



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2018 – 11:09 pm GMT

PDB ID : 2C39
Title : RNase PH core of the archaeal exosome in complex with ADP
Authors : Lorentzen, E.; Conti, E.
Deposited on : 2005-10-05
Resolution : 3.30 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
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

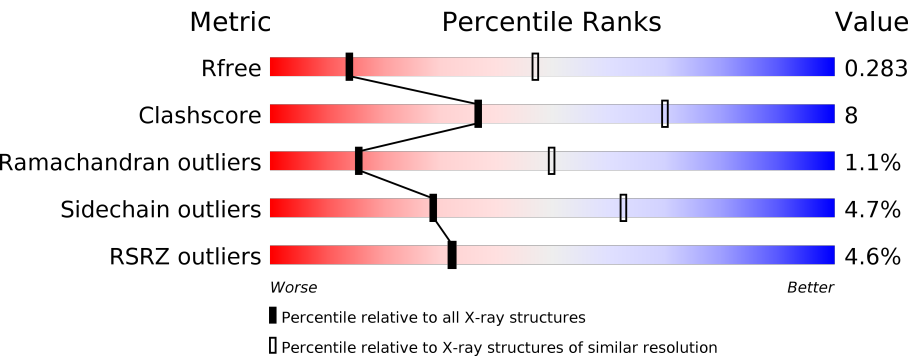
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	111664	1168 (3.36-3.24)
Clashscore	122126	1022 (3.34-3.26)
Ramachandran outliers	120053	1004 (3.34-3.26)
Sidechain outliers	120020	1003 (3.34-3.26)
RSRZ outliers	108989	1133 (3.36-3.24)

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. 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>81%13%5%</div></div>
1	C	275	<div><div>2%</div><div>75%19%5%</div></div>
1	E	275	<div><div>2%</div><div>77%17%5%</div></div>
1	G	275	<div><div>5%</div><div>77%16%5%</div></div>
1	I	275	<div><div>7%</div><div>78%16%5%</div></div>
1	K	275	<div><div>2%</div><div>73%21%5%</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 3 unique types of molecules in this entry. The entry contains 45814 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 PROBABLE EXOSOME COMPLEX EXONUCLEASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			1944	1239	320	380	5			
1	C	260	Total	C	N	O	S	0	0	0
			1947	1243	321	378	5			
1	E	260	Total	C	N	O	S	0	0	0
			1968	1253	325	385	5			
1	G	260	Total	C	N	O	S	0	0	0
			1961	1250	323	383	5			
1	I	260	Total	C	N	O	S	0	0	0
			1954	1247	323	379	5			
1	K	260	Total	C	N	O	S	0	0	0
			1958	1249	323	381	5			
1	M	260	Total	C	N	O	S	0	0	0
			1960	1249	324	382	5			
1	O	260	Total	C	N	O	S	0	0	0
			1951	1246	323	377	5			
1	Q	260	Total	C	N	O	S	0	0	0
			1953	1245	322	381	5			
1	S	259	Total	C	N	O	S	0	0	0
			1955	1245	323	382	5			
1	U	255	Total	C	N	O	S	0	0	0
			1908	1219	317	367	5			
1	W	259	Total	C	N	O	S	0	0	0
			1950	1245	322	378	5			

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

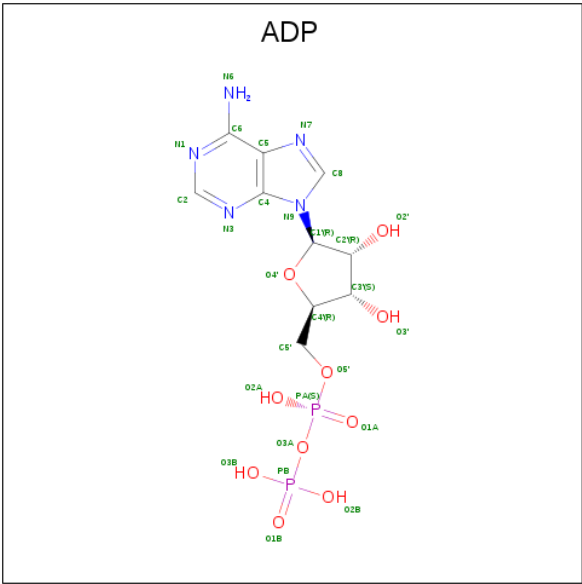
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	241	Total	C	N	O	S	0	0	0
			1812	1145	317	340	10			
2	D	248	Total	C	N	O	S	0	0	0
			1900	1198	330	360	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	241	Total	C	N	O	S	0	0	0
			1838	1161	317	350	10			
2	H	230	Total	C	N	O	S	0	0	0
			1732	1094	302	327	9			
2	J	241	Total	C	N	O	S	0	0	0
			1844	1165	321	348	10			
2	L	247	Total	C	N	O	S	0	0	0
			1890	1194	328	357	11			
2	N	239	Total	C	N	O	S	0	0	0
			1809	1144	313	342	10			
2	P	248	Total	C	N	O	S	0	0	0
			1904	1202	332	358	12			
2	R	248	Total	C	N	O	S	0	0	0
			1880	1188	332	348	12			
2	T	248	Total	C	N	O	S	0	0	0
			1884	1193	328	351	12			
2	V	239	Total	C	N	O	S	0	0	0
			1815	1148	318	339	10			
2	X	239	Total	C	N	O	S	0	0	0
			1821	1148	315	348	10			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



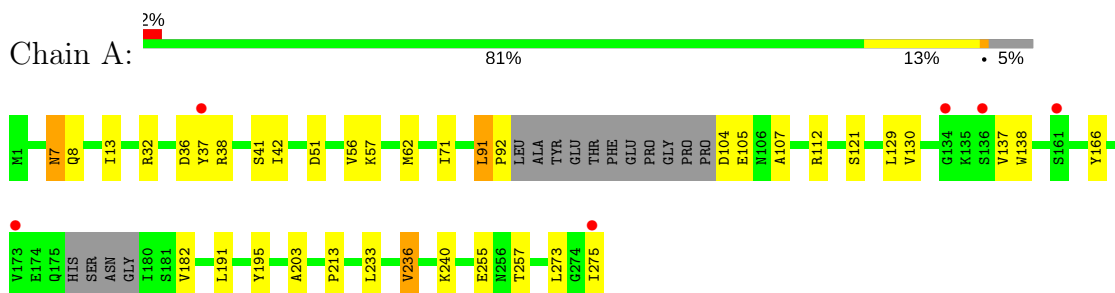
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	F	1	Total	C	O	P		0	0
			17	5	10	2			
3	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	J	1	Total	O	P			0	0
			9	7	2				
3	L	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	N	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	P	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	R	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	T	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	V	1	Total	C	O	P		0	0
			17	5	10	2			
3	X	1	Total	C	O	P		0	0
			17	5	10	2			

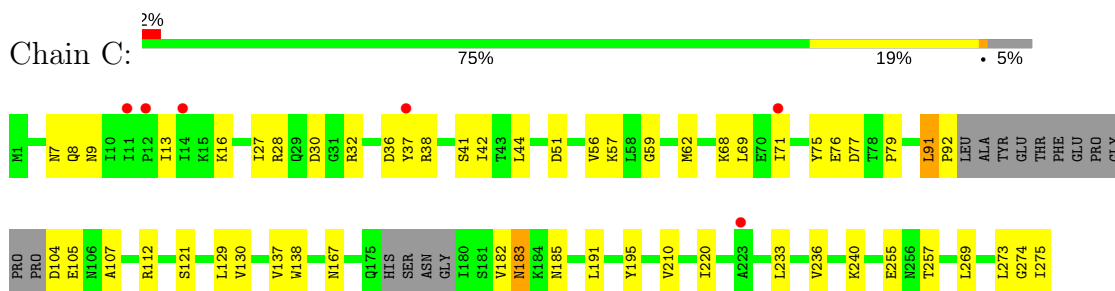
3 Residue-property plots [i](#)

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.

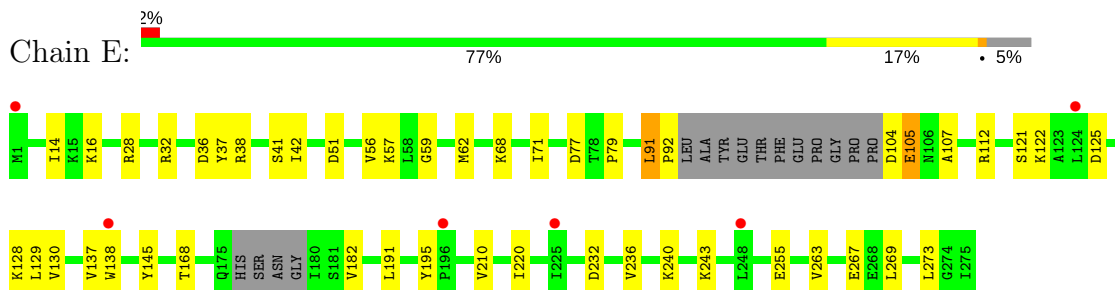
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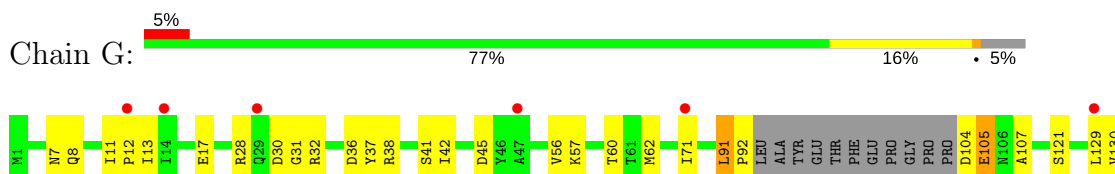
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• Molecule 1: PROBABLE EXOSOME COMPLEX EXONUCLEASE 2

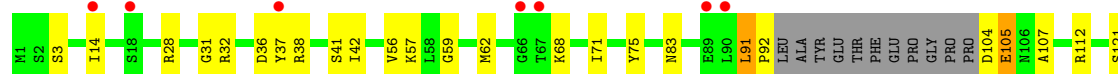
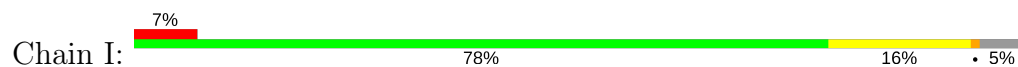


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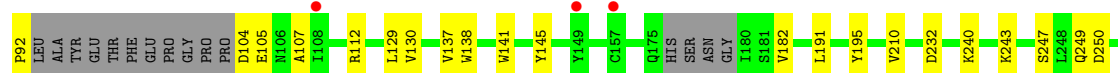
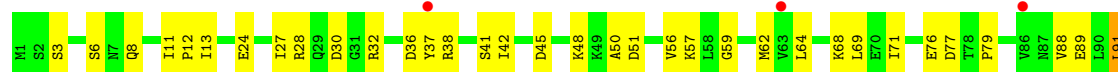




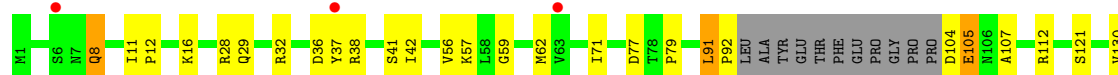
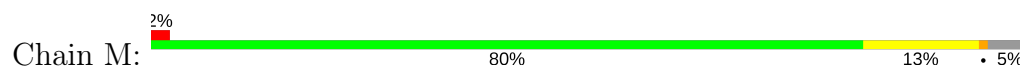
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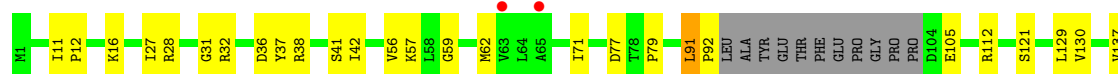
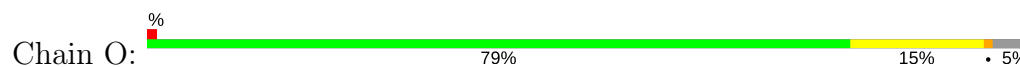
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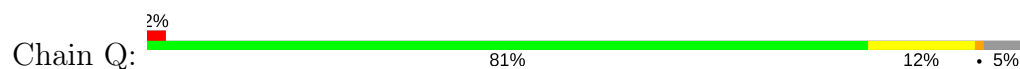
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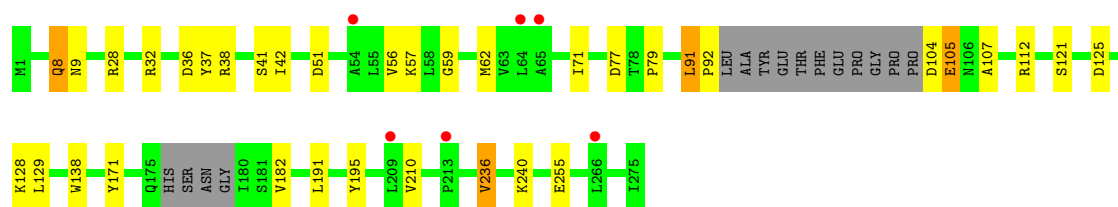


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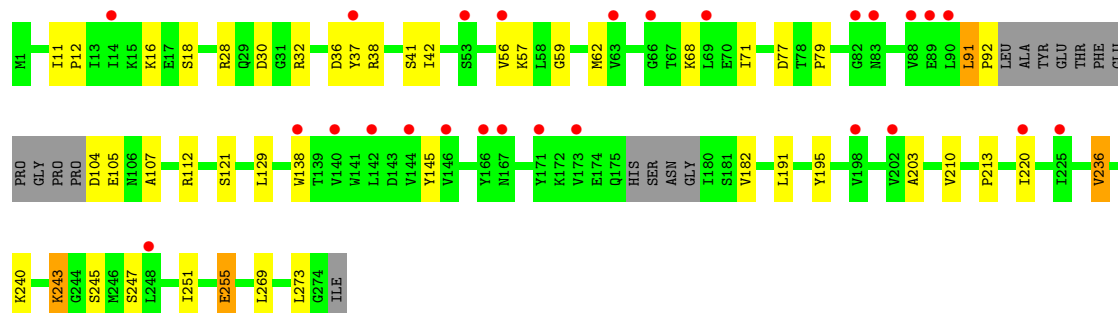
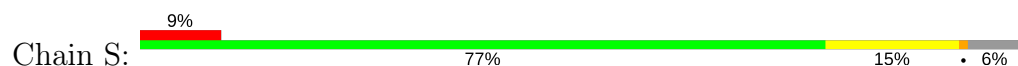


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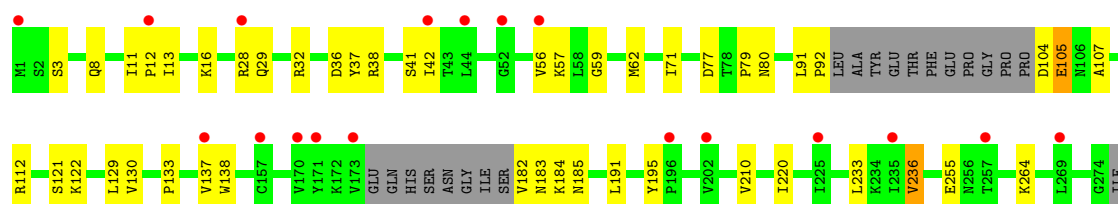
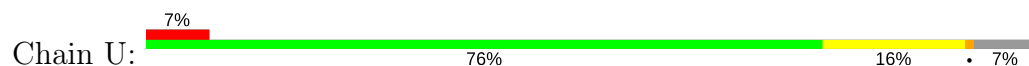




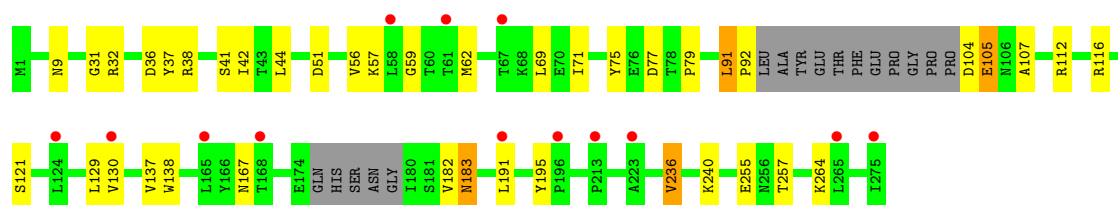
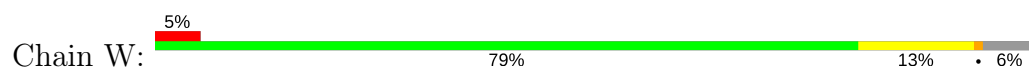
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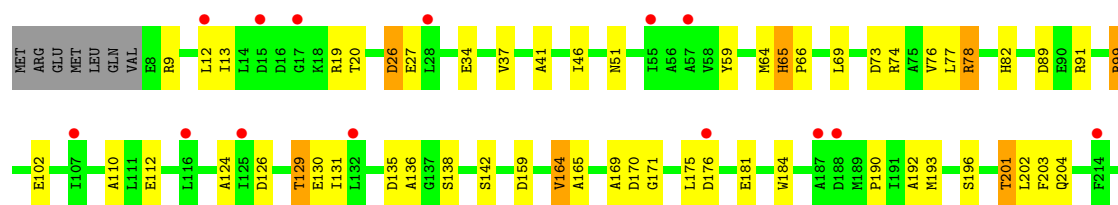
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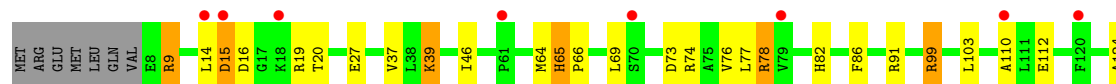


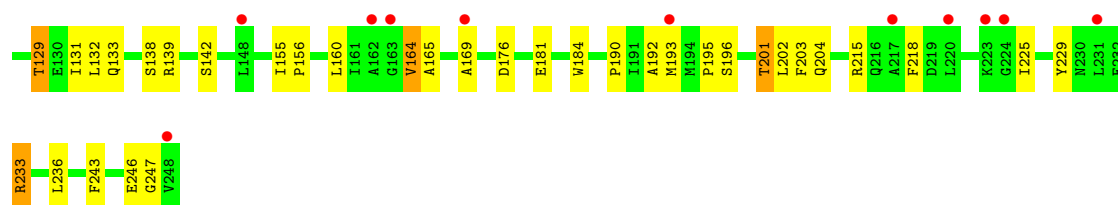
• Molecule 1: PROBABLE EXOSOME COMPLEX EXONUCLEASE 2



• Molecule 2: PROBABLE EXOSOME COMPLEX EXONUCLEASE 1







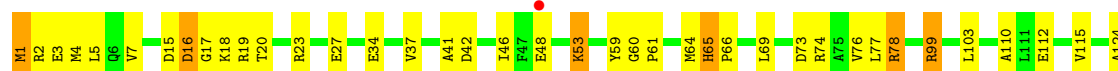
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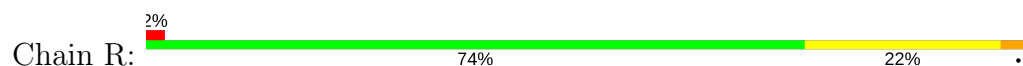
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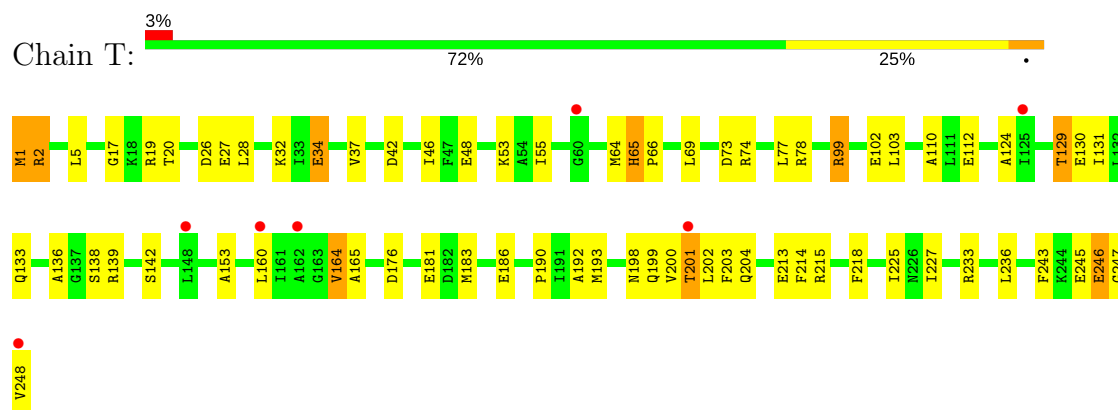
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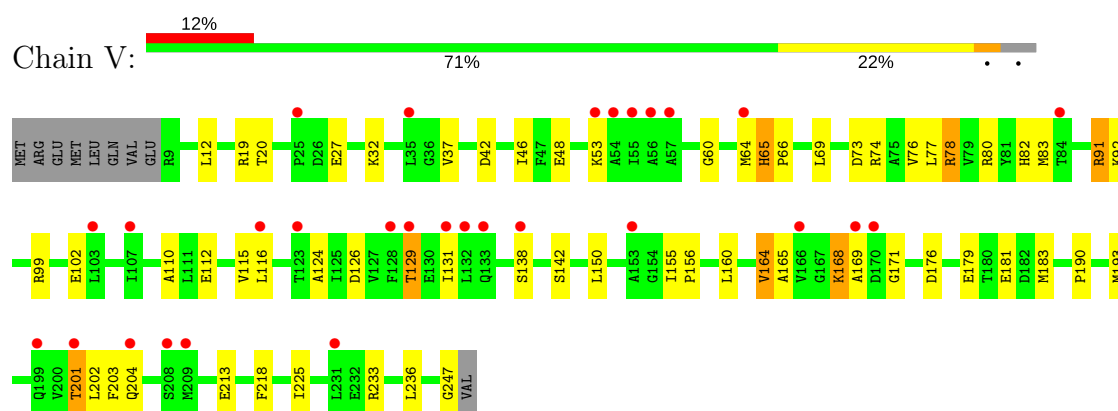
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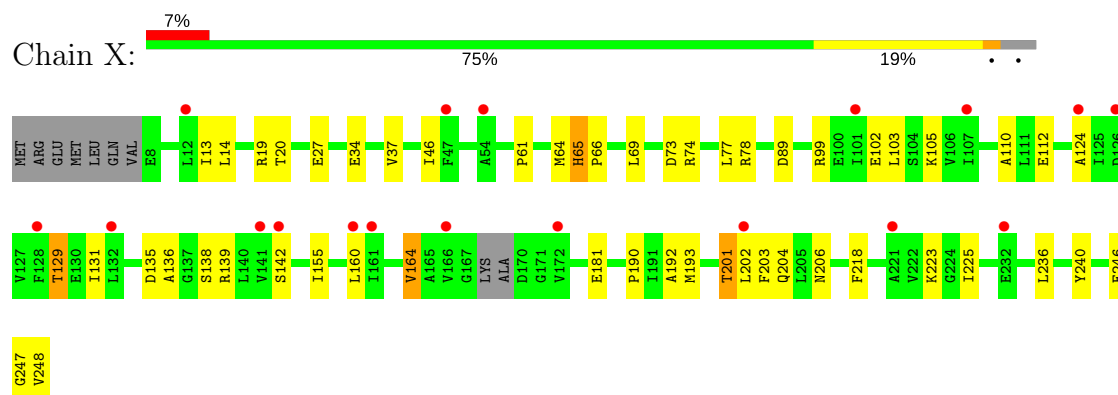
• Molecule 2: PROBABLE EXOSOME COMPLEX EXONUCLEASE 1



• Molecule 2: PROBABLE EXOSOME COMPLEX EXONUCLEASE 1



• Molecule 2: PROBABLE EXOSOME COMPLEX EXONUCLEASE 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	206.20Å 214.00Å 432.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	93.25 – 3.30 93.06 – 3.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (93.25-3.30) 93.5 (93.06-3.30)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.274 , 0.295 0.265 , 0.283	Depositor DCC
R_{free} test set	4015 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	86.3	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 21.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.048 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	45814	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.35% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.47	0/1969	0.58	0/2678
1	C	0.54	0/1972	0.59	0/2680
1	E	0.47	0/1993	0.58	0/2706
1	G	0.49	0/1986	0.57	0/2697
1	I	0.44	0/1979	0.56	0/2688
1	K	0.54	0/1983	0.60	0/2693
1	M	0.49	0/1985	0.58	0/2696
1	O	0.52	0/1976	0.60	0/2684
1	Q	0.49	0/1978	0.58	0/2688
1	S	0.47	0/1980	0.58	0/2690
1	U	0.43	0/1933	0.58	0/2628
1	W	0.47	0/1975	0.57	0/2682
2	B	0.45	0/1840	0.60	0/2494
2	D	0.51	0/1928	0.64	0/2606
2	F	0.47	0/1866	0.60	0/2524
2	H	0.45	0/1757	0.59	0/2377
2	J	0.46	0/1872	0.58	0/2530
2	L	0.51	0/1918	0.65	0/2592
2	N	0.48	0/1837	0.60	0/2487
2	P	0.51	0/1932	0.65	0/2609
2	R	0.50	0/1908	0.65	1/2578 (0.0%)
2	T	0.49	0/1912	0.63	0/2584
2	V	0.47	0/1843	0.60	0/2494
2	X	0.46	0/1848	0.60	0/2501
All	All	0.48	0/46170	0.60	1/62586 (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
2	D	0	2
2	L	0	1
2	P	0	1
2	R	0	2
2	T	0	1
All	All	0	7

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	R	4	MET	N-CA-C	-5.96	94.91	111.00

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	1	MET	Peptide
2	D	17	GLY	Peptide
2	L	17	GLY	Peptide
2	P	17	GLY	Peptide
2	R	5	LEU	Peptide

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	1944	0	1969	20	0
1	C	1947	0	1982	30	0
1	E	1968	0	2013	35	0
1	G	1961	0	2003	33	0
1	I	1954	0	1997	33	0
1	K	1958	0	2001	35	0
1	M	1960	0	2003	20	0
1	O	1951	0	1995	23	0
1	Q	1953	0	1988	23	0
1	S	1955	0	1996	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	U	1908	0	1950	26	0
1	W	1950	0	1997	25	0
2	B	1812	0	1810	41	0
2	D	1900	0	1920	45	0
2	F	1838	0	1852	47	0
2	H	1732	0	1740	49	0
2	J	1844	0	1870	47	0
2	L	1890	0	1915	50	0
2	N	1809	0	1817	41	0
2	P	1904	0	1938	47	0
2	R	1880	0	1904	39	0
2	T	1884	0	1913	49	0
2	V	1815	0	1836	41	0
2	X	1821	0	1820	31	0
3	B	27	0	12	5	0
3	D	27	0	12	3	0
3	F	17	0	7	1	0
3	H	27	0	12	2	0
3	J	9	0	0	1	0
3	L	27	0	12	3	0
3	N	27	0	12	3	0
3	P	27	0	12	3	0
3	R	27	0	12	0	0
3	T	27	0	12	3	0
3	V	17	0	7	2	0
3	X	17	0	7	0	0
All	All	45814	0	46346	777	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 8.

The worst 5 of 777 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:T:1:MET:H2	2:T:2:ARG:HA	1.24	1.00
2:T:1:MET:N	2:T:2:ARG:HA	1.75	1.00
1:E:243:LYS:HG2	2:F:112:GLU:OE1	1.61	0.98
1:G:249:GLN:H	1:G:249:GLN:HE21	1.18	0.90
2:P:99:ARG:NH1	3:P:404:ADP:O2A	2.07	0.87

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	254/275 (92%)	241 (95%)	10 (4%)	3 (1%)	14	47
1	C	254/275 (92%)	240 (94%)	8 (3%)	6 (2%)	6	32
1	E	254/275 (92%)	241 (95%)	11 (4%)	2 (1%)	21	55
1	G	254/275 (92%)	239 (94%)	11 (4%)	4 (2%)	11	41
1	I	254/275 (92%)	242 (95%)	10 (4%)	2 (1%)	21	55
1	K	254/275 (92%)	240 (94%)	11 (4%)	3 (1%)	14	47
1	M	254/275 (92%)	240 (94%)	11 (4%)	3 (1%)	14	47
1	O	254/275 (92%)	245 (96%)	7 (3%)	2 (1%)	21	55
1	Q	254/275 (92%)	238 (94%)	13 (5%)	3 (1%)	14	47
1	S	253/275 (92%)	242 (96%)	9 (4%)	2 (1%)	21	55
1	U	249/275 (90%)	236 (95%)	11 (4%)	2 (1%)	21	55
1	W	253/275 (92%)	241 (95%)	9 (4%)	3 (1%)	14	47
2	B	239/248 (96%)	221 (92%)	15 (6%)	3 (1%)	13	45
2	D	246/248 (99%)	231 (94%)	10 (4%)	5 (2%)	8	37
2	F	239/248 (96%)	226 (95%)	10 (4%)	3 (1%)	13	45
2	H	226/248 (91%)	216 (96%)	8 (4%)	2 (1%)	19	53
2	J	239/248 (96%)	225 (94%)	10 (4%)	4 (2%)	10	40
2	L	245/248 (99%)	231 (94%)	13 (5%)	1 (0%)	36	69
2	N	237/248 (96%)	224 (94%)	12 (5%)	1 (0%)	36	69
2	P	246/248 (99%)	230 (94%)	13 (5%)	3 (1%)	14	47
2	R	246/248 (99%)	230 (94%)	13 (5%)	3 (1%)	14	47
2	T	246/248 (99%)	233 (95%)	11 (4%)	2 (1%)	21	55
2	V	237/248 (96%)	218 (92%)	15 (6%)	4 (2%)	10	40
2	X	235/248 (95%)	223 (95%)	11 (5%)	1 (0%)	36	69
All	All	5922/6276 (94%)	5593 (94%)	262 (4%)	67 (1%)	16	50

5 of 67 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	8	GLN
2	J	15	ASP
2	P	16	ASP
1	Q	8	GLN
2	V	91	ARG

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	212/242 (88%)	202 (95%)	10 (5%)	29	62
1	C	212/242 (88%)	204 (96%)	8 (4%)	36	67
1	E	218/242 (90%)	213 (98%)	5 (2%)	53	78
1	G	216/242 (89%)	206 (95%)	10 (5%)	29	63
1	I	214/242 (88%)	209 (98%)	5 (2%)	53	78
1	K	215/242 (89%)	204 (95%)	11 (5%)	26	60
1	M	216/242 (89%)	206 (95%)	10 (5%)	29	63
1	O	213/242 (88%)	205 (96%)	8 (4%)	36	67
1	Q	214/242 (88%)	208 (97%)	6 (3%)	47	74
1	S	216/242 (89%)	208 (96%)	8 (4%)	37	68
1	U	208/242 (86%)	199 (96%)	9 (4%)	32	65
1	W	214/242 (88%)	207 (97%)	7 (3%)	41	71
2	B	186/208 (89%)	176 (95%)	10 (5%)	24	58
2	D	200/208 (96%)	186 (93%)	14 (7%)	16	48
2	F	193/208 (93%)	182 (94%)	11 (6%)	23	56
2	H	179/208 (86%)	169 (94%)	10 (6%)	23	57
2	J	194/208 (93%)	184 (95%)	10 (5%)	25	59
2	L	199/208 (96%)	187 (94%)	12 (6%)	21	54
2	N	188/208 (90%)	182 (97%)	6 (3%)	42	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	201/208 (97%)	186 (92%)	15 (8%)	15	44
2	R	194/208 (93%)	184 (95%)	10 (5%)	25	59
2	T	196/208 (94%)	182 (93%)	14 (7%)	16	47
2	V	189/208 (91%)	182 (96%)	7 (4%)	37	68
2	X	191/208 (92%)	180 (94%)	11 (6%)	22	55
All	All	4878/5400 (90%)	4651 (95%)	227 (5%)	29	62

5 of 227 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	257	THR
2	N	20	THR
1	W	37	TYR
2	L	20	THR
2	L	233	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
2	L	40	ASN
2	L	178	ASN
1	S	29	GLN
2	J	82	HIS
2	T	82	HIS

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

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	B	404	-	25,29,29	1.24	4 (16%)	25,45,45	1.66	2 (8%)
3	ADP	D	404	2	25,29,29	1.18	3 (12%)	25,45,45	2.00	3 (12%)
3	ADP	F	404	-	16,17,29	1.66	3 (18%)	18,26,45	1.17	1 (5%)
3	ADP	H	404	-	25,29,29	1.10	2 (8%)	25,45,45	1.79	3 (12%)
3	ADP	J	404	-	8,8,29	1.27	2 (25%)	9,13,45	1.23	1 (11%)
3	ADP	L	404	-	25,29,29	1.12	2 (8%)	25,45,45	1.92	4 (16%)
3	ADP	N	404	-	25,29,29	1.22	3 (12%)	25,45,45	1.72	3 (12%)
3	ADP	P	404	-	25,29,29	1.12	3 (12%)	25,45,45	2.10	4 (16%)
3	ADP	R	404	2	25,29,29	1.20	3 (12%)	25,45,45	1.61	4 (16%)
3	ADP	T	404	-	25,29,29	1.05	2 (8%)	25,45,45	1.74	4 (16%)
3	ADP	V	404	-	16,17,29	0.96	1 (6%)	18,26,45	1.27	2 (11%)
3	ADP	X	404	-	16,17,29	1.89	2 (12%)	18,26,45	1.53	3 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	B	404	-	-	0/12/32/32	0/3/3/3
3	ADP	D	404	2	-	0/12/32/32	0/3/3/3
3	ADP	F	404	-	-	0/12/25/32	0/1/1/3
3	ADP	H	404	-	-	0/12/32/32	0/3/3/3
3	ADP	J	404	-	-	0/6/6/32	0/0/0/3
3	ADP	L	404	-	-	0/12/32/32	0/3/3/3
3	ADP	N	404	-	-	0/12/32/32	0/3/3/3
3	ADP	P	404	-	-	0/12/32/32	0/3/3/3
3	ADP	R	404	2	-	0/12/32/32	0/3/3/3
3	ADP	T	404	-	-	0/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	V	404	-	-	0/12/25/32	0/1/1/3
3	ADP	X	404	-	-	0/12/25/32	0/1/1/3

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	404	ADP	C8-N9	-2.07	1.34	1.36
3	J	404	ADP	PB-O3A	2.04	1.63	1.60
3	T	404	ADP	C2-N3	2.06	1.35	1.32
3	F	404	ADP	PB-O3A	2.09	1.63	1.60
3	J	404	ADP	PA-O3A	2.10	1.63	1.60

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	404	ADP	N3-C2-N1	-7.64	122.33	128.86
3	D	404	ADP	N3-C2-N1	-7.09	122.80	128.86
3	N	404	ADP	N3-C2-N1	-6.80	123.05	128.86
3	H	404	ADP	N3-C2-N1	-6.65	123.17	128.86
3	B	404	ADP	N3-C2-N1	-6.49	123.31	128.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	404	ADP	5	0
3	D	404	ADP	3	0
3	F	404	ADP	1	0
3	H	404	ADP	2	0
3	J	404	ADP	1	0
3	L	404	ADP	3	0
3	N	404	ADP	3	0
3	P	404	ADP	3	0
3	T	404	ADP	3	0
3	V	404	ADP	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	260/275 (94%)	0.57	6 (2%) 60 59	46, 53, 67, 74	0
1	C	260/275 (94%)	0.68	6 (2%) 60 59	46, 53, 67, 75	0
1	E	260/275 (94%)	0.59	6 (2%) 60 59	46, 53, 67, 74	0
1	G	260/275 (94%)	0.64	14 (5%) 26 25	46, 53, 67, 74	0
1	I	260/275 (94%)	0.67	18 (6%) 17 18	46, 53, 67, 73	0
1	K	260/275 (94%)	0.75	6 (2%) 60 59	46, 53, 67, 75	0
1	M	260/275 (94%)	0.63	6 (2%) 60 59	46, 53, 67, 75	0
1	O	260/275 (94%)	0.69	3 (1%) 79 78	46, 53, 67, 75	0
1	Q	260/275 (94%)	0.64	6 (2%) 60 59	46, 53, 67, 74	0
1	S	259/275 (94%)	0.73	26 (10%) 7 7	46, 53, 67, 73	0
1	U	255/275 (92%)	0.72	18 (7%) 16 17	46, 53, 67, 73	0
1	W	259/275 (94%)	0.74	13 (5%) 29 28	46, 53, 67, 75	0
2	B	241/248 (97%)	0.75	16 (6%) 18 19	46, 52, 68, 80	0
2	D	248/248 (100%)	0.68	8 (3%) 47 46	45, 52, 68, 80	0
2	F	241/248 (97%)	0.65	11 (4%) 32 32	46, 52, 68, 80	0
2	H	230/248 (92%)	0.86	23 (10%) 7 7	46, 52, 69, 80	0
2	J	241/248 (97%)	0.78	19 (7%) 12 13	46, 52, 68, 80	0
2	L	247/248 (99%)	0.67	5 (2%) 65 64	45, 52, 68, 80	0
2	N	239/248 (96%)	0.65	4 (1%) 70 68	46, 52, 69, 79	0
2	P	248/248 (100%)	0.71	6 (2%) 59 56	45, 52, 68, 80	0
2	R	248/248 (100%)	0.65	4 (1%) 72 70	45, 52, 69, 80	0
2	T	248/248 (100%)	0.67	7 (2%) 53 52	45, 52, 69, 79	0
2	V	239/248 (96%)	0.92	29 (12%) 4 4	46, 52, 68, 79	0
2	X	239/248 (96%)	0.68	18 (7%) 14 15	46, 52, 69, 79	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	6022/6276 (95%)	0.70	278 (4%) 32 32	45, 52, 68, 80	0

The worst 5 of 278 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	U	171	TYR	5.0
2	V	132	LEU	4.7
2	L	248	VAL	4.6
1	S	138	TRP	4.5
1	S	90	LEU	4.4

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, 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(Å ²)	Q<0.9
3	ADP	H	404	27/27	0.86	0.24	116,117,119,119	0
3	ADP	V	404	17/27	0.86	0.28	90,93,95,95	0
3	ADP	F	404	17/27	0.88	0.22	91,94,95,95	0
3	ADP	X	404	17/27	0.88	0.20	86,87,89,89	0
3	ADP	J	404	9/27	0.92	0.14	100,100,101,101	0
3	ADP	N	404	27/27	0.92	0.25	59,62,64,64	0
3	ADP	B	404	27/27	0.93	0.20	79,90,95,95	0
3	ADP	R	404	27/27	0.95	0.22	47,55,58,58	0
3	ADP	L	404	27/27	0.95	0.23	52,54,56,58	0
3	ADP	D	404	27/27	0.95	0.25	48,50,51,51	0
3	ADP	T	404	27/27	0.96	0.24	55,60,63,63	0
3	ADP	P	404	27/27	0.97	0.23	33,39,41,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.