



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 02:30 AM UTC

PDB ID : 7RDB / pdb_00007rdb
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

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
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

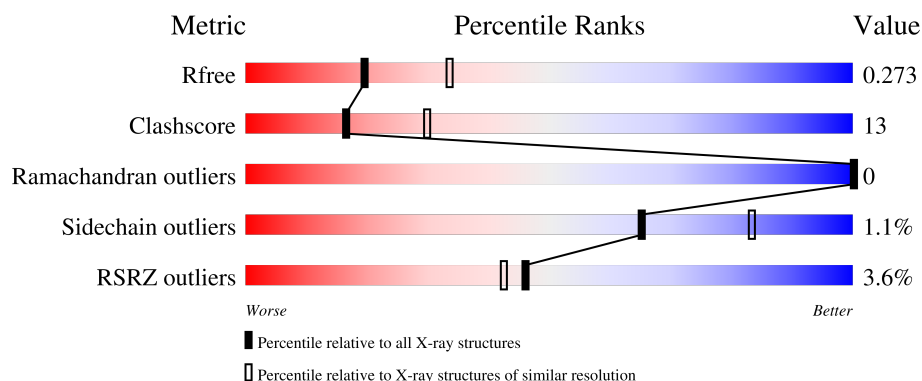
1 Overall quality at a glance

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}	180053	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (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 ≥ 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	0% 76% 23% .
1	B	122	2% 75% 25% .
1	C	122	77% 22% .
1	D	122	4% 80% 19% .
1	E	122	2% 83% 16% .

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Mol	Chain	Length	Quality of chain
1	F	122	
1	G	122	
1	H	122	
1	I	122	
1	J	122	
1	K	122	
1	L	122	
1	M	122	
1	N	122	
1	O	122	
1	P	122	
1	Q	122	
1	R	122	
1	S	122	
1	T	122	
1	U	122	
1	V	122	
1	W	122	
1	X	122	

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

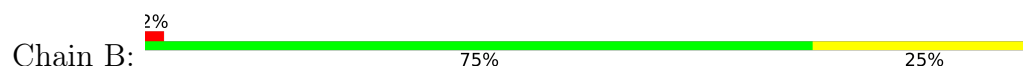
- Molecule 2 is water.

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

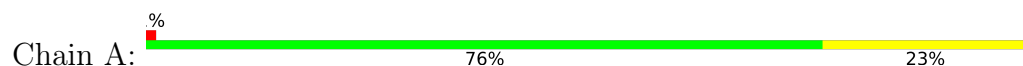
3 Residue-property plots

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.

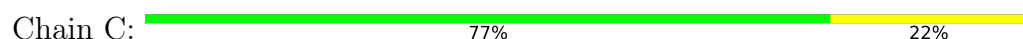
• Molecule 1: Tetraspanin-15



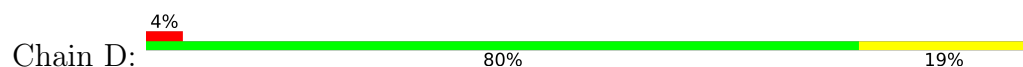
• Molecule 1: Tetraspanin-15



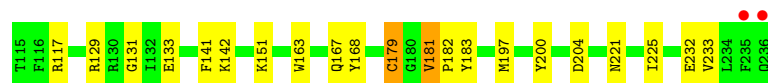
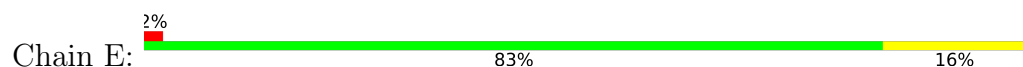
• Molecule 1: Tetraspanin-15



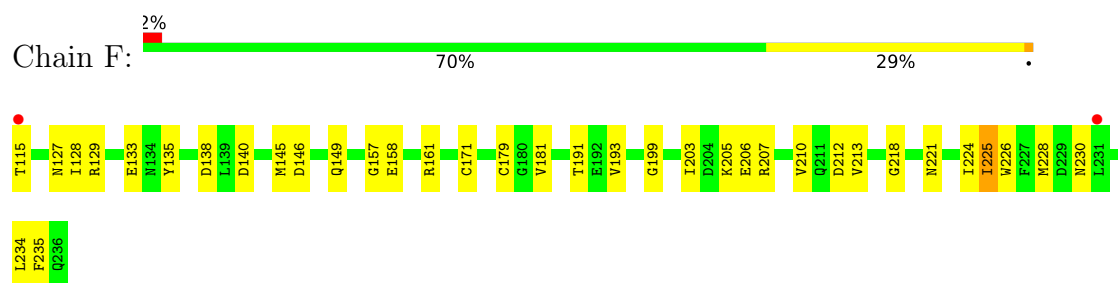
• Molecule 1: Tetraspanin-15



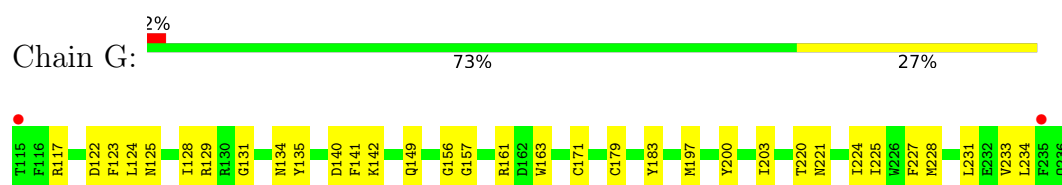
• Molecule 1: Tetraspanin-15



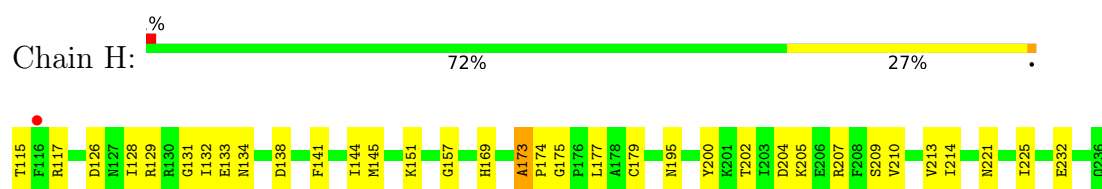
• Molecule 1: Tetraspanin-15



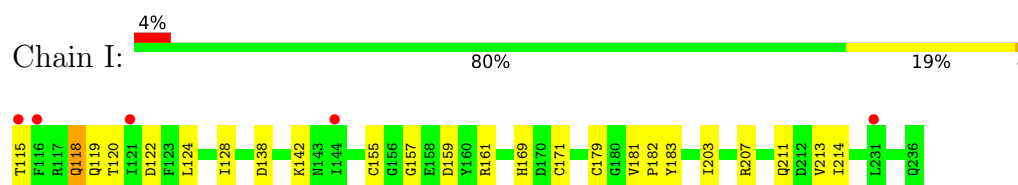
• Molecule 1: Tetraspanin-15



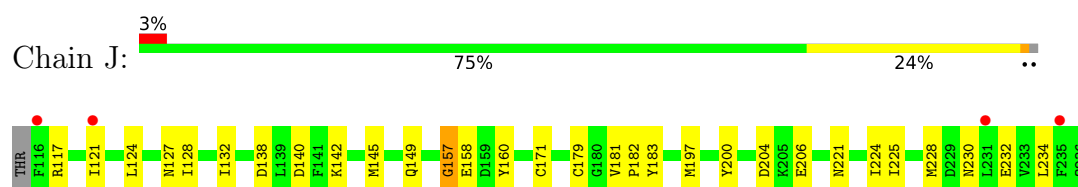
• Molecule 1: Tetraspanin-15



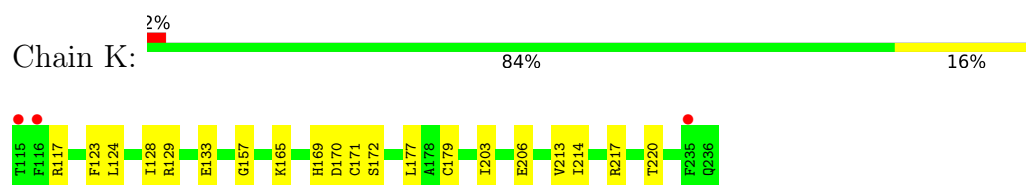
• Molecule 1: Tetraspanin-15



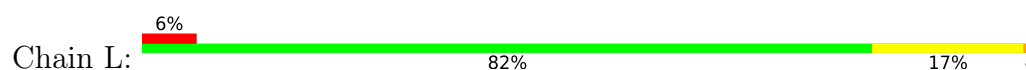
• Molecule 1: Tetraspanin-15



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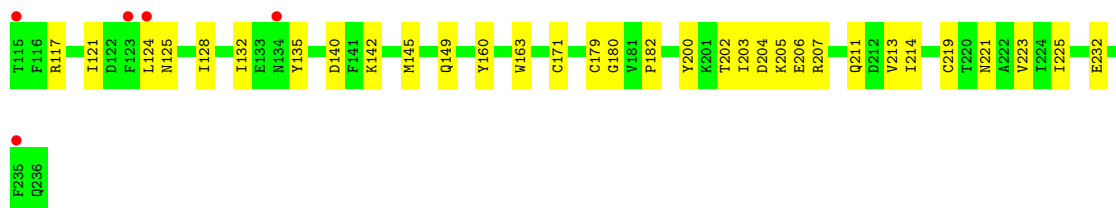
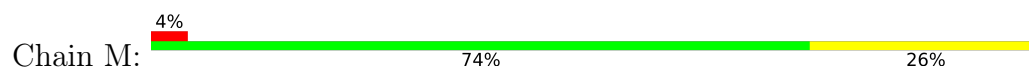


• Molecule 1: Tetraspanin-15

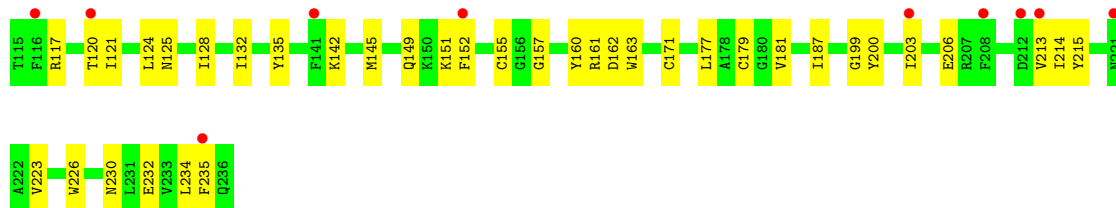




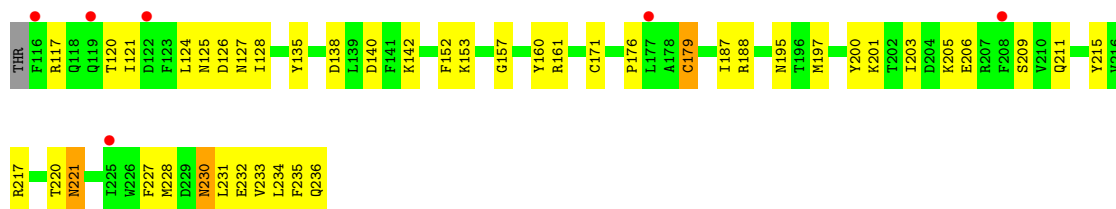
• Molecule 1: Tetraspanin-15



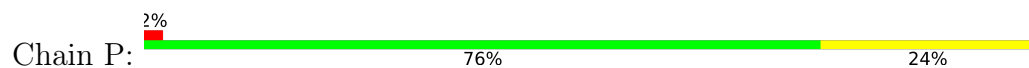
• Molecule 1: Tetraspanin-15



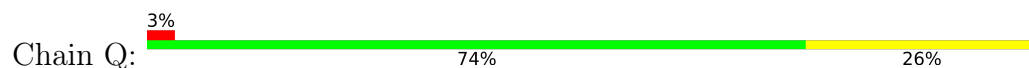
• Molecule 1: Tetraspanin-15

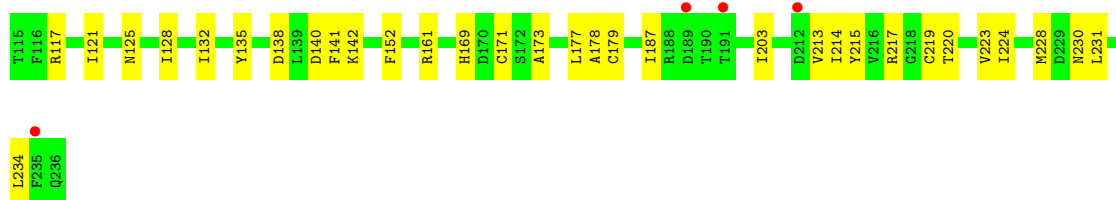


• Molecule 1: Tetraspanin-15

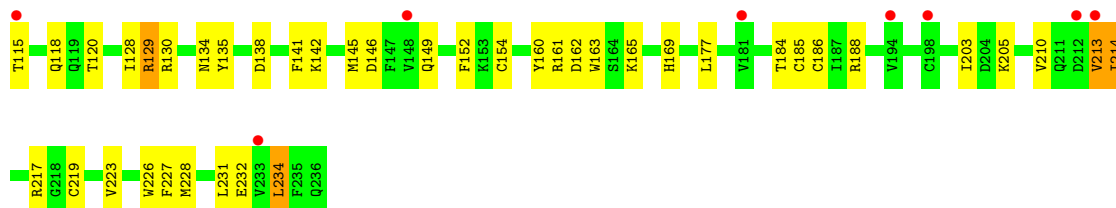


• Molecule 1: Tetraspanin-15





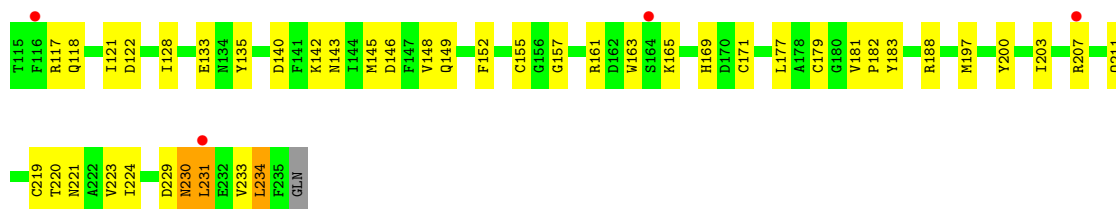
- Molecule 1: Tetraspanin-15



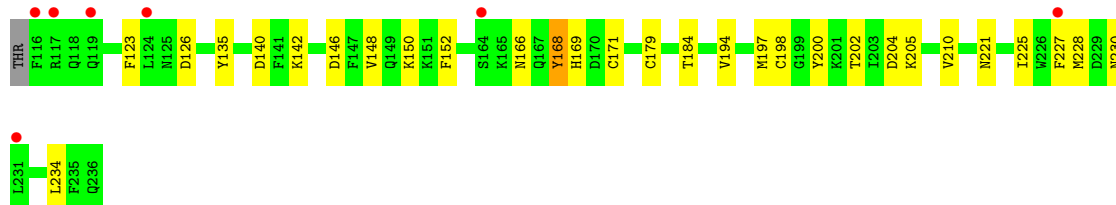
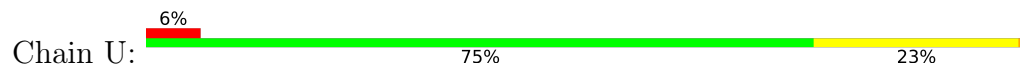
- Molecule 1: Tetraspanin-15



- Molecule 1: Tetraspanin-15

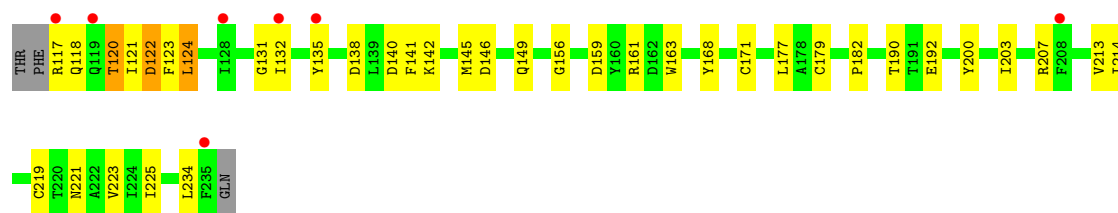


- Molecule 1: Tetraspanin-15

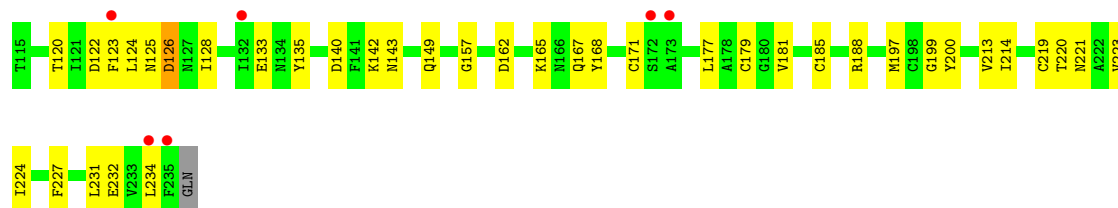


- Molecule 1: Tetraspanin-15

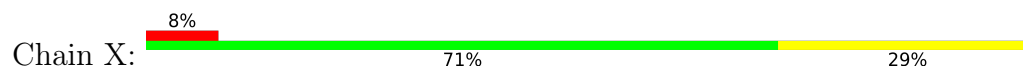




● Molecule 1: Tetraspanin-15



● Molecule 1: Tetraspanin-15



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122+SVN	Depositor
R, R_{free}	0.235 , 0.273 0.235 , 0.273	Depositor DCC
R_{free} test set	1971 reflections (1.73%)	wwPDB-VP
Wilson B-factor (Å ²)	76.7	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 60.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	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 ²)	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.*

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	0.60	0/993	0.91	3/1346 (0.2%)
1	B	0.59	0/977	0.77	0/1326
1	C	0.54	1/969 (0.1%)	0.81	3/1317 (0.2%)
1	D	0.86	0/969	0.81	2/1314 (0.2%)
1	E	0.66	0/969	0.83	2/1315 (0.2%)
1	F	0.76	0/993	0.99	6/1346 (0.4%)
1	G	0.69	0/990	0.91	1/1341 (0.1%)
1	H	0.68	0/966	1.16	9/1310 (0.7%)
1	I	0.60	0/977	0.88	2/1323 (0.2%)
1	J	0.58	3/952 (0.3%)	0.81	1/1293 (0.1%)
1	K	0.66	1/973 (0.1%)	0.86	1/1320 (0.1%)
1	L	0.45	0/967	0.80	2/1313 (0.2%)
1	M	0.43	0/988	0.83	0/1338
1	N	0.46	0/974	0.78	0/1321
1	O	0.79	1/969 (0.1%)	1.00	2/1312 (0.2%)
1	P	0.72	0/970	0.81	1/1317 (0.1%)
1	Q	0.44	0/958	0.74	1/1300 (0.1%)
1	R	0.81	4/978 (0.4%)	0.91	4/1325 (0.3%)
1	S	0.72	0/962	0.88	1/1307 (0.1%)
1	T	0.59	0/970	0.90	4/1316 (0.3%)
1	U	0.49	0/951	0.70	0/1293
1	V	0.53	0/927	0.85	2/1263 (0.2%)
1	W	0.67	0/935	0.90	4/1273 (0.3%)
1	X	0.80	6/921 (0.7%)	0.86	2/1260 (0.2%)
All	All	0.64	16/23198 (0.1%)	0.87	53/31489 (0.2%)

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 (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	158	GLU	CD-OE2	7.72	1.40	1.25
1	R	129	ARG	CD-NE	7.23	1.56	1.46
1	X	206	GLU	CD-OE1	6.24	1.37	1.25
1	O	179	CYS	N-CA	-6.13	1.37	1.46
1	X	158	GLU	CD-OE1	6.13	1.37	1.25
1	X	206	GLU	CD-OE2	6.13	1.37	1.25
1	J	157	GLY	CA-C	-6.10	1.48	1.51
1	C	150	LYS	CE-NZ	5.84	1.66	1.49
1	X	206	GLU	CB-CG	5.81	1.69	1.52
1	R	129	ARG	NE-CZ	5.53	1.39	1.33
1	R	129	ARG	CB-CG	5.34	1.68	1.52
1	K	165	LYS	CD-CE	5.33	1.68	1.52
1	J	158	GLU	CD-OE1	5.33	1.35	1.25
1	R	129	ARG	CZ-NH2	5.15	1.40	1.33
1	X	158	GLU	CB-CG	5.12	1.67	1.52
1	J	158	GLU	CD-OE2	5.06	1.34	1.25

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	173	ALA	CA-C-N	11.62	131.95	119.05
1	H	173	ALA	C-N-CA	11.62	131.95	119.05
1	H	175	GLY	CA-C-N	11.33	131.63	119.05
1	H	175	GLY	C-N-CA	11.33	131.63	119.05
1	L	207	ARG	CD-NE-CZ	10.85	139.59	124.40
1	H	207	ARG	N-CA-C	9.13	121.23	111.28
1	H	213	VAL	N-CA-C	8.78	120.57	111.00
1	L	207	ARG	NE-CZ-NH2	-8.67	111.40	119.20
1	V	207	ARG	N-CA-C	8.64	120.70	111.28
1	H	205	LYS	N-CA-C	8.63	123.81	113.28
1	V	203	ILE	N-CA-C	7.12	117.25	110.42
1	Q	203	ILE	N-CA-C	7.01	117.01	110.42
1	S	209	SER	N-CA-C	-6.95	103.44	112.68
1	T	231	LEU	N-CA-C	6.76	118.31	111.07
1	E	181	VAL	CA-C-N	6.76	126.74	119.78
1	E	181	VAL	C-N-CA	6.76	126.74	119.78
1	X	158	GLU	CB-CG-CD	-6.71	101.18	112.60
1	F	207	ARG	N-CA-C	6.67	118.55	111.28
1	R	205	LYS	N-CA-C	6.66	122.32	112.94
1	G	129	ARG	CB-CG-CD	-6.48	96.40	111.30
1	R	214	ILE	N-CA-C	6.46	118.02	108.65
1	H	210	VAL	N-CA-C	6.18	118.10	112.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	205	LYS	N-CA-C	6.12	121.57	112.94
1	F	210	VAL	N-CA-C	6.12	118.77	112.90
1	D	121	ILE	CB-CA-C	-6.08	103.93	112.14
1	O	179	CYS	CB-CA-C	6.06	119.98	111.86
1	O	228	MET	N-CA-C	5.85	117.33	111.07
1	C	150	LYS	CA-CB-CG	-5.83	102.43	114.10
1	W	133	GLU	CA-C-N	-5.82	113.88	122.83
1	W	133	GLU	C-N-CA	-5.82	113.88	122.83
1	I	169	HIS	CA-C-N	5.78	129.32	120.82
1	I	169	HIS	C-N-CA	5.78	129.32	120.82
1	X	206	GLU	CB-CG-CD	-5.64	103.02	112.60
1	A	171	CYS	CA-CB-SG	5.62	127.33	114.40
1	T	233	VAL	CB-CA-C	-5.59	104.59	112.14
1	R	210	VAL	N-CA-C	5.58	118.36	112.83
1	R	213	VAL	N-CA-C	5.57	120.93	109.34
1	J	158	GLU	CB-CG-CD	-5.52	103.22	112.60
1	P	221	ASN	CB-CA-C	5.49	119.29	109.29
1	A	132	ILE	CA-C-N	-5.42	111.66	121.14
1	A	132	ILE	C-N-CA	-5.42	111.66	121.14
1	C	215	TYR	CA-C-N	-5.32	117.18	122.77
1	C	215	TYR	C-N-CA	-5.32	117.18	122.77
1	T	234	LEU	N-CA-C	5.28	117.04	111.28
1	D	144	ILE	CB-CA-C	-5.24	105.06	112.14
1	K	165	LYS	CD-CE-NZ	-5.20	95.26	111.90
1	F	213	VAL	N-CA-C	-5.10	107.86	112.96
1	W	125	ASN	CA-C-N	-5.10	112.19	120.71
1	W	125	ASN	C-N-CA	-5.10	112.19	120.71
1	T	233	VAL	N-CA-C	5.05	115.77	110.62
1	H	214	ILE	CB-CA-C	-5.05	101.77	110.30
1	F	127	ASN	CA-C-N	-5.04	111.62	120.29
1	F	127	ASN	C-N-CA	-5.04	111.62	120.29

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 ⓘ

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	22	0
1	B	956	0	870	23	1
1	C	950	0	857	24	0
1	D	949	0	869	20	0
1	E	950	0	869	14	1
1	F	972	0	898	25	4
1	G	970	0	895	26	0
1	H	948	0	862	24	0
1	I	958	0	886	16	0
1	J	934	0	842	21	1
1	K	954	0	871	15	0
1	L	948	0	860	21	0
1	M	966	0	890	22	1
1	N	954	0	871	36	0
1	O	950	0	880	45	2
1	P	950	0	858	20	4
1	Q	939	0	847	24	1
1	R	958	0	880	30	1
1	S	943	0	854	32	3
1	T	950	0	871	39	0
1	U	931	0	835	20	3
1	V	908	0	801	32	1
1	W	917	0	825	24	2
1	X	902	0	763	32	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	22771	0	20644	561	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 13.

All (561) 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	1.09
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:S:187:ILE:CD1	1:S:213:VAL:C	2.38	0.90
1:O:201:LYS:N	1:O:201:LYS:HD2	1.85	0.89
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:131:GLY:C	1:D:141:PHE:CE2	2.67	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:D:131:GLY:C	1:D:141:PHE:CZ	2.68	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:U:227:PHE:HD1	1:U:228:MET:HE2	1.57	0.70
1:A:144:ILE:HD11	1:G:228:MET:HE1	1.72	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:S:234:LEU:C	1:S:235:PHE:HD1	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:234:LEU:C	1:F:235:PHE:HD1	2.09	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
1:S:191:THR:HA	1:V:221:ASN:HD21	1.65	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:O:205:LYS:O	1:O:206:GLU:HB2	2.01	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:G:227:PHE:CD2	1:G:228:MET:HE2	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:U:227:PHE:CD1	1:U:228:MET:HE2	2.41	0.55
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:G:227:PHE:HD2	1:G:228:MET:HE2	1.71	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:C:115:THR:C	1:C:117:ARG:H	2.16	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
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: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:H:151:LYS:HD3	1:H:151:LYS:C	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:169:HIS:HE1	1:T:177:LEU:HD22	1.74	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:V:145:MET:HE3	1:V:149:GLN:HG3	1.92	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:P:140:ASP:HA	1:R:228:MET:HE2	1.92	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
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:P:141:PHE:CD1	1:P:141:PHE:C	2.89	0.50
1:R:152:PHE:O	1:R:217:ARG:NH2	2.42	0.50
1:R:128:ILE:HG23	1:R:145:MET:HE1	1.93	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:X:227:PHE:CD1	1:X:227:PHE:C	2.90	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:115:THR:C	1:H:117:ARG:H	2.21	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:F:115:THR:O	1:F:115:THR:OG1	2.21	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:133:GLU:HG2	1:T:165:LYS:HZ1	1.78	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:M:232:GLU:CD	1:M:232:GLU:H	2.22	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
1:G:123:PHE:CD2	1:G:124:LEU:HD12	2.50	0.47
1:U:135:TYR:OH	1:U:146:ASP:OD1	2.28	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:C:221:ASN:O	1:C:222:ALA:C	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:118:GLN:C	1:I:118:GLN:CD	2.84	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:140:ASP:CA	1:R:228:MET:HE2	2.46	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:J:232:GLU:CD	1:J:232:GLU:H	2.24	0.45
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:F:228:MET:HE2	1:T:140:ASP:HA	1.98	0.45
1:P:179:CYS:HA	1:P:203:ILE:HD12	1.98	0.45
1:T:145:MET:HE3	1:T:145:MET:HB3	1.85	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:C:151:LYS:HD3	1:C:151:LYS:C	2.42	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
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:144:ILE:HG13	1:P:228:MET:HE1	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:Q:125:ASN:CG	1:Q:220:THR:HG21	2.42	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:R:145:MET:HE3	1:R:149:GLN:HE21	1.83	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:C:115:THR:C	1:C:117:ARG:N	2.77	0.43
1:E:131:GLY:C	1:E:141:PHE:CE2	2.97	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:R:227:PHE:C	1:R:227:PHE:CD1	2.96	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:C:228:MET:HE2	1:G:140:ASP:HA	2.00	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: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:C:131:GLY:C	1:C:141:PHE:CE2	2.98	0.42
1:H:128:ILE:HD11	1:H:157:GLY:N	2.35	0.42
1:H:195:ASN:OD1	1:H:195:ASN:C	2.63	0.42
1:I:207:ARG:O	1:I:211:GLN:HG3	2.20	0.42
1:S:128:ILE:HD11	1:S:156:GLY:C	2.44	0.42
1:T:207:ARG:O	1:T:211:GLN:HG2	2.20	0.42
1:X:117:ARG:O	1:X:118:GLN:C	2.62	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:R:145:MET:HE3	1:R:149:GLN:NE2	2.35	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: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:128:ILE:HD11	1:G:156:GLY:C	2.45	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:U:204:ASP:OD1	1:U:204:ASP:C	2.64	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:J:124:LEU:HD22	1:J:124:LEU:C	2.45	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: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:N:226:TRP:NE1	1:N:230:ASN:HD21	2.20	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:X:220:THR:C	1:X:223:VAL:HG12	2.45	0.40
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:V:141:PHE:CD1	1:V:141:PHE:C	2.99	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: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
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%)	68	85
1	E	101/112 (90%)	100 (99%)	1 (1%)	68	85
1	F	106/112 (95%)	104 (98%)	2 (2%)	50	74
1	G	105/112 (94%)	105 (100%)	0	100	100
1	H	101/112 (90%)	100 (99%)	1 (1%)	68	85
1	I	102/112 (91%)	100 (98%)	2 (2%)	48	73

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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%)	101 (100%)	0	100	100
1	O	101/112 (90%)	99 (98%)	2 (2%)	48	73
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%)	28	52
1	S	99/112 (88%)	95 (96%)	4 (4%)	28	51
1	T	102/112 (91%)	100 (98%)	2 (2%)	48	73
1	U	97/112 (87%)	96 (99%)	1 (1%)	68	85
1	V	94/112 (84%)	90 (96%)	4 (4%)	26	49
1	W	95/112 (85%)	93 (98%)	2 (2%)	47	72
1	X	88/112 (79%)	88 (100%)	0	100	100
All	All	2406/2688 (90%)	2380 (99%)	26 (1%)	65	83

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	179	CYS
1	E	179	CYS
1	F	221	ASN
1	F	225	ILE
1	H	179	CYS
1	I	118	GLN
1	I	122	ASP
1	O	221	ASN
1	O	230	ASN
1	R	120	THR
1	R	213	VAL
1	R	231	LEU
1	R	234	LEU
1	S	115	THR
1	S	120	THR
1	S	121	ILE
1	S	128	ILE

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Mol	Chain	Res	Type
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	W	126	ASP
1	W	140	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	127	ASN
1	B	230	ASN
1	A	118	GLN
1	C	221	ASN
1	D	167	GLN
1	E	221	ASN
1	F	134	ASN
1	G	119	GLN
1	G	149	GLN
1	G	230	ASN
1	I	230	ASN
1	J	118	GLN
1	J	230	ASN
1	L	149	GLN
1	N	125	ASN
1	N	221	ASN
1	N	230	ASN
1	O	166	ASN
1	O	221	ASN
1	P	118	GLN
1	Q	118	GLN
1	Q	134	ASN
1	S	230	ASN
1	T	127	ASN
1	T	166	ASN
1	T	169	HIS
1	T	230	ASN
1	V	118	GLN
1	V	149	GLN

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Mol	Chain	Res	Type
1	V	221	ASN
1	W	143	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	122/122 (100%)	0.25	1 (0%) 82 80	52, 71, 101, 115	0
1	B	122/122 (100%)	0.23	2 (1%) 70 68	57, 76, 107, 117	0
1	C	122/122 (100%)	0.11	0 100 100	54, 74, 115, 134	0
1	D	121/122 (99%)	0.33	5 (4%) 41 38	60, 79, 114, 144	0
1	E	122/122 (100%)	0.26	2 (1%) 70 68	59, 78, 117, 138	0
1	F	122/122 (100%)	0.24	2 (1%) 70 68	57, 76, 108, 128	0
1	G	122/122 (100%)	0.45	2 (1%) 70 68	59, 83, 111, 140	0
1	H	122/122 (100%)	0.24	1 (0%) 82 80	58, 78, 119, 135	0
1	I	122/122 (100%)	0.43	5 (4%) 41 38	63, 87, 115, 126	0
1	J	121/122 (99%)	0.39	4 (3%) 49 46	64, 83, 136, 146	0
1	K	122/122 (100%)	0.37	3 (2%) 58 55	61, 92, 122, 143	0
1	L	122/122 (100%)	0.54	7 (5%) 29 26	68, 88, 130, 148	0
1	M	122/122 (100%)	0.45	5 (4%) 41 38	69, 91, 126, 154	0
1	N	122/122 (100%)	0.82	10 (8%) 17 15	73, 102, 129, 137	0
1	O	121/122 (99%)	0.70	6 (4%) 34 31	74, 110, 153, 167	0
1	P	122/122 (100%)	0.43	2 (1%) 70 68	72, 101, 132, 151	0
1	Q	122/122 (100%)	0.50	4 (3%) 49 46	74, 98, 125, 155	0
1	R	122/122 (100%)	0.75	8 (6%) 24 22	81, 104, 133, 151	0
1	S	122/122 (100%)	0.49	3 (2%) 58 55	74, 105, 138, 162	0
1	T	121/122 (99%)	0.58	4 (3%) 49 46	77, 110, 129, 134	0
1	U	121/122 (99%)	0.70	7 (5%) 29 26	87, 104, 149, 167	0
1	V	119/122 (97%)	0.66	7 (5%) 28 25	85, 111, 151, 163	0
1	W	121/122 (99%)	0.72	6 (4%) 34 31	83, 115, 147, 156	0
1	X	122/122 (100%)	0.80	10 (8%) 17 15	96, 129, 156, 171	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
All	All	2919/2928 (99%)	0.48	106 (3%)	46	42	52, 94, 138, 171	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	V	135	TYR	4.9
1	O	116	PHE	4.4
1	J	116	PHE	4.2
1	U	116	PHE	4.0
1	W	235	PHE	3.5
1	J	235	PHE	3.4
1	Q	235	PHE	3.3
1	R	148	VAL	3.3
1	N	221	ASN	3.2
1	S	231	LEU	3.2
1	O	177	LEU	3.1
1	M	115	THR	3.0
1	G	235	PHE	3.0
1	P	115	THR	3.0
1	R	198	CYS	3.0
1	H	116	PHE	2.9
1	X	189	ASP	2.9
1	L	116	PHE	2.9
1	T	116	PHE	2.9
1	I	231	LEU	2.8
1	U	124	LEU	2.8
1	N	212	ASP	2.8
1	V	208	PHE	2.8
1	D	225	ILE	2.7
1	X	213	VAL	2.7
1	F	115	THR	2.7
1	D	141	PHE	2.7
1	E	235	PHE	2.7
1	U	231	LEU	2.7
1	N	116	PHE	2.7
1	P	235	PHE	2.7
1	N	152	PHE	2.6
1	W	173	ALA	2.6
1	D	235	PHE	2.6
1	L	181	VAL	2.6
1	T	207	ARG	2.5
1	D	124	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	O	119	GLN	2.5
1	V	119	GLN	2.5
1	Q	212	ASP	2.5
1	V	132	ILE	2.5
1	U	119	GLN	2.5
1	U	117	ARG	2.5
1	I	144	ILE	2.4
1	O	225	ILE	2.4
1	V	128	ILE	2.4
1	B	225	ILE	2.4
1	J	121	ILE	2.4
1	V	117	ARG	2.4
1	I	116	PHE	2.4
1	R	233	VAL	2.4
1	X	115	THR	2.4
1	X	212	ASP	2.4
1	O	208	PHE	2.4
1	L	115	THR	2.3
1	G	115	THR	2.3
1	L	203	ILE	2.3
1	N	235	PHE	2.3
1	S	124	LEU	2.3
1	F	231	LEU	2.3
1	K	235	PHE	2.3
1	M	123	PHE	2.3
1	A	171	CYS	2.3
1	E	236	GLN	2.2
1	U	164	SER	2.2
1	B	116	PHE	2.2
1	X	219	CYS	2.2
1	Q	191	THR	2.2
1	R	115	THR	2.2
1	T	231	LEU	2.2
1	W	172	SER	2.2
1	O	122	ASP	2.2
1	N	208	PHE	2.2
1	X	235	PHE	2.2
1	D	223	VAL	2.2
1	N	213	VAL	2.2
1	R	213	VAL	2.2
1	N	203	ILE	2.2
1	T	164	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	L	206	GLU	2.2
1	K	116	PHE	2.2
1	S	235	PHE	2.2
1	X	223	VAL	2.2
1	I	115	THR	2.2
1	J	231	LEU	2.2
1	V	235	PHE	2.2
1	R	194	VAL	2.1
1	L	191	THR	2.1
1	N	141	PHE	2.1
1	X	123	PHE	2.1
1	L	124	LEU	2.1
1	X	207	ARG	2.1
1	X	122	ASP	2.1
1	R	181	VAL	2.1
1	M	124	LEU	2.1
1	M	134	ASN	2.1
1	W	132	ILE	2.1
1	U	227	PHE	2.0
1	I	121	ILE	2.0
1	K	115	THR	2.0
1	M	235	PHE	2.0
1	W	123	PHE	2.0
1	W	234	LEU	2.0
1	N	120	THR	2.0
1	Q	189	ASP	2.0
1	R	212	ASP	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 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.