



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 30, 2021 – 09:16 AM EDT

PDB ID : 7RDB  
Title : Crystal structure of Tspan15 large extracellular loop (Tspan15 LEL)  
Authors : Lipper, C.H.; Gabriel, K.H.; Seegar, T.C.M.; Durr, K.L.; Tomlinson, M.G.; Blacklow, S.C.  
Deposited on : 2021-07-09  
Resolution : 2.52 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](mailto: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.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

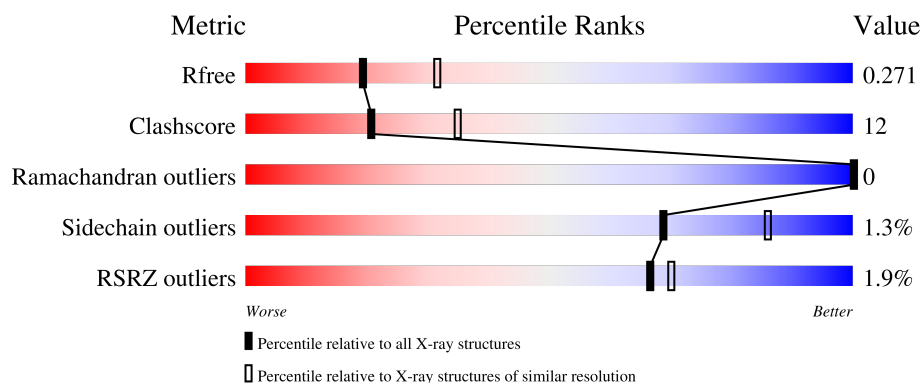
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.52 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))
$R_{free}$	130704	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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  $\geq 3$ , 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	122	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>22%</div> <div>.</div> </div> </div>
1	B	122	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>25%</div> <div>.</div> </div> </div>
1	C	122	<div> <div></div> <div> <div></div> <div>79%</div> <div>20%</div> <div>.</div> </div> </div>
1	D	122	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>17%</div> <div>.</div> </div> </div>
1	E	122	<div> <div></div> <div> <div></div> <div>84%</div> <div>15%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	122	<div> <div></div> <div>75%</div> <div>23%</div> <div></div> </div>
1	G	122	<div> <div></div> <div>74%</div> <div>25%</div> <div></div> </div>
1	H	122	<div> <div></div> <div>77%</div> <div>23%</div> <div></div> </div>
1	I	122	<div> <div>2%</div> <div></div> <div>81%</div> <div>19%</div> <div></div> </div>
1	J	122	<div> <div></div> <div>75%</div> <div>21%</div> <div></div> </div>
1	K	122	<div> <div>2%</div> <div></div> <div>84%</div> <div>16%</div> <div></div> </div>
1	L	122	<div> <div>3%</div> <div></div> <div>82%</div> <div>16%</div> <div></div> </div>
1	M	122	<div> <div>2%</div> <div></div> <div>72%</div> <div>28%</div> <div></div> </div>
1	N	122	<div> <div>4%</div> <div></div> <div>68%</div> <div>31%</div> <div></div> </div>
1	O	122	<div> <div>2%</div> <div></div> <div>63%</div> <div>30%</div> <div>6%</div> </div>
1	P	122	<div> <div>2%</div> <div></div> <div>77%</div> <div>23%</div> <div></div> </div>
1	Q	122	<div> <div></div> <div>75%</div> <div>25%</div> <div></div> </div>
1	R	122	<div> <div>5%</div> <div></div> <div>70%</div> <div>27%</div> <div></div> </div>
1	S	122	<div> <div>2%</div> <div></div> <div>72%</div> <div>25%</div> <div></div> </div>
1	T	122	<div> <div></div> <div>65%</div> <div>34%</div> <div></div> </div>
1	U	122	<div> <div>3%</div> <div></div> <div>77%</div> <div>20%</div> <div></div> </div>
1	V	122	<div> <div>2%</div> <div></div> <div>68%</div> <div>26%</div> <div></div> </div>
1	W	122	<div> <div>5%</div> <div></div> <div>69%</div> <div>29%</div> <div></div> </div>
1	X	122	<div> <div>7%</div> <div></div> <div>72%</div> <div>26%</div> <div></div> </div>

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 22771 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 Tetraspanin-15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	122	Total	C	N	O	S	0	0	0
			956	606	156	183	11			
1	A	122	Total	C	N	O	S	0	0	0
			973	610	162	190	11			
1	C	122	Total	C	N	O	S	0	0	0
			950	596	158	185	11			
1	D	121	Total	C	N	O	S	0	0	0
			949	599	159	180	11			
1	E	122	Total	C	N	O	S	0	0	0
			950	597	160	182	11			
1	F	122	Total	C	N	O	S	0	0	0
			972	615	160	186	11			
1	G	122	Total	C	N	O	S	0	0	0
			970	610	163	186	11			
1	H	122	Total	C	N	O	S	0	0	0
			948	592	159	186	11			
1	I	122	Total	C	N	O	S	0	0	0
			958	602	164	181	11			
1	J	121	Total	C	N	O	S	0	0	0
			934	585	156	182	11			
1	K	122	Total	C	N	O	S	0	0	0
			954	599	159	185	11			
1	L	122	Total	C	N	O	S	0	0	0
			948	596	156	185	11			
1	M	122	Total	C	N	O	S	0	0	0
			966	615	160	180	11			
1	N	122	Total	C	N	O	S	0	0	0
			954	602	160	181	11			
1	O	121	Total	C	N	O	S	0	0	0
			950	598	162	179	11			
1	P	122	Total	C	N	O	S	0	0	0
			950	599	158	182	11			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	122	Total	C	N	O	S	0	0	0
			939	591	156	181	11			
1	R	122	Total	C	N	O	S	0	0	0
			958	605	160	182	11			
1	S	122	Total	C	N	O	S	0	0	0
			943	593	158	181	11			
1	T	121	Total	C	N	O	S	0	0	0
			950	601	156	182	11			
1	U	121	Total	C	N	O	S	0	0	0
			931	589	153	178	11			
1	V	119	Total	C	N	O	S	0	0	0
			908	570	151	176	11			
1	W	121	Total	C	N	O	S	0	0	0
			917	578	152	176	11			
1	X	122	Total	C	N	O	S	0	0	0
			902	568	147	177	10			

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	118	GLN	ASN	engineered mutation	UNP O95858
B	189	ASP	ASN	engineered mutation	UNP O95858
B	231	LEU	-	expression tag	UNP O95858
B	232	GLU	-	expression tag	UNP O95858
B	233	VAL	-	expression tag	UNP O95858
B	234	LEU	-	expression tag	UNP O95858
B	235	PHE	-	expression tag	UNP O95858
B	236	GLN	-	expression tag	UNP O95858
A	118	GLN	ASN	engineered mutation	UNP O95858
A	189	ASP	ASN	engineered mutation	UNP O95858
A	231	LEU	-	expression tag	UNP O95858
A	232	GLU	-	expression tag	UNP O95858
A	233	VAL	-	expression tag	UNP O95858
A	234	LEU	-	expression tag	UNP O95858
A	235	PHE	-	expression tag	UNP O95858
A	236	GLN	-	expression tag	UNP O95858
C	118	GLN	ASN	engineered mutation	UNP O95858
C	189	ASP	ASN	engineered mutation	UNP O95858
C	231	LEU	-	expression tag	UNP O95858
C	232	GLU	-	expression tag	UNP O95858
C	233	VAL	-	expression tag	UNP O95858
C	234	LEU	-	expression tag	UNP O95858
C	235	PHE	-	expression tag	UNP O95858

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Chain	Residue	Modelled	Actual	Comment	Reference
C	236	GLN	-	expression tag	UNP 095858
D	118	GLN	ASN	engineered mutation	UNP 095858
D	189	ASP	ASN	engineered mutation	UNP 095858
D	231	LEU	-	expression tag	UNP 095858
D	232	GLU	-	expression tag	UNP 095858
D	233	VAL	-	expression tag	UNP 095858
D	234	LEU	-	expression tag	UNP 095858
D	235	PHE	-	expression tag	UNP 095858
D	236	GLN	-	expression tag	UNP 095858
E	118	GLN	ASN	engineered mutation	UNP 095858
E	189	ASP	ASN	engineered mutation	UNP 095858
E	231	LEU	-	expression tag	UNP 095858
E	232	GLU	-	expression tag	UNP 095858
E	233	VAL	-	expression tag	UNP 095858
E	234	LEU	-	expression tag	UNP 095858
E	235	PHE	-	expression tag	UNP 095858
E	236	GLN	-	expression tag	UNP 095858
F	118	GLN	ASN	engineered mutation	UNP 095858
F	189	ASP	ASN	engineered mutation	UNP 095858
F	231	LEU	-	expression tag	UNP 095858
F	232	GLU	-	expression tag	UNP 095858
F	233	VAL	-	expression tag	UNP 095858
F	234	LEU	-	expression tag	UNP 095858
F	235	PHE	-	expression tag	UNP 095858
F	236	GLN	-	expression tag	UNP 095858
G	118	GLN	ASN	engineered mutation	UNP 095858
G	189	ASP	ASN	engineered mutation	UNP 095858
G	231	LEU	-	expression tag	UNP 095858
G	232	GLU	-	expression tag	UNP 095858
G	233	VAL	-	expression tag	UNP 095858
G	234	LEU	-	expression tag	UNP 095858
G	235	PHE	-	expression tag	UNP 095858
G	236	GLN	-	expression tag	UNP 095858
H	118	GLN	ASN	engineered mutation	UNP 095858
H	189	ASP	ASN	engineered mutation	UNP 095858
H	231	LEU	-	expression tag	UNP 095858
H	232	GLU	-	expression tag	UNP 095858
H	233	VAL	-	expression tag	UNP 095858
H	234	LEU	-	expression tag	UNP 095858
H	235	PHE	-	expression tag	UNP 095858
H	236	GLN	-	expression tag	UNP 095858
I	118	GLN	ASN	engineered mutation	UNP 095858

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Chain	Residue	Modelled	Actual	Comment	Reference
I	189	ASP	ASN	engineered mutation	UNP 095858
I	231	LEU	-	expression tag	UNP 095858
I	232	GLU	-	expression tag	UNP 095858
I	233	VAL	-	expression tag	UNP 095858
I	234	LEU	-	expression tag	UNP 095858
I	235	PHE	-	expression tag	UNP 095858
I	236	GLN	-	expression tag	UNP 095858
J	118	GLN	ASN	engineered mutation	UNP 095858
J	189	ASP	ASN	engineered mutation	UNP 095858
J	231	LEU	-	expression tag	UNP 095858
J	232	GLU	-	expression tag	UNP 095858
J	233	VAL	-	expression tag	UNP 095858
J	234	LEU	-	expression tag	UNP 095858
J	235	PHE	-	expression tag	UNP 095858
J	236	GLN	-	expression tag	UNP 095858
K	118	GLN	ASN	engineered mutation	UNP 095858
K	189	ASP	ASN	engineered mutation	UNP 095858
K	231	LEU	-	expression tag	UNP 095858
K	232	GLU	-	expression tag	UNP 095858
K	233	VAL	-	expression tag	UNP 095858
K	234	LEU	-	expression tag	UNP 095858
K	235	PHE	-	expression tag	UNP 095858
K	236	GLN	-	expression tag	UNP 095858
L	118	GLN	ASN	engineered mutation	UNP 095858
L	189	ASP	ASN	engineered mutation	UNP 095858
L	231	LEU	-	expression tag	UNP 095858
L	232	GLU	-	expression tag	UNP 095858
L	233	VAL	-	expression tag	UNP 095858
L	234	LEU	-	expression tag	UNP 095858
L	235	PHE	-	expression tag	UNP 095858
L	236	GLN	-	expression tag	UNP 095858
M	118	GLN	ASN	engineered mutation	UNP 095858
M	189	ASP	ASN	engineered mutation	UNP 095858
M	231	LEU	-	expression tag	UNP 095858
M	232	GLU	-	expression tag	UNP 095858
M	233	VAL	-	expression tag	UNP 095858
M	234	LEU	-	expression tag	UNP 095858
M	235	PHE	-	expression tag	UNP 095858
M	236	GLN	-	expression tag	UNP 095858
N	118	GLN	ASN	engineered mutation	UNP 095858
N	189	ASP	ASN	engineered mutation	UNP 095858
N	231	LEU	-	expression tag	UNP 095858

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Chain	Residue	Modelled	Actual	Comment	Reference
N	232	GLU	-	expression tag	UNP 095858
N	233	VAL	-	expression tag	UNP 095858
N	234	LEU	-	expression tag	UNP 095858
N	235	PHE	-	expression tag	UNP 095858
N	236	GLN	-	expression tag	UNP 095858
O	118	GLN	ASN	engineered mutation	UNP 095858
O	189	ASP	ASN	engineered mutation	UNP 095858
O	231	LEU	-	expression tag	UNP 095858
O	232	GLU	-	expression tag	UNP 095858
O	233	VAL	-	expression tag	UNP 095858
O	234	LEU	-	expression tag	UNP 095858
O	235	PHE	-	expression tag	UNP 095858
O	236	GLN	-	expression tag	UNP 095858
P	118	GLN	ASN	engineered mutation	UNP 095858
P	189	ASP	ASN	engineered mutation	UNP 095858
P	231	LEU	-	expression tag	UNP 095858
P	232	GLU	-	expression tag	UNP 095858
P	233	VAL	-	expression tag	UNP 095858
P	234	LEU	-	expression tag	UNP 095858
P	235	PHE	-	expression tag	UNP 095858
P	236	GLN	-	expression tag	UNP 095858
Q	118	GLN	ASN	engineered mutation	UNP 095858
Q	189	ASP	ASN	engineered mutation	UNP 095858
Q	231	LEU	-	expression tag	UNP 095858
Q	232	GLU	-	expression tag	UNP 095858
Q	233	VAL	-	expression tag	UNP 095858
Q	234	LEU	-	expression tag	UNP 095858
Q	235	PHE	-	expression tag	UNP 095858
Q	236	GLN	-	expression tag	UNP 095858
R	118	GLN	ASN	engineered mutation	UNP 095858
R	189	ASP	ASN	engineered mutation	UNP 095858
R	231	LEU	-	expression tag	UNP 095858
R	232	GLU	-	expression tag	UNP 095858
R	233	VAL	-	expression tag	UNP 095858
R	234	LEU	-	expression tag	UNP 095858
R	235	PHE	-	expression tag	UNP 095858
R	236	GLN	-	expression tag	UNP 095858
S	118	GLN	ASN	engineered mutation	UNP 095858
S	189	ASP	ASN	engineered mutation	UNP 095858
S	231	LEU	-	expression tag	UNP 095858
S	232	GLU	-	expression tag	UNP 095858
S	233	VAL	-	expression tag	UNP 095858

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Chain	Residue	Modelled	Actual	Comment	Reference
S	234	LEU	-	expression tag	UNP 095858
S	235	PHE	-	expression tag	UNP 095858
S	236	GLN	-	expression tag	UNP 095858
T	118	GLN	ASN	engineered mutation	UNP 095858
T	189	ASP	ASN	engineered mutation	UNP 095858
T	231	LEU	-	expression tag	UNP 095858
T	232	GLU	-	expression tag	UNP 095858
T	233	VAL	-	expression tag	UNP 095858
T	234	LEU	-	expression tag	UNP 095858
T	235	PHE	-	expression tag	UNP 095858
T	236	GLN	-	expression tag	UNP 095858
U	118	GLN	ASN	engineered mutation	UNP 095858
U	189	ASP	ASN	engineered mutation	UNP 095858
U	231	LEU	-	expression tag	UNP 095858
U	232	GLU	-	expression tag	UNP 095858
U	233	VAL	-	expression tag	UNP 095858
U	234	LEU	-	expression tag	UNP 095858
U	235	PHE	-	expression tag	UNP 095858
U	236	GLN	-	expression tag	UNP 095858
V	118	GLN	ASN	engineered mutation	UNP 095858
V	189	ASP	ASN	engineered mutation	UNP 095858
V	231	LEU	-	expression tag	UNP 095858
V	232	GLU	-	expression tag	UNP 095858
V	233	VAL	-	expression tag	UNP 095858
V	234	LEU	-	expression tag	UNP 095858
V	235	PHE	-	expression tag	UNP 095858
V	236	GLN	-	expression tag	UNP 095858
W	118	GLN	ASN	engineered mutation	UNP 095858
W	189	ASP	ASN	engineered mutation	UNP 095858
W	231	LEU	-	expression tag	UNP 095858
W	232	GLU	-	expression tag	UNP 095858
W	233	VAL	-	expression tag	UNP 095858
W	234	LEU	-	expression tag	UNP 095858
W	235	PHE	-	expression tag	UNP 095858
W	236	GLN	-	expression tag	UNP 095858
X	118	GLN	ASN	engineered mutation	UNP 095858
X	189	ASP	ASN	engineered mutation	UNP 095858
X	231	LEU	-	expression tag	UNP 095858
X	232	GLU	-	expression tag	UNP 095858
X	233	VAL	-	expression tag	UNP 095858
X	234	LEU	-	expression tag	UNP 095858
X	235	PHE	-	expression tag	UNP 095858

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Chain	Residue	Modelled	Actual	Comment	Reference
X	236	GLN	-	expression tag	UNP O95858

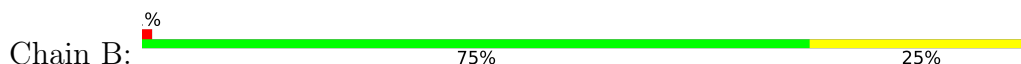
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	5	Total O 5 5	0	0
2	A	4	Total O 4 4	0	0
2	C	6	Total O 6 6	0	0
2	D	1	Total O 1 1	0	0
2	E	4	Total O 4 4	0	0
2	F	6	Total O 6 6	0	0
2	G	3	Total O 3 3	0	0
2	H	4	Total O 4 4	0	0
2	I	3	Total O 3 3	0	0
2	J	1	Total O 1 1	0	0
2	L	2	Total O 2 2	0	0
2	M	1	Total O 1 1	0	0
2	V	1	Total O 1 1	0	0

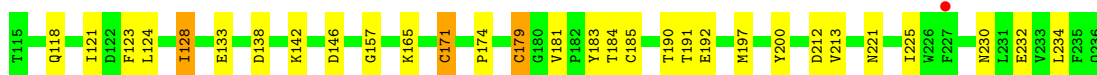
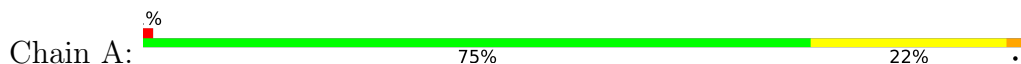
### 3 Residue-property plots [i](#)

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.

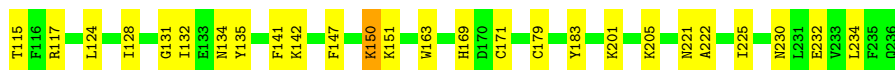
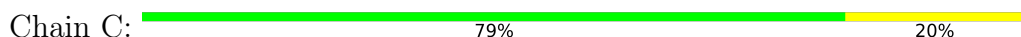
- Molecule 1: Tetraspanin-15



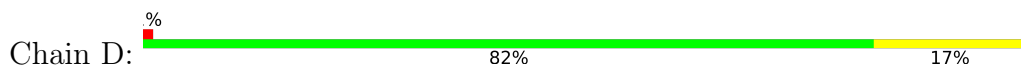
- Molecule 1: Tetraspanin-15



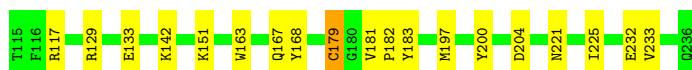
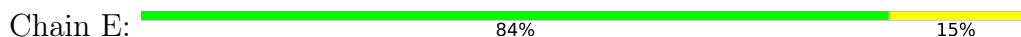
- Molecule 1: Tetraspanin-15



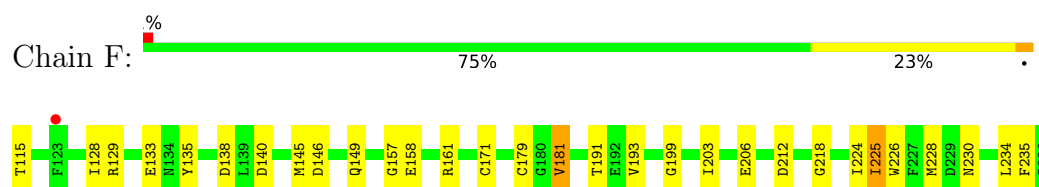
- Molecule 1: Tetraspanin-15



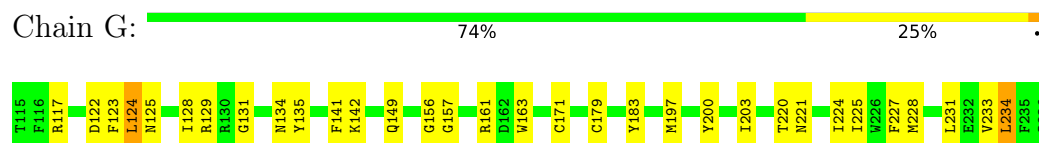
- Molecule 1: Tetraspanin-15



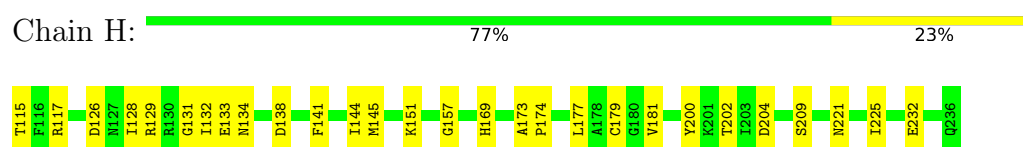
- Molecule 1: Tetraspanin-15



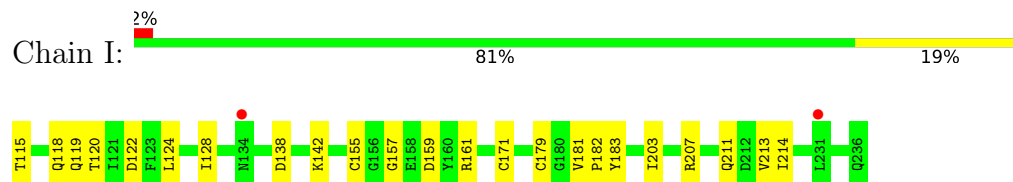
- Molecule 1: Tetraspanin-15



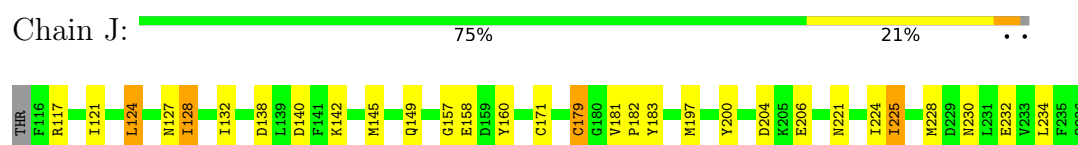
- Molecule 1: Tetraspanin-15



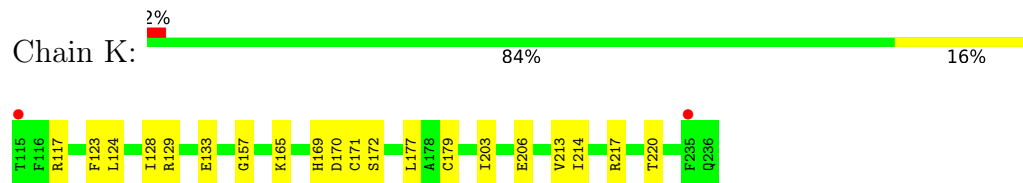
- Molecule 1: Tetraspanin-15



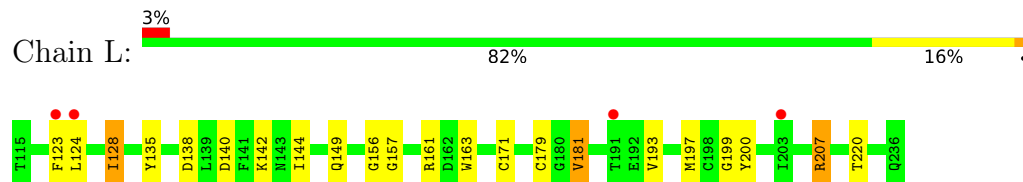
- Molecule 1: Tetraspanin-15



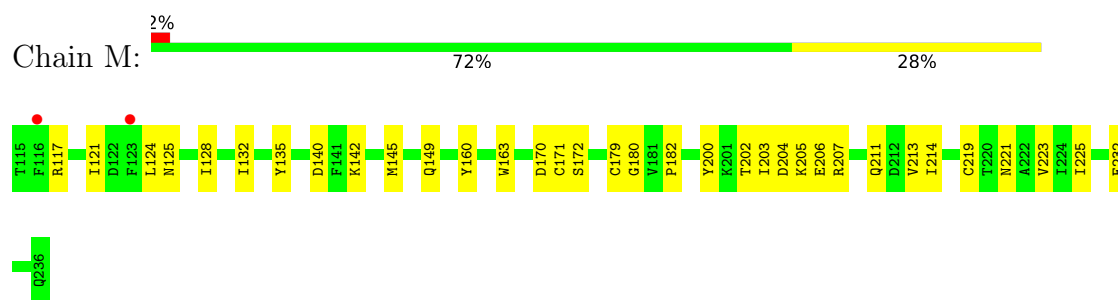
- Molecule 1: Tetraspanin-15



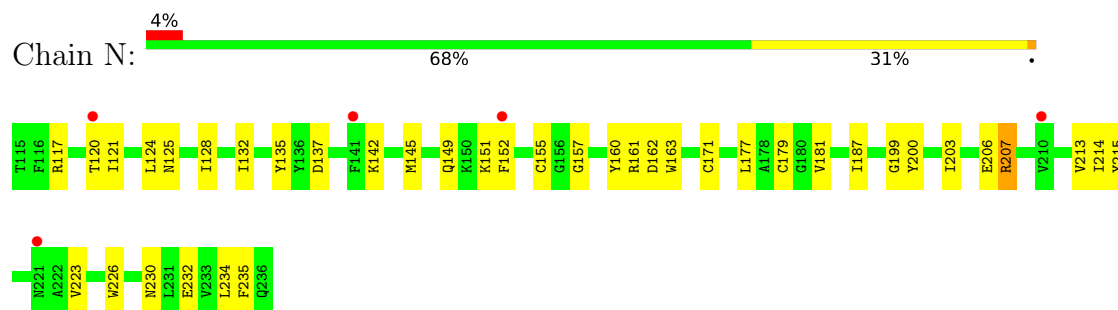
- Molecule 1: Tetraspanin-15



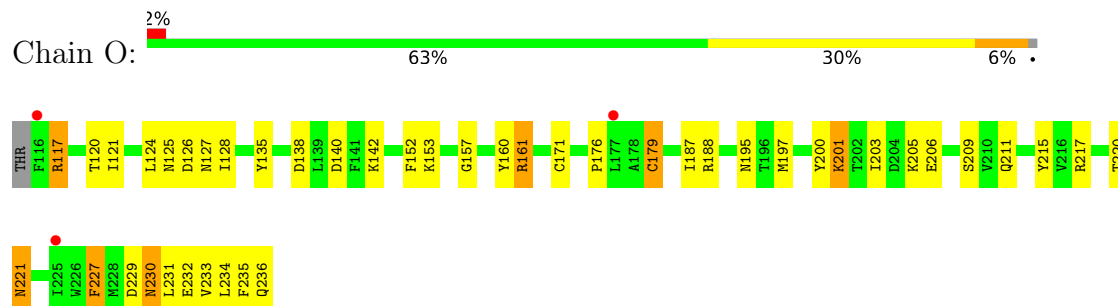
- Molecule 1: Tetraspanin-15



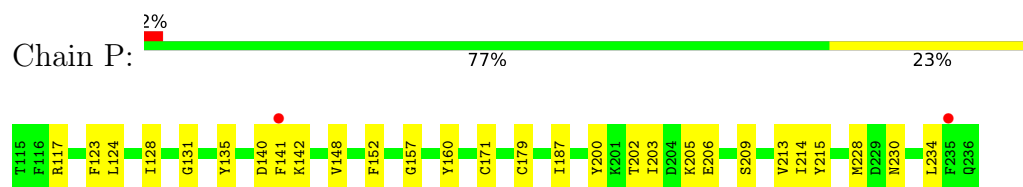
- Molecule 1: Tetraspanin-15



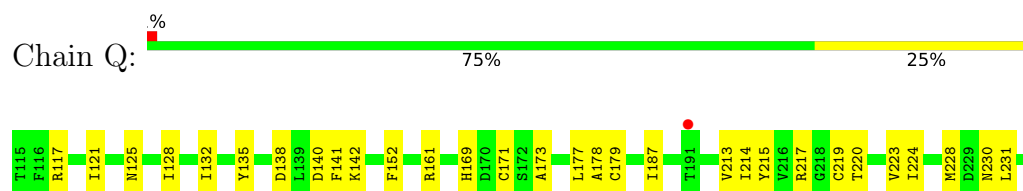
- Molecule 1: Tetraspanin-15



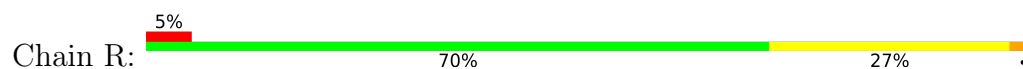
- Molecule 1: Tetraspanin-15

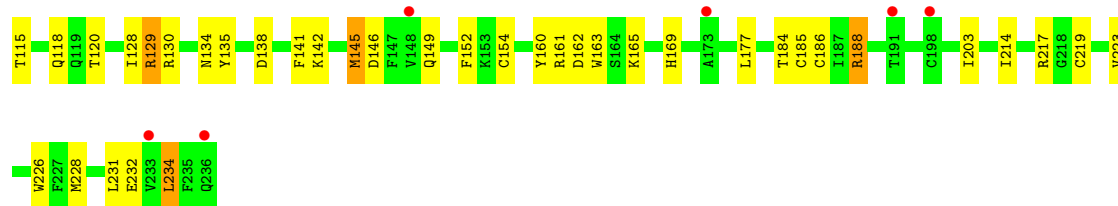


- Molecule 1: Tetraspanin-15

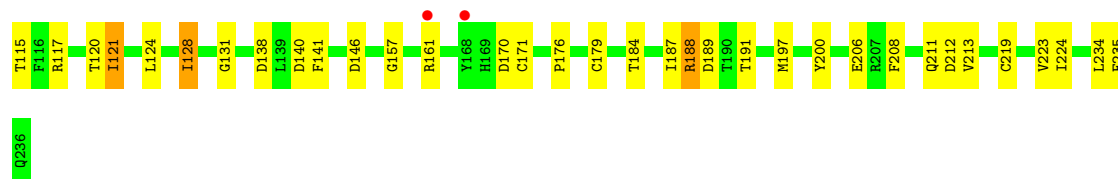
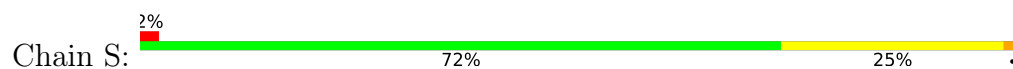


- Molecule 1: Tetraspanin-15

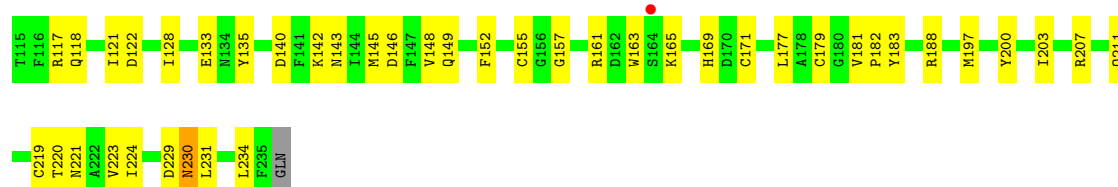




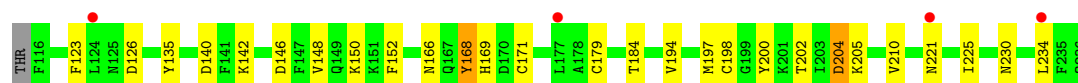
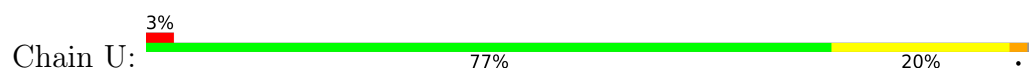
• Molecule 1: Tetraspanin-15



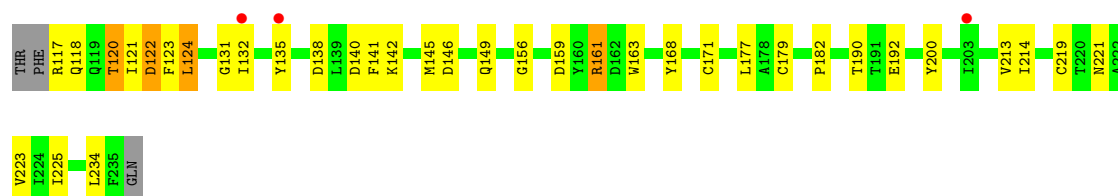
• Molecule 1: Tetraspanin-15



• Molecule 1: Tetraspanin-15

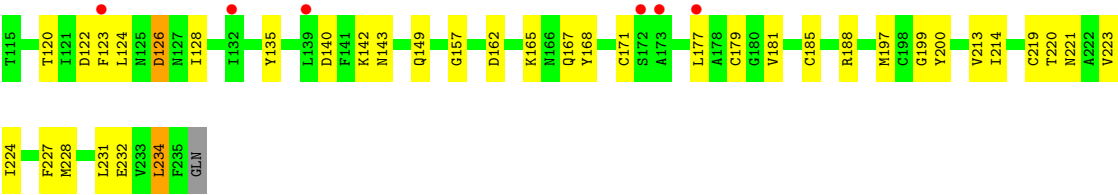


• Molecule 1: Tetraspanin-15

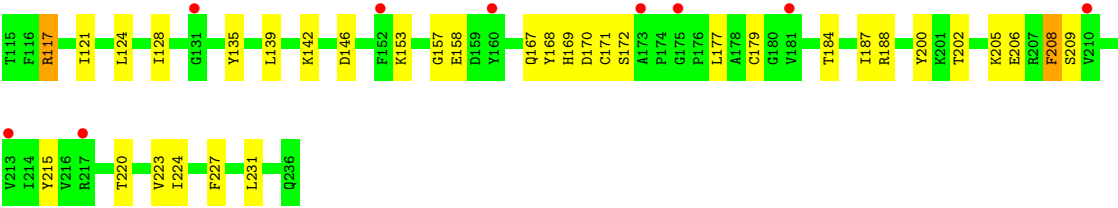


• Molecule 1: Tetraspanin-15





● Molecule 1: Tetraspanin-15



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.57Å 91.95Å 112.38Å 87.55° 86.52° 86.24°	Depositor
Resolution (Å)	48.67 – 2.52 48.67 – 2.52	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.67-2.52) 99.4 (48.67-2.52)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.42 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122+SVN	Depositor
R, $R_{free}$	0.235 , 0.273 0.232 , 0.271	Depositor DCC
$R_{free}$ test set	1971 reflections (1.76%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	76.7	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 58.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	22771	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.70	3/993 (0.3%)	0.87	3/1346 (0.2%)
1	B	0.62	0/977	0.75	0/1326
1	C	0.59	1/969 (0.1%)	0.75	0/1317
1	D	0.69	0/969	0.70	0/1314
1	E	0.60	0/969	0.75	0/1315
1	F	0.62	0/993	0.82	1/1346 (0.1%)
1	G	0.65	0/990	0.87	3/1341 (0.2%)
1	H	0.62	0/966	0.83	1/1310 (0.1%)
1	I	0.56	0/977	0.79	0/1323
1	J	0.71	4/952 (0.4%)	0.79	3/1293 (0.2%)
1	K	0.62	1/973 (0.1%)	0.77	1/1320 (0.1%)
1	L	0.55	0/967	0.91	4/1313 (0.3%)
1	M	0.49	0/988	0.75	0/1338
1	N	0.52	0/974	0.79	3/1321 (0.2%)
1	O	0.71	2/969 (0.2%)	0.85	2/1312 (0.2%)
1	P	0.56	0/970	0.70	0/1317
1	Q	0.47	0/958	0.64	0/1300
1	R	0.70	4/978 (0.4%)	0.81	1/1325 (0.1%)
1	S	0.61	0/962	0.79	3/1307 (0.2%)
1	T	0.54	0/970	0.76	0/1316
1	U	0.51	0/951	0.73	1/1293 (0.1%)
1	V	0.48	0/927	0.67	0/1263
1	W	0.60	0/935	0.82	2/1273 (0.2%)
1	X	1.04	8/921 (0.9%)	0.82	1/1260 (0.1%)
All	All	0.63	23/23198 (0.1%)	0.78	29/31489 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	158	GLU	CD-OE2	13.05	1.40	1.25
1	X	206	GLU	CD-OE1	10.50	1.37	1.25
1	X	158	GLU	CD-OE1	10.32	1.37	1.25
1	X	206	GLU	CD-OE2	10.32	1.37	1.25
1	X	206	GLU	CB-CG	9.33	1.69	1.52
1	J	158	GLU	CD-OE1	8.93	1.35	1.25
1	J	158	GLU	CD-OE2	8.47	1.34	1.25
1	X	158	GLU	CB-CG	8.25	1.67	1.52
1	O	179	CYS	CB-SG	8.06	1.96	1.82
1	J	179	CYS	CB-SG	-7.95	1.68	1.82
1	A	133	GLU	CD-OE2	7.59	1.34	1.25
1	C	150	LYS	CE-NZ	7.12	1.66	1.49
1	K	165	LYS	CD-CE	6.87	1.68	1.51
1	J	158	GLU	CG-CD	-6.47	1.42	1.51
1	R	129	ARG	CB-CG	5.90	1.68	1.52
1	R	129	ARG	CD-NE	5.83	1.56	1.46
1	X	208	PHE	CE1-CZ	5.83	1.48	1.37
1	A	179	CYS	CB-SG	-5.71	1.72	1.81
1	O	201	LYS	CE-NZ	5.56	1.62	1.49
1	R	129	ARG	CG-CD	5.49	1.65	1.51
1	A	185	CYS	CB-SG	5.47	1.91	1.82
1	R	129	ARG	CZ-NH2	5.46	1.40	1.33
1	X	208	PHE	CE2-CZ	5.25	1.47	1.37

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	207	ARG	NE-CZ-NH2	-17.80	111.40	120.30
1	L	207	ARG	CD-NE-CZ	11.42	139.59	123.60
1	N	207	ARG	NE-CZ-NH2	-7.90	116.35	120.30
1	N	207	ARG	NE-CZ-NH1	7.63	124.11	120.30
1	A	171	CYS	CA-CB-SG	7.41	127.33	114.00
1	K	165	LYS	CD-CE-NZ	-7.15	95.26	111.70
1	W	234	LEU	CA-CB-CG	6.97	131.32	115.30
1	O	201	LYS	CD-CE-NZ	-6.78	96.12	111.70
1	X	117	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	S	188	ARG	NE-CZ-NH2	6.17	123.38	120.30
1	S	189	ASP	CB-CG-OD1	6.06	123.75	118.30
1	J	124	LEU	CB-CG-CD1	6.05	121.29	111.00
1	U	204	ASP	CB-CG-OD2	-5.94	112.96	118.30
1	G	129	ARG	CB-CG-CD	-5.85	96.40	111.60
1	L	128	ILE	CG1-CB-CG2	-5.84	98.55	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	234	LEU	CA-CB-CG	5.73	128.49	115.30
1	W	228	MET	CG-SD-CE	5.70	109.32	100.20
1	G	124	LEU	CB-CG-CD2	-5.59	101.50	111.00
1	S	188	ARG	NE-CZ-NH1	-5.57	117.51	120.30
1	J	225	ILE	CG1-CB-CG2	-5.48	99.35	111.40
1	O	117	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	128	ILE	CG1-CB-CG2	-5.41	99.49	111.40
1	A	181	VAL	CG1-CB-CG2	5.38	119.52	110.90
1	R	145	MET	CG-SD-CE	5.38	108.82	100.20
1	J	128	ILE	CG1-CB-CG2	-5.26	99.83	111.40
1	L	181	VAL	CG1-CB-CG2	5.25	119.30	110.90
1	N	137	ASP	CB-CG-OD1	-5.08	113.72	118.30
1	F	181	VAL	CG1-CB-CG2	5.07	119.01	110.90
1	H	181	VAL	CG1-CB-CG2	5.01	118.92	110.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	207	ARG	Sidechain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	973	0	890	21	0
1	B	956	0	870	23	1
1	C	950	0	857	21	0
1	D	949	0	869	20	0
1	E	950	0	869	13	1
1	F	972	0	898	24	4
1	G	970	0	895	22	0
1	H	948	0	862	23	0
1	I	958	0	886	15	0
1	J	934	0	842	20	1
1	K	954	0	871	15	0
1	L	948	0	860	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	966	0	890	23	1
1	N	954	0	871	35	0
1	O	950	0	880	45	2
1	P	950	0	858	19	4
1	Q	939	0	847	23	1
1	R	958	0	880	26	1
1	S	943	0	854	31	3
1	T	950	0	871	36	0
1	U	931	0	835	16	3
1	V	908	0	801	31	1
1	W	917	0	825	24	2
1	X	902	0	763	30	1
2	A	4	0	0	0	0
2	B	5	0	0	0	0
2	C	6	0	0	0	0
2	D	1	0	0	0	0
2	E	4	0	0	0	0
2	F	6	0	0	0	0
2	G	3	0	0	0	0
2	H	4	0	0	0	0
2	I	3	0	0	0	0
2	J	1	0	0	0	0
2	L	2	0	0	0	0
2	M	1	0	0	0	0
2	V	1	0	0	1	0
All	All	22771	0	20644	535	13

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 12.

All (535) 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:S:187:ILE:CD1	1:S:213:VAL:O	1.86	1.23
1:S:187:ILE:HD12	1:S:213:VAL:O	0.97	1.11
1:S:187:ILE:HD12	1:S:213:VAL:C	1.77	1.04
1:O:195:ASN:ND2	1:O:197:MET:HB2	1.70	1.04
1:O:171:CYS:HA	1:O:179:CYS:HB2	1.47	0.96
1:S:128:ILE:HD11	1:S:157:GLY:CA	1.96	0.95
1:O:233:VAL:HA	1:O:236:GLN:OXT	1.69	0.91
1:O:201:LYS:N	1:O:201:LYS:HD2	1.85	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:128:ILE:HD11	1:T:157:GLY:HA2	1.53	0.88
1:S:128:ILE:HD11	1:S:157:GLY:N	1.90	0.86
1:N:152:PHE:CD2	1:N:223:VAL:HG22	2.10	0.86
1:S:187:ILE:CD1	1:S:213:VAL:C	2.38	0.85
1:A:128:ILE:HD11	1:A:157:GLY:HA2	1.55	0.84
1:H:173:ALA:HB1	1:H:174:PRO:HD2	1.57	0.84
1:O:195:ASN:HD21	1:O:197:MET:HB2	1.43	0.83
1:S:176:PRO:HB2	1:S:200:TYR:HE2	1.45	0.81
1:L:149:GLN:HE21	1:L:156:GLY:H	1.27	0.81
1:L:140:ASP:OD2	1:M:117:ARG:NH1	2.12	0.81
1:N:152:PHE:CE2	1:N:223:VAL:HG22	2.14	0.81
1:D:131:GLY:HA3	1:D:141:PHE:CE1	2.16	0.80
1:N:160:TYR:OH	1:N:206:GLU:O	1.98	0.80
1:B:208:PHE:CD1	1:F:206:GLU:HG2	2.18	0.79
1:S:128:ILE:CD1	1:S:157:GLY:CA	2.62	0.78
1:F:161:ARG:HG2	1:F:203:ILE:HG23	1.65	0.78
1:R:138:ASP:HB3	1:R:141:PHE:HD2	1.50	0.77
1:K:117:ARG:HG3	1:K:117:ARG:HH11	1.48	0.77
1:V:190:THR:HG22	1:V:192:GLU:H	1.48	0.76
1:O:221:ASN:HD22	1:O:221:ASN:H	1.33	0.76
1:N:177:LEU:HD23	1:N:200:TYR:HE1	1.51	0.76
1:X:220:THR:O	1:X:223:VAL:HG12	1.86	0.75
1:Q:138:ASP:HB3	1:Q:141:PHE:HD1	1.51	0.75
1:G:149:GLN:HE21	1:G:156:GLY:H	1.34	0.75
1:V:168:TYR:O	2:V:301:HOH:O	2.05	0.75
1:L:149:GLN:HE22	1:L:163:TRP:HE1	1.30	0.75
1:J:128:ILE:HD11	1:J:157:GLY:HA2	1.70	0.73
1:H:128:ILE:HD11	1:H:157:GLY:CA	2.19	0.72
1:K:117:ARG:HG3	1:K:117:ARG:NH1	2.01	0.72
1:L:161:ARG:CZ	1:O:209:SER:HB2	2.19	0.71
1:X:117:ARG:O	1:X:121:ILE:HG12	1.91	0.71
1:J:160:TYR:OH	1:J:206:GLU:O	2.09	0.70
1:F:226:TRP:O	1:F:230:ASN:ND2	2.24	0.70
1:Q:187:ILE:HG13	1:Q:215:TYR:CE1	2.26	0.70
1:C:230:ASN:O	1:C:234:LEU:HG	1.92	0.70
1:F:129:ARG:O	1:F:133:GLU:HG3	1.92	0.70
1:L:149:GLN:NE2	1:L:156:GLY:H	1.90	0.70
1:A:128:ILE:HD11	1:A:157:GLY:CA	2.20	0.69
1:R:145:MET:O	1:R:149:GLN:HG3	1.93	0.69
1:I:128:ILE:HD11	1:I:157:GLY:CA	2.22	0.69
1:D:131:GLY:C	1:D:141:PHE:CE2	2.67	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:206:GLU:OE1	1:S:206:GLU:HA	1.93	0.68
1:G:183:TYR:OH	1:L:142:LYS:HE3	1.92	0.68
1:X:124:LEU:HD22	1:X:220:THR:HG23	1.75	0.68
1:O:171:CYS:SG	1:O:203:ILE:HD11	2.34	0.68
1:L:128:ILE:HD11	1:L:157:GLY:HA2	1.76	0.68
1:K:170:ASP:OD1	1:K:172:SER:OG	2.12	0.68
1:D:131:GLY:C	1:D:141:PHE:CZ	2.68	0.67
1:X:121:ILE:HD12	1:X:224:ILE:HD11	1.75	0.67
1:X:128:ILE:HD11	1:X:157:GLY:CA	2.24	0.67
1:K:128:ILE:HD11	1:K:157:GLY:CA	2.25	0.67
1:O:176:PRO:O	1:O:201:LYS:NZ	2.27	0.67
1:P:123:PHE:HD2	1:P:124:LEU:HD12	1.58	0.67
1:W:177:LEU:HD23	1:W:200:TYR:HE1	1.60	0.66
1:R:128:ILE:HG23	1:R:145:MET:HE1	1.77	0.66
1:V:135:TYR:OH	1:V:146:ASP:OD1	2.07	0.66
1:V:149:GLN:HE21	1:V:156:GLY:H	1.43	0.66
1:E:232:GLU:OE1	1:E:232:GLU:N	2.27	0.66
1:U:194:VAL:HG13	1:U:198:CYS:HB3	1.78	0.66
1:U:166:ASN:HB3	1:U:169:HIS:HB2	1.77	0.65
1:M:171:CYS:HA	1:M:179:CYS:HB2	1.78	0.65
1:O:125:ASN:OD1	1:O:220:THR:HG21	1.96	0.65
1:K:206:GLU:OE1	1:K:206:GLU:HA	1.96	0.65
1:R:138:ASP:HB3	1:R:141:PHE:CD2	2.32	0.65
1:G:149:GLN:HE22	1:G:163:TRP:HE1	1.45	0.65
1:N:128:ILE:HD11	1:N:157:GLY:CA	2.27	0.65
1:T:128:ILE:HD11	1:T:157:GLY:CA	2.27	0.65
1:M:128:ILE:O	1:M:132:ILE:HG13	1.97	0.65
1:J:171:CYS:HA	1:J:179:CYS:HB2	1.79	0.64
1:V:171:CYS:HA	1:V:179:CYS:HB2	1.80	0.64
1:B:153:LYS:HG2	1:B:215:TYR:CZ	2.31	0.64
1:X:187:ILE:HG13	1:X:215:TYR:CE1	2.32	0.64
1:W:128:ILE:HD11	1:W:157:GLY:HA2	1.79	0.64
1:F:128:ILE:HD11	1:F:157:GLY:CA	2.28	0.64
1:J:124:LEU:O	1:J:124:LEU:HD22	1.98	0.64
1:N:117:ARG:O	1:N:121:ILE:HG12	1.98	0.64
1:N:157:GLY:N	1:N:162:ASP:OD2	2.30	0.64
1:Q:219:CYS:O	1:Q:223:VAL:HG23	1.98	0.64
1:W:128:ILE:HD11	1:W:157:GLY:CA	2.28	0.64
1:O:124:LEU:O	1:O:128:ILE:HG12	1.98	0.64
1:T:171:CYS:HA	1:T:179:CYS:HB2	1.80	0.64
1:P:160:TYR:OH	1:P:206:GLU:O	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:149:GLN:OE1	1:W:185:CYS:SG	2.56	0.64
1:O:206:GLU:O	1:O:209:SER:OG	2.16	0.63
1:N:151:LYS:HD3	1:N:152:PHE:HE1	1.62	0.63
1:I:213:VAL:HG12	1:I:214:ILE:HG23	1.80	0.63
1:P:128:ILE:HD11	1:P:157:GLY:HA2	1.81	0.63
1:G:220:THR:O	1:G:224:ILE:HG12	1.97	0.63
1:C:221:ASN:O	1:C:225:ILE:HG12	1.99	0.62
1:D:213:VAL:HG12	1:D:214:ILE:HG23	1.81	0.62
1:P:171:CYS:HA	1:P:179:CYS:HB2	1.81	0.62
1:B:201:LYS:O	1:B:205:LYS:HE3	1.99	0.62
1:L:181:VAL:HG12	1:L:199:GLY:HA3	1.81	0.62
1:V:132:ILE:HG23	1:V:163:TRP:CZ3	2.33	0.62
1:N:213:VAL:HG12	1:N:214:ILE:HG23	1.82	0.62
1:V:117:ARG:O	1:V:120:THR:HG23	1.99	0.62
1:T:148:VAL:HG13	1:T:152:PHE:HD2	1.65	0.62
1:G:128:ILE:HD11	1:G:157:GLY:N	2.15	0.61
1:N:128:ILE:O	1:N:132:ILE:HD12	2.00	0.61
1:X:171:CYS:HA	1:X:179:CYS:HB2	1.82	0.61
1:T:169:HIS:CE1	1:T:177:LEU:HD22	2.35	0.61
1:W:220:THR:O	1:W:224:ILE:HG13	2.01	0.61
1:D:189:ASP:HA	1:F:225:ILE:HD12	1.81	0.61
1:X:121:ILE:CD1	1:X:224:ILE:HD11	2.31	0.61
1:J:197:MET:HG2	1:J:200:TYR:CE2	2.36	0.61
1:H:209:SER:HB3	1:X:208:PHE:CZ	2.36	0.61
1:W:171:CYS:HA	1:W:179:CYS:HB2	1.81	0.60
1:D:142:LYS:HE3	1:T:183:TYR:CZ	2.34	0.60
1:H:169:HIS:CE1	1:H:177:LEU:HD22	2.36	0.60
1:V:213:VAL:HG12	1:V:214:ILE:HG23	1.81	0.60
1:X:146:ASP:HB3	1:X:184:THR:HG21	1.83	0.60
1:A:212:ASP:OD1	1:A:213:VAL:HG23	2.02	0.60
1:I:138:ASP:OD2	1:Q:117:ARG:HB2	2.01	0.60
1:J:117:ARG:HG2	1:J:121:ILE:HD11	1.82	0.60
1:N:171:CYS:HA	1:N:179:CYS:HB2	1.83	0.60
1:O:157:GLY:O	1:O:220:THR:HG23	2.02	0.60
1:S:191:THR:HG22	1:V:221:ASN:ND2	2.16	0.60
1:B:205:LYS:NZ	1:F:158:GLU:OE2	2.34	0.60
1:O:231:LEU:HD12	1:O:234:LEU:HD12	1.83	0.60
1:D:131:GLY:O	1:D:141:PHE:CE2	2.55	0.60
1:G:231:LEU:O	1:G:234:LEU:HG	2.02	0.60
1:O:117:ARG:HA	1:O:120:THR:HG22	1.83	0.60
1:Q:128:ILE:O	1:Q:132:ILE:HG13	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:191:THR:HA	1:V:221:ASN:HD21	1.65	0.59
1:O:205:LYS:O	1:O:206:GLU:HB2	2.01	0.59
1:D:131:GLY:HA3	1:D:141:PHE:CZ	2.37	0.59
1:K:124:LEU:HD12	1:K:220:THR:HG23	1.83	0.59
1:N:232:GLU:OE1	1:N:232:GLU:N	2.33	0.59
1:O:117:ARG:O	1:O:121:ILE:HG13	2.02	0.59
1:T:220:THR:O	1:T:224:ILE:HG12	2.02	0.59
1:E:142:LYS:HE3	1:J:183:TYR:CZ	2.37	0.59
1:L:140:ASP:O	1:L:144:ILE:HG13	2.02	0.59
1:N:226:TRP:NE1	1:N:230:ASN:ND2	2.50	0.59
1:O:235:PHE:HD1	1:O:235:PHE:N	2.01	0.59
1:P:230:ASN:O	1:P:234:LEU:HG	2.03	0.59
1:N:135:TYR:O	1:N:142:LYS:HB2	2.02	0.59
1:S:128:ILE:HD11	1:S:157:GLY:HA3	1.82	0.59
1:W:213:VAL:HG12	1:W:214:ILE:HG23	1.85	0.59
1:Q:138:ASP:HB3	1:Q:141:PHE:CD1	2.35	0.58
1:H:128:ILE:HD11	1:H:157:GLY:HA2	1.85	0.58
1:E:197:MET:HG2	1:E:200:TYR:CE2	2.38	0.58
1:T:117:ARG:O	1:T:121:ILE:HG12	2.04	0.58
1:W:219:CYS:O	1:W:223:VAL:HG23	2.04	0.58
1:C:131:GLY:HA3	1:C:141:PHE:CZ	2.37	0.58
1:V:121:ILE:HA	1:V:124:LEU:HD12	1.85	0.58
1:O:221:ASN:H	1:O:221:ASN:ND2	1.99	0.58
1:Q:125:ASN:OD1	1:Q:220:THR:HG21	2.04	0.58
1:R:161:ARG:HG2	1:R:203:ILE:HG23	1.86	0.57
1:R:149:GLN:HB3	1:R:154:CYS:O	2.03	0.57
1:V:219:CYS:O	1:V:223:VAL:HG23	2.04	0.57
1:R:129:ARG:CZ	1:R:129:ARG:HB2	2.33	0.57
1:U:168:TYR:N	1:U:168:TYR:CD1	2.72	0.57
1:A:138:ASP:OD2	1:G:117:ARG:HD2	2.04	0.57
1:S:234:LEU:C	1:S:235:PHE:HD1	2.08	0.57
1:B:138:ASP:HB3	1:B:141:PHE:HD2	1.70	0.57
1:N:155:CYS:SG	1:N:181:VAL:HG21	2.44	0.57
1:A:197:MET:HG2	1:A:200:TYR:CE2	2.40	0.57
1:G:122:ASP:O	1:G:125:ASN:N	2.38	0.57
1:M:213:VAL:HG12	1:M:214:ILE:HG23	1.87	0.57
1:N:128:ILE:HD11	1:N:157:GLY:HA2	1.87	0.57
1:O:235:PHE:N	1:O:235:PHE:CD1	2.72	0.57
1:D:143:ASN:OD1	1:T:188:ARG:NH2	2.32	0.56
1:O:233:VAL:HG22	1:O:233:VAL:O	2.05	0.56
1:P:128:ILE:CD1	1:P:157:GLY:HA2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:160:TYR:HE1	1:R:203:ILE:HA	1.70	0.56
1:B:213:VAL:HG12	1:B:214:ILE:HG23	1.87	0.56
1:E:233:VAL:HG12	1:E:233:VAL:O	2.04	0.56
1:H:138:ASP:OD2	1:P:117:ARG:HB2	2.04	0.56
1:C:131:GLY:O	1:C:134:ASN:N	2.39	0.56
1:F:234:LEU:C	1:F:235:PHE:HD1	2.09	0.56
1:Q:213:VAL:HG12	1:Q:214:ILE:HG23	1.86	0.56
1:T:161:ARG:HG2	1:T:203:ILE:HG23	1.88	0.56
1:C:232:GLU:HG2	1:M:232:GLU:HG2	1.87	0.56
1:D:142:LYS:HE3	1:T:183:TYR:OH	2.06	0.56
1:N:181:VAL:O	1:N:199:GLY:HA3	2.06	0.56
1:T:221:ASN:O	1:T:224:ILE:N	2.39	0.56
1:V:149:GLN:HE22	1:V:163:TRP:HE1	1.54	0.56
1:Q:171:CYS:HA	1:Q:179:CYS:HB2	1.88	0.56
1:O:232:GLU:O	1:O:236:GLN:OXT	2.23	0.56
1:L:197:MET:HG2	1:L:200:TYR:CE2	2.41	0.55
1:M:124:LEU:O	1:M:128:ILE:HG12	2.05	0.55
1:V:138:ASP:OD2	1:V:140:ASP:HB2	2.05	0.55
1:X:121:ILE:HD12	1:X:224:ILE:CD1	2.36	0.55
1:W:177:LEU:HD23	1:W:200:TYR:CE1	2.41	0.55
1:N:160:TYR:CE1	1:N:161:ARG:HG3	2.41	0.55
1:R:186:CYS:HA	1:R:214:ILE:HG22	1.88	0.55
1:F:115:THR:O	1:F:115:THR:OG1	2.21	0.55
1:X:139:LEU:HD12	1:X:139:LEU:H	1.70	0.55
1:M:121:ILE:HG22	1:M:125:ASN:ND2	2.22	0.55
1:O:195:ASN:HD22	1:O:197:MET:HB2	1.65	0.55
1:V:145:MET:HE3	1:V:149:GLN:HG3	1.89	0.55
1:R:135:TYR:O	1:R:142:LYS:HB2	2.07	0.55
1:G:131:GLY:HA3	1:G:141:PHE:CE1	2.22	0.54
1:W:123:PHE:CD2	1:W:124:LEU:HD12	2.42	0.54
1:C:150:LYS:O	1:C:150:LYS:HG2	2.07	0.54
1:M:207:ARG:O	1:M:211:GLN:HG3	2.08	0.54
1:B:158:GLU:N	1:B:162:ASP:OD2	2.39	0.54
1:C:131:GLY:HA3	1:C:141:PHE:CE1	2.43	0.54
1:V:117:ARG:CB	1:V:120:THR:CG2	2.86	0.54
1:X:169:HIS:CE1	1:X:177:LEU:HD12	2.42	0.54
1:S:128:ILE:CD1	1:S:157:GLY:HA3	2.36	0.54
1:V:190:THR:HG22	1:V:192:GLU:N	2.21	0.54
1:B:117:ARG:O	1:B:121:ILE:HG12	2.07	0.54
1:G:149:GLN:NE2	1:G:156:GLY:H	2.04	0.54
1:H:151:LYS:O	1:H:151:LYS:HD3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:146:ASP:HB3	1:S:184:THR:HG21	1.90	0.54
1:X:170:ASP:OD2	1:X:172:SER:OG	2.20	0.54
1:O:124:LEU:HD12	1:O:124:LEU:H	1.73	0.54
1:W:120:THR:HA	1:W:123:PHE:HB3	1.89	0.54
1:B:208:PHE:CE1	1:F:206:GLU:CG	2.91	0.53
1:G:183:TYR:CZ	1:L:142:LYS:HE3	2.43	0.53
1:J:128:ILE:HD11	1:J:157:GLY:CA	2.35	0.53
1:S:128:ILE:CD1	1:S:157:GLY:HA2	2.37	0.53
1:P:140:ASP:O	1:R:228:MET:HE1	2.08	0.53
1:G:161:ARG:HD3	1:G:203:ILE:O	2.08	0.53
1:X:231:LEU:HD12	1:X:231:LEU:O	2.07	0.53
1:N:151:LYS:HG2	1:N:152:PHE:HD1	1.73	0.53
1:O:126:ASP:OD1	1:O:127:ASN:N	2.42	0.53
1:O:205:LYS:O	1:O:209:SER:OG	2.17	0.53
1:N:121:ILE:HG22	1:N:125:ASN:ND2	2.23	0.53
1:S:131:GLY:HA3	1:S:141:PHE:CZ	2.44	0.53
1:P:135:TYR:CE1	1:P:142:LYS:HG3	2.44	0.52
1:Q:121:ILE:HG22	1:Q:125:ASN:ND2	2.24	0.52
1:N:121:ILE:HG22	1:N:125:ASN:HD21	1.74	0.52
1:E:221:ASN:O	1:E:225:ILE:HG23	2.08	0.52
1:N:145:MET:O	1:N:149:GLN:HG3	2.10	0.52
1:R:146:ASP:HB3	1:R:184:THR:HG21	1.91	0.52
1:T:169:HIS:HE1	1:T:177:LEU:HD22	1.74	0.52
1:H:144:ILE:HG13	1:P:228:MET:HE1	1.92	0.52
1:X:128:ILE:HD11	1:X:157:GLY:HA3	1.91	0.52
1:R:149:GLN:OE1	1:R:185:CYS:SG	2.68	0.52
1:X:139:LEU:HD12	1:X:139:LEU:N	2.25	0.52
1:A:190:THR:OG1	1:A:192:GLU:HG2	2.10	0.52
1:A:230:ASN:O	1:A:234:LEU:HG	2.09	0.52
1:G:161:ARG:NH2	1:J:204:ASP:OD2	2.43	0.52
1:U:221:ASN:O	1:U:225:ILE:HG23	2.11	0.51
1:G:135:TYR:O	1:G:142:LYS:HB2	2.10	0.51
1:H:173:ALA:CB	1:H:174:PRO:HD2	2.27	0.51
1:B:142:LYS:HE3	1:C:183:TYR:CZ	2.45	0.51
1:F:171:CYS:HA	1:F:179:CYS:HB2	1.92	0.51
1:H:209:SER:HB3	1:X:208:PHE:CE1	2.44	0.51
1:T:234:LEU:N	1:T:234:LEU:HD23	2.26	0.51
1:U:168:TYR:H	1:U:168:TYR:HD1	1.57	0.51
1:X:153:LYS:HA	1:X:215:TYR:CE2	2.45	0.51
1:A:123:PHE:HD2	1:A:124:LEU:HD12	1.75	0.51
1:H:204:ASP:OD1	1:H:204:ASP:N	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:230:ASN:N	1:T:230:ASN:HD22	2.09	0.51
1:S:187:ILE:HG22	1:S:188:ARG:H	1.76	0.51
1:W:167:GLN:HG2	1:W:168:TYR:CD1	2.46	0.51
1:J:128:ILE:O	1:J:132:ILE:HG13	2.11	0.51
1:D:120:THR:O	1:D:124:LEU:HG	2.11	0.51
1:Q:152:PHE:O	1:Q:217:ARG:NH2	2.43	0.51
1:U:148:VAL:HG13	1:U:152:PHE:HD2	1.76	0.51
1:W:162:ASP:O	1:W:165:LYS:HG2	2.10	0.51
1:X:200:TYR:O	1:X:202:THR:HG23	2.11	0.51
1:N:187:ILE:HG13	1:N:215:TYR:CE1	2.46	0.51
1:A:118:GLN:HA	1:A:121:ILE:HG12	1.93	0.50
1:K:213:VAL:HG13	1:K:214:ILE:HG23	1.93	0.50
1:U:230:ASN:O	1:U:234:LEU:HG	2.11	0.50
1:R:152:PHE:O	1:R:217:ARG:NH2	2.42	0.50
1:C:171:CYS:HA	1:C:179:CYS:HB2	1.93	0.50
1:F:128:ILE:HD11	1:F:157:GLY:N	2.26	0.50
1:R:219:CYS:O	1:R:223:VAL:HG23	2.11	0.50
1:U:197:MET:HG2	1:U:200:TYR:CE2	2.47	0.50
1:I:128:ILE:HD11	1:I:157:GLY:HA2	1.94	0.50
1:Q:135:TYR:O	1:Q:142:LYS:HB2	2.12	0.50
1:T:197:MET:HG2	1:T:200:TYR:CE2	2.47	0.50
1:V:131:GLY:HA3	1:V:141:PHE:CZ	2.47	0.50
1:A:124:LEU:O	1:A:128:ILE:HG23	2.12	0.49
1:M:145:MET:O	1:M:149:GLN:HG3	2.11	0.49
1:S:170:ASP:OD1	1:S:171:CYS:N	2.45	0.49
1:S:187:ILE:HD13	1:S:212:ASP:O	2.13	0.49
1:O:128:ILE:HD11	1:O:220:THR:HG22	1.94	0.49
1:O:231:LEU:HA	1:O:234:LEU:HG	1.95	0.49
1:B:197:MET:HG2	1:B:200:TYR:CE2	2.47	0.49
1:O:221:ASN:ND2	1:O:221:ASN:N	2.60	0.49
1:C:115:THR:C	1:C:117:ARG:H	2.16	0.49
1:L:123:PHE:CD2	1:L:124:LEU:HD12	2.47	0.49
1:X:124:LEU:CD2	1:X:220:THR:OG1	2.61	0.49
1:I:159:ASP:OD2	1:I:161:ARG:NH2	2.45	0.49
1:O:153:LYS:HG2	1:O:215:TYR:CZ	2.48	0.49
1:O:233:VAL:CA	1:O:236:GLN:OXT	2.54	0.49
1:O:230:ASN:OD1	1:O:230:ASN:N	2.45	0.49
1:P:213:VAL:HG13	1:P:214:ILE:HG23	1.94	0.49
1:R:135:TYR:CD1	1:R:163:TRP:HH2	2.30	0.49
1:S:188:ARG:O	1:S:188:ARG:HG3	2.13	0.49
1:T:230:ASN:N	1:T:230:ASN:ND2	2.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:131:GLY:HA3	1:V:141:PHE:CE2	2.48	0.48
1:E:183:TYR:CZ	1:J:142:LYS:HE3	2.48	0.48
1:S:219:CYS:O	1:S:223:VAL:HG23	2.12	0.48
1:B:115:THR:O	1:B:117:ARG:N	2.44	0.48
1:C:201:LYS:O	1:C:205:LYS:HE3	2.13	0.48
1:T:165:LYS:HD2	1:T:165:LYS:O	2.13	0.48
1:K:128:ILE:HD11	1:K:157:GLY:N	2.29	0.48
1:D:131:GLY:CA	1:D:141:PHE:CZ	2.96	0.48
1:H:128:ILE:O	1:H:132:ILE:HG13	2.13	0.48
1:O:201:LYS:HD2	1:O:201:LYS:H	1.73	0.48
1:G:128:ILE:HD11	1:G:157:GLY:CA	2.44	0.48
1:U:123:PHE:O	1:U:126:ASP:HB3	2.14	0.48
1:H:151:LYS:HD3	1:H:151:LYS:C	2.34	0.48
1:M:179:CYS:HA	1:M:203:ILE:HD12	1.95	0.48
1:F:212:ASP:OD1	1:F:212:ASP:N	2.28	0.48
1:V:221:ASN:O	1:V:225:ILE:HG12	2.13	0.48
1:W:197:MET:HG2	1:W:200:TYR:CE2	2.49	0.48
1:L:138:ASP:OD2	1:M:117:ARG:HD2	2.14	0.47
1:M:135:TYR:O	1:M:142:LYS:HB2	2.14	0.47
1:W:135:TYR:CE1	1:W:142:LYS:HG3	2.49	0.47
1:Q:128:ILE:HD11	1:Q:220:THR:HG23	1.95	0.47
1:Q:138:ASP:OD1	1:Q:140:ASP:HB2	2.14	0.47
1:O:160:TYR:CZ	1:O:161:ARG:HD2	2.49	0.47
1:O:227:PHE:HD1	1:O:227:PHE:O	1.97	0.47
1:Q:224:ILE:O	1:Q:228:MET:HG2	2.14	0.47
1:S:208:PHE:HA	1:S:211:GLN:HB2	1.96	0.47
1:T:135:TYR:O	1:T:142:LYS:HB2	2.13	0.47
1:K:171:CYS:HA	1:K:179:CYS:HB2	1.96	0.47
1:R:145:MET:HB3	1:R:149:GLN:HE21	1.79	0.47
1:X:124:LEU:HD22	1:X:220:THR:CG2	2.44	0.47
1:X:167:GLN:HG3	1:X:168:TYR:CD1	2.50	0.47
1:A:221:ASN:O	1:A:225:ILE:HG23	2.14	0.47
1:C:117:ARG:HH11	1:L:193:VAL:HG12	1.78	0.47
1:D:167:GLN:HG3	1:D:168:TYR:CD1	2.49	0.47
1:G:233:VAL:O	1:G:234:LEU:HD23	2.13	0.47
1:R:130:ARG:O	1:R:134:ASN:ND2	2.46	0.47
1:S:128:ILE:HD13	1:S:157:GLY:HA2	1.97	0.47
1:F:181:VAL:HG12	1:F:199:GLY:HA3	1.96	0.47
1:L:171:CYS:HA	1:L:179:CYS:HB2	1.97	0.47
1:V:141:PHE:CE1	1:V:145:MET:HG3	2.50	0.47
1:W:181:VAL:N	1:W:199:GLY:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:123:PHE:CD2	1:G:124:LEU:HD12	2.50	0.47
1:B:124:LEU:O	1:B:128:ILE:HG12	2.15	0.46
1:B:208:PHE:CE1	1:F:206:GLU:HG2	2.49	0.46
1:B:235:PHE:O	1:B:236:GLN:OXT	2.33	0.46
1:K:123:PHE:CD1	1:K:124:LEU:HD23	2.50	0.46
1:O:138:ASP:OD1	1:O:140:ASP:HB2	2.15	0.46
1:Q:117:ARG:O	1:Q:121:ILE:HG12	2.15	0.46
1:V:135:TYR:O	1:V:142:LYS:HB2	2.15	0.46
1:A:171:CYS:HA	1:A:179:CYS:HB2	1.97	0.46
1:T:148:VAL:HG13	1:T:152:PHE:CD2	2.46	0.46
1:D:183:TYR:CZ	1:T:142:LYS:HE3	2.51	0.46
1:M:180:GLY:O	1:M:203:ILE:HD11	2.16	0.46
1:J:138:ASP:OD1	1:J:140:ASP:HB2	2.14	0.46
1:N:230:ASN:O	1:N:234:LEU:HG	2.16	0.46
1:Q:121:ILE:O	1:Q:125:ASN:ND2	2.48	0.46
1:J:181:VAL:HG22	1:J:182:PRO:HD2	1.97	0.46
1:P:187:ILE:HG12	1:P:215:TYR:CE1	2.51	0.46
1:B:183:TYR:CZ	1:C:142:LYS:HE3	2.50	0.46
1:W:221:ASN:HA	1:W:224:ILE:HD12	1.97	0.46
1:X:220:THR:O	1:X:223:VAL:CG1	2.59	0.46
1:P:141:PHE:CD1	1:P:141:PHE:C	2.89	0.46
1:H:129:ARG:O	1:H:133:GLU:HG3	2.15	0.46
1:K:117:ARG:HH11	1:K:117:ARG:CG	2.16	0.46
1:L:135:TYR:O	1:L:142:LYS:HB2	2.16	0.45
1:N:151:LYS:HG2	1:N:152:PHE:CD1	2.51	0.45
1:V:122:ASP:OD1	1:V:122:ASP:N	2.41	0.45
1:K:179:CYS:HA	1:K:203:ILE:HD12	1.98	0.45
1:P:148:VAL:HG13	1:P:152:PHE:HD2	1.82	0.45
1:T:157:GLY:O	1:T:220:THR:HG22	2.16	0.45
1:A:118:GLN:OE1	1:A:121:ILE:HD11	2.17	0.45
1:V:177:LEU:HD23	1:V:200:TYR:HE1	1.81	0.45
1:X:227:PHE:CD1	1:X:227:PHE:C	2.90	0.45
1:P:179:CYS:HA	1:P:203:ILE:HD12	1.98	0.45
1:W:123:PHE:HD2	1:W:124:LEU:HD12	1.80	0.45
1:C:151:LYS:O	1:C:151:LYS:HD3	2.17	0.45
1:F:138:ASP:OD1	1:F:140:ASP:HB2	2.17	0.45
1:P:128:ILE:HD11	1:P:157:GLY:CA	2.46	0.45
1:X:121:ILE:CD1	1:X:224:ILE:CD1	2.93	0.45
1:M:204:ASP:OD2	1:M:205:LYS:NZ	2.48	0.45
1:M:219:CYS:O	1:M:223:VAL:HG23	2.17	0.45
1:A:191:THR:O	1:Q:117:ARG:NH2	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:169:HIS:CE1	1:K:177:LEU:HD22	2.52	0.45
1:T:133:GLU:HG2	1:T:165:LYS:NZ	2.32	0.45
1:T:155:CYS:SG	1:T:181:VAL:HG21	2.57	0.45
1:B:124:LEU:HB2	1:B:220:THR:HG23	1.98	0.44
1:H:115:THR:C	1:H:117:ARG:H	2.21	0.44
1:I:115:THR:N	1:I:119:GLN:HG3	2.32	0.44
1:N:128:ILE:HD11	1:N:157:GLY:N	2.31	0.44
1:T:181:VAL:HG22	1:T:182:PRO:HD2	1.98	0.44
1:E:181:VAL:HB	1:E:182:PRO:HD2	2.00	0.44
1:B:234:LEU:HD23	1:B:234:LEU:HA	1.63	0.44
1:S:138:ASP:OD1	1:S:140:ASP:HB2	2.17	0.44
1:X:187:ILE:HG13	1:X:215:TYR:CD1	2.52	0.44
1:A:128:ILE:HG21	1:A:128:ILE:HD13	1.65	0.44
1:C:124:LEU:O	1:C:128:ILE:HG12	2.17	0.44
1:S:161:ARG:NE	1:S:206:GLU:OE2	2.51	0.44
1:R:160:TYR:CE1	1:R:203:ILE:HA	2.51	0.44
1:X:169:HIS:HE1	1:X:177:LEU:HD12	1.82	0.44
1:O:152:PHE:O	1:O:217:ARG:NH2	2.50	0.44
1:B:159:ASP:OD2	1:B:161:ARG:NH2	2.51	0.43
1:E:151:LYS:NZ	1:N:235:PHE:O	2.51	0.43
1:F:158:GLU:O	1:F:218:GLY:HA3	2.18	0.43
1:P:131:GLY:HA3	1:P:141:PHE:CZ	2.52	0.43
1:B:225:ILE:HG13	1:B:226:TRP:N	2.33	0.43
1:A:146:ASP:HB3	1:A:184:THR:HG21	2.00	0.43
1:O:187:ILE:HD11	1:O:211:GLN:O	2.18	0.43
1:R:169:HIS:CE1	1:R:177:LEU:HD22	2.53	0.43
1:S:124:LEU:HD12	1:S:124:LEU:HA	1.78	0.43
1:T:118:GLN:O	1:T:122:ASP:N	2.39	0.43
1:L:124:LEU:HD22	1:L:220:THR:HG23	2.00	0.43
1:O:128:ILE:HD13	1:O:128:ILE:HG21	1.79	0.43
1:Q:173:ALA:HB3	1:Q:178:ALA:HB2	2.00	0.43
1:U:204:ASP:OD1	1:U:205:LYS:N	2.51	0.43
1:W:227:PHE:CD1	1:W:234:LEU:HD11	2.54	0.43
1:E:179:CYS:SG	1:E:204:ASP:OD2	2.77	0.43
1:S:121:ILE:HD11	1:S:224:ILE:CD1	2.48	0.43
1:P:200:TYR:O	1:P:202:THR:HG23	2.18	0.43
1:F:128:ILE:HD11	1:F:157:GLY:HA3	2.00	0.43
1:N:181:VAL:HG11	1:N:214:ILE:HD13	1.99	0.43
1:T:231:LEU:HD12	1:T:231:LEU:HA	1.73	0.43
1:M:121:ILE:HG22	1:M:125:ASN:HD21	1.82	0.43
1:M:170:ASP:OD1	1:M:172:SER:OG	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:152:PHE:CD1	1:N:152:PHE:N	2.87	0.43
1:R:115:THR:CB	1:R:118:GLN:HB2	2.48	0.43
1:U:202:THR:HB	1:U:210:VAL:HG11	1.99	0.43
1:V:118:GLN:OE1	1:V:122:ASP:OD1	2.37	0.43
1:C:135:TYR:O	1:C:142:LYS:HB2	2.18	0.43
1:D:161:ARG:HE	1:D:161:ARG:HB2	1.29	0.43
1:D:188:ARG:NH1	1:T:143:ASN:OD1	2.39	0.43
1:H:141:PHE:CE2	1:H:145:MET:HG2	2.54	0.43
1:P:205:LYS:O	1:P:209:SER:OG	2.36	0.43
1:S:128:ILE:HD13	1:S:157:GLY:CA	2.47	0.43
1:T:220:THR:HG23	1:T:221:ASN:N	2.34	0.43
1:G:227:PHE:CE2	1:G:228:MET:HE1	2.54	0.43
1:X:205:LYS:O	1:X:209:SER:HB2	2.19	0.43
1:A:165:LYS:NZ	1:D:204:ASP:HB2	2.33	0.42
1:E:163:TRP:CZ2	1:E:182:PRO:HG2	2.54	0.42
1:K:217:ARG:O	1:K:217:ARG:HG3	2.19	0.42
1:N:120:THR:O	1:N:124:LEU:HD12	2.19	0.42
1:A:174:PRO:HG3	1:N:161:ARG:HB3	2.01	0.42
1:G:221:ASN:O	1:G:225:ILE:HG23	2.19	0.42
1:M:232:GLU:H	1:M:232:GLU:CD	2.22	0.42
1:U:146:ASP:HB3	1:U:184:THR:HG21	2.01	0.42
1:V:159:ASP:OD1	1:V:161:ARG:HG2	2.18	0.42
1:W:122:ASP:O	1:W:126:ASP:OD1	2.37	0.42
1:W:231:LEU:HA	1:W:234:LEU:HD12	2.01	0.42
1:H:131:GLY:HA3	1:H:141:PHE:CZ	2.54	0.42
1:I:128:ILE:HD11	1:I:157:GLY:N	2.34	0.42
1:M:221:ASN:O	1:M:225:ILE:HG23	2.19	0.42
1:V:163:TRP:CZ2	1:V:182:PRO:HG2	2.55	0.42
1:F:135:TYR:OH	1:F:146:ASP:OD1	2.31	0.42
1:F:161:ARG:HD3	1:F:203:ILE:O	2.19	0.42
1:F:228:MET:HG3	1:T:140:ASP:OD1	2.19	0.42
1:Q:169:HIS:CE1	1:Q:177:LEU:HD12	2.54	0.42
1:E:142:LYS:HE3	1:J:183:TYR:CE2	2.54	0.42
1:C:128:ILE:O	1:C:132:ILE:HG13	2.20	0.42
1:T:163:TRP:CZ2	1:T:182:PRO:HG2	2.54	0.42
1:D:153:LYS:HG2	1:D:215:TYR:CZ	2.55	0.42
1:R:232:GLU:OE1	1:R:232:GLU:N	2.39	0.42
1:T:145:MET:O	1:T:149:GLN:HG3	2.19	0.42
1:H:128:ILE:HD11	1:H:157:GLY:N	2.35	0.42
1:I:207:ARG:O	1:I:211:GLN:HG3	2.20	0.42
1:T:207:ARG:O	1:T:211:GLN:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:TRP:O	1:C:169:HIS:HB2	2.20	0.42
1:H:221:ASN:O	1:H:225:ILE:HG23	2.20	0.42
1:I:181:VAL:HG22	1:I:182:PRO:HD2	2.01	0.41
1:L:124:LEU:O	1:L:128:ILE:HG23	2.20	0.41
1:L:128:ILE:HG21	1:L:128:ILE:HD13	1.78	0.41
1:O:179:CYS:HA	1:O:203:ILE:HD11	2.01	0.41
1:B:232:GLU:OE1	1:B:232:GLU:N	2.38	0.41
1:H:131:GLY:O	1:H:134:ASN:N	2.42	0.41
1:H:200:TYR:O	1:H:202:THR:HG23	2.20	0.41
1:M:132:ILE:HG23	1:M:163:TRP:CE3	2.56	0.41
1:T:219:CYS:O	1:T:223:VAL:HG23	2.19	0.41
1:C:221:ASN:O	1:C:222:ALA:C	2.56	0.41
1:E:167:GLN:HG3	1:E:168:TYR:CD1	2.55	0.41
1:F:145:MET:O	1:F:149:GLN:HG3	2.20	0.41
1:J:124:LEU:O	1:J:127:ASN:N	2.49	0.41
1:K:129:ARG:O	1:K:133:GLU:HG3	2.20	0.41
1:M:163:TRP:CZ2	1:M:182:PRO:HG2	2.55	0.41
1:N:161:ARG:HG2	1:N:203:ILE:HG23	2.01	0.41
1:U:148:VAL:HG13	1:U:152:PHE:CD2	2.54	0.41
1:D:159:ASP:OD2	1:D:161:ARG:NH2	2.54	0.41
1:G:131:GLY:O	1:G:134:ASN:N	2.53	0.41
1:I:171:CYS:HA	1:I:179:CYS:HB2	2.02	0.41
1:J:145:MET:O	1:J:149:GLN:HG3	2.20	0.41
1:N:128:ILE:HG21	1:N:128:ILE:HD13	1.88	0.41
1:R:234:LEU:HA	1:R:234:LEU:HD13	1.60	0.41
1:U:135:TYR:O	1:U:142:LYS:HB2	2.20	0.41
1:D:152:PHE:O	1:D:217:ARG:NH2	2.54	0.41
1:G:197:MET:HG2	1:G:200:TYR:CZ	2.55	0.41
1:M:160:TYR:OH	1:M:206:GLU:O	2.37	0.41
1:S:191:THR:HA	1:V:221:ASN:ND2	2.33	0.41
1:G:171:CYS:HA	1:G:179:CYS:HB2	2.02	0.41
1:I:155:CYS:SG	1:I:181:VAL:HG21	2.61	0.41
1:J:224:ILE:O	1:J:228:MET:HG2	2.20	0.41
1:W:128:ILE:HG21	1:W:128:ILE:HD13	1.88	0.41
1:W:167:GLN:HG2	1:W:168:TYR:HD1	1.84	0.41
1:B:200:TYR:O	1:B:202:THR:HG23	2.21	0.41
1:I:120:THR:O	1:I:124:LEU:HD13	2.21	0.41
1:L:123:PHE:HD2	1:L:124:LEU:HD12	1.86	0.41
1:N:117:ARG:O	1:N:120:THR:HG22	2.21	0.41
1:N:132:ILE:HG23	1:N:163:TRP:CE3	2.55	0.41
1:O:195:ASN:OD1	1:O:195:ASN:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:231:LEU:HD12	1:Q:231:LEU:O	2.21	0.41
1:T:135:TYR:OH	1:T:146:ASP:OD1	2.32	0.41
1:W:188:ARG:HA	1:W:188:ARG:HD2	1.96	0.41
1:A:232:GLU:HA	1:C:147:PHE:CE1	2.55	0.41
1:E:129:ARG:O	1:E:133:GLU:HG3	2.21	0.41
1:F:224:ILE:O	1:F:228:MET:HG2	2.21	0.41
1:H:126:ASP:OD1	1:H:129:ARG:NH1	2.54	0.41
1:H:232:GLU:OE1	1:H:232:GLU:N	2.36	0.41
1:J:230:ASN:O	1:J:234:LEU:HG	2.20	0.41
1:J:232:GLU:H	1:J:232:GLU:CD	2.24	0.41
1:O:135:TYR:O	1:O:142:LYS:HB2	2.21	0.41
1:Q:230:ASN:O	1:Q:234:LEU:HG	2.21	0.41
1:R:146:ASP:CB	1:R:184:THR:HG21	2.51	0.41
1:R:162:ASP:O	1:R:165:LYS:HG2	2.21	0.41
1:V:121:ILE:HA	1:V:124:LEU:CD1	2.51	0.41
1:A:183:TYR:CZ	1:I:142:LYS:HE3	2.55	0.41
1:I:161:ARG:HA	1:I:203:ILE:HG23	2.02	0.41
1:Q:128:ILE:HD13	1:Q:128:ILE:HG21	1.80	0.41
1:T:118:GLN:O	1:T:121:ILE:N	2.54	0.41
1:L:128:ILE:HD11	1:L:157:GLY:CA	2.49	0.40
1:O:197:MET:HG2	1:O:200:TYR:CE2	2.56	0.40
1:O:201:LYS:N	1:O:201:LYS:CD	2.71	0.40
1:S:197:MET:HA	1:S:200:TYR:CD1	2.57	0.40
1:X:135:TYR:CE2	1:X:142:LYS:HE2	2.56	0.40
1:J:221:ASN:O	1:J:225:ILE:HG23	2.21	0.40
1:O:201:LYS:O	1:O:205:LYS:HD2	2.22	0.40
1:U:150:LYS:HE2	1:U:150:LYS:HB3	1.85	0.40
1:A:142:LYS:HE3	1:I:183:TYR:CZ	2.57	0.40
1:U:171:CYS:HA	1:U:179:CYS:HB2	2.04	0.40
1:V:124:LEU:H	1:V:124:LEU:HG	1.63	0.40
1:B:208:PHE:CD1	1:F:206:GLU:CG	2.96	0.40
1:C:151:LYS:HD3	1:C:151:LYS:C	2.42	0.40
1:M:200:TYR:O	1:M:202:THR:HG23	2.22	0.40
1:R:152:PHE:HE1	1:R:226:TRP:CG	2.38	0.40
1:V:234:LEU:HD23	1:V:234:LEU:HA	1.89	0.40

All (13) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:140:ASP:OD2	1:S:117:ARG:NH2[1_564]	1.90	0.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:188:ARG:NH2	1:W:143:ASN:OD1[1_556]	1.91	0.29
1:U:150:LYS:NZ	1:W:232:GLU:OE2[1_465]	1.93	0.27
1:U:140:ASP:OD1	1:X:188:ARG:NH2[1_554]	1.97	0.23
1:Q:161:ARG:NH1	1:S:170:ASP:OD2[1_554]	1.99	0.21
1:B:140:ASP:OD2	1:E:117:ARG:NH2[1_455]	2.01	0.19
1:R:188:ARG:NH1	1:V:140:ASP:OD1[1_565]	2.01	0.19
1:O:117:ARG:NH2	1:U:140:ASP:OD2[1_556]	2.02	0.18
1:O:188:ARG:NH2	1:P:140:ASP:OD1[1_455]	2.02	0.18
1:F:191:THR:O	1:P:117:ARG:NH2[1_554]	2.04	0.16
1:J:117:ARG:NH1	1:M:140:ASP:OD2[1_655]	2.04	0.16
1:F:193:VAL:CG2	1:P:117:ARG:CD[1_554]	2.06	0.14
1:F:193:VAL:CG2	1:P:117:ARG:NE[1_554]	2.11	0.09

## 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	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
1	B	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
1	C	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
1	D	119/122 (98%)	112 (94%)	7 (6%)	0	100	100
1	E	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
1	F	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
1	G	120/122 (98%)	104 (87%)	16 (13%)	0	100	100
1	H	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
1	I	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
1	J	119/122 (98%)	109 (92%)	10 (8%)	0	100	100
1	K	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
1	L	120/122 (98%)	110 (92%)	10 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
1	N	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
1	O	119/122 (98%)	113 (95%)	6 (5%)	0	100	100
1	P	120/122 (98%)	109 (91%)	11 (9%)	0	100	100
1	Q	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
1	R	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
1	S	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
1	T	119/122 (98%)	114 (96%)	5 (4%)	0	100	100
1	U	119/122 (98%)	114 (96%)	5 (4%)	0	100	100
1	V	117/122 (96%)	113 (97%)	4 (3%)	0	100	100
1	W	119/122 (98%)	113 (95%)	6 (5%)	0	100	100
1	X	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
All	All	2871/2928 (98%)	2698 (94%)	173 (6%)	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 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	106/112 (95%)	106 (100%)	0	100	100
1	B	102/112 (91%)	102 (100%)	0	100	100
1	C	101/112 (90%)	101 (100%)	0	100	100
1	D	101/112 (90%)	100 (99%)	1 (1%)	76	89
1	E	101/112 (90%)	100 (99%)	1 (1%)	76	89
1	F	106/112 (95%)	105 (99%)	1 (1%)	78	91
1	G	105/112 (94%)	105 (100%)	0	100	100
1	H	101/112 (90%)	100 (99%)	1 (1%)	76	89
1	I	102/112 (91%)	100 (98%)	2 (2%)	55	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	98/112 (88%)	98 (100%)	0	100	100
1	K	102/112 (91%)	102 (100%)	0	100	100
1	L	101/112 (90%)	101 (100%)	0	100	100
1	M	103/112 (92%)	103 (100%)	0	100	100
1	N	101/112 (90%)	100 (99%)	1 (1%)	76	89
1	O	101/112 (90%)	96 (95%)	5 (5%)	24	44
1	P	100/112 (89%)	100 (100%)	0	100	100
1	Q	98/112 (88%)	98 (100%)	0	100	100
1	R	102/112 (91%)	98 (96%)	4 (4%)	32	55
1	S	99/112 (88%)	94 (95%)	5 (5%)	24	43
1	T	102/112 (91%)	100 (98%)	2 (2%)	55	78
1	U	97/112 (87%)	96 (99%)	1 (1%)	76	89
1	V	94/112 (84%)	89 (95%)	5 (5%)	22	40
1	W	95/112 (85%)	93 (98%)	2 (2%)	53	76
1	X	88/112 (79%)	88 (100%)	0	100	100
All	All	2406/2688 (90%)	2375 (99%)	31 (1%)	69	86

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	179	CYS
1	E	179	CYS
1	F	225	ILE
1	H	179	CYS
1	I	118	GLN
1	I	122	ASP
1	N	207	ARG
1	O	161	ARG
1	O	221	ASN
1	O	227	PHE
1	O	229	ASP
1	O	230	ASN
1	R	120	THR
1	R	188	ARG
1	R	231	LEU
1	R	234	LEU
1	S	115	THR

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Mol	Chain	Res	Type
1	S	120	THR
1	S	121	ILE
1	S	128	ILE
1	S	179	CYS
1	T	229	ASP
1	T	230	ASN
1	U	168	TYR
1	V	120	THR
1	V	122	ASP
1	V	123	PHE
1	V	124	LEU
1	V	161	ARG
1	W	126	ASP
1	W	140	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	221	ASN
1	G	119	GLN
1	G	149	GLN
1	K	118	GLN
1	L	149	GLN
1	N	127	ASN
1	N	230	ASN
1	O	221	ASN
1	P	118	GLN
1	R	149	GLN
1	T	127	ASN
1	T	230	ASN
1	U	143	ASN
1	V	149	GLN
1	V	221	ASN
1	W	143	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	122/122 (100%)	0.24	1 (0%) 86 88	52, 71, 101, 115	0
1	B	122/122 (100%)	0.03	1 (0%) 86 88	57, 76, 107, 117	0
1	C	122/122 (100%)	-0.19	0 100 100	54, 74, 115, 134	0
1	D	121/122 (99%)	-0.03	1 (0%) 86 88	60, 79, 114, 144	0
1	E	122/122 (100%)	-0.07	0 100 100	59, 78, 117, 138	0
1	F	122/122 (100%)	0.14	1 (0%) 86 88	57, 76, 108, 128	0
1	G	122/122 (100%)	0.15	0 100 100	59, 83, 111, 140	0
1	H	122/122 (100%)	-0.06	0 100 100	58, 78, 119, 135	0
1	I	122/122 (100%)	0.09	2 (1%) 72 74	63, 87, 115, 126	0
1	J	121/122 (99%)	0.08	0 100 100	64, 83, 136, 146	0
1	K	122/122 (100%)	-0.11	2 (1%) 72 74	61, 92, 122, 143	0
1	L	122/122 (100%)	0.09	4 (3%) 46 50	68, 88, 130, 148	0
1	M	122/122 (100%)	0.10	2 (1%) 72 74	69, 91, 126, 154	0
1	N	122/122 (100%)	0.35	5 (4%) 37 41	73, 102, 129, 137	0
1	O	121/122 (99%)	0.15	3 (2%) 57 61	74, 110, 153, 167	0
1	P	122/122 (100%)	0.08	2 (1%) 72 74	72, 101, 132, 151	0
1	Q	122/122 (100%)	0.08	1 (0%) 86 88	74, 98, 125, 155	0
1	R	122/122 (100%)	0.28	6 (4%) 29 32	81, 104, 133, 151	0
1	S	122/122 (100%)	0.06	2 (1%) 72 74	74, 105, 138, 162	0
1	T	121/122 (99%)	0.13	1 (0%) 86 88	77, 110, 129, 134	0
1	U	121/122 (99%)	0.29	4 (3%) 46 50	87, 104, 149, 167	0
1	V	119/122 (97%)	0.30	3 (2%) 57 61	85, 111, 151, 163	0
1	W	121/122 (99%)	0.23	6 (4%) 28 31	83, 115, 147, 156	0
1	X	122/122 (100%)	0.24	9 (7%) 14 15	96, 129, 156, 171	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	2919/2928 (99%)	0.11	56 (1%) 66 70	52, 94, 138, 171	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	V	132	ILE	4.9
1	W	173	ALA	4.7
1	V	203	ILE	4.4
1	V	135	TYR	4.1
1	P	235	PHE	3.9
1	M	116	PHE	3.4
1	O	177	LEU	3.4
1	F	123	PHE	3.2
1	W	123	PHE	3.1
1	X	181	VAL	3.1
1	N	141	PHE	3.0
1	X	213	VAL	2.9
1	O	225	ILE	2.8
1	N	210	VAL	2.7
1	K	115	THR	2.6
1	T	164	SER	2.6
1	Q	191	THR	2.5
1	N	152	PHE	2.5
1	W	139	LEU	2.5
1	X	131	GLY	2.5
1	B	177	LEU	2.4
1	L	124	LEU	2.4
1	I	134	ASN	2.4
1	R	236	GLN	2.4
1	X	152	PHE	2.4
1	O	116	PHE	2.3
1	W	177	LEU	2.3
1	U	124	LEU	2.3
1	D	141	PHE	2.3
1	R	173	ALA	2.2
1	W	132	ILE	2.2
1	X	173	ALA	2.2
1	N	221	ASN	2.2
1	K	235	PHE	2.2
1	U	234	LEU	2.2
1	R	198	CYS	2.2
1	L	123	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	U	221	ASN	2.2
1	X	175	GLY	2.2
1	S	161	ARG	2.2
1	L	191	THR	2.1
1	N	120	THR	2.1
1	U	177	LEU	2.1
1	R	148	VAL	2.1
1	P	141	PHE	2.1
1	I	231	LEU	2.1
1	W	172	SER	2.1
1	L	203	ILE	2.1
1	A	227	PHE	2.1
1	R	233	VAL	2.0
1	R	191	THR	2.0
1	M	123	PHE	2.0
1	X	210	VAL	2.0
1	X	217	ARG	2.0
1	S	168	TYR	2.0
1	X	160	TYR	2.0

## 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 monosaccharides 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.