



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 07:57 PM UTC

PDB ID : 6KOI / pdb_00006koi
Title : Crystal structure of SNX11-PXe domain in dimer form.
Authors : Xu, T.; Xu, J.; Liu, J.
Deposited on : 2019-08-11
Resolution : 3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (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

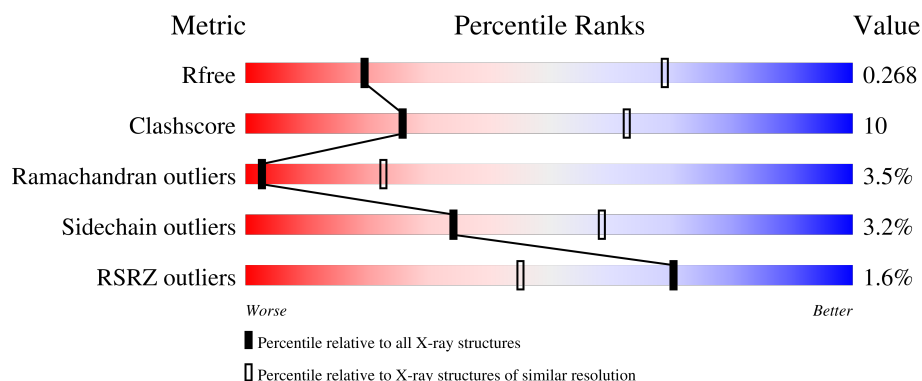
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	160	
1	B	160	
1	C	160	
1	D	160	
1	E	160	

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Mol	Chain	Length	Quality of chain
1	F	160	
1	G	160	
1	H	160	
1	I	160	
1	J	160	
1	K	160	
1	L	160	
1	M	160	
1	N	160	
1	O	160	
1	P	160	
1	Q	160	
1	R	160	
1	S	160	
1	T	160	
1	U	160	
1	V	160	
1	W	160	
1	X	160	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 25878 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 Sorting nexin-11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	124	Total	C	N	O	S	0	0	0
			1018	651	183	182	2			
1	B	140	Total	C	N	O	S	0	0	0
			1142	722	207	209	2			
1	C	126	Total	C	N	O	S	0	0	0
			1036	661	186	187	2			
1	D	147	Total	C	N	O	S	0	0	0
			1197	758	214	221	2			
1	E	125	Total	C	N	O	S	0	0	0
			1027	656	185	184	2			
1	F	138	Total	C	N	O	S	0	0	0
			1126	712	205	205	2			
1	G	126	Total	C	N	O	S	0	0	0
			1036	661	186	187	2			
1	H	144	Total	C	N	O	S	0	0	0
			1170	740	211	215	2			
1	I	125	Total	C	N	O	S	0	0	0
			1027	656	184	185	2			
1	J	141	Total	C	N	O	S	0	0	0
			1151	727	208	212	2			
1	K	117	Total	C	N	O	S	0	0	0
			971	621	176	172	2			
1	L	143	Total	C	N	O	S	0	0	0
			1164	737	210	213	2			
1	M	125	Total	C	N	O	S	0	0	0
			1027	656	185	184	2			
1	N	141	Total	C	N	O	S	0	0	0
			1148	725	208	211	2			
1	O	118	Total	C	N	O	S	0	0	0
			973	622	176	173	2			
1	P	141	Total	C	N	O	S	0	0	0
			1146	724	208	210	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	122	Total	C	N	O	S	0	0	0
			1005	644	181	178	2			
1	R	139	Total	C	N	O	S	Se	0	0
			1130	715	206	205	2	2		
1	S	124	Total	C	N	O	S		0	0
			1018	651	183	182	2			
1	T	143	Total	C	N	O	S	Se	0	0
			1164	737	210	213	2	2		
1	U	121	Total	C	N	O	S		0	0
			999	637	181	179	2			
1	V	130	Total	C	N	O	S	Se	0	0
			1065	673	195	193	2	2		
1	W	121	Total	C	N	O	S		0	0
			992	630	180	180	2			
1	X	141	Total	C	N	O	S	Se	0	0
			1146	724	208	210	2	2		

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	159	LEU	-	expression tag	UNP Q9Y5W9
A	160	GLU	-	expression tag	UNP Q9Y5W9
A	161	HIS	-	expression tag	UNP Q9Y5W9
A	162	HIS	-	expression tag	UNP Q9Y5W9
A	163	HIS	-	expression tag	UNP Q9Y5W9
A	164	HIS	-	expression tag	UNP Q9Y5W9
A	165	HIS	-	expression tag	UNP Q9Y5W9
A	166	HIS	-	expression tag	UNP Q9Y5W9
B	159	LEU	-	expression tag	UNP Q9Y5W9
B	160	GLU	-	expression tag	UNP Q9Y5W9
B	161	HIS	-	expression tag	UNP Q9Y5W9
B	162	HIS	-	expression tag	UNP Q9Y5W9
B	163	HIS	-	expression tag	UNP Q9Y5W9
B	164	HIS	-	expression tag	UNP Q9Y5W9
B	165	HIS	-	expression tag	UNP Q9Y5W9
B	166	HIS	-	expression tag	UNP Q9Y5W9
C	159	LEU	-	expression tag	UNP Q9Y5W9
C	160	GLU	-	expression tag	UNP Q9Y5W9
C	161	HIS	-	expression tag	UNP Q9Y5W9
C	162	HIS	-	expression tag	UNP Q9Y5W9
C	163	HIS	-	expression tag	UNP Q9Y5W9
C	164	HIS	-	expression tag	UNP Q9Y5W9
C	165	HIS	-	expression tag	UNP Q9Y5W9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	166	HIS	-	expression tag	UNP Q9Y5W9
D	159	LEU	-	expression tag	UNP Q9Y5W9
D	160	GLU	-	expression tag	UNP Q9Y5W9
D	161	HIS	-	expression tag	UNP Q9Y5W9
D	162	HIS	-	expression tag	UNP Q9Y5W9
D	163	HIS	-	expression tag	UNP Q9Y5W9
D	164	HIS	-	expression tag	UNP Q9Y5W9
D	165	HIS	-	expression tag	UNP Q9Y5W9
D	166	HIS	-	expression tag	UNP Q9Y5W9
E	159	LEU	-	expression tag	UNP Q9Y5W9
E	160	GLU	-	expression tag	UNP Q9Y5W9
E	161	HIS	-	expression tag	UNP Q9Y5W9
E	162	HIS	-	expression tag	UNP Q9Y5W9
E	163	HIS	-	expression tag	UNP Q9Y5W9
E	164	HIS	-	expression tag	UNP Q9Y5W9
E	165	HIS	-	expression tag	UNP Q9Y5W9
E	166	HIS	-	expression tag	UNP Q9Y5W9
F	159	LEU	-	expression tag	UNP Q9Y5W9
F	160	GLU	-	expression tag	UNP Q9Y5W9
F	161	HIS	-	expression tag	UNP Q9Y5W9
F	162	HIS	-	expression tag	UNP Q9Y5W9
F	163	HIS	-	expression tag	UNP Q9Y5W9
F	164	HIS	-	expression tag	UNP Q9Y5W9
F	165	HIS	-	expression tag	UNP Q9Y5W9
F	166	HIS	-	expression tag	UNP Q9Y5W9
G	159	LEU	-	expression tag	UNP Q9Y5W9
G	160	GLU	-	expression tag	UNP Q9Y5W9
G	161	HIS	-	expression tag	UNP Q9Y5W9
G	162	HIS	-	expression tag	UNP Q9Y5W9
G	163	HIS	-	expression tag	UNP Q9Y5W9
G	164	HIS	-	expression tag	UNP Q9Y5W9
G	165	HIS	-	expression tag	UNP Q9Y5W9
G	166	HIS	-	expression tag	UNP Q9Y5W9
H	159	LEU	-	expression tag	UNP Q9Y5W9
H	160	GLU	-	expression tag	UNP Q9Y5W9
H	161	HIS	-	expression tag	UNP Q9Y5W9
H	162	HIS	-	expression tag	UNP Q9Y5W9
H	163	HIS	-	expression tag	UNP Q9Y5W9
H	164	HIS	-	expression tag	UNP Q9Y5W9
H	165	HIS	-	expression tag	UNP Q9Y5W9
H	166	HIS	-	expression tag	UNP Q9Y5W9
I	159	LEU	-	expression tag	UNP Q9Y5W9

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Chain	Residue	Modelled	Actual	Comment	Reference
I	160	GLU	-	expression tag	UNP Q9Y5W9
I	161	HIS	-	expression tag	UNP Q9Y5W9
I	162	HIS	-	expression tag	UNP Q9Y5W9
I	163	HIS	-	expression tag	UNP Q9Y5W9
I	164	HIS	-	expression tag	UNP Q9Y5W9
I	165	HIS	-	expression tag	UNP Q9Y5W9
I	166	HIS	-	expression tag	UNP Q9Y5W9
J	159	LEU	-	expression tag	UNP Q9Y5W9
J	160	GLU	-	expression tag	UNP Q9Y5W9
J	161	HIS	-	expression tag	UNP Q9Y5W9
J	162	HIS	-	expression tag	UNP Q9Y5W9
J	163	HIS	-	expression tag	UNP Q9Y5W9
J	164	HIS	-	expression tag	UNP Q9Y5W9
J	165	HIS	-	expression tag	UNP Q9Y5W9
J	166	HIS	-	expression tag	UNP Q9Y5W9
K	159	LEU	-	expression tag	UNP Q9Y5W9
K	160	GLU	-	expression tag	UNP Q9Y5W9
K	161	HIS	-	expression tag	UNP Q9Y5W9
K	162	HIS	-	expression tag	UNP Q9Y5W9
K	163	HIS	-	expression tag	UNP Q9Y5W9
K	164	HIS	-	expression tag	UNP Q9Y5W9
K	165	HIS	-	expression tag	UNP Q9Y5W9
K	166	HIS	-	expression tag	UNP Q9Y5W9
L	159	LEU	-	expression tag	UNP Q9Y5W9
L	160	GLU	-	expression tag	UNP Q9Y5W9
L	161	HIS	-	expression tag	UNP Q9Y5W9
L	162	HIS	-	expression tag	UNP Q9Y5W9
L	163	HIS	-	expression tag	UNP Q9Y5W9
L	164	HIS	-	expression tag	UNP Q9Y5W9
L	165	HIS	-	expression tag	UNP Q9Y5W9
L	166	HIS	-	expression tag	UNP Q9Y5W9
M	159	LEU	-	expression tag	UNP Q9Y5W9
M	160	GLU	-	expression tag	UNP Q9Y5W9
M	161	HIS	-	expression tag	UNP Q9Y5W9
M	162	HIS	-	expression tag	UNP Q9Y5W9
M	163	HIS	-	expression tag	UNP Q9Y5W9
M	164	HIS	-	expression tag	UNP Q9Y5W9
M	165	HIS	-	expression tag	UNP Q9Y5W9
M	166	HIS	-	expression tag	UNP Q9Y5W9
N	159	LEU	-	expression tag	UNP Q9Y5W9
N	160	GLU	-	expression tag	UNP Q9Y5W9
N	161	HIS	-	expression tag	UNP Q9Y5W9

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Chain	Residue	Modelled	Actual	Comment	Reference
N	162	HIS	-	expression tag	UNP Q9Y5W9
N	163	HIS	-	expression tag	UNP Q9Y5W9
N	164	HIS	-	expression tag	UNP Q9Y5W9
N	165	HIS	-	expression tag	UNP Q9Y5W9
N	166	HIS	-	expression tag	UNP Q9Y5W9
O	159	LEU	-	expression tag	UNP Q9Y5W9
O	160	GLU	-	expression tag	UNP Q9Y5W9
O	161	HIS	-	expression tag	UNP Q9Y5W9
O	162	HIS	-	expression tag	UNP Q9Y5W9
O	163	HIS	-	expression tag	UNP Q9Y5W9
O	164	HIS	-	expression tag	UNP Q9Y5W9
O	165	HIS	-	expression tag	UNP Q9Y5W9
O	166	HIS	-	expression tag	UNP Q9Y5W9
P	159	LEU	-	expression tag	UNP Q9Y5W9
P	160	GLU	-	expression tag	UNP Q9Y5W9
P	161	HIS	-	expression tag	UNP Q9Y5W9
P	162	HIS	-	expression tag	UNP Q9Y5W9
P	163	HIS	-	expression tag	UNP Q9Y5W9
P	164	HIS	-	expression tag	UNP Q9Y5W9
P	165	HIS	-	expression tag	UNP Q9Y5W9
P	166	HIS	-	expression tag	UNP Q9Y5W9
Q	159	LEU	-	expression tag	UNP Q9Y5W9
Q	160	GLU	-	expression tag	UNP Q9Y5W9
Q	161	HIS	-	expression tag	UNP Q9Y5W9
Q	162	HIS	-	expression tag	UNP Q9Y5W9
Q	163	HIS	-	expression tag	UNP Q9Y5W9
Q	164	HIS	-	expression tag	UNP Q9Y5W9
Q	165	HIS	-	expression tag	UNP Q9Y5W9
Q	166	HIS	-	expression tag	UNP Q9Y5W9
R	159	LEU	-	expression tag	UNP Q9Y5W9
R	160	GLU	-	expression tag	UNP Q9Y5W9
R	161	HIS	-	expression tag	UNP Q9Y5W9
R	162	HIS	-	expression tag	UNP Q9Y5W9
R	163	HIS	-	expression tag	UNP Q9Y5W9
R	164	HIS	-	expression tag	UNP Q9Y5W9
R	165	HIS	-	expression tag	UNP Q9Y5W9
R	166	HIS	-	expression tag	UNP Q9Y5W9
S	159	LEU	-	expression tag	UNP Q9Y5W9
S	160	GLU	-	expression tag	UNP Q9Y5W9
S	161	HIS	-	expression tag	UNP Q9Y5W9
S	162	HIS	-	expression tag	UNP Q9Y5W9
S	163	HIS	-	expression tag	UNP Q9Y5W9

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Chain	Residue	Modelled	Actual	Comment	Reference
S	164	HIS	-	expression tag	UNP Q9Y5W9
S	165	HIS	-	expression tag	UNP Q9Y5W9
S	166	HIS	-	expression tag	UNP Q9Y5W9
T	159	LEU	-	expression tag	UNP Q9Y5W9
T	160	GLU	-	expression tag	UNP Q9Y5W9
T	161	HIS	-	expression tag	UNP Q9Y5W9
T	162	HIS	-	expression tag	UNP Q9Y5W9
T	163	HIS	-	expression tag	UNP Q9Y5W9
T	164	HIS	-	expression tag	UNP Q9Y5W9
T	165	HIS	-	expression tag	UNP Q9Y5W9
T	166	HIS	-	expression tag	UNP Q9Y5W9
U	159	LEU	-	expression tag	UNP Q9Y5W9
U	160	GLU	-	expression tag	UNP Q9Y5W9
U	161	HIS	-	expression tag	UNP Q9Y5W9
U	162	HIS	-	expression tag	UNP Q9Y5W9
U	163	HIS	-	expression tag	UNP Q9Y5W9
U	164	HIS	-	expression tag	UNP Q9Y5W9
U	165	HIS	-	expression tag	UNP Q9Y5W9
U	166	HIS	-	expression tag	UNP Q9Y5W9
V	159	LEU	-	expression tag	UNP Q9Y5W9
V	160	GLU	-	expression tag	UNP Q9Y5W9
V	161	HIS	-	expression tag	UNP Q9Y5W9
V	162	HIS	-	expression tag	UNP Q9Y5W9
V	163	HIS	-	expression tag	UNP Q9Y5W9
V	164	HIS	-	expression tag	UNP Q9Y5W9
V	165	HIS	-	expression tag	UNP Q9Y5W9
V	166	HIS	-	expression tag	UNP Q9Y5W9
W	159	LEU	-	expression tag	UNP Q9Y5W9
W	160	GLU	-	expression tag	UNP Q9Y5W9
W	161	HIS	-	expression tag	UNP Q9Y5W9
W	162	HIS	-	expression tag	UNP Q9Y5W9
W	163	HIS	-	expression tag	UNP Q9Y5W9
W	164	HIS	-	expression tag	UNP Q9Y5W9
W	165	HIS	-	expression tag	UNP Q9Y5W9
W	166	HIS	-	expression tag	UNP Q9Y5W9
X	159	LEU	-	expression tag	UNP Q9Y5W9
X	160	GLU	-	expression tag	UNP Q9Y5W9
X	161	HIS	-	expression tag	UNP Q9Y5W9
X	162	HIS	-	expression tag	UNP Q9Y5W9
X	163	HIS	-	expression tag	UNP Q9Y5W9
X	164	HIS	-	expression tag	UNP Q9Y5W9
X	165	HIS	-	expression tag	UNP Q9Y5W9

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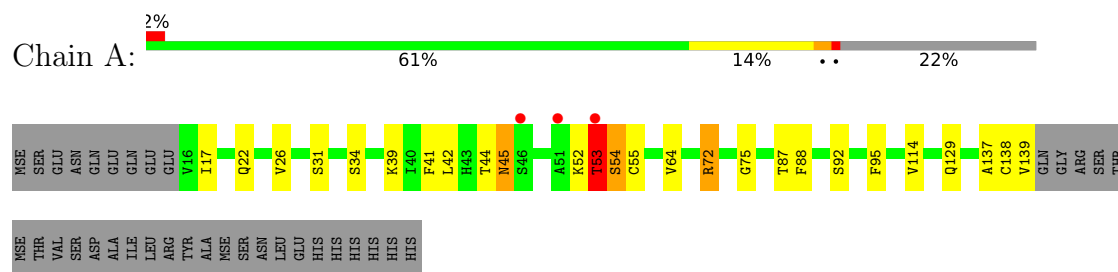
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Chain	Residue	Modelled	Actual	Comment	Reference
X	166	HIS	-	expression tag	UNP Q9Y5W9

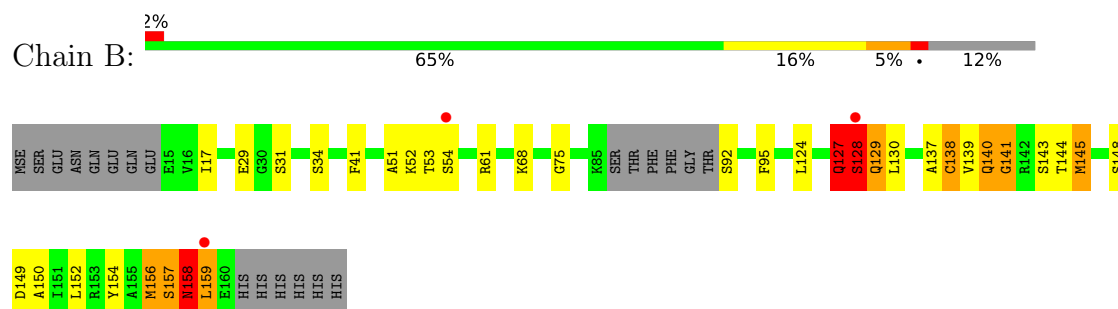
3 Residue-property plots [i](#)

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.

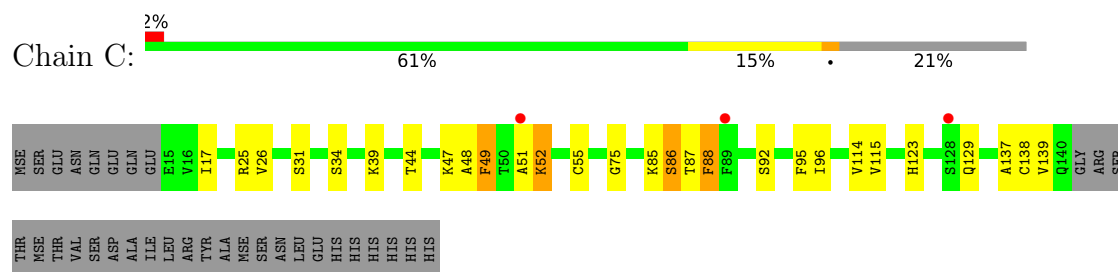
• Molecule 1: Sorting nexin-11



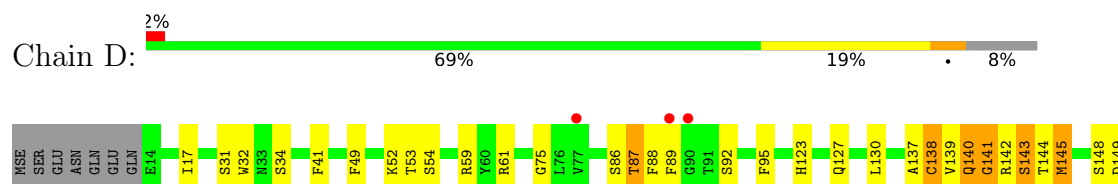
• Molecule 1: Sorting nexin-11

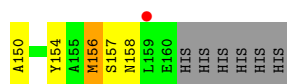


• Molecule 1: Sorting nexin-11



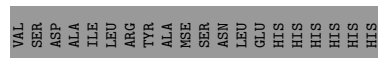
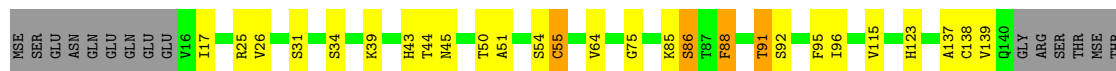
• Molecule 1: Sorting nexin-11





- Molecule 1: Sorting nexin-11

Chain E: 61% 14% 22%



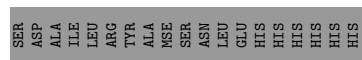
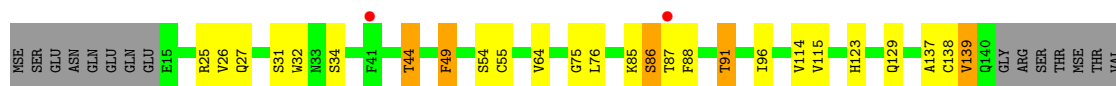
- Molecule 1: Sorting nexin-11

Chain F: 64% 19% 14%



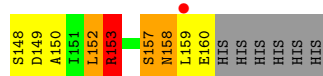
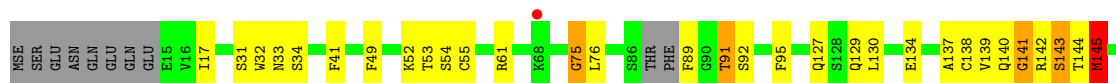
- Molecule 1: Sorting nexin-11

Chain G: 62% 13% 21%



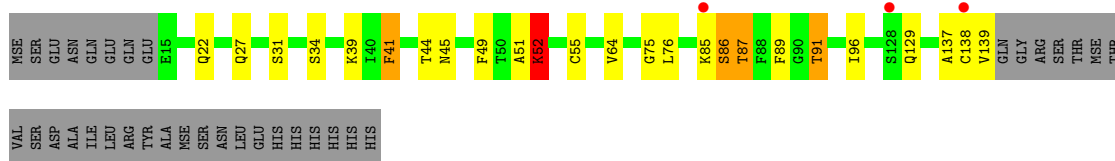
- Molecule 1: Sorting nexin-11

Chain H: 65% 19% 10%

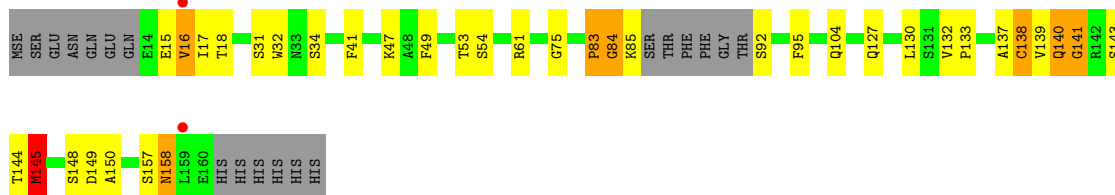


- Molecule 1: Sorting nexin-11

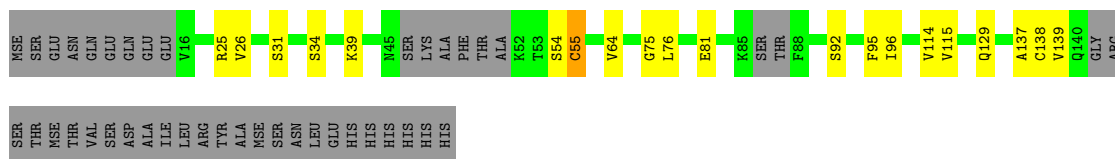
Chain I: 62% 12% 22%



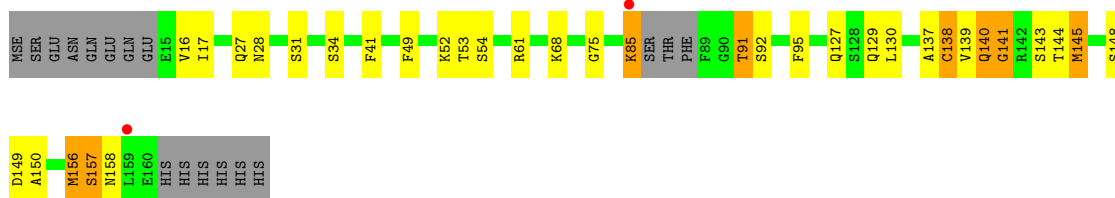
• Molecule 1: Sorting nexin-11



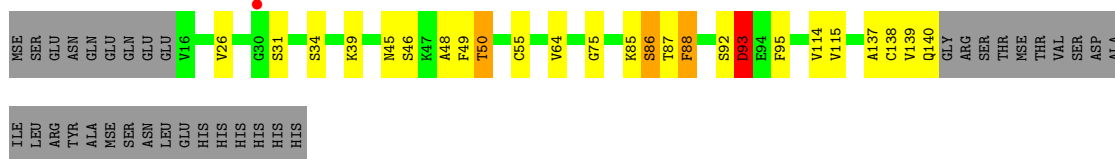
• Molecule 1: Sorting nexin-11



• Molecule 1: Sorting nexin-11

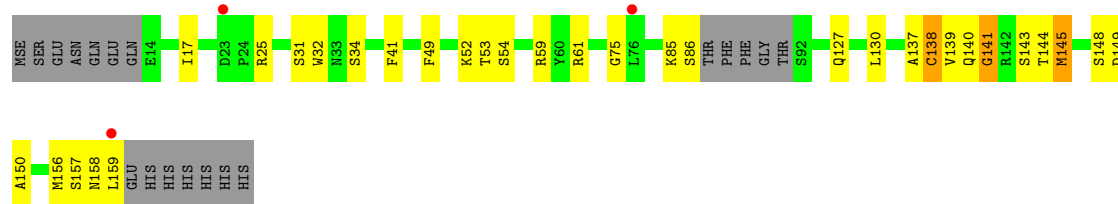


• Molecule 1: Sorting nexin-11

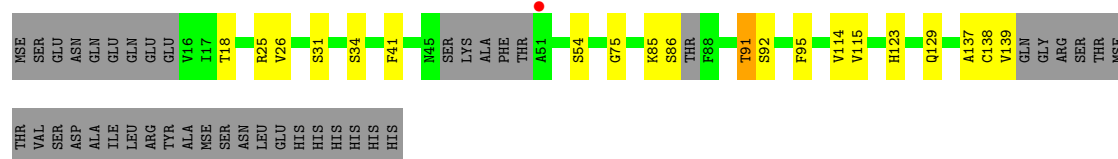


• Molecule 1: Sorting nexin-11

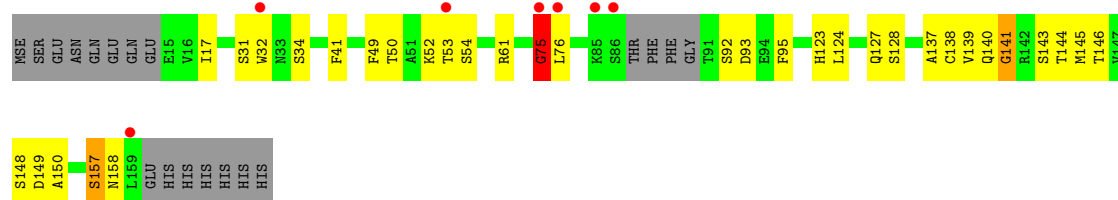




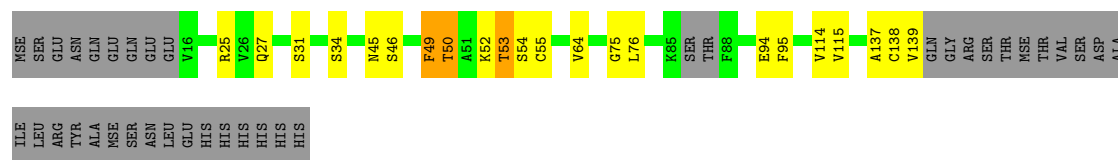
● Molecule 1: Sorting nexin-11



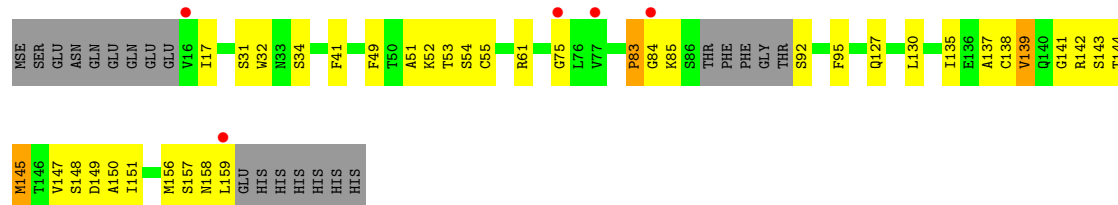
● Molecule 1: Sorting nexin-11



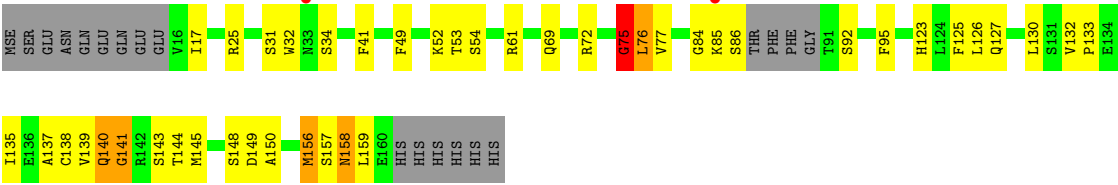
● Molecule 1: Sorting nexin-11



● Molecule 1: Sorting nexin-11



● Molecule 1: Sorting nexin-11



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	142.04Å 190.43Å 237.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.87 – 3.50 65.87 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (65.87-3.50) 99.0 (65.87-3.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 3.49Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.234 , 0.265 0.238 , 0.268	Depositor DCC
R_{free} test set	3921 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	102.0	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 92.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	25878	wwPDB-VP
Average B, all atoms (Å ²)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% 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	1.28	7/1040 (0.7%)	1.60	5/1406 (0.4%)
1	B	1.01	0/1160	1.53	5/1562 (0.3%)
1	C	1.06	2/1058 (0.2%)	1.49	5/1430 (0.3%)
1	D	1.05	0/1218	1.54	6/1642 (0.4%)
1	E	1.04	1/1049 (0.1%)	1.47	3/1418 (0.2%)
1	F	1.04	0/1144	1.52	4/1540 (0.3%)
1	G	1.01	0/1058	1.45	3/1430 (0.2%)
1	H	1.08	1/1189 (0.1%)	1.57	10/1601 (0.6%)
1	I	1.06	1/1049 (0.1%)	1.56	9/1418 (0.6%)
1	J	1.06	3/1169 (0.3%)	1.49	3/1574 (0.2%)
1	K	0.99	0/990	1.42	1/1335 (0.1%)
1	L	1.05	1/1183 (0.1%)	1.53	6/1593 (0.4%)
1	M	1.09	1/1049 (0.1%)	1.49	2/1418 (0.1%)
1	N	1.03	0/1166	1.46	1/1570 (0.1%)
1	O	0.98	0/992	1.43	2/1338 (0.1%)
1	P	1.05	1/1164 (0.1%)	1.47	2/1568 (0.1%)
1	Q	1.06	2/1026 (0.2%)	1.45	2/1385 (0.1%)
1	R	1.06	1/1148 (0.1%)	1.47	1/1546 (0.1%)
1	S	1.02	0/1040	1.44	1/1406 (0.1%)
1	T	1.04	0/1183	1.50	7/1594 (0.4%)
1	U	1.05	1/1019 (0.1%)	1.48	2/1375 (0.1%)
1	V	1.01	0/1081	1.54	8/1455 (0.5%)
1	W	1.05	1/1011 (0.1%)	1.48	1/1366 (0.1%)
1	X	1.05	2/1164 (0.2%)	1.45	2/1568 (0.1%)
All	All	1.05	25/26350 (0.1%)	1.49	91/35538 (0.3%)

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	A	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	1
1	G	0	2
1	H	0	1
1	I	0	1
1	J	0	1
1	R	0	3
1	W	0	2
All	All	0	17

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	72	ARG	NE-CZ	10.49	1.44	1.33
1	A	72	ARG	CZ-NH2	10.43	1.47	1.33
1	A	72	ARG	CZ-NH1	9.47	1.46	1.32
1	M	50	THR	C-O	8.72	1.34	1.23
1	A	53	THR	CA-C	8.53	1.58	1.53
1	I	45	ASN	C-O	8.53	1.34	1.24
1	L	27	GLN	C-O	8.39	1.33	1.24
1	Q	45	ASN	C-O	7.85	1.33	1.24
1	W	46	SER	C-O	-7.82	1.14	1.24
1	H	75	GLY	C-O	-7.30	1.14	1.23
1	J	84	GLY	C-O	-7.14	1.14	1.23
1	A	53	THR	N-CA	6.82	1.52	1.46
1	A	72	ARG	CG-CD	6.45	1.71	1.52
1	P	75	GLY	C-O	-6.40	1.15	1.23
1	Q	49	PHE	C-O	6.30	1.30	1.24
1	R	85	LYS	N-CA	6.29	1.51	1.46
1	J	17	ILE	C-O	6.16	1.30	1.24
1	J	83	PRO	C-O	-6.09	1.16	1.24
1	U	85	LYS	C-O	6.08	1.31	1.24
1	X	75	GLY	C-O	5.58	1.31	1.23
1	A	53	THR	C-O	5.46	1.30	1.24
1	C	51	ALA	C-O	-5.39	1.17	1.24
1	E	45	ASN	C-O	5.31	1.30	1.24
1	C	52	LYS	CA-C	5.10	1.59	1.52
1	X	84	GLY	C-O	5.09	1.28	1.23

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	27	GLN	N-CA-C	15.93	128.34	110.97
1	A	72	ARG	NE-CZ-NH1	-14.47	107.03	121.50
1	V	43	HIS	CA-C-N	11.57	143.64	121.54
1	V	43	HIS	C-N-CA	11.57	143.64	121.54
1	D	143	SER	CA-C-N	10.78	141.80	123.91
1	D	143	SER	C-N-CA	10.78	141.80	123.91
1	H	143	SER	CA-C-N	10.77	141.78	123.91
1	H	143	SER	C-N-CA	10.77	141.78	123.91
1	F	143	SER	CA-C-N	10.71	141.69	123.91
1	F	143	SER	C-N-CA	10.71	141.69	123.91
1	B	128	SER	N-CA-CB	10.48	128.19	110.49
1	W	49	PHE	CA-CB-CG	10.27	124.07	113.80
1	A	72	ARG	CD-NE-CZ	-9.83	110.64	124.40
1	U	45	ASN	CB-CA-C	9.32	125.06	110.14
1	L	27	GLN	CA-C-O	-9.25	111.29	121.00
1	A	53	THR	CB-CA-C	8.97	129.72	116.53
1	B	127	GLN	N-CA-C	-8.95	92.85	108.69
1	J	83	PRO	CA-C-O	-8.75	106.75	119.00
1	U	53	THR	CA-CB-OG1	8.60	122.50	109.60
1	D	156	MSE	CG-SE-CE	8.59	117.82	98.92
1	F	143	SER	O-C-N	8.23	130.99	123.26
1	D	143	SER	O-C-N	8.15	131.44	123.29
1	A	72	ARG	NE-CZ-NH2	8.02	126.42	119.20
1	I	51	ALA	CA-C-N	8.01	136.84	121.54
1	I	51	ALA	C-N-CA	8.01	136.84	121.54
1	H	143	SER	O-C-N	7.99	131.65	123.26
1	M	93	ASP	CA-CB-CG	7.96	120.56	112.60
1	A	54	SER	N-CA-CB	7.96	123.94	110.49
1	H	152	LEU	N-CA-C	-7.86	97.27	109.76
1	V	44	THR	CA-CB-CG2	7.63	123.47	110.50
1	I	49	PHE	CA-C-N	7.56	135.97	121.54
1	I	49	PHE	C-N-CA	7.56	135.97	121.54
1	C	49	PHE	CA-C-O	-7.51	109.77	120.51
1	H	76	LEU	N-CA-CB	-7.36	100.73	110.88
1	E	50	THR	CA-CB-OG1	-7.30	98.65	109.60
1	H	145	MSE	CG-SE-CE	7.23	114.83	98.92
1	J	18	THR	CA-CB-OG1	7.13	120.29	109.60
1	V	44	THR	CA-C-N	6.94	132.73	122.74
1	V	44	THR	C-N-CA	6.94	132.73	122.74
1	C	52	LYS	N-CA-C	6.91	125.52	110.80
1	S	46	SER	CA-C-O	-6.82	113.15	121.06
1	B	156	MSE	CG-SE-CE	6.80	113.88	98.92
1	R	145	MSE	CG-SE-CE	6.79	113.87	98.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	28	ASN	CA-C-O	-6.76	113.20	121.58
1	X	156	MSE	CG-SE-CE	6.71	113.69	98.92
1	O	18	THR	CA-CB-OG1	6.65	119.58	109.60
1	D	145	MSE	CG-SE-CE	6.64	113.53	98.92
1	J	145	MSE	CG-SE-CE	6.60	113.44	98.92
1	L	156	MSE	CG-SE-CE	6.56	113.36	98.92
1	Q	50	THR	CA-CB-OG1	-6.46	99.92	109.60
1	K	54	SER	CA-CB-OG	-6.36	98.37	111.10
1	G	44	THR	CA-C-O	-6.34	113.86	120.70
1	T	140	GLN	CB-CA-C	6.28	122.91	110.42
1	B	145	MSE	CG-SE-CE	6.25	112.68	98.92
1	B	129	GLN	N-CA-C	-5.98	105.82	112.57
1	C	48	ALA	N-CA-CB	5.98	121.09	111.65
1	T	140	GLN	CA-C-O	-5.90	112.08	120.51
1	P	76	LEU	N-CA-CB	-5.86	102.80	110.88
1	L	145	MSE	CG-SE-CE	5.83	111.75	98.92
1	H	153	ARG	CA-C-O	-5.76	112.28	120.51
1	I	49	PHE	O-C-N	5.75	128.59	122.38
1	C	88	PHE	CA-C-O	-5.73	112.85	119.78
1	D	143	SER	N-CA-C	5.69	116.79	108.14
1	T	140	GLN	N-CA-CB	-5.68	100.89	110.49
1	I	91	THR	CA-CB-OG1	5.67	118.10	109.60
1	V	44	THR	CB-CA-C	5.67	121.70	110.42
1	E	88	PHE	CA-C-O	-5.66	112.94	119.78
1	Q	54	SER	CA-CB-OG	-5.61	99.87	111.10
1	T	145	MSE	CG-SE-CE	5.61	111.25	98.92
1	H	143	SER	N-CA-C	5.60	116.77	108.60
1	G	91	THR	CA-CB-OG1	5.55	117.92	109.60
1	L	91	THR	CA-CB-OG1	5.54	117.92	109.60
1	V	43	HIS	O-C-N	5.54	130.11	123.13
1	M	140	GLN	CA-C-O	-5.50	111.44	120.80
1	I	52	LYS	N-CA-CB	5.49	119.76	110.49
1	H	89	PHE	CB-CA-C	5.40	120.36	110.10
1	T	92	SER	N-CA-C	5.40	122.30	110.80
1	V	156	MSE	CG-SE-CE	5.34	110.67	98.92
1	I	51	ALA	O-C-N	5.32	128.03	121.33
1	C	51	ALA	CA-C-O	-5.27	113.91	119.97
1	E	91	THR	CA-CB-OG1	5.27	117.51	109.60
1	X	145	MSE	CG-SE-CE	5.26	110.50	98.92
1	H	91	THR	CA-CB-OG1	5.25	117.47	109.60
1	N	156	MSE	CG-SE-CE	5.22	110.41	98.92
1	T	156	MSE	CG-SE-CE	5.20	110.36	98.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	89	PHE	CA-C-O	-5.13	113.18	120.51
1	P	145	MSE	CG-SE-CE	5.12	110.20	98.92
1	O	91	THR	CA-CB-OG1	5.11	117.27	109.60
1	G	139	VAL	CA-C-O	-5.09	114.42	120.78
1	T	92	SER	CA-C-O	5.08	127.77	120.51
1	F	129	GLN	N-CA-C	-5.01	106.91	112.57

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	22	GLN	Sidechain
1	A	45	ASN	Mainchain,Peptide
1	A	53	THR	Mainchain
1	A	72	ARG	Sidechain
1	B	127	GLN	Mainchain
1	D	140	GLN	Peptide
1	G	44	THR	Mainchain
1	G	49	PHE	Peptide
1	H	158	ASN	Peptide
1	I	44	THR	Peptide
1	J	83	PRO	Peptide
1	R	83	PRO	Mainchain,Peptide
1	R	84	GLY	Peptide
1	W	46	SER	Peptide
1	W	50	THR	Mainchain

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	1018	0	1028	21	0
1	B	1142	0	1154	25	0
1	C	1036	0	1042	35	0
1	D	1197	0	1201	45	0
1	E	1027	0	1036	29	0
1	F	1126	0	1139	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1036	0	1042	28	0
1	H	1170	0	1178	39	0
1	I	1027	0	1034	21	0
1	J	1151	0	1160	31	1
1	K	971	0	978	28	0
1	L	1164	0	1173	33	0
1	M	1027	0	1036	21	0
1	N	1148	0	1159	25	1
1	O	973	0	980	14	0
1	P	1146	0	1160	23	1
1	Q	1005	0	1015	25	1
1	R	1130	0	1147	41	0
1	S	1018	0	1028	27	0
1	T	1164	0	1176	40	0
1	U	999	0	1009	23	0
1	V	1065	0	1075	28	0
1	W	992	0	998	21	0
1	X	1146	0	1160	38	0
All	All	25878	0	26108	496	2

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 10.

All (496) 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:K:129:GLN:HE22	1:L:137:ALA:CB	1.62	1.12
1:I:39:LYS:HD2	1:J:138:CYS:SG	1.95	1.05
1:K:39:LYS:HD2	1:L:138:CYS:SG	1.99	1.02
1:B:152:LEU:O	1:B:156:MSE:HG3	1.64	0.97
1:Q:95:PHE:HD2	1:R:156:MSE:HE3	1.30	0.94
1:I:96:ILE:HG21	1:J:144:THR:HG21	1.53	0.91
1:T:86:SER:O	1:T:88:PHE:N	2.02	0.90
1:C:26:VAL:H	1:D:143:SER:HB3	1.33	0.90
1:C:95:PHE:HD2	1:D:156:MSE:HE2	1.36	0.89
1:E:26:VAL:H	1:F:143:SER:HB3	1.38	0.88
1:R:147:VAL:HB	1:R:151:ILE:HD11	1.53	0.88
1:K:129:GLN:NE2	1:L:137:ALA:HB1	1.88	0.87
1:K:129:GLN:NE2	1:L:137:ALA:CB	2.36	0.87
1:G:26:VAL:H	1:H:143:SER:HB3	1.38	0.87
1:G:96:ILE:HG21	1:H:144:THR:HG21	1.54	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:SER:HB2	1:D:61:ARG:HD3	1.57	0.86
1:K:129:GLN:HE22	1:L:137:ALA:HB1	1.41	0.86
1:S:96:ILE:HG21	1:T:144:THR:HG21	1.60	0.84
1:B:124:LEU:O	1:B:127:GLN:O	1.95	0.84
1:I:55:CYS:HB3	1:J:130:LEU:HD11	1.61	0.83
1:S:95:PHE:HD2	1:T:156:MSE:HE2	1.42	0.83
1:Q:95:PHE:CD2	1:R:156:MSE:HE3	2.15	0.81
1:J:15:GLU:O	1:J:16:VAL:O	1.99	0.81
1:K:26:VAL:HG23	1:L:144:THR:HG22	1.63	0.79
1:E:96:ILE:HG21	1:F:144:THR:HG21	1.65	0.79
1:B:157:SER:O	1:B:158:ASN:O	2.01	0.78
1:S:48:ALA:HB2	1:U:81:GLU:OE1	1.85	0.76
1:Q:52:LYS:O	1:Q:53:THR:O	2.04	0.76
1:I:22:GLN:OE1	1:I:41:PHE:HD2	1.68	0.76
1:V:139:VAL:O	1:V:139:VAL:HG13	1.86	0.75
1:C:96:ILE:HG21	1:D:144:THR:HG21	1.69	0.75
1:C:26:VAL:H	1:D:143:SER:CB	1.99	0.75
1:A:39:LYS:HE2	1:B:138:CYS:SG	2.27	0.75
1:U:25:ARG:HH22	1:V:139:VAL:HG23	1.52	0.74
1:G:27:GLN:OE1	1:H:140:GLN:HB3	1.87	0.74
1:U:95:PHE:HD2	1:V:156:MSE:HE2	1.53	0.74
1:N:25:ARG:NH1	1:V:29:GLU:OE2	2.20	0.74
1:D:89:PHE:CG	1:D:89:PHE:O	2.41	0.74
1:K:95:PHE:HD2	1:L:156:MSE:HE2	1.53	0.74
1:R:139:VAL:O	1:R:139:VAL:HG23	1.86	0.73
1:W:95:PHE:HD2	1:X:156:MSE:HE2	1.52	0.73
1:X:139:VAL:HG13	1:X:139:VAL:O	1.87	0.73
1:C:39:LYS:HD2	1:D:138:CYS:SG	2.30	0.72
1:K:64:VAL:HG11	1:P:32:TRP:NE1	2.04	0.72
1:M:88:PHE:CE1	1:M:95:PHE:HB2	2.26	0.71
1:H:159:LEU:HD23	1:H:160:GLU:N	2.06	0.71
1:D:89:PHE:O	1:D:89:PHE:CD1	2.45	0.70
1:I:22:GLN:OE1	1:I:41:PHE:CD2	2.44	0.70
1:K:64:VAL:HG11	1:P:32:TRP:CD1	2.27	0.69
1:S:96:ILE:HG12	1:T:156:MSE:HE3	1.74	0.69
1:W:96:ILE:HG12	1:X:156:MSE:HE3	1.75	0.69
1:E:26:VAL:H	1:F:143:SER:CB	2.04	0.69
1:E:92:SER:OG	1:F:153:ARG:NH1	2.26	0.69
1:F:32:TRP:CD1	1:M:64:VAL:HG11	2.28	0.69
1:T:88:PHE:O	1:T:91:THR:HG23	1.92	0.68
1:M:26:VAL:HG23	1:N:144:THR:HG22	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:SER:CB	1:D:61:ARG:HD3	2.24	0.67
1:C:95:PHE:CD2	1:D:156:MSE:HE2	2.23	0.67
1:U:96:ILE:CD1	1:V:156:MSE:HE3	2.24	0.67
1:E:17:ILE:HG23	1:E:44:THR:HG22	1.77	0.67
1:G:34:SER:O	1:H:158:ASN:ND2	2.24	0.67
1:W:55:CYS:HB3	1:X:130:LEU:HD11	1.77	0.66
1:K:34:SER:O	1:L:158:ASN:ND2	2.26	0.66
1:G:26:VAL:H	1:H:143:SER:CB	2.05	0.66
1:L:157:SER:HB2	1:P:61:ARG:HD3	1.77	0.66
1:S:95:PHE:CD2	1:T:156:MSE:HE2	2.28	0.65
1:A:45:ASN:OD1	1:A:45:ASN:O	2.15	0.65
1:L:61:ARG:HD3	1:V:157:SER:CB	2.27	0.65
1:H:157:SER:HB2	1:J:61:ARG:HD3	1.80	0.64
1:W:26:VAL:HG23	1:X:144:THR:HG22	1.80	0.64
1:E:55:CYS:HB2	1:F:130:LEU:HD11	1.79	0.64
1:F:146:THR:O	1:F:146:THR:HG22	1.98	0.64
1:Q:25:ARG:HG2	1:R:144:THR:HG22	1.80	0.64
1:K:96:ILE:HG12	1:L:156:MSE:HE3	1.79	0.63
1:A:26:VAL:HG23	1:B:144:THR:HG22	1.80	0.63
1:M:45:ASN:OD1	1:M:45:ASN:O	2.16	0.63
1:E:39:LYS:HD2	1:F:138:CYS:SG	2.39	0.62
1:M:93:ASP:OD2	1:N:145:MSE:HE3	1.99	0.62
1:S:17:ILE:HG23	1:S:44:THR:HG22	1.81	0.62
1:H:144:THR:O	1:H:144:THR:HG22	1.98	0.62
1:U:96:ILE:HG12	1:V:156:MSE:HE3	1.79	0.62
1:A:17:ILE:CD1	1:A:44:THR:OG1	2.47	0.62
1:P:124:LEU:O	1:P:128:SER:OG	2.10	0.62
1:F:17:ILE:HD12	1:F:111:LEU:HB3	1.82	0.62
1:F:157:SER:OG	1:X:61:ARG:HD3	1.98	0.62
1:D:144:THR:HG22	1:D:144:THR:O	2.00	0.61
1:N:61:ARG:HD3	1:X:157:SER:CB	2.30	0.61
1:D:154:TYR:O	1:T:61:ARG:NH2	2.32	0.61
1:G:55:CYS:HB3	1:H:130:LEU:HD11	1.81	0.61
1:H:148:SER:C	1:H:150:ALA:H	2.08	0.61
1:R:147:VAL:CB	1:R:151:ILE:HD11	2.27	0.61
1:T:148:SER:C	1:T:150:ALA:H	2.09	0.61
1:C:114:VAL:HG12	1:G:115:VAL:CG2	2.31	0.61
1:K:129:GLN:HE22	1:L:137:ALA:HB3	1.63	0.61
1:N:148:SER:C	1:N:150:ALA:H	2.09	0.61
1:A:41:PHE:CE1	1:A:55:CYS:SG	2.94	0.61
1:F:148:SER:C	1:F:150:ALA:H	2.09	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:SER:C	1:B:150:ALA:H	2.09	0.61
1:C:114:VAL:HG12	1:G:115:VAL:HG23	1.83	0.61
1:T:117:LEU:O	1:T:123:HIS:CE1	2.54	0.60
1:D:148:SER:C	1:D:150:ALA:H	2.09	0.60
1:J:148:SER:C	1:J:150:ALA:H	2.09	0.60
1:L:61:ARG:HD3	1:V:157:SER:OG	2.01	0.60
1:L:148:SER:C	1:L:150:ALA:H	2.10	0.60
1:P:148:SER:C	1:P:150:ALA:H	2.10	0.60
1:X:148:SER:C	1:X:150:ALA:H	2.09	0.60
1:J:144:THR:O	1:J:144:THR:HG22	2.02	0.59
1:V:148:SER:C	1:V:150:ALA:H	2.08	0.59
1:H:152:LEU:O	1:H:153:ARG:CB	2.49	0.59
1:T:144:THR:O	1:T:144:THR:HG22	2.01	0.59
1:C:96:ILE:HG12	1:D:156:MSE:HE3	1.84	0.59
1:T:87:THR:HG22	1:T:87:THR:O	2.02	0.59
1:N:61:ARG:HD3	1:X:157:SER:OG	2.01	0.59
1:H:157:SER:CB	1:J:61:ARG:HD3	2.33	0.59
1:F:144:THR:O	1:F:144:THR:HG22	2.01	0.59
1:K:39:LYS:CD	1:L:138:CYS:SG	2.84	0.59
1:D:87:THR:O	1:D:87:THR:HG22	2.02	0.58
1:H:61:ARG:HD3	1:R:157:SER:OG	2.03	0.58
1:L:61:ARG:HD3	1:V:157:SER:HB3	1.85	0.58
1:R:148:SER:C	1:R:150:ALA:H	2.09	0.58
1:W:17:ILE:HG23	1:W:44:THR:HG22	1.85	0.58
1:F:32:TRP:NE1	1:M:64:VAL:HG11	2.18	0.58
1:O:25:ARG:HD3	1:P:140:GLN:O	2.03	0.58
1:U:26:VAL:HG23	1:V:144:THR:HG22	1.85	0.58
1:P:157:SER:HB2	1:V:61:ARG:HD3	1.84	0.58
1:S:27:GLN:OE1	1:T:140:GLN:HB3	2.04	0.58
1:H:61:ARG:HD3	1:R:157:SER:CB	2.34	0.58
1:H:152:LEU:O	1:H:153:ARG:HB3	2.03	0.58
1:A:64:VAL:HG11	1:D:32:TRP:CD1	2.38	0.57
1:B:29:GLU:OE2	1:X:25:ARG:NH1	2.37	0.57
1:C:123:HIS:HD2	1:G:76:LEU:HD12	1.69	0.57
1:C:17:ILE:HG23	1:C:44:THR:HG22	1.87	0.57
1:F:124:LEU:O	1:F:128:SER:OG	2.10	0.57
1:C:55:CYS:HB2	1:D:130:LEU:HD11	1.86	0.57
1:Q:25:ARG:HA	1:R:144:THR:HA	1.86	0.57
1:I:41:PHE:CE1	1:I:55:CYS:SG	2.98	0.57
1:E:88:PHE:CE2	1:E:95:PHE:HB2	2.40	0.57
1:P:146:THR:O	1:P:146:THR:HG22	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:95:PHE:CD2	1:V:156:MSE:HE2	2.37	0.56
1:R:147:VAL:HB	1:R:151:ILE:CD1	2.30	0.56
1:K:95:PHE:CD2	1:L:156:MSE:HE2	2.37	0.56
1:R:135:ILE:O	1:R:139:VAL:HG13	2.06	0.56
1:J:157:SER:OG	1:R:61:ARG:HD3	2.05	0.56
1:W:95:PHE:CD2	1:X:156:MSE:HE2	2.36	0.56
1:J:157:SER:CB	1:R:61:ARG:HD3	2.35	0.56
1:V:135:ILE:O	1:V:139:VAL:HG12	2.05	0.56
1:Q:27:GLN:HE22	1:R:141:GLY:CA	2.19	0.56
1:R:141:GLY:C	1:R:143:SER:H	2.15	0.55
1:O:41:PHE:CE2	1:P:50:THR:HG21	2.41	0.55
1:K:96:ILE:CD1	1:L:156:MSE:HE3	2.36	0.55
1:N:61:ARG:HD3	1:X:157:SER:HB3	1.89	0.55
1:S:96:ILE:CD1	1:T:156:MSE:HE3	2.37	0.55
1:E:25:ARG:HH11	1:F:142:ARG:HA	1.71	0.55
1:B:61:ARG:NE	1:T:154:TYR:O	2.32	0.55
1:U:96:ILE:CG1	1:V:156:MSE:HE3	2.37	0.54
1:D:88:PHE:CE2	1:D:95:PHE:HB2	2.43	0.54
1:E:17:ILE:HG23	1:E:44:THR:CG2	2.37	0.54
1:P:49:PHE:CD1	1:P:123:HIS:CE1	2.95	0.54
1:D:157:SER:OG	1:T:61:ARG:HD3	2.08	0.54
1:W:96:ILE:CD1	1:X:156:MSE:HE3	2.36	0.54
1:C:25:ARG:HH11	1:D:142:ARG:HA	1.72	0.53
1:S:17:ILE:HG23	1:S:44:THR:CG2	2.38	0.53
1:U:92:SER:OG	1:V:153:ARG:CZ	2.57	0.53
1:F:61:ARG:HD3	1:N:157:SER:CB	2.37	0.53
1:X:135:ILE:O	1:X:139:VAL:HG12	2.07	0.53
1:D:49:PHE:CD1	1:D:123:HIS:CE1	2.97	0.53
1:W:55:CYS:CB	1:X:130:LEU:HD11	2.38	0.53
1:X:49:PHE:CD1	1:X:123:HIS:CE1	2.97	0.53
1:F:61:ARG:HD3	1:N:157:SER:HB3	1.90	0.53
1:H:61:ARG:HD3	1:R:157:SER:HB3	1.89	0.53
1:T:117:LEU:O	1:T:123:HIS:HE1	1.92	0.53
1:B:61:ARG:HD2	1:T:157:SER:OG	2.08	0.53
1:K:55:CYS:HB2	1:L:130:LEU:HD11	1.91	0.53
1:W:96:ILE:CG1	1:X:156:MSE:HE3	2.39	0.52
1:S:55:CYS:HB3	1:T:130:LEU:HD11	1.92	0.52
1:J:157:SER:HB3	1:R:61:ARG:HD3	1.91	0.52
1:K:25:ARG:HH22	1:L:139:VAL:HG13	1.75	0.52
1:X:75:GLY:O	1:X:77:VAL:N	2.42	0.52
1:F:61:ARG:HD3	1:N:157:SER:OG	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:86:SER:O	1:I:87:THR:OG1	2.25	0.52
1:Q:25:ARG:HB3	1:R:141:GLY:HA3	1.90	0.52
1:W:17:ILE:HG23	1:W:44:THR:CG2	2.40	0.52
1:A:64:VAL:HG11	1:D:32:TRP:NE1	2.25	0.52
1:T:143:SER:HB3	1:T:146:THR:HG22	1.91	0.52
1:B:152:LEU:O	1:B:156:MSE:CG	2.49	0.51
1:S:96:ILE:HG13	1:T:144:THR:CG2	2.41	0.51
1:E:25:ARG:HA	1:F:143:SER:HB2	1.92	0.51
1:I:55:CYS:CB	1:J:130:LEU:HD11	2.37	0.51
1:S:27:GLN:CD	1:T:140:GLN:HB3	2.35	0.51
1:S:96:ILE:CG1	1:T:156:MSE:HE3	2.39	0.51
1:X:139:VAL:O	1:X:139:VAL:CG1	2.58	0.51
1:I:41:PHE:HE1	1:I:55:CYS:SG	2.33	0.51
1:X:125:PHE:HD1	1:X:126:LEU:HD12	1.75	0.51
1:C:137:ALA:C	1:C:139:VAL:H	2.19	0.51
1:A:114:VAL:HG12	1:E:115:VAL:CG2	2.41	0.51
1:C:17:ILE:HG23	1:C:44:THR:CG2	2.41	0.51
1:G:137:ALA:C	1:G:139:VAL:H	2.19	0.51
1:A:88:PHE:CE2	1:A:95:PHE:HB2	2.46	0.51
1:C:55:CYS:CB	1:D:130:LEU:HD11	2.41	0.51
1:C:88:PHE:CE2	1:C:95:PHE:HB2	2.46	0.51
1:H:32:TRP:CD1	1:Q:64:VAL:HG11	2.45	0.51
1:W:137:ALA:C	1:W:139:VAL:H	2.19	0.51
1:B:159:LEU:HD12	1:D:59:ARG:HH12	1.75	0.51
1:J:137:ALA:C	1:J:139:VAL:H	2.19	0.51
1:E:25:ARG:HH22	1:F:139:VAL:HG13	1.77	0.50
1:E:64:VAL:HG11	1:X:32:TRP:CD1	2.46	0.50
1:I:96:ILE:HG13	1:J:144:THR:CG2	2.42	0.50
1:I:137:ALA:C	1:I:139:VAL:H	2.20	0.50
1:M:137:ALA:C	1:M:139:VAL:H	2.20	0.50
1:H:137:ALA:C	1:H:139:VAL:H	2.20	0.50
1:S:114:VAL:HG12	1:U:115:VAL:CG2	2.42	0.50
1:X:75:GLY:C	1:X:77:VAL:N	2.68	0.50
1:P:137:ALA:C	1:P:139:VAL:H	2.20	0.50
1:Q:27:GLN:HE22	1:R:141:GLY:N	2.10	0.50
1:D:137:ALA:C	1:D:139:VAL:H	2.20	0.50
1:E:137:ALA:C	1:E:139:VAL:H	2.19	0.49
1:U:137:ALA:C	1:U:139:VAL:H	2.19	0.49
1:X:137:ALA:C	1:X:139:VAL:H	2.20	0.49
1:B:137:ALA:C	1:B:139:VAL:H	2.20	0.49
1:U:96:ILE:HD11	1:V:156:MSE:HE3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:137:ALA:C	1:F:139:VAL:H	2.20	0.49
1:T:137:ALA:C	1:T:139:VAL:H	2.20	0.49
1:V:137:ALA:C	1:V:139:VAL:H	2.20	0.49
1:N:137:ALA:C	1:N:139:VAL:H	2.20	0.49
1:S:137:ALA:C	1:S:139:VAL:H	2.20	0.49
1:J:84:GLY:O	1:J:85:LYS:C	2.56	0.49
1:O:137:ALA:C	1:O:139:VAL:H	2.20	0.49
1:K:137:ALA:C	1:K:139:VAL:H	2.19	0.49
1:Q:137:ALA:C	1:Q:139:VAL:H	2.20	0.49
1:R:141:GLY:O	1:R:143:SER:N	2.46	0.49
1:S:55:CYS:CB	1:T:130:LEU:HD11	2.43	0.49
1:T:144:THR:O	1:T:144:THR:CG2	2.61	0.49
1:L:157:SER:CB	1:P:61:ARG:HD3	2.43	0.49
1:U:39:LYS:HD2	1:V:138:CYS:SG	2.53	0.49
1:O:41:PHE:HE2	1:P:50:THR:HG21	1.78	0.48
1:R:148:SER:O	1:R:151:ILE:HG12	2.12	0.48
1:C:25:ARG:HA	1:D:143:SER:HB2	1.95	0.48
1:E:39:LYS:CG	1:F:138:CYS:SG	3.01	0.48
1:U:17:ILE:HG23	1:U:44:THR:HG22	1.94	0.48
1:A:137:ALA:C	1:A:139:VAL:H	2.21	0.48
1:S:27:GLN:NE2	1:T:140:GLN:HB3	2.28	0.48
1:V:139:VAL:O	1:V:139:VAL:CG1	2.57	0.48
1:O:114:VAL:HG12	1:Q:115:VAL:CG2	2.43	0.48
1:R:137:ALA:C	1:R:139:VAL:H	2.20	0.48
1:L:137:ALA:C	1:L:139:VAL:H	2.20	0.48
1:N:59:ARG:NH1	1:X:159:LEU:HD11	2.28	0.48
1:E:25:ARG:HA	1:F:143:SER:CB	2.44	0.48
1:K:96:ILE:CG1	1:L:156:MSE:HE3	2.41	0.48
1:T:86:SER:C	1:T:88:PHE:H	2.11	0.48
1:Q:27:GLN:NE2	1:R:141:GLY:CA	2.77	0.48
1:Q:55:CYS:CB	1:R:130:LEU:HD11	2.44	0.48
1:E:26:VAL:N	1:F:143:SER:HB3	2.19	0.47
1:L:85:LYS:HD3	1:V:153:ARG:NH1	2.29	0.47
1:A:34:SER:O	1:B:158:ASN:ND2	2.47	0.47
1:A:42:LEU:O	1:A:53:THR:O	2.30	0.47
1:O:26:VAL:HG23	1:P:144:THR:HG22	1.95	0.47
1:S:96:ILE:HG13	1:T:144:THR:HG21	1.97	0.47
1:C:26:VAL:N	1:D:143:SER:HB3	2.15	0.47
1:U:41:PHE:HE1	1:U:53:THR:HG22	1.79	0.47
1:H:144:THR:O	1:H:144:THR:CG2	2.62	0.47
1:B:154:TYR:O	1:D:61:ARG:NH1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:THR:O	1:D:144:THR:CG2	2.62	0.47
1:J:144:THR:O	1:J:144:THR:CG2	2.61	0.47
1:L:68:LYS:HE3	1:U:30:GLY:O	2.15	0.47
1:P:157:SER:CB	1:V:61:ARG:HD3	2.44	0.47
1:M:49:PHE:CE2	1:M:50:THR:HG23	2.49	0.47
1:X:75:GLY:O	1:X:76:LEU:C	2.57	0.47
1:C:115:VAL:CG2	1:K:114:VAL:HG12	2.45	0.47
1:G:25:ARG:HH11	1:H:142:ARG:HA	1.78	0.47
1:H:140:GLN:O	1:H:141:GLY:O	2.32	0.47
1:S:25:ARG:HH22	1:T:139:VAL:HG13	1.80	0.47
1:U:17:ILE:HG23	1:U:44:THR:CG2	2.44	0.47
1:B:140:GLN:O	1:B:141:GLY:O	2.33	0.47
1:Q:55:CYS:HB3	1:R:130:LEU:HD11	1.97	0.47
1:X:75:GLY:C	1:X:77:VAL:H	2.22	0.47
1:X:140:GLN:O	1:X:141:GLY:O	2.32	0.47
1:B:61:ARG:HD2	1:T:157:SER:CB	2.44	0.47
1:Q:50:THR:HG21	1:R:55:CYS:HB2	1.97	0.47
1:J:140:GLN:O	1:J:141:GLY:O	2.33	0.47
1:K:25:ARG:HD3	1:L:140:GLN:O	2.16	0.46
1:P:140:GLN:O	1:P:141:GLY:O	2.33	0.46
1:C:25:ARG:HH22	1:D:139:VAL:HG13	1.80	0.46
1:H:159:LEU:HD23	1:H:160:GLU:H	1.78	0.46
1:F:140:GLN:O	1:F:141:GLY:O	2.33	0.46
1:D:49:PHE:HB3	1:D:127:GLN:HE22	1.81	0.46
1:D:140:GLN:O	1:D:141:GLY:O	2.33	0.46
1:J:49:PHE:HB3	1:J:127:GLN:HE22	1.80	0.46
1:R:49:PHE:HB3	1:R:127:GLN:HE22	1.80	0.46
1:R:141:GLY:C	1:R:143:SER:N	2.72	0.46
1:X:49:PHE:HB3	1:X:127:GLN:HE22	1.81	0.46
1:F:49:PHE:HB3	1:F:127:GLN:HE22	1.81	0.46
1:N:140:GLN:O	1:N:141:GLY:O	2.34	0.46
1:F:17:ILE:HG22	1:F:44:THR:OG1	2.15	0.46
1:M:55:CYS:CB	1:N:130:LEU:HD11	2.45	0.46
1:T:49:PHE:HB3	1:T:127:GLN:HE22	1.81	0.46
1:P:49:PHE:HB3	1:P:127:GLN:HE22	1.81	0.46
1:T:140:GLN:O	1:T:141:GLY:O	2.34	0.46
1:L:140:GLN:O	1:L:141:GLY:O	2.34	0.46
1:M:85:LYS:O	1:M:86:SER:C	2.59	0.46
1:N:148:SER:C	1:N:150:ALA:N	2.74	0.46
1:A:17:ILE:HD12	1:A:44:THR:OG1	2.16	0.45
1:E:55:CYS:CB	1:F:130:LEU:HD11	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:144:THR:O	1:F:144:THR:CG2	2.64	0.45
1:R:148:SER:C	1:R:150:ALA:N	2.74	0.45
1:J:148:SER:C	1:J:150:ALA:N	2.74	0.45
1:M:49:PHE:CD2	1:M:50:THR:HG23	2.51	0.45
1:T:88:PHE:O	1:T:91:THR:CG2	2.61	0.45
1:V:148:SER:C	1:V:150:ALA:N	2.74	0.45
1:W:34:SER:O	1:X:158:ASN:OD1	2.34	0.45
1:H:49:PHE:HB3	1:H:127:GLN:HE22	1.81	0.45
1:A:44:THR:CG2	1:A:52:LYS:HB2	2.46	0.45
1:G:25:ARG:HA	1:H:143:SER:CB	2.46	0.45
1:M:55:CYS:HB2	1:N:130:LEU:HD11	1.99	0.45
1:Q:27:GLN:OE1	1:R:141:GLY:HA2	2.17	0.45
1:C:31:SER:O	1:C:34:SER:HB2	2.17	0.45
1:G:123:HIS:HD2	1:K:76:LEU:HD12	1.81	0.45
1:L:31:SER:O	1:L:34:SER:HB2	2.17	0.45
1:P:31:SER:O	1:P:34:SER:HB2	2.17	0.45
1:X:85:LYS:O	1:X:86:SER:C	2.60	0.45
1:D:31:SER:O	1:D:34:SER:HB2	2.17	0.45
1:L:49:PHE:HB3	1:L:127:GLN:HE22	1.81	0.45
1:K:31:SER:O	1:K:34:SER:HB2	2.17	0.45
1:I:31:SER:O	1:I:34:SER:HB2	2.17	0.45
1:E:39:LYS:HG3	1:F:138:CYS:SG	2.56	0.45
1:H:31:SER:O	1:H:34:SER:HB2	2.17	0.45
1:O:31:SER:O	1:O:34:SER:HB2	2.17	0.45
1:Q:27:GLN:CD	1:R:141:GLY:HA2	2.42	0.45
1:A:31:SER:O	1:A:34:SER:HB2	2.17	0.44
1:B:31:SER:O	1:B:34:SER:HB2	2.17	0.44
1:M:31:SER:O	1:M:34:SER:HB2	2.17	0.44
1:X:31:SER:O	1:X:34:SER:HB2	2.17	0.44
1:S:115:VAL:CG2	1:W:114:VAL:HG12	2.46	0.44
1:G:26:VAL:N	1:H:143:SER:HB3	2.19	0.44
1:G:31:SER:O	1:G:34:SER:HB2	2.17	0.44
1:J:31:SER:O	1:J:34:SER:HB2	2.17	0.44
1:N:31:SER:O	1:N:34:SER:HB2	2.17	0.44
1:U:114:VAL:HG12	1:W:115:VAL:CG2	2.48	0.44
1:W:31:SER:O	1:W:34:SER:HB2	2.17	0.44
1:A:17:ILE:HD13	1:A:44:THR:OG1	2.17	0.44
1:F:157:SER:CB	1:X:61:ARG:HD3	2.47	0.44
1:S:114:VAL:HG12	1:U:115:VAL:HG21	2.00	0.44
1:N:85:LYS:O	1:N:86:SER:C	2.60	0.44
1:S:85:LYS:O	1:S:86:SER:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:140:GLN:O	1:V:141:GLY:O	2.35	0.44
1:A:114:VAL:HG12	1:E:115:VAL:HG23	2.00	0.44
1:V:31:SER:O	1:V:34:SER:HB2	2.17	0.44
1:E:31:SER:O	1:E:34:SER:HB2	2.17	0.44
1:G:49:PHE:CE1	1:K:81:GLU:OE1	2.71	0.44
1:M:115:VAL:HG21	1:Q:114:VAL:HG12	2.00	0.44
1:N:49:PHE:HB3	1:N:127:GLN:HE22	1.81	0.44
1:Q:31:SER:O	1:Q:34:SER:HB2	2.17	0.44
1:G:129:GLN:NE2	1:H:134:GLU:CD	2.75	0.44
1:P:148:SER:C	1:P:150:ALA:N	2.75	0.44
1:Q:46:SER:HB3	1:Q:49:PHE:HD2	1.83	0.44
1:S:115:VAL:HG21	1:W:114:VAL:HG12	1.99	0.44
1:C:25:ARG:NH1	1:D:142:ARG:HA	2.33	0.44
1:G:85:LYS:O	1:G:86:SER:C	2.60	0.44
1:G:114:VAL:HG12	1:K:115:VAL:CG2	2.48	0.44
1:I:34:SER:O	1:J:158:ASN:OD1	2.36	0.44
1:S:31:SER:O	1:S:34:SER:HB2	2.17	0.44
1:B:128:SER:HB3	1:B:130:LEU:HG	1.99	0.43
1:F:144:THR:O	1:F:145:MSE:HG3	2.17	0.43
1:U:31:SER:O	1:U:34:SER:HB2	2.17	0.43
1:E:85:LYS:O	1:E:86:SER:C	2.61	0.43
1:O:85:LYS:O	1:O:86:SER:C	2.60	0.43
1:C:85:LYS:O	1:C:86:SER:C	2.60	0.43
1:R:31:SER:O	1:R:34:SER:HB2	2.17	0.43
1:T:31:SER:O	1:T:34:SER:HB2	2.17	0.43
1:T:148:SER:C	1:T:150:ALA:N	2.74	0.43
1:I:39:LYS:HE3	1:I:41:PHE:CZ	2.53	0.43
1:O:114:VAL:HG12	1:Q:115:VAL:HG23	1.99	0.43
1:B:148:SER:C	1:B:150:ALA:N	2.74	0.43
1:C:55:CYS:O	1:C:129:GLN:NE2	2.51	0.43
1:D:86:SER:C	1:D:88:PHE:H	2.26	0.43
1:F:31:SER:O	1:F:34:SER:HB2	2.17	0.43
1:B:41:PHE:HE1	1:B:53:THR:HG23	1.83	0.43
1:I:85:LYS:O	1:I:86:SER:C	2.61	0.43
1:H:148:SER:C	1:H:150:ALA:N	2.74	0.43
1:M:39:LYS:HD2	1:N:138:CYS:SG	2.59	0.43
1:R:41:PHE:HE1	1:R:53:THR:HG23	1.83	0.43
1:G:55:CYS:CB	1:H:130:LEU:HD11	2.49	0.43
1:J:41:PHE:HE1	1:J:53:THR:HG23	1.84	0.43
1:L:41:PHE:HE1	1:L:53:THR:HG23	1.84	0.43
1:M:45:ASN:CG	1:M:48:ALA:HA	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:41:PHE:HE1	1:N:53:THR:HG23	1.84	0.43
1:T:87:THR:O	1:T:87:THR:CG2	2.65	0.43
1:F:148:SER:C	1:F:150:ALA:N	2.75	0.42
1:G:129:GLN:NE2	1:H:134:GLU:OE2	2.52	0.42
1:X:41:PHE:HE1	1:X:53:THR:HG23	1.84	0.42
1:X:69:GLN:HE22	1:X:72:ARG:NH1	2.17	0.42
1:H:55:CYS:O	1:H:129:GLN:NE2	2.52	0.42
1:J:137:ALA:O	1:J:139:VAL:N	2.53	0.42
1:W:137:ALA:O	1:W:139:VAL:N	2.53	0.42
1:E:123:HIS:HD2	1:I:76:LEU:HD12	1.84	0.42
1:G:25:ARG:HA	1:H:143:SER:HB2	2.00	0.42
1:H:137:ALA:O	1:H:139:VAL:N	2.53	0.42
1:T:92:SER:O	1:T:95:PHE:N	2.53	0.42
1:H:41:PHE:HE1	1:H:53:THR:HG23	1.84	0.42
1:B:51:ALA:CB	1:B:54:SER:OG	2.68	0.42
1:C:39:LYS:CD	1:D:138:CYS:SG	3.06	0.42
1:C:137:ALA:O	1:C:139:VAL:N	2.53	0.42
1:F:94:GLU:N	1:F:94:GLU:OE1	2.53	0.42
1:T:137:ALA:O	1:T:139:VAL:N	2.53	0.42
1:U:137:ALA:O	1:U:139:VAL:N	2.53	0.42
1:X:137:ALA:C	1:X:139:VAL:N	2.78	0.42
1:B:137:ALA:O	1:B:139:VAL:N	2.53	0.42
1:E:43:HIS:HE1	1:E:51:ALA:HB1	1.85	0.42
1:M:114:VAL:HG12	1:O:115:VAL:CG2	2.50	0.42
1:B:92:SER:O	1:B:95:PHE:N	2.53	0.42
1:F:41:PHE:HE1	1:F:53:THR:HG23	1.84	0.42
1:G:137:ALA:C	1:G:139:VAL:N	2.78	0.42
1:G:137:ALA:O	1:G:139:VAL:N	2.53	0.42
1:K:137:ALA:C	1:K:139:VAL:N	2.78	0.42
1:K:137:ALA:O	1:K:139:VAL:N	2.53	0.42
1:W:137:ALA:C	1:W:139:VAL:N	2.78	0.42
1:F:137:ALA:C	1:F:139:VAL:N	2.78	0.42
1:F:137:ALA:O	1:F:139:VAL:N	2.53	0.42
1:I:137:ALA:O	1:I:139:VAL:N	2.53	0.42
1:L:137:ALA:O	1:L:139:VAL:N	2.53	0.42
1:M:137:ALA:C	1:M:139:VAL:N	2.78	0.42
1:N:32:TRP:NE1	1:W:64:VAL:HG11	2.35	0.42
1:O:137:ALA:C	1:O:139:VAL:N	2.78	0.42
1:S:92:SER:O	1:S:95:PHE:N	2.53	0.42
1:V:137:ALA:O	1:V:139:VAL:N	2.53	0.42
1:X:137:ALA:O	1:X:139:VAL:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:ARG:HA	1:D:143:SER:CB	2.49	0.41
1:R:137:ALA:C	1:R:139:VAL:N	2.78	0.41
1:R:142:ARG:NE	1:R:142:ARG:HA	2.35	0.41
1:E:137:ALA:C	1:E:139:VAL:N	2.78	0.41
1:G:86:SER:O	1:G:88:PHE:CD2	2.74	0.41
1:H:157:SER:OG	1:J:61:ARG:HD3	2.20	0.41
1:P:137:ALA:O	1:P:139:VAL:N	2.53	0.41
1:T:41:PHE:HE1	1:T:53:THR:HG23	1.84	0.41
1:T:137:ALA:C	1:T:139:VAL:N	2.78	0.41
1:H:92:SER:O	1:H:95:PHE:N	2.53	0.41
1:I:96:ILE:CG2	1:J:144:THR:HG21	2.37	0.41
1:P:92:SER:O	1:P:95:PHE:N	2.54	0.41
1:D:41:PHE:HE1	1:D:53:THR:HG23	1.84	0.41
1:D:137:ALA:O	1:D:139:VAL:N	2.53	0.41
1:E:137:ALA:O	1:E:139:VAL:N	2.53	0.41
1:G:32:TRP:O	1:J:61:ARG:NH2	2.41	0.41
1:G:64:VAL:HG11	1:J:32:TRP:CD1	2.55	0.41
1:N:144:THR:C	1:N:145:MSE:HG2	2.45	0.41
1:O:123:HIS:HD2	1:Q:76:LEU:HD12	1.86	0.41
1:R:137:ALA:O	1:R:139:VAL:N	2.53	0.41
1:A:137:ALA:O	1:A:139:VAL:N	2.54	0.41
1:C:92:SER:O	1:C:95:PHE:N	2.54	0.41
1:D:137:ALA:C	1:D:139:VAL:N	2.78	0.41
1:I:137:ALA:C	1:I:139:VAL:N	2.78	0.41
1:R:51:ALA:CB	1:R:54:SER:OG	2.68	0.41
1:V:137:ALA:C	1:V:139:VAL:N	2.78	0.41
1:A:114:VAL:HG12	1:E:115:VAL:HG21	2.03	0.41
1:E:92:SER:O	1:E:95:PHE:N	2.54	0.41
1:I:27:GLN:OE1	1:J:140:GLN:HB3	2.21	0.41
1:L:137:ALA:C	1:L:139:VAL:N	2.78	0.41
1:M:137:ALA:O	1:M:139:VAL:N	2.53	0.41
1:S:137:ALA:O	1:S:139:VAL:N	2.53	0.41
1:A:137:ALA:C	1:A:139:VAL:N	2.79	0.41
1:C:25:ARG:NH1	1:D:142:ARG:HG2	2.36	0.41
1:J:92:SER:O	1:J:95:PHE:N	2.53	0.41
1:L:92:SER:O	1:L:95:PHE:N	2.54	0.41
1:P:41:PHE:HE1	1:P:53:THR:HG23	1.85	0.41
1:W:92:SER:O	1:W:95:PHE:N	2.54	0.41
1:C:47:LYS:HB3	1:C:49:PHE:HB2	2.02	0.41
1:D:148:SER:C	1:D:150:ALA:N	2.74	0.41
1:O:137:ALA:O	1:O:139:VAL:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:92:SER:O	1:X:95:PHE:N	2.54	0.41
1:A:92:SER:O	1:A:95:PHE:N	2.54	0.41
1:C:137:ALA:C	1:C:139:VAL:N	2.78	0.41
1:K:92:SER:O	1:K:95:PHE:N	2.54	0.41
1:M:92:SER:O	1:M:95:PHE:N	2.54	0.41
1:M:115:VAL:CG2	1:Q:114:VAL:HG12	2.51	0.41
1:N:137:ALA:C	1:N:139:VAL:N	2.78	0.41
1:N:137:ALA:O	1:N:139:VAL:N	2.53	0.41
1:Q:137:ALA:O	1:Q:139:VAL:N	2.53	0.41
1:S:137:ALA:C	1:S:139:VAL:N	2.78	0.41
1:C:114:VAL:HG12	1:G:115:VAL:HG21	2.01	0.41
1:C:39:LYS:CG	1:D:138:CYS:SG	3.09	0.40
1:D:92:SER:O	1:D:95:PHE:N	2.54	0.40
1:Q:137:ALA:C	1:Q:139:VAL:N	2.78	0.40
1:C:39:LYS:HG3	1:D:138:CYS:SG	2.61	0.40
1:F:68:LYS:HG2	1:F:72:ARG:HH12	1.86	0.40
1:F:144:THR:C	1:F:145:MSE:HG3	2.46	0.40
1:H:33:ASN:HD22	1:R:159:LEU:HD11	1.86	0.40
1:H:144:THR:C	1:H:145:MSE:HG2	2.45	0.40
1:I:64:VAL:HG11	1:R:32:TRP:NE1	2.36	0.40
1:O:92:SER:O	1:O:95:PHE:N	2.54	0.40
1:R:92:SER:O	1:R:95:PHE:N	2.53	0.40
1:U:30:GLY:O	1:V:154:TYR:CE2	2.74	0.40
1:U:92:SER:O	1:U:95:PHE:N	2.54	0.40
1:X:132:VAL:HB	1:X:133:PRO:HD3	2.03	0.40
1:H:137:ALA:C	1:H:139:VAL:N	2.78	0.40
1:J:144:THR:O	1:J:145:MSE:HG2	2.22	0.40
1:P:137:ALA:C	1:P:139:VAL:N	2.78	0.40
1:W:49:PHE:CD2	1:W:52:LYS:HD3	2.56	0.40
1:J:132:VAL:HB	1:J:133:PRO:HD3	2.04	0.40

All (2) 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:J:104:GLN:NE2	1:Q:94:GLU:OE2[4_555]	1.20	1.00
1:N:150:ALA:CB	1:P:75:GLY:O[3_444]	1.64	0.56

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	122/160 (76%)	103 (84%)	15 (12%)	4 (3%)	3	23
1	B	136/160 (85%)	116 (85%)	13 (10%)	7 (5%)	1	15
1	C	124/160 (78%)	102 (82%)	17 (14%)	5 (4%)	2	19
1	D	145/160 (91%)	128 (88%)	12 (8%)	5 (3%)	3	23
1	E	123/160 (77%)	104 (85%)	16 (13%)	3 (2%)	4	29
1	F	134/160 (84%)	119 (89%)	11 (8%)	4 (3%)	3	25
1	G	124/160 (78%)	106 (86%)	14 (11%)	4 (3%)	3	24
1	H	140/160 (88%)	120 (86%)	15 (11%)	5 (4%)	2	22
1	I	123/160 (77%)	104 (85%)	14 (11%)	5 (4%)	2	19
1	J	137/160 (86%)	118 (86%)	13 (10%)	6 (4%)	2	17
1	K	111/160 (69%)	99 (89%)	10 (9%)	2 (2%)	6	34
1	L	139/160 (87%)	119 (86%)	15 (11%)	5 (4%)	2	22
1	M	123/160 (77%)	106 (86%)	12 (10%)	5 (4%)	2	19
1	N	137/160 (86%)	119 (87%)	13 (10%)	5 (4%)	2	22
1	O	112/160 (70%)	101 (90%)	9 (8%)	2 (2%)	6	34
1	P	137/160 (86%)	120 (88%)	11 (8%)	6 (4%)	2	17
1	Q	118/160 (74%)	101 (86%)	14 (12%)	3 (2%)	4	28
1	R	135/160 (84%)	116 (86%)	15 (11%)	4 (3%)	3	25
1	S	122/160 (76%)	106 (87%)	12 (10%)	4 (3%)	3	23
1	T	139/160 (87%)	120 (86%)	12 (9%)	7 (5%)	1	15
1	U	117/160 (73%)	100 (86%)	14 (12%)	3 (3%)	4	27
1	V	124/160 (78%)	105 (85%)	13 (10%)	6 (5%)	2	16
1	W	117/160 (73%)	101 (86%)	13 (11%)	3 (3%)	4	27
1	X	137/160 (86%)	118 (86%)	13 (10%)	6 (4%)	2	17
All	All	3076/3840 (80%)	2651 (86%)	316 (10%)	109 (4%)	3	23

All (109) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	SER
1	A	87	THR
1	B	128	SER
1	B	141	GLY
1	B	158	ASN
1	C	52	LYS
1	D	141	GLY
1	E	86	SER
1	F	141	GLY
1	G	87	THR
1	H	153	ARG
1	I	86	SER
1	J	16	VAL
1	J	141	GLY
1	M	87	THR
1	N	141	GLY
1	Q	53	THR
1	S	87	THR
1	T	87	THR
1	U	87	THR
1	V	44	THR
1	W	46	SER
1	X	76	LEU
1	A	75	GLY
1	B	75	GLY
1	C	75	GLY
1	C	86	SER
1	D	75	GLY
1	D	87	THR
1	E	75	GLY
1	F	75	GLY
1	G	75	GLY
1	G	86	SER
1	H	75	GLY
1	H	141	GLY
1	I	52	LYS
1	I	75	GLY
1	I	87	THR
1	J	75	GLY
1	K	75	GLY
1	L	75	GLY
1	L	141	GLY

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Mol	Chain	Res	Type
1	M	75	GLY
1	M	86	SER
1	N	75	GLY
1	O	75	GLY
1	P	75	GLY
1	P	141	GLY
1	P	149	ASP
1	Q	75	GLY
1	R	75	GLY
1	R	83	PRO
1	S	75	GLY
1	S	86	SER
1	T	75	GLY
1	T	141	GLY
1	U	75	GLY
1	V	75	GLY
1	V	141	GLY
1	W	75	GLY
1	X	75	GLY
1	X	141	GLY
1	B	149	ASP
1	C	87	THR
1	D	149	ASP
1	H	149	ASP
1	J	149	ASP
1	L	149	ASP
1	N	149	ASP
1	P	93	ASP
1	T	143	SER
1	T	149	ASP
1	B	143	SER
1	C	138	CYS
1	D	138	CYS
1	E	138	CYS
1	F	138	CYS
1	F	149	ASP
1	G	138	CYS
1	I	138	CYS
1	J	143	SER
1	K	138	CYS
1	M	46	SER
1	M	138	CYS

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Mol	Chain	Res	Type
1	N	138	CYS
1	P	138	CYS
1	R	138	CYS
1	R	149	ASP
1	S	138	CYS
1	U	138	CYS
1	V	143	SER
1	V	149	ASP
1	W	138	CYS
1	X	143	SER
1	X	149	ASP
1	A	138	CYS
1	B	138	CYS
1	H	138	CYS
1	J	138	CYS
1	L	138	CYS
1	L	143	SER
1	N	143	SER
1	O	138	CYS
1	P	143	SER
1	Q	138	CYS
1	T	93	ASP
1	T	138	CYS
1	V	138	CYS
1	X	138	CYS

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	115/145 (79%)	114 (99%)	1 (1%)	70	76
1	B	129/145 (89%)	120 (93%)	9 (7%)	14	39
1	C	117/145 (81%)	117 (100%)	0	100	100
1	D	135/145 (93%)	130 (96%)	5 (4%)	30	56
1	E	116/145 (80%)	113 (97%)	3 (3%)	40	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	127/145 (88%)	123 (97%)	4 (3%)	35	59
1	G	117/145 (81%)	115 (98%)	2 (2%)	53	70
1	H	132/145 (91%)	126 (96%)	6 (4%)	24	50
1	I	116/145 (80%)	112 (97%)	4 (3%)	32	57
1	J	130/145 (90%)	125 (96%)	5 (4%)	29	55
1	K	110/145 (76%)	109 (99%)	1 (1%)	70	76
1	L	131/145 (90%)	121 (92%)	10 (8%)	12	37
1	M	116/145 (80%)	114 (98%)	2 (2%)	53	70
1	N	130/145 (90%)	124 (95%)	6 (5%)	24	50
1	O	110/145 (76%)	107 (97%)	3 (3%)	39	62
1	P	130/145 (90%)	125 (96%)	5 (4%)	29	55
1	Q	113/145 (78%)	113 (100%)	0	100	100
1	R	128/145 (88%)	123 (96%)	5 (4%)	28	54
1	S	115/145 (79%)	115 (100%)	0	100	100
1	T	132/145 (91%)	125 (95%)	7 (5%)	20	47
1	U	114/145 (79%)	111 (97%)	3 (3%)	40	62
1	V	121/145 (83%)	115 (95%)	6 (5%)	22	48
1	W	112/145 (77%)	110 (98%)	2 (2%)	51	69
1	X	130/145 (90%)	125 (96%)	5 (4%)	29	55
All	All	2926/3480 (84%)	2832 (97%)	94 (3%)	34	59

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	GLN
1	B	17	ILE
1	B	52	LYS
1	B	68	LYS
1	B	129	GLN
1	B	140	GLN
1	B	145	MSE
1	B	157	SER
1	B	158	ASN
1	B	159	LEU
1	D	17	ILE

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Mol	Chain	Res	Type
1	D	52	LYS
1	D	54	SER
1	D	145	MSE
1	D	158	ASN
1	E	54	SER
1	E	55	CYS
1	E	91	THR
1	F	54	SER
1	F	140	GLN
1	F	149	ASP
1	F	158	ASN
1	G	54	SER
1	G	91	THR
1	H	17	ILE
1	H	52	LYS
1	H	54	SER
1	H	91	THR
1	H	145	MSE
1	H	157	SER
1	I	41	PHE
1	I	52	LYS
1	I	91	THR
1	I	129	GLN
1	J	47	LYS
1	J	54	SER
1	J	140	GLN
1	J	145	MSE
1	J	158	ASN
1	K	55	CYS
1	L	16	VAL
1	L	17	ILE
1	L	52	LYS
1	L	54	SER
1	L	85	LYS
1	L	91	THR
1	L	129	GLN
1	L	140	GLN
1	L	145	MSE
1	L	157	SER
1	M	88	PHE
1	M	93	ASP
1	N	17	ILE

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Mol	Chain	Res	Type
1	N	52	LYS
1	N	54	SER
1	N	145	MSE
1	N	158	ASN
1	N	159	LEU
1	O	54	SER
1	O	91	THR
1	O	129	GLN
1	P	17	ILE
1	P	52	LYS
1	P	54	SER
1	P	157	SER
1	P	158	ASN
1	R	17	ILE
1	R	52	LYS
1	R	139	VAL
1	R	145	MSE
1	R	158	ASN
1	T	17	ILE
1	T	52	LYS
1	T	54	SER
1	T	145	MSE
1	T	149	ASP
1	T	157	SER
1	T	158	ASN
1	U	45	ASN
1	U	47	LYS
1	U	53	THR
1	V	17	ILE
1	V	54	SER
1	V	129	GLN
1	V	140	GLN
1	V	149	ASP
1	V	158	ASN
1	W	54	SER
1	W	129	GLN
1	X	17	ILE
1	X	52	LYS
1	X	54	SER
1	X	140	GLN
1	X	158	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (139)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	43	HIS
1	A	45	ASN
1	A	69	GLN
1	A	73	ASN
1	A	121	GLN
1	A	123	HIS
1	A	127	GLN
1	B	28	ASN
1	B	69	GLN
1	B	73	ASN
1	B	121	GLN
1	C	28	ASN
1	C	69	GLN
1	C	73	ASN
1	C	121	GLN
1	C	123	HIS
1	C	127	GLN
1	D	28	ASN
1	D	69	GLN
1	D	73	ASN
1	D	121	GLN
1	D	127	GLN
1	D	158	ASN
1	E	28	ASN
1	E	43	HIS
1	E	69	GLN
1	E	73	ASN
1	E	121	GLN
1	E	123	HIS
1	E	127	GLN
1	F	28	ASN
1	F	69	GLN
1	F	73	ASN
1	F	121	GLN
1	F	127	GLN
1	F	158	ASN
1	G	28	ASN
1	G	43	HIS
1	G	69	GLN
1	G	73	ASN
1	G	121	GLN

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Mol	Chain	Res	Type
1	G	123	HIS
1	G	127	GLN
1	H	28	ASN
1	H	69	GLN
1	H	73	ASN
1	H	121	GLN
1	H	127	GLN
1	I	28	ASN
1	I	69	GLN
1	I	73	ASN
1	I	121	GLN
1	I	123	HIS
1	I	127	GLN
1	J	28	ASN
1	J	69	GLN
1	J	73	ASN
1	J	121	GLN
1	J	127	GLN
1	J	158	ASN
1	K	28	ASN
1	K	69	GLN
1	K	73	ASN
1	K	121	GLN
1	K	123	HIS
1	K	129	GLN
1	L	28	ASN
1	L	69	GLN
1	L	73	ASN
1	L	121	GLN
1	L	127	GLN
1	M	28	ASN
1	M	45	ASN
1	M	69	GLN
1	M	73	ASN
1	M	121	GLN
1	N	28	ASN
1	N	69	GLN
1	N	73	ASN
1	N	121	GLN
1	N	127	GLN
1	O	28	ASN
1	O	69	GLN

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Mol	Chain	Res	Type
1	O	73	ASN
1	O	121	GLN
1	O	123	HIS
1	O	127	GLN
1	P	28	ASN
1	P	69	GLN
1	P	73	ASN
1	P	121	GLN
1	P	127	GLN
1	Q	27	GLN
1	Q	28	ASN
1	Q	69	GLN
1	Q	73	ASN
1	Q	121	GLN
1	Q	123	HIS
1	R	28	ASN
1	R	45	ASN
1	R	69	GLN
1	R	73	ASN
1	R	121	GLN
1	R	127	GLN
1	S	28	ASN
1	S	43	HIS
1	S	69	GLN
1	S	73	ASN
1	S	121	GLN
1	S	123	HIS
1	S	127	GLN
1	T	28	ASN
1	T	69	GLN
1	T	73	ASN
1	T	121	GLN
1	T	127	GLN
1	T	140	GLN
1	U	28	ASN
1	U	69	GLN
1	U	73	ASN
1	U	121	GLN
1	U	123	HIS
1	V	28	ASN
1	V	69	GLN
1	V	73	ASN

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Mol	Chain	Res	Type
1	V	121	GLN
1	V	158	ASN
1	W	28	ASN
1	W	69	GLN
1	W	73	ASN
1	W	121	GLN
1	W	123	HIS
1	W	127	GLN
1	X	28	ASN
1	X	69	GLN
1	X	121	GLN
1	X	127	GLN
1	X	158	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	124/160 (77%)	0.03	3 (2%) 59 35	63, 95, 159, 217	0
1	B	138/160 (86%)	0.24	3 (2%) 62 37	68, 120, 173, 184	0
1	C	126/160 (78%)	0.17	3 (2%) 59 35	68, 104, 170, 206	0
1	D	145/160 (90%)	0.10	4 (2%) 55 32	66, 110, 165, 201	0
1	E	125/160 (78%)	-0.05	0 100 100	71, 105, 177, 217	0
1	F	136/160 (85%)	0.10	1 (0%) 84 63	78, 131, 170, 180	0
1	G	126/160 (78%)	0.08	2 (1%) 70 45	60, 97, 173, 212	0
1	H	142/160 (88%)	0.01	2 (1%) 73 48	64, 102, 154, 215	0
1	I	125/160 (78%)	0.04	3 (2%) 59 35	60, 94, 159, 204	0
1	J	139/160 (86%)	0.09	2 (1%) 73 48	64, 105, 154, 186	0
1	K	117/160 (73%)	-0.02	0 100 100	72, 103, 155, 194	0
1	L	141/160 (88%)	0.05	2 (1%) 73 48	69, 121, 167, 188	0
1	M	125/160 (78%)	-0.00	1 (0%) 82 60	74, 105, 169, 220	0
1	N	139/160 (86%)	0.15	3 (2%) 62 37	79, 135, 177, 195	0
1	O	118/160 (73%)	0.09	1 (0%) 82 60	77, 108, 165, 182	0
1	P	139/160 (86%)	0.33	7 (5%) 34 19	65, 122, 164, 200	0
1	Q	122/160 (76%)	-0.02	0 100 100	66, 100, 167, 205	0
1	R	137/160 (85%)	0.28	5 (3%) 46 25	70, 119, 166, 199	0
1	S	124/160 (77%)	0.02	3 (2%) 59 35	90, 123, 191, 211	0
1	T	141/160 (88%)	0.31	1 (0%) 84 63	92, 147, 184, 200	0
1	U	121/160 (75%)	0.07	1 (0%) 82 60	86, 120, 169, 193	0
1	V	128/160 (80%)	0.22	2 (1%) 70 45	92, 148, 185, 204	0
1	W	121/160 (75%)	0.00	0 100 100	87, 122, 173, 199	0
1	X	139/160 (86%)	0.16	2 (1%) 73 48	86, 131, 187, 206	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	3138/3840 (81%)	0.11	51 (1%) 70 45	60, 116, 176, 220	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	51	ALA	4.9
1	R	159	LEU	4.2
1	O	51	ALA	4.2
1	P	159	LEU	4.0
1	N	159	LEU	3.5
1	B	128	SER	3.4
1	P	75	GLY	3.2
1	C	128	SER	3.1
1	U	128	SER	3.1
1	P	76	LEU	3.0
1	J	159	LEU	3.0
1	N	76	LEU	2.9
1	P	53	THR	2.9
1	V	159	LEU	2.9
1	A	51	ALA	2.7
1	L	159	LEU	2.5
1	V	32	TRP	2.5
1	B	54	SER	2.5
1	L	85	LYS	2.5
1	S	51	ALA	2.4
1	P	85	LYS	2.4
1	A	53	THR	2.4
1	B	159	LEU	2.4
1	D	89	PHE	2.3
1	H	159	LEU	2.3
1	X	85	LYS	2.3
1	I	128	SER	2.3
1	D	159	LEU	2.3
1	A	46	SER	2.3
1	C	89	PHE	2.3
1	P	86	SER	2.3
1	D	90	GLY	2.3
1	H	68	LYS	2.3
1	R	75	GLY	2.3
1	X	33	ASN	2.2
1	R	84	GLY	2.2
1	S	88	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	138	CYS	2.2
1	P	32	TRP	2.1
1	J	16	VAL	2.1
1	G	87	THR	2.1
1	G	41	PHE	2.1
1	T	51	ALA	2.1
1	R	16	VAL	2.1
1	I	85	LYS	2.1
1	D	77	VAL	2.1
1	N	23	ASP	2.0
1	S	89	PHE	2.0
1	R	77	VAL	2.0
1	M	30	GLY	2.0
1	F	159	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.