



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 13, 2018 – 11:02 pm GMT

PDB ID : 5O7X
Title : CRYSTAL STRUCTURE OF S. CEREVISIAE CORE FACTOR AT 3.2A RESOLUTION
Authors : Engel, C.; Gubbey, T.; Neyer, S.; Sainsbury, S.; Oberthuer, C.; Baejen, C.; Bernecky, C.; Cramer, P.
Deposited on : 2017-06-09
Resolution : 3.20 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	:	trunk31020
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)	:	trunk31020

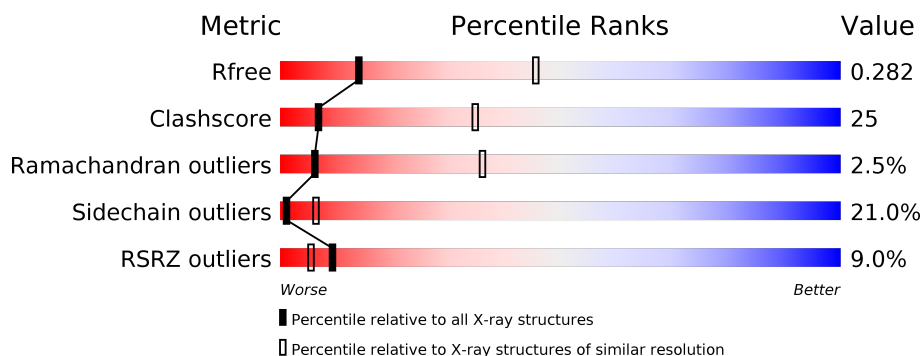
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1121 (3.22-3.18)
Clashscore	122126	1091 (3.20-3.20)
Ramachandran outliers	120053	1074 (3.20-3.20)
Sidechain outliers	120020	1073 (3.20-3.20)
RSRZ outliers	108989	1083 (3.22-3.18)

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	894	<div> <div>7%</div> <div> <div></div> <div>30%</div> <div>27%</div> <div>9%</div> <div>•</div> <div>33%</div> </div> </div>
1	D	894	<div> <div>6%</div> <div> <div></div> <div>30%</div> <div>27%</div> <div>9%</div> <div>•</div> <div>33%</div> </div> </div>
1	G	894	<div> <div>7%</div> <div> <div></div> <div>30%</div> <div>27%</div> <div>9%</div> <div>•</div> <div>33%</div> </div> </div>
1	J	894	<div> <div>6%</div> <div> <div></div> <div>30%</div> <div>27%</div> <div>9%</div> <div>•</div> <div>33%</div> </div> </div>
1	M	894	<div> <div>6%</div> <div> <div></div> <div>30%</div> <div>27%</div> <div>9%</div> <div>•</div> <div>33%</div> </div> </div>
1	P	894	<div> <div>7%</div> <div> <div></div> <div>30%</div> <div>27%</div> <div>9%</div> <div>•</div> <div>33%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	B	514	
2	E	514	
2	H	514	
2	K	514	
2	N	514	
2	Q	514	
3	C	507	
3	F	507	
3	I	507	
3	L	507	
3	O	507	
3	R	507	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	A	1005	-	-	-	X
4	SO4	D	1004	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 63438 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 RNA polymerase I-specific transcription initiation factor RRN6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	598	Total	C	N	O	S	0	0	0
			4856	3092	824	929	11			
1	D	598	Total	C	N	O	S	0	0	0
			4856	3092	824	929	11			
1	G	598	Total	C	N	O	S	0	0	0
			4856	3092	824	929	11			
1	J	598	Total	C	N	O	S	0	0	0
			4856	3092	824	929	11			
1	M	598	Total	C	N	O	S	0	0	0
			4856	3092	824	929	11			
1	P	598	Total	C	N	O	S	0	0	0
			4856	3092	824	929	11			

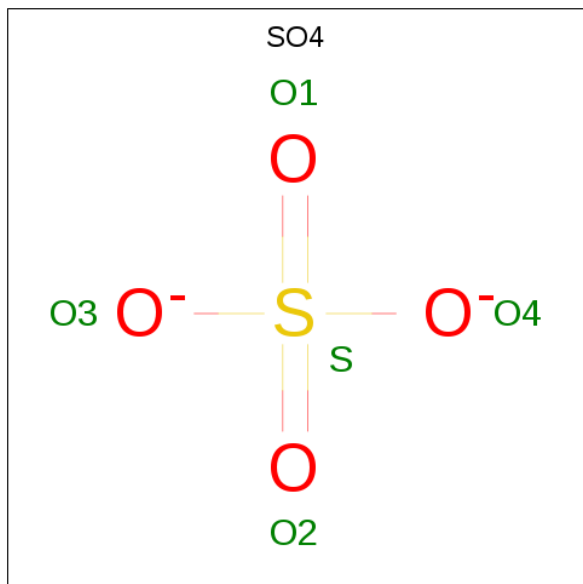
- Molecule 2 is a protein called RNA polymerase I-specific transcription initiation factor RRN7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	377	Total	C	N	O	S	0	0	0
			3156	2055	526	559	16			
2	E	377	Total	C	N	O	S	0	0	0
			3156	2055	526	559	16			
2	H	377	Total	C	N	O	S	0	0	0
			3156	2055	526	559	16			
2	K	377	Total	C	N	O	S	0	0	0
			3156	2055	526	559	16			
2	N	377	Total	C	N	O	S	0	0	0
			3156	2055	526	559	16			
2	Q	377	Total	C	N	O	S	0	0	0
			3156	2055	526	559	16			

- Molecule 3 is a protein called RNA polymerase I-specific transcription initiation factor RRN11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	303	Total	C	N	O	S	0	0	0
			2535	1634	456	434	11			
3	F	303	Total	C	N	O	S	0	0	0
			2535	1634	456	434	11			
3	I	303	Total	C	N	O	S	0	0	0
			2535	1634	456	434	11			
3	L	303	Total	C	N	O	S	0	0	0
			2535	1634	456	434	11			
3	O	303	Total	C	N	O	S	0	0	0
			2535	1634	456	434	11			
3	R	303	Total	C	N	O	S	0	0	0
			2535	1634	456	434	11			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	K	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		
4	M	1	Total	O	S	0	0
			5	4	1		
4	M	1	Total	O	S	0	0
			5	4	1		
4	M	1	Total	O	S	0	0
			5	4	1		
4	M	1	Total	O	S	0	0
			5	4	1		
4	O	1	Total	O	S	0	0
			5	4	1		
4	P	1	Total	O	S	0	0
			5	4	1		
4	P	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	P	1	Total	O	S	0	0
			5	4	1		
4	P	1	Total	O	S	0	0
			5	4	1		
4	P	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	P	1	Total	Mg	0	0
			1	1		
5	G	1	Total	Mg	0	0
			1	1		
5	J	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		
5	A	1	Total	Mg	0	0
			1	1		
5	M	1	Total	Mg	0	0
			1	1		

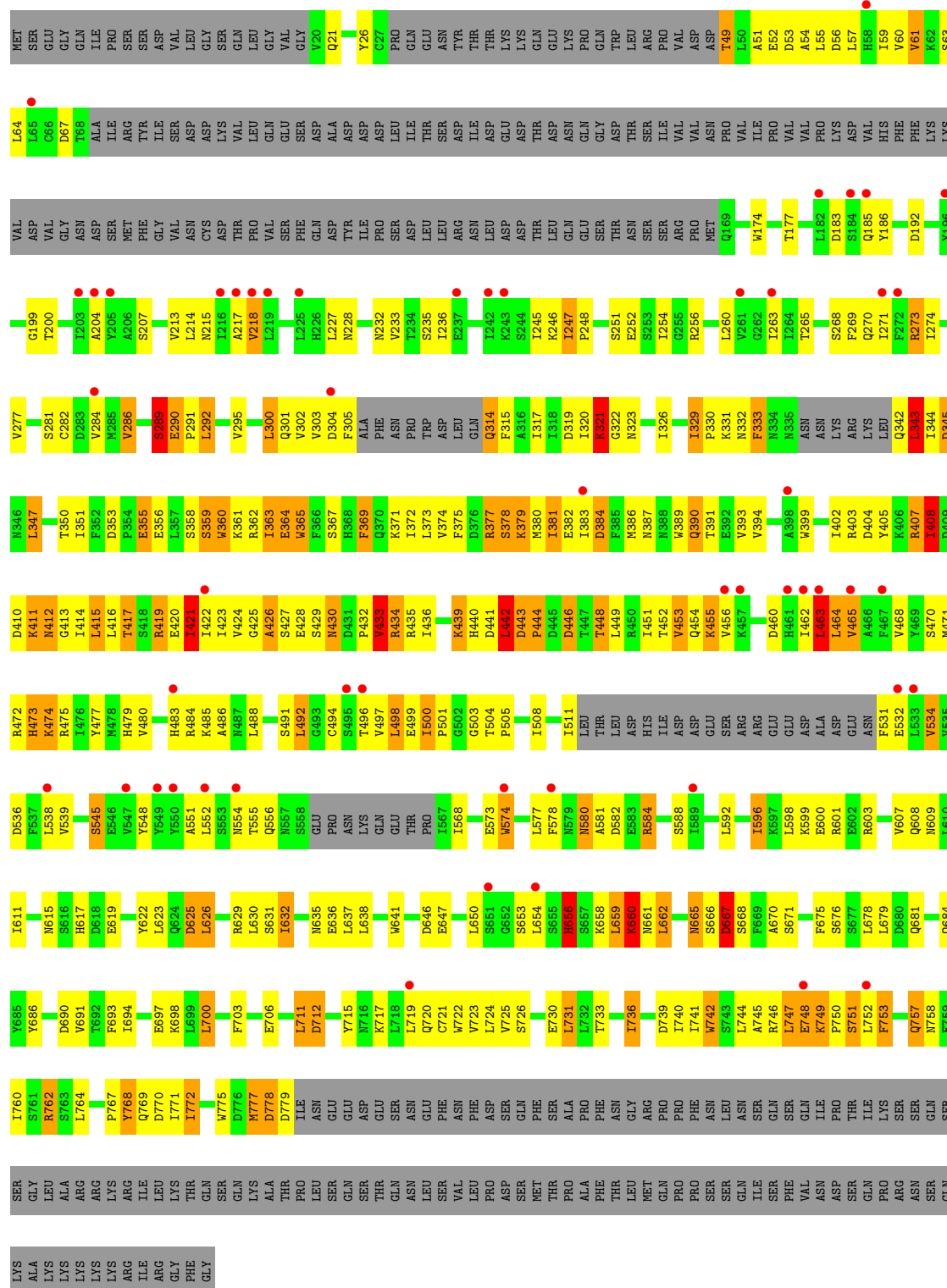
Chain G:



ASN
SER
GLN
LYS
LYS
ALA
GLN
LYS
LYS
LYS
LYS
ARG
ARG
ILE
GLY
PHE
GLY

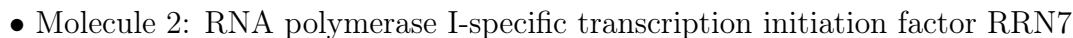
• Molecule 1: RNA polymerase I-specific transcription initiation factor RRN6

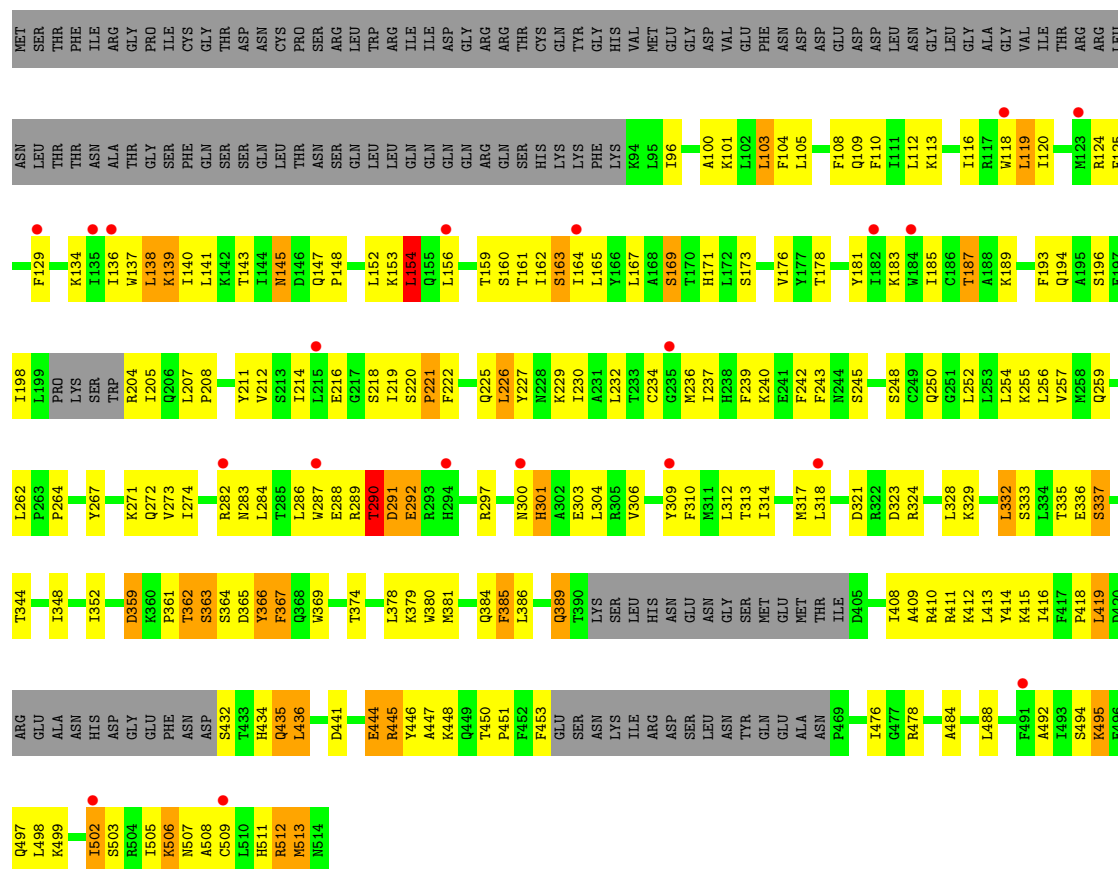
Chain J:  6% 30% 27% 9% 33%



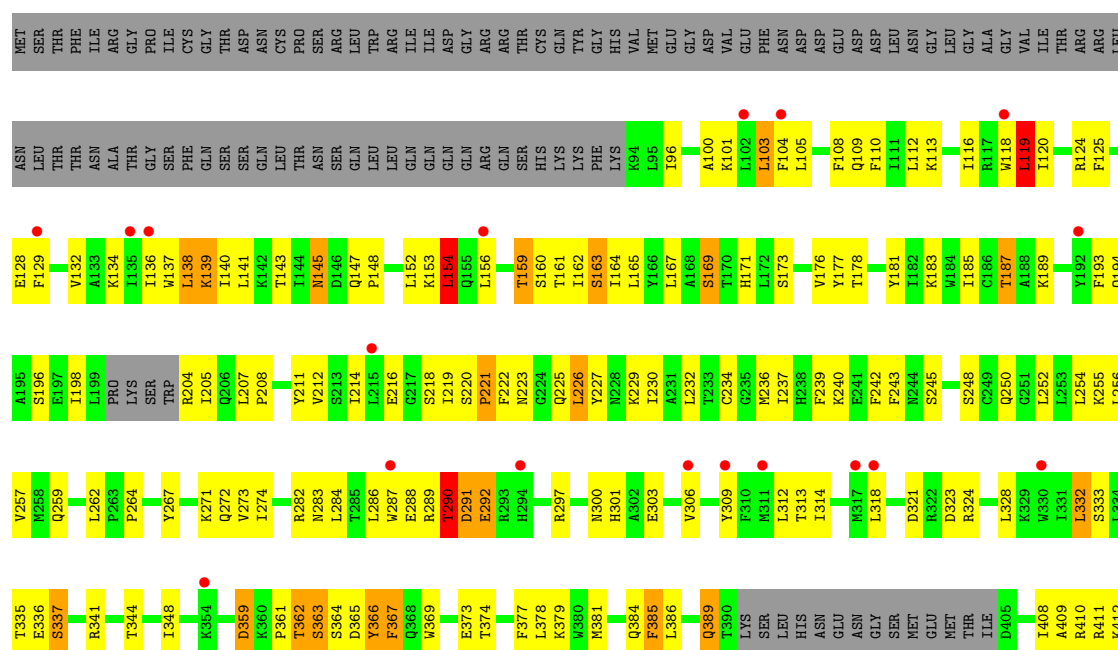
[illegible]

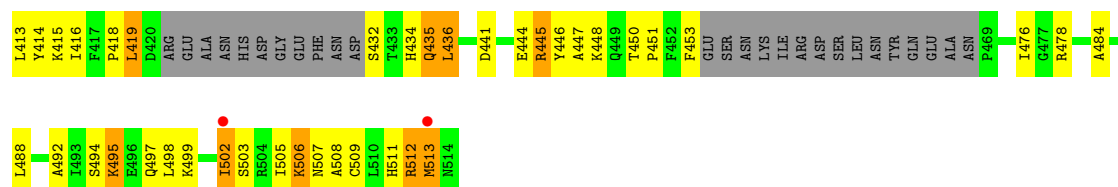
- Molecule 1: RNA polymerase I-specific transcription initiation factor RRN6



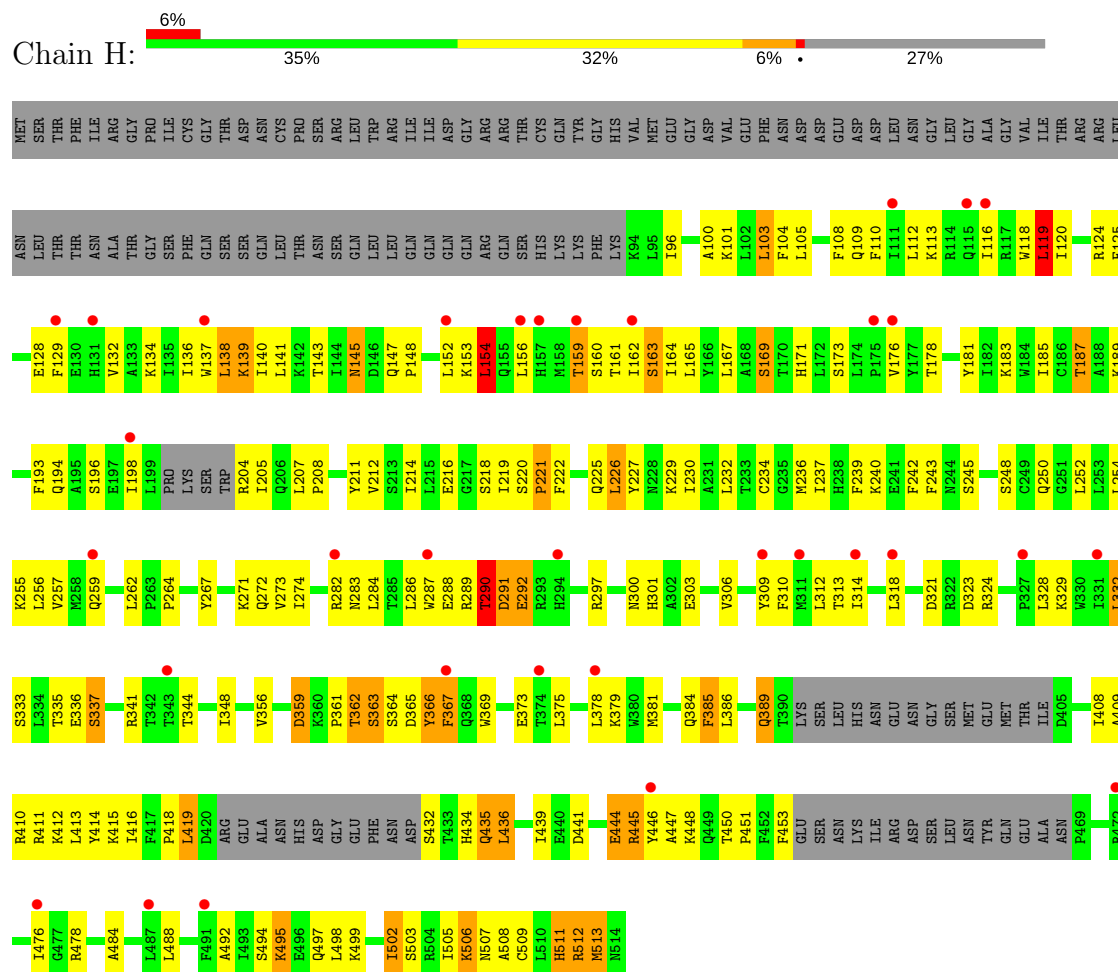


• Molecule 2: RNA polymerase I-specific transcription initiation factor RRN7

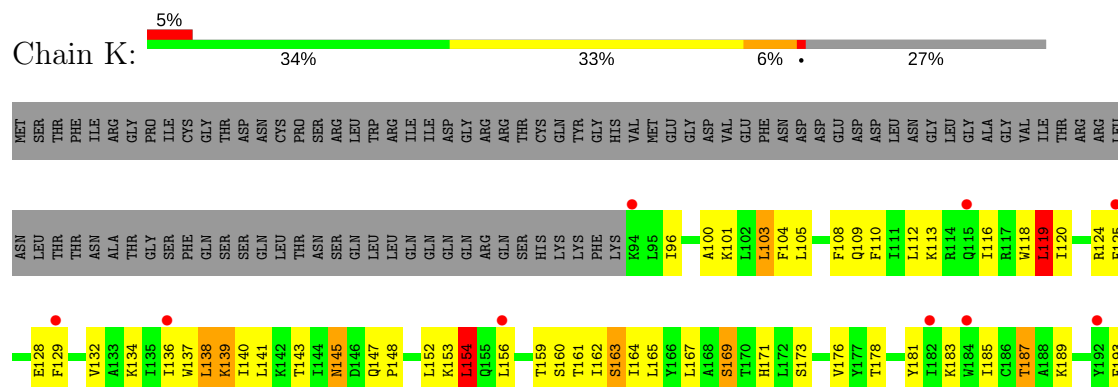


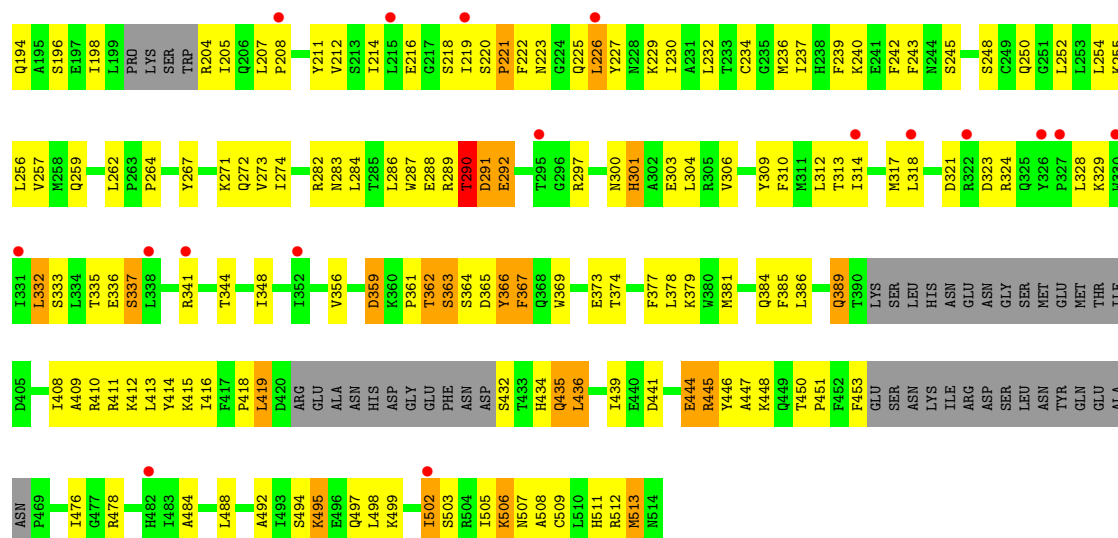


• Molecule 2: RNA polymerase I-specific transcription initiation factor RRN7

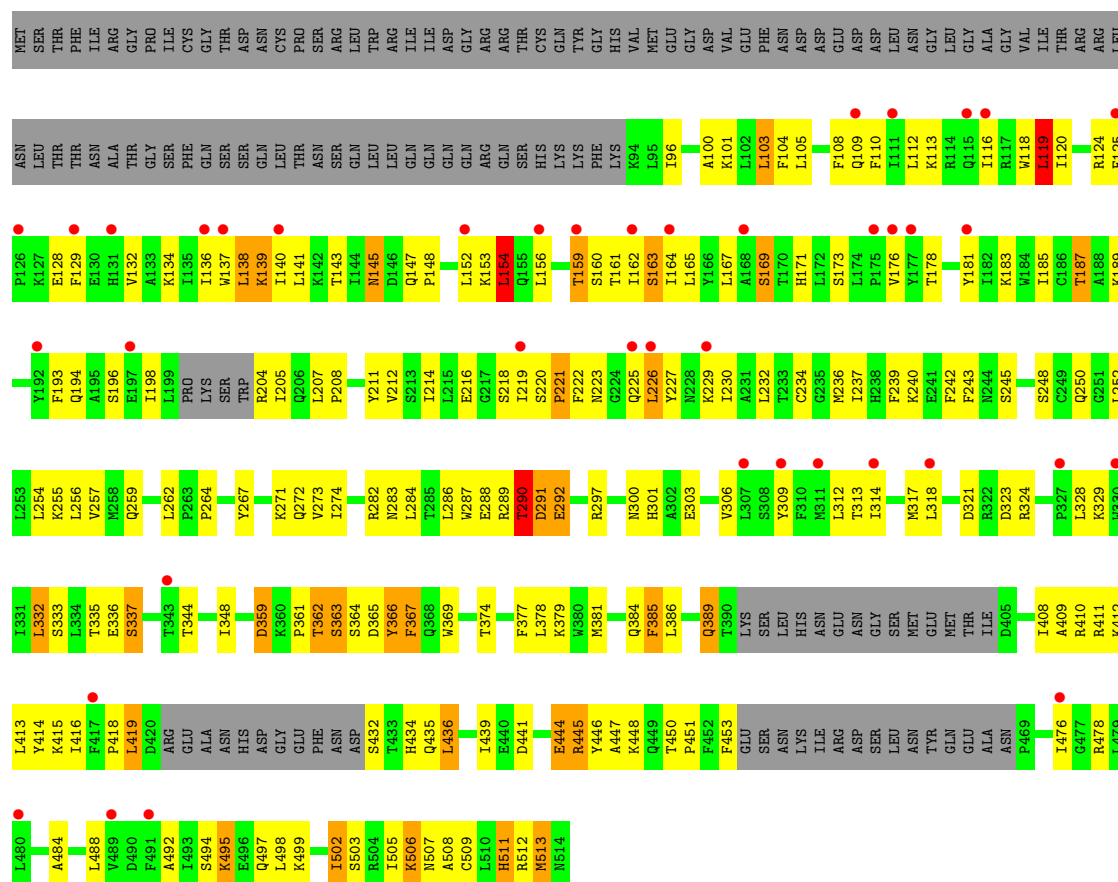


• Molecule 2: RNA polymerase I-specific transcription initiation factor RRN7



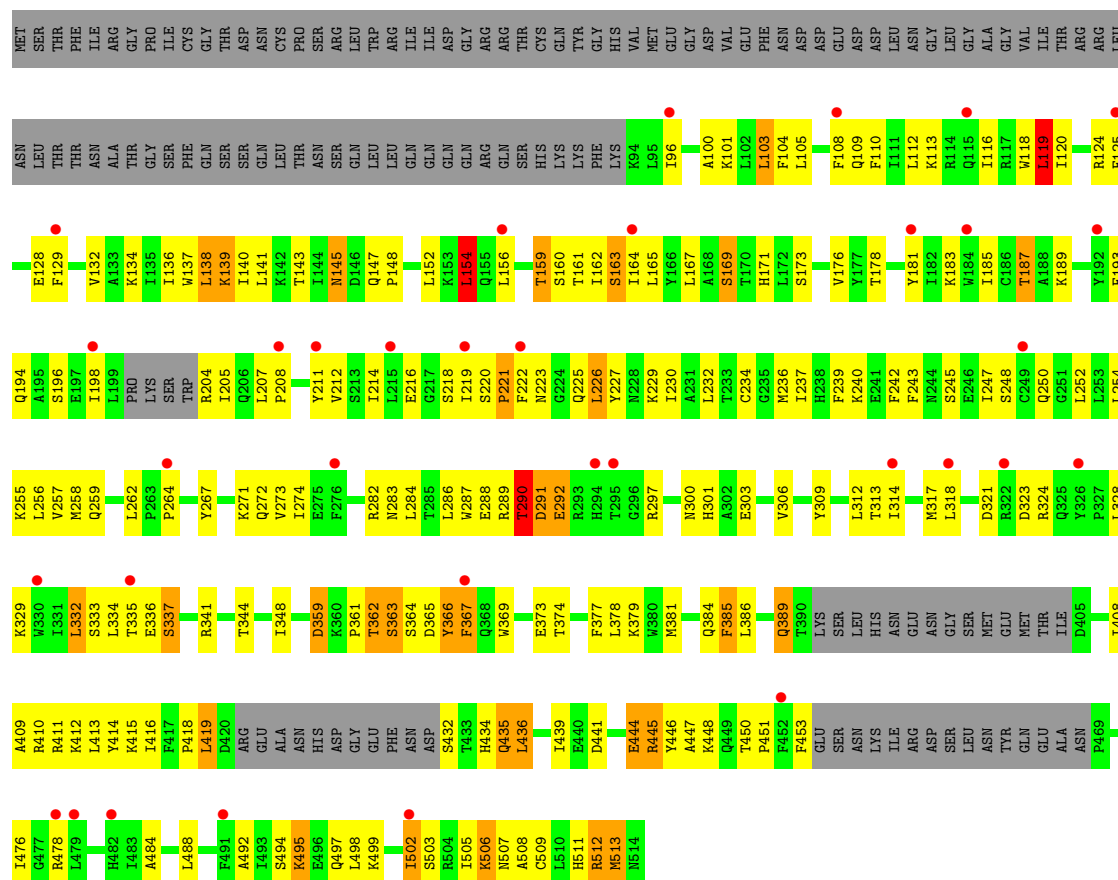


• Molecule 2: RNA polymerase I-specific transcription initiation factor RRN7

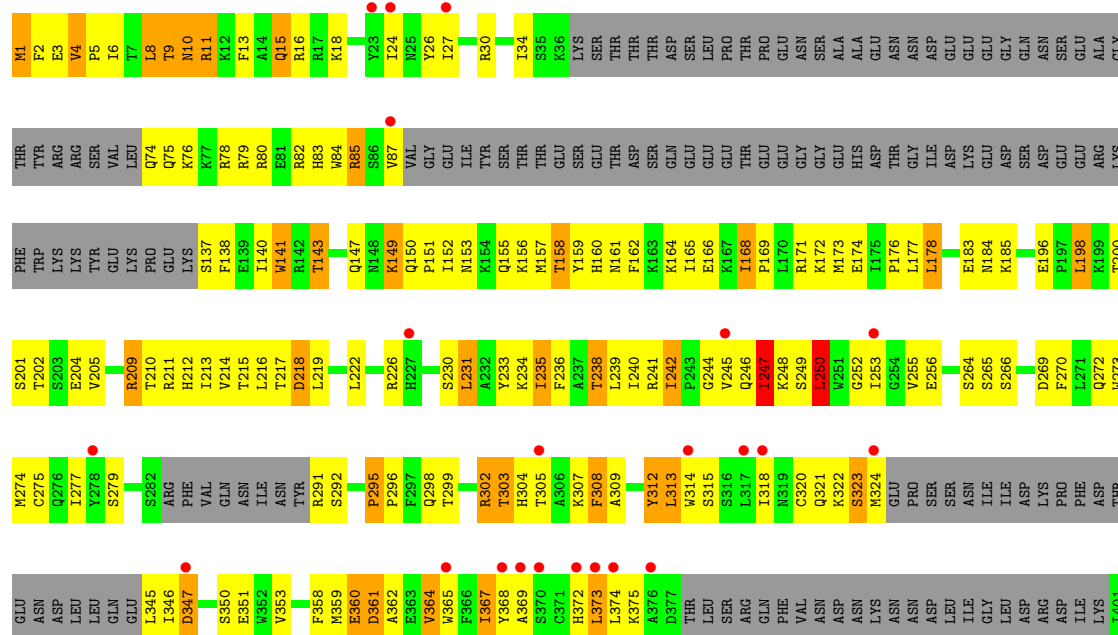
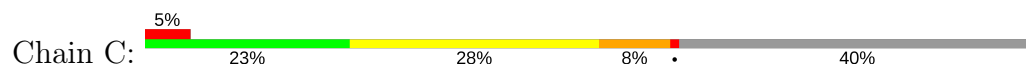


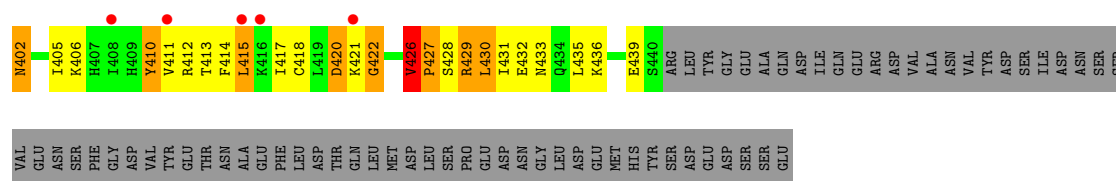
• Molecule 2: RNA polymerase I-specific transcription initiation factor RRN7



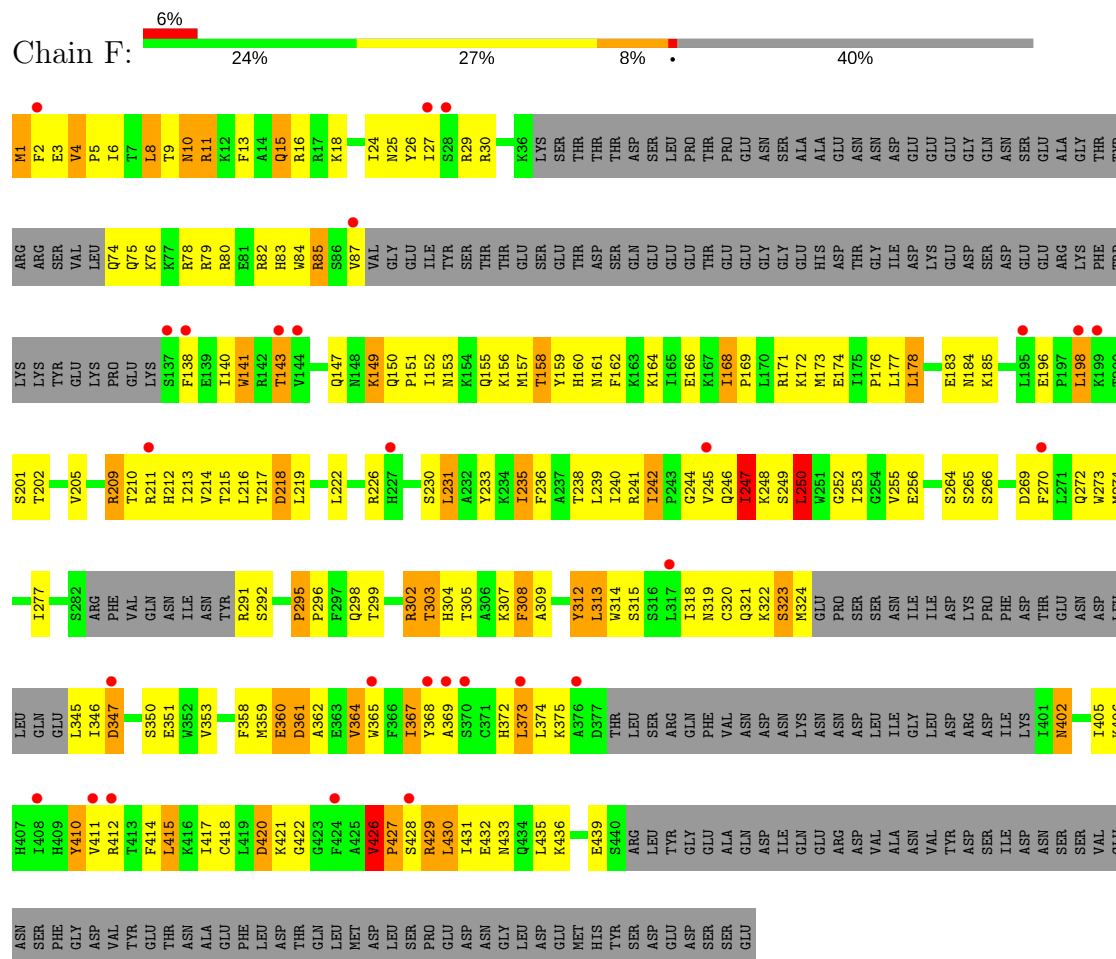


• Molecule 3: RNA polymerase I-specific transcription initiation factor RRN11

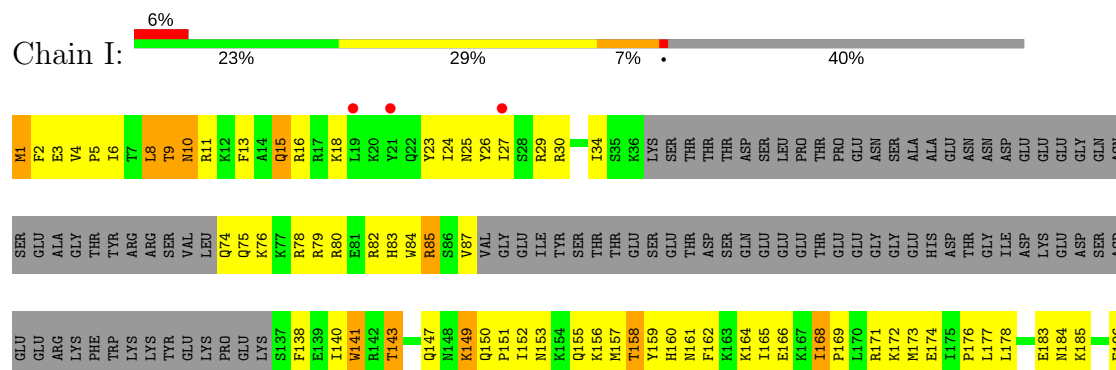


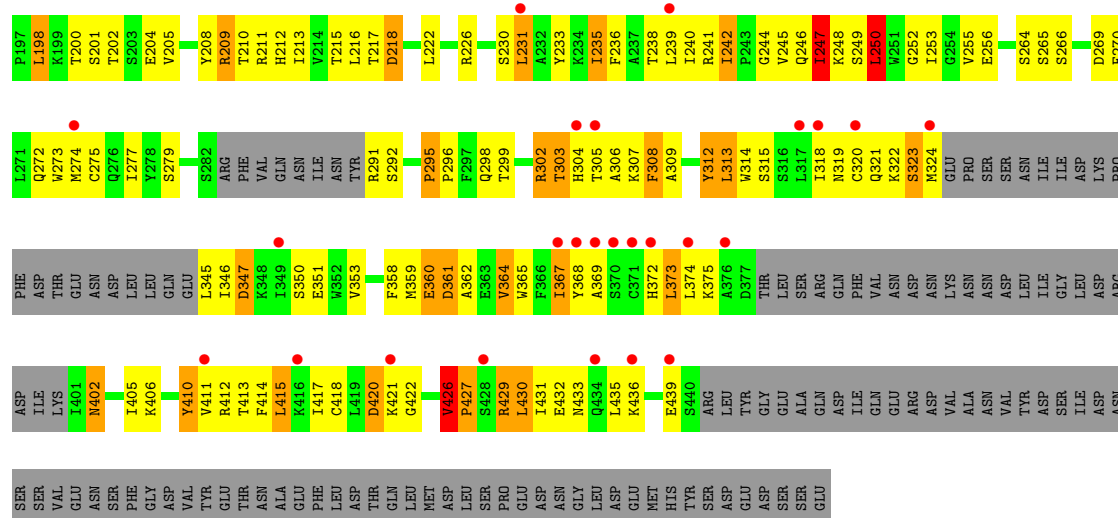


• Molecule 3: RNA polymerase I-specific transcription initiation factor RRN11

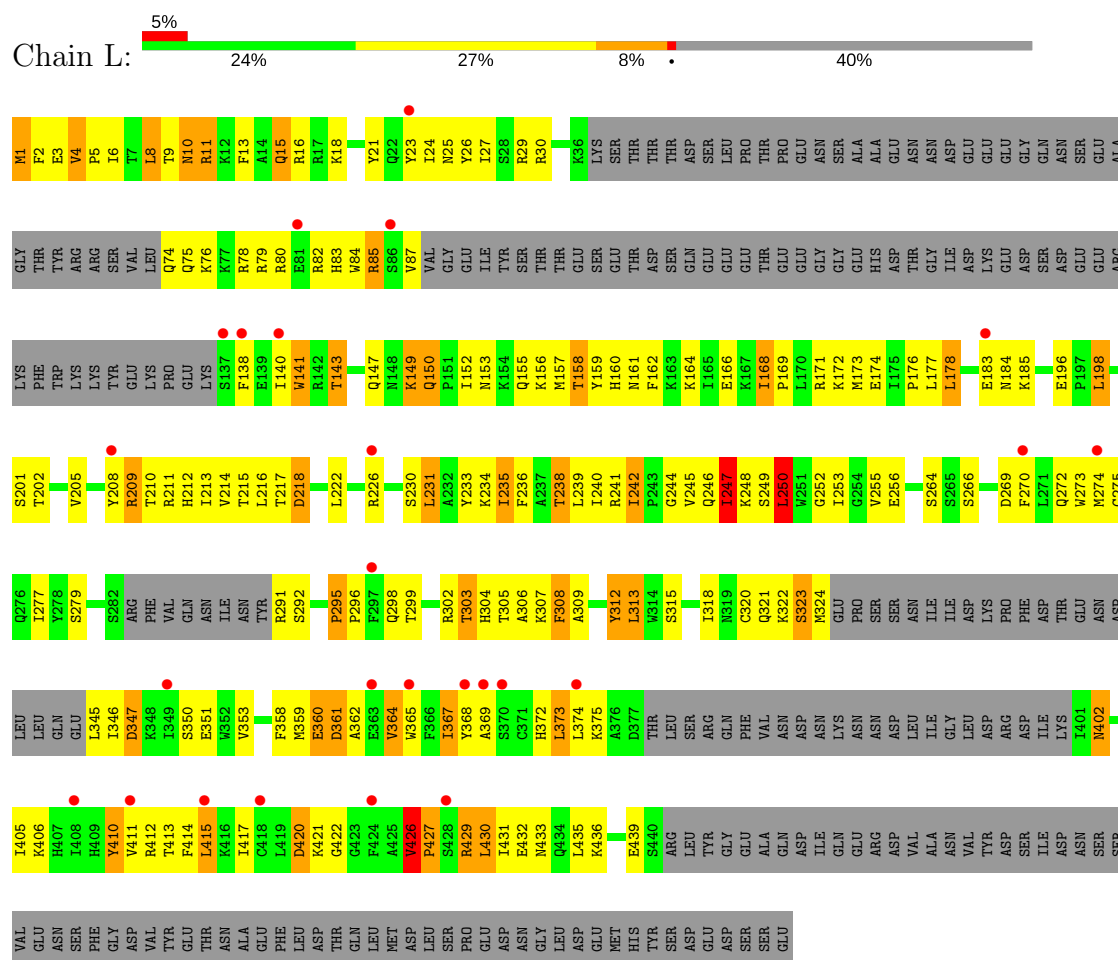


• Molecule 3: RNA polymerase I-specific transcription initiation factor RRN11

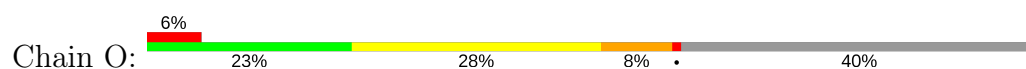


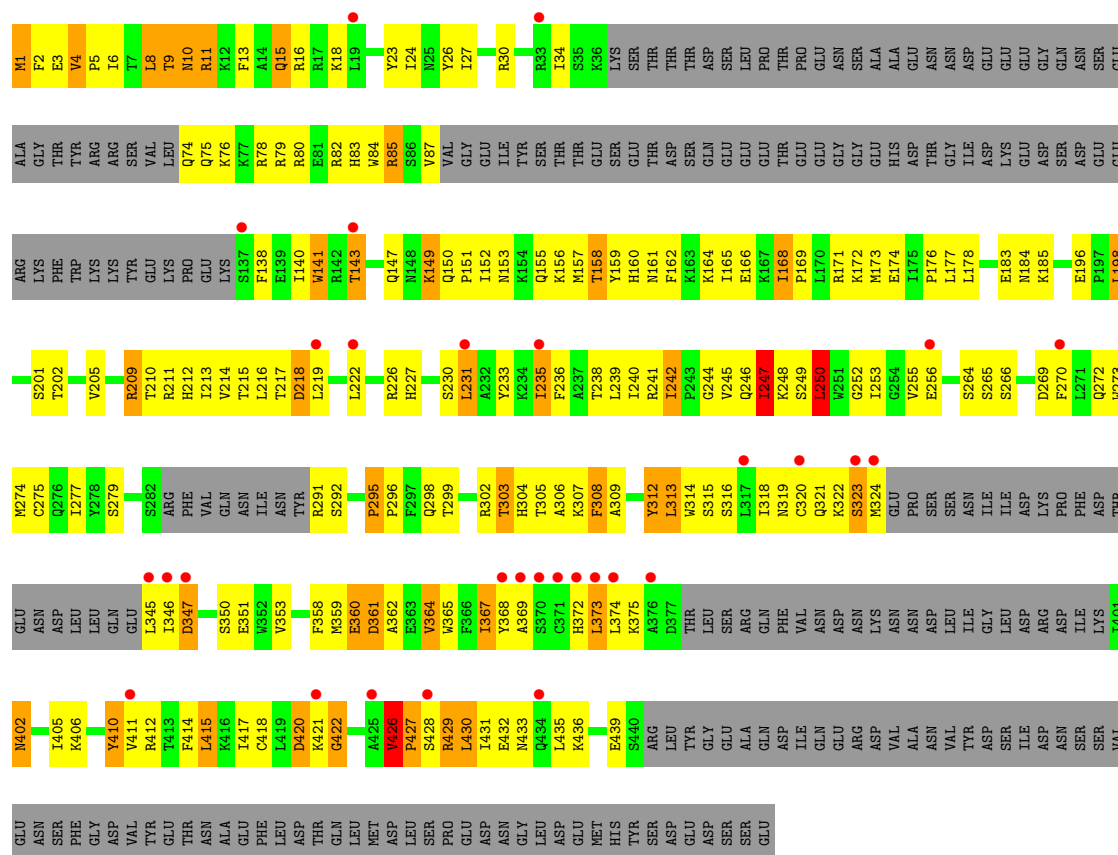


• Molecule 3: RNA polymerase I-specific transcription initiation factor RRN11

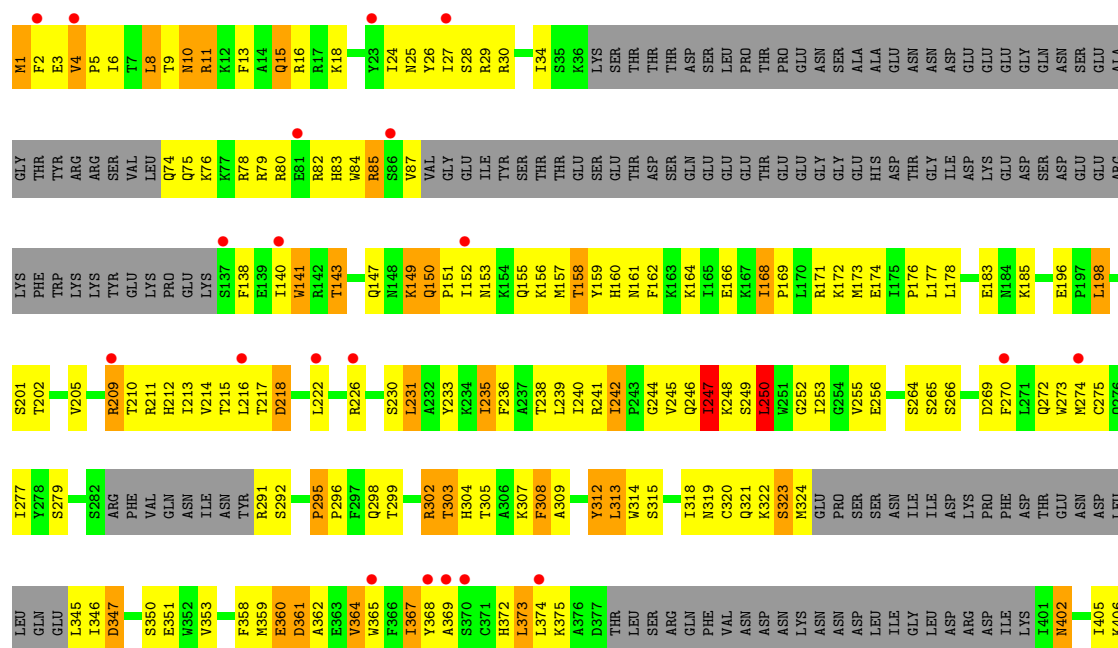
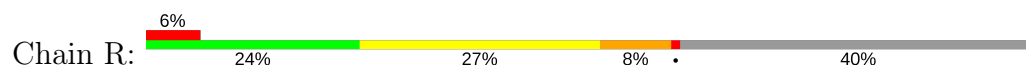


• Molecule 3: RNA polymerase I-specific transcription initiation factor RRN11





● Molecule 3: RNA polymerase I-specific transcription initiation factor RRN11





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	109.07Å 109.14Å 385.64Å 90.02° 90.01° 59.98°	Depositor
Resolution (Å)	54.57 – 3.20 54.57 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.9 (54.57-3.20) 98.7 (54.57-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 3.19Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.254 , 0.283 0.254 , 0.282	Depositor DCC
R_{free} test set	7461 reflections (2.97%)	wwPDB-VP
Wilson B-factor (Å ²)	127.2	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 147.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.418 for k,-h+k,l 0.418 for h-k,h,l 0.410 for -h+k,-h,l 0.410 for -k,h-k,l 0.033 for h,h-k,-l 0.033 for -k,-h,-l 0.418 for -h,-k,l 0.033 for -h+k,k,-l 0.033 for h-k,-k,-l 0.033 for -h,-h+k,-l 0.034 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	63438	wwPDB-VP
Average B, all atoms (Å ²)	149.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% 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: MG, SO4

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	0.40	0/4954	0.63	2/6707 (0.0%)
1	D	0.40	0/4954	0.63	2/6707 (0.0%)
1	G	0.40	0/4954	0.63	2/6707 (0.0%)
1	J	0.41	0/4954	0.63	2/6707 (0.0%)
1	M	0.40	0/4954	0.63	2/6707 (0.0%)
1	P	0.40	0/4954	0.63	2/6707 (0.0%)
2	B	0.37	0/3231	0.57	2/4362 (0.0%)
2	E	0.38	0/3231	0.57	2/4362 (0.0%)
2	H	0.38	0/3231	0.57	2/4362 (0.0%)
2	K	0.38	0/3231	0.57	2/4362 (0.0%)
2	N	0.38	0/3231	0.57	2/4362 (0.0%)
2	Q	0.37	0/3231	0.57	2/4362 (0.0%)
3	C	0.36	0/2592	0.57	2/3486 (0.1%)
3	F	0.36	0/2592	0.57	2/3486 (0.1%)
3	I	0.36	0/2592	0.57	1/3486 (0.0%)
3	L	0.36	0/2592	0.57	2/3486 (0.1%)
3	O	0.36	0/2592	0.57	1/3486 (0.0%)
3	R	0.36	0/2592	0.57	1/3486 (0.0%)
All	All	0.39	0/64662	0.60	33/87330 (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	A	0	10
1	D	0	10
1	G	0	10
1	J	0	10
1	M	0	10

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	P	0	10
2	B	0	3
2	E	0	3
2	H	0	3
2	K	0	2
2	N	0	3
2	Q	0	3
3	C	0	4
3	F	0	4
3	I	0	4
3	L	0	3
3	O	0	4
3	R	0	4
All	All	0	100

There are no bond length outliers.

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	250	LEU	CA-CB-CG	8.02	133.75	115.30
3	L	250	LEU	CA-CB-CG	7.96	133.60	115.30
3	F	250	LEU	CA-CB-CG	7.88	133.44	115.30
3	R	250	LEU	CA-CB-CG	7.88	133.44	115.30
3	I	250	LEU	CA-CB-CG	7.85	133.35	115.30

There are no chirality outliers.

5 of 100 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	289	SER	Peptide
1	A	333	PHE	Peptide
1	A	365	TRP	Peptide
1	A	393	VAL	Peptide
1	A	408	ILE	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	4856	0	4790	270	0
1	D	4856	0	4790	270	0
1	G	4856	0	4790	273	0
1	J	4856	0	4790	265	0
1	M	4856	0	4790	280	0
1	P	4856	0	4790	276	0
2	B	3156	0	3205	159	0
2	E	3156	0	3205	160	0
2	H	3156	0	3205	168	0
2	K	3156	0	3205	160	0
2	N	3156	0	3205	169	0
2	Q	3156	0	3205	166	0
3	C	2535	0	2609	134	0
3	F	2535	0	2609	130	0
3	I	2535	0	2609	134	0
3	L	2535	0	2609	129	0
3	O	2535	0	2609	136	0
3	R	2535	0	2609	129	0
4	A	25	0	0	1	0
4	D	20	0	0	1	0
4	F	5	0	0	0	0
4	G	15	0	0	1	0
4	H	5	0	0	0	0
4	I	5	0	0	0	0
4	J	15	0	0	1	0
4	K	5	0	0	0	0
4	L	5	0	0	0	0
4	M	20	0	0	1	0
4	O	5	0	0	0	0
4	P	25	0	0	1	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
5	G	1	0	0	0	0
5	J	1	0	0	0	0
5	M	1	0	0	0	0
5	P	1	0	0	0	0
All	All	63438	0	63624	3145	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 25.

The worst 5 of 3145 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:D:622:TYR:O	1:D:626:LEU:HB2	1.52	1.09
2:E:134:LYS:O	2:E:138:LEU:HB2	1.54	1.08
2:H:134:LYS:O	2:H:138:LEU:HB2	1.54	1.08
1:G:622:TYR:O	1:G:626:LEU:HB2	1.53	1.07
1:J:622:TYR:O	1:J:626:LEU:HB2	1.53	1.07

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	584/894 (65%)	499 (85%)	65 (11%)	20 (3%)	4	27
1	D	584/894 (65%)	500 (86%)	63 (11%)	21 (4%)	4	26
1	G	584/894 (65%)	500 (86%)	62 (11%)	22 (4%)	3	24
1	J	584/894 (65%)	500 (86%)	62 (11%)	22 (4%)	3	24
1	M	584/894 (65%)	498 (85%)	65 (11%)	21 (4%)	4	26
1	P	584/894 (65%)	499 (85%)	65 (11%)	20 (3%)	4	27
2	B	367/514 (71%)	323 (88%)	40 (11%)	4 (1%)	16	56
2	E	367/514 (71%)	321 (88%)	42 (11%)	4 (1%)	16	56
2	H	367/514 (71%)	320 (87%)	43 (12%)	4 (1%)	16	56
2	K	367/514 (71%)	322 (88%)	41 (11%)	4 (1%)	16	56
2	N	367/514 (71%)	322 (88%)	41 (11%)	4 (1%)	16	56
2	Q	367/514 (71%)	321 (88%)	42 (11%)	4 (1%)	16	56
3	C	291/507 (57%)	244 (84%)	40 (14%)	7 (2%)	6	37
3	F	291/507 (57%)	248 (85%)	37 (13%)	6 (2%)	8	40
3	I	291/507 (57%)	246 (84%)	39 (13%)	6 (2%)	8	40
3	L	291/507 (57%)	246 (84%)	39 (13%)	6 (2%)	8	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	O	291/507 (57%)	245 (84%)	39 (13%)	7 (2%)	6	37
3	R	291/507 (57%)	248 (85%)	37 (13%)	6 (2%)	8	40
All	All	7452/11490 (65%)	6402 (86%)	862 (12%)	188 (2%)	6	36

5 of 188 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	321	LYS
1	A	332	ASN
1	A	444	PRO
1	A	501	PRO
1	A	752	LEU

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	552/828 (67%)	423 (77%)	129 (23%)	1	3
1	D	552/828 (67%)	422 (76%)	130 (24%)	1	3
1	G	552/828 (67%)	425 (77%)	127 (23%)	1	4
1	J	552/828 (67%)	424 (77%)	128 (23%)	1	4
1	M	552/828 (67%)	424 (77%)	128 (23%)	1	4
1	P	552/828 (67%)	425 (77%)	127 (23%)	1	4
2	B	354/476 (74%)	298 (84%)	56 (16%)	3	13
2	E	354/476 (74%)	297 (84%)	57 (16%)	2	12
2	H	354/476 (74%)	297 (84%)	57 (16%)	2	12
2	K	354/476 (74%)	297 (84%)	57 (16%)	2	12
2	N	354/476 (74%)	297 (84%)	57 (16%)	2	12
2	Q	354/476 (74%)	297 (84%)	57 (16%)	2	12
3	C	286/474 (60%)	221 (77%)	65 (23%)	1	4
3	F	286/474 (60%)	221 (77%)	65 (23%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	I	286/474 (60%)	220 (77%)	66 (23%)	1	4
3	L	286/474 (60%)	222 (78%)	64 (22%)	1	4
3	O	286/474 (60%)	220 (77%)	66 (23%)	1	4
3	R	286/474 (60%)	221 (77%)	65 (23%)	1	4
All	All	7152/10668 (67%)	5651 (79%)	1501 (21%)	1	6

5 of 1501 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	453	PHE
1	J	615	ASN
2	Q	147	GLN
3	I	143	THR
1	J	247	ILE

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

Mol	Chain	Res	Type
1	G	757	GLN
2	H	389	GLN
2	N	171	HIS
1	G	656	HIS
1	P	301	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 36 ligands modelled in this entry, 6 are monoatomic - leaving 30 for Mogul analysis.

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
4	SO4	A	1001	-	4,4,4	0.27	0	6,6,6	0.22	0
4	SO4	A	1002	-	4,4,4	0.17	0	6,6,6	0.24	0
4	SO4	A	1003	-	4,4,4	0.18	0	6,6,6	0.18	0
4	SO4	A	1004	-	4,4,4	0.17	0	6,6,6	0.10	0
4	SO4	A	1005	-	4,4,4	0.16	0	6,6,6	0.11	0
4	SO4	D	1001	-	4,4,4	0.27	0	6,6,6	0.21	0
4	SO4	D	1002	-	4,4,4	0.19	0	6,6,6	0.23	0
4	SO4	D	1003	-	4,4,4	0.17	0	6,6,6	0.11	0
4	SO4	D	1004	-	4,4,4	0.14	0	6,6,6	0.11	0
4	SO4	F	601	-	4,4,4	0.16	0	6,6,6	0.10	0
4	SO4	G	901	-	4,4,4	0.17	0	6,6,6	0.24	0
4	SO4	G	902	-	4,4,4	0.17	0	6,6,6	0.16	0
4	SO4	G	903	-	4,4,4	0.15	0	6,6,6	0.11	0
4	SO4	H	1001	-	4,4,4	0.29	0	6,6,6	0.25	0
4	SO4	I	601	-	4,4,4	0.18	0	6,6,6	0.10	0
4	SO4	J	1001	-	4,4,4	0.25	0	6,6,6	0.25	0
4	SO4	J	1002	-	4,4,4	0.17	0	6,6,6	0.17	0
4	SO4	J	1003	-	4,4,4	0.15	0	6,6,6	0.12	0
4	SO4	K	601	-	4,4,4	0.18	0	6,6,6	0.20	0
4	SO4	L	601	-	4,4,4	0.16	0	6,6,6	0.11	0
4	SO4	M	1001	-	4,4,4	0.25	0	6,6,6	0.34	0
4	SO4	M	1002	-	4,4,4	0.18	0	6,6,6	0.20	0
4	SO4	M	1003	-	4,4,4	0.17	0	6,6,6	0.15	0
4	SO4	M	1004	-	4,4,4	0.15	0	6,6,6	0.11	0
4	SO4	O	601	-	4,4,4	0.17	0	6,6,6	0.13	0
4	SO4	P	1001	-	4,4,4	0.27	0	6,6,6	0.32	0
4	SO4	P	1002	-	4,4,4	0.17	0	6,6,6	0.21	0
4	SO4	P	1003	-	4,4,4	0.19	0	6,6,6	0.14	0
4	SO4	P	1004	-	4,4,4	0.17	0	6,6,6	0.14	0
4	SO4	P	1005	-	4,4,4	0.15	0	6,6,6	0.11	0

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
4	SO4	A	1001	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1002	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1003	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1004	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1005	-	-	0/0/0/0	0/0/0/0
4	SO4	D	1001	-	-	0/0/0/0	0/0/0/0
4	SO4	D	1002	-	-	0/0/0/0	0/0/0/0
4	SO4	D	1003	-	-	0/0/0/0	0/0/0/0
4	SO4	D	1004	-	-	0/0/0/0	0/0/0/0
4	SO4	F	601	-	-	0/0/0/0	0/0/0/0
4	SO4	G	901	-	-	0/0/0/0	0/0/0/0
4	SO4	G	902	-	-	0/0/0/0	0/0/0/0
4	SO4	G	903	-	-	0/0/0/0	0/0/0/0
4	SO4	H	1001	-	-	0/0/0/0	0/0/0/0
4	SO4	I	601	-	-	0/0/0/0	0/0/0/0
4	SO4	J	1001	-	-	0/0/0/0	0/0/0/0
4	SO4	J	1002	-	-	0/0/0/0	0/0/0/0
4	SO4	J	1003	-	-	0/0/0/0	0/0/0/0
4	SO4	K	601	-	-	0/0/0/0	0/0/0/0
4	SO4	L	601	-	-	0/0/0/0	0/0/0/0
4	SO4	M	1001	-	-	0/0/0/0	0/0/0/0
4	SO4	M	1002	-	-	0/0/0/0	0/0/0/0
4	SO4	M	1003	-	-	0/0/0/0	0/0/0/0
4	SO4	M	1004	-	-	0/0/0/0	0/0/0/0
4	SO4	O	601	-	-	0/0/0/0	0/0/0/0
4	SO4	P	1001	-	-	0/0/0/0	0/0/0/0
4	SO4	P	1002	-	-	0/0/0/0	0/0/0/0
4	SO4	P	1003	-	-	0/0/0/0	0/0/0/0
4	SO4	P	1004	-	-	0/0/0/0	0/0/0/0
4	SO4	P	1005	-	-	0/0/0/0	0/0/0/0

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.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1005	SO4	1	0
4	D	1004	SO4	1	0
4	G	903	SO4	1	0
4	J	1003	SO4	1	0
4	M	1004	SO4	1	0
4	P	1005	SO4	1	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	598/894 (66%)	0.47	60 (10%) 7 4	85, 143, 228, 326	0
1	D	598/894 (66%)	0.51	55 (9%) 9 5	86, 145, 228, 326	0
1	G	598/894 (66%)	0.51	63 (10%) 6 4	83, 145, 229, 339	0
1	J	598/894 (66%)	0.47	52 (8%) 10 6	85, 144, 226, 317	0
1	M	598/894 (66%)	0.50	57 (9%) 8 5	86, 146, 230, 331	0
1	P	598/894 (66%)	0.52	61 (10%) 7 4	86, 144, 230, 328	0
2	B	377/514 (73%)	0.46	20 (5%) 26 14	78, 128, 210, 294	0
2	E	377/514 (73%)	0.43	20 (5%) 26 14	79, 129, 217, 279	0
2	H	377/514 (73%)	0.57	33 (8%) 10 5	79, 128, 210, 283	0
2	K	377/514 (73%)	0.41	26 (6%) 17 9	79, 130, 214, 287	0
2	N	377/514 (73%)	0.53	40 (10%) 6 4	79, 127, 207, 284	0
2	Q	377/514 (73%)	0.52	34 (9%) 9 5	79, 129, 211, 286	0
3	C	303/507 (59%)	0.50	27 (8%) 9 5	82, 158, 242, 312	0
3	F	303/507 (59%)	0.58	28 (9%) 9 5	84, 158, 248, 318	0
3	I	303/507 (59%)	0.53	28 (9%) 9 5	83, 154, 241, 324	0
3	L	303/507 (59%)	0.49	25 (8%) 11 6	83, 160, 241, 326	0
3	O	303/507 (59%)	0.49	30 (9%) 7 4	84, 156, 244, 313	0
3	R	303/507 (59%)	0.45	28 (9%) 9 5	83, 155, 242, 334	0
All	All	7668/11490 (66%)	0.50	687 (8%) 9 5	78, 141, 230, 339	0

The worst 5 of 687 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	324	MET	16.6
1	M	532	GLU	11.2
1	D	196	TYR	10.3

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Mol	Chain	Res	Type	RSRZ
3	I	369	ALA	9.7
3	L	424	PHE	9.2

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
5	MG	P	1006	1/1	0.23	0.28	108,108,108,108	0
4	SO4	D	1004	5/5	0.33	0.58	172,284,325,366	0
4	SO4	M	1004	5/5	0.36	0.38	164,293,328,365	0
4	SO4	A	1005	5/5	0.39	0.46	161,270,297,338	0
5	MG	J	1004	1/1	0.53	0.26	106,106,106,106	0
4	SO4	J	1003	5/5	0.57	0.26	166,284,321,362	0
4	SO4	G	903	5/5	0.62	0.23	164,281,309,354	0
5	MG	A	1006	1/1	0.67	0.23	107,107,107,107	0
4	SO4	M	1002	5/5	0.69	0.27	169,171,179,191	0
4	SO4	P	1005	5/5	0.71	0.18	166,296,344,363	0
4	SO4	O	601	5/5	0.77	0.24	101,215,246,246	0
4	SO4	P	1002	5/5	0.80	0.30	166,168,172,186	0
5	MG	G	904	1/1	0.81	0.34	108,108,108,108	0
5	MG	D	1005	1/1	0.84	0.17	107,107,107,107	0
4	SO4	I	601	5/5	0.86	0.22	98,191,239,244	0
4	SO4	A	1003	5/5	0.86	0.15	98,142,149,150	0
4	SO4	K	601	5/5	0.86	0.20	165,172,176,184	0
5	MG	M	1005	1/1	0.87	0.32	108,108,108,108	0
4	SO4	G	902	5/5	0.87	0.15	117,133,146,149	0
4	SO4	A	1002	5/5	0.87	0.21	163,169,175,184	0
4	SO4	G	901	5/5	0.88	0.34	153,155,162,180	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	D	1002	5/5	0.88	0.18	144,165,173,183	0
4	SO4	P	1003	5/5	0.88	0.17	111,150,158,158	0
4	SO4	L	601	5/5	0.89	0.22	101,201,236,237	0
4	SO4	F	601	5/5	0.89	0.22	99,179,235,237	0
4	SO4	J	1002	5/5	0.91	0.16	106,127,143,149	0
4	SO4	A	1004	5/5	0.91	0.30	95,186,233,252	0
4	SO4	D	1003	5/5	0.92	0.17	104,134,141,147	0
4	SO4	P	1004	5/5	0.92	0.27	96,187,207,226	0
4	SO4	A	1001	5/5	0.93	0.22	96,110,115,123	0
4	SO4	D	1001	5/5	0.94	0.19	94,106,110,111	0
4	SO4	M	1001	5/5	0.94	0.28	92,110,119,130	0
4	SO4	M	1003	5/5	0.96	0.14	107,162,234,240	0
4	SO4	P	1001	5/5	0.96	0.19	94,105,113,126	0
4	SO4	H	1001	5/5	0.97	0.25	92,92,108,112	0
4	SO4	J	1001	5/5	0.98	0.18	94,108,113,120	0

6.5 Other polymers ⓘ

There are no such residues in this entry.