



wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 03:38 am BST

PDB ID : 3PIF
Title : Crystal structure of the 5'->3' exoribonuclease Xrn1, E178Q mutant in Complex with Manganese
Authors : Chang, J.H.; Xiang, S.; Tong, L.
Deposited on : 2010-11-06
Resolution : 2.92 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

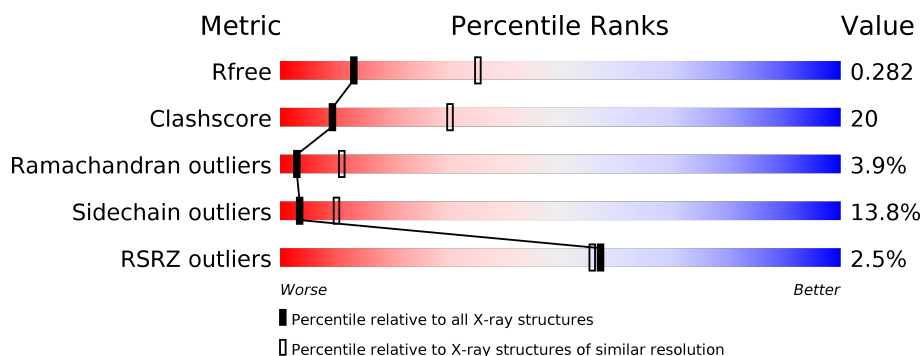
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.92 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	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

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 on 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	1155	<div> <div>2%</div> <div> <div></div> <div>57%</div> <div>27%</div> <div>7%</div> <div>8%</div> </div> </div>
1	B	1155	<div> <div>2%</div> <div> <div></div> <div>52%</div> <div>32%</div> <div>7%</div> <div>9%</div> </div> </div>
1	C	1155	<div> <div>2%</div> <div> <div></div> <div>55%</div> <div>30%</div> <div>6%</div> <div>8%</div> </div> </div>
1	D	1155	<div> <div>3%</div> <div> <div></div> <div>52%</div> <div>30%</div> <div>6%</div> <div>11%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 34013 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 5'->3' EXORIBONUCLEASE (xrn1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1057	Total	C	N	O	S	0	0	0
			8549	5509	1438	1579	23			
1	B	1056	Total	C	N	O	S	0	0	0
			8535	5501	1436	1575	23			
1	C	1066	Total	C	N	O	S	0	0	0
			8605	5543	1446	1593	23			
1	D	1023	Total	C	N	O	S	0	0	0
			8320	5365	1397	1535	23			

There are 188 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	178	GLN	GLU	ENGINEERED MUTATION	UNP Q6CJ09
A	469	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	470	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	471	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	472	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	473	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	474	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	475	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	476	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	477	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	478	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	479	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	480	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	481	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	482	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	483	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	484	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	485	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	486	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	487	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1036	UNK	-	SEE REMARK 999	UNP Q6CJ09

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1037	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1038	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1039	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1040	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1041	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1042	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1043	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1044	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1045	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1046	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1047	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1048	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1049	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1050	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1051	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1052	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1053	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1054	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1246	LEU	-	EXPRESSION TAG	UNP Q6CJ09
A	1247	GLU	-	EXPRESSION TAG	UNP Q6CJ09
A	1248	HIS	-	EXPRESSION TAG	UNP Q6CJ09
A	1249	HIS	-	EXPRESSION TAG	UNP Q6CJ09
A	1250	HIS	-	EXPRESSION TAG	UNP Q6CJ09
A	1251	HIS	-	EXPRESSION TAG	UNP Q6CJ09
A	1252	HIS	-	EXPRESSION TAG	UNP Q6CJ09
A	1253	HIS	-	EXPRESSION TAG	UNP Q6CJ09
B	178	GLN	GLU	ENGINEERED MUTATION	UNP Q6CJ09
B	469	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	470	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	471	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	472	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	473	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	474	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	475	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	476	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	477	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	478	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	479	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	480	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	481	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	482	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	483	UNK	-	SEE REMARK 999	UNP Q6CJ09

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Chain	Residue	Modelled	Actual	Comment	Reference
B	484	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	485	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	486	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	487	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1036	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1037	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1038	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1039	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1040	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1041	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1042	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1043	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1044	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1045	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1046	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1047	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1048	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1049	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1050	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1051	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1052	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1053	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1054	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1246	LEU	-	EXPRESSION TAG	UNP Q6CJ09
B	1247	GLU	-	EXPRESSION TAG	UNP Q6CJ09
B	1248	HIS	-	EXPRESSION TAG	UNP Q6CJ09
B	1249	HIS	-	EXPRESSION TAG	UNP Q6CJ09
B	1250	HIS	-	EXPRESSION TAG	UNP Q6CJ09
B	1251	HIS	-	EXPRESSION TAG	UNP Q6CJ09
B	1252	HIS	-	EXPRESSION TAG	UNP Q6CJ09
B	1253	HIS	-	EXPRESSION TAG	UNP Q6CJ09
C	178	GLN	GLU	ENGINEERED MUTATION	UNP Q6CJ09
C	469	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	470	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	471	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	472	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	473	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	474	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	475	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	476	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	477	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	478	UNK	-	SEE REMARK 999	UNP Q6CJ09

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Chain	Residue	Modelled	Actual	Comment	Reference
C	479	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	480	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	481	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	482	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	483	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	484	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	485	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	486	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	487	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1036	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1037	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1038	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1039	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1040	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1041	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1042	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1043	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1044	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1045	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1046	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1047	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1048	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1049	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1050	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1051	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1052	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1053	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1054	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1246	LEU	-	EXPRESSION TAG	UNP Q6CJ09
C	1247	GLU	-	EXPRESSION TAG	UNP Q6CJ09
C	1248	HIS	-	EXPRESSION TAG	UNP Q6CJ09
C	1249	HIS	-	EXPRESSION TAG	UNP Q6CJ09
C	1250	HIS	-	EXPRESSION TAG	UNP Q6CJ09
C	1251	HIS	-	EXPRESSION TAG	UNP Q6CJ09
C	1252	HIS	-	EXPRESSION TAG	UNP Q6CJ09
C	1253	HIS	-	EXPRESSION TAG	UNP Q6CJ09
D	178	GLN	GLU	ENGINEERED MUTATION	UNP Q6CJ09
D	469	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	470	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	471	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	472	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	473	UNK	-	SEE REMARK 999	UNP Q6CJ09

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Chain	Residue	Modelled	Actual	Comment	Reference
D	474	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	475	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	476	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	477	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	478	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	479	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	480	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	481	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	482	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	483	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	484	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	485	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	486	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	487	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1036	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1037	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1038	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1039	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1040	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1041	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1042	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1043	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1044	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1045	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1046	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1047	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1048	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1049	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1050	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1051	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1052	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1053	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1054	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1246	LEU	-	EXPRESSION TAG	UNP Q6CJ09
D	1247	GLU	-	EXPRESSION TAG	UNP Q6CJ09
D	1248	HIS	-	EXPRESSION TAG	UNP Q6CJ09
D	1249	HIS	-	EXPRESSION TAG	UNP Q6CJ09
D	1250	HIS	-	EXPRESSION TAG	UNP Q6CJ09
D	1251	HIS	-	EXPRESSION TAG	UNP Q6CJ09
D	1252	HIS	-	EXPRESSION TAG	UNP Q6CJ09
D	1253	HIS	-	EXPRESSION TAG	UNP Q6CJ09

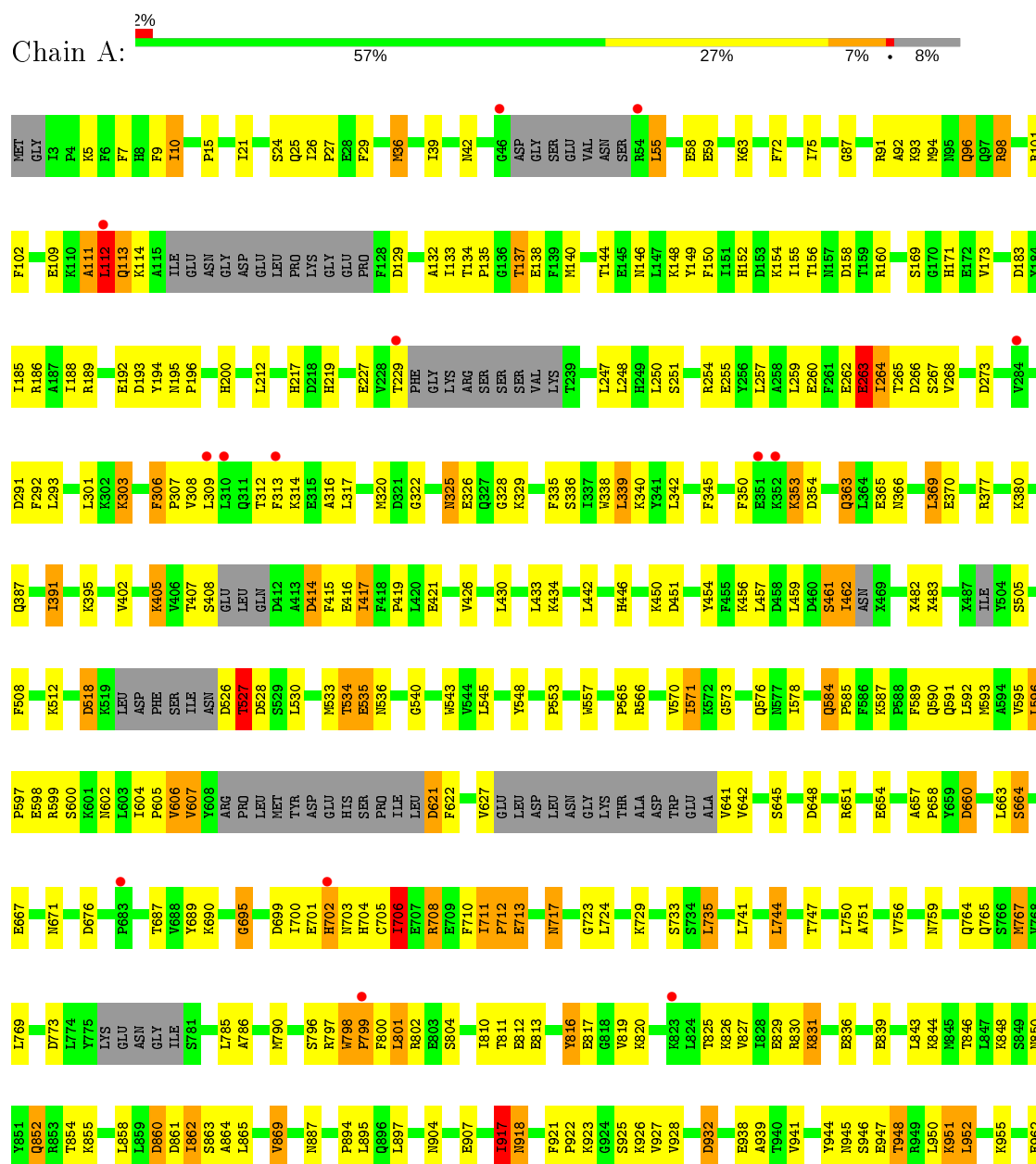
- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

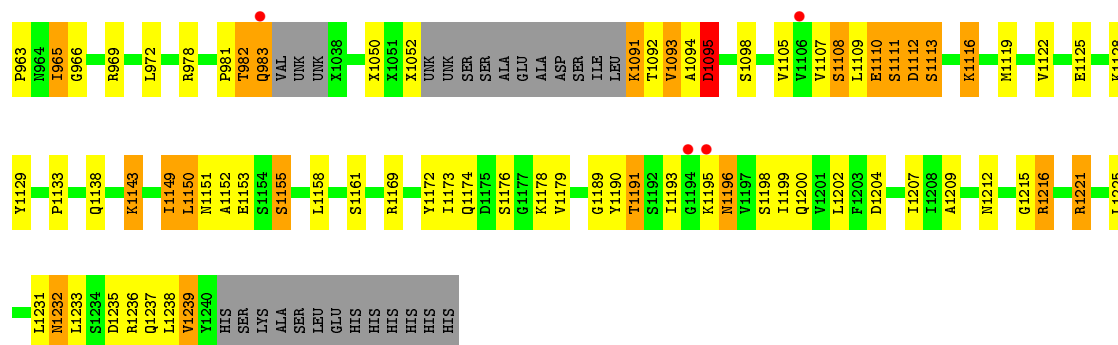
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	Mn 1	0	0
2	A	1	Total 1	Mn 1	0	0
2	D	1	Total 1	Mn 1	0	0
2	C	1	Total 1	Mn 1	0	0

3 Residue-property plots [i](#)

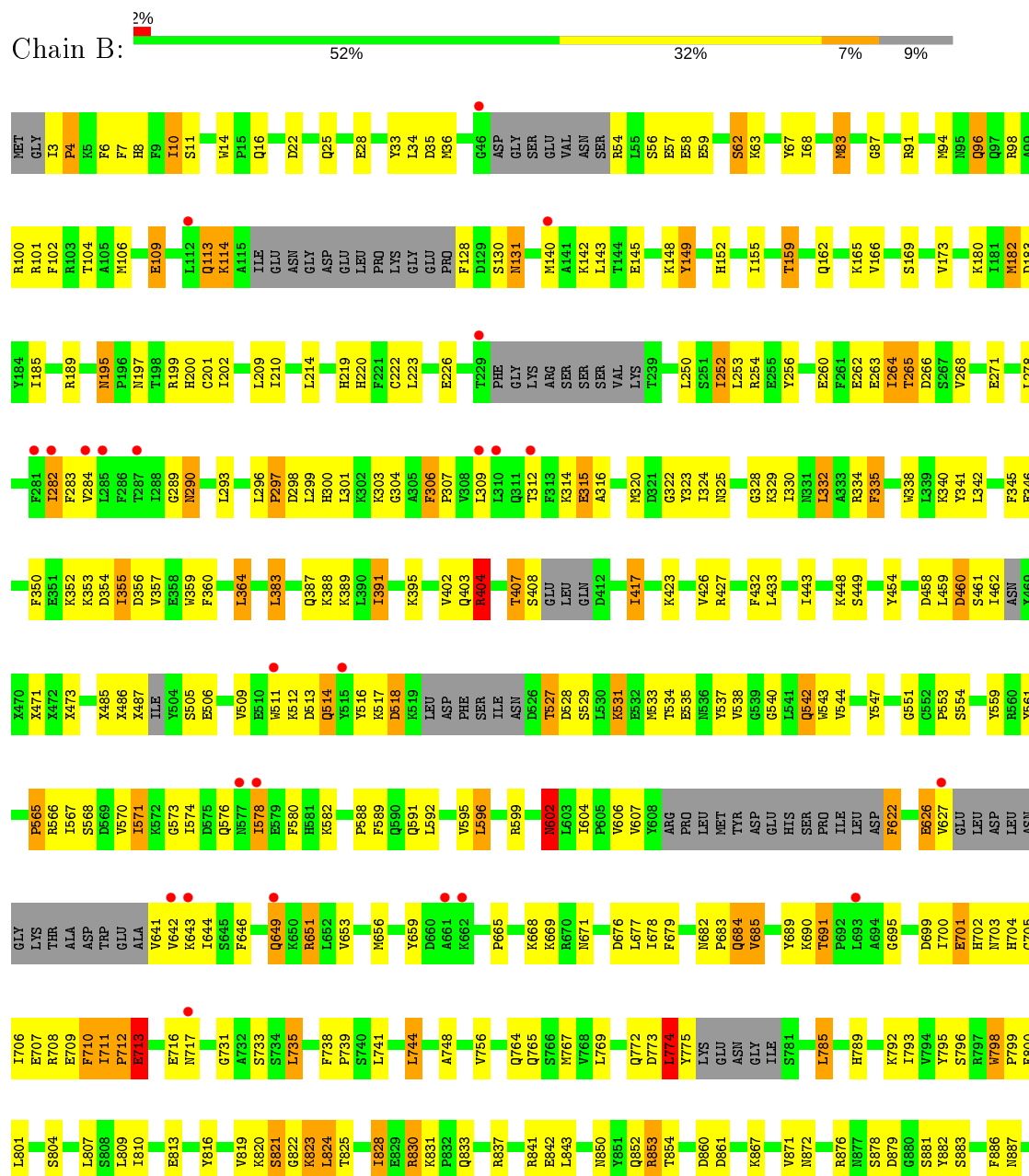
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: 5'->3' EXORIBONUCLEASE (xrn1)



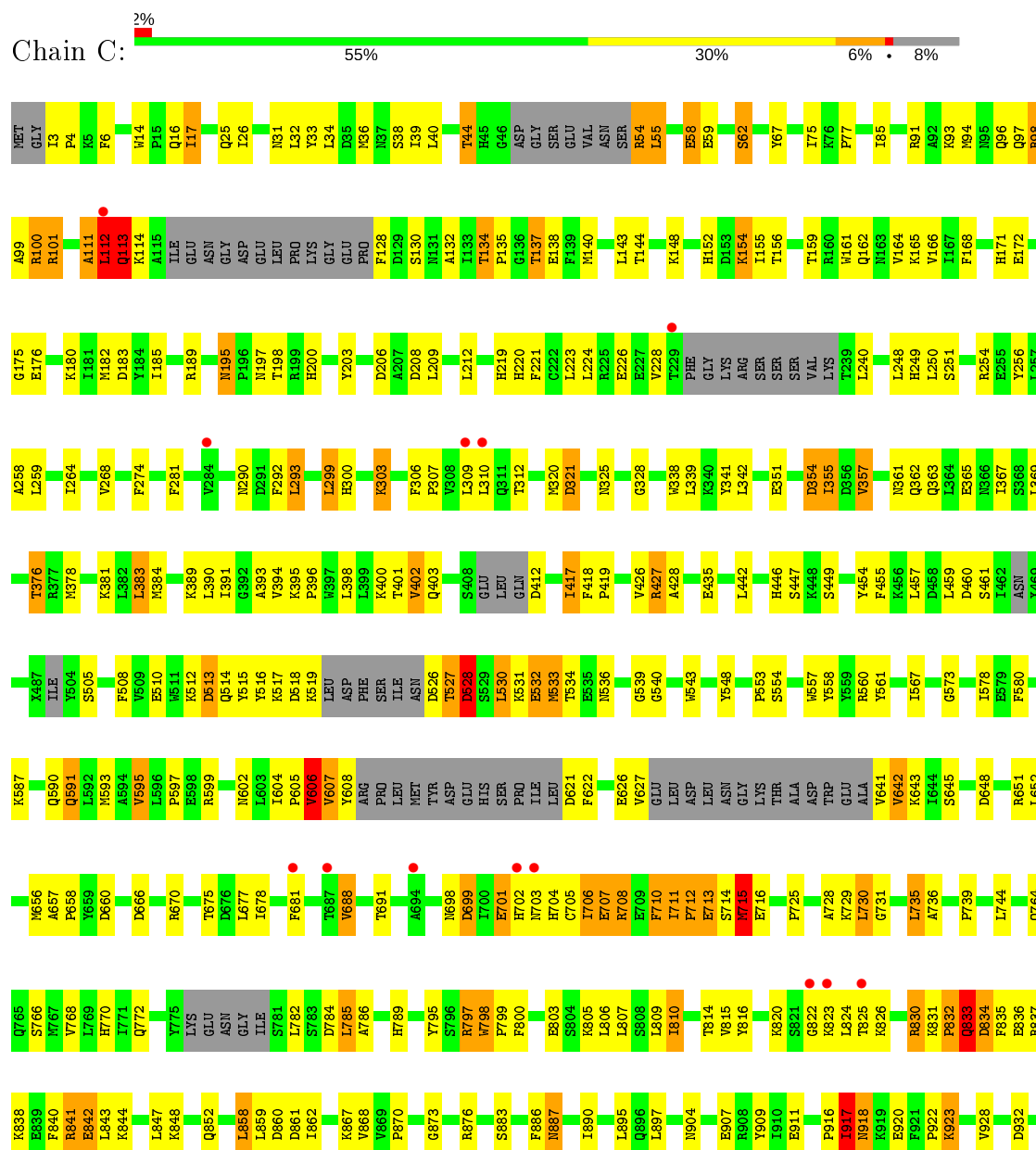


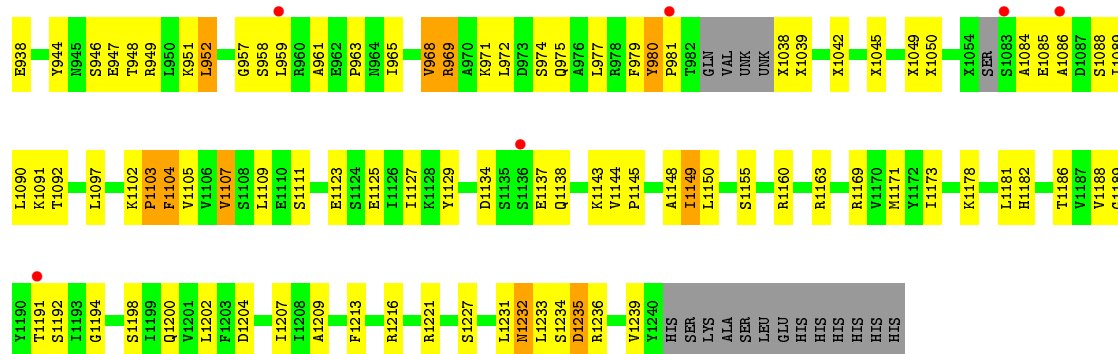
• Molecule 1: 5'->3' EXORIBONUCLEASE (xrn1)



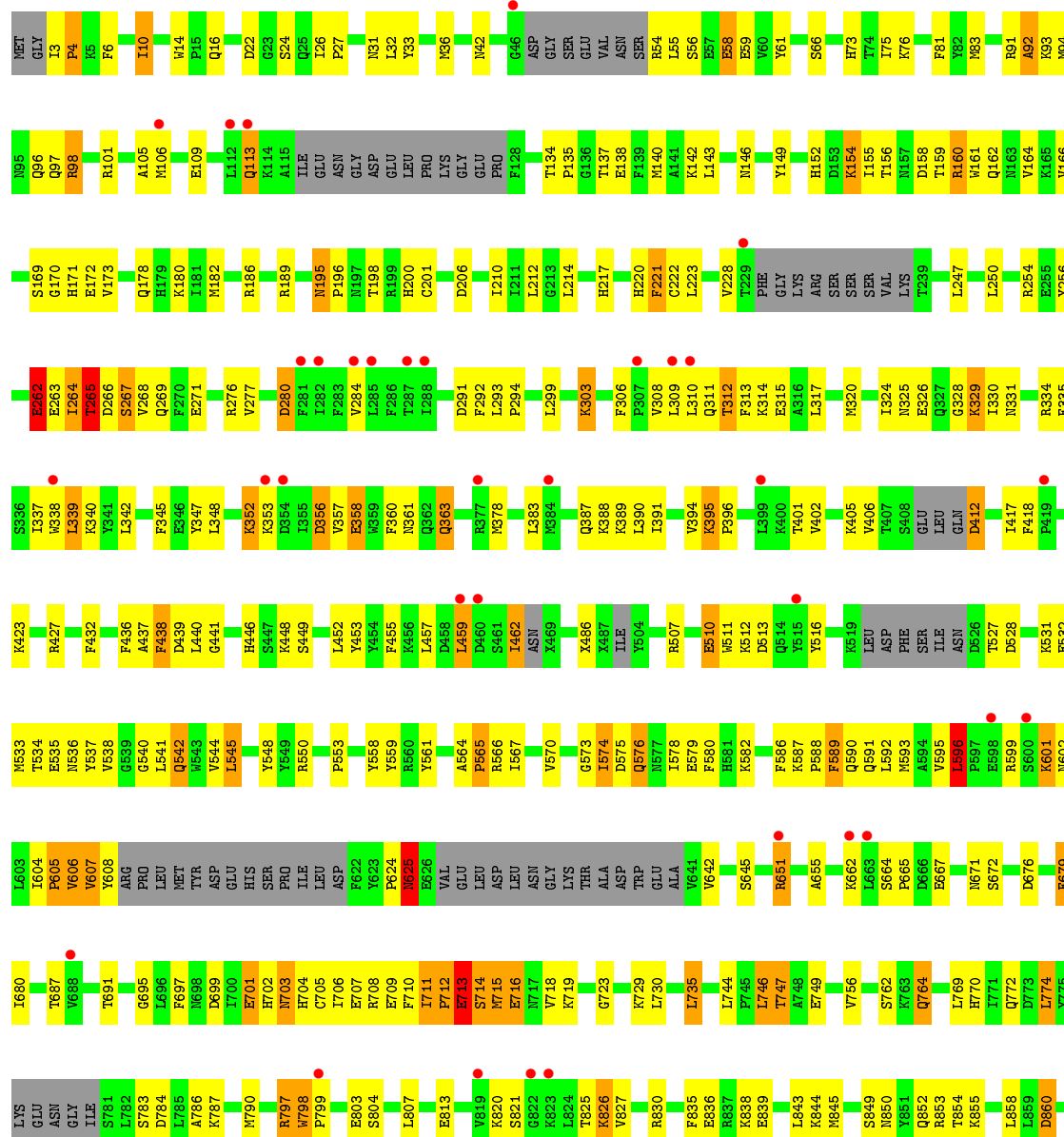


• Molecule 1: 5'->3' EXORIBONUCLEASE (xrn1)





• Molecule 1: 5'->3' EXORIBONUCLEASE (xrn1)





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	116.27Å 132.58Å 144.07Å 109.92° 105.81° 104.00°	Depositor
Resolution (Å)	30.00 – 2.92 29.05 – 2.92	Depositor EDS
% Data completeness (in resolution range)	96.1 (30.00-2.92) 96.1 (29.05-2.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.248 , 0.284 0.245 , 0.282	Depositor DCC
R_{free} test set	7614 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	73.6	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,h+k+l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	34013	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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

Bond lengths and bond angles in the following residue types are not validated in this section: MN

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	0.85	3/8567 (0.0%)	0.88	5/11553 (0.0%)
1	B	0.84	2/8543 (0.0%)	0.89	4/11521 (0.0%)
1	C	0.77	0/8613	0.81	7/11616 (0.1%)
1	D	0.70	1/8409 (0.0%)	0.80	4/11337 (0.0%)
All	All	0.79	6/34132 (0.0%)	0.84	20/46027 (0.0%)

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	C	0	2
1	D	0	1
All	All	0	3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	598	GLU	CG-CD	7.86	1.63	1.51
1	A	598	GLU	CB-CG	7.25	1.66	1.52
1	A	705	CYS	CB-SG	7.23	1.94	1.82
1	B	709	GLU	CB-CG	7.18	1.65	1.52
1	B	1153	GLU	CG-CD	5.90	1.60	1.51

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	774	LEU	CA-CB-CG	7.08	131.59	115.30
1	D	950	LEU	CA-CB-CG	6.76	130.86	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	35	ASP	CB-CG-OD1	6.56	124.20	118.30
1	A	865	LEU	CA-CB-CG	6.33	129.87	115.30
1	A	706	ILE	CB-CA-C	-6.13	99.34	111.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	797	ARG	Peptide
1	C	980	TYR	Peptide
1	D	860	ASP	Peptide

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	8549	0	8404	346	0
1	B	8535	0	8385	367	0
1	C	8605	0	8452	314	0
1	D	8320	0	8233	315	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
All	All	34013	0	33474	1333	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

The worst 5 of 1333 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:A:798:TRP:HB3	1:A:799:PRO:CD	1.73	1.19
1:C:917:ILE:H	1:C:917:ILE:CD1	1.51	1.18
1:B:36:MET:HE3	1:B:83:MET:HG2	1.21	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:917:ILE:N	1:C:917:ILE:HD13	1.61	1.14
1:B:264:ILE:HG21	1:B:268:VAL:HG13	1.23	1.14

There are no symmetry-related clashes.

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	1001/1155 (87%)	867 (87%)	98 (10%)	36 (4%)	3	13
1	B	998/1155 (86%)	839 (84%)	113 (11%)	46 (5%)	2	8
1	C	1008/1155 (87%)	855 (85%)	118 (12%)	35 (4%)	3	13
1	D	982/1155 (85%)	827 (84%)	117 (12%)	38 (4%)	3	11
All	All	3989/4620 (86%)	3388 (85%)	446 (11%)	155 (4%)	3	11

5 of 155 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	111	ALA
1	A	112	LEU
1	A	263	GLU
1	A	265	THR
1	A	353	LYS

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	922/1004 (92%)	799 (87%)	123 (13%)	4	11
1	B	919/1004 (92%)	787 (86%)	132 (14%)	3	9
1	C	927/1004 (92%)	804 (87%)	123 (13%)	4	11
1	D	905/1004 (90%)	775 (86%)	130 (14%)	3	9
All	All	3673/4016 (92%)	3165 (86%)	508 (14%)	3	10

5 of 508 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	979	PHE
1	C	339	LEU
1	D	813	GLU
1	B	1110	GLU
1	C	25	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 121 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	964	ASN
1	C	220	HIS
1	D	625	ASN
1	B	1196	ASN
1	C	96	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	1023/1155 (88%)	-0.28	18 (1%) 68 67	44, 66, 97, 117	0
1	B	1020/1155 (88%)	-0.16	27 (2%) 56 53	36, 72, 124, 140	0
1	C	1030/1155 (89%)	-0.11	19 (1%) 68 67	51, 81, 109, 133	0
1	D	1004/1155 (86%)	0.01	39 (3%) 39 36	51, 87, 131, 151	0
All	All	4077/4620 (88%)	-0.14	103 (2%) 57 56	36, 76, 121, 151	0

The worst 5 of 103 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	112	LEU	6.0
1	B	627	VAL	5.8
1	A	229	THR	4.2
1	B	662	LYS	4.2
1	C	823	LYS	4.0

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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MN	A	1254	1/1	0.97	0.16	67,67,67,67	0
2	MN	B	1254	1/1	0.97	0.14	67,67,67,67	0
2	MN	D	1254	1/1	0.98	0.21	75,75,75,75	0
2	MN	C	1254	1/1	0.99	0.17	66,66,66,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.