1349	0	1407	8	0
1	BA	1349	0	1407	8	0
1	BB	1349	0	1407	8	0
1	C	1349	0	1407	8	0
1	DA	1349	0	1407	8	0
1	DB	1349	0	1407	10	0
1	E	1349	0	1407	7	0
1	FA	1349	0	1407	7	0
1	FB	1349	0	1407	7	0
1	G	1349	0	1407	7	0
1	HA	1349	0	1407	8	0
1	HB	1349	0	1407	8	0
1	I	1349	0	1407	8	0
1	JA	1349	0	1407	8	0
1	JB	1349	0	1407	6	0
1	K	1349	0	1407	8	0
1	LA	1349	0	1407	7	0
1	LB	1349	0	1407	7	0
1	M	1349	0	1407	8	0
1	NA	1349	0	1407	8	0
1	NB	1349	0	1407	9	0
1	O	1349	0	1407	9	0
1	PA	1349	0	1407	8	0
1	PB	1349	0	1407	7	0
1	Q	1349	0	1407	7	0
1	RA	1349	0	1407	7	0
1	RB	1349	0	1407	9	0
1	S	1349	0	1407	8	0
1	TA	1349	0	1407	9	0
1	TB	1349	0	1407	8	0
1	V	1349	0	1407	12	0
1	VA	1349	0	1407	6	0
1	X	1349	0	1407	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	XA	1349	0	1407	7	0
1	Z	1349	0	1407	9	0
1	ZA	1349	0	1407	9	0
2	AA	1353	0	1385	8	0
2	AB	1353	0	1385	9	0
2	B	1353	0	1385	9	0
2	CA	1353	0	1385	11	0
2	CB	1353	0	1385	8	0
2	D	1353	0	1385	10	0
2	EA	1353	0	1385	8	0
2	EB	1353	0	1385	11	0
2	F	1353	0	1385	9	0
2	GA	1353	0	1385	10	0
2	GB	1353	0	1385	7	0
2	H	1353	0	1385	9	0
2	IA	1353	0	1385	8	0
2	IB	1353	0	1385	9	0
2	J	1353	0	1385	10	0
2	KA	1353	0	1385	8	0
2	KB	1353	0	1385	9	0
2	L	1353	0	1385	9	0
2	MA	1353	0	1385	9	0
2	MB	1353	0	1385	8	0
2	N	1353	0	1385	10	0
2	OA	1353	0	1385	7	0
2	OB	1353	0	1385	10	0
2	P	1353	0	1385	9	0
2	QA	1353	0	1385	9	0
2	QB	1353	0	1385	9	0
2	R	1353	0	1385	8	0
2	SA	1353	0	1385	8	0
2	SB	1353	0	1385	9	0
2	T	1353	0	1385	9	0
2	UA	1353	0	1385	10	0
2	UB	1353	0	1385	11	0
2	W	1353	0	1385	13	0
2	WA	1353	0	1385	8	0
2	Y	1353	0	1385	8	0
2	YA	1353	0	1385	10	0
All	All	97272	0	100512	464	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 2.

All (464) 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:V:160:ILE:HG22	1:V:164:ARG:NH2	1.97	0.80
1:HB:160:ILE:HG22	1:HB:164:ARG:NH2	1.97	0.80
1:RA:160:ILE:HG22	1:RA:164:ARG:NH2	1.97	0.80
1:BB:160:ILE:HG22	1:BB:164:ARG:NH2	1.97	0.80
1:DA:160:ILE:HG22	1:DA:164:ARG:NH2	1.97	0.80
1:DB:160:ILE:HG22	1:DB:164:ARG:NH2	1.97	0.80
1:NA:160:ILE:HG22	1:NA:164:ARG:NH2	1.97	0.80
1:BA:160:ILE:HG22	1:BA:164:ARG:NH2	1.97	0.80
1:FA:160:ILE:HG22	1:FA:164:ARG:NH2	1.97	0.80
1:HA:160:ILE:HG22	1:HA:164:ARG:NH2	1.97	0.80
1:NB:160:ILE:HG22	1:NB:164:ARG:NH2	1.97	0.80
1:TA:160:ILE:HG22	1:TA:164:ARG:NH2	1.97	0.80
1:VA:160:ILE:HG22	1:VA:164:ARG:NH2	1.97	0.80
1:I:160:ILE:HG22	1:I:164:ARG:NH2	1.97	0.80
1:Q:160:ILE:HG22	1:Q:164:ARG:NH2	1.97	0.80
1:Z:160:ILE:HG22	1:Z:164:ARG:NH2	1.97	0.80
1:K:160:ILE:HG22	1:K:164:ARG:NH2	1.97	0.80
1:C:160:ILE:HG22	1:C:164:ARG:NH2	1.97	0.80
1:E:160:ILE:HG22	1:E:164:ARG:NH2	1.97	0.80
1:FB:160:ILE:HG22	1:FB:164:ARG:NH2	1.97	0.80
1:G:160:ILE:HG22	1:G:164:ARG:NH2	1.97	0.80
1:JB:160:ILE:HG22	1:JB:164:ARG:NH2	1.97	0.80
1:LA:160:ILE:HG22	1:LA:164:ARG:NH2	1.97	0.80
1:PB:160:ILE:HG22	1:PB:164:ARG:NH2	1.97	0.80
1:XA:160:ILE:HG22	1:XA:164:ARG:NH2	1.97	0.80
1:LB:160:ILE:HG22	1:LB:164:ARG:NH2	1.97	0.80
1:M:160:ILE:HG22	1:M:164:ARG:NH2	1.97	0.80
1:O:160:ILE:HG22	1:O:164:ARG:NH2	1.97	0.80
1:RB:160:ILE:HG22	1:RB:164:ARG:NH2	1.97	0.80
1:JA:160:ILE:HG22	1:JA:164:ARG:NH2	1.97	0.80
1:PA:160:ILE:HG22	1:PA:164:ARG:NH2	1.97	0.80
1:X:160:ILE:HG22	1:X:164:ARG:NH2	1.97	0.80
1:TB:160:ILE:HG22	1:TB:164:ARG:NH2	1.97	0.79
1:A:160:ILE:HG22	1:A:164:ARG:NH2	1.97	0.79
1:S:160:ILE:HG22	1:S:164:ARG:NH2	1.97	0.79
1:ZA:160:ILE:HG22	1:ZA:164:ARG:NH2	1.97	0.79
1:VA:165:TYR:OH	2:WA:196:ARG:NH1	2.20	0.74
1:BA:165:TYR:OH	2:CA:196:ARG:NH1	2.20	0.74
1:DB:165:TYR:OH	2:EB:196:ARG:NH1	2.20	0.74
1:HB:165:TYR:OH	2:IB:196:ARG:NH1	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:165:TYR:OH	2:AA:196:ARG:NH1	2.20	0.74
1:BB:165:TYR:OH	2:CB:196:ARG:NH1	2.20	0.74
1:FA:165:TYR:OH	2:GA:196:ARG:NH1	2.20	0.74
1:K:165:TYR:OH	2:L:196:ARG:NH1	2.20	0.74
1:NA:165:TYR:OH	2:OA:196:ARG:NH1	2.20	0.74
1:V:165:TYR:OH	2:W:196:ARG:NH1	2.20	0.74
1:NB:165:TYR:OH	2:OB:196:ARG:NH1	2.20	0.74
1:FB:165:TYR:OH	2:GB:196:ARG:NH1	2.20	0.74
1:LB:165:TYR:OH	2:MB:196:ARG:NH1	2.20	0.74
1:RA:165:TYR:OH	2:SA:196:ARG:NH1	2.20	0.74
1:O:165:TYR:OH	2:P:196:ARG:NH1	2.20	0.74
1:A:165:TYR:OH	2:B:196:ARG:NH1	2.20	0.74
1:RB:165:TYR:OH	2:SB:196:ARG:NH1	2.20	0.74
1:JA:165:TYR:OH	2:KA:196:ARG:NH1	2.20	0.74
1:M:165:TYR:OH	2:N:196:ARG:NH1	2.20	0.73
1:TB:165:TYR:OH	2:UB:196:ARG:NH1	2.20	0.73
1:ZA:165:TYR:OH	2:AB:196:ARG:NH1	2.20	0.73
1:S:165:TYR:OH	2:T:196:ARG:NH1	2.20	0.73
1:JB:165:TYR:OH	2:KB:196:ARG:NH1	2.20	0.73
1:E:165:TYR:OH	2:F:196:ARG:NH1	2.20	0.73
1:XA:165:TYR:OH	2:YA:196:ARG:NH1	2.20	0.73
1:C:165:TYR:OH	2:D:196:ARG:NH1	2.20	0.73
1:PB:165:TYR:OH	2:QB:196:ARG:NH1	2.20	0.73
1:TA:165:TYR:OH	2:UA:196:ARG:NH1	2.20	0.73
1:X:165:TYR:OH	2:Y:196:ARG:NH1	2.20	0.73
1:G:165:TYR:OH	2:H:196:ARG:NH1	2.20	0.73
1:PA:165:TYR:OH	2:QA:196:ARG:NH1	2.20	0.73
1:I:165:TYR:OH	2:J:196:ARG:NH1	2.20	0.72
1:LA:165:TYR:OH	2:MA:196:ARG:NH1	2.20	0.72
1:HA:165:TYR:OH	2:IA:196:ARG:NH1	2.20	0.72
1:Q:165:TYR:OH	2:R:196:ARG:NH1	2.20	0.72
1:DA:165:TYR:OH	2:EA:196:ARG:NH1	2.20	0.72
1:I:160:ILE:CG2	1:I:164:ARG:NH2	2.65	0.60
1:LA:160:ILE:CG2	1:LA:164:ARG:NH2	2.64	0.60
1:Q:160:ILE:CG2	1:Q:164:ARG:NH2	2.64	0.60
1:TA:160:ILE:CG2	1:TA:164:ARG:NH2	2.65	0.60
1:G:160:ILE:CG2	1:G:164:ARG:NH2	2.64	0.60
1:X:160:ILE:CG2	1:X:164:ARG:NH2	2.65	0.60
1:DA:160:ILE:CG2	1:DA:164:ARG:NH2	2.64	0.60
1:HA:160:ILE:CG2	1:HA:164:ARG:NH2	2.65	0.60
1:HB:14:ASN:ND2	1:HB:116:GLU:OE1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:NB:14:ASN:ND2	1:NB:116:GLU:OE1	2.35	0.60
1:V:160:ILE:CG2	1:V:164:ARG:NH2	2.65	0.60
1:BA:14:ASN:ND2	1:BA:116:GLU:OE1	2.35	0.60
1:BB:14:ASN:ND2	1:BB:116:GLU:OE1	2.35	0.60
1:K:14:ASN:ND2	1:K:116:GLU:OE1	2.35	0.60
1:LB:14:ASN:ND2	1:LB:116:GLU:OE1	2.35	0.60
1:O:14:ASN:ND2	1:O:116:GLU:OE1	2.35	0.60
1:RA:14:ASN:ND2	1:RA:116:GLU:OE1	2.35	0.60
1:RA:160:ILE:CG2	1:RA:164:ARG:NH2	2.65	0.60
1:V:14:ASN:ND2	1:V:116:GLU:OE1	2.35	0.60
1:VA:14:ASN:ND2	1:VA:116:GLU:OE1	2.35	0.60
1:Z:14:ASN:ND2	1:Z:116:GLU:OE1	2.35	0.60
1:A:14:ASN:ND2	1:A:116:GLU:OE1	2.35	0.59
1:BB:160:ILE:CG2	1:BB:164:ARG:NH2	2.65	0.59
1:DB:14:ASN:ND2	1:DB:116:GLU:OE1	2.35	0.59
1:DB:160:ILE:CG2	1:DB:164:ARG:NH2	2.65	0.59
1:FB:14:ASN:ND2	1:FB:116:GLU:OE1	2.35	0.59
1:HB:160:ILE:CG2	1:HB:164:ARG:NH2	2.65	0.59
1:JA:14:ASN:ND2	1:JA:116:GLU:OE1	2.35	0.59
1:NA:14:ASN:ND2	1:NA:116:GLU:OE1	2.35	0.59
1:NB:160:ILE:CG2	1:NB:164:ARG:NH2	2.65	0.59
1:RB:14:ASN:ND2	1:RB:116:GLU:OE1	2.35	0.59
1:FA:14:ASN:ND2	1:FA:116:GLU:OE1	2.35	0.59
1:Z:160:ILE:CG2	1:Z:164:ARG:NH2	2.65	0.59
1:BA:160:ILE:CG2	1:BA:164:ARG:NH2	2.65	0.59
1:M:14:ASN:ND2	1:M:116:GLU:OE1	2.35	0.59
1:PA:160:ILE:CG2	1:PA:164:ARG:NH2	2.65	0.59
1:VA:160:ILE:CG2	1:VA:164:ARG:NH2	2.65	0.59
1:C:160:ILE:CG2	1:C:164:ARG:NH2	2.65	0.59
1:NA:160:ILE:CG2	1:NA:164:ARG:NH2	2.65	0.59
1:RB:160:ILE:CG2	1:RB:164:ARG:NH2	2.65	0.59
1:TB:14:ASN:ND2	1:TB:116:GLU:OE1	2.35	0.59
1:JB:14:ASN:ND2	1:JB:116:GLU:OE1	2.35	0.59
1:M:160:ILE:CG2	1:M:164:ARG:NH2	2.64	0.59
1:O:160:ILE:CG2	1:O:164:ARG:NH2	2.65	0.59
1:S:14:ASN:ND2	1:S:116:GLU:OE1	2.35	0.59
1:ZA:14:ASN:ND2	1:ZA:116:GLU:OE1	2.35	0.59
1:E:14:ASN:ND2	1:E:116:GLU:OE1	2.35	0.59
1:FA:160:ILE:CG2	1:FA:164:ARG:NH2	2.64	0.59
1:JA:160:ILE:CG2	1:JA:164:ARG:NH2	2.64	0.59
1:FB:160:ILE:CG2	1:FB:164:ARG:NH2	2.65	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LB:160:ILE:CG2	1:LB:164:ARG:NH2	2.64	0.59
1:XA:14:ASN:ND2	1:XA:116:GLU:OE1	2.35	0.59
1:TB:160:ILE:CG2	1:TB:164:ARG:NH2	2.65	0.59
1:A:160:ILE:CG2	1:A:164:ARG:NH2	2.65	0.59
1:C:14:ASN:ND2	1:C:116:GLU:OE1	2.35	0.59
1:K:160:ILE:CG2	1:K:164:ARG:NH2	2.65	0.59
1:PA:14:ASN:ND2	1:PA:116:GLU:OE1	2.35	0.59
1:PB:14:ASN:ND2	1:PB:116:GLU:OE1	2.35	0.59
1:G:14:ASN:ND2	1:G:116:GLU:OE1	2.35	0.59
1:HA:14:ASN:ND2	1:HA:116:GLU:OE1	2.35	0.58
1:X:14:ASN:ND2	1:X:116:GLU:OE1	2.35	0.58
1:DA:14:ASN:ND2	1:DA:116:GLU:OE1	2.35	0.58
1:S:160:ILE:CG2	1:S:164:ARG:NH2	2.65	0.58
1:TA:14:ASN:ND2	1:TA:116:GLU:OE1	2.35	0.58
1:I:14:ASN:ND2	1:I:116:GLU:OE1	2.35	0.58
1:LA:14:ASN:ND2	1:LA:116:GLU:OE1	2.35	0.58
1:Q:14:ASN:ND2	1:Q:116:GLU:OE1	2.35	0.58
1:ZA:160:ILE:CG2	1:ZA:164:ARG:NH2	2.64	0.58
1:E:160:ILE:CG2	1:E:164:ARG:NH2	2.65	0.58
1:JB:160:ILE:CG2	1:JB:164:ARG:NH2	2.65	0.58
1:PB:160:ILE:CG2	1:PB:164:ARG:NH2	2.65	0.58
1:XA:160:ILE:CG2	1:XA:164:ARG:NH2	2.65	0.57
2:P:33:LYS:HA	2:P:36:ILE:HD12	1.87	0.57
2:AB:33:LYS:HA	2:AB:36:ILE:HD12	1.87	0.57
2:D:33:LYS:HA	2:D:36:ILE:HD12	1.87	0.57
2:J:33:LYS:HA	2:J:36:ILE:HD12	1.87	0.57
2:T:33:LYS:HA	2:T:36:ILE:HD12	1.87	0.57
2:MA:33:LYS:HA	2:MA:36:ILE:HD12	1.87	0.57
2:QA:33:LYS:HA	2:QA:36:ILE:HD12	1.87	0.57
2:QB:33:LYS:HA	2:QB:36:ILE:HD12	1.87	0.57
2:SB:33:LYS:HA	2:SB:36:ILE:HD12	1.87	0.57
2:UA:33:LYS:HA	2:UA:36:ILE:HD12	1.87	0.57
2:F:33:LYS:HA	2:F:36:ILE:HD12	1.87	0.57
2:GB:33:LYS:HA	2:GB:36:ILE:HD12	1.87	0.57
2:KB:33:LYS:HA	2:KB:36:ILE:HD12	1.87	0.57
2:J:75:VAL:HG21	2:AB:136:MET:HG2	1.86	0.57
2:MB:33:LYS:HA	2:MB:36:ILE:HD12	1.87	0.57
2:R:33:LYS:HA	2:R:36:ILE:HD12	1.87	0.57
2:YA:33:LYS:HA	2:YA:36:ILE:HD12	1.87	0.57
2:CB:33:LYS:HA	2:CB:36:ILE:HD12	1.87	0.57
2:EB:33:LYS:HA	2:EB:36:ILE:HD12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:WA:33:LYS:HA	2:WA:36:ILE:HD12	1.87	0.56
2:AA:33:LYS:HA	2:AA:36:ILE:HD12	1.87	0.56
2:OB:33:LYS:HA	2:OB:36:ILE:HD12	1.87	0.56
2:L:33:LYS:HA	2:L:36:ILE:HD12	1.87	0.56
2:GA:33:LYS:HA	2:GA:36:ILE:HD12	1.87	0.56
2:L:75:VAL:HG21	2:W:136:MET:HG2	1.86	0.56
2:IB:33:LYS:HA	2:IB:36:ILE:HD12	1.87	0.56
2:N:33:LYS:HA	2:N:36:ILE:HD12	1.87	0.56
2:SA:33:LYS:HA	2:SA:36:ILE:HD12	1.87	0.56
2:H:33:LYS:HA	2:H:36:ILE:HD12	1.87	0.56
2:UB:33:LYS:HA	2:UB:36:ILE:HD12	1.87	0.56
2:W:33:LYS:HA	2:W:36:ILE:HD12	1.87	0.56
2:CA:33:LYS:HA	2:CA:36:ILE:HD12	1.87	0.56
2:IA:33:LYS:HA	2:IA:36:ILE:HD12	1.87	0.56
2:OA:33:LYS:HA	2:OA:36:ILE:HD12	1.87	0.56
2:KA:33:LYS:HA	2:KA:36:ILE:HD12	1.87	0.56
2:Y:33:LYS:HA	2:Y:36:ILE:HD12	1.87	0.56
2:EA:33:LYS:HA	2:EA:36:ILE:HD12	1.87	0.55
2:B:33:LYS:HA	2:B:36:ILE:HD12	1.87	0.55
2:W:75:VAL:HG21	2:UB:136:MET:HG2	1.90	0.53
1:NA:54:ILE:HD12	1:BB:78:LEU:HD23	1.90	0.52
1:E:54:ILE:HD12	1:PA:78:LEU:HD23	1.93	0.51
2:CA:115:MET:HB3	2:EB:135:THR:HG21	1.93	0.50
1:V:21:ARG:HD3	2:EB:127:VAL:HG21	1.94	0.49
1:V:78:LEU:HD23	1:DB:54:ILE:HD12	1.94	0.49
2:B:75:VAL:HG21	2:CA:136:MET:HG2	1.95	0.48
2:L:136:MET:HG2	2:AB:75:VAL:HG21	1.93	0.48
1:V:77:ASP:OD1	1:DB:58:HIS:NE2	2.46	0.48
1:XA:54:ILE:HD12	1:ZA:78:LEU:HD23	1.95	0.48
2:T:136:MET:HG2	2:UA:75:VAL:HG21	1.96	0.48
1:O:78:LEU:HD23	1:Z:54:ILE:HD12	1.96	0.48
1:FA:78:LEU:HD23	1:FB:54:ILE:HD12	1.95	0.47
1:V:73:GLU:HG2	1:DB:51:ARG:NH1	2.29	0.47
2:Y:136:MET:HG2	2:EA:75:VAL:HG21	1.97	0.47
2:EB:75:VAL:HG21	2:SB:136:MET:HG2	1.96	0.47
1:NB:54:ILE:HD12	1:RB:78:LEU:HD23	1.97	0.47
1:V:50:GLU:HG2	1:NB:74:LEU:HD21	1.97	0.47
2:CA:75:VAL:HG21	2:OB:136:MET:HG2	1.96	0.46
2:B:136:MET:HG2	2:H:75:VAL:HG21	1.98	0.46
2:P:136:MET:HG2	2:WA:75:VAL:HG21	1.97	0.46
2:H:136:MET:HG2	2:IA:75:VAL:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:136:MET:HG2	2:IB:75:VAL:HG21	1.97	0.46
2:QA:75:VAL:HG21	2:UA:136:MET:HG2	1.97	0.46
1:X:78:LEU:HD23	1:TA:54:ILE:HD12	1.97	0.45
2:EA:25:CYS:SG	2:EA:61:GLN:NE2	2.90	0.45
2:AB:78:ARG:HE	2:MB:122:PHE:HB3	1.82	0.45
2:SB:25:CYS:SG	2:SB:61:GLN:NE2	2.90	0.45
2:AB:25:CYS:SG	2:AB:61:GLN:NE2	2.90	0.45
2:IA:25:CYS:SG	2:IA:61:GLN:NE2	2.90	0.45
2:P:25:CYS:SG	2:P:61:GLN:NE2	2.90	0.45
2:QB:25:CYS:SG	2:QB:61:GLN:NE2	2.90	0.45
2:T:25:CYS:SG	2:T:61:GLN:NE2	2.90	0.45
2:QA:122:PHE:HB3	2:UB:78:ARG:HE	1.81	0.45
2:J:25:CYS:SG	2:J:61:GLN:NE2	2.90	0.45
2:N:25:CYS:SG	2:N:61:GLN:NE2	2.90	0.45
2:N:75:VAL:HG21	2:IA:136:MET:HG2	1.99	0.45
2:UA:25:CYS:SG	2:UA:61:GLN:NE2	2.90	0.45
2:YA:25:CYS:SG	2:YA:61:GLN:NE2	2.90	0.45
2:CB:25:CYS:SG	2:CB:61:GLN:NE2	2.90	0.45
2:D:136:MET:HG2	2:P:75:VAL:HG21	1.98	0.45
2:D:78:ARG:HE	2:R:122:PHE:HB3	1.82	0.45
2:EB:25:CYS:SG	2:EB:61:GLN:NE2	2.90	0.45
2:MA:115:MET:HB3	2:UA:135:THR:HG21	1.98	0.45
2:UB:25:CYS:SG	2:UB:61:GLN:NE2	2.90	0.45
2:WA:25:CYS:SG	2:WA:61:GLN:NE2	2.90	0.45
2:Y:75:VAL:HG21	2:KA:136:MET:HG2	1.99	0.45
2:F:25:CYS:SG	2:F:61:GLN:NE2	2.90	0.45
2:KB:25:CYS:SG	2:KB:61:GLN:NE2	2.90	0.45
2:MA:25:CYS:SG	2:MA:61:GLN:NE2	2.90	0.45
2:R:25:CYS:SG	2:R:61:GLN:NE2	2.90	0.45
2:W:78:ARG:HE	2:SB:122:PHE:HB3	1.81	0.45
1:BA:113:GLU:HG3	1:BA:114:VAL:HG22	1.99	0.45
2:D:25:CYS:SG	2:D:61:GLN:NE2	2.90	0.45
2:GB:25:CYS:SG	2:GB:61:GLN:NE2	2.90	0.45
2:IB:25:CYS:SG	2:IB:61:GLN:NE2	2.90	0.45
2:MB:25:CYS:SG	2:MB:61:GLN:NE2	2.90	0.45
2:QA:25:CYS:SG	2:QA:61:GLN:NE2	2.90	0.45
1:VA:113:GLU:HG3	1:VA:114:VAL:HG22	1.99	0.45
1:NA:113:GLU:HG3	1:NA:114:VAL:HG22	1.99	0.45
2:SA:25:CYS:SG	2:SA:61:GLN:NE2	2.90	0.45
2:Y:25:CYS:SG	2:Y:61:GLN:NE2	2.90	0.45
2:YA:75:VAL:HG21	2:MB:136:MET:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BB:113:GLU:HG3	1:BB:114:VAL:HG22	1.99	0.44
1:DB:113:GLU:HG3	1:DB:114:VAL:HG22	1.99	0.44
2:H:25:CYS:SG	2:H:61:GLN:NE2	2.90	0.44
1:HB:113:GLU:HG3	1:HB:114:VAL:HG22	1.99	0.44
1:K:113:GLU:HG3	1:K:114:VAL:HG22	1.99	0.44
2:L:25:CYS:SG	2:L:61:GLN:NE2	2.90	0.44
1:LB:113:GLU:HG3	1:LB:114:VAL:HG22	1.99	0.44
2:OB:25:CYS:SG	2:OB:61:GLN:NE2	2.90	0.44
2:QA:136:MET:HG2	2:SB:75:VAL:HG21	1.98	0.44
1:V:113:GLU:HG3	1:V:114:VAL:HG22	1.99	0.44
2:W:25:CYS:SG	2:W:61:GLN:NE2	2.90	0.44
2:AA:25:CYS:SG	2:AA:61:GLN:NE2	2.90	0.44
1:DA:54:ILE:HD12	1:LA:78:LEU:HD23	1.98	0.44
1:FA:113:GLU:HG3	1:FA:114:VAL:HG22	1.99	0.44
1:FB:113:GLU:HG3	1:FB:114:VAL:HG22	1.99	0.44
2:GA:25:CYS:SG	2:GA:61:GLN:NE2	2.90	0.44
1:RA:113:GLU:HG3	1:RA:114:VAL:HG22	1.99	0.44
1:Z:113:GLU:HG3	1:Z:114:VAL:HG22	1.99	0.44
1:NB:113:GLU:HG3	1:NB:114:VAL:HG22	1.99	0.44
1:Q:113:GLU:HG3	1:Q:114:VAL:HG22	1.99	0.44
1:A:113:GLU:HG3	1:A:114:VAL:HG22	1.99	0.44
2:B:25:CYS:SG	2:B:61:GLN:NE2	2.90	0.44
1:C:54:ILE:HD12	1:HA:78:LEU:HD23	1.99	0.44
2:CA:25:CYS:SG	2:CA:61:GLN:NE2	2.90	0.44
1:DA:113:GLU:HG3	1:DA:114:VAL:HG22	1.99	0.44
1:JA:113:GLU:HG3	1:JA:114:VAL:HG22	1.99	0.44
1:LA:113:GLU:HG3	1:LA:114:VAL:HG22	1.99	0.44
1:RB:113:GLU:HG3	1:RB:114:VAL:HG22	1.99	0.44
1:S:113:GLU:HG3	1:S:114:VAL:HG22	1.99	0.44
1:HA:113:GLU:HG3	1:HA:114:VAL:HG22	1.99	0.44
1:Z:78:LEU:HD23	1:HB:54:ILE:HD12	2.00	0.44
1:JB:113:GLU:HG3	1:JB:114:VAL:HG22	1.99	0.44
2:KA:25:CYS:SG	2:KA:61:GLN:NE2	2.90	0.44
2:MA:75:VAL:HG21	2:QB:136:MET:HG2	1.99	0.44
1:O:113:GLU:HG3	1:O:114:VAL:HG22	1.99	0.44
2:OA:25:CYS:SG	2:OA:61:GLN:NE2	2.90	0.44
1:ZA:113:GLU:HG3	1:ZA:114:VAL:HG22	1.99	0.44
1:E:113:GLU:HG3	1:E:114:VAL:HG22	1.99	0.44
1:X:113:GLU:HG3	1:X:114:VAL:HG22	1.99	0.44
1:G:113:GLU:HG3	1:G:114:VAL:HG22	1.99	0.44
2:D:135:THR:HG21	2:KB:115:MET:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:135:THR:HG21	2:R:115:MET:HB3	2.00	0.43
1:PB:113:GLU:HG3	1:PB:114:VAL:HG22	1.99	0.43
1:RB:54:ILE:HD12	1:TB:78:LEU:HD23	2.00	0.43
1:TB:113:GLU:HG3	1:TB:114:VAL:HG22	1.99	0.43
1:XA:113:GLU:HG3	1:XA:114:VAL:HG22	1.99	0.43
2:GA:115:MET:HB3	2:OA:135:THR:HG21	1.99	0.43
1:M:113:GLU:HG3	1:M:114:VAL:HG22	1.99	0.43
1:C:113:GLU:HG3	1:C:114:VAL:HG22	1.99	0.43
2:F:75:VAL:HG21	2:MA:136:MET:HG2	2.00	0.43
2:IA:138:SER:HA	2:IA:141:THR:HG23	2.01	0.43
2:QB:138:SER:HA	2:QB:141:THR:HG23	2.01	0.43
2:EA:138:SER:HA	2:EA:141:THR:HG23	2.01	0.43
1:I:113:GLU:HG3	1:I:114:VAL:HG22	1.99	0.43
2:J:191:ARG:HG2	2:J:194:ARG:HH21	1.84	0.43
1:PA:113:GLU:HG3	1:PA:114:VAL:HG22	1.99	0.43
1:TA:113:GLU:HG3	1:TA:114:VAL:HG22	1.99	0.43
2:IA:191:ARG:HG2	2:IA:194:ARG:HH21	1.84	0.43
2:QA:138:SER:HA	2:QA:141:THR:HG23	2.01	0.43
2:QA:191:ARG:HG2	2:QA:194:ARG:HH21	1.84	0.43
2:UA:191:ARG:HG2	2:UA:194:ARG:HH21	1.84	0.43
2:YA:138:SER:HA	2:YA:141:THR:HG23	2.01	0.43
2:D:191:ARG:HG2	2:D:194:ARG:HH21	1.84	0.43
2:EA:136:MET:HG2	2:UB:75:VAL:HG21	2.00	0.43
2:EA:191:ARG:HG2	2:EA:194:ARG:HH21	1.84	0.43
1:E:164:ARG:HD3	2:F:195:LEU:HD11	2.01	0.43
2:J:78:ARG:HE	2:YA:122:PHE:HB3	1.84	0.43
2:KB:191:ARG:HG2	2:KB:194:ARG:HH21	1.84	0.43
1:RB:164:ARG:HD3	2:SB:195:LEU:HD11	2.01	0.43
2:D:138:SER:HA	2:D:141:THR:HG23	2.01	0.42
2:F:191:ARG:HG2	2:F:194:ARG:HH21	1.84	0.42
1:JB:164:ARG:HD3	2:KB:195:LEU:HD11	2.01	0.42
1:O:164:ARG:HD3	2:P:195:LEU:HD11	2.01	0.42
2:AA:75:VAL:HG21	2:KB:136:MET:HG2	2.00	0.42
1:BB:164:ARG:HD3	2:CB:195:LEU:HD11	2.01	0.42
2:D:75:VAL:HG21	2:J:136:MET:HG2	2.00	0.42
1:DB:164:ARG:HD3	2:EB:195:LEU:HD11	2.01	0.42
2:H:138:SER:HA	2:H:141:THR:HG23	2.01	0.42
1:S:54:ILE:HD12	1:JA:78:LEU:HD23	2.00	0.42
2:MA:191:ARG:HG2	2:MA:194:ARG:HH21	1.84	0.42
2:R:138:SER:HA	2:R:141:THR:HG23	2.01	0.42
1:VA:164:ARG:HD3	2:WA:195:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:138:SER:HA	2:Y:141:THR:HG23	2.01	0.42
2:B:122:PHE:HB3	2:YA:78:ARG:HE	1.83	0.42
2:MA:138:SER:HA	2:MA:141:THR:HG23	2.01	0.42
1:NB:164:ARG:HD3	2:OB:195:LEU:HD11	2.01	0.42
2:QB:191:ARG:HG2	2:QB:194:ARG:HH21	1.84	0.42
2:R:191:ARG:HG2	2:R:194:ARG:HH21	1.84	0.42
2:W:122:PHE:HB3	2:CA:78:ARG:HE	1.84	0.42
2:YA:191:ARG:HG2	2:YA:194:ARG:HH21	1.84	0.42
2:W:115:MET:HB3	2:OB:135:THR:HG21	2.00	0.42
2:SB:138:SER:HA	2:SB:141:THR:HG23	2.01	0.42
1:Z:164:ARG:HD3	2:AA:195:LEU:HD11	2.01	0.42
2:GB:138:SER:HA	2:GB:141:THR:HG23	2.01	0.42
2:N:138:SER:HA	2:N:141:THR:HG23	2.01	0.42
2:P:138:SER:HA	2:P:141:THR:HG23	2.01	0.42
2:T:138:SER:HA	2:T:141:THR:HG23	2.01	0.42
2:AB:138:SER:HA	2:AB:141:THR:HG23	2.01	0.42
1:C:164:ARG:HD3	2:D:195:LEU:HD11	2.01	0.42
2:MB:138:SER:HA	2:MB:141:THR:HG23	2.01	0.42
2:UB:138:SER:HA	2:UB:141:THR:HG23	2.01	0.42
2:CA:191:ARG:HG2	2:CA:194:ARG:HH21	1.84	0.42
2:KA:115:MET:HB3	2:GB:135:THR:HG21	2.01	0.42
2:H:191:ARG:HG2	2:H:194:ARG:HH21	1.84	0.42
1:HB:164:ARG:HD3	2:IB:195:LEU:HD11	2.01	0.42
2:L:191:ARG:HG2	2:L:194:ARG:HH21	1.84	0.42
1:PA:164:ARG:HD3	2:QA:195:LEU:HD11	2.01	0.42
2:SA:135:THR:HG21	2:CB:115:MET:HB3	2.01	0.42
2:GA:75:VAL:HG21	2:SA:136:MET:HG2	2.00	0.42
2:WA:115:MET:HB3	2:IB:135:THR:HG21	2.01	0.42
2:AB:191:ARG:HG2	2:AB:194:ARG:HH21	1.84	0.42
2:CB:191:ARG:HG2	2:CB:194:ARG:HH21	1.84	0.42
2:EB:191:ARG:HG2	2:EB:194:ARG:HH21	1.84	0.42
2:GA:191:ARG:HG2	2:GA:194:ARG:HH21	1.84	0.42
1:M:78:LEU:HD23	1:O:54:ILE:HD12	2.02	0.42
1:LA:164:ARG:HD3	2:MA:195:LEU:HD11	2.01	0.42
2:N:191:ARG:HG2	2:N:194:ARG:HH21	1.84	0.42
1:Q:164:ARG:HD3	2:R:195:LEU:HD11	2.01	0.42
2:T:135:THR:HG21	2:QB:115:MET:HB3	2.01	0.42
2:T:191:ARG:HG2	2:T:194:ARG:HH21	1.84	0.42
2:WA:191:ARG:HG2	2:WA:194:ARG:HH21	1.84	0.42
1:JA:160:ILE:CG2	1:JA:164:ARG:HH22	2.33	0.42
2:L:115:MET:HB3	2:CA:135:THR:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:OA:191:ARG:HG2	2:OA:194:ARG:HH21	1.84	0.42
1:V:164:ARG:HD3	2:W:195:LEU:HD11	2.01	0.42
1:A:160:ILE:CG2	1:A:164:ARG:HH22	2.33	0.42
2:CB:138:SER:HA	2:CB:141:THR:HG23	2.01	0.42
1:TB:160:ILE:CG2	1:TB:164:ARG:HH22	2.33	0.42
2:UB:191:ARG:HG2	2:UB:194:ARG:HH21	1.84	0.42
1:X:50:GLU:HG2	1:PB:74:LEU:HD21	2.01	0.42
2:AA:191:ARG:HG2	2:AA:194:ARG:HH21	1.84	0.41
2:EB:138:SER:HA	2:EB:141:THR:HG23	2.01	0.41
2:F:136:MET:HG2	2:OB:75:VAL:HG21	2.01	0.41
2:L:138:SER:HA	2:L:141:THR:HG23	2.01	0.41
1:M:160:ILE:CG2	1:M:164:ARG:HH22	2.33	0.41
1:O:160:ILE:CG2	1:O:164:ARG:HH22	2.33	0.41
1:RA:164:ARG:HD3	2:SA:195:LEU:HD11	2.01	0.41
1:RB:160:ILE:CG2	1:RB:164:ARG:HH22	2.33	0.41
2:SB:191:ARG:HG2	2:SB:194:ARG:HH21	1.84	0.41
2:WA:138:SER:HA	2:WA:141:THR:HG23	2.01	0.41
2:Y:191:ARG:HG2	2:Y:194:ARG:HH21	1.84	0.41
2:B:191:ARG:HG2	2:B:194:ARG:HH21	1.84	0.41
1:K:54:ILE:HD12	1:BA:78:LEU:HD23	2.03	0.41
1:G:160:ILE:CG2	1:G:164:ARG:HH22	2.33	0.41
2:KA:191:ARG:HG2	2:KA:194:ARG:HH21	1.84	0.41
1:LB:164:ARG:HD3	2:MB:195:LEU:HD11	2.01	0.41
2:OB:191:ARG:HG2	2:OB:194:ARG:HH21	1.84	0.41
2:P:191:ARG:HG2	2:P:194:ARG:HH21	1.84	0.41
2:UA:138:SER:HA	2:UA:141:THR:HG23	2.01	0.41
2:H:115:MET:HB3	2:YA:135:THR:HG21	2.02	0.41
1:BA:164:ARG:HD3	2:CA:195:LEU:HD11	2.01	0.41
1:FB:164:ARG:HD3	2:GB:195:LEU:HD11	2.01	0.41
2:GA:138:SER:HA	2:GA:141:THR:HG23	2.01	0.41
2:GA:78:ARG:HE	2:CB:122:PHE:HB3	1.85	0.41
2:J:138:SER:HA	2:J:141:THR:HG23	2.01	0.41
1:K:164:ARG:HD3	2:L:195:LEU:HD11	2.01	0.41
1:NA:164:ARG:HD3	2:OA:195:LEU:HD11	2.01	0.41
1:PB:164:ARG:HD3	2:QB:195:LEU:HD11	2.01	0.41
1:X:160:ILE:CG2	1:X:164:ARG:HH22	2.33	0.41
1:DA:164:ARG:HD3	2:EA:195:LEU:HD11	2.01	0.41
2:F:138:SER:HA	2:F:141:THR:HG23	2.01	0.41
1:S:164:ARG:HD3	2:T:195:LEU:HD11	2.01	0.41
1:XA:164:ARG:HD3	2:YA:195:LEU:HD11	2.01	0.41
1:ZA:164:ARG:HD3	2:AB:195:LEU:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BB:160:ILE:CG2	1:BB:164:ARG:HH22	2.33	0.41
1:DA:160:ILE:CG2	1:DA:164:ARG:HH22	2.33	0.41
1:DB:160:ILE:CG2	1:DB:164:ARG:HH22	2.33	0.41
1:FA:164:ARG:HD3	2:GA:195:LEU:HD11	2.01	0.41
1:G:164:ARG:HD3	2:H:195:LEU:HD11	2.01	0.41
1:HA:164:ARG:HD3	2:IA:195:LEU:HD11	2.01	0.41
2:IB:138:SER:HA	2:IB:141:THR:HG23	2.01	0.41
2:P:122:PHE:HB3	2:IB:78:ARG:HE	1.85	0.41
1:M:164:ARG:HD3	2:N:195:LEU:HD11	2.01	0.41
2:SA:138:SER:HA	2:SA:141:THR:HG23	2.01	0.41
1:TB:164:ARG:HD3	2:UB:195:LEU:HD11	2.01	0.41
2:UA:78:ARG:HE	2:QB:122:PHE:HB3	1.85	0.41
1:A:164:ARG:HD3	2:B:195:LEU:HD11	2.01	0.41
1:A:74:LEU:HD21	1:ZA:50:GLU:HG2	2.02	0.41
2:B:138:SER:HA	2:B:141:THR:HG23	2.01	0.41
1:HA:160:ILE:CG2	1:HA:164:ARG:HH22	2.33	0.41
1:K:78:LEU:HD23	1:LB:54:ILE:HD12	2.02	0.41
2:KA:138:SER:HA	2:KA:141:THR:HG23	2.01	0.41
1:JA:164:ARG:HD3	2:KA:195:LEU:HD11	2.01	0.41
2:F:135:THR:HG21	2:UB:115:MET:HB3	2.02	0.41
1:ZA:160:ILE:CG2	1:ZA:164:ARG:HH22	2.33	0.41
1:C:160:ILE:CG2	1:C:164:ARG:HH22	2.33	0.41
2:W:121:GLN:HE22	2:EB:100:ASP:HB2	1.86	0.41
1:I:164:ARG:HD3	2:J:195:LEU:HD11	2.01	0.41
2:KB:138:SER:HA	2:KB:141:THR:HG23	2.01	0.41
1:S:160:ILE:CG2	1:S:164:ARG:HH22	2.33	0.41
2:SA:191:ARG:HG2	2:SA:194:ARG:HH21	1.84	0.41
2:W:138:SER:HA	2:W:141:THR:HG23	2.01	0.41
1:X:164:ARG:HD3	2:Y:195:LEU:HD11	2.01	0.41
1:I:160:ILE:CG2	1:I:164:ARG:HH22	2.33	0.41
2:W:191:ARG:HG2	2:W:194:ARG:HH21	1.84	0.41
2:IB:191:ARG:HG2	2:IB:194:ARG:HH21	1.84	0.41
1:NA:160:ILE:CG2	1:NA:164:ARG:HH22	2.33	0.41
2:OB:138:SER:HA	2:OB:141:THR:HG23	2.01	0.41
1:PA:160:ILE:CG2	1:PA:164:ARG:HH22	2.33	0.41
1:I:78:LEU:HD23	1:Q:54:ILE:HD12	2.02	0.41
1:TA:160:ILE:CG2	1:TA:164:ARG:HH22	2.33	0.41
1:TA:164:ARG:HD3	2:UA:195:LEU:HD11	2.01	0.41
1:X:73:GLU:HG2	1:TA:51:ARG:NH1	2.36	0.41
2:AA:138:SER:HA	2:AA:141:THR:HG23	2.01	0.41
1:BA:160:ILE:CG2	1:BA:164:ARG:HH22	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CA:138:SER:HA	2:CA:141:THR:HG23	2.01	0.41
2:OA:138:SER:HA	2:OA:141:THR:HG23	2.01	0.41
2:OB:78:ARG:HE	2:UB:122:PHE:HB3	1.87	0.40
1:V:160:ILE:CG2	1:V:164:ARG:HH22	2.33	0.40
2:W:121:GLN:HB3	2:EB:99:MET:HE2	2.02	0.40
2:N:115:MET:HB3	2:KB:135:THR:HG21	2.03	0.40
1:RA:160:ILE:CG2	1:RA:164:ARG:HH22	2.33	0.40
1:Z:160:ILE:CG2	1:Z:164:ARG:HH22	2.33	0.40
2:GB:191:ARG:HG2	2:GB:194:ARG:HH21	1.84	0.40
1:HB:160:ILE:CG2	1:HB:164:ARG:HH22	2.33	0.40
2:T:75:VAL:HG21	2:GA:136:MET:HG2	2.02	0.40
2:MB:191:ARG:HG2	2:MB:194:ARG:HH21	1.84	0.40
1:NB:160:ILE:CG2	1:NB:164:ARG:HH22	2.33	0.40
2:N:122:PHE:HB3	2:AA:78:ARG:HE	1.87	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	A	163/366 (44%)	161 (99%)	2 (1%)	0	100	100
1	BA	163/366 (44%)	161 (99%)	2 (1%)	0	100	100
1	BB	163/366 (44%)	161 (99%)	2 (1%)	0	100	100
1	C	163/366 (44%)	161 (99%)	2 (1%)	0	100	100
1	DA	163/366 (44%)	161 (99%)	2 (1%)	0	100	100
1	DB	163/366 (44%)	161 (99%)	2 (1%)	0	100	100
1	E	163/366 (44%)	161 (99%)	2 (1%)	0	100	100
1	FA	163/366 (44%)	161 (99%)	2 (1%)	0	100	100
1	FB	163/366 (44%)	161 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	163/366 (44%)	161 (99%)	2 (1%)	0	100	100
1	HA	163/366 (44%)	161 (99%)	2 (1%)	0	100	100
1	HB	163/366 (44%)	161 (99%)	2 (1%)	0	100	100
1	I	163/366 (44%)	161 (99%)	2 (1%)	0	100	100
1	JA	163/366 (44%)	161 (99%)	2 (1%)	0	100	100
1	JB	163/366 (44%)	161 (99%)	2 (1%)	0	100	100
1	K	163/366 (44%)	161 (99%)	2 (1%)	0	100	100
1	LA	163/366 (44%)	161 (99%)	2 (1%)	0	100	100
1	LB	163/366 (44%)	161 (99%)	2 (1%)	0	100	100
1	M	163/366 (44%)	161 (99%)	2 (1%)	0	100	100
1	NA	163/366 (44%)	161 (99%)	2 (1%)	0	100	100
1	NB	163/366 (44%)	161 (99%)	2 (1%)	0	100	100
1	O	163/366 (44%)	161 (99%)	2 (1%)	0	100	100
1	PA	163/366 (44%)	161 (99%)	2 (1%)	0	100	100
1	PB	163/366 (44%)	161 (99%)	2 (1%)	0	100	100
1	Q	163/366 (44%)	161 (99%)	2 (1%)	0	100	100
1	RA	163/366 (44%)	161 (99%)	2 (1%)	0	100	100
1	RB	163/366 (44%)	161 (99%)	2 (1%)	0	100	100
1	S	163/366 (44%)	161 (99%)	2 (1%)	0	100	100
1	TA	163/366 (44%)	161 (99%)	2 (1%)	0	100	100
1	TB	163/366 (44%)	161 (99%)	2 (1%)	0	100	100
1	V	163/366 (44%)	161 (99%)	2 (1%)	0	100	100
1	VA	163/366 (44%)	161 (99%)	2 (1%)	0	100	100
1	X	163/366 (44%)	161 (99%)	2 (1%)	0	100	100
1	XA	163/366 (44%)	161 (99%)	2 (1%)	0	100	100
1	Z	163/366 (44%)	161 (99%)	2 (1%)	0	100	100
1	ZA	163/366 (44%)	161 (99%)	2 (1%)	0	100	100
2	AA	170/199 (85%)	169 (99%)	1 (1%)	0	100	100
2	AB	170/199 (85%)	169 (99%)	1 (1%)	0	100	100
2	B	170/199 (85%)	169 (99%)	1 (1%)	0	100	100
2	CA	170/199 (85%)	169 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	CB	170/199 (85%)	169 (99%)	1 (1%)	0	100	100
2	D	170/199 (85%)	169 (99%)	1 (1%)	0	100	100
2	EA	170/199 (85%)	169 (99%)	1 (1%)	0	100	100
2	EB	170/199 (85%)	169 (99%)	1 (1%)	0	100	100
2	F	170/199 (85%)	169 (99%)	1 (1%)	0	100	100
2	GA	170/199 (85%)	169 (99%)	1 (1%)	0	100	100
2	GB	170/199 (85%)	169 (99%)	1 (1%)	0	100	100
2	H	170/199 (85%)	169 (99%)	1 (1%)	0	100	100
2	IA	170/199 (85%)	169 (99%)	1 (1%)	0	100	100
2	IB	170/199 (85%)	169 (99%)	1 (1%)	0	100	100
2	J	170/199 (85%)	169 (99%)	1 (1%)	0	100	100
2	KA	170/199 (85%)	169 (99%)	1 (1%)	0	100	100
2	KB	170/199 (85%)	169 (99%)	1 (1%)	0	100	100
2	L	170/199 (85%)	169 (99%)	1 (1%)	0	100	100
2	MA	170/199 (85%)	169 (99%)	1 (1%)	0	100	100
2	MB	170/199 (85%)	169 (99%)	1 (1%)	0	100	100
2	N	170/199 (85%)	169 (99%)	1 (1%)	0	100	100
2	OA	170/199 (85%)	169 (99%)	1 (1%)	0	100	100
2	OB	170/199 (85%)	169 (99%)	1 (1%)	0	100	100
2	P	170/199 (85%)	169 (99%)	1 (1%)	0	100	100
2	QA	170/199 (85%)	169 (99%)	1 (1%)	0	100	100
2	QB	170/199 (85%)	169 (99%)	1 (1%)	0	100	100
2	R	170/199 (85%)	169 (99%)	1 (1%)	0	100	100
2	SA	170/199 (85%)	169 (99%)	1 (1%)	0	100	100
2	SB	170/199 (85%)	169 (99%)	1 (1%)	0	100	100
2	T	170/199 (85%)	169 (99%)	1 (1%)	0	100	100
2	UA	170/199 (85%)	169 (99%)	1 (1%)	0	100	100
2	UB	170/199 (85%)	169 (99%)	1 (1%)	0	100	100
2	W	170/199 (85%)	169 (99%)	1 (1%)	0	100	100
2	WA	170/199 (85%)	169 (99%)	1 (1%)	0	100	100
2	Y	170/199 (85%)	169 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	YA	170/199 (85%)	169 (99%)	1 (1%)	0	100	100
All	All	11988/20340 (59%)	11880 (99%)	108 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	144/309 (47%)	142 (99%)	2 (1%)	69	90
1	BA	144/309 (47%)	142 (99%)	2 (1%)	69	90
1	BB	144/309 (47%)	142 (99%)	2 (1%)	69	90
1	C	144/309 (47%)	142 (99%)	2 (1%)	69	90
1	DA	144/309 (47%)	142 (99%)	2 (1%)	69	90
1	DB	144/309 (47%)	142 (99%)	2 (1%)	69	90
1	E	144/309 (47%)	142 (99%)	2 (1%)	69	90
1	FA	144/309 (47%)	142 (99%)	2 (1%)	69	90
1	FB	144/309 (47%)	142 (99%)	2 (1%)	69	90
1	G	144/309 (47%)	142 (99%)	2 (1%)	69	90
1	HA	144/309 (47%)	142 (99%)	2 (1%)	69	90
1	HB	144/309 (47%)	142 (99%)	2 (1%)	69	90
1	I	144/309 (47%)	142 (99%)	2 (1%)	69	90
1	JA	144/309 (47%)	142 (99%)	2 (1%)	69	90
1	JB	144/309 (47%)	142 (99%)	2 (1%)	69	90
1	K	144/309 (47%)	142 (99%)	2 (1%)	69	90
1	LA	144/309 (47%)	142 (99%)	2 (1%)	69	90
1	LB	144/309 (47%)	142 (99%)	2 (1%)	69	90
1	M	144/309 (47%)	142 (99%)	2 (1%)	69	90
1	NA	144/309 (47%)	142 (99%)	2 (1%)	69	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	NB	144/309 (47%)	142 (99%)	2 (1%)	69	90
1	O	144/309 (47%)	142 (99%)	2 (1%)	69	90
1	PA	144/309 (47%)	142 (99%)	2 (1%)	69	90
1	PB	144/309 (47%)	142 (99%)	2 (1%)	69	90
1	Q	144/309 (47%)	142 (99%)	2 (1%)	69	90
1	RA	144/309 (47%)	142 (99%)	2 (1%)	69	90
1	RB	144/309 (47%)	142 (99%)	2 (1%)	69	90
1	S	144/309 (47%)	142 (99%)	2 (1%)	69	90
1	TA	144/309 (47%)	142 (99%)	2 (1%)	69	90
1	TB	144/309 (47%)	142 (99%)	2 (1%)	69	90
1	V	144/309 (47%)	142 (99%)	2 (1%)	69	90
1	VA	144/309 (47%)	142 (99%)	2 (1%)	69	90
1	X	144/309 (47%)	142 (99%)	2 (1%)	69	90
1	XA	144/309 (47%)	142 (99%)	2 (1%)	69	90
1	Z	144/309 (47%)	142 (99%)	2 (1%)	69	90
1	ZA	144/309 (47%)	142 (99%)	2 (1%)	69	90
2	AA	146/169 (86%)	145 (99%)	1 (1%)	85	96
2	AB	146/169 (86%)	145 (99%)	1 (1%)	85	96
2	B	146/169 (86%)	145 (99%)	1 (1%)	85	96
2	CA	146/169 (86%)	145 (99%)	1 (1%)	85	96
2	CB	146/169 (86%)	145 (99%)	1 (1%)	85	96
2	D	146/169 (86%)	145 (99%)	1 (1%)	85	96
2	EA	146/169 (86%)	145 (99%)	1 (1%)	85	96
2	EB	146/169 (86%)	145 (99%)	1 (1%)	85	96
2	F	146/169 (86%)	145 (99%)	1 (1%)	85	96
2	GA	146/169 (86%)	145 (99%)	1 (1%)	85	96
2	GB	146/169 (86%)	145 (99%)	1 (1%)	85	96
2	H	146/169 (86%)	145 (99%)	1 (1%)	85	96
2	IA	146/169 (86%)	145 (99%)	1 (1%)	85	96
2	IB	146/169 (86%)	145 (99%)	1 (1%)	85	96
2	J	146/169 (86%)	145 (99%)	1 (1%)	85	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	KA	146/169 (86%)	145 (99%)	1 (1%)	85	96
2	KB	146/169 (86%)	145 (99%)	1 (1%)	85	96
2	L	146/169 (86%)	145 (99%)	1 (1%)	85	96
2	MA	146/169 (86%)	145 (99%)	1 (1%)	85	96
2	MB	146/169 (86%)	145 (99%)	1 (1%)	85	96
2	N	146/169 (86%)	145 (99%)	1 (1%)	85	96
2	OA	146/169 (86%)	145 (99%)	1 (1%)	85	96
2	OB	146/169 (86%)	145 (99%)	1 (1%)	85	96
2	P	146/169 (86%)	145 (99%)	1 (1%)	85	96
2	QA	146/169 (86%)	145 (99%)	1 (1%)	85	96
2	QB	146/169 (86%)	145 (99%)	1 (1%)	85	96
2	R	146/169 (86%)	145 (99%)	1 (1%)	85	96
2	SA	146/169 (86%)	145 (99%)	1 (1%)	85	96
2	SB	146/169 (86%)	145 (99%)	1 (1%)	85	96
2	T	146/169 (86%)	145 (99%)	1 (1%)	85	96
2	UA	146/169 (86%)	145 (99%)	1 (1%)	85	96
2	UB	146/169 (86%)	145 (99%)	1 (1%)	85	96
2	W	146/169 (86%)	145 (99%)	1 (1%)	85	96
2	WA	146/169 (86%)	145 (99%)	1 (1%)	85	96
2	Y	146/169 (86%)	145 (99%)	1 (1%)	85	96
2	YA	146/169 (86%)	145 (99%)	1 (1%)	85	96
All	All	10440/17208 (61%)	10332 (99%)	108 (1%)	80	94

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	165	TYR
1	S	172	ASN
2	T	151	MET
1	A	165	TYR
1	A	172	ASN
2	B	151	MET
1	C	165	TYR
1	C	172	ASN
2	D	151	MET

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Mol	Chain	Res	Type
1	E	165	TYR
1	E	172	ASN
2	F	151	MET
1	G	165	TYR
1	G	172	ASN
2	H	151	MET
1	I	165	TYR
1	I	172	ASN
2	J	151	MET
1	K	165	TYR
1	K	172	ASN
2	L	151	MET
1	M	165	TYR
1	M	172	ASN
2	N	151	MET
1	O	165	TYR
1	O	172	ASN
2	P	151	MET
1	Q	165	TYR
1	Q	172	ASN
2	R	151	MET
1	V	165	TYR
1	V	172	ASN
2	W	151	MET
1	X	165	TYR
1	X	172	ASN
2	Y	151	MET
1	Z	165	TYR
1	Z	172	ASN
2	AA	151	MET
1	BA	165	TYR
1	BA	172	ASN
2	CA	151	MET
1	DA	165	TYR
1	DA	172	ASN
2	EA	151	MET
1	FA	165	TYR
1	FA	172	ASN
2	GA	151	MET
1	HA	165	TYR
1	HA	172	ASN
2	IA	151	MET

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Mol	Chain	Res	Type
1	JA	165	TYR
1	JA	172	ASN
2	KA	151	MET
1	LA	165	TYR
1	LA	172	ASN
2	MA	151	MET
1	NA	165	TYR
1	NA	172	ASN
2	OA	151	MET
1	PA	165	TYR
1	PA	172	ASN
2	QA	151	MET
1	RA	165	TYR
1	RA	172	ASN
2	SA	151	MET
1	TA	165	TYR
1	TA	172	ASN
2	UA	151	MET
1	VA	165	TYR
1	VA	172	ASN
2	WA	151	MET
1	XA	165	TYR
1	XA	172	ASN
2	YA	151	MET
1	ZA	165	TYR
1	ZA	172	ASN
2	AB	151	MET
1	BB	165	TYR
1	BB	172	ASN
2	CB	151	MET
1	DB	165	TYR
1	DB	172	ASN
2	EB	151	MET
1	FB	165	TYR
1	FB	172	ASN
2	GB	151	MET
1	HB	165	TYR
1	HB	172	ASN
2	IB	151	MET
1	JB	165	TYR
1	JB	172	ASN
2	KB	151	MET

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Mol	Chain	Res	Type
1	LB	165	TYR
1	LB	172	ASN
2	MB	151	MET
1	NB	165	TYR
1	NB	172	ASN
2	OB	151	MET
1	PB	165	TYR
1	PB	172	ASN
2	QB	151	MET
1	RB	165	TYR
1	RB	172	ASN
2	SB	151	MET
1	TB	165	TYR
1	TB	172	ASN
2	UB	151	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	S	14	ASN
2	T	61	GLN
1	A	14	ASN
2	B	61	GLN
1	C	14	ASN
2	D	61	GLN
1	E	14	ASN
2	F	61	GLN
1	G	14	ASN
2	H	61	GLN
1	I	14	ASN
2	J	61	GLN
1	K	14	ASN
2	L	61	GLN
1	M	14	ASN
2	N	61	GLN
1	O	14	ASN
2	P	61	GLN
1	Q	14	ASN
2	R	61	GLN
1	V	14	ASN
2	W	61	GLN
1	X	14	ASN

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Mol	Chain	Res	Type
2	Y	61	GLN
1	Z	14	ASN
2	AA	61	GLN
2	CA	61	GLN
1	DA	14	ASN
2	EA	61	GLN
1	FA	14	ASN
2	GA	61	GLN
1	HA	14	ASN
2	IA	61	GLN
1	JA	14	ASN
2	KA	61	GLN
1	LA	14	ASN
2	OA	61	GLN
1	PA	14	ASN
2	QA	61	GLN
2	SA	61	GLN
1	TA	14	ASN
2	UA	61	GLN
2	WA	61	GLN
1	XA	14	ASN
2	YA	61	GLN
1	ZA	14	ASN
2	AB	61	GLN
2	CB	61	GLN
2	EB	61	GLN
1	FB	14	ASN
2	GB	61	GLN
1	HB	14	ASN
2	IB	61	GLN
1	JB	14	ASN
2	KB	61	GLN
1	LB	14	ASN
2	MB	61	GLN
1	NB	14	ASN
2	OB	61	GLN
1	PB	14	ASN
2	QB	61	GLN
1	RB	14	ASN
2	SB	61	GLN
1	TB	14	ASN
2	UB	61	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.