Full wwPDB X-ray Structure Validation Report (i)

Nov 16, 2023 – 03:45 AM JST

PDB ID	:	6KOI
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 (i) 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 (1)) were used in the production of this report:

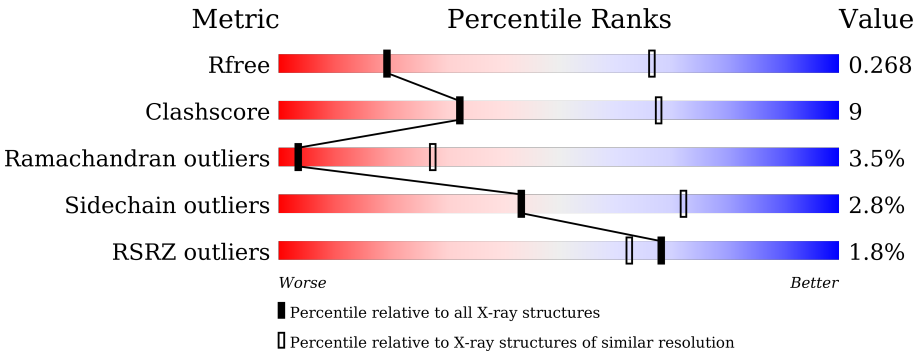
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 <=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	61% 14% 22%
1	B	160	2% 66% 16% 12%
1	C	160	2% 62% 16% 21%
1	D	160	% 70% 17% 5% 8%
1	E	160	2% 62% 14% 22%
1	F	160	2% 64% 19% 14%

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Mol	Chain	Length	Quality of chain
1	G	160	2% 62% 15% 21%
1	H	160	67% 18% 5% 10%
1	I	160	63% 12% 22%
1	J	160	65% 19% 12%
1	K	160	61% 12% 27%
1	L	160	69% 16% 11%
1	M	160	64% 11% 22%
1	N	160	71% 16% 12%
1	O	160	62% 12% 26%
1	P	160	3% 69% 16% 12%
1	Q	160	62% 14% 24%
1	R	160	2% 65% 20% 13%
1	S	160	65% 12% 22%
1	T	160	68% 16% 6% 11%
1	U	160	61% 14% 24%
1	V	160	6% 65% 13% 19%
1	W	160	2% 62% 13% 24%
1	X	160	4% 62% 24% 12%

2 Entry composition (i)

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

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

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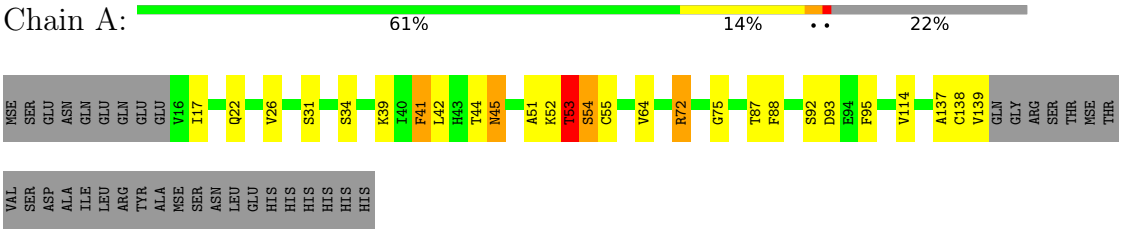
Chain	Residue	Modelled	Actual	Comment	Reference
X	166	HIS	-	expression tag	UNP Q9Y5W9

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.

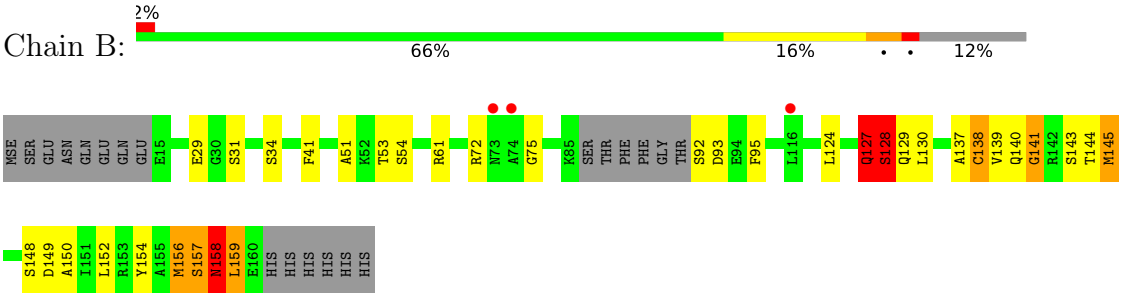
• Molecule 1: Sorting nexin-11

Chain A:



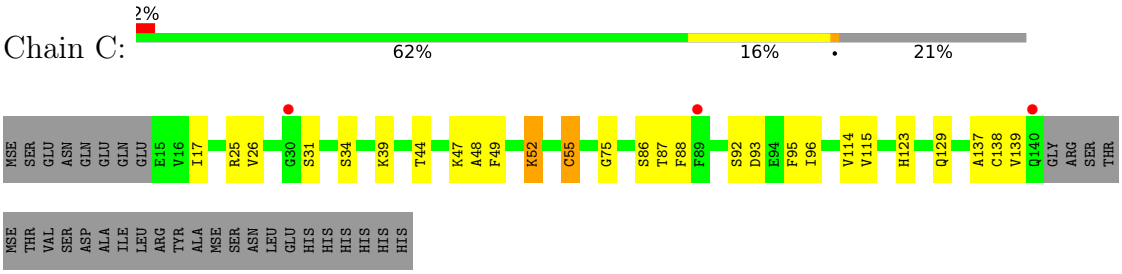
• Molecule 1: Sorting nexin-11

Chain B:



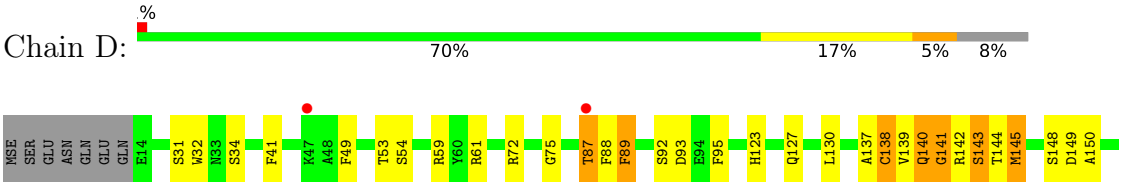
• Molecule 1: Sorting nexin-11

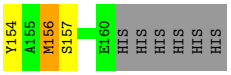
Chain C:



• Molecule 1: Sorting nexin-11

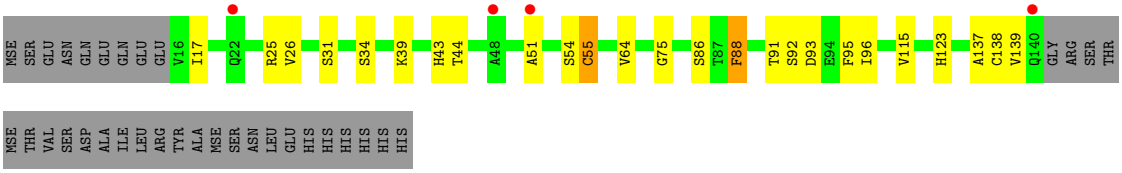
Chain D:





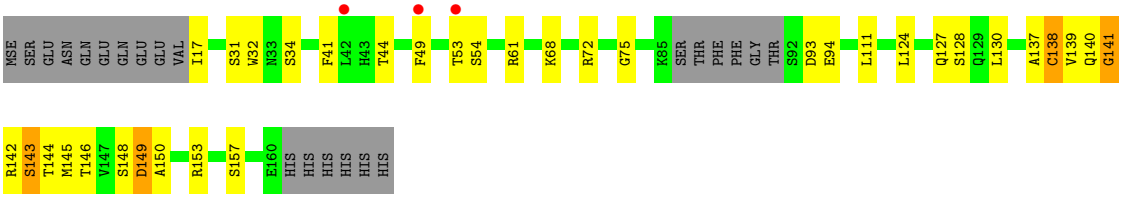
• Molecule 1: Sorting nexin-11

Chain E:



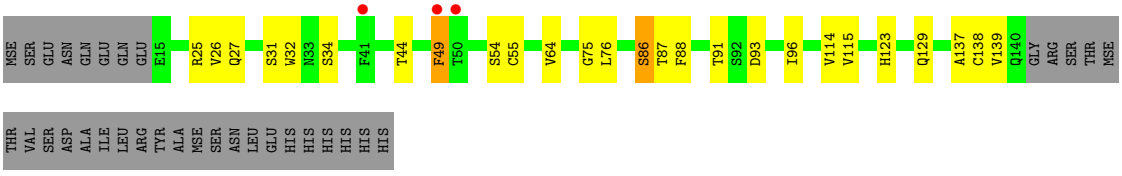
• Molecule 1: Sorting nexin-11

Chain F:



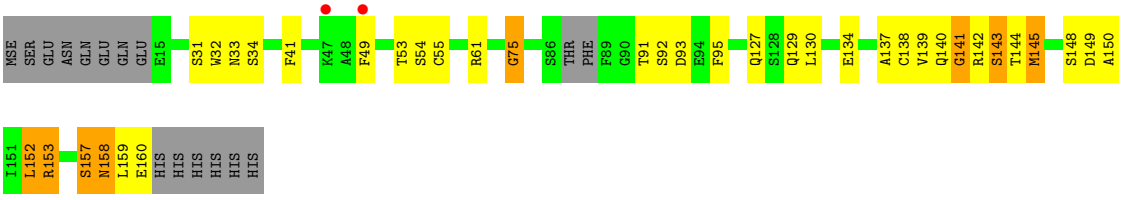
• Molecule 1: Sorting nexin-11

Chain G:



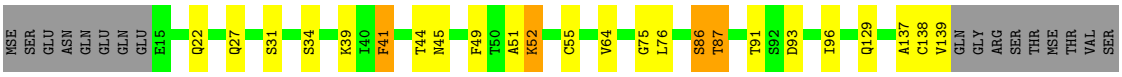
• Molecule 1: Sorting nexin-11

Chain H:



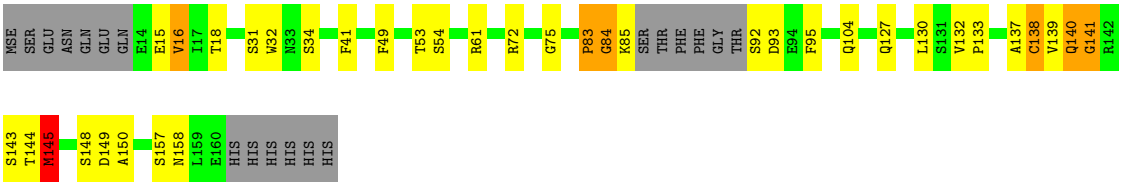
• Molecule 1: Sorting nexin-11

Chain I:



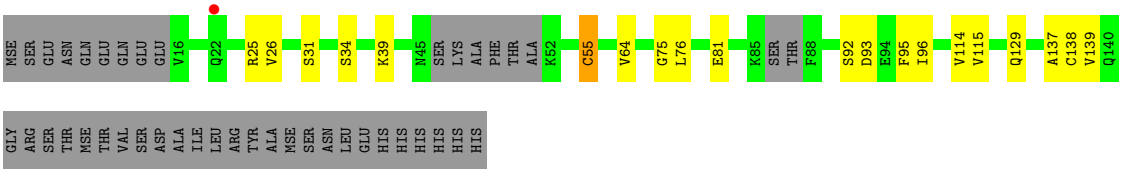
• Molecule 1: Sorting nexin-11

Chain J:



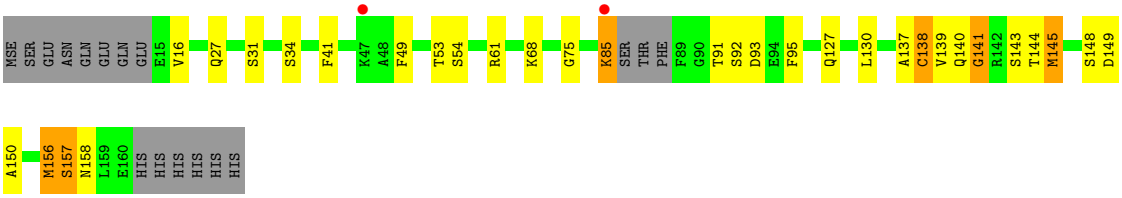
• Molecule 1: Sorting nexin-11

Chain K:



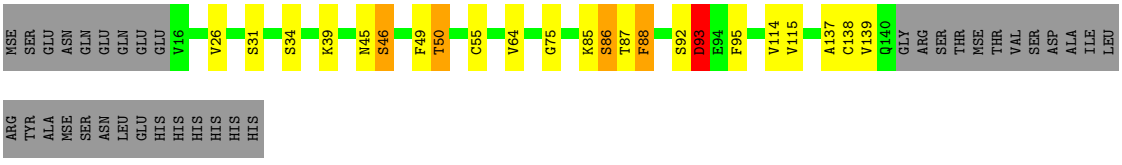
• Molecule 1: Sorting nexin-11

Chain L:



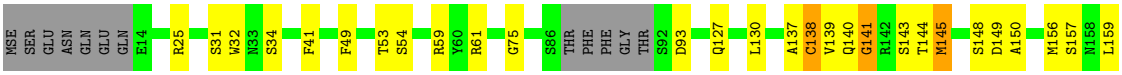
• Molecule 1: Sorting nexin-11

Chain M:



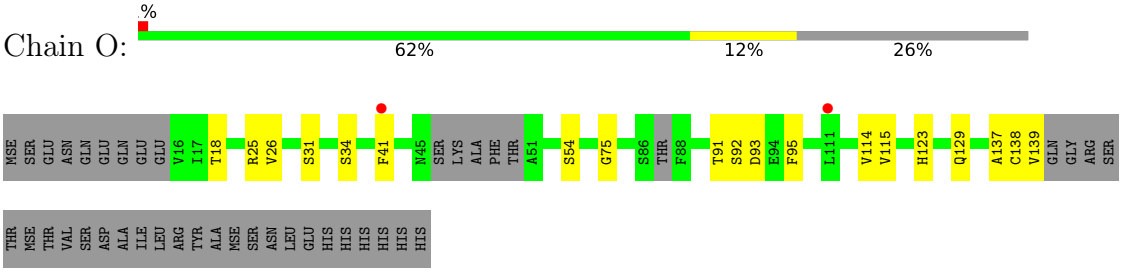
• Molecule 1: Sorting nexin-11

Chain N:



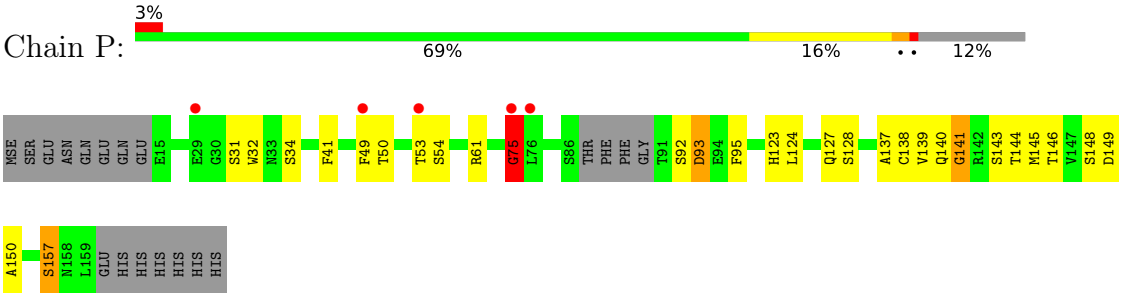
• Molecule 1: Sorting nexin-11

Chain O:



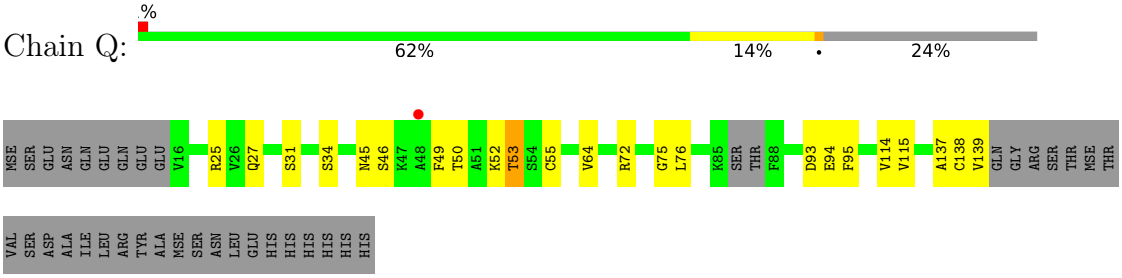
• Molecule 1: Sorting nexin-11

Chain P:



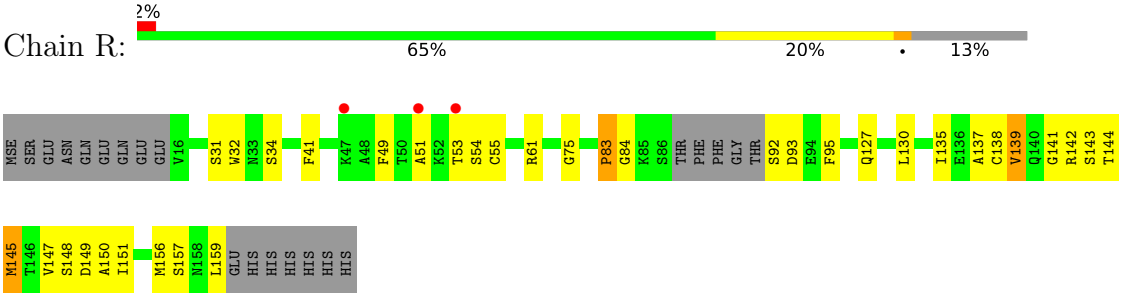
• Molecule 1: Sorting nexin-11

Chain Q:



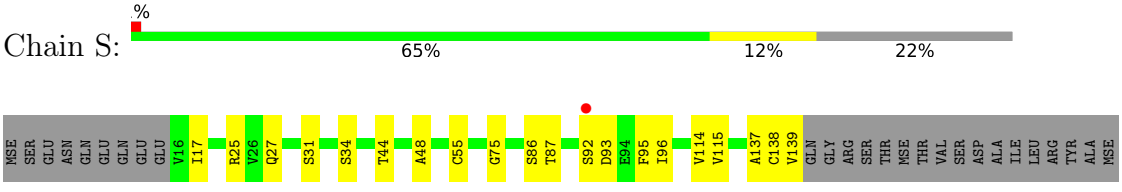
• Molecule 1: Sorting nexin-11

Chain R:



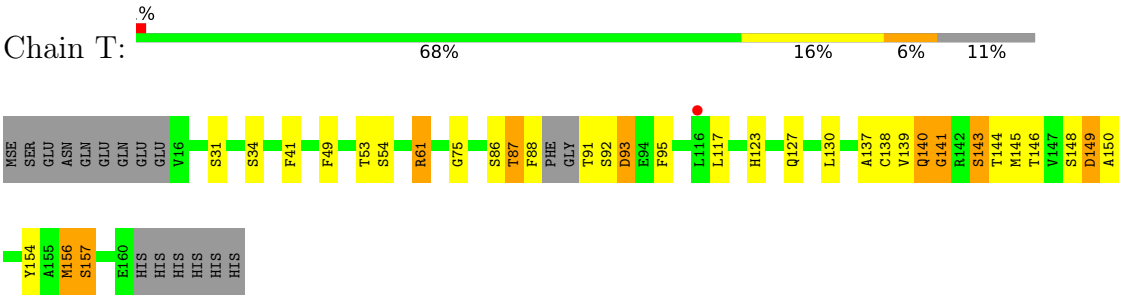
• Molecule 1: Sorting nexin-11

Chain S:



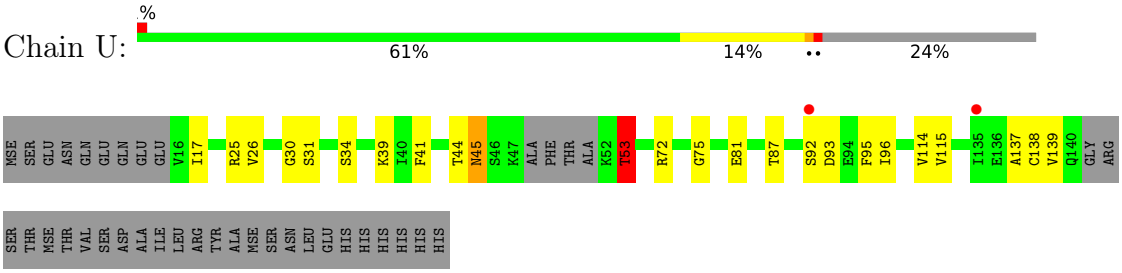
• Molecule 1: Sorting nexin-11

Chain T:



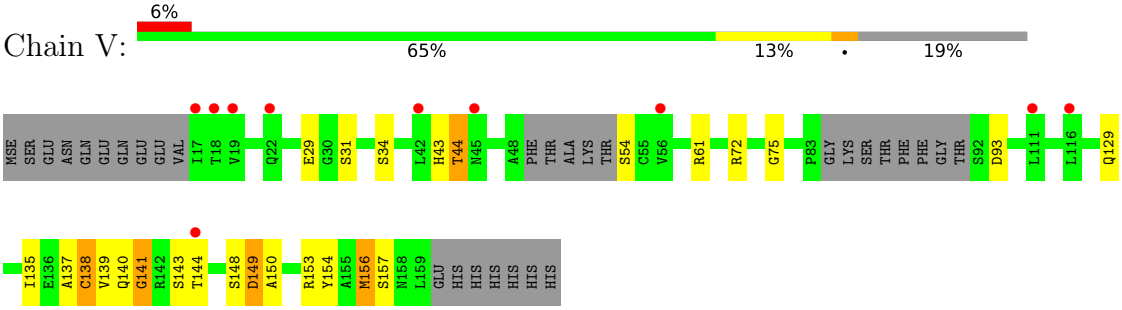
• Molecule 1: Sorting nexin-11

Chain U:



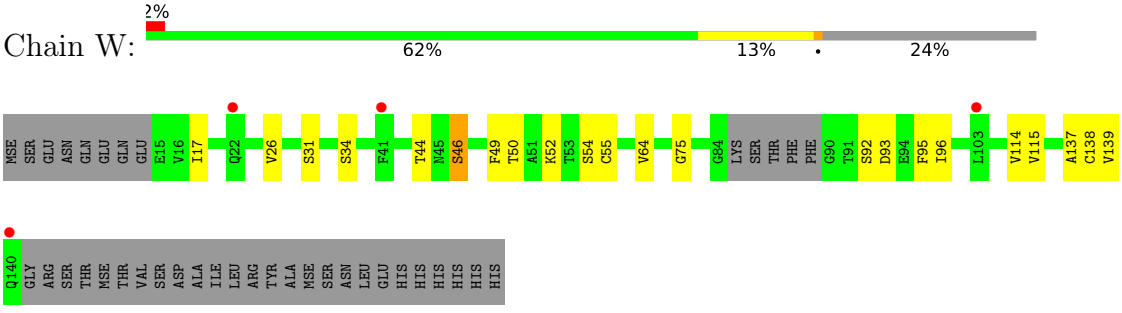
• Molecule 1: Sorting nexin-11

Chain V:



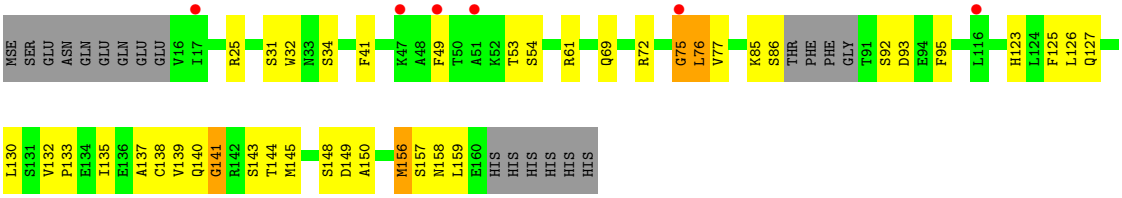
• Molecule 1: Sorting nexin-11

Chain W:



• Molecule 1: Sorting nexin-11

Chain X:


MSE SER GLU ASN GLN GLU GLN GLU GLU V16 I17 R25 S31 W32 N33 S34 F41 K47 A48 F49 T50 A51 K52 T53 S54 R61 Q69 R72 G75 L76 V77 K85 S86 THR PHE PHE GLY T91 S92 D93 E94 F95 L116 H123 L124 F125 L126 Q127
L130 S131 V132 P133 E134 I135 E136 A137 C138 V139 Q140 G141 R142 S143 T144 M145 S148 D149 A150 M156 S157 N158 L159 E160 HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

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 65.79 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (65.87-3.50) 99.1 (65.79-3.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (4.85%)	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)	0.33 , 79.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.95	4/1040 (0.4%)	1.22	6/1406 (0.4%)
1	B	0.67	0/1160	0.94	5/1562 (0.3%)
1	C	0.69	0/1058	0.89	2/1430 (0.1%)
1	D	0.68	0/1218	0.90	5/1642 (0.3%)
1	E	0.69	0/1049	0.84	0/1418
1	F	0.68	0/1144	0.84	2/1540 (0.1%)
1	G	0.66	0/1058	0.82	0/1430
1	H	0.72	1/1189 (0.1%)	0.92	4/1601 (0.2%)
1	I	0.69	1/1049 (0.1%)	0.89	3/1418 (0.2%)
1	J	0.71	1/1169 (0.1%)	0.86	5/1574 (0.3%)
1	K	0.67	0/990	0.78	0/1335
1	L	0.69	1/1183 (0.1%)	0.86	3/1593 (0.2%)
1	M	0.72	2/1049 (0.2%)	0.85	1/1418 (0.1%)
1	N	0.68	0/1166	0.80	1/1570 (0.1%)
1	O	0.65	0/992	0.79	1/1338 (0.1%)
1	P	0.70	1/1164 (0.1%)	0.83	1/1568 (0.1%)
1	Q	0.70	1/1026 (0.1%)	0.82	1/1385 (0.1%)
1	R	0.69	0/1148	0.84	1/1546 (0.1%)
1	S	0.67	0/1040	0.80	0/1406
1	T	0.67	0/1183	0.88	4/1594 (0.3%)
1	U	0.69	0/1019	0.87	3/1375 (0.2%)
1	V	0.66	0/1081	0.92	4/1455 (0.3%)
1	W	0.68	0/1011	0.83	0/1366
1	X	0.70	0/1164	0.80	2/1568 (0.1%)
All	All	0.70	12/26350 (0.0%)	0.87	54/35538 (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	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 (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	72	ARG	CZ-NH2	10.74	1.47	1.33
1	A	72	ARG	CZ-NH1	9.97	1.46	1.33
1	A	72	ARG	NE-CZ	8.87	1.44	1.33
1	A	72	ARG	CG-CD	7.93	1.71	1.51
1	H	75	GLY	C-O	-5.99	1.14	1.23
1	I	45	ASN	C-O	5.99	1.34	1.23
1	M	50	THR	C-O	5.97	1.34	1.23
1	J	84	GLY	C-O	-5.86	1.14	1.23
1	Q	45	ASN	C-O	5.54	1.33	1.23
1	L	27	GLN	C-O	5.46	1.33	1.23
1	P	75	GLY	C-O	-5.23	1.15	1.23
1	M	46	SER	CA-CB	-5.17	1.45	1.52

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	72	ARG	NE-CZ-NH1	-26.54	107.03	120.30
1	A	72	ARG	NE-CZ-NH2	12.23	126.42	120.30
1	B	128	SER	N-CA-CB	11.80	128.19	110.50
1	V	72	ARG	NE-CZ-NH2	-10.24	115.18	120.30
1	A	72	ARG	CD-NE-CZ	-9.26	110.64	123.60
1	A	54	SER	N-CA-CB	8.96	123.94	110.50
1	V	43	HIS	C-N-CA	8.78	143.64	121.70
1	D	156	MSE	CG-SE-CE	8.60	117.82	98.90
1	D	143	SER	C-N-CA	8.04	141.80	121.70
1	H	143	SER	C-N-CA	8.03	141.78	121.70
1	F	143	SER	C-N-CA	8.00	141.69	121.70
1	V	44	THR	CA-CB-CG2	7.91	123.47	112.40
1	C	48	ALA	N-CA-CB	7.85	121.09	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	U	45	ASN	CB-CA-C	7.33	125.06	110.40
1	H	145	MSE	CG-SE-CE	7.24	114.83	98.90
1	D	72	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	B	156	MSE	CG-SE-CE	6.81	113.88	98.90
1	R	145	MSE	CG-SE-CE	6.81	113.87	98.90
1	B	127	GLN	N-CA-C	-6.72	92.85	111.00
1	X	156	MSE	CG-SE-CE	6.72	113.69	98.90
1	A	53	THR	CB-CA-C	6.71	129.72	111.60
1	J	72	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	D	145	MSE	CG-SE-CE	6.65	113.53	98.90
1	J	145	MSE	CG-SE-CE	6.61	113.44	98.90
1	L	156	MSE	CG-SE-CE	6.57	113.36	98.90
1	M	93	ASP	CB-CG-OD1	-6.51	112.44	118.30
1	U	53	THR	CA-CB-OG1	6.43	122.50	109.00
1	L	27	GLN	N-CA-C	6.42	128.34	111.00
1	B	72	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	B	145	MSE	CG-SE-CE	6.26	112.68	98.90
1	T	140	GLN	CB-CA-C	6.26	122.91	110.40
1	I	51	ALA	C-N-CA	6.05	136.84	121.70
1	U	72	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	L	145	MSE	CG-SE-CE	5.84	111.75	98.90
1	I	49	PHE	C-N-CA	5.71	135.97	121.70
1	T	145	MSE	CG-SE-CE	5.62	111.25	98.90
1	J	83	PRO	CA-C-O	-5.60	106.75	120.20
1	H	143	SER	O-C-N	5.59	131.65	122.70
1	D	143	SER	O-C-N	5.46	131.44	122.70
1	A	51	ALA	N-CA-CB	5.44	117.72	110.10
1	T	140	GLN	N-CA-CB	-5.39	100.89	110.60
1	C	52	LYS	N-CA-C	5.38	125.52	111.00
1	J	18	THR	CA-CB-OG1	5.38	120.29	109.00
1	V	156	MSE	CG-SE-CE	5.35	110.67	98.90
1	J	83	PRO	CA-C-N	5.30	126.80	116.20
1	X	145	MSE	CG-SE-CE	5.27	110.50	98.90
1	N	156	MSE	CG-SE-CE	5.23	110.41	98.90
1	T	156	MSE	CG-SE-CE	5.21	110.36	98.90
1	F	143	SER	O-C-N	5.18	130.99	122.70
1	P	145	MSE	CG-SE-CE	5.13	110.20	98.90
1	I	52	LYS	N-CA-CB	5.09	119.76	110.60
1	Q	72	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	H	152	LEU	N-CA-C	-5.08	97.27	111.00
1	O	18	THR	CA-CB-OG1	5.04	119.58	109.00

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	Peptide,Mainchain
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	Peptide,Mainchain
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	20	0
1	B	1142	0	1154	24	0
1	C	1036	0	1042	33	0
1	D	1197	0	1201	42	0
1	E	1027	0	1036	27	0
1	F	1126	0	1139	37	0
1	G	1036	0	1042	25	0
1	H	1170	0	1178	36	0
1	I	1027	0	1034	19	0
1	J	1151	0	1160	31	1
1	K	971	0	978	27	0
1	L	1164	0	1173	32	0
1	M	1027	0	1036	19	0
1	N	1148	0	1159	21	1
1	O	973	0	980	12	0
1	P	1146	0	1160	21	1
1	Q	1005	0	1015	23	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	1130	0	1147	40	0
1	S	1018	0	1028	25	0
1	T	1164	0	1176	38	0
1	U	999	0	1009	23	0
1	V	1065	0	1075	27	0
1	W	992	0	998	20	0
1	X	1146	0	1160	38	0
All	All	25878	0	26108	457	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 9.

All (457) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:R:139:VAL:O	1:R:139:VAL:HG23	1.86	0.74
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:R:147:VAL:CB	1:R:151:ILE:HD11	2.27	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:A:41:PHE:CE1	1:A:55:CYS:SG	2.94	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:L:61:ARG:HD3	1:V:157:SER:OG	2.01	0.60
1:J:144:THR:O	1:J:144:THR:HG22	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:U:95:PHE:CD2	1:V:156:MSE:HE2	2.37	0.56
1:H:148:SER:C	1:H:150:ALA:H	2.08	0.56
1:R:147:VAL:HB	1:R:151:ILE:CD1	2.30	0.56
1:J:148:SER:C	1:J:150:ALA:H	2.09	0.56
1:N:148:SER:C	1:N:150:ALA:H	2.09	0.56
1:X:148:SER:C	1:X:150:ALA:H	2.09	0.56
1:F:148:SER:C	1:F:150:ALA:H	2.09	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:B:148:SER:C	1:B:150:ALA:H	2.09	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:T:148:SER:C	1:T:150:ALA:H	2.09	0.56
1:V:135:ILE:O	1:V:139:VAL:HG12	2.05	0.56
1:D:148:SER:C	1:D:150:ALA:H	2.09	0.56
1:Q:27:GLN:HE22	1:R:141:GLY:CA	2.19	0.56
1:L:148:SER:C	1:L:150:ALA:H	2.10	0.55
1:P:148:SER:C	1:P:150:ALA:H	2.10	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:V:148:SER:C	1:V:150:ALA:H	2.08	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:R:148:SER:C	1:R:150:ALA:H	2.09	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:125:PHE:HD1	1:X:126:LEU:HD12	1.75	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: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:B:159:LEU:HD12	1:D:59:ARG:HH12	1.75	0.51
1:R:141:GLY:C	1:R:143:SER:H	2.15	0.50
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:S:114:VAL:HG12	1:U:115:VAL:CG2	2.42	0.50
1:Q:27:GLN:HE22	1:R:141:GLY:N	2.10	0.50
1:U:96:ILE:HD11	1:V:156:MSE:HE3	1.95	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:S:27:GLN:CD	1:T:140:GLN:HB3	2.35	0.46
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:C:137:ALA:C	1:C:139:VAL:H	2.19	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:G:137:ALA:C	1:G:139:VAL:H	2.19	0.46
1:R:49:PHE:HB3	1:R:127:GLN:HE22	1.80	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:J:137:ALA:C	1:J:139:VAL:H	2.19	0.46
1:N:140:GLN:O	1:N:141:GLY:O	2.34	0.46
1:W:137:ALA:C	1:W:139:VAL:H	2.19	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:R:139:VAL:O	1:R:139:VAL:CG2	2.56	0.46
1:T:140:GLN:O	1:T:141:GLY:O	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:140:GLN:O	1:L:141:GLY:O	2.34	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
1:F:144:THR:O	1:F:144:THR:CG2	2.64	0.45
1:M:49:PHE:CD2	1:M:50:THR:HG23	2.51	0.45
1:N:137:ALA:C	1:N:139:VAL:H	2.20	0.45
1:T:88:PHE:O	1:T:91:THR:CG2	2.61	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:M:137:ALA:C	1:M:139:VAL:H	2.20	0.45
1:A:44:THR:CG2	1:A:52:LYS:HB2	2.46	0.45
1:P:137:ALA:C	1:P:139:VAL:H	2.20	0.45
1:X:75:GLY:C	1:X:77:VAL:N	2.68	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:U:137:ALA:C	1:U:139:VAL:H	2.19	0.45
1:C:31:SER:O	1:C:34:SER:HB2	2.17	0.45
1:E:137:ALA:C	1:E:139:VAL:H	2.19	0.45
1:G:123:HIS:HD2	1:K:76:LEU:HD12	1.81	0.45
1:I:137:ALA:C	1:I:139:VAL:H	2.20	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:V:137:ALA:C	1:V:139:VAL:H	2.20	0.45
1:B:137:ALA:C	1:B:139:VAL:H	2.20	0.45
1:D:31:SER:O	1:D:34:SER:HB2	2.17	0.45
1:D:137:ALA:C	1:D:139:VAL:H	2.20	0.45
1:L:49:PHE:HB3	1:L:127:GLN:HE22	1.81	0.45
1:X:137:ALA:C	1:X:139:VAL:H	2.20	0.45
1:K:31:SER:O	1:K:34:SER:HB2	2.17	0.45
1:K:137:ALA:C	1:K:139:VAL:H	2.19	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: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:H:137:ALA:C	1:H:139:VAL:H	2.20	0.44
1:M:31:SER:O	1:M:34:SER:HB2	2.17	0.44
1:T:137:ALA:C	1:T:139:VAL:H	2.20	0.44
1:X:31:SER:O	1:X:34:SER:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:115:VAL:CG2	1:W:114:VAL:HG12	2.46	0.44
1:S:137:ALA:C	1:S:139:VAL:H	2.20	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:J:84:GLY:O	1:J:85:LYS:C	2.56	0.44
1:N:31:SER:O	1:N:34:SER:HB2	2.17	0.44
1:O:137:ALA:C	1:O:139:VAL:H	2.20	0.44
1:Q:137:ALA:C	1:Q:139:VAL:H	2.20	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: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: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: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:A:137:ALA:C	1:A:139:VAL:H	2.21	0.43
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:L:137:ALA:C	1:L:139:VAL:H	2.20	0.43
1:U:31:SER:O	1:U:34:SER:HB2	2.17	0.43
1:F:137:ALA:C	1:F:139:VAL:H	2.20	0.43
1:R:137:ALA:C	1:R:139:VAL:H	2.20	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: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:C:55:CYS:O	1:C:129:GLN:NE2	2.51	0.43
1:F:31:SER:O	1:F:34:SER:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:PHE:HE1	1:B:53:THR:HG23	1.83	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:N:41:PHE:HE1	1:N:53:THR:HG23	1.84	0.43
1:R:141:GLY:C	1:R:143:SER:N	2.72	0.43
1:T:87:THR:O	1:T:87:THR:CG2	2.65	0.43
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:75:GLY:O	1:X:76:LEU:C	2.57	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:X:75:GLY:C	1:X:77:VAL:H	2.22	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: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:O	1:G:139:VAL:N	2.53	0.42
1:K:137:ALA:O	1:K:139:VAL:N	2.53	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:N:32:TRP:NE1	1:W:64:VAL:HG11	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:137:ALA:O	1:X:139:VAL:N	2.53	0.42
1:C:25:ARG:HA	1:D:143:SER:CB	2.49	0.41
1:R:142:ARG:NE	1:R:142:ARG:HA	2.35	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: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: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:R:51:ALA:CB	1:R:54:SER:OG	2.68	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: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: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:M:85:LYS:O	1:M:86:SER:C	2.59	0.41
1:O:137:ALA:O	1:O:139:VAL:N	2.53	0.41
1:T:86:SER:C	1:T:88:PHE:H	2.11	0.41
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:J:148:SER:C	1:J:150:ALA:N	2.74	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:O	1:N:139:VAL:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:137:ALA:O	1:Q:139:VAL:N	2.53	0.41
1:R:148:SER:C	1:R:150:ALA:N	2.74	0.41
1:V:148:SER:C	1:V:150:ALA:N	2.74	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: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:H:33:ASN:HD22	1:R:159:LEU:HD11	1.86	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:J:144:THR:O	1:J:145:MSE:HG2	2.22	0.40
1:X:85:LYS:O	1:X:86:SER:C	2.60	0.40
1:W:49:PHE:CD2	1:W:52:LYS:HD3	2.56	0.40
1:H:148:SER:C	1:H:150:ALA:N	2.74	0.40
1:J:132:VAL:HB	1:J:133:PRO:HD3	2.04	0.40
1:X:148:SER:C	1:X:150:ALA:N	2.74	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 (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	4	28
1	B	136/160 (85%)	116 (85%)	13 (10%)	7 (5%)	2	19
1	C	124/160 (78%)	102 (82%)	17 (14%)	5 (4%)	3	24
1	D	145/160 (91%)	128 (88%)	12 (8%)	5 (3%)	3	28
1	E	123/160 (77%)	104 (85%)	16 (13%)	3 (2%)	6	35
1	F	134/160 (84%)	119 (89%)	11 (8%)	4 (3%)	4	30
1	G	124/160 (78%)	106 (86%)	14 (11%)	4 (3%)	4	29
1	H	140/160 (88%)	120 (86%)	15 (11%)	5 (4%)	3	26
1	I	123/160 (77%)	104 (85%)	14 (11%)	5 (4%)	3	23
1	J	137/160 (86%)	118 (86%)	13 (10%)	6 (4%)	2	21
1	K	111/160 (69%)	99 (89%)	10 (9%)	2 (2%)	8	41
1	L	139/160 (87%)	119 (86%)	15 (11%)	5 (4%)	3	26
1	M	123/160 (77%)	106 (86%)	12 (10%)	5 (4%)	3	23
1	N	137/160 (86%)	119 (87%)	13 (10%)	5 (4%)	3	26
1	O	112/160 (70%)	101 (90%)	9 (8%)	2 (2%)	8	41
1	P	137/160 (86%)	120 (88%)	11 (8%)	6 (4%)	2	21
1	Q	118/160 (74%)	101 (86%)	14 (12%)	3 (2%)	5	34
1	R	135/160 (84%)	116 (86%)	15 (11%)	4 (3%)	4	30
1	S	122/160 (76%)	106 (87%)	12 (10%)	4 (3%)	4	28
1	T	139/160 (87%)	120 (86%)	12 (9%)	7 (5%)	2	19
1	U	117/160 (73%)	100 (86%)	14 (12%)	3 (3%)	5	33
1	V	124/160 (78%)	105 (85%)	13 (10%)	6 (5%)	2	20
1	W	117/160 (73%)	101 (86%)	13 (11%)	3 (3%)	5	33
1	X	137/160 (86%)	118 (86%)	13 (10%)	6 (4%)	2	21
All	All	3076/3840 (80%)	2651 (86%)	316 (10%)	109 (4%)	3	27

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

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Mol	Chain	Res	Type
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
1	M	75	GLY
1	M	86	SER
1	N	75	GLY
1	O	75	GLY
1	P	75	GLY
1	P	141	GLY

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Mol	Chain	Res	Type
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
1	N	138	CYS
1	P	138	CYS
1	R	138	CYS
1	R	149	ASP
1	S	138	CYS
1	U	138	CYS

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Mol	Chain	Res	Type
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 (i)

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%)	113 (98%)	2 (2%)	60	82
1	B	129/145 (89%)	123 (95%)	6 (5%)	26	60
1	C	117/145 (81%)	115 (98%)	2 (2%)	60	82
1	D	135/145 (93%)	131 (97%)	4 (3%)	41	71
1	E	116/145 (80%)	111 (96%)	5 (4%)	29	62
1	F	127/145 (88%)	124 (98%)	3 (2%)	49	76
1	G	117/145 (81%)	114 (97%)	3 (3%)	46	74
1	H	132/145 (91%)	127 (96%)	5 (4%)	33	65
1	I	116/145 (80%)	112 (97%)	4 (3%)	37	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	130/145 (90%)	126 (97%)	4 (3%)	40	70
1	K	110/145 (76%)	108 (98%)	2 (2%)	59	81
1	L	131/145 (90%)	124 (95%)	7 (5%)	22	55
1	M	116/145 (80%)	114 (98%)	2 (2%)	60	82
1	N	130/145 (90%)	126 (97%)	4 (3%)	40	70
1	O	110/145 (76%)	106 (96%)	4 (4%)	35	66
1	P	130/145 (90%)	127 (98%)	3 (2%)	50	77
1	Q	113/145 (78%)	112 (99%)	1 (1%)	78	90
1	R	128/145 (88%)	125 (98%)	3 (2%)	50	77
1	S	115/145 (79%)	114 (99%)	1 (1%)	78	90
1	T	132/145 (91%)	127 (96%)	5 (4%)	33	65
1	U	114/145 (79%)	111 (97%)	3 (3%)	46	74
1	V	121/145 (83%)	117 (97%)	4 (3%)	38	68
1	W	112/145 (77%)	110 (98%)	2 (2%)	59	81
1	X	130/145 (90%)	128 (98%)	2 (2%)	65	84
All	All	2926/3480 (84%)	2845 (97%)	81 (3%)	43	72

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	PHE
1	A	93	ASP
1	B	93	ASP
1	B	129	GLN
1	B	145	MSE
1	B	157	SER
1	B	158	ASN
1	B	159	LEU
1	C	55	CYS
1	C	93	ASP
1	D	54	SER
1	D	89	PHE
1	D	93	ASP
1	D	145	MSE
1	E	54	SER
1	E	55	CYS
1	E	88	PHE

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Mol	Chain	Res	Type
1	E	91	THR
1	E	93	ASP
1	F	54	SER
1	F	93	ASP
1	F	149	ASP
1	G	54	SER
1	G	91	THR
1	G	93	ASP
1	H	54	SER
1	H	91	THR
1	H	93	ASP
1	H	145	MSE
1	H	157	SER
1	I	41	PHE
1	I	91	THR
1	I	93	ASP
1	I	129	GLN
1	J	54	SER
1	J	93	ASP
1	J	140	GLN
1	J	145	MSE
1	K	55	CYS
1	K	93	ASP
1	L	16	VAL
1	L	54	SER
1	L	85	LYS
1	L	91	THR
1	L	93	ASP
1	L	145	MSE
1	L	157	SER
1	M	88	PHE
1	M	93	ASP
1	N	54	SER
1	N	93	ASP
1	N	145	MSE
1	N	159	LEU
1	O	54	SER
1	O	91	THR
1	O	93	ASP
1	O	129	GLN
1	P	54	SER
1	P	93	ASP

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Mol	Chain	Res	Type
1	P	157	SER
1	Q	93	ASP
1	R	93	ASP
1	R	139	VAL
1	R	145	MSE
1	S	93	ASP
1	T	54	SER
1	T	61	ARG
1	T	93	ASP
1	T	149	ASP
1	T	157	SER
1	U	45	ASN
1	U	53	THR
1	U	93	ASP
1	V	54	SER
1	V	93	ASP
1	V	129	GLN
1	V	149	ASP
1	W	54	SER
1	W	93	ASP
1	X	54	SER
1	X	93	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (109) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	69	GLN
1	A	73	ASN
1	A	121	GLN
1	A	123	HIS
1	B	69	GLN
1	B	73	ASN
1	B	121	GLN
1	C	69	GLN
1	C	73	ASN
1	C	121	GLN
1	C	123	HIS
1	D	69	GLN
1	D	73	ASN
1	D	121	GLN
1	D	127	GLN

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Mol	Chain	Res	Type
1	D	158	ASN
1	E	43	HIS
1	E	69	GLN
1	E	73	ASN
1	E	121	GLN
1	E	123	HIS
1	F	69	GLN
1	F	73	ASN
1	F	121	GLN
1	F	127	GLN
1	F	158	ASN
1	G	43	HIS
1	G	69	GLN
1	G	73	ASN
1	G	121	GLN
1	G	123	HIS
1	H	69	GLN
1	H	73	ASN
1	H	121	GLN
1	H	127	GLN
1	I	69	GLN
1	I	73	ASN
1	I	121	GLN
1	I	123	HIS
1	J	69	GLN
1	J	73	ASN
1	J	121	GLN
1	J	127	GLN
1	J	158	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	45	ASN
1	M	69	GLN
1	M	73	ASN

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Mol	Chain	Res	Type
1	M	121	GLN
1	N	69	GLN
1	N	73	ASN
1	N	121	GLN
1	N	127	GLN
1	N	158	ASN
1	O	69	GLN
1	O	73	ASN
1	O	121	GLN
1	O	123	HIS
1	P	69	GLN
1	P	73	ASN
1	P	121	GLN
1	P	127	GLN
1	P	158	ASN
1	Q	27	GLN
1	Q	69	GLN
1	Q	73	ASN
1	Q	121	GLN
1	Q	123	HIS
1	R	69	GLN
1	R	73	ASN
1	R	121	GLN
1	R	127	GLN
1	R	158	ASN
1	S	69	GLN
1	S	73	ASN
1	S	121	GLN
1	S	123	HIS
1	S	127	GLN
1	T	69	GLN
1	T	73	ASN
1	T	121	GLN
1	T	127	GLN
1	T	158	ASN
1	U	69	GLN
1	U	73	ASN
1	U	121	GLN
1	U	123	HIS
1	V	69	GLN
1	V	73	ASN
1	V	121	GLN

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Mol	Chain	Res	Type
1	V	158	ASN
1	W	69	GLN
1	W	73	ASN
1	W	121	GLN
1	W	123	HIS
1	X	69	GLN
1	X	121	GLN
1	X	127	GLN
1	X	158	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	0.22	0 100 100	63, 95, 159, 217	0
1	B	138/160 (86%)	0.39	3 (2%) 62 56	68, 120, 173, 184	0
1	C	126/160 (78%)	0.36	3 (2%) 59 53	68, 104, 170, 206	0
1	D	145/160 (90%)	0.17	2 (1%) 75 69	66, 110, 165, 201	0
1	E	125/160 (78%)	0.33	4 (3%) 47 42	71, 105, 177, 217	0
1	F	136/160 (85%)	0.22	3 (2%) 62 56	78, 131, 170, 180	0
1	G	126/160 (78%)	0.29	3 (2%) 59 53	60, 97, 173, 212	0
1	H	142/160 (88%)	0.19	2 (1%) 75 69	64, 102, 154, 215	0
1	I	125/160 (78%)	0.28	0 100 100	60, 94, 159, 204	0
1	J	139/160 (86%)	0.07	0 100 100	64, 105, 154, 186	0
1	K	117/160 (73%)	0.27	1 (0%) 84 79	72, 103, 155, 194	0
1	L	141/160 (88%)	0.14	2 (1%) 75 69	69, 121, 167, 188	0
1	M	125/160 (78%)	0.19	0 100 100	74, 105, 169, 220	0
1	N	139/160 (86%)	0.11	0 100 100	79, 135, 177, 195	0
1	O	118/160 (73%)	0.39	2 (1%) 70 64	77, 108, 165, 182	0
1	P	139/160 (86%)	0.35	5 (3%) 42 38	65, 122, 164, 200	0
1	Q	122/160 (76%)	0.30	1 (0%) 86 81	66, 100, 167, 205	0
1	R	137/160 (85%)	0.30	3 (2%) 62 56	70, 119, 166, 199	0
1	S	124/160 (77%)	0.16	1 (0%) 86 81	90, 123, 191, 211	0
1	T	141/160 (88%)	0.31	1 (0%) 87 83	92, 147, 184, 200	0
1	U	121/160 (75%)	0.36	2 (1%) 70 64	86, 120, 169, 193	0
1	V	128/160 (80%)	0.43	10 (7%) 13 13	92, 148, 185, 204	0
1	W	121/160 (75%)	0.34	4 (3%) 46 41	87, 122, 173, 199	0
1	X	139/160 (86%)	0.41	6 (4%) 35 31	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%)	0.27	58 (1%) 68 62	60, 116, 176, 220	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	140	GLN	7.1
1	V	111	LEU	4.1
1	P	49	PHE	3.8
1	R	51	ALA	3.7
1	G	49	PHE	3.5
1	X	49	PHE	3.4
1	P	76	LEU	3.3
1	E	140	GLN	3.2
1	P	53	THR	3.2
1	P	75	GLY	3.2
1	F	53	THR	3.2
1	V	45	ASN	3.2
1	V	19	VAL	3.2
1	E	51	ALA	3.1
1	X	47	LYS	3.0
1	C	89	PHE	3.0
1	B	116	LEU	2.8
1	U	135	ILE	2.8
1	V	144	THR	2.8
1	D	47	LYS	2.8
1	G	50	THR	2.8
1	V	17	ILE	2.7
1	E	22	GLN	2.7
1	B	73	ASN	2.7
1	W	41	PHE	2.7
1	W	140	GLN	2.6
1	B	74	ALA	2.6
1	W	103	LEU	2.5
1	L	85	LYS	2.5
1	O	41	PHE	2.5
1	X	51	ALA	2.4
1	C	30	GLY	2.4
1	V	56	VAL	2.4
1	Q	48	ALA	2.4
1	R	47	LYS	2.4
1	X	75	GLY	2.4
1	S	92	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	T	116	LEU	2.3
1	F	49	PHE	2.3
1	H	49	PHE	2.3
1	L	47	LYS	2.3
1	X	116	LEU	2.3
1	V	22	GLN	2.2
1	V	18	THR	2.2
1	V	42	LEU	2.2
1	F	42	LEU	2.2
1	H	47	LYS	2.2
1	G	41	PHE	2.2
1	P	29	GLU	2.1
1	O	111	LEU	2.1
1	R	53	THR	2.1
1	U	92	SER	2.1
1	W	22	GLN	2.1
1	X	17	ILE	2.1
1	E	48	ALA	2.1
1	K	22	GLN	2.1
1	D	87	THR	2.0
1	V	116	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.