



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 20, 2026 – 06:29 PM EDT

PDB ID : 9NIP / pdb_00009nip
Title : Mycobacterium tuberculosis Small RNA-Binding protein (SRB)
Authors : Mai, J.; Ly, A.; Ng, D.; Moraes, T.F.; Liu, J.
Deposited on : 2025-02-26
Resolution : 2.62 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

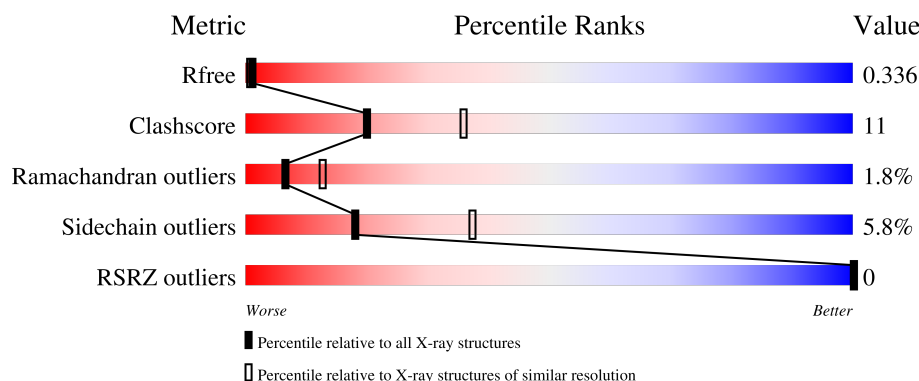
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.62 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	83	
1	B	83	
1	C	83	
1	D	83	
1	E	83	

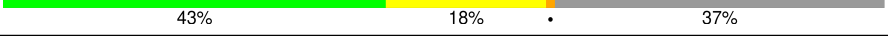
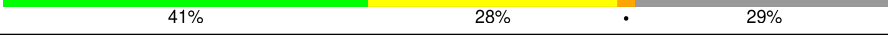
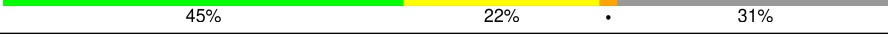
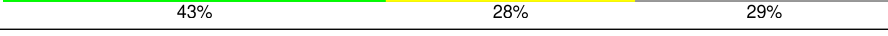
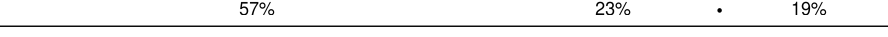
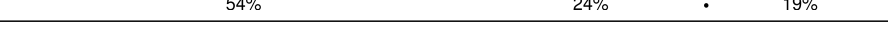
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Mol	Chain	Length	Quality of chain
1	F	83	
1	G	83	
1	H	83	
1	I	83	
1	J	83	
1	K	83	
1	L	83	
1	M	83	
1	N	83	
1	O	83	
1	P	83	
1	Q	83	
1	R	83	
1	S	83	
1	T	83	
1	U	83	
1	V	83	
1	W	83	
1	X	83	
1	Y	83	
1	Z	83	
1	a	83	
1	b	83	
1	c	83	
1	d	83	

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Mol	Chain	Length	Quality of chain
1	e	83	
1	f	83	
1	g	83	
1	h	83	
1	i	83	
1	j	83	
1	k	83	
1	l	83	
1	m	83	
1	n	83	
1	o	83	
1	p	83	
1	q	83	
1	r	83	
1	s	83	
1	t	83	
1	u	83	
1	v	83	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23282 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Small RNA-Binding protein (SRB).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	65	Total	C	N	O	Se	0	0	0
			486	304	82	99	1			
1	B	66	Total	C	N	O	Se	0	0	0
			500	313	89	97	1			
1	C	66	Total	C	N	O	Se	0	0	0
			489	304	86	98	1			
1	D	66	Total	C	N	O	Se	0	0	0
			497	311	86	99	1			
1	E	66	Total	C	N	O	Se	0	0	0
			507	315	89	102	1			
1	F	66	Total	C	N	O	Se	0	0	0
			489	306	86	96	1			
1	G	66	Total	C	N	O	Se	0	0	0
			486	303	80	102	1			
1	H	68	Total	C	N	O	Se	0	0	0
			520	322	91	106	1			
1	I	63	Total	C	N	O	Se	0	0	0
			477	298	83	95	1			
1	J	59	Total	C	N	O	Se	0	0	0
			444	279	73	91	1			
1	K	60	Total	C	N	O	Se	0	0	0
			465	291	83	90	1			
1	L	60	Total	C	N	O	Se	0	0	0
			459	288	80	90	1			
1	M	63	Total	C	N	O	Se	0	0	0
			479	301	86	91	1			
1	N	55	Total	C	N	O	Se	0	0	0
			405	251	68	85	1			
1	O	57	Total	C	N	O	Se	0	0	0
			436	274	74	87	1			
1	P	61	Total	C	N	O	Se	0	0	0
			458	285	81	91	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	64	Total	C	N	O	Se	0	0	0
			482	301	84	96	1			
1	R	64	Total	C	N	O	Se	0	0	0
			462	291	77	93	1			
1	S	65	Total	C	N	O	Se	0	0	0
			482	306	88	87	1			
1	T	66	Total	C	N	O	Se	0	0	0
			475	300	80	94	1			
1	U	66	Total	C	N	O	Se	0	0	0
			511	318	91	101	1			
1	V	67	Total	C	N	O	Se	0	0	0
			512	318	90	103	1			
1	W	63	Total	C	N	O	Se	0	0	0
			475	299	83	92	1			
1	X	64	Total	C	N	O	Se	0	0	0
			470	297	81	91	1			
1	Y	66	Total	C	N	O	Se	0	0	0
			494	309	86	98	1			
1	Z	67	Total	C	N	O	Se	0	0	0
			506	315	87	103	1			
1	a	67	Total	C	N	O	Se	0	0	0
			511	318	90	102	1			
1	b	67	Total	C	N	O	Se	0	0	0
			503	314	87	101	1			
1	c	68	Total	C	N	O	Se	0	0	0
			514	320	91	102	1			
1	d	67	Total	C	N	O	Se	0	0	0
			512	318	90	103	1			
1	e	62	Total	C	N	O	Se	0	0	0
			463	291	79	92	1			
1	f	66	Total	C	N	O	Se	0	0	0
			498	309	86	102	1			
1	g	54	Total	C	N	O	Se	0	0	0
			412	258	70	83	1			
1	h	59	Total	C	N	O	Se	0	0	0
			445	277	76	91	1			
1	i	52	Total	C	N	O	Se	0	0	0
			382	239	62	80	1			
1	j	59	Total	C	N	O	Se	0	0	0
			445	278	75	91	1			
1	k	57	Total	C	N	O	Se	0	0	0
			443	277	79	86	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	l	60	Total	C	N	O	Se	0	0	0
			450	284	74	91	1			
1	m	59	Total	C	N	O	Se	0	0	0
			443	280	70	92	1			
1	n	58	Total	C	N	O	Se	0	0	0
			447	281	78	87	1			
1	o	67	Total	C	N	O	Se	0	0	0
			504	314	87	102	1			
1	p	65	Total	C	N	O	Se	0	0	0
			491	307	88	95	1			
1	q	66	Total	C	N	O	Se	0	0	0
			493	308	86	98	1			
1	r	67	Total	C	N	O	Se	0	0	0
			515	319	90	105	1			
1	s	67	Total	C	N	O	Se	0	0	0
			522	324	94	103	1			
1	t	67	Total	C	N	O	Se	0	0	0
			512	318	90	103	1			
1	u	66	Total	C	N	O	Se	0	0	0
			499	312	89	97	1			
1	v	66	Total	C	N	O	Se	0	0	0
			501	312	86	102	1			

There are 480 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MSE	-	initiating methionine	UNP Q6MWZ8
A	-6	GLY	-	expression tag	UNP Q6MWZ8
A	-5	HIS	-	expression tag	UNP Q6MWZ8
A	-4	HIS	-	expression tag	UNP Q6MWZ8
A	-3	HIS	-	expression tag	UNP Q6MWZ8
A	-2	HIS	-	expression tag	UNP Q6MWZ8
A	-1	HIS	-	expression tag	UNP Q6MWZ8
A	0	HIS	-	expression tag	UNP Q6MWZ8
A	1	VAL	-	expression tag	UNP Q6MWZ8
A	51	MSE	LEU	engineered mutation	UNP Q6MWZ8
B	-7	MSE	-	initiating methionine	UNP Q6MWZ8
B	-6	GLY	-	expression tag	UNP Q6MWZ8
B	-5	HIS	-	expression tag	UNP Q6MWZ8
B	-4	HIS	-	expression tag	UNP Q6MWZ8
B	-3	HIS	-	expression tag	UNP Q6MWZ8
B	-2	HIS	-	expression tag	UNP Q6MWZ8
B	-1	HIS	-	expression tag	UNP Q6MWZ8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	HIS	-	expression tag	UNP Q6MWZ8
B	1	VAL	-	expression tag	UNP Q6MWZ8
B	51	MSE	LEU	engineered mutation	UNP Q6MWZ8
C	-7	MSE	-	initiating methionine	UNP Q6MWZ8
C	-6	GLY	-	expression tag	UNP Q6MWZ8
C	-5	HIS	-	expression tag	UNP Q6MWZ8
C	-4	HIS	-	expression tag	UNP Q6MWZ8
C	-3	HIS	-	expression tag	UNP Q6MWZ8
C	-2	HIS	-	expression tag	UNP Q6MWZ8
C	-1	HIS	-	expression tag	UNP Q6MWZ8
C	0	HIS	-	expression tag	UNP Q6MWZ8
C	1	VAL	-	expression tag	UNP Q6MWZ8
C	51	MSE	LEU	engineered mutation	UNP Q6MWZ8
D	-7	MSE	-	initiating methionine	UNP Q6MWZ8
D	-6	GLY	-	expression tag	UNP Q6MWZ8
D	-5	HIS	-	expression tag	UNP Q6MWZ8
D	-4	HIS	-	expression tag	UNP Q6MWZ8
D	-3	HIS	-	expression tag	UNP Q6MWZ8
D	-2	HIS	-	expression tag	UNP Q6MWZ8
D	-1	HIS	-	expression tag	UNP Q6MWZ8
D	0	HIS	-	expression tag	UNP Q6MWZ8
D	1	VAL	-	expression tag	UNP Q6MWZ8
D	51	MSE	LEU	engineered mutation	UNP Q6MWZ8
E	-7	MSE	-	initiating methionine	UNP Q6MWZ8
E	-6	GLY	-	expression tag	UNP Q6MWZ8
E	-5	HIS	-	expression tag	UNP Q6MWZ8
E	-4	HIS	-	expression tag	UNP Q6MWZ8
E	-3	HIS	-	expression tag	UNP Q6MWZ8
E	-2	HIS	-	expression tag	UNP Q6MWZ8
E	-1	HIS	-	expression tag	UNP Q6MWZ8
E	0	HIS	-	expression tag	UNP Q6MWZ8
E	1	VAL	-	expression tag	UNP Q6MWZ8
E	51	MSE	LEU	engineered mutation	UNP Q6MWZ8
F	-7	MSE	-	initiating methionine	UNP Q6MWZ8
F	-6	GLY	-	expression tag	UNP Q6MWZ8
F	-5	HIS	-	expression tag	UNP Q6MWZ8
F	-4	HIS	-	expression tag	UNP Q6MWZ8
F	-3	HIS	-	expression tag	UNP Q6MWZ8
F	-2	HIS	-	expression tag	UNP Q6MWZ8
F	-1	HIS	-	expression tag	UNP Q6MWZ8
F	0	HIS	-	expression tag	UNP Q6MWZ8
F	1	VAL	-	expression tag	UNP Q6MWZ8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	51	MSE	LEU	engineered mutation	UNP Q6MWZ8
G	-7	MSE	-	initiating methionine	UNP Q6MWZ8
G	-6	GLY	-	expression tag	UNP Q6MWZ8
G	-5	HIS	-	expression tag	UNP Q6MWZ8
G	-4	HIS	-	expression tag	UNP Q6MWZ8
G	-3	HIS	-	expression tag	UNP Q6MWZ8
G	-2	HIS	-	expression tag	UNP Q6MWZ8
G	-1	HIS	-	expression tag	UNP Q6MWZ8
G	0	HIS	-	expression tag	UNP Q6MWZ8
G	1	VAL	-	expression tag	UNP Q6MWZ8
G	51	MSE	LEU	engineered mutation	UNP Q6MWZ8
H	-7	MSE	-	initiating methionine	UNP Q6MWZ8
H	-6	GLY	-	expression tag	UNP Q6MWZ8
H	-5	HIS	-	expression tag	UNP Q6MWZ8
H	-4	HIS	-	expression tag	UNP Q6MWZ8
H	-3	HIS	-	expression tag	UNP Q6MWZ8
H	-2	HIS	-	expression tag	UNP Q6MWZ8
H	-1	HIS	-	expression tag	UNP Q6MWZ8
H	0	HIS	-	expression tag	UNP Q6MWZ8
H	1	VAL	-	expression tag	UNP Q6MWZ8
H	51	MSE	LEU	engineered mutation	UNP Q6MWZ8
I	-7	MSE	-	initiating methionine	UNP Q6MWZ8
I	-6	GLY	-	expression tag	UNP Q6MWZ8
I	-5	HIS	-	expression tag	UNP Q6MWZ8
I	-4	HIS	-	expression tag	UNP Q6MWZ8
I	-3	HIS	-	expression tag	UNP Q6MWZ8
I	-2	HIS	-	expression tag	UNP Q6MWZ8
I	-1	HIS	-	expression tag	UNP Q6MWZ8
I	0	HIS	-	expression tag	UNP Q6MWZ8
I	1	VAL	-	expression tag	UNP Q6MWZ8
I	51	MSE	LEU	engineered mutation	UNP Q6MWZ8
J	-7	MSE	-	initiating methionine	UNP Q6MWZ8
J	-6	GLY	-	expression tag	UNP Q6MWZ8
J	-5	HIS	-	expression tag	UNP Q6MWZ8
J	-4	HIS	-	expression tag	UNP Q6MWZ8
J	-3	HIS	-	expression tag	UNP Q6MWZ8
J	-2	HIS	-	expression tag	UNP Q6MWZ8
J	-1	HIS	-	expression tag	UNP Q6MWZ8
J	0	HIS	-	expression tag	UNP Q6MWZ8
J	1	VAL	-	expression tag	UNP Q6MWZ8
J	51	MSE	LEU	engineered mutation	UNP Q6MWZ8
K	-7	MSE	-	initiating methionine	UNP Q6MWZ8

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-6	GLY	-	expression tag	UNP Q6MWZ8
K	-5	HIS	-	expression tag	UNP Q6MWZ8
K	-4	HIS	-	expression tag	UNP Q6MWZ8
K	-3	HIS	-	expression tag	UNP Q6MWZ8
K	-2	HIS	-	expression tag	UNP Q6MWZ8
K	-1	HIS	-	expression tag	UNP Q6MWZ8
K	0	HIS	-	expression tag	UNP Q6MWZ8
K	1	VAL	-	expression tag	UNP Q6MWZ8
K	51	MSE	LEU	engineered mutation	UNP Q6MWZ8
L	-7	MSE	-	initiating methionine	UNP Q6MWZ8
L	-6	GLY	-	expression tag	UNP Q6MWZ8
L	-5	HIS	-	expression tag	UNP Q6MWZ8
L	-4	HIS	-	expression tag	UNP Q6MWZ8
L	-3	HIS	-	expression tag	UNP Q6MWZ8
L	-2	HIS	-	expression tag	UNP Q6MWZ8
L	-1	HIS	-	expression tag	UNP Q6MWZ8
L	0	HIS	-	expression tag	UNP Q6MWZ8
L	1	VAL	-	expression tag	UNP Q6MWZ8
L	51	MSE	LEU	engineered mutation	UNP Q6MWZ8
M	-7	MSE	-	initiating methionine	UNP Q6MWZ8
M	-6	GLY	-	expression tag	UNP Q6MWZ8
M	-5	HIS	-	expression tag	UNP Q6MWZ8
M	-4	HIS	-	expression tag	UNP Q6MWZ8
M	-3	HIS	-	expression tag	UNP Q6MWZ8
M	-2	HIS	-	expression tag	UNP Q6MWZ8
M	-1	HIS	-	expression tag	UNP Q6MWZ8
M	0	HIS	-	expression tag	UNP Q6MWZ8
M	1	VAL	-	expression tag	UNP Q6MWZ8
M	51	MSE	LEU	engineered mutation	UNP Q6MWZ8
N	-7	MSE	-	initiating methionine	UNP Q6MWZ8
N	-6	GLY	-	expression tag	UNP Q6MWZ8
N	-5	HIS	-	expression tag	UNP Q6MWZ8
N	-4	HIS	-	expression tag	UNP Q6MWZ8
N	-3	HIS	-	expression tag	UNP Q6MWZ8
N	-2	HIS	-	expression tag	UNP Q6MWZ8
N	-1	HIS	-	expression tag	UNP Q6MWZ8
N	0	HIS	-	expression tag	UNP Q6MWZ8
N	1	VAL	-	expression tag	UNP Q6MWZ8
N	51	MSE	LEU	engineered mutation	UNP Q6MWZ8
O	-7	MSE	-	initiating methionine	UNP Q6MWZ8
O	-6	GLY	-	expression tag	UNP Q6MWZ8
O	-5	HIS	-	expression tag	UNP Q6MWZ8

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Chain	Residue	Modelled	Actual	Comment	Reference
O	-4	HIS	-	expression tag	UNP Q6MWZ8
O	-3	HIS	-	expression tag	UNP Q6MWZ8
O	-2	HIS	-	expression tag	UNP Q6MWZ8
O	-1	HIS	-	expression tag	UNP Q6MWZ8
O	0	HIS	-	expression tag	UNP Q6MWZ8
O	1	VAL	-	expression tag	UNP Q6MWZ8
O	51	MSE	LEU	engineered mutation	UNP Q6MWZ8
P	-7	MSE	-	initiating methionine	UNP Q6MWZ8
P	-6	GLY	-	expression tag	UNP Q6MWZ8
P	-5	HIS	-	expression tag	UNP Q6MWZ8
P	-4	HIS	-	expression tag	UNP Q6MWZ8
P	-3	HIS	-	expression tag	UNP Q6MWZ8
P	-2	HIS	-	expression tag	UNP Q6MWZ8
P	-1	HIS	-	expression tag	UNP Q6MWZ8
P	0	HIS	-	expression tag	UNP Q6MWZ8
P	1	VAL	-	expression tag	UNP Q6MWZ8
P	51	MSE	LEU	engineered mutation	UNP Q6MWZ8
Q	-7	MSE	-	initiating methionine	UNP Q6MWZ8
Q	-6	GLY	-	expression tag	UNP Q6MWZ8
Q	-5	HIS	-	expression tag	UNP Q6MWZ8
Q	-4	HIS	-	expression tag	UNP Q6MWZ8
Q	-3	HIS	-	expression tag	UNP Q6MWZ8
Q	-2	HIS	-	expression tag	UNP Q6MWZ8
Q	-1	HIS	-	expression tag	UNP Q6MWZ8
Q	0	HIS	-	expression tag	UNP Q6MWZ8
Q	1	VAL	-	expression tag	UNP Q6MWZ8
Q	51	MSE	LEU	engineered mutation	UNP Q6MWZ8
R	-7	MSE	-	initiating methionine	UNP Q6MWZ8
R	-6	GLY	-	expression tag	UNP Q6MWZ8
R	-5	HIS	-	expression tag	UNP Q6MWZ8
R	-4	HIS	-	expression tag	UNP Q6MWZ8
R	-3	HIS	-	expression tag	UNP Q6MWZ8
R	-2	HIS	-	expression tag	UNP Q6MWZ8
R	-1	HIS	-	expression tag	UNP Q6MWZ8
R	0	HIS	-	expression tag	UNP Q6MWZ8
R	1	VAL	-	expression tag	UNP Q6MWZ8
R	51	MSE	LEU	engineered mutation	UNP Q6MWZ8
S	-7	MSE	-	initiating methionine	UNP Q6MWZ8
S	-6	GLY	-	expression tag	UNP Q6MWZ8
S	-5	HIS	-	expression tag	UNP Q6MWZ8
S	-4	HIS	-	expression tag	UNP Q6MWZ8
S	-3	HIS	-	expression tag	UNP Q6MWZ8

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Chain	Residue	Modelled	Actual	Comment	Reference
S	-2	HIS	-	expression tag	UNP Q6MWZ8
S	-1	HIS	-	expression tag	UNP Q6MWZ8
S	0	HIS	-	expression tag	UNP Q6MWZ8
S	1	VAL	-	expression tag	UNP Q6MWZ8
S	51	MSE	LEU	engineered mutation	UNP Q6MWZ8
T	-7	MSE	-	initiating methionine	UNP Q6MWZ8
T	-6	GLY	-	expression tag	UNP Q6MWZ8
T	-5	HIS	-	expression tag	UNP Q6MWZ8
T	-4	HIS	-	expression tag	UNP Q6MWZ8
T	-3	HIS	-	expression tag	UNP Q6MWZ8
T	-2	HIS	-	expression tag	UNP Q6MWZ8
T	-1	HIS	-	expression tag	UNP Q6MWZ8
T	0	HIS	-	expression tag	UNP Q6MWZ8
T	1	VAL	-	expression tag	UNP Q6MWZ8
T	51	MSE	LEU	engineered mutation	UNP Q6MWZ8
U	-7	MSE	-	initiating methionine	UNP Q6MWZ8
U	-6	GLY	-	expression tag	UNP Q6MWZ8
U	-5	HIS	-	expression tag	UNP Q6MWZ8
U	-4	HIS	-	expression tag	UNP Q6MWZ8
U	-3	HIS	-	expression tag	UNP Q6MWZ8
U	-2	HIS	-	expression tag	UNP Q6MWZ8
U	-1	HIS	-	expression tag	UNP Q6MWZ8
U	0	HIS	-	expression tag	UNP Q6MWZ8
U	1	VAL	-	expression tag	UNP Q6MWZ8
U	51	MSE	LEU	engineered mutation	UNP Q6MWZ8
V	-7	MSE	-	initiating methionine	UNP Q6MWZ8
V	-6	GLY	-	expression tag	UNP Q6MWZ8
V	-5	HIS	-	expression tag	UNP Q6MWZ8
V	-4	HIS	-	expression tag	UNP Q6MWZ8
V	-3	HIS	-	expression tag	UNP Q6MWZ8
V	-2	HIS	-	expression tag	UNP Q6MWZ8
V	-1	HIS	-	expression tag	UNP Q6MWZ8
V	0	HIS	-	expression tag	UNP Q6MWZ8
V	1	VAL	-	expression tag	UNP Q6MWZ8
V	51	MSE	LEU	engineered mutation	UNP Q6MWZ8
W	-7	MSE	-	initiating methionine	UNP Q6MWZ8
W	-6	GLY	-	expression tag	UNP Q6MWZ8
W	-5	HIS	-	expression tag	UNP Q6MWZ8
W	-4	HIS	-	expression tag	UNP Q6MWZ8
W	-3	HIS	-	expression tag	UNP Q6MWZ8
W	-2	HIS	-	expression tag	UNP Q6MWZ8
W	-1	HIS	-	expression tag	UNP Q6MWZ8

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Chain	Residue	Modelled	Actual	Comment	Reference
W	0	HIS	-	expression tag	UNP Q6MWZ8
W	1	VAL	-	expression tag	UNP Q6MWZ8
W	51	MSE	LEU	engineered mutation	UNP Q6MWZ8
X	-7	MSE	-	initiating methionine	UNP Q6MWZ8
X	-6	GLY	-	expression tag	UNP Q6MWZ8
X	-5	HIS	-	expression tag	UNP Q6MWZ8
X	-4	HIS	-	expression tag	UNP Q6MWZ8
X	-3	HIS	-	expression tag	UNP Q6MWZ8
X	-2	HIS	-	expression tag	UNP Q6MWZ8
X	-1	HIS	-	expression tag	UNP Q6MWZ8
X	0	HIS	-	expression tag	UNP Q6MWZ8
X	1	VAL	-	expression tag	UNP Q6MWZ8
X	51	MSE	LEU	engineered mutation	UNP Q6MWZ8
Y	-7	MSE	-	initiating methionine	UNP Q6MWZ8
Y	-6	GLY	-	expression tag	UNP Q6MWZ8
Y	-5	HIS	-	expression tag	UNP Q6MWZ8
Y	-4	HIS	-	expression tag	UNP Q6MWZ8
Y	-3	HIS	-	expression tag	UNP Q6MWZ8
Y	-2	HIS	-	expression tag	UNP Q6MWZ8
Y	-1	HIS	-	expression tag	UNP Q6MWZ8
Y	0	HIS	-	expression tag	UNP Q6MWZ8
Y	1	VAL	-	expression tag	UNP Q6MWZ8
Y	51	MSE	LEU	engineered mutation	UNP Q6MWZ8
Z	-7	MSE	-	initiating methionine	UNP Q6MWZ8
Z	-6	GLY	-	expression tag	UNP Q6MWZ8
Z	-5	HIS	-	expression tag	UNP Q6MWZ8
Z	-4	HIS	-	expression tag	UNP Q6MWZ8
Z	-3	HIS	-	expression tag	UNP Q6MWZ8
Z	-2	HIS	-	expression tag	UNP Q6MWZ8
Z	-1	HIS	-	expression tag	UNP Q6MWZ8
Z	0	HIS	-	expression tag	UNP Q6MWZ8
Z	1	VAL	-	expression tag	UNP Q6MWZ8
Z	51	MSE	LEU	engineered mutation	UNP Q6MWZ8
a	-7	MSE	-	initiating methionine	UNP Q6MWZ8
a	-6	GLY	-	expression tag	UNP Q6MWZ8
a	-5	HIS	-	expression tag	UNP Q6MWZ8
a	-4	HIS	-	expression tag	UNP Q6MWZ8
a	-3	HIS	-	expression tag	UNP Q6MWZ8
a	-2	HIS	-	expression tag	UNP Q6MWZ8
a	-1	HIS	-	expression tag	UNP Q6MWZ8
a	0	HIS	-	expression tag	UNP Q6MWZ8
a	1	VAL	-	expression tag	UNP Q6MWZ8

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Chain	Residue	Modelled	Actual	Comment	Reference
a	51	MSE	LEU	engineered mutation	UNP Q6MWZ8
b	-7	MSE	-	initiating methionine	UNP Q6MWZ8
b	-6	GLY	-	expression tag	UNP Q6MWZ8
b	-5	HIS	-	expression tag	UNP Q6MWZ8
b	-4	HIS	-	expression tag	UNP Q6MWZ8
b	-3	HIS	-	expression tag	UNP Q6MWZ8
b	-2	HIS	-	expression tag	UNP Q6MWZ8
b	-1	HIS	-	expression tag	UNP Q6MWZ8
b	0	HIS	-	expression tag	UNP Q6MWZ8
b	1	VAL	-	expression tag	UNP Q6MWZ8
b	51	MSE	LEU	engineered mutation	UNP Q6MWZ8
c	-7	MSE	-	initiating methionine	UNP Q6MWZ8
c	-6	GLY	-	expression tag	UNP Q6MWZ8
c	-5	HIS	-	expression tag	UNP Q6MWZ8
c	-4	HIS	-	expression tag	UNP Q6MWZ8
c	-3	HIS	-	expression tag	UNP Q6MWZ8
c	-2	HIS	-	expression tag	UNP Q6MWZ8
c	-1	HIS	-	expression tag	UNP Q6MWZ8
c	0	HIS	-	expression tag	UNP Q6MWZ8
c	1	VAL	-	expression tag	UNP Q6MWZ8
c	51	MSE	LEU	engineered mutation	UNP Q6MWZ8
d	-7	MSE	-	initiating methionine	UNP Q6MWZ8
d	-6	GLY	-	expression tag	UNP Q6MWZ8
d	-5	HIS	-	expression tag	UNP Q6MWZ8
d	-4	HIS	-	expression tag	UNP Q6MWZ8
d	-3	HIS	-	expression tag	UNP Q6MWZ8
d	-2	HIS	-	expression tag	UNP Q6MWZ8
d	-1	HIS	-	expression tag	UNP Q6MWZ8
d	0	HIS	-	expression tag	UNP Q6MWZ8
d	1	VAL	-	expression tag	UNP Q6MWZ8
d	51	MSE	LEU	engineered mutation	UNP Q6MWZ8
e	-7	MSE	-	initiating methionine	UNP Q6MWZ8
e	-6	GLY	-	expression tag	UNP Q6MWZ8
e	-5	HIS	-	expression tag	UNP Q6MWZ8
e	-4	HIS	-	expression tag	UNP Q6MWZ8
e	-3	HIS	-	expression tag	UNP Q6MWZ8
e	-2	HIS	-	expression tag	UNP Q6MWZ8
e	-1	HIS	-	expression tag	UNP Q6MWZ8
e	0	HIS	-	expression tag	UNP Q6MWZ8
e	1	VAL	-	expression tag	UNP Q6MWZ8
e	51	MSE	LEU	engineered mutation	UNP Q6MWZ8
f	-7	MSE	-	initiating methionine	UNP Q6MWZ8

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Chain	Residue	Modelled	Actual	Comment	Reference
f	-6	GLY	-	expression tag	UNP Q6MWZ8
f	-5	HIS	-	expression tag	UNP Q6MWZ8
f	-4	HIS	-	expression tag	UNP Q6MWZ8
f	-3	HIS	-	expression tag	UNP Q6MWZ8
f	-2	HIS	-	expression tag	UNP Q6MWZ8
f	-1	HIS	-	expression tag	UNP Q6MWZ8
f	0	HIS	-	expression tag	UNP Q6MWZ8
f	1	VAL	-	expression tag	UNP Q6MWZ8
f	51	MSE	LEU	engineered mutation	UNP Q6MWZ8
g	-7	MSE	-	initiating methionine	UNP Q6MWZ8
g	-6	GLY	-	expression tag	UNP Q6MWZ8
g	-5	HIS	-	expression tag	UNP Q6MWZ8
g	-4	HIS	-	expression tag	UNP Q6MWZ8
g	-3	HIS	-	expression tag	UNP Q6MWZ8
g	-2	HIS	-	expression tag	UNP Q6MWZ8
g	-1	HIS	-	expression tag	UNP Q6MWZ8
g	0	HIS	-	expression tag	UNP Q6MWZ8
g	1	VAL	-	expression tag	UNP Q6MWZ8
g	51	MSE	LEU	engineered mutation	UNP Q6MWZ8
h	-7	MSE	-	initiating methionine	UNP Q6MWZ8
h	-6	GLY	-	expression tag	UNP Q6MWZ8
h	-5	HIS	-	expression tag	UNP Q6MWZ8
h	-4	HIS	-	expression tag	UNP Q6MWZ8
h	-3	HIS	-	expression tag	UNP Q6MWZ8
h	-2	HIS	-	expression tag	UNP Q6MWZ8
h	-1	HIS	-	expression tag	UNP Q6MWZ8
h	0	HIS	-	expression tag	UNP Q6MWZ8
h	1	VAL	-	expression tag	UNP Q6MWZ8
h	51	MSE	LEU	engineered mutation	UNP Q6MWZ8
i	-7	MSE	-	initiating methionine	UNP Q6MWZ8
i	-6	GLY	-	expression tag	UNP Q6MWZ8
i	-5	HIS	-	expression tag	UNP Q6MWZ8
i	-4	HIS	-	expression tag	UNP Q6MWZ8
i	-3	HIS	-	expression tag	UNP Q6MWZ8
i	-2	HIS	-	expression tag	UNP Q6MWZ8
i	-1	HIS	-	expression tag	UNP Q6MWZ8
i	0	HIS	-	expression tag	UNP Q6MWZ8
i	1	VAL	-	expression tag	UNP Q6MWZ8
i	51	MSE	LEU	engineered mutation	UNP Q6MWZ8
j	-7	MSE	-	initiating methionine	UNP Q6MWZ8
j	-6	GLY	-	expression tag	UNP Q6MWZ8
j	-5	HIS	-	expression tag	UNP Q6MWZ8

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Chain	Residue	Modelled	Actual	Comment	Reference
j	-4	HIS	-	expression tag	UNP Q6MWZ8
j	-3	HIS	-	expression tag	UNP Q6MWZ8
j	-2	HIS	-	expression tag	UNP Q6MWZ8
j	-1	HIS	-	expression tag	UNP Q6MWZ8
j	0	HIS	-	expression tag	UNP Q6MWZ8
j	1	VAL	-	expression tag	UNP Q6MWZ8
j	51	MSE	LEU	engineered mutation	UNP Q6MWZ8
k	-7	MSE	-	initiating methionine	UNP Q6MWZ8
k	-6	GLY	-	expression tag	UNP Q6MWZ8
k	-5	HIS	-	expression tag	UNP Q6MWZ8
k	-4	HIS	-	expression tag	UNP Q6MWZ8
k	-3	HIS	-	expression tag	UNP Q6MWZ8
k	-2	HIS	-	expression tag	UNP Q6MWZ8
k	-1	HIS	-	expression tag	UNP Q6MWZ8
k	0	HIS	-	expression tag	UNP Q6MWZ8
k	1	VAL	-	expression tag	UNP Q6MWZ8
k	51	MSE	LEU	engineered mutation	UNP Q6MWZ8
l	-7	MSE	-	initiating methionine	UNP Q6MWZ8
l	-6	GLY	-	expression tag	UNP Q6MWZ8
l	-5	HIS	-	expression tag	UNP Q6MWZ8
l	-4	HIS	-	expression tag	UNP Q6MWZ8
l	-3	HIS	-	expression tag	UNP Q6MWZ8
l	-2	HIS	-	expression tag	UNP Q6MWZ8
l	-1	HIS	-	expression tag	UNP Q6MWZ8
l	0	HIS	-	expression tag	UNP Q6MWZ8
l	1	VAL	-	expression tag	UNP Q6MWZ8
l	51	MSE	LEU	engineered mutation	UNP Q6MWZ8
m	-7	MSE	-	initiating methionine	UNP Q6MWZ8
m	-6	GLY	-	expression tag	UNP Q6MWZ8
m	-5	HIS	-	expression tag	UNP Q6MWZ8
m	-4	HIS	-	expression tag	UNP Q6MWZ8
m	-3	HIS	-	expression tag	UNP Q6MWZ8
m	-2	HIS	-	expression tag	UNP Q6MWZ8
m	-1	HIS	-	expression tag	UNP Q6MWZ8
m	0	HIS	-	expression tag	UNP Q6MWZ8
m	1	VAL	-	expression tag	UNP Q6MWZ8
m	51	MSE	LEU	engineered mutation	UNP Q6MWZ8
n	-7	MSE	-	initiating methionine	UNP Q6MWZ8
n	-6	GLY	-	expression tag	UNP Q6MWZ8
n	-5	HIS	-	expression tag	UNP Q6MWZ8
n	-4	HIS	-	expression tag	UNP Q6MWZ8
n	-3	HIS	-	expression tag	UNP Q6MWZ8

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Chain	Residue	Modelled	Actual	Comment	Reference
n	-2	HIS	-	expression tag	UNP Q6MWZ8
n	-1	HIS	-	expression tag	UNP Q6MWZ8
n	0	HIS	-	expression tag	UNP Q6MWZ8
n	1	VAL	-	expression tag	UNP Q6MWZ8
n	51	MSE	LEU	engineered mutation	UNP Q6MWZ8
o	-7	MSE	-	initiating methionine	UNP Q6MWZ8
o	-6	GLY	-	expression tag	UNP Q6MWZ8
o	-5	HIS	-	expression tag	UNP Q6MWZ8
o	-4	HIS	-	expression tag	UNP Q6MWZ8
o	-3	HIS	-	expression tag	UNP Q6MWZ8
o	-2	HIS	-	expression tag	UNP Q6MWZ8
o	-1	HIS	-	expression tag	UNP Q6MWZ8
o	0	HIS	-	expression tag	UNP Q6MWZ8
o	1	VAL	-	expression tag	UNP Q6MWZ8
o	51	MSE	LEU	engineered mutation	UNP Q6MWZ8
p	-7	MSE	-	initiating methionine	UNP Q6MWZ8
p	-6	GLY	-	expression tag	UNP Q6MWZ8
p	-5	HIS	-	expression tag	UNP Q6MWZ8
p	-4	HIS	-	expression tag	UNP Q6MWZ8
p	-3	HIS	-	expression tag	UNP Q6MWZ8
p	-2	HIS	-	expression tag	UNP Q6MWZ8
p	-1	HIS	-	expression tag	UNP Q6MWZ8
p	0	HIS	-	expression tag	UNP Q6MWZ8
p	1	VAL	-	expression tag	UNP Q6MWZ8
p	51	MSE	LEU	engineered mutation	UNP Q6MWZ8
q	-7	MSE	-	initiating methionine	UNP Q6MWZ8
q	-6	GLY	-	expression tag	UNP Q6MWZ8
q	-5	HIS	-	expression tag	UNP Q6MWZ8
q	-4	HIS	-	expression tag	UNP Q6MWZ8
q	-3	HIS	-	expression tag	UNP Q6MWZ8
q	-2	HIS	-	expression tag	UNP Q6MWZ8
q	-1	HIS	-	expression tag	UNP Q6MWZ8
q	0	HIS	-	expression tag	UNP Q6MWZ8
q	1	VAL	-	expression tag	UNP Q6MWZ8
q	51	MSE	LEU	engineered mutation	UNP Q6MWZ8
r	-7	MSE	-	initiating methionine	UNP Q6MWZ8
r	-6	GLY	-	expression tag	UNP Q6MWZ8
r	-5	HIS	-	expression tag	UNP Q6MWZ8
r	-4	HIS	-	expression tag	UNP Q6MWZ8
r	-3	HIS	-	expression tag	UNP Q6MWZ8
r	-2	HIS	-	expression tag	UNP Q6MWZ8
r	-1	HIS	-	expression tag	UNP Q6MWZ8

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Chain	Residue	Modelled	Actual	Comment	Reference
r	0	HIS	-	expression tag	UNP Q6MWZ8
r	1	VAL	-	expression tag	UNP Q6MWZ8
r	51	MSE	LEU	engineered mutation	UNP Q6MWZ8
s	-7	MSE	-	initiating methionine	UNP Q6MWZ8
s	-6	GLY	-	expression tag	UNP Q6MWZ8
s	-5	HIS	-	expression tag	UNP Q6MWZ8
s	-4	HIS	-	expression tag	UNP Q6MWZ8
s	-3	HIS	-	expression tag	UNP Q6MWZ8
s	-2	HIS	-	expression tag	UNP Q6MWZ8
s	-1	HIS	-	expression tag	UNP Q6MWZ8
s	0	HIS	-	expression tag	UNP Q6MWZ8
s	1	VAL	-	expression tag	UNP Q6MWZ8
s	51	MSE	LEU	engineered mutation	UNP Q6MWZ8
t	-7	MSE	-	initiating methionine	UNP Q6MWZ8
t	-6	GLY	-	expression tag	UNP Q6MWZ8
t	-5	HIS	-	expression tag	UNP Q6MWZ8
t	-4	HIS	-	expression tag	UNP Q6MWZ8
t	-3	HIS	-	expression tag	UNP Q6MWZ8
t	-2	HIS	-	expression tag	UNP Q6MWZ8
t	-1	HIS	-	expression tag	UNP Q6MWZ8
t	0	HIS	-	expression tag	UNP Q6MWZ8
t	1	VAL	-	expression tag	UNP Q6MWZ8
t	51	MSE	LEU	engineered mutation	UNP Q6MWZ8
u	-7	MSE	-	initiating methionine	UNP Q6MWZ8
u	-6	GLY	-	expression tag	UNP Q6MWZ8
u	-5	HIS	-	expression tag	UNP Q6MWZ8
u	-4	HIS	-	expression tag	UNP Q6MWZ8
u	-3	HIS	-	expression tag	UNP Q6MWZ8
u	-2	HIS	-	expression tag	UNP Q6MWZ8
u	-1	HIS	-	expression tag	UNP Q6MWZ8
u	0	HIS	-	expression tag	UNP Q6MWZ8
u	1	VAL	-	expression tag	UNP Q6MWZ8
u	51	MSE	LEU	engineered mutation	UNP Q6MWZ8
v	-7	MSE	-	initiating methionine	UNP Q6MWZ8
v	-6	GLY	-	expression tag	UNP Q6MWZ8
v	-5	HIS	-	expression tag	UNP Q6MWZ8
v	-4	HIS	-	expression tag	UNP Q6MWZ8
v	-3	HIS	-	expression tag	UNP Q6MWZ8
v	-2	HIS	-	expression tag	UNP Q6MWZ8
v	-1	HIS	-	expression tag	UNP Q6MWZ8
v	0	HIS	-	expression tag	UNP Q6MWZ8
v	1	VAL	-	expression tag	UNP Q6MWZ8

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Chain	Residue	Modelled	Actual	Comment	Reference
v	51	MSE	LEU	engineered mutation	UNP Q6MWZ8

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	11	Total O 11 11	0	0
2	B	8	Total O 8 8	0	0
2	C	10	Total O 10 10	0	0
2	D	9	Total O 9 9	0	0
2	E	10	Total O 10 10	0	0
2	F	9	Total O 9 9	0	0
2	G	9	Total O 9 9	0	0
2	H	11	Total O 11 11	0	0
2	I	5	Total O 5 5	0	0
2	J	3	Total O 3 3	0	0
2	K	8	Total O 8 8	0	0
2	L	4	Total O 4 4	0	0
2	N	4	Total O 4 4	0	0
2	O	5	Total O 5 5	0	0
2	P	4	Total O 4 4	0	0
2	Q	11	Total O 11 11	0	0
2	R	10	Total O 10 10	0	0
2	S	8	Total O 8 8	0	0
2	T	9	Total O 9 9	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	U	11	Total O 11 11	0	0
2	V	8	Total O 8 8	0	0
2	W	13	Total O 13 13	0	0
2	X	11	Total O 11 11	0	0
2	Y	6	Total O 6 6	0	0
2	Z	6	Total O 6 6	0	0
2	a	7	Total O 7 7	0	0
2	b	9	Total O 9 9	0	0
2	c	5	Total O 5 5	0	0
2	d	6	Total O 6 6	0	0
2	e	8	Total O 8 8	0	0
2	f	6	Total O 6 6	0	0
2	g	2	Total O 2 2	0	0
2	h	2	Total O 2 2	0	0
2	i	4	Total O 4 4	0	0
2	j	1	Total O 1 1	0	0
2	k	1	Total O 1 1	0	0
2	m	1	Total O 1 1	0	0
2	o	6	Total O 6 6	0	0
2	p	5	Total O 5 5	0	0
2	q	8	Total O 8 8	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	r	6	Total 6	O 6	0	0
2	s	9	Total 9	O 9	0	0
2	t	5	Total 5	O 5	0	0
2	u	11	Total 11	O 11	0	0
2	v	6	Total 6	O 6	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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

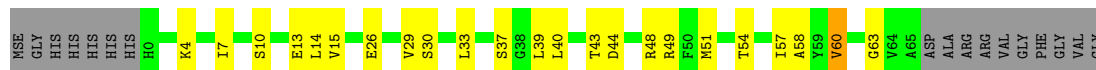
• Molecule 1: Small RNA-Binding protein (SRB)

Chain A: 



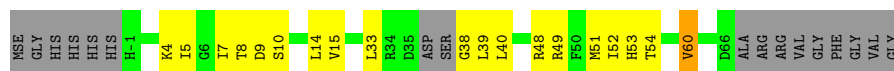
• Molecule 1: Small RNA-Binding protein (SRB)

Chain B: 



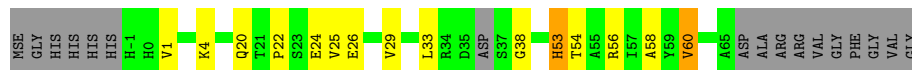
• Molecule 1: Small RNA-Binding protein (SRB)

Chain C: 



• Molecule 1: Small RNA-Binding protein (SRB)

Chain D: 



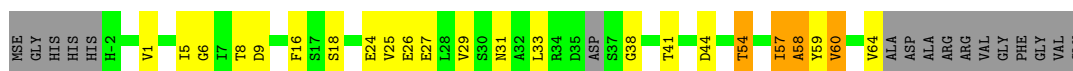
• Molecule 1: Small RNA-Binding protein (SRB)

Chain E: 



• Molecule 1: Small RNA-Binding protein (SRB)

Chain F: 



- Molecule 1: Small RNA-Binding protein (SRB)



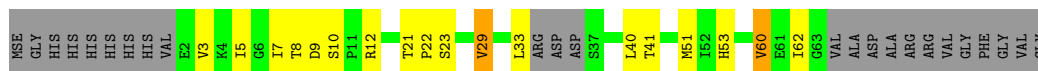
- Molecule 1: Small RNA-Binding protein (SRB)



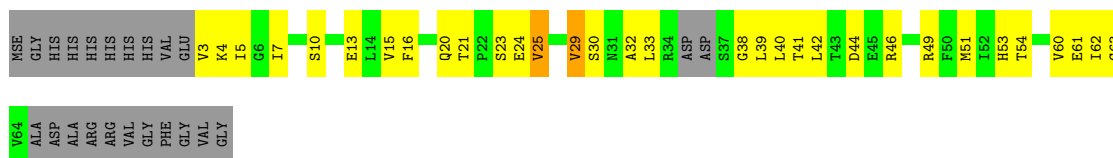
- Molecule 1: Small RNA-Binding protein (SRB)



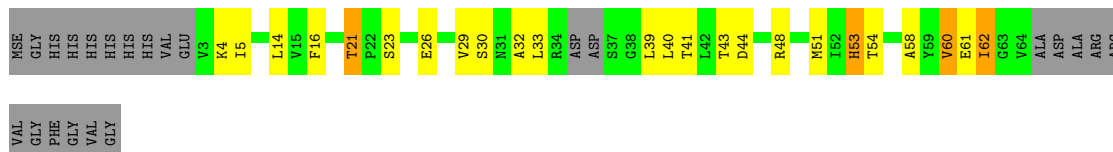
- Molecule 1: Small RNA-Binding protein (SRB)



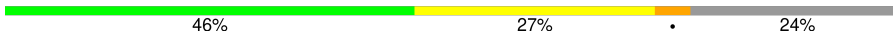
- Molecule 1: Small RNA-Binding protein (SRB)

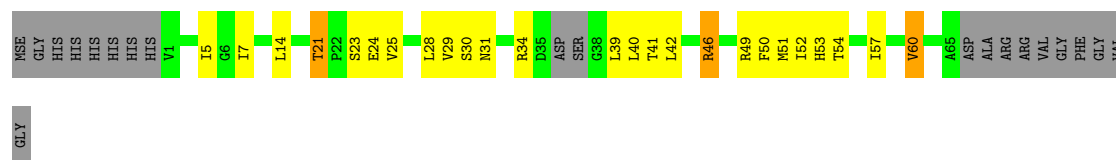


- Molecule 1: Small RNA-Binding protein (SRB)



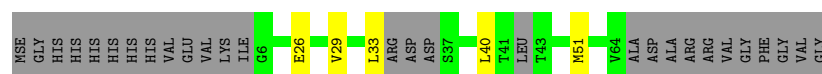
- Molecule 1: Small RNA-Binding protein (SRB)

Chain M: 

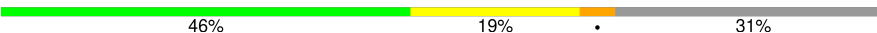


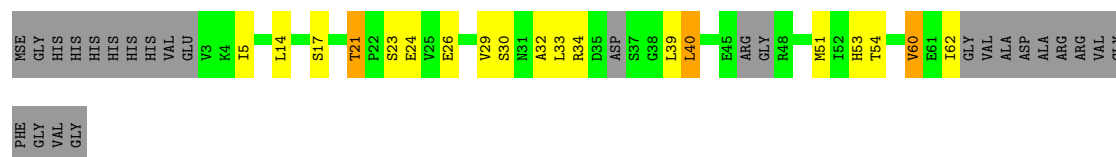
- Molecule 1: Small RNA-Binding protein (SRB)

Chain N: 



- Molecule 1: Small RNA-Binding protein (SRB)

Chain O: 



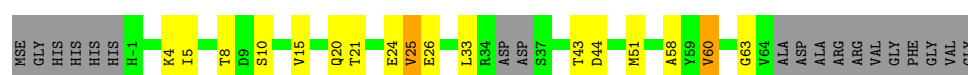
- Molecule 1: Small RNA-Binding protein (SRB)

Chain P: 



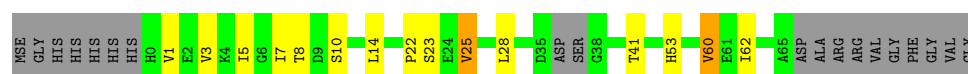
- Molecule 1: Small RNA-Binding protein (SRB)

Chain Q: 



- Molecule 1: Small RNA-Binding protein (SRB)

Chain R: 



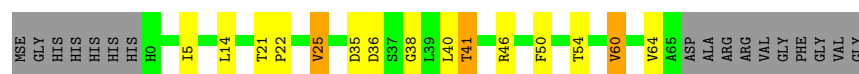
- Molecule 1: Small RNA-Binding protein (SRB)

Chain S:  58% 19% 22%



- Molecule 1: Small RNA-Binding protein (SRB)

Chain T:  61% 14% 20%



- Molecule 1: Small RNA-Binding protein (SRB)

Chain U:  59% 19% 20%



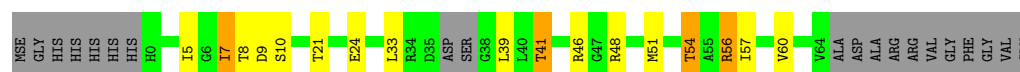
- Molecule 1: Small RNA-Binding protein (SRB)

Chain V:  61% 17% 19%



- Molecule 1: Small RNA-Binding protein (SRB)

Chain W:  55% 16% 5% 24%



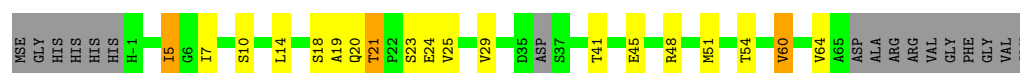
- Molecule 1: Small RNA-Binding protein (SRB)

Chain X:  55% 20% 23%



- Molecule 1: Small RNA-Binding protein (SRB)

Chain Y:  57% 19% 20%



- Molecule 1: Small RNA-Binding protein (SRB)

Chain Z: 



- Molecule 1: Small RNA-Binding protein (SRB)

Chain a: 



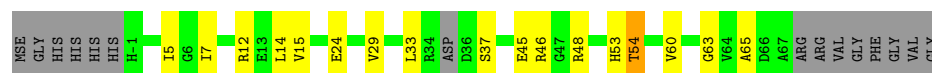
- Molecule 1: Small RNA-Binding protein (SRB)

Chain b: 



- Molecule 1: Small RNA-Binding protein (SRB)

Chain c: 



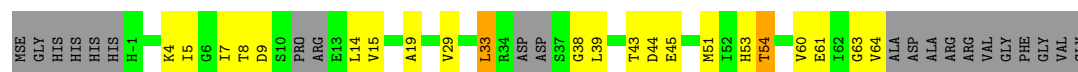
- Molecule 1: Small RNA-Binding protein (SRB)

Chain d: 



- Molecule 1: Small RNA-Binding protein (SRB)

Chain e: 

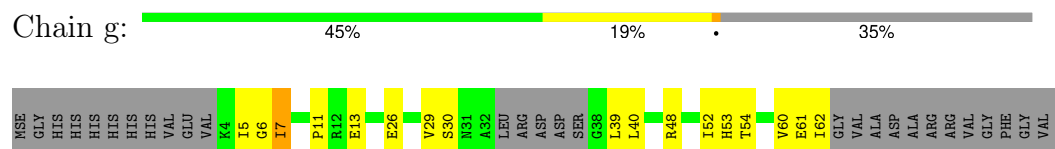


- Molecule 1: Small RNA-Binding protein (SRB)

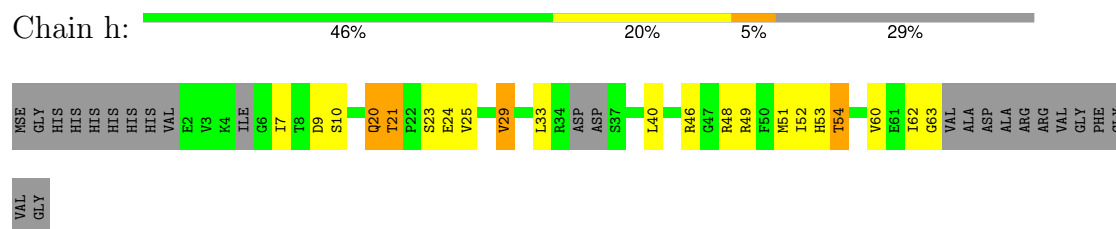
Chain f: 



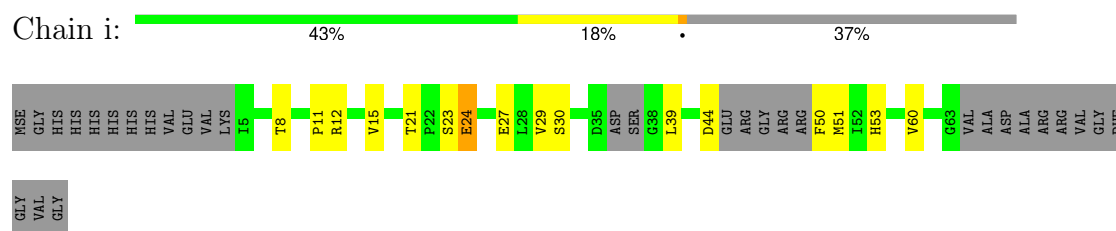
- Molecule 1: Small RNA-Binding protein (SRB)



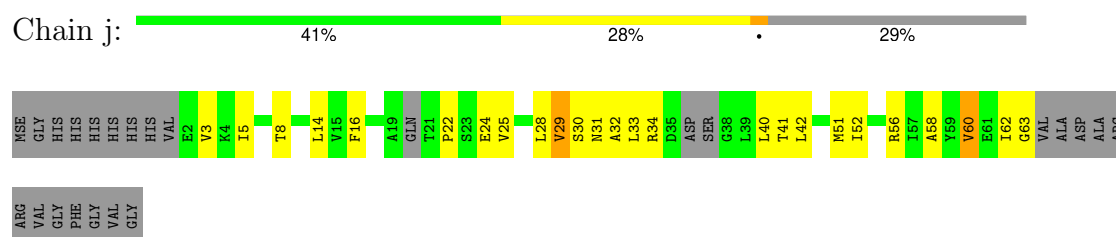
• Molecule 1: Small RNA-Binding protein (SRB)



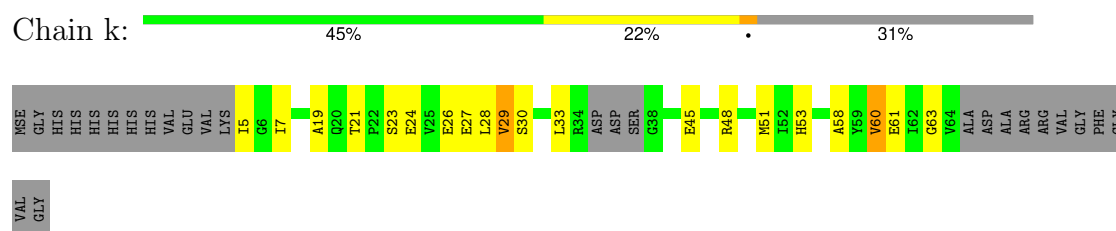
• Molecule 1: Small RNA-Binding protein (SRB)



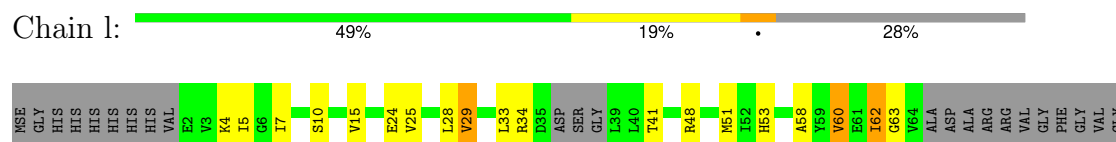
• Molecule 1: Small RNA-Binding protein (SRB)



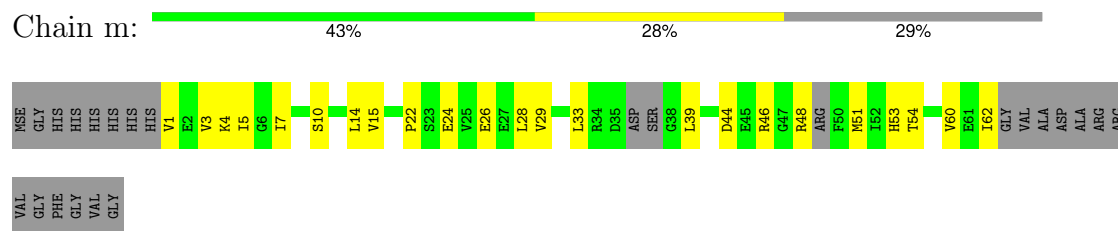
• Molecule 1: Small RNA-Binding protein (SRB)



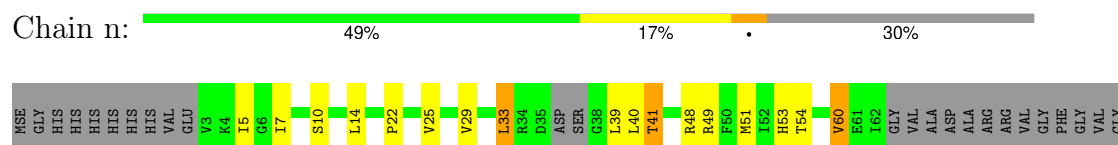
• Molecule 1: Small RNA-Binding protein (SRB)



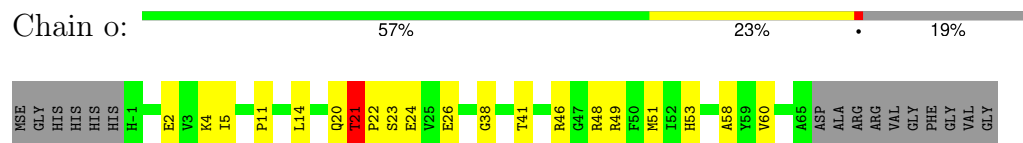
- Molecule 1: Small RNA-Binding protein (SRB)



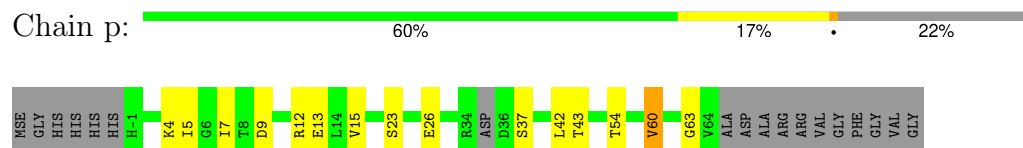
- Molecule 1: Small RNA-Binding protein (SRB)



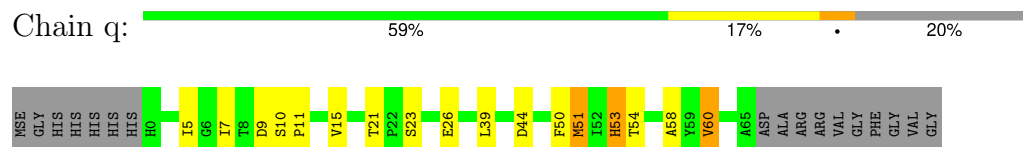
- Molecule 1: Small RNA-Binding protein (SRB)



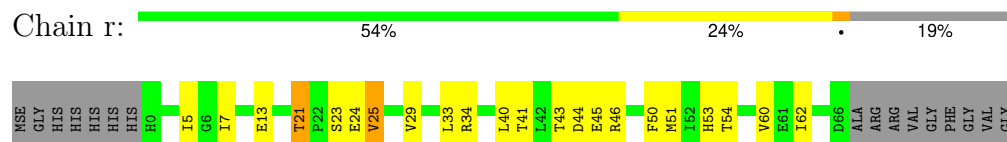
- Molecule 1: Small RNA-Binding protein (SRB)



- Molecule 1: Small RNA-Binding protein (SRB)

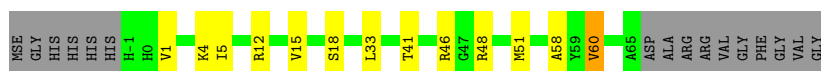


- Molecule 1: Small RNA-Binding protein (SRB)



- Molecule 1: Small RNA-Binding protein (SRB)

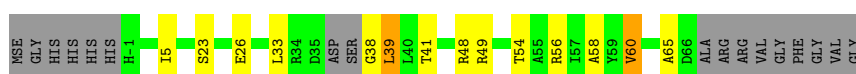




• Molecule 1: Small RNA-Binding protein (SRB)



• Molecule 1: Small RNA-Binding protein (SRB)



• Molecule 1: Small RNA-Binding protein (SRB)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	87.98Å 87.99Å 122.49Å 90.02° 90.03° 90.03°	Depositor
Resolution (Å)	41.40 – 2.62 41.40 – 2.62	Depositor EDS
% Data completeness (in resolution range)	99.3 (41.40-2.62) 99.3 (41.40-2.62)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.275 , 0.335 0.273 , 0.336	Depositor DCC
R_{free} test set	5410 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	50.7	Xtriage
Anisotropy	0.626	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 25.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.447 for k,-h,l 0.447 for -k,h,l 0.447 for h,-k,-l 0.448 for -h,k,-l 0.440 for -h,-k,l 0.440 for k,h,-l 0.457 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	23282	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.67 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.0385e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.17	0/490	0.38	0/664
1	B	0.17	0/504	0.45	0/681
1	C	0.20	0/491	0.43	0/663
1	D	0.17	0/500	0.37	0/675
1	E	0.20	0/511	0.44	0/690
1	F	0.18	0/492	0.44	0/664
1	G	0.21	0/490	0.45	0/665
1	H	0.16	0/524	0.42	0/708
1	I	0.16	0/481	0.38	0/650
1	J	0.14	0/447	0.32	0/603
1	K	0.20	0/468	0.40	0/629
1	L	0.16	0/462	0.40	0/622
1	M	0.21	0/482	0.46	0/650
1	N	0.13	0/407	0.36	0/548
1	O	0.30	0/438	0.61	0/589
1	P	0.14	0/460	0.38	0/620
1	Q	0.26	0/485	0.50	0/654
1	R	0.16	0/465	0.47	0/631
1	S	0.15	0/485	0.40	0/652
1	T	0.21	0/479	0.48	0/651
1	U	0.17	0/515	0.37	0/694
1	V	0.26	0/516	0.48	0/697
1	W	0.21	0/478	0.40	0/645
1	X	0.20	0/473	0.46	0/640
1	Y	0.30	0/497	0.43	0/671
1	Z	0.16	0/510	0.44	0/690
1	a	0.17	0/514	0.42	0/693
1	b	0.17	0/507	0.37	0/686
1	c	0.23	0/517	0.43	0/697
1	d	0.16	0/516	0.41	0/697
1	e	0.17	0/464	0.43	0/624
1	f	0.15	0/502	0.41	0/679
1	g	0.12	0/415	0.34	0/560
1	h	0.16	0/447	0.43	0/600

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	i	0.10	0/383	0.27	0/517
1	j	0.15	0/447	0.43	0/601
1	k	0.13	0/446	0.38	0/600
1	l	0.13	0/453	0.38	0/613
1	m	0.18	0/445	0.35	0/601
1	n	0.14	0/450	0.45	0/606
1	o	0.17	0/508	0.44	0/687
1	p	0.16	0/494	0.41	0/666
1	q	0.18	0/497	0.44	0/673
1	r	0.18	0/519	0.42	0/701
1	s	0.18	0/528	0.40	0/713
1	t	0.17	0/516	0.42	0/697
1	u	0.18	0/502	0.48	0/677
1	v	0.20	0/505	0.47	0/683
All	All	0.18	0/23125	0.42	0/31217

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	486	0	482	16	0
1	B	500	0	503	19	0
1	C	489	0	484	16	0
1	D	497	0	493	12	0
1	E	507	0	510	19	0
1	F	489	0	480	17	0
1	G	486	0	468	16	0
1	H	520	0	516	11	0
1	I	477	0	477	15	0
1	J	444	0	438	14	0
1	K	465	0	476	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	459	0	465	18	0
1	M	479	0	487	19	0
1	N	405	0	380	5	0
1	O	436	0	431	16	0
1	P	458	0	460	11	0
1	Q	482	0	478	13	0
1	R	462	0	443	8	0
1	S	482	0	492	9	0
1	T	475	0	465	8	0
1	U	511	0	511	9	0
1	V	512	0	512	10	0
1	W	475	0	478	16	0
1	X	470	0	468	18	0
1	Y	494	0	492	10	0
1	Z	506	0	501	7	0
1	a	511	0	511	13	0
1	b	503	0	499	9	0
1	c	514	0	514	14	0
1	d	512	0	512	8	0
1	e	463	0	462	16	0
1	f	498	0	487	8	0
1	g	412	0	404	14	0
1	h	445	0	432	20	0
1	i	382	0	368	16	0
1	j	445	0	432	18	0
1	k	443	0	449	18	0
1	l	450	0	441	24	0
1	m	443	0	434	22	0
1	n	447	0	450	15	0
1	o	504	0	496	12	0
1	p	491	0	494	14	0
1	q	493	0	491	14	0
1	r	515	0	514	14	0
1	s	522	0	522	12	0
1	t	512	0	512	12	0
1	u	499	0	500	7	0
1	v	501	0	499	13	0
2	A	11	0	0	2	0
2	B	8	0	0	0	0
2	C	10	0	0	0	0
2	D	9	0	0	0	0
2	E	10	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	9	0	0	1	0
2	G	9	0	0	2	0
2	H	11	0	0	1	0
2	I	5	0	0	0	0
2	J	3	0	0	0	0
2	K	8	0	0	0	0
2	L	4	0	0	0	0
2	N	4	0	0	0	0
2	O	5	0	0	0	0
2	P	4	0	0	1	0
2	Q	11	0	0	2	0
2	R	10	0	0	2	0
2	S	8	0	0	0	0
2	T	9	0	0	0	0
2	U	11	0	0	1	0
2	V	8	0	0	0	0
2	W	13	0	0	2	0
2	X	11	0	0	0	0
2	Y	6	0	0	0	0
2	Z	6	0	0	0	0
2	a	7	0	0	0	0
2	b	9	0	0	0	0
2	c	5	0	0	0	0
2	d	6	0	0	0	0
2	e	8	0	0	2	0
2	f	6	0	0	0	0
2	g	2	0	0	0	0
2	h	2	0	0	0	0
2	i	4	0	0	0	0
2	j	1	0	0	0	0
2	k	1	0	0	0	0
2	m	1	0	0	1	0
2	o	6	0	0	0	0
2	p	5	0	0	0	0
2	q	8	0	0	3	0
2	r	6	0	0	1	0
2	s	9	0	0	0	0
2	t	5	0	0	0	0
2	u	11	0	0	0	0
2	v	6	0	0	0	0
All	All	23282	0	22813	520	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 11.

All (520) 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:r:21:THR:HG22	1:r:24:GLU:HG3	1.46	0.96
1:Y:21:THR:HG22	1:Y:24:GLU:HG3	1.50	0.91
1:K:32:ALA:HB3	1:K:40:LEU:HD12	1.53	0.90
1:Q:20:GLN:HB3	2:Q:101:HOH:O	1.76	0.85
1:M:21:THR:HG23	1:M:23:SER:H	1.43	0.84
1:Q:24:GLU:HB2	2:Q:101:HOH:O	1.78	0.82
1:b:33:LEU:HD22	1:c:53:HIS:HE1	1.45	0.81
1:N:29:VAL:HG12	1:N:40:LEU:HD11	1.66	0.78
1:B:29:VAL:HG11	1:B:60:VAL:HG11	1.65	0.78
1:Y:48:ARG:HG2	1:f:63:GLY:HA2	1.66	0.78
1:I:21:THR:HG23	1:I:23:SER:H	1.47	0.78
1:g:29:VAL:HG11	1:g:60:VAL:HG21	1.64	0.77
1:D:29:VAL:HG11	1:D:60:VAL:HG11	1.66	0.77
1:O:21:THR:HG23	1:O:23:SER:H	1.50	0.77
1:K:29:VAL:HG11	1:K:60:VAL:HG21	1.67	0.76
1:s:4:LYS:HG2	1:s:15:VAL:HG12	1.67	0.76
1:J:5:ILE:HG12	1:J:60:VAL:HG13	1.68	0.75
1:f:29:VAL:HG11	1:f:60:VAL:HG21	1.69	0.75
1:u:5:ILE:HG12	1:u:60:VAL:HG13	1.70	0.74
1:E:29:VAL:HG11	1:E:60:VAL:HG11	1.70	0.74
1:L:5:ILE:HG12	1:L:60:VAL:HG13	1.70	0.74
1:M:29:VAL:HG22	1:M:40:LEU:HD11	1.71	0.73
1:f:5:ILE:HG12	1:f:60:VAL:HG12	1.69	0.73
1:s:5:ILE:HG12	1:s:60:VAL:HG13	1.70	0.73
1:L:21:THR:HG23	1:L:23:SER:H	1.54	0.72
1:I:5:ILE:HG12	1:I:60:VAL:HG13	1.71	0.72
1:h:46:ARG:HH22	1:o:46:ARG:HB3	1.54	0.71
1:j:29:VAL:HG11	1:j:60:VAL:HG21	1.71	0.71
1:q:5:ILE:HG12	1:q:60:VAL:HG13	1.72	0.71
1:K:29:VAL:HA	1:K:40:LEU:HD11	1.72	0.71
1:O:62:ILE:HG22	1:P:49:ARG:HB2	1.72	0.70
1:B:39:LEU:HD11	1:B:51:MSE:HB3	1.72	0.70
1:b:5:ILE:HG12	1:b:60:VAL:HG13	1.74	0.69
1:r:7:ILE:HG21	1:s:58:ALA:HB1	1.75	0.69
1:i:29:VAL:HG11	1:i:60:VAL:HG21	1.75	0.69
1:a:21:THR:HG22	1:a:24:GLU:H	1.59	0.68
1:P:29:VAL:HG21	1:P:60:VAL:HG21	1.74	0.68
1:v:21:THR:HG22	1:v:24:GLU:HG3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:v:21:THR:HG23	1:v:23:SER:H	1.58	0.68
1:V:9:ASP:HB2	1:V:56:ARG:HH22	1.59	0.68
1:P:5:ILE:HG12	1:P:60:VAL:HG12	1.74	0.67
1:Z:5:ILE:HG12	1:Z:60:VAL:HG13	1.75	0.67
1:M:5:ILE:HG12	1:M:60:VAL:HG13	1.76	0.67
1:Z:4:LYS:HG2	1:Z:15:VAL:HG12	1.77	0.67
1:K:4:LYS:HB3	1:K:13:GLU:OE2	1.95	0.67
1:n:41:THR:HG23	1:n:51:MSE:HG2	1.76	0.66
1:m:1:VAL:HG11	1:m:22:PRO:HG3	1.77	0.66
1:a:21:THR:HG23	1:a:23:SER:H	1.61	0.66
1:m:5:ILE:HG12	1:m:60:VAL:HG12	1.76	0.66
1:K:21:THR:HG23	1:K:23:SER:H	1.59	0.66
1:o:58:ALA:HB1	1:v:7:ILE:HG21	1.77	0.66
1:m:29:VAL:HG21	1:m:60:VAL:HG21	1.78	0.66
1:E:9:ASP:HB2	1:E:56:ARG:HH22	1.60	0.66
1:l:5:ILE:HG12	1:l:60:VAL:HG12	1.78	0.66
1:I:21:THR:HG22	1:I:24:GLU:HG3	1.78	0.66
1:t:5:ILE:HG12	1:t:60:VAL:HG13	1.77	0.65
1:a:5:ILE:HG12	1:a:60:VAL:HG13	1.77	0.65
1:L:33:LEU:HA	1:L:54:THR:HG21	1.78	0.65
1:c:29:VAL:HG11	1:c:60:VAL:HG21	1.79	0.64
1:Y:7:ILE:HG21	1:f:58:ALA:HB1	1.79	0.64
1:g:6:GLY:HA2	1:g:13:GLU:HG2	1.80	0.64
1:p:7:ILE:HG21	1:q:58:ALA:HB1	1.79	0.64
1:E:5:ILE:HG21	1:E:52:ILE:HD13	1.79	0.64
1:n:5:ILE:HG12	1:n:60:VAL:HG13	1.78	0.64
1:I:29:VAL:HG22	1:I:40:LEU:HD11	1.80	0.64
1:O:29:VAL:HG22	1:O:40:LEU:HD11	1.79	0.64
1:e:33:LEU:HD23	1:e:54:THR:HG22	1.80	0.64
1:o:48:ARG:HG2	1:p:63:GLY:HA2	1.80	0.64
1:A:5:ILE:HG12	1:A:60:VAL:HG13	1.80	0.63
1:S:41:THR:HG22	1:S:51:MSE:HG2	1.80	0.63
1:U:4:LYS:HG2	1:U:15:VAL:HG22	1.78	0.63
1:h:21:THR:HG23	1:h:23:SER:H	1.64	0.63
1:O:21:THR:HG22	1:O:24:GLU:H	1.64	0.63
1:Y:19:ALA:HB2	1:Y:45:GLU:HG3	1.80	0.62
1:v:41:THR:HA	1:v:50:PHE:O	1.98	0.62
1:g:61:GLU:HG2	1:h:48:ARG:HD2	1.82	0.62
1:j:33:LEU:HD22	1:k:53:HIS:NE2	2.15	0.62
1:F:54:THR:HA	1:F:57:ILE:HD12	1.82	0.61
1:k:33:LEU:HD22	1:l:53:HIS:NE2	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:q:53:HIS:HA	2:q:101:HOH:O	2.00	0.61
1:g:53:HIS:NE2	1:n:33:LEU:HD22	2.15	0.61
1:k:60:VAL:HG23	1:l:51:MSE:HB2	1.81	0.61
1:m:24:GLU:O	1:m:28:LEU:HD23	2.00	0.61
1:J:33:LEU:HD12	1:K:39:LEU:HD22	1.83	0.61
1:m:7:ILE:HB	1:m:10:SER:HB2	1.83	0.61
1:k:19:ALA:HB2	1:k:45:GLU:HG2	1.82	0.60
1:U:5:ILE:HG12	1:U:60:VAL:HG13	1.82	0.60
1:e:5:ILE:HG12	2:e:101:HOH:O	2.01	0.60
1:i:21:THR:HG23	1:i:24:GLU:H	1.66	0.60
1:l:60:VAL:HG23	1:m:51:MSE:HB2	1.83	0.60
1:l:62:ILE:HG23	1:l:63:GLY:H	1.65	0.60
1:m:44:ASP:HB3	1:m:48:ARG:H	1.66	0.60
1:I:3:VAL:HG23	1:I:4:LYS:HG3	1.83	0.60
1:W:39:LEU:HD23	1:X:34:ARG:HH21	1.67	0.60
1:K:39:LEU:HD21	1:K:51:MSE:HE2	1.84	0.60
1:A:53:HIS:CE1	1:H:33:LEU:HD22	2.36	0.59
1:J:33:LEU:HD22	1:K:53:HIS:HE1	1.67	0.59
1:P:50:PHE:HB3	1:P:52:ILE:HD11	1.84	0.59
1:L:16:PHE:HB2	1:L:44:ASP:OD1	2.02	0.59
1:S:4:LYS:HG2	1:S:15:VAL:HG22	1.83	0.59
1:J:21:THR:HG23	1:J:23:SER:H	1.67	0.59
1:k:63:GLY:HA3	1:l:48:ARG:HG2	1.85	0.59
1:l:7:ILE:HB	1:l:10:SER:HB2	1.83	0.59
1:c:5:ILE:HG12	1:c:60:VAL:HG12	1.85	0.59
1:q:39:LEU:HA	2:q:101:HOH:O	2.03	0.59
1:s:48:ARG:HG2	1:t:64:VAL:HG13	1.85	0.59
1:F:5:ILE:HG12	1:F:60:VAL:HG13	1.85	0.58
1:Q:26:GLU:HG3	1:X:51:MSE:SE	2.53	0.58
1:r:51:MSE:HE3	1:s:60:VAL:HB	1.84	0.58
1:n:7:ILE:HB	1:n:10:SER:HB2	1.85	0.58
1:n:29:VAL:O	1:n:33:LEU:HG	2.02	0.58
1:D:1:VAL:HG11	1:D:22:PRO:HG3	1.85	0.58
1:K:30:SER:HB3	1:L:51:MSE:HE1	1.85	0.58
1:o:20:GLN:O	1:o:24:GLU:HB3	2.03	0.58
1:r:45:GLU:HG3	1:r:46:ARG:HE	1.69	0.58
1:T:38:GLY:HA2	1:T:54:THR:OG1	2.04	0.58
1:V:9:ASP:HB2	1:V:56:ARG:NH2	2.19	0.58
1:i:11:PRO:HB2	1:q:11:PRO:HB2	1.84	0.58
1:C:5:ILE:HG12	1:C:60:VAL:HG13	1.85	0.58
1:I:53:HIS:NE2	1:P:33:LEU:HD22	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:GLU:HG3	1:E:51:MSE:SE	2.54	0.57
1:h:7:ILE:HB	1:h:10:SER:HB2	1.86	0.57
1:m:53:HIS:HB3	2:m:101:HOH:O	2.03	0.57
1:p:5:ILE:HG12	1:p:60:VAL:HG13	1.86	0.57
1:T:5:ILE:HG12	1:T:60:VAL:HG13	1.86	0.57
1:K:39:LEU:HD11	1:K:51:MSE:HB3	1.87	0.56
1:l:33:LEU:HD22	1:m:53:HIS:NE2	2.20	0.56
1:Y:29:VAL:HG11	1:Y:60:VAL:HG11	1.88	0.56
1:k:23:SER:O	1:k:27:GLU:HG2	2.05	0.56
1:E:24:GLU:HB2	2:E:101:HOH:O	2.04	0.56
1:e:63:GLY:HA2	1:f:48:ARG:HG3	1.86	0.56
1:h:33:LEU:HD22	1:i:53:HIS:NE2	2.21	0.56
1:q:39:LEU:HD23	1:r:34:ARG:HH21	1.71	0.56
1:E:4:LYS:O	1:E:60:VAL:HA	2.07	0.55
1:g:29:VAL:HG22	1:g:40:LEU:HD21	1.88	0.55
1:V:53:HIS:NE2	1:W:33:LEU:HD22	2.21	0.55
1:N:26:GLU:HG3	1:O:51:MSE:SE	2.56	0.55
1:R:28:LEU:HB2	2:R:102:HOH:O	2.04	0.55
1:m:60:VAL:HG23	1:n:51:MSE:HB2	1.89	0.55
1:W:7:ILE:HB	1:W:10:SER:HB2	1.88	0.55
1:i:15:VAL:HG21	1:q:15:VAL:HG11	1.88	0.55
1:Q:51:MSE:HE3	1:R:60:VAL:HB	1.88	0.55
1:N:33:LEU:HD22	1:O:53:HIS:CE1	2.42	0.55
1:O:60:VAL:HG13	1:P:51:MSE:HB2	1.89	0.55
1:n:7:ILE:HD11	1:n:14:LEU:HD23	1.89	0.55
1:B:4:LYS:HG2	1:B:15:VAL:HG22	1.89	0.55
1:t:44:ASP:OD2	1:t:48:ARG:HD2	2.07	0.55
1:X:5:ILE:HG12	1:X:60:VAL:HG13	1.88	0.55
1:g:54:THR:O	1:h:53:HIS:HE1	1.90	0.55
1:Q:63:GLY:HA2	1:X:48:ARG:HG2	1.87	0.54
1:A:12:ARG:HE	1:A:13:GLU:H	1.55	0.54
1:f:7:ILE:HA	1:f:56:ARG:O	2.06	0.54
1:h:62:ILE:HG23	1:h:63:GLY:H	1.72	0.54
1:C:33:LEU:HD22	1:D:53:HIS:CE1	2.42	0.54
1:b:58:ALA:HB1	1:c:7:ILE:HG21	1.89	0.54
1:I:51:MSE:HB2	1:P:60:VAL:HG23	1.90	0.54
1:l:48:ARG:HH21	1:s:46:ARG:HH12	1.55	0.54
1:t:33:LEU:HD21	1:t:57:ILE:HD12	1.89	0.54
1:K:5:ILE:HG12	1:K:60:VAL:HG12	1.90	0.54
1:m:26:GLU:HG2	1:n:51:MSE:SE	2.57	0.54
1:r:53:HIS:NE2	1:s:33:LEU:HD22	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:7:ILE:HD11	1:R:14:LEU:HG	1.90	0.54
1:h:29:VAL:HG22	1:h:40:LEU:HD21	1.88	0.54
1:A:38:GLY:O	1:A:53:HIS:HA	2.08	0.54
1:X:29:VAL:HG22	1:X:40:LEU:HD21	1.90	0.54
1:h:29:VAL:O	1:h:33:LEU:HG	2.07	0.54
1:q:7:ILE:HB	1:q:10:SER:HB3	1.90	0.54
1:A:7:ILE:HG21	1:H:58:ALA:HB1	1.90	0.53
1:I:4:LYS:HB3	1:I:13:GLU:OE2	2.08	0.53
1:Z:58:ALA:HB1	1:a:7:ILE:HG21	1.90	0.53
1:J:29:VAL:O	1:J:33:LEU:HG	2.08	0.53
1:X:32:ALA:C	1:X:34:ARG:H	2.16	0.53
1:X:38:GLY:HA2	1:X:54:THR:OG1	2.08	0.53
1:r:5:ILE:HG12	1:r:60:VAL:HG13	1.89	0.53
1:K:7:ILE:HB	1:K:10:SER:HB3	1.88	0.53
1:Q:33:LEU:HD22	1:X:53:HIS:NE2	2.23	0.53
1:o:38:GLY:O	1:o:53:HIS:HA	2.08	0.53
1:J:8:THR:HG22	1:J:9:ASP:OD2	2.08	0.53
1:I:16:PHE:HB2	1:I:44:ASP:OD1	2.08	0.53
1:G:8:THR:HG22	1:H:56:ARG:HE	1.74	0.53
1:l:25:VAL:HG21	1:l:62:ILE:HD13	1.91	0.53
1:d:44:ASP:OD2	1:d:48:ARG:HD2	2.09	0.53
1:s:1:VAL:HG13	1:s:18:SER:HB3	1.91	0.53
1:G:38:GLY:O	1:G:53:HIS:HA	2.09	0.53
1:e:5:ILE:HB	1:e:14:LEU:HB2	1.91	0.53
1:j:24:GLU:O	1:j:28:LEU:HD23	2.08	0.53
1:B:7:ILE:HB	1:B:10:SER:HB3	1.89	0.52
1:E:13:GLU:HA	2:E:102:HOH:O	2.09	0.52
1:F:26:GLU:HG3	1:G:51:MSE:SE	2.59	0.52
1:O:29:VAL:HG11	1:O:60:VAL:HG11	1.90	0.52
1:l:63:GLY:HA2	1:m:48:ARG:HA	1.92	0.52
1:G:5:ILE:HG21	1:G:52:ILE:HD13	1.90	0.52
1:G:33:LEU:HD22	1:H:53:HIS:CE1	2.44	0.52
1:L:39:LEU:HD21	1:L:51:MSE:HE2	1.91	0.52
1:X:9:ASP:HB2	1:X:56:ARG:HH22	1.73	0.52
1:S:23:SER:O	1:S:27:GLU:HG2	2.09	0.52
1:u:56:ARG:HE	1:v:8:THR:HG21	1.75	0.52
1:L:29:VAL:HG21	1:L:60:VAL:HG21	1.92	0.52
1:E:4:LYS:HD3	1:E:13:GLU:OE2	2.10	0.52
1:L:4:LYS:HB2	1:L:61:GLU:HB3	1.91	0.52
1:Y:60:VAL:HG13	1:Z:51:MSE:HB2	1.92	0.52
1:e:60:VAL:HG13	2:e:101:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:m:33:LEU:HD22	1:n:53:HIS:NE2	2.25	0.52
1:C:38:GLY:HA2	1:C:54:THR:OG1	2.09	0.52
1:M:25:VAL:HG22	1:M:28:LEU:HD12	1.92	0.52
1:X:38:GLY:O	1:X:53:HIS:HA	2.10	0.52
1:N:29:VAL:O	1:N:33:LEU:HG	2.09	0.52
1:i:39:LEU:HD21	1:i:51:MSE:HE2	1.91	0.51
1:J:29:VAL:HG22	1:J:40:LEU:HD21	1.92	0.51
1:F:27:GLU:OE2	1:p:42:LEU:HA	2.10	0.51
1:c:48:ARG:HH12	1:j:31:ASN:ND2	2.07	0.51
1:t:38:GLY:O	1:t:53:HIS:HA	2.10	0.51
1:G:8:THR:CG2	1:H:56:ARG:HE	2.23	0.51
1:P:29:VAL:O	1:P:33:LEU:HG	2.10	0.51
1:c:5:ILE:HB	1:c:14:LEU:HB2	1.93	0.51
1:a:33:LEU:HD21	1:a:57:ILE:HD12	1.91	0.51
1:W:5:ILE:HG12	1:W:60:VAL:HG13	1.93	0.51
1:W:8:THR:HG23	1:W:56:ARG:C	2.36	0.51
1:g:11:PRO:HB2	1:o:11:PRO:HB2	1.93	0.51
1:G:13:GLU:HB2	1:O:34:ARG:HE	1.75	0.51
1:K:20:GLN:HB3	1:K:24:GLU:HB3	1.93	0.51
1:a:41:THR:HA	1:a:50:PHE:O	2.11	0.51
1:r:40:LEU:HD12	2:r:102:HOH:O	2.10	0.51
1:t:7:ILE:HG21	1:u:58:ALA:HB1	1.92	0.51
1:D:58:ALA:HB1	1:E:7:ILE:HG21	1.92	0.51
1:L:58:ALA:HB1	1:M:7:ILE:HG21	1.93	0.51
1:v:21:THR:HG22	1:v:24:GLU:H	1.76	0.51
1:D:33:LEU:HD22	1:E:53:HIS:NE2	2.25	0.50
1:j:5:ILE:HG23	1:j:14:LEU:HB2	1.92	0.50
1:E:20:GLN:HB3	2:E:101:HOH:O	2.10	0.50
1:e:19:ALA:HB2	1:e:45:GLU:HG2	1.93	0.50
1:F:31:ASN:OD1	1:p:43:THR:HG21	2.10	0.50
1:G:57:ILE:HG23	2:G:101:HOH:O	2.11	0.50
1:n:29:VAL:HG22	1:n:40:LEU:HD21	1.93	0.50
1:i:23:SER:O	1:i:27:GLU:HG2	2.11	0.50
1:B:58:ALA:HB1	1:C:7:ILE:HG21	1.94	0.50
1:B:33:LEU:HD22	1:C:53:HIS:NE2	2.27	0.50
1:c:24:GLU:OE1	1:c:24:GLU:HA	2.10	0.50
1:F:27:GLU:OE2	1:p:42:LEU:HD23	2.12	0.50
1:Q:4:LYS:HG2	1:Q:15:VAL:HG22	1.94	0.50
1:q:51:MSE:HE1	1:r:62:ILE:HD12	1.92	0.50
1:h:20:GLN:O	1:h:21:THR:HB	2.12	0.49
1:T:21:THR:O	1:T:25:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:34:ARG:HD3	2:U:103:HOH:O	2.11	0.49
1:c:33:LEU:HD23	1:c:54:THR:HG22	1.94	0.49
1:K:63:GLY:HA2	1:L:48:ARG:HG2	1.94	0.49
1:H:38:GLY:O	1:H:53:HIS:HA	2.12	0.49
1:e:38:GLY:O	1:e:53:HIS:HA	2.13	0.49
1:e:7:ILE:C	1:e:9:ASP:H	2.21	0.49
1:o:2:GLU:OE2	1:o:4:LYS:HE3	2.11	0.49
1:T:41:THR:HA	1:T:50:PHE:O	2.13	0.49
1:Y:41:THR:HG23	1:Y:51:MSE:HG2	1.95	0.49
1:v:60:VAL:O	1:v:61:GLU:HB3	2.12	0.49
1:E:13:GLU:HG3	2:E:102:HOH:O	2.12	0.49
1:c:63:GLY:HA2	1:d:48:ARG:HG2	1.94	0.49
1:l:33:LEU:HD22	1:m:53:HIS:HE2	1.78	0.49
1:V:7:ILE:HD11	1:V:14:LEU:HG	1.95	0.49
1:M:5:ILE:HG21	1:M:52:ILE:HD13	1.95	0.49
1:M:21:THR:HG22	1:M:24:GLU:HG3	1.94	0.49
1:V:38:GLY:O	1:V:53:HIS:HA	2.13	0.49
2:F:104:HOH:O	1:G:53:HIS:HB2	2.12	0.48
1:E:15:VAL:O	1:M:34:ARG:HD2	2.13	0.48
1:A:60:VAL:HB	1:B:51:MSE:HE3	1.96	0.48
1:K:38:GLY:H	1:K:54:THR:HG21	1.79	0.48
1:X:29:VAL:O	1:X:33:LEU:HD13	2.13	0.48
1:K:21:THR:O	1:K:25:VAL:HG23	2.13	0.48
1:k:26:GLU:HG3	1:l:51:MSE:SE	2.63	0.48
1:H:41:THR:HA	1:H:50:PHE:O	2.14	0.48
1:S:16:PHE:HB2	1:S:44:ASP:OD1	2.13	0.48
1:S:51:MSE:HE3	1:T:60:VAL:HB	1.96	0.48
1:a:4:LYS:HG2	1:a:15:VAL:HG22	1.96	0.48
1:A:41:THR:HA	1:A:50:PHE:O	2.14	0.48
1:O:21:THR:HG22	1:O:24:GLU:HG3	1.96	0.48
1:e:4:LYS:HG2	1:e:15:VAL:HG12	1.96	0.48
1:E:4:LYS:HG2	1:E:15:VAL:HG22	1.96	0.47
1:p:4:LYS:HE2	1:p:13:GLU:OE1	2.14	0.47
1:I:33:LEU:HD22	1:J:53:HIS:NE2	2.29	0.47
1:u:49:ARG:HD2	1:v:26:GLU:OE2	2.13	0.47
1:l:29:VAL:O	1:l:33:LEU:HG	2.13	0.47
1:M:31:ASN:ND2	1:M:34:ARG:HH21	2.12	0.47
1:a:30:SER:O	1:a:34:ARG:HG2	2.13	0.47
1:d:33:LEU:HD21	1:d:57:ILE:HD12	1.97	0.47
1:l:48:ARG:HH21	1:s:46:ARG:NH1	2.12	0.47
1:t:41:THR:HG23	1:t:51:MSE:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:33:LEU:HG	1:M:53:HIS:NE2	2.29	0.47
1:M:30:SER:OG	1:N:51:MSE:HE1	2.15	0.47
1:c:45:GLU:HG3	1:c:46:ARG:HG3	1.96	0.47
1:k:5:ILE:HD12	1:k:61:GLU:H	1.80	0.47
1:l:58:ALA:HB1	1:m:7:ILE:HG21	1.97	0.47
1:o:49:ARG:HH12	1:p:23:SER:HA	1.80	0.47
1:J:62:ILE:HB	1:K:49:ARG:HB2	1.96	0.47
1:j:16:PHE:HZ	1:j:42:LEU:HD22	1.80	0.47
1:C:38:GLY:O	1:C:53:HIS:HA	2.15	0.47
1:I:30:SER:OG	1:J:51:MSE:HE1	2.15	0.47
1:g:48:ARG:CZ	1:v:48:ARG:HH21	2.27	0.47
1:h:33:LEU:HA	1:h:54:THR:HG21	1.96	0.47
1:K:4:LYS:HG2	1:K:15:VAL:HG22	1.97	0.47
1:M:31:ASN:HD22	1:M:34:ARG:HH21	1.63	0.47
1:X:33:LEU:H	1:X:54:THR:HG21	1.80	0.47
1:s:51:MSE:HE1	1:t:30:SER:HB3	1.97	0.46
1:g:62:ILE:HG22	1:h:49:ARG:HB2	1.97	0.46
1:B:26:GLU:HG3	1:C:51:MSE:SE	2.65	0.46
1:W:33:LEU:HD21	1:W:57:ILE:HD12	1.97	0.46
1:d:4:LYS:HG2	1:d:15:VAL:HG22	1.98	0.46
1:g:7:ILE:HD11	1:g:52:ILE:HD11	1.97	0.46
1:r:41:THR:HA	1:r:50:PHE:O	2.16	0.46
1:J:33:LEU:HD22	1:K:53:HIS:CE1	2.50	0.46
1:K:3:VAL:HG22	1:K:62:ILE:HD13	1.98	0.46
1:S:49:ARG:HH21	1:T:22:PRO:HB2	1.80	0.46
1:l:4:LYS:HG2	1:l:15:VAL:HG13	1.98	0.46
1:F:6:GLY:O	1:F:58:ALA:HB3	2.16	0.46
1:O:30:SER:OG	1:P:51:MSE:HE1	2.15	0.46
1:W:51:MSE:HE3	1:X:60:VAL:HB	1.98	0.46
1:k:24:GLU:O	1:k:28:LEU:HD23	2.16	0.46
1:l:48:ARG:NH2	1:s:46:ARG:HH12	2.13	0.46
1:m:4:LYS:HG2	1:m:15:VAL:HG22	1.98	0.46
1:F:29:VAL:O	1:F:33:LEU:HD13	2.16	0.46
1:Y:18:SER:OG	1:Y:20:GLN:HB2	2.16	0.46
1:b:27:GLU:HG2	1:b:31:ASN:OD1	2.16	0.46
1:f:21:THR:C	1:f:23:SER:H	2.23	0.46
1:n:33:LEU:HA	1:n:54:THR:HG21	1.97	0.46
1:v:38:GLY:O	1:v:53:HIS:HA	2.16	0.46
1:C:33:LEU:HD22	1:D:53:HIS:HE1	1.81	0.46
1:H:5:ILE:HG12	1:H:60:VAL:HG13	1.98	0.46
1:k:30:SER:OG	1:l:51:MSE:HE1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:k:58:ALA:HB1	1:l:7:ILE:HG21	1.98	0.46
1:E:9:ASP:HB2	1:E:56:ARG:NH2	2.29	0.46
1:I:25:VAL:HG23	1:I:62:ILE:HD13	1.98	0.46
1:B:33:LEU:HD21	1:B:57:ILE:HD12	1.98	0.45
1:m:46:ARG:HH12	1:t:48:ARG:HH21	1.63	0.45
1:C:8:THR:CG2	1:D:56:ARG:HD2	2.45	0.45
1:c:12:ARG:HD2	1:c:12:ARG:HA	1.76	0.45
1:k:61:GLU:OE2	1:l:48:ARG:NH1	2.48	0.45
1:X:32:ALA:O	1:X:33:LEU:HB2	2.17	0.45
1:A:6:GLY:HA2	2:A:103:HOH:O	2.16	0.45
1:L:5:ILE:HB	1:L:14:LEU:HB2	1.99	0.45
1:j:29:VAL:O	1:j:33:LEU:HG	2.16	0.45
1:u:49:ARG:O	1:v:61:GLU:HA	2.16	0.45
1:U:23:SER:O	1:U:27:GLU:HG2	2.17	0.45
1:A:13:GLU:HA	2:A:103:HOH:O	2.15	0.45
1:O:62:ILE:HD12	1:O:62:ILE:HA	1.83	0.45
1:Q:8:THR:HB	1:X:56:ARG:NH2	2.32	0.45
1:U:29:VAL:HG22	1:U:40:LEU:HD21	1.99	0.45
1:U:56:ARG:HA	1:U:56:ARG:NE	2.31	0.45
1:b:33:LEU:HD21	1:b:57:ILE:HD12	1.98	0.45
1:i:12:ARG:NH2	1:p:12:ARG:HD2	2.31	0.45
1:l:24:GLU:O	1:l:28:LEU:HD23	2.15	0.45
1:m:62:ILE:HG22	1:n:49:ARG:HB2	1.97	0.45
1:T:5:ILE:HB	1:T:14:LEU:HB2	1.99	0.45
1:A:53:HIS:HB2	2:H:101:HOH:O	2.15	0.45
1:M:7:ILE:HD11	1:M:14:LEU:HG	1.98	0.45
1:c:15:VAL:HG21	1:j:34:ARG:NH2	2.32	0.45
1:p:9:ASP:HB3	1:q:9:ASP:OD1	2.16	0.45
1:v:5:ILE:HB	1:v:14:LEU:HB2	1.99	0.45
1:F:38:GLY:HA2	1:F:54:THR:OG1	2.17	0.45
1:e:61:GLU:OE2	1:f:48:ARG:HD3	2.17	0.45
1:q:54:THR:N	2:q:101:HOH:O	2.48	0.45
1:C:4:LYS:HG2	1:C:15:VAL:HG22	1.98	0.45
1:G:54:THR:O	1:G:57:ILE:HB	2.17	0.45
1:S:29:VAL:O	1:S:33:LEU:HD13	2.17	0.45
1:V:38:GLY:HA2	1:V:54:THR:OG1	2.17	0.45
1:e:7:ILE:HD11	1:e:14:LEU:HG	1.99	0.45
1:a:33:LEU:HD23	1:a:54:THR:HG22	1.99	0.44
1:b:33:LEU:HD22	1:c:53:HIS:CE1	2.37	0.44
1:j:63:GLY:HA2	1:k:48:ARG:HD3	1.99	0.44
1:k:29:VAL:O	1:k:33:LEU:HG	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:l:33:LEU:HD12	1:m:39:LEU:HD22	1.98	0.44
1:p:12:ARG:HG2	1:p:13:GLU:N	2.32	0.44
1:t:21:THR:HG23	1:t:24:GLU:H	1.82	0.44
1:Q:58:ALA:HB1	1:X:7:ILE:HG21	2.00	0.44
1:R:7:ILE:HB	1:R:10:SER:HB3	1.98	0.44
1:U:12:ARG:HG2	1:U:13:GLU:H	1.82	0.44
1:a:43:THR:HG22	1:a:44:ASP:O	2.17	0.44
1:m:33:LEU:HD23	1:m:54:THR:HG23	1.99	0.44
1:F:57:ILE:O	1:F:59:TYR:N	2.49	0.44
1:o:5:ILE:HB	1:o:14:LEU:HB2	1.99	0.44
1:B:63:GLY:HA2	1:C:48:ARG:HG2	1.99	0.44
1:L:41:THR:HG23	1:L:51:MSE:HG2	1.99	0.44
1:O:26:GLU:HG3	1:P:51:MSE:SE	2.67	0.44
1:R:1:VAL:HG21	1:R:22:PRO:HD3	2.00	0.44
1:W:54:THR:N	2:W:102:HOH:O	2.50	0.44
1:i:8:THR:HG21	1:j:56:ARG:HE	1.83	0.44
1:M:54:THR:HA	1:M:57:ILE:HG13	1.99	0.44
1:d:7:ILE:HB	1:d:10:SER:HB3	2.00	0.44
1:D:38:GLY:HA2	1:D:54:THR:OG1	2.18	0.44
1:G:13:GLU:H	1:O:34:ARG:HE	1.66	0.44
1:q:44:ASP:HB2	1:q:50:PHE:HE1	1.83	0.44
1:A:22:PRO:HB2	1:B:49:ARG:HH21	1.83	0.44
1:h:21:THR:O	1:h:25:VAL:HG22	2.18	0.44
1:j:60:VAL:HG23	1:k:51:MSE:HB2	1.98	0.44
1:L:30:SER:OG	1:M:51:MSE:HE1	2.18	0.44
1:Y:5:ILE:HB	1:Y:14:LEU:HB2	2.00	0.44
1:G:5:ILE:HG12	1:G:60:VAL:HG13	2.00	0.43
1:G:38:GLY:HA2	1:G:54:THR:OG1	2.17	0.43
1:U:56:ARG:HD2	1:V:8:THR:CG2	2.48	0.43
1:m:5:ILE:HB	1:m:14:LEU:HB2	1.99	0.43
1:D:20:GLN:HB3	1:D:24:GLU:HB2	1.98	0.43
1:W:46:ARG:NH2	1:W:48:ARG:HH12	2.15	0.43
1:F:54:THR:O	1:F:57:ILE:HB	2.19	0.43
1:d:58:ALA:HB1	1:e:7:ILE:HG21	2.00	0.43
1:r:29:VAL:O	1:r:33:LEU:HG	2.17	0.43
1:t:35:ASP:O	1:t:36:ASP:OD1	2.37	0.43
1:Q:10:SER:HB2	2:R:101:HOH:O	2.19	0.43
1:Z:27:GLU:HG2	1:Z:31:ASN:OD1	2.18	0.43
1:l:29:VAL:HG11	1:l:60:VAL:HG21	2.00	0.43
1:n:39:LEU:HD21	1:n:51:MSE:HE2	2.00	0.43
1:B:30:SER:HB2	1:C:51:MSE:HE1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:32:ALA:CB	1:K:40:LEU:HD12	2.36	0.43
1:R:5:ILE:HB	1:R:14:LEU:HB2	2.01	0.43
1:U:33:LEU:HD21	1:U:57:ILE:HD12	2.01	0.43
1:W:41:THR:HG23	1:W:51:MSE:CG	2.48	0.43
1:h:21:THR:CG2	1:h:24:GLU:H	2.32	0.43
1:E:7:ILE:HD11	1:E:14:LEU:HG	2.01	0.43
1:Q:21:THR:O	1:Q:25:VAL:HG23	2.18	0.43
1:W:33:LEU:HD23	1:W:54:THR:HG22	2.00	0.43
1:A:48:ARG:HH22	1:I:31:ASN:ND2	2.16	0.43
1:F:64:VAL:HG11	1:G:46:ARG:O	2.18	0.43
1:K:46:ARG:HD3	1:K:46:ARG:HA	1.86	0.43
1:K:33:LEU:HD22	1:L:53:HIS:CE1	2.54	0.43
1:P:33:LEU:HA	1:P:54:THR:HG21	2.00	0.43
1:g:39:LEU:HD12	1:g:52:ILE:O	2.19	0.43
1:h:40:LEU:HB3	1:h:52:ILE:CG2	2.49	0.43
1:g:30:SER:OG	1:h:51:MSE:HE1	2.19	0.42
1:h:33:LEU:HD12	1:i:39:LEU:HD22	2.00	0.42
1:B:51:MSE:HE3	1:B:51:MSE:HB2	1.98	0.42
1:E:21:THR:N	2:E:101:HOH:O	2.51	0.42
1:M:41:THR:O	1:M:42:LEU:HD23	2.18	0.42
1:Q:5:ILE:HG12	1:Q:60:VAL:HG13	2.01	0.42
1:Z:38:GLY:O	1:Z:53:HIS:HA	2.20	0.42
1:k:21:THR:HG23	1:k:24:GLU:OE2	2.20	0.42
1:m:44:ASP:OD2	1:m:46:ARG:NE	2.49	0.42
1:O:32:ALA:HB3	1:O:40:LEU:HD12	2.00	0.42
1:j:22:PRO:HA	1:j:25:VAL:HG22	2.00	0.42
1:u:38:GLY:O	1:u:39:LEU:HB2	2.18	0.42
1:A:8:THR:HG23	1:A:56:ARG:C	2.45	0.42
1:H:33:LEU:HD23	1:H:54:THR:HG22	2.00	0.42
1:S:38:GLY:HA2	1:S:54:THR:OG1	2.19	0.42
1:e:29:VAL:HG21	1:e:60:VAL:HG11	2.01	0.42
1:C:14:LEU:HD13	1:C:52:ILE:HD11	2.02	0.42
1:r:21:THR:O	1:r:25:VAL:HG23	2.19	0.42
1:r:51:MSE:HE3	1:r:51:MSE:HB2	1.88	0.42
1:A:12:ARG:HD2	1:A:12:ARG:HA	1.86	0.42
1:R:3:VAL:HG21	1:R:25:VAL:HG11	2.01	0.42
1:W:39:LEU:HA	2:W:102:HOH:O	2.19	0.42
1:C:7:ILE:HD11	1:C:14:LEU:HD12	2.02	0.42
1:I:31:ASN:HA	1:I:34:ARG:HG2	2.02	0.42
1:K:4:LYS:HB2	1:K:61:GLU:HB3	2.01	0.42
1:L:26:GLU:HG3	1:M:51:MSE:SE	2.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:62:ILE:HB	1:M:49:ARG:HB2	2.02	0.42
1:a:26:GLU:HG3	1:b:51:MSE:SE	2.70	0.42
1:e:43:THR:HG22	1:e:44:ASP:O	2.20	0.42
1:i:44:ASP:HB2	1:i:50:PHE:HE1	1.84	0.42
1:j:30:SER:HB2	1:k:51:MSE:HE1	2.02	0.42
1:o:20:GLN:O	1:o:21:THR:HG22	2.20	0.42
1:F:8:THR:O	1:F:9:ASP:HB2	2.19	0.41
1:n:22:PRO:HA	1:n:25:VAL:HG22	2.02	0.41
1:o:51:MSE:SE	1:p:26:GLU:HG3	2.70	0.41
1:B:43:THR:HG22	1:B:44:ASP:O	2.21	0.41
1:E:35:ASP:OD1	1:E:36:ASP:N	2.53	0.41
1:G:57:ILE:HG22	2:G:102:HOH:O	2.19	0.41
1:K:41:THR:O	1:K:42:LEU:HD12	2.20	0.41
1:V:56:ARG:HA	1:V:56:ARG:HD2	1.72	0.41
1:X:9:ASP:HB2	1:X:56:ARG:NH2	2.35	0.41
1:i:12:ARG:NH1	1:p:12:ARG:HD2	2.35	0.41
1:j:3:VAL:HG22	1:j:62:ILE:HD13	2.02	0.41
1:j:40:LEU:O	1:j:52:ILE:HG22	2.21	0.41
1:r:43:THR:HG22	1:r:44:ASP:O	2.20	0.41
1:B:37:SER:C	1:B:39:LEU:H	2.28	0.41
1:V:43:THR:HG22	1:V:44:ASP:O	2.20	0.41
1:v:29:VAL:O	1:v:33:LEU:HG	2.21	0.41
1:D:4:LYS:O	1:D:60:VAL:HA	2.20	0.41
1:H:13:GLU:HB2	2:P:101:HOH:O	2.21	0.41
1:W:9:ASP:HB3	1:X:9:ASP:HA	2.03	0.41
1:a:30:SER:OG	1:b:51:MSE:HE1	2.20	0.41
1:g:26:GLU:HG3	1:h:51:MSE:SE	2.71	0.41
1:i:39:LEU:HD11	1:i:51:MSE:HB3	2.02	0.41
1:F:24:GLU:OE2	1:q:26:GLU:OE2	2.38	0.41
1:p:4:LYS:HG2	1:p:15:VAL:HG22	2.01	0.41
1:A:59:TYR:CG	1:B:14:LEU:HD11	2.56	0.41
1:L:32:ALA:HB3	1:L:40:LEU:HD12	2.02	0.41
1:O:5:ILE:HB	1:O:14:LEU:HB2	2.02	0.41
1:d:8:THR:O	1:e:9:ASP:HB3	2.21	0.41
1:d:21:THR:HG23	1:d:23:SER:H	1.84	0.41
1:j:32:ALA:HB2	1:j:40:LEU:HD13	2.03	0.41
1:F:33:LEU:HD11	1:F:57:ILE:HD13	2.01	0.41
1:J:7:ILE:HB	1:J:10:SER:HB3	2.03	0.41
1:Q:43:THR:HG22	1:Q:44:ASP:O	2.21	0.41
1:W:46:ARG:CZ	1:W:48:ARG:HH12	2.34	0.41
1:j:58:ALA:HB1	1:k:7:ILE:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:LEU:HD12	1:C:39:LEU:HA	1.90	0.41
1:D:60:VAL:HG13	1:E:51:MSE:HB2	2.03	0.41
1:F:1:VAL:HG12	1:F:18:SER:HB3	2.02	0.41
1:M:21:THR:HG22	1:M:24:GLU:H	1.86	0.41
1:T:40:LEU:O	1:T:41:THR:O	2.39	0.41
1:W:39:LEU:HA	1:W:39:LEU:HD12	1.85	0.41
1:s:12:ARG:NH1	1:t:13:GLU:OE2	2.54	0.41
1:A:64:VAL:HG13	1:B:48:ARG:HG3	2.02	0.41
1:R:25:VAL:O	1:R:62:ILE:HD11	2.21	0.41
1:b:33:LEU:HB3	1:c:53:HIS:CE1	2.55	0.41
1:h:40:LEU:HB3	1:h:52:ILE:HG22	2.02	0.41
1:B:29:VAL:HG22	1:B:40:LEU:HD21	2.04	0.40
1:I:59:TYR:OH	1:J:12:ARG:HD2	2.21	0.40
1:W:21:THR:OG1	1:W:24:GLU:HB2	2.21	0.40
1:Y:64:VAL:HG11	1:Z:46:ARG:O	2.22	0.40
1:e:39:LEU:HD11	1:e:51:MSE:HB3	2.04	0.40
1:o:21:THR:HA	1:o:22:PRO:HD3	1.92	0.40
1:G:30:SER:HB2	1:H:51:MSE:HE1	2.02	0.40
1:J:22:PRO:HB3	1:J:62:ILE:CG2	2.50	0.40
1:K:16:PHE:HB2	1:K:44:ASP:OD1	2.21	0.40
1:a:-1:HIS:O	1:a:19:ALA:HA	2.21	0.40
1:i:21:THR:HG22	1:i:24:GLU:HB2	2.02	0.40
1:q:50:PHE:O	1:q:51:MSE:C	2.64	0.40
1:B:26:GLU:OE1	1:C:49:ARG:HD3	2.22	0.40
1:V:5:ILE:HG21	1:V:52:ILE:HD13	2.02	0.40
1:h:33:LEU:HD22	1:i:53:HIS:CE1	2.56	0.40
1:F:16:PHE:HB2	1:F:44:ASP:OD1	2.21	0.40
1:S:1:VAL:HG21	1:S:22:PRO:HG3	2.03	0.40
1:g:5:ILE:HG12	1:g:60:VAL:HG12	2.04	0.40
1:i:30:SER:OG	1:j:51:MSE:HE1	2.22	0.40
1:n:48:ARG:HH21	1:u:48:ARG:NH2	2.19	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	63/83 (76%)	61 (97%)	2 (3%)	0	100	100
1	B	64/83 (77%)	59 (92%)	4 (6%)	1 (2%)	7	15
1	C	62/83 (75%)	59 (95%)	2 (3%)	1 (2%)	7	15
1	D	62/83 (75%)	57 (92%)	5 (8%)	0	100	100
1	E	64/83 (77%)	61 (95%)	2 (3%)	1 (2%)	7	15
1	F	62/83 (75%)	57 (92%)	4 (6%)	1 (2%)	7	15
1	G	64/83 (77%)	63 (98%)	0	1 (2%)	7	15
1	H	66/83 (80%)	63 (96%)	2 (3%)	1 (2%)	8	16
1	I	61/83 (74%)	58 (95%)	3 (5%)	0	100	100
1	J	55/83 (66%)	53 (96%)	2 (4%)	0	100	100
1	K	56/83 (68%)	54 (96%)	2 (4%)	0	100	100
1	L	56/83 (68%)	55 (98%)	1 (2%)	0	100	100
1	M	59/83 (71%)	55 (93%)	2 (3%)	2 (3%)	3	4
1	N	49/83 (59%)	47 (96%)	2 (4%)	0	100	100
1	O	51/83 (61%)	44 (86%)	5 (10%)	2 (4%)	2	3
1	P	57/83 (69%)	53 (93%)	3 (5%)	1 (2%)	6	13
1	Q	60/83 (72%)	59 (98%)	1 (2%)	0	100	100
1	R	60/83 (72%)	55 (92%)	3 (5%)	2 (3%)	3	4
1	S	61/83 (74%)	59 (97%)	2 (3%)	0	100	100
1	T	64/83 (77%)	54 (84%)	6 (9%)	4 (6%)	1	1
1	U	62/83 (75%)	60 (97%)	2 (3%)	0	100	100
1	V	65/83 (78%)	60 (92%)	3 (5%)	2 (3%)	3	5
1	W	59/83 (71%)	58 (98%)	1 (2%)	0	100	100
1	X	60/83 (72%)	57 (95%)	3 (5%)	0	100	100
1	Y	62/83 (75%)	59 (95%)	2 (3%)	1 (2%)	7	15
1	Z	65/83 (78%)	60 (92%)	2 (3%)	3 (5%)	2	2
1	a	63/83 (76%)	61 (97%)	2 (3%)	0	100	100
1	b	65/83 (78%)	64 (98%)	1 (2%)	0	100	100
1	c	64/83 (77%)	59 (92%)	3 (5%)	2 (3%)	3	5
1	d	65/83 (78%)	62 (95%)	1 (2%)	2 (3%)	3	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	e	56/83 (68%)	53 (95%)	1 (2%)	2 (4%)	2	3
1	f	64/83 (77%)	60 (94%)	1 (2%)	3 (5%)	2	2
1	g	50/83 (60%)	48 (96%)	1 (2%)	1 (2%)	6	11
1	h	53/83 (64%)	48 (91%)	3 (6%)	2 (4%)	2	3
1	i	46/83 (55%)	45 (98%)	1 (2%)	0	100	100
1	j	53/83 (64%)	51 (96%)	1 (2%)	1 (2%)	6	12
1	k	53/83 (64%)	51 (96%)	2 (4%)	0	100	100
1	l	56/83 (68%)	53 (95%)	1 (2%)	2 (4%)	2	3
1	m	53/83 (64%)	52 (98%)	1 (2%)	0	100	100
1	n	54/83 (65%)	51 (94%)	2 (4%)	1 (2%)	6	12
1	o	65/83 (78%)	62 (95%)	1 (2%)	2 (3%)	3	5
1	p	61/83 (74%)	59 (97%)	1 (2%)	1 (2%)	7	15
1	q	64/83 (77%)	59 (92%)	3 (5%)	2 (3%)	3	5
1	r	65/83 (78%)	59 (91%)	5 (8%)	1 (2%)	8	16
1	s	65/83 (78%)	63 (97%)	2 (3%)	0	100	100
1	t	65/83 (78%)	60 (92%)	4 (6%)	1 (2%)	8	16
1	u	62/83 (75%)	55 (89%)	3 (5%)	4 (6%)	1	1
1	v	64/83 (77%)	57 (89%)	5 (8%)	2 (3%)	3	5
All	All	2875/3984 (72%)	2712 (94%)	111 (4%)	52 (2%)	6	13

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	8	THR
1	H	23	SER
1	P	46	ARG
1	R	8	THR
1	R	23	SER
1	T	41	THR
1	u	39	LEU
1	v	41	THR
1	M	46	ARG
1	M	50	PHE
1	T	35	ASP
1	T	46	ARG
1	V	36	ASP

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Mol	Chain	Res	Type
1	d	8	THR
1	g	7	ILE
1	n	33	LEU
1	o	23	SER
1	q	51	MSE
1	r	23	SER
1	u	23	SER
1	u	65	ALA
1	C	9	ASP
1	E	9	ASP
1	F	58	ALA
1	V	9	ASP
1	Y	23	SER
1	Z	23	SER
1	f	7	ILE
1	l	34	ARG
1	p	37	SER
1	B	13	GLU
1	O	17	SER
1	O	33	LEU
1	Z	0	HIS
1	Z	33	LEU
1	c	37	SER
1	f	33	LEU
1	j	8	THR
1	u	33	LEU
1	v	61	GLU
1	T	36	ASP
1	c	65	ALA
1	d	36	ASP
1	e	33	LEU
1	q	23	SER
1	e	8	THR
1	h	20	GLN
1	t	36	ASP
1	f	22	PRO
1	o	21	THR
1	h	21	THR
1	l	62	ILE

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 X-ray entries followed by that with respect to entries of similar resolution.

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	53/67 (79%)	51 (96%)	2 (4%)	29	54
1	B	53/67 (79%)	51 (96%)	2 (4%)	29	54
1	C	52/67 (78%)	49 (94%)	3 (6%)	18	37
1	D	53/67 (79%)	50 (94%)	3 (6%)	18	38
1	E	56/67 (84%)	51 (91%)	5 (9%)	9	19
1	F	51/67 (76%)	46 (90%)	5 (10%)	7	15
1	G	52/67 (78%)	46 (88%)	6 (12%)	5	10
1	H	57/67 (85%)	52 (91%)	5 (9%)	9	19
1	I	52/67 (78%)	48 (92%)	4 (8%)	12	25
1	J	49/67 (73%)	45 (92%)	4 (8%)	10	22
1	K	52/67 (78%)	50 (96%)	2 (4%)	29	54
1	L	51/67 (76%)	46 (90%)	5 (10%)	7	15
1	M	51/67 (76%)	47 (92%)	4 (8%)	11	25
1	N	43/67 (64%)	43 (100%)	0	100	100
1	O	48/67 (72%)	43 (90%)	5 (10%)	7	13
1	P	50/67 (75%)	47 (94%)	3 (6%)	17	36
1	Q	52/67 (78%)	50 (96%)	2 (4%)	29	54
1	R	47/67 (70%)	43 (92%)	4 (8%)	10	21
1	S	51/67 (76%)	48 (94%)	3 (6%)	18	36
1	T	49/67 (73%)	46 (94%)	3 (6%)	17	35
1	U	56/67 (84%)	52 (93%)	4 (7%)	13	29
1	V	56/67 (84%)	52 (93%)	4 (7%)	13	29
1	W	51/67 (76%)	47 (92%)	4 (8%)	11	25
1	X	49/67 (73%)	45 (92%)	4 (8%)	10	22
1	Y	53/67 (79%)	47 (89%)	6 (11%)	5	11
1	Z	55/67 (82%)	52 (94%)	3 (6%)	19	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	55/67 (82%)	52 (94%)	3 (6%)	19	39
1	b	54/67 (81%)	53 (98%)	1 (2%)	50	74
1	c	55/67 (82%)	54 (98%)	1 (2%)	51	75
1	d	56/67 (84%)	53 (95%)	3 (5%)	20	40
1	e	50/67 (75%)	48 (96%)	2 (4%)	28	53
1	f	54/67 (81%)	53 (98%)	1 (2%)	50	74
1	g	45/67 (67%)	45 (100%)	0	100	100
1	h	48/67 (72%)	44 (92%)	4 (8%)	10	22
1	i	42/67 (63%)	41 (98%)	1 (2%)	43	69
1	j	48/67 (72%)	45 (94%)	3 (6%)	16	34
1	k	49/67 (73%)	47 (96%)	2 (4%)	27	52
1	l	49/67 (73%)	46 (94%)	3 (6%)	17	35
1	m	49/67 (73%)	48 (98%)	1 (2%)	48	73
1	n	49/67 (73%)	47 (96%)	2 (4%)	27	52
1	o	54/67 (81%)	50 (93%)	4 (7%)	13	27
1	p	53/67 (79%)	51 (96%)	2 (4%)	29	54
1	q	53/67 (79%)	50 (94%)	3 (6%)	18	38
1	r	57/67 (85%)	53 (93%)	4 (7%)	14	29
1	s	58/67 (87%)	56 (97%)	2 (3%)	32	58
1	t	56/67 (84%)	55 (98%)	1 (2%)	51	75
1	u	53/67 (79%)	49 (92%)	4 (8%)	12	26
1	v	55/67 (82%)	53 (96%)	2 (4%)	31	56
All	All	2484/3216 (77%)	2340 (94%)	144 (6%)	18	37

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

Mol	Chain	Res	Type
1	A	49	ARG
1	A	60	VAL
1	B	54	THR
1	B	60	VAL
1	C	10	SER
1	C	40	LEU
1	C	60	VAL

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Mol	Chain	Res	Type
1	D	25	VAL
1	D	53	HIS
1	D	60	VAL
1	E	21	THR
1	E	25	VAL
1	E	54	THR
1	E	60	VAL
1	E	64	VAL
1	F	25	VAL
1	F	41	THR
1	F	54	THR
1	F	57	ILE
1	F	60	VAL
1	G	8	THR
1	G	41	THR
1	G	54	THR
1	G	57	ILE
1	G	60	VAL
1	G	64	VAL
1	H	10	SER
1	H	25	VAL
1	H	39	LEU
1	H	54	THR
1	H	60	VAL
1	I	21	THR
1	I	29	VAL
1	I	39	LEU
1	I	60	VAL
1	J	3	VAL
1	J	29	VAL
1	J	41	THR
1	J	60	VAL
1	K	25	VAL
1	K	29	VAL
1	L	21	THR
1	L	43	THR
1	L	53	HIS
1	L	60	VAL
1	L	62	ILE
1	M	21	THR
1	M	39	LEU
1	M	46	ARG

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Mol	Chain	Res	Type
1	M	60	VAL
1	O	21	THR
1	O	39	LEU
1	O	40	LEU
1	O	54	THR
1	O	60	VAL
1	P	39	LEU
1	P	41	THR
1	P	42	LEU
1	Q	25	VAL
1	Q	60	VAL
1	R	25	VAL
1	R	41	THR
1	R	53	HIS
1	R	60	VAL
1	S	5	ILE
1	S	25	VAL
1	S	54	THR
1	T	25	VAL
1	T	60	VAL
1	T	64	VAL
1	U	10	SER
1	U	25	VAL
1	U	41	THR
1	U	60	VAL
1	V	10	SER
1	V	41	THR
1	V	54	THR
1	V	60	VAL
1	W	7	ILE
1	W	41	THR
1	W	54	THR
1	W	56	ARG
1	X	10	SER
1	X	21	THR
1	X	41	THR
1	X	60	VAL
1	Y	5	ILE
1	Y	10	SER
1	Y	21	THR
1	Y	25	VAL
1	Y	54	THR

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Mol	Chain	Res	Type
1	Y	60	VAL
1	Z	13	GLU
1	Z	54	THR
1	Z	60	VAL
1	a	21	THR
1	a	41	THR
1	a	60	VAL
1	b	60	VAL
1	c	54	THR
1	d	41	THR
1	d	49	ARG
1	d	60	VAL
1	e	54	THR
1	e	64	VAL
1	f	41	THR
1	h	9	ASP
1	h	29	VAL
1	h	54	THR
1	h	60	VAL
1	i	24	GLU
1	j	29	VAL
1	j	41	THR
1	j	60	VAL
1	k	29	VAL
1	k	60	VAL
1	l	29	VAL
1	l	41	THR
1	l	60	VAL
1	m	3	VAL
1	n	41	THR
1	n	60	VAL
1	o	21	THR
1	o	26	GLU
1	o	41	THR
1	o	60	VAL
1	p	54	THR
1	p	60	VAL
1	q	21	THR
1	q	53	HIS
1	q	60	VAL
1	r	13	GLU
1	r	21	THR

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Mol	Chain	Res	Type
1	r	25	VAL
1	r	54	THR
1	s	41	THR
1	s	60	VAL
1	t	60	VAL
1	u	26	GLU
1	u	41	THR
1	u	54	THR
1	u	60	VAL
1	v	21	THR
1	v	25	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	HIS
1	B	53	HIS
1	G	20	GLN
1	G	53	HIS
1	I	31	ASN
1	K	53	HIS
1	L	31	ASN
1	M	31	ASN
1	O	20	GLN
1	O	53	HIS
1	Q	31	ASN
1	Q	53	HIS
1	U	0	HIS
1	V	20	GLN
1	a	20	GLN
1	a	53	HIS
1	c	53	HIS
1	e	20	GLN
1	h	31	ASN
1	h	53	HIS
1	i	20	GLN
1	j	31	ASN
1	n	31	ASN
1	o	20	GLN
1	u	20	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 oligosaccharides 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 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	64/83 (77%)	-1.30	0 100 100	48, 60, 92, 102	0
1	B	65/83 (78%)	-1.37	0 100 100	43, 59, 91, 99	0
1	C	65/83 (78%)	-1.30	0 100 100	46, 62, 91, 105	0
1	D	65/83 (78%)	-1.35	0 100 100	42, 59, 91, 94	0
1	E	65/83 (78%)	-1.33	0 100 100	46, 61, 96, 114	0
1	F	65/83 (78%)	-1.29	0 100 100	43, 61, 94, 100	0
1	G	65/83 (78%)	-1.32	0 100 100	44, 62, 92, 98	0
1	H	67/83 (80%)	-1.28	0 100 100	42, 57, 91, 99	0
1	I	62/83 (74%)	-1.29	0 100 100	65, 86, 110, 119	0
1	J	58/83 (69%)	-1.25	0 100 100	68, 94, 112, 114	0
1	K	59/83 (71%)	-1.23	0 100 100	62, 90, 116, 133	0
1	L	59/83 (71%)	-1.22	0 100 100	73, 93, 112, 121	0
1	M	62/83 (74%)	-1.16	0 100 100	67, 95, 123, 137	0
1	N	54/83 (65%)	-1.22	0 100 100	67, 89, 103, 113	0
1	O	56/83 (67%)	-1.26	0 100 100	72, 91, 110, 115	0
1	P	60/83 (72%)	-1.20	0 100 100	70, 93, 112, 115	0
1	Q	63/83 (75%)	-1.29	0 100 100	38, 56, 84, 90	0
1	R	63/83 (75%)	-1.33	0 100 100	43, 60, 88, 105	0
1	S	64/83 (77%)	-1.27	0 100 100	45, 60, 86, 97	0
1	T	65/83 (78%)	-1.39	0 100 100	43, 60, 88, 100	0
1	U	65/83 (78%)	-1.32	0 100 100	42, 57, 90, 99	0
1	V	66/83 (79%)	-1.29	0 100 100	48, 66, 101, 110	0
1	W	62/83 (74%)	-1.28	0 100 100	42, 58, 85, 99	0
1	X	63/83 (75%)	-1.30	0 100 100	46, 58, 85, 99	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	Y	65/83 (78%)	-1.31	0	35, 57, 84, 89	0
1	Z	66/83 (79%)	-1.39	0	34, 50, 71, 79	0
1	a	66/83 (79%)	-1.29	0	36, 58, 82, 97	0
1	b	66/83 (79%)	-1.46	0	34, 52, 71, 79	0
1	c	67/83 (80%)	-1.34	0	36, 58, 86, 103	0
1	d	66/83 (79%)	-1.44	0	34, 50, 76, 79	0
1	e	61/83 (73%)	-1.36	0	31, 55, 75, 79	0
1	f	65/83 (78%)	-1.44	0	35, 50, 67, 82	0
1	g	53/83 (63%)	-1.16	0	80, 96, 130, 133	0
1	h	58/83 (69%)	-1.23	0	79, 100, 126, 128	0
1	i	51/83 (61%)	-1.14	0	80, 96, 119, 125	0
1	j	58/83 (69%)	-1.26	0	80, 101, 115, 121	0
1	k	56/83 (67%)	-1.19	0	84, 97, 114, 116	0
1	l	59/83 (71%)	-1.21	0	81, 101, 114, 119	0
1	m	58/83 (69%)	-1.15	0	81, 96, 113, 119	0
1	n	57/83 (68%)	-1.19	0	75, 92, 112, 116	0
1	o	66/83 (79%)	-1.33	0	33, 51, 71, 78	0
1	p	64/83 (77%)	-1.27	0	35, 57, 77, 104	0
1	q	65/83 (78%)	-1.34	0	35, 51, 75, 80	0
1	r	66/83 (79%)	-1.37	0	32, 57, 83, 100	0
1	s	66/83 (79%)	-1.36	0	35, 53, 79, 87	0
1	t	66/83 (79%)	-1.36	0	32, 56, 83, 94	0
1	u	65/83 (78%)	-1.31	0	33, 50, 71, 84	0
1	v	65/83 (78%)	-1.24	0	35, 55, 86, 95	0
All	All	2997/3984 (75%)	-1.30	0	31, 67, 109, 137	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.