



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 28, 2020 – 09:35 pm BST

PDB ID : 2BR2  
Title : RNase PH core of the archaeal exosome  
Authors : lorentzen, E.; Fribourg, S.; Conti, E.  
Deposited on : 2005-04-30  
Resolution : 2.80 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

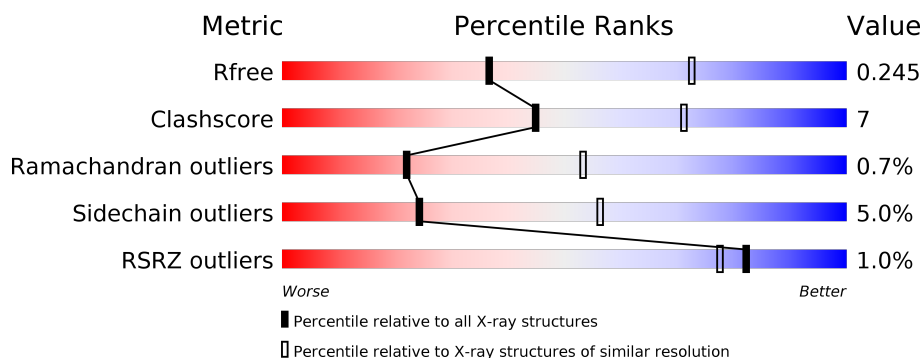
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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.






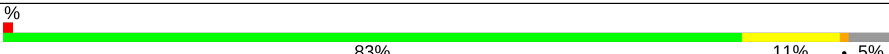
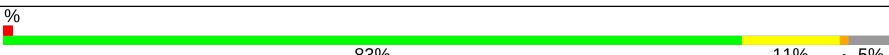
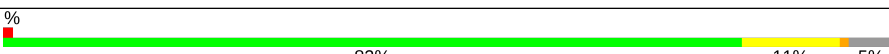
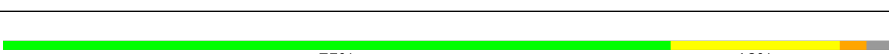
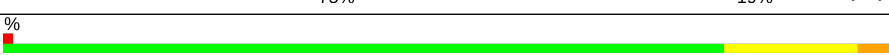

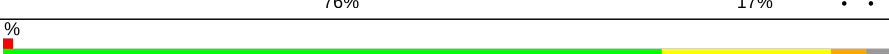
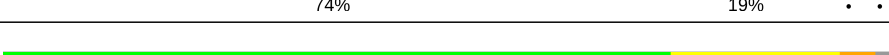

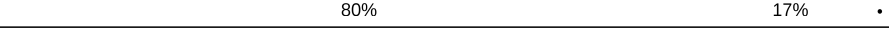
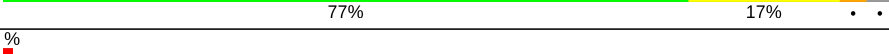




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	275	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>• 5%</div> </div> </div>
1	C	275	<div> <div></div> <div> <div>81%</div> <div>13%</div> <div>• 5%</div> </div> </div>
1	E	275	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>• 5%</div> </div> </div>
1	G	275	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>11%</div> <div>5%</div> </div> </div>
1	I	275	<div> <div></div> <div> <div>81%</div> <div>13%</div> <div>• 5%</div> </div> </div>
1	K	275	<div> <div></div> <div> <div>81%</div> <div>13%</div> <div>• 5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	M	275	
1	O	275	
1	Q	275	
1	S	275	
1	U	275	
1	W	275	
2	B	248	
2	D	248	
2	F	248	
2	H	248	
2	J	248	
2	L	248	
2	N	248	
2	P	248	
2	R	248	
2	T	248	
2	V	248	
2	X	248	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 46287 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 EXOSOME COMPLEX EXONUCLEASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			1960	1248	323	384	5			
1	C	260	Total	C	N	O	S	0	0	0
			1972	1255	325	387	5			
1	E	260	Total	C	N	O	S	0	0	0
			1968	1253	324	386	5			
1	G	260	Total	C	N	O	S	0	0	0
			1964	1251	324	384	5			
1	I	260	Total	C	N	O	S	0	0	0
			1961	1250	323	383	5			
1	K	260	Total	C	N	O	S	0	0	0
			1964	1251	324	384	5			
1	M	260	Total	C	N	O	S	0	0	0
			1972	1255	325	387	5			
1	O	260	Total	C	N	O	S	0	0	0
			1968	1253	325	385	5			
1	Q	260	Total	C	N	O	S	0	0	0
			1968	1253	325	385	5			
1	S	260	Total	C	N	O	S	0	0	0
			1967	1253	324	385	5			
1	U	260	Total	C	N	O	S	0	0	0
			1968	1253	325	385	5			
1	W	260	Total	C	N	O	S	0	0	0
			1968	1253	324	386	5			

- Molecule 2 is a protein called EXOSOME COMPLEX EXONUCLEASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	241	Total	C	N	O	S	0	0	0
			1863	1175	322	356	10			
2	D	247	Total	C	N	O	S	0	0	0
			1905	1202	329	363	11			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	241	Total	C	N	O	S	0	0	0
			1863	1175	322	356	10			
2	H	241	Total	C	N	O	S	0	0	0
			1863	1175	322	356	10			
2	J	241	Total	C	N	O	S	0	0	0
			1863	1175	322	356	10			
2	L	247	Total	C	N	O	S	0	0	0
			1909	1204	329	365	11			
2	N	241	Total	C	N	O	S	0	0	0
			1863	1175	322	356	10			
2	P	248	Total	C	N	O	S	0	0	0
			1907	1204	327	364	12			
2	R	245	Total	C	N	O	S	0	0	0
			1889	1192	327	359	11			
2	T	247	Total	C	N	O	S	0	0	0
			1905	1202	329	363	11			
2	V	244	Total	C	N	O	S	0	0	0
			1883	1189	325	359	10			
2	X	241	Total	C	N	O	S	0	0	0
			1863	1175	322	356	10			

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	1	Total	Cl	0	0
			1	1		
3	J	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		
3	H	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		
3	V	1	Total	Cl	0	0
			1	1		
3	T	1	Total	Cl	0	0
			1	1		
3	N	1	Total	Cl	0	0
			1	1		
3	X	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	R	1	Total 1	Cl 1	0	0
3	L	1	Total 1	Cl 1	0	0
3	F	1	Total 1	Cl 1	0	0
3	M	1	Total 1	Cl 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	6	Total 6	O 6	0	0
4	B	5	Total 5	O 5	0	0
4	C	4	Total 4	O 4	0	0
4	D	1	Total 1	O 1	0	0
4	E	6	Total 6	O 6	0	0
4	F	4	Total 4	O 4	0	0
4	G	2	Total 2	O 2	0	0
4	H	3	Total 3	O 3	0	0
4	I	1	Total 1	O 1	0	0
4	J	5	Total 5	O 5	0	0
4	K	3	Total 3	O 3	0	0
4	L	3	Total 3	O 3	0	0
4	M	8	Total 8	O 8	0	0
4	N	4	Total 4	O 4	0	0
4	O	9	Total 9	O 9	0	0

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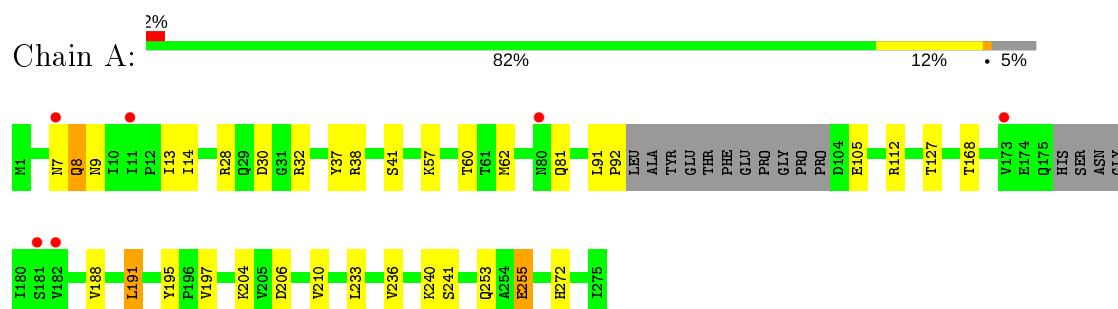
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	P	6	Total 6	O 6	0	0
4	Q	4	Total 4	O 4	0	0
4	R	5	Total 5	O 5	0	0
4	S	6	Total 6	O 6	0	0
4	T	4	Total 4	O 4	0	0
4	U	3	Total 3	O 3	0	0
4	V	3	Total 3	O 3	0	0
4	W	2	Total 2	O 2	0	0
4	X	1	Total 1	O 1	0	0

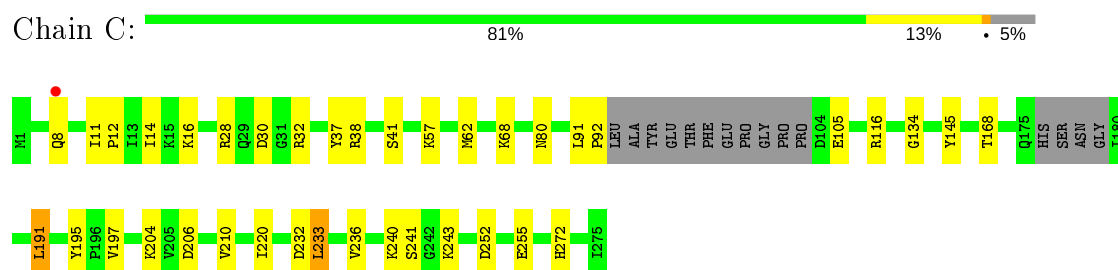
### 3 Residue-property plots [i](#)

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.

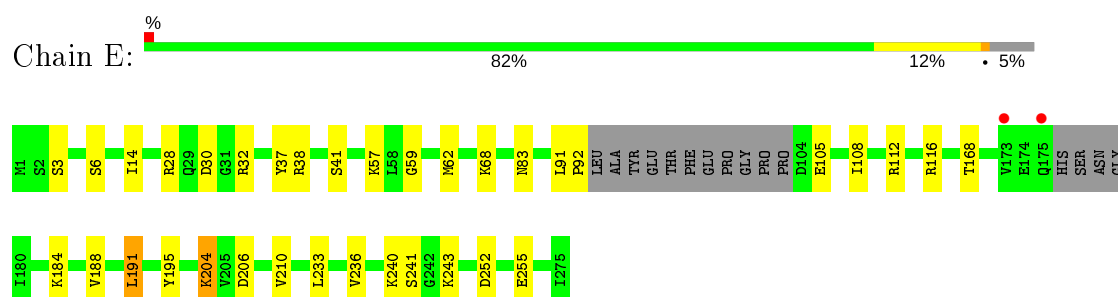
#### • Molecule 1: EXOSOME COMPLEX EXONUCLEASE 2



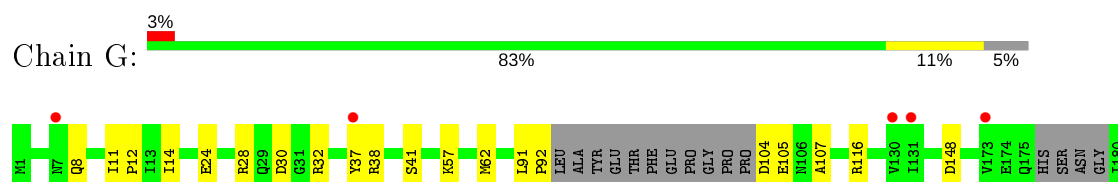
#### • Molecule 1: EXOSOME COMPLEX EXONUCLEASE 2



#### • Molecule 1: EXOSOME COMPLEX EXONUCLEASE 2



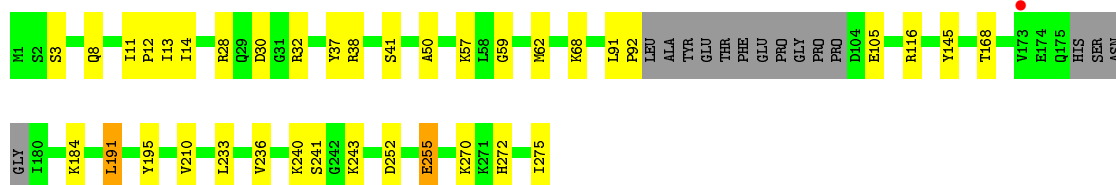
#### • Molecule 1: EXOSOME COMPLEX EXONUCLEASE 2





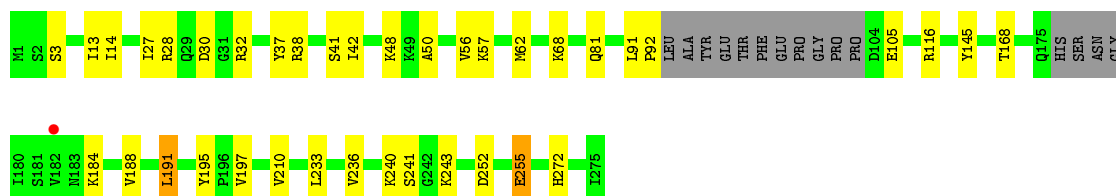
• Molecule 1: EXOSOME COMPLEX EXONUCLEASE 2

Chain I: 81% 13% • 5%



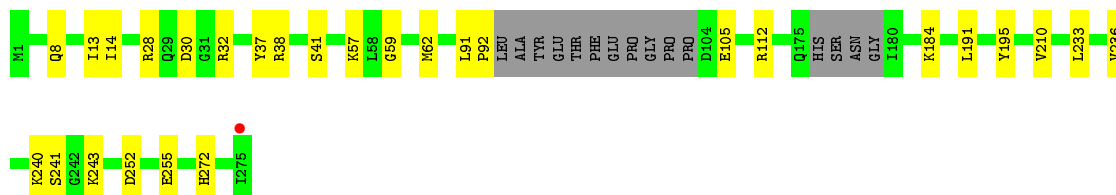
• Molecule 1: EXOSOME COMPLEX EXONUCLEASE 2

Chain K: 81% 13% • 5%



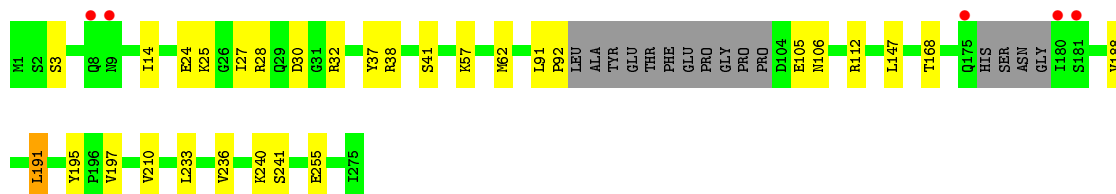
• Molecule 1: EXOSOME COMPLEX EXONUCLEASE 2

Chain M: 84% 10% 5%



• Molecule 1: EXOSOME COMPLEX EXONUCLEASE 2

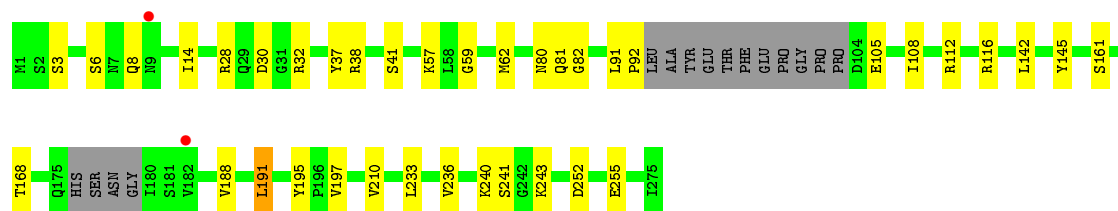
Chain O: 84% 11% 5%



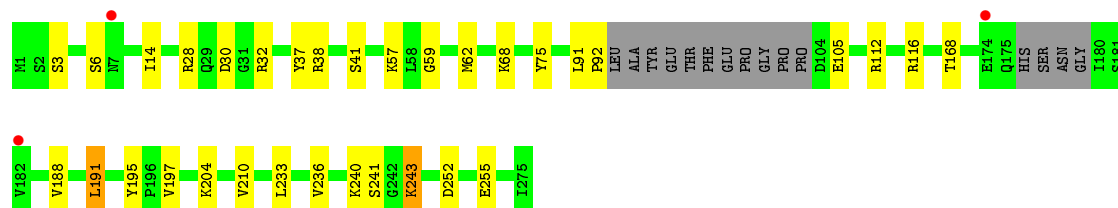
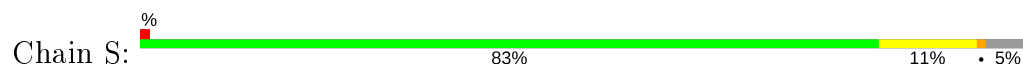
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Chain Q: 81% 13% 5%

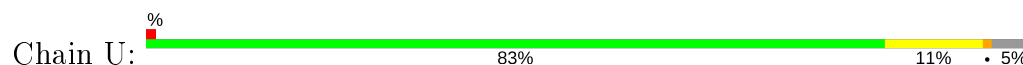




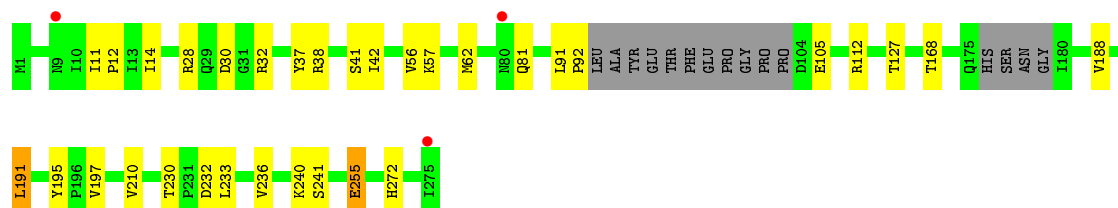
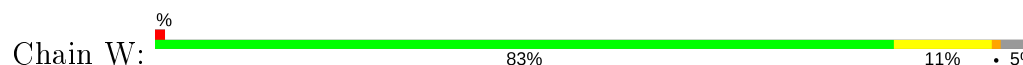
• Molecule 1: EXOSOME COMPLEX EXONUCLEASE 2



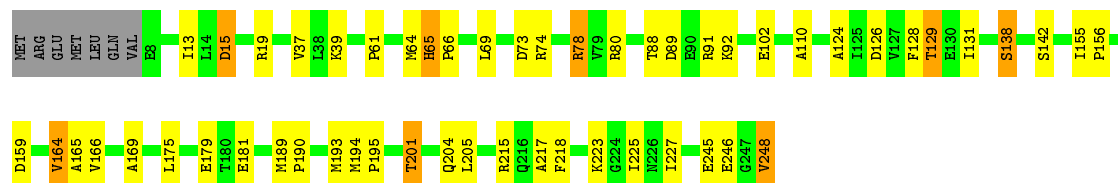
• Molecule 1: EXOSOME COMPLEX EXONUCLEASE 2



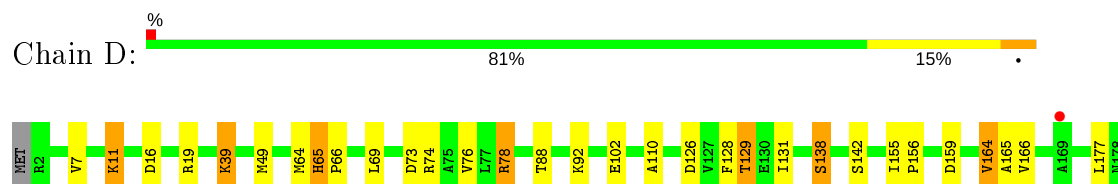
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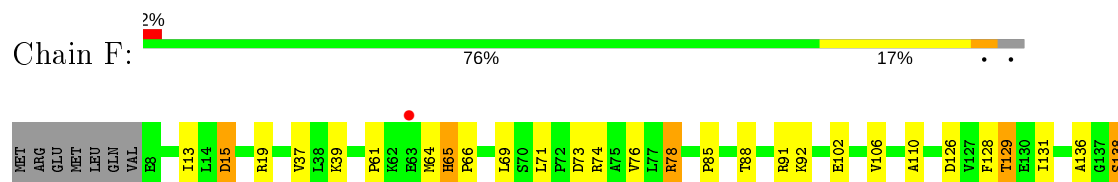
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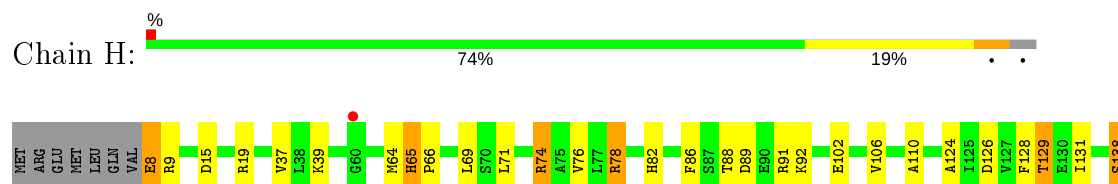
• Molecule 2: EXOSOME COMPLEX EXONUCLEASE 1



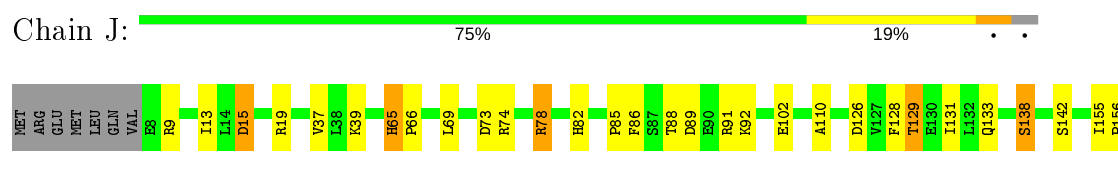
- Molecule 2: EXOSOME COMPLEX EXONUCLEASE 1



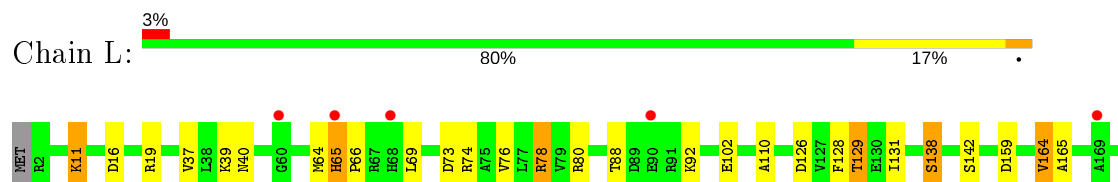
- Molecule 2: EXOSOME COMPLEX EXONUCLEASE 1



- Molecule 2: EXOSOME COMPLEX EXONUCLEASE 1



- Molecule 2: EXOSOME COMPLEX EXONUCLEASE 1





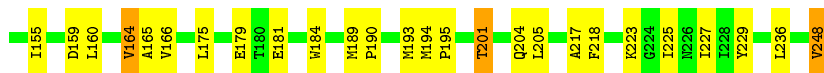
• Molecule 2: EXOSOME COMPLEX EXONUCLEASE 1

Chain N: 77% 17%



• Molecule 2: EXOSOME COMPLEX EXONUCLEASE 1

Chain P: 76% 21%



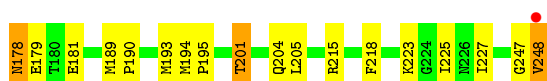
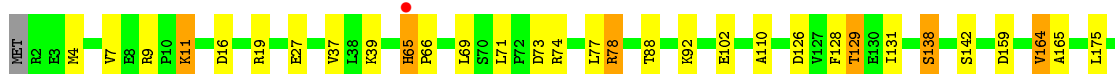
• Molecule 2: EXOSOME COMPLEX EXONUCLEASE 1

Chain R: 76% 19%



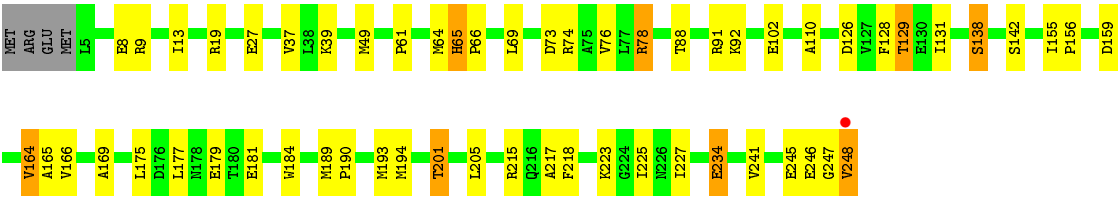
• Molecule 2: EXOSOME COMPLEX EXONUCLEASE 1

Chain T: 80% 16%

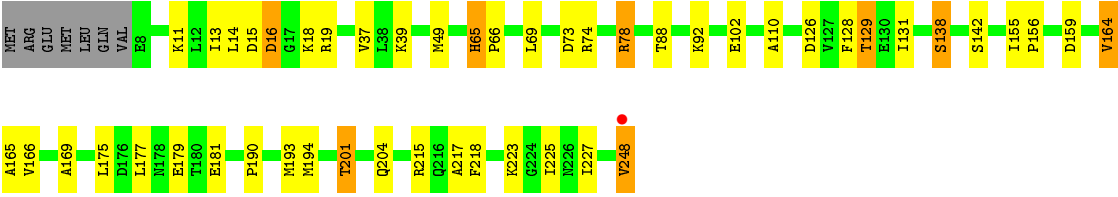
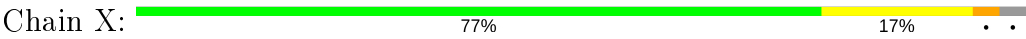


• Molecule 2: EXOSOME COMPLEX EXONUCLEASE 1

Chain V: 75% 20%



• Molecule 2: EXOSOME COMPLEX EXONUCLEASE 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	206.88Å 212.72Å 434.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	218.22 – 2.80 217.03 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (218.22-2.80) 99.7 (217.03-2.80)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.81 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.215 , 0.237 0.227 , 0.245	Depositor DCC
$R_{free}$ test set	7031 reflections (3.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.3	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 33.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.033 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	46287	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.64% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.46	0/1985	0.57	0/2697
1	C	0.50	0/1997	0.58	0/2711
1	E	0.48	0/1993	0.58	0/2706
1	G	0.47	0/1989	0.59	0/2701
1	I	0.47	0/1986	0.60	0/2697
1	K	0.51	0/1989	0.59	0/2701
1	M	0.47	0/1997	0.58	0/2711
1	O	0.51	1/1993 (0.1%)	0.62	0/2706
1	Q	0.48	0/1993	0.59	0/2706
1	S	0.48	0/1992	0.60	0/2706
1	U	0.48	0/1993	0.58	0/2706
1	W	0.47	0/1993	0.57	0/2706
2	B	0.48	0/1891	0.65	0/2553
2	D	0.46	0/1933	0.64	0/2610
2	F	0.48	0/1891	0.66	1/2553 (0.0%)
2	H	0.46	0/1891	0.65	1/2553 (0.0%)
2	J	0.48	0/1891	0.64	1/2553 (0.0%)
2	L	0.48	0/1937	0.65	0/2615
2	N	0.48	0/1891	0.65	1/2553 (0.0%)
2	P	0.49	0/1935	0.65	0/2613
2	R	0.51	0/1917	0.69	3/2588 (0.1%)
2	T	0.49	0/1933	0.67	1/2610 (0.0%)
2	V	0.47	0/1911	0.64	0/2581
2	X	0.46	0/1891	0.63	0/2553
All	All	0.48	1/46812 (0.0%)	0.62	8/63389 (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	O	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	25	LYS	C-N	5.08	1.42	1.33

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	202	LEU	CA-CB-CG	6.75	130.83	115.30
2	H	202	LEU	CA-CB-CG	6.36	129.93	115.30
2	R	9	ARG	N-CA-CB	5.46	120.44	110.60
2	R	177	LEU	CA-CB-CG	5.44	127.82	115.30
2	R	8	GLU	C-N-CA	5.36	135.09	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	O	24	GLU	Mainchain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1960	0	1996	20	0
1	C	1972	0	2017	21	0
1	E	1968	0	2011	21	0
1	G	1964	0	2007	15	0
1	I	1961	0	2003	26	0
1	K	1964	0	2007	28	0
1	M	1972	0	2017	16	0
1	O	1968	0	2013	19	0
1	Q	1968	0	2013	25	0
1	S	1967	0	2011	22	0
1	U	1968	0	2013	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	W	1968	0	2011	16	0
2	B	1863	0	1895	36	0
2	D	1905	0	1936	33	0
2	F	1863	0	1895	35	0
2	H	1863	0	1895	39	0
2	J	1863	0	1895	47	0
2	L	1909	0	1940	36	0
2	N	1863	0	1895	34	0
2	P	1907	0	1937	41	0
2	R	1889	0	1921	40	0
2	T	1905	0	1936	37	0
2	V	1883	0	1917	36	0
2	X	1863	0	1895	28	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
3	J	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	1	0
3	N	1	0	0	0	0
3	P	1	0	0	0	0
3	R	1	0	0	0	0
3	T	1	0	0	0	0
3	V	1	0	0	0	0
3	X	1	0	0	0	0
4	A	6	0	0	2	0
4	B	5	0	0	2	0
4	C	4	0	0	1	0
4	D	1	0	0	0	0
4	E	6	0	0	1	0
4	F	4	0	0	0	0
4	G	2	0	0	0	0
4	H	3	0	0	0	0
4	I	1	0	0	1	0
4	J	5	0	0	0	0
4	K	3	0	0	1	0
4	L	3	0	0	2	0
4	M	8	0	0	2	0
4	N	4	0	0	0	0
4	O	9	0	0	3	0
4	P	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Q	4	0	0	1	0
4	R	5	0	0	0	0
4	S	6	0	0	0	0
4	T	4	0	0	0	0
4	U	3	0	0	0	0
4	V	3	0	0	0	0
4	W	2	0	0	1	0
4	X	1	0	0	0	0
All	All	46287	0	47076	610	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 7.

The worst 5 of 610 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)
2:P:110:ALA:HB1	2:P:201:THR:HG23	1.45	0.99
1:A:272:HIS:HD2	4:A:2001:HOH:O	1.49	0.94
2:T:110:ALA:HB1	2:T:201:THR:HG23	1.50	0.91
2:N:110:ALA:HB1	2:N:201:THR:HG23	1.50	0.91
2:L:110:ALA:HB1	2:L:201:THR:HG23	1.54	0.90

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	254/275 (92%)	245 (96%)	7 (3%)	2 (1%)	19 49
1	C	254/275 (92%)	245 (96%)	7 (3%)	2 (1%)	19 49
1	E	254/275 (92%)	247 (97%)	6 (2%)	1 (0%)	34 66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	254/275 (92%)	247 (97%)	5 (2%)	2 (1%)	19	49
1	I	254/275 (92%)	243 (96%)	9 (4%)	2 (1%)	19	49
1	K	254/275 (92%)	245 (96%)	8 (3%)	1 (0%)	34	66
1	M	254/275 (92%)	244 (96%)	9 (4%)	1 (0%)	34	66
1	O	254/275 (92%)	245 (96%)	8 (3%)	1 (0%)	34	66
1	Q	254/275 (92%)	243 (96%)	9 (4%)	2 (1%)	19	49
1	S	254/275 (92%)	248 (98%)	5 (2%)	1 (0%)	34	66
1	U	254/275 (92%)	244 (96%)	8 (3%)	2 (1%)	19	49
1	W	254/275 (92%)	247 (97%)	6 (2%)	1 (0%)	34	66
2	B	239/248 (96%)	227 (95%)	11 (5%)	1 (0%)	34	66
2	D	245/248 (99%)	231 (94%)	12 (5%)	2 (1%)	19	49
2	F	239/248 (96%)	228 (95%)	9 (4%)	2 (1%)	19	49
2	H	239/248 (96%)	227 (95%)	11 (5%)	1 (0%)	34	66
2	J	239/248 (96%)	228 (95%)	10 (4%)	1 (0%)	34	66
2	L	245/248 (99%)	230 (94%)	13 (5%)	2 (1%)	19	49
2	N	239/248 (96%)	227 (95%)	11 (5%)	1 (0%)	34	66
2	P	246/248 (99%)	232 (94%)	12 (5%)	2 (1%)	19	49
2	R	243/248 (98%)	226 (93%)	13 (5%)	4 (2%)	9	31
2	T	245/248 (99%)	229 (94%)	14 (6%)	2 (1%)	19	49
2	V	242/248 (98%)	229 (95%)	11 (4%)	2 (1%)	19	49
2	X	239/248 (96%)	227 (95%)	11 (5%)	1 (0%)	34	66
All	All	5948/6276 (95%)	5684 (96%)	225 (4%)	39 (1%)	22	53

5 of 39 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	105	GLU
1	C	105	GLU
1	E	105	GLU
1	G	105	GLU
1	I	105	GLU

### 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	216/242 (89%)	207 (96%)	9 (4%)	30	63
1	C	219/242 (90%)	210 (96%)	9 (4%)	30	64
1	E	218/242 (90%)	210 (96%)	8 (4%)	34	68
1	G	217/242 (90%)	208 (96%)	9 (4%)	30	64
1	I	216/242 (89%)	210 (97%)	6 (3%)	43	77
1	K	217/242 (90%)	208 (96%)	9 (4%)	30	64
1	M	219/242 (90%)	212 (97%)	7 (3%)	39	73
1	O	218/242 (90%)	210 (96%)	8 (4%)	34	68
1	Q	218/242 (90%)	208 (95%)	10 (5%)	27	60
1	S	218/242 (90%)	208 (95%)	10 (5%)	27	60
1	U	218/242 (90%)	208 (95%)	10 (5%)	27	60
1	W	218/242 (90%)	210 (96%)	8 (4%)	34	68
2	B	199/208 (96%)	188 (94%)	11 (6%)	21	52
2	D	203/208 (98%)	190 (94%)	13 (6%)	17	45
2	F	199/208 (96%)	186 (94%)	13 (6%)	17	44
2	H	199/208 (96%)	186 (94%)	13 (6%)	17	44
2	J	199/208 (96%)	187 (94%)	12 (6%)	19	48
2	L	204/208 (98%)	192 (94%)	12 (6%)	19	49
2	N	199/208 (96%)	188 (94%)	11 (6%)	21	52
2	P	203/208 (98%)	191 (94%)	12 (6%)	19	49
2	R	201/208 (97%)	191 (95%)	10 (5%)	24	56
2	T	203/208 (98%)	190 (94%)	13 (6%)	17	45
2	V	201/208 (97%)	188 (94%)	13 (6%)	17	44
2	X	199/208 (96%)	185 (93%)	14 (7%)	15	40
All	All	5021/5400 (93%)	4771 (95%)	250 (5%)	24	56

5 of 250 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	37	VAL
2	N	201	THR
1	W	195	TYR
2	L	129	THR
1	M	191	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
2	L	178	ASN
1	M	272	HIS
1	W	272	HIS
1	M	9	ASN
1	M	81	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 13 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 [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	260/275 (94%)	0.20	6 (2%) 60 51	23, 32, 46, 60	0
1	C	260/275 (94%)	0.19	1 (0%) 92 91	24, 32, 46, 58	0
1	E	260/275 (94%)	0.15	2 (0%) 86 81	24, 32, 46, 57	0
1	G	260/275 (94%)	0.23	8 (3%) 49 39	24, 32, 46, 58	0
1	I	260/275 (94%)	0.12	1 (0%) 92 91	24, 32, 46, 57	0
1	K	260/275 (94%)	0.21	1 (0%) 92 91	24, 32, 46, 58	0
1	M	260/275 (94%)	0.16	1 (0%) 92 91	24, 32, 46, 58	0
1	O	260/275 (94%)	0.27	5 (1%) 66 59	24, 32, 46, 59	0
1	Q	260/275 (94%)	0.19	2 (0%) 86 81	24, 32, 46, 59	0
1	S	260/275 (94%)	0.15	3 (1%) 79 73	24, 32, 46, 57	0
1	U	260/275 (94%)	0.15	3 (1%) 79 73	24, 32, 46, 58	0
1	W	260/275 (94%)	0.15	3 (1%) 79 73	24, 32, 46, 57	0
2	B	241/248 (97%)	0.17	0 100 100	25, 31, 46, 59	0
2	D	247/248 (99%)	0.20	3 (1%) 79 73	22, 30, 46, 59	0
2	F	241/248 (97%)	0.17	4 (1%) 70 63	25, 31, 47, 59	0
2	H	241/248 (97%)	0.17	3 (1%) 79 73	25, 31, 46, 59	0
2	J	241/248 (97%)	0.16	0 100 100	25, 31, 46, 59	0
2	L	247/248 (99%)	0.21	7 (2%) 53 43	22, 31, 46, 59	0
2	N	241/248 (97%)	0.15	1 (0%) 92 91	25, 31, 46, 59	0
2	P	248/248 (100%)	0.19	2 (0%) 86 81	23, 30, 46, 59	0
2	R	245/248 (98%)	0.28	3 (1%) 79 73	23, 31, 46, 59	0
2	T	247/248 (99%)	0.20	2 (0%) 86 81	23, 31, 46, 59	0
2	V	244/248 (98%)	0.17	1 (0%) 92 91	25, 31, 46, 59	0
2	X	241/248 (97%)	0.16	1 (0%) 92 91	25, 31, 46, 59	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	6044/6276 (96%)	0.18	63 (1%) 82 77	22, 31, 47, 60	0

The worst 5 of 63 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	248	VAL	4.6
2	F	247	GLY	3.9
1	G	181	SER	3.6
1	E	175	GLN	3.4
1	U	275	ILE	3.4

## 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 carbohydrates in this entry.

## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
3	CL	D	1249	1/1	0.76	0.15	49,49,49,49	0
3	CL	L	1249	1/1	0.84	0.20	45,45,45,45	0
3	CL	N	1249	1/1	0.85	0.19	56,56,56,56	0
3	CL	B	1249	1/1	0.86	0.20	67,67,67,67	0
3	CL	F	1249	1/1	0.90	0.17	48,48,48,48	0
3	CL	X	1249	1/1	0.90	0.16	43,43,43,43	0
3	CL	P	1249	1/1	0.93	0.09	59,59,59,59	0
3	CL	V	1249	1/1	0.94	0.17	52,52,52,52	0
3	CL	T	1249	1/1	0.94	0.14	50,50,50,50	0
3	CL	M	1276	1/1	0.94	0.12	45,45,45,45	0
3	CL	J	1249	1/1	0.95	0.17	47,47,47,47	0
3	CL	R	1249	1/1	0.95	0.15	46,46,46,46	0
3	CL	H	1249	1/1	0.96	0.17	52,52,52,52	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.