



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 10, 2017 – 01:13 PM EDT

PDB ID : 5OKZ
Title : Crystal Strucrure of the Mpp6 Exosome complex
Authors : Falk, S.; Ebert, J.; Conti, E.
Deposited on : unknown
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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

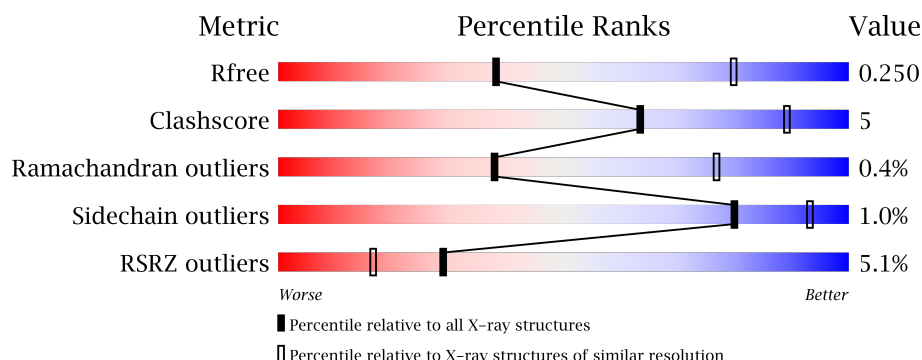
1 Overall quality at a glance

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.



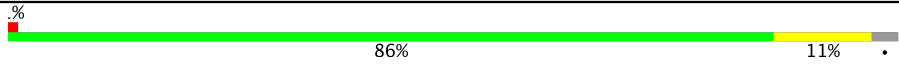

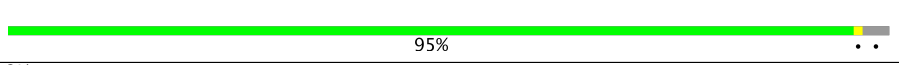

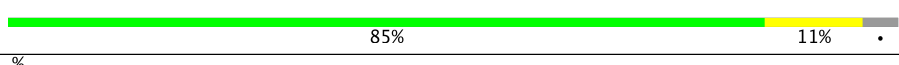
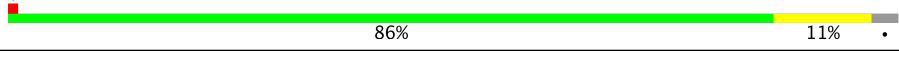
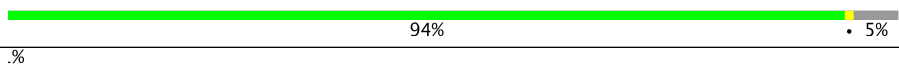

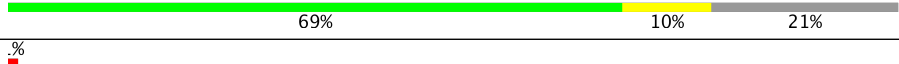


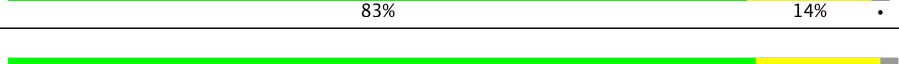
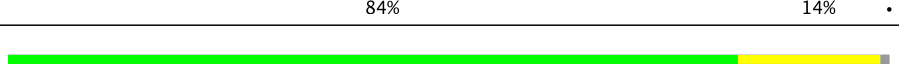
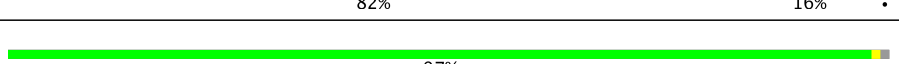
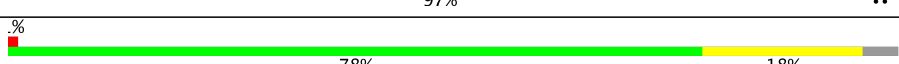
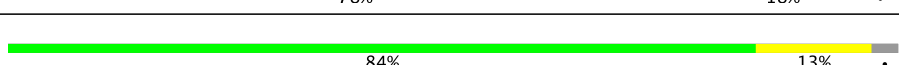
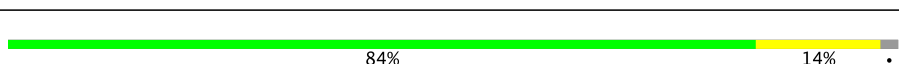
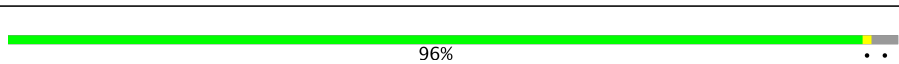
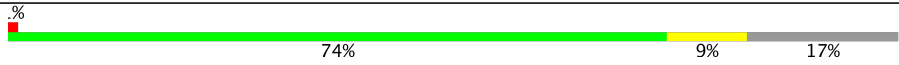


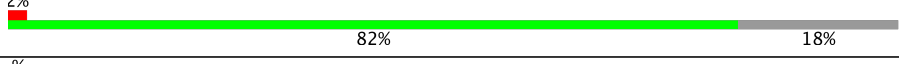
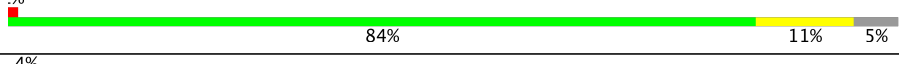


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)

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	I	295	<div> <div>27%</div> <div> <div></div> <div>52%</div> <div>8%</div> <div>40%</div> </div> </div>
1	S	295	<div> <div>35%</div> <div> <div></div> <div>64%</div> <div>6%</div> <div>29%</div> </div> </div>
1	c	295	<div> <div>26%</div> <div> <div></div> <div>67%</div> <div></div> <div>33%</div> </div> </div>
1	m	295	<div> <div>20%</div> <div> <div></div> <div>64%</div> <div></div> <div>36%</div> </div> </div>
2	A	305	<div> <div></div> <div> <div></div> <div>86%</div> <div>10%</div> <div>...</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	K	305	
2	U	305	
2	e	305	
3	B	249	
3	L	249	
3	V	249	
3	f	249	
4	C	394	
4	M	394	
4	W	394	
4	g	394	
5	D	226	
5	N	226	
5	X	226	
5	h	226	
6	E	268	
6	O	268	
6	Y	268	
6	i	268	
7	F	250	
7	P	250	
7	Z	250	
7	j	250	
8	G	244	
8	Q	244	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	a	244	<div><div></div><div>16%</div><div>92%</div><div>7%</div></div>
8	k	244	<div><div></div><div>5%</div><div>92%</div><div>7%</div></div>
9	H	316	<div><div></div><div>%</div><div>72%</div><div>11%</div><div>16%</div></div>
9	R	316	<div><div></div><div>2%</div><div>74%</div><div>10%</div><div>16%</div></div>
9	b	316	<div><div></div><div></div><div>80%</div><div></div><div>17%</div></div>
9	l	316	<div><div></div><div>2%</div><div>83%</div><div></div><div>15%</div></div>
10	J	190	<div><div></div><div>%</div><div>10%</div><div>89%</div></div>
10	T	190	<div><div></div><div></div><div>96%</div></div>
10	d	190	<div><div></div><div></div><div>96%</div></div>
10	n	190	<div><div></div><div>%</div><div>5%</div><div>95%</div></div>

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 67168 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 component CSL4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	m	190	Total	C	N	O	S	0	0	0
			1425	892	254	273	6			
1	I	178	Total	C	N	O	S	0	0	0
			1317	825	233	252	7			
1	S	208	Total	C	N	O	S	0	0	0
			1554	975	274	297	8			
1	c	197	Total	C	N	O	S	0	0	0
			1463	915	261	280	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
m	-2	GLY	-	expression tag	UNP P53859
m	-1	PRO	-	expression tag	UNP P53859
m	0	HIS	-	expression tag	UNP P53859
I	-2	GLY	-	expression tag	UNP P53859
I	-1	PRO	-	expression tag	UNP P53859
I	0	HIS	-	expression tag	UNP P53859
S	-2	GLY	-	expression tag	UNP P53859
S	-1	PRO	-	expression tag	UNP P53859
S	0	HIS	-	expression tag	UNP P53859
c	-2	GLY	-	expression tag	UNP P53859
c	-1	PRO	-	expression tag	UNP P53859
c	0	HIS	-	expression tag	UNP P53859

- Molecule 2 is a protein called Exosome complex component RRP45.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	295	Total	C	N	O	S	0	0	0
			2244	1410	384	434	16			
2	K	295	Total	C	N	O	S	0	0	0
			2244	1410	384	434	16			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	U	295	Total	C	N	O	S	0	0	0
			2244	1410	384	434	16			
2	e	295	Total	C	N	O	S	0	0	0
			2248	1413	385	434	16			

- Molecule 3 is a protein called Exosome complex component SKI6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	242	Total	C	N	O	S	0	0	0
			1830	1145	325	353	7			
3	L	238	Total	C	N	O	S	0	0	0
			1797	1126	316	347	8			
3	V	241	Total	C	N	O	S	0	0	0
			1851	1158	332	353	8			
3	f	237	Total	C	N	O	S	0	1	0
			1832	1145	328	351	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP P46948
B	-1	PRO	-	expression tag	UNP P46948
B	0	HIS	-	expression tag	UNP P46948
L	-2	GLY	-	expression tag	UNP P46948
L	-1	PRO	-	expression tag	UNP P46948
L	0	HIS	-	expression tag	UNP P46948
V	-2	GLY	-	expression tag	UNP P46948
V	-1	PRO	-	expression tag	UNP P46948
V	0	HIS	-	expression tag	UNP P46948
f	-2	GLY	-	expression tag	UNP P46948
f	-1	PRO	-	expression tag	UNP P46948
f	0	HIS	-	expression tag	UNP P46948

- Molecule 4 is a protein called Exosome complex component RRP43.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	313	Total	C	N	O	S	0	0	0
			2335	1478	404	444	9			
4	M	310	Total	C	N	O	S	0	0	0
			2283	1439	398	436	10			
4	W	319	Total	C	N	O	S	0	0	0
			2400	1518	416	455	11			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	g	317	Total	C	N	O	S	0	1	0
			2376	1508	417	441	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	363	MET	VAL	conflict	UNP P25359
M	363	MET	VAL	conflict	UNP P25359
W	363	MET	VAL	conflict	UNP P25359
g	363	MET	VAL	conflict	UNP P25359

- Molecule 5 is a protein called Exosome complex component RRP46.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	221	Total	C	N	O	S	0	0	0
			1649	1040	279	321	9			
5	N	222	Total	C	N	O	S	0	0	0
			1666	1050	280	327	9			
5	X	223	Total	C	N	O	S	0	0	0
			1704	1071	289	334	10			
5	h	223	Total	C	N	O	S	0	0	0
			1703	1071	289	333	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	ALA	-	expression tag	UNP P53256
D	-1	ALA	-	expression tag	UNP P53256
D	0	SER	-	expression tag	UNP P53256
N	-2	ALA	-	expression tag	UNP P53256
N	-1	ALA	-	expression tag	UNP P53256
N	0	SER	-	expression tag	UNP P53256
X	-2	ALA	-	expression tag	UNP P53256
X	-1	ALA	-	expression tag	UNP P53256
X	0	SER	-	expression tag	UNP P53256
h	-2	ALA	-	expression tag	UNP P53256
h	-1	ALA	-	expression tag	UNP P53256
h	0	SER	-	expression tag	UNP P53256

- Molecule 6 is a protein called Exosome complex component RRP42.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	257	Total	C	N	O	S	0	0	0
			1894	1209	318	363	4			
6	O	260	Total	C	N	O	S	0	0	0
			1941	1241	323	372	5			
6	Y	263	Total	C	N	O	S	0	0	0
			1974	1257	328	384	5			
6	i	261	Total	C	N	O	S	0	0	0
			1981	1269	327	380	5			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP Q12277
E	-1	PRO	-	expression tag	UNP Q12277
E	0	HIS	-	expression tag	UNP Q12277
E	138	ILE	VAL	conflict	UNP Q12277
O	-2	GLY	-	expression tag	UNP Q12277
O	-1	PRO	-	expression tag	UNP Q12277
O	0	HIS	-	expression tag	UNP Q12277
O	138	ILE	VAL	conflict	UNP Q12277
Y	-2	GLY	-	expression tag	UNP Q12277
Y	-1	PRO	-	expression tag	UNP Q12277
Y	0	HIS	-	expression tag	UNP Q12277
Y	138	ILE	VAL	conflict	UNP Q12277
i	-2	GLY	-	expression tag	UNP Q12277
i	-1	PRO	-	expression tag	UNP Q12277
i	0	HIS	-	expression tag	UNP Q12277
i	138	ILE	VAL	conflict	UNP Q12277

- Molecule 7 is a protein called Exosome complex component MTR3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	F	207	Total	C	N	O	S	0	0	0
			1517	956	256	295	10			
7	P	208	Total	C	N	O	S	0	0	0
			1515	956	257	292	10			
7	Z	208	Total	C	N	O	S	0	0	0
			1531	966	259	296	10			
7	j	206	Total	C	N	O	S	0	0	0
			1506	953	253	290	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	161	THR	MET	conflict	UNP P48240
P	161	THR	MET	conflict	UNP P48240
Z	161	THR	MET	conflict	UNP P48240
j	161	THR	MET	conflict	UNP P48240

- Molecule 8 is a protein called Exosome complex component RRP40.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	G	231	Total	C	N	O	S	0	0	0
			1696	1088	275	322	11			
8	Q	207	Total	C	N	O	S	0	0	0
			1550	984	257	300	9			
8	a	227	Total	C	N	O	S	0	0	0
			1744	1112	285	336	11			
8	k	226	Total	C	N	O	S	0	0	0
			1615	1040	268	297	10			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-3	GLY	-	expression tag	UNP Q08285
G	-2	PRO	-	expression tag	UNP Q08285
G	-1	ASP	-	expression tag	UNP Q08285
G	0	SER	-	expression tag	UNP Q08285
Q	-3	GLY	-	expression tag	UNP Q08285
Q	-2	PRO	-	expression tag	UNP Q08285
Q	-1	ASP	-	expression tag	UNP Q08285
Q	0	SER	-	expression tag	UNP Q08285
a	-3	GLY	-	expression tag	UNP Q08285
a	-2	PRO	-	expression tag	UNP Q08285
a	-1	ASP	-	expression tag	UNP Q08285
a	0	SER	-	expression tag	UNP Q08285
k	-3	GLY	-	expression tag	UNP Q08285
k	-2	PRO	-	expression tag	UNP Q08285
k	-1	ASP	-	expression tag	UNP Q08285
k	0	SER	-	expression tag	UNP Q08285

- Molecule 9 is a protein called Exosome complex component RRP4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	267	Total	C	N	O	S	0	0	0
			2013	1262	361	380	10			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	R	265	Total 2019	C 1263	N 360	O 386	S 10	0	0	0
9	b	262	Total 1993	C 1250	N 357	O 375	S 11	0	0	0
9	l	268	Total 2020	C 1268	N 361	O 380	S 11	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	44	THR	-	expression tag	UNP P38792
H	45	GLY	-	expression tag	UNP P38792
H	46	GLY	-	expression tag	UNP P38792
H	47	ARG	-	expression tag	UNP P38792
H	48	SER	-	expression tag	UNP P38792
H	49	MET	-	expression tag	UNP P38792
R	44	THR	-	expression tag	UNP P38792
R	45	GLY	-	expression tag	UNP P38792
R	46	GLY	-	expression tag	UNP P38792
R	47	ARG	-	expression tag	UNP P38792
R	48	SER	-	expression tag	UNP P38792
R	49	MET	-	expression tag	UNP P38792
b	44	THR	-	expression tag	UNP P38792
b	45	GLY	-	expression tag	UNP P38792
b	46	GLY	-	expression tag	UNP P38792
b	47	ARG	-	expression tag	UNP P38792
b	48	SER	-	expression tag	UNP P38792
b	49	MET	-	expression tag	UNP P38792
l	44	THR	-	expression tag	UNP P38792
l	45	GLY	-	expression tag	UNP P38792
l	46	GLY	-	expression tag	UNP P38792
l	47	ARG	-	expression tag	UNP P38792
l	48	SER	-	expression tag	UNP P38792
l	49	MET	-	expression tag	UNP P38792

- Molecule 10 is a protein called M-phase phosphoprotein 6 homolog.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	20	Total 139	C 89	N 25	O 25	0	0	0
10	T	7	Total 46	C 27	N 10	O 9	0	0	0

Continued on next page...

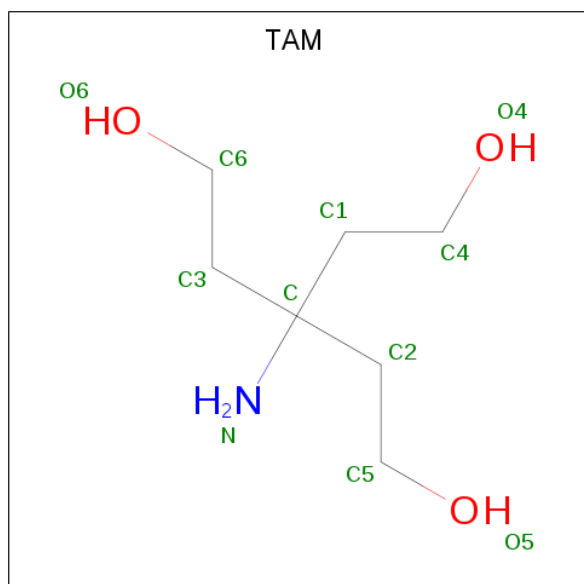
Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	d	7	Total	C	N	O	0	0	0
			46	27	10	9			
10	n	10	Total	C	N	O	0	0	0
			70	44	14	12			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	-3	GLY	-	expression tag	UNP P53725
J	-2	PRO	-	expression tag	UNP P53725
J	-1	ASP	-	expression tag	UNP P53725
J	0	SER	-	expression tag	UNP P53725
T	-3	GLY	-	expression tag	UNP P53725
T	-2	PRO	-	expression tag	UNP P53725
T	-1	ASP	-	expression tag	UNP P53725
T	0	SER	-	expression tag	UNP P53725
d	-3	GLY	-	expression tag	UNP P53725
d	-2	PRO	-	expression tag	UNP P53725
d	-1	ASP	-	expression tag	UNP P53725
d	0	SER	-	expression tag	UNP P53725
n	-3	GLY	-	expression tag	UNP P53725
n	-2	PRO	-	expression tag	UNP P53725
n	-1	ASP	-	expression tag	UNP P53725
n	0	SER	-	expression tag	UNP P53725

- Molecule 11 is TRIS(HYDROXYETHYL)AMINOMETHANE (three-letter code: TAM) (formula: $C_7H_{17}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C N O 11 7 1 3	0	0
11	K	1	Total C N O 11 7 1 3	0	0
11	U	1	Total C N O 11 7 1 3	0	0
11	e	1	Total C N O 11 7 1 3	0	0

- Molecule 12 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	G	1	Total Cl 1 1	0	0
12	H	1	Total Cl 1 1	0	0
12	b	1	Total Cl 1 1	0	0
12	R	2	Total Cl 2 2	0	0
12	l	1	Total Cl 1 1	0	0
12	f	1	Total Cl 1 1	0	0

- Molecule 13 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	O	1	Total Mg 1 1	0	0
13	g	1	Total Mg 1 1	0	0

- Molecule 14 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	4	Total O 4 4	0	0
14	B	9	Total O 9 9	0	0
14	C	8	Total O 8 8	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	D	7	Total O 7 7	0	0
14	E	2	Total O 2 2	0	0
14	G	3	Total O 3 3	0	0
14	H	3	Total O 3 3	0	0
14	L	2	Total O 2 2	0	0
14	N	2	Total O 2 2	0	0
14	O	7	Total O 7 7	0	0
14	P	2	Total O 2 2	0	0
14	R	3	Total O 3 3	0	0
14	U	13	Total O 13 13	0	0
14	V	12	Total O 12 12	0	0
14	W	6	Total O 6 6	0	0
14	X	7	Total O 7 7	0	0
14	Y	6	Total O 6 6	0	0
14	Z	2	Total O 2 2	0	0
14	b	11	Total O 11 11	0	0
14	e	8	Total O 8 8	0	0
14	f	4	Total O 4 4	0	0
14	g	5	Total O 5 5	0	0
14	h	3	Total O 3 3	0	0
14	i	2	Total O 2 2	0	0

Continued on next page...

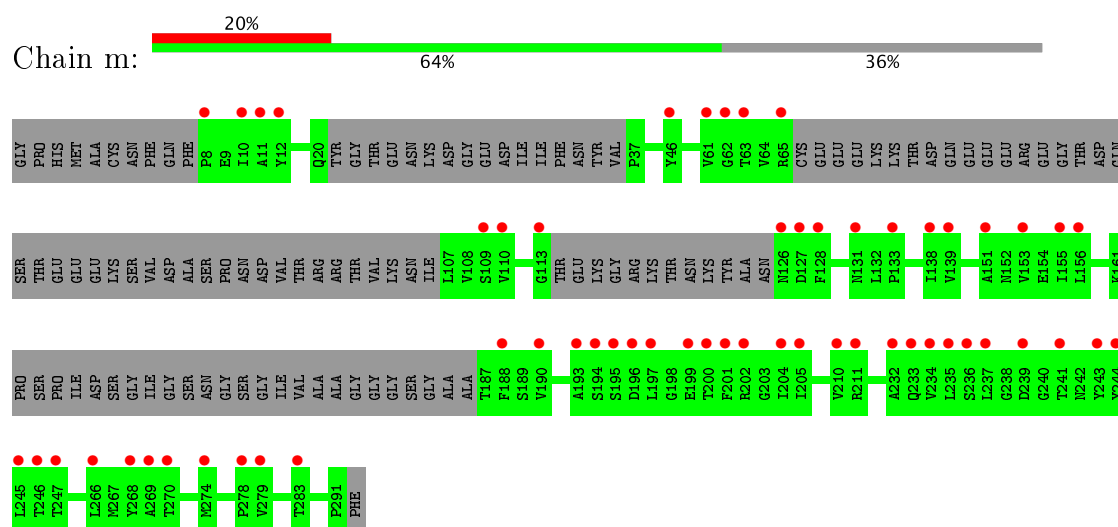
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	j	1	Total	O	0	0
			1	1		
14	l	8	Total	O	0	0
			8	8		

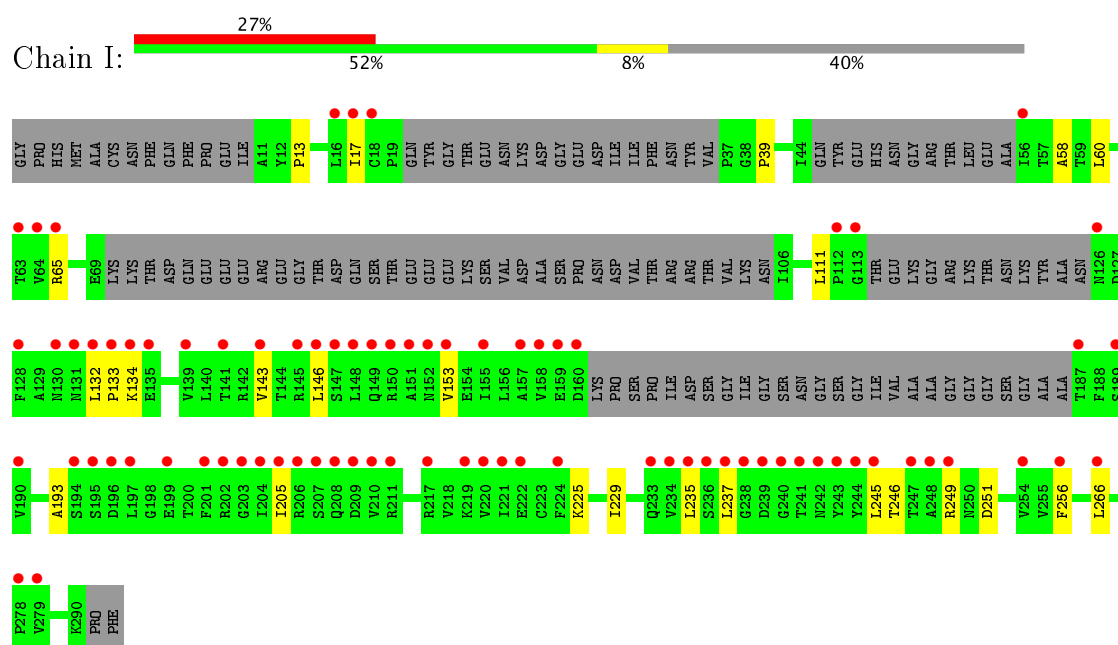
3 Residue-property plots [i](#)

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 component CSL4



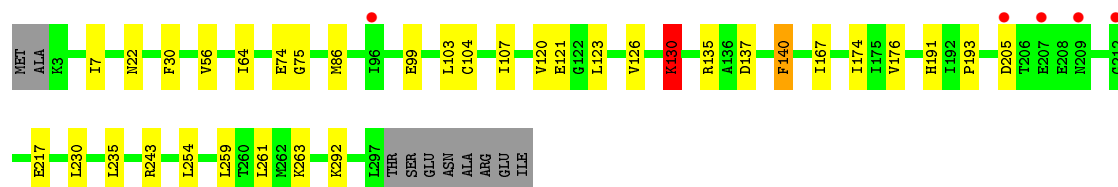
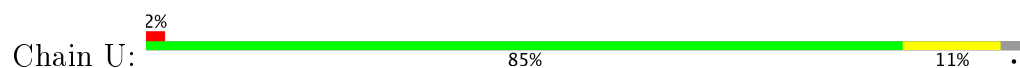
• Molecule 1: Exosome complex component CSL4



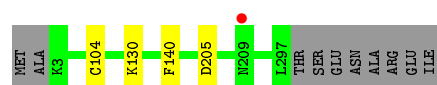
• Molecule 1: Exosome complex component CSL4



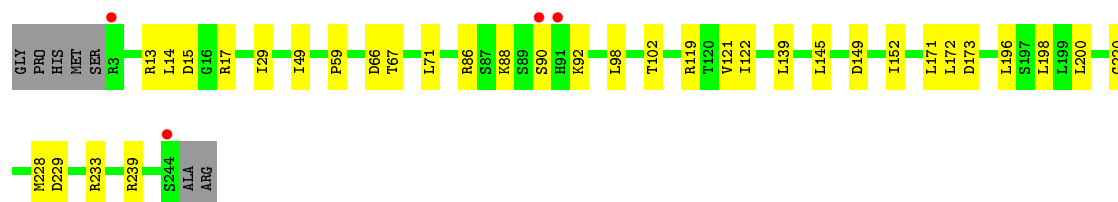
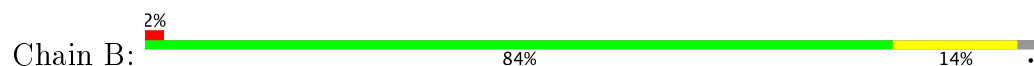
- Molecule 2: Exosome complex component RRP45



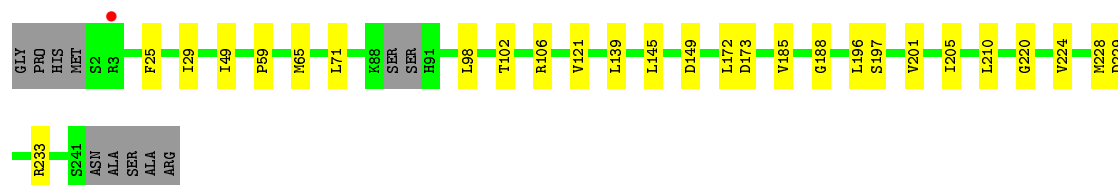
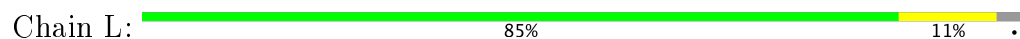
- Molecule 2: Exosome complex component RRP45



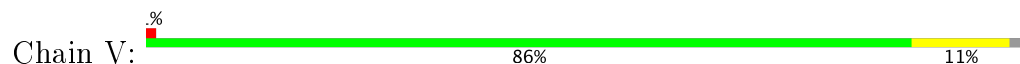
- Molecule 3: Exosome complex component SKI6



- Molecule 3: Exosome complex component SKI6



- Molecule 3: Exosome complex component SKI6





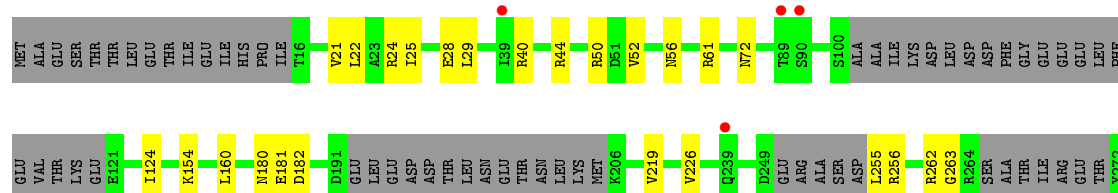
- Molecule 3: Exosome complex component SKI6

Chain f: 94% 5%



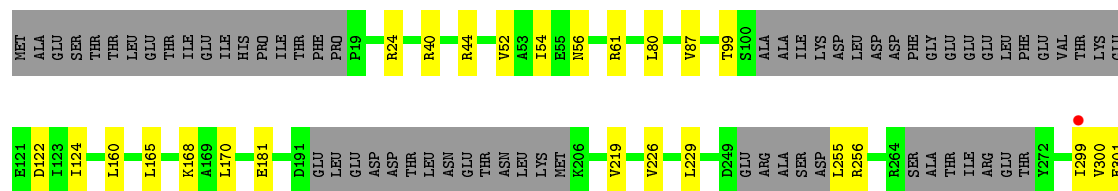
- Molecule 4: Exosome complex component RRP43

Chain C: 70% 10% 21%



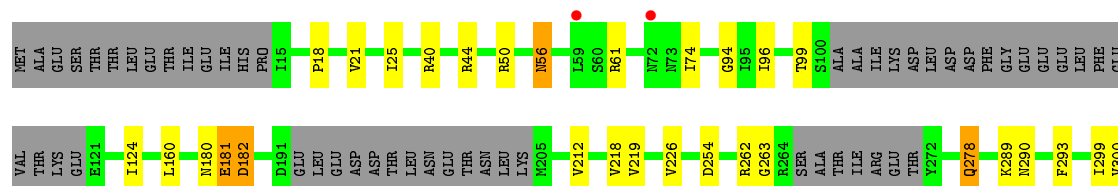
- Molecule 4: Exosome complex component RRP43

Chain M: 69% 10% 21%



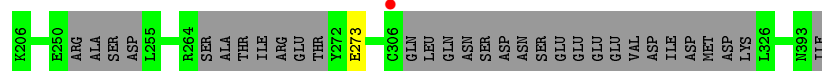
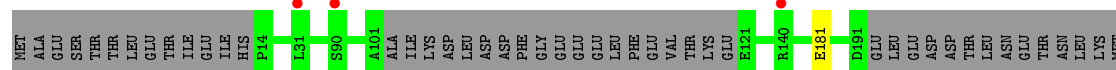
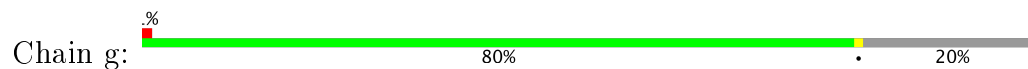
- Molecule 4: Exosome complex component RRP43

Chain W: 69% 11% 19%

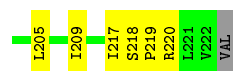
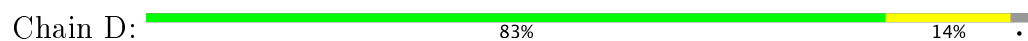




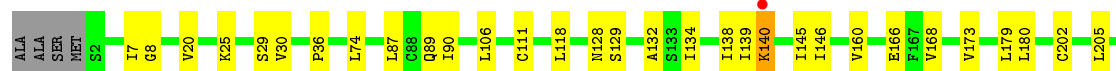
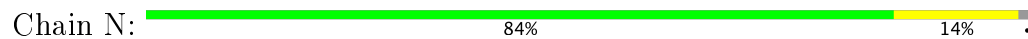
- Molecule 4: Exosome complex component RRP43



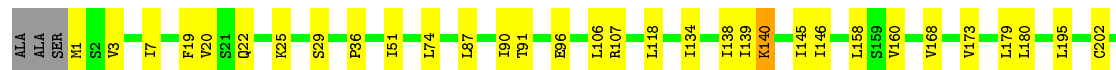
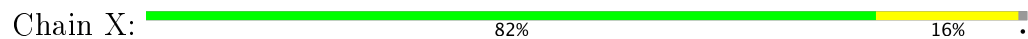
- Molecule 5: Exosome complex component RRP46



- Molecule 5: Exosome complex component RRP46



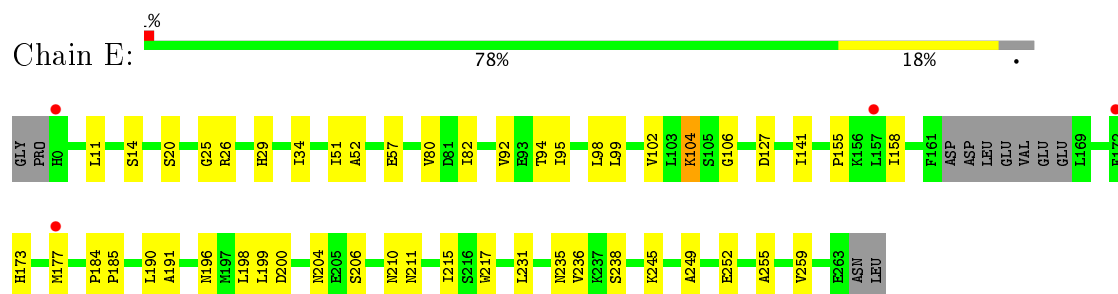
- Molecule 5: Exosome complex component RRP46



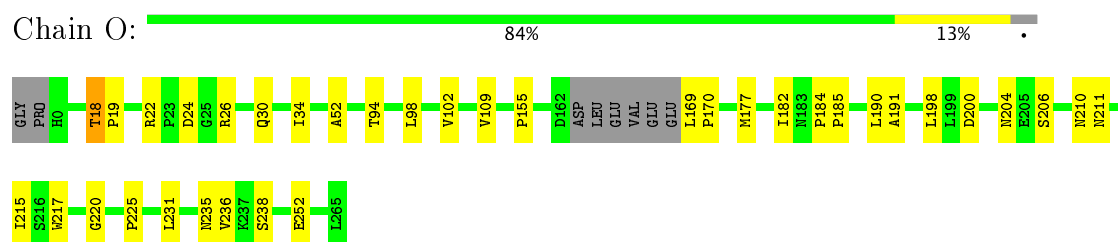
- Molecule 5: Exosome complex component RRP46



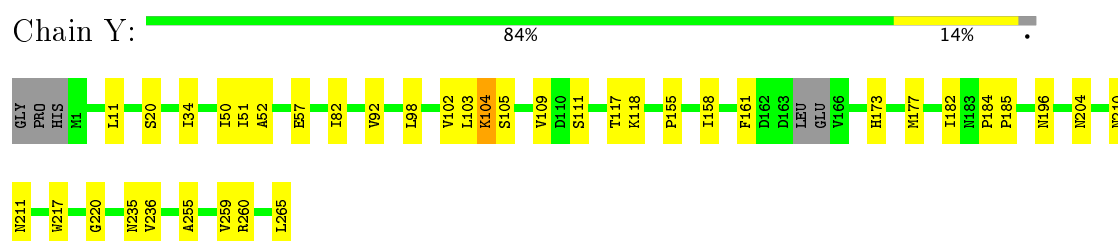
- Molecule 6: Exosome complex component RRP42



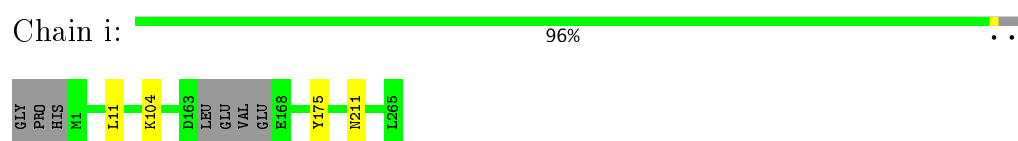
- Molecule 6: Exosome complex component RRP42



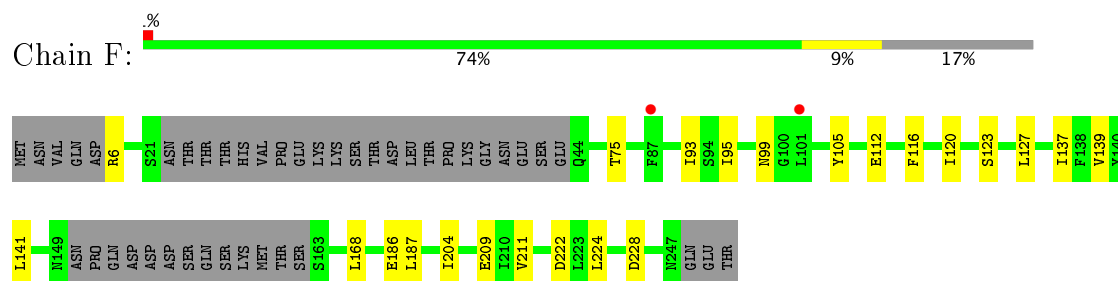
- Molecule 6: Exosome complex component RRP42



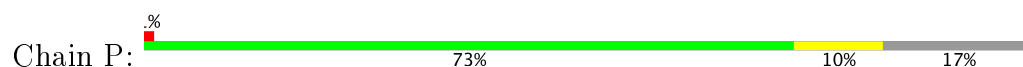
- Molecule 6: Exosome complex component RRP42

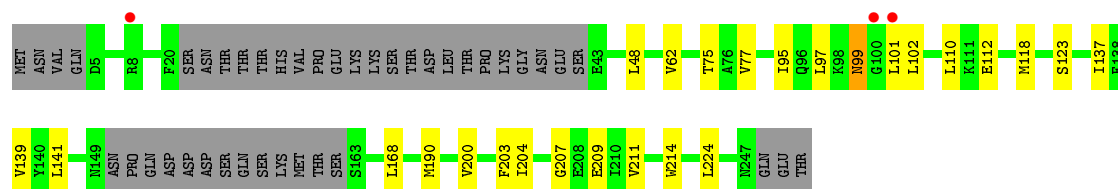


- Molecule 7: Exosome complex component MTR3

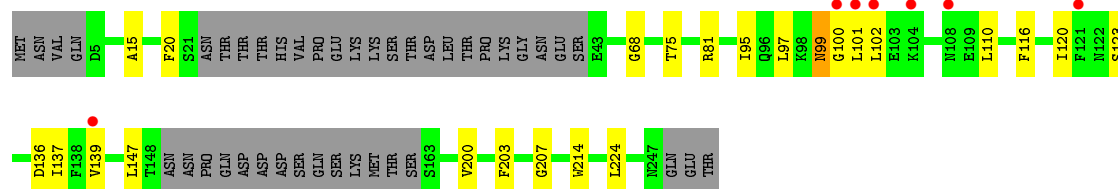


- Molecule 7: Exosome complex component MTR3

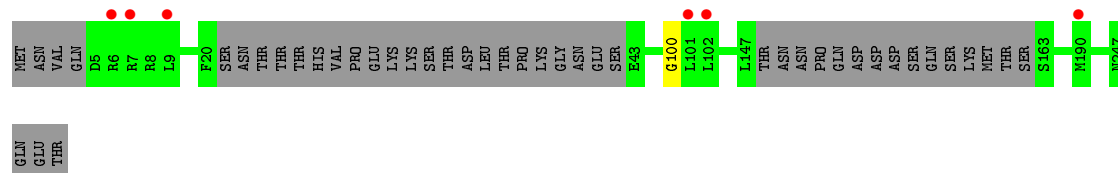
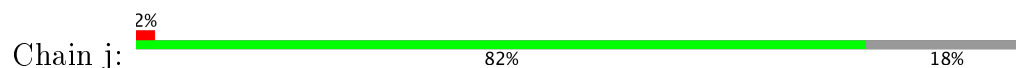




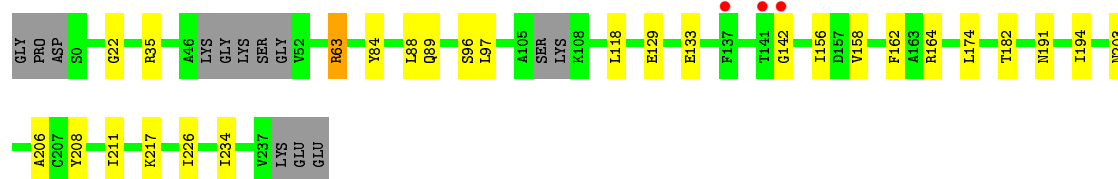
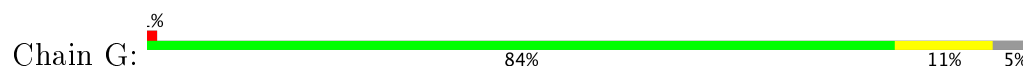
- Molecule 7: Exosome complex component MTR3



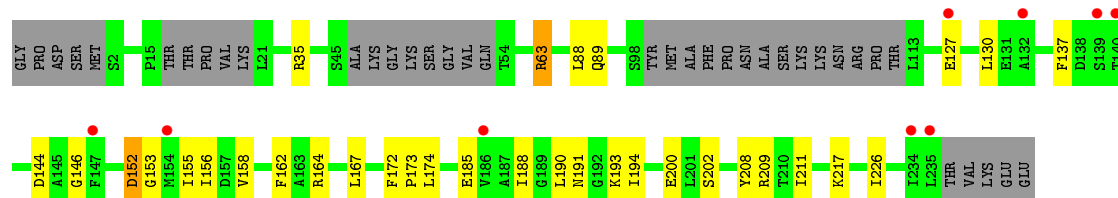
- Molecule 7: Exosome complex component MTR3



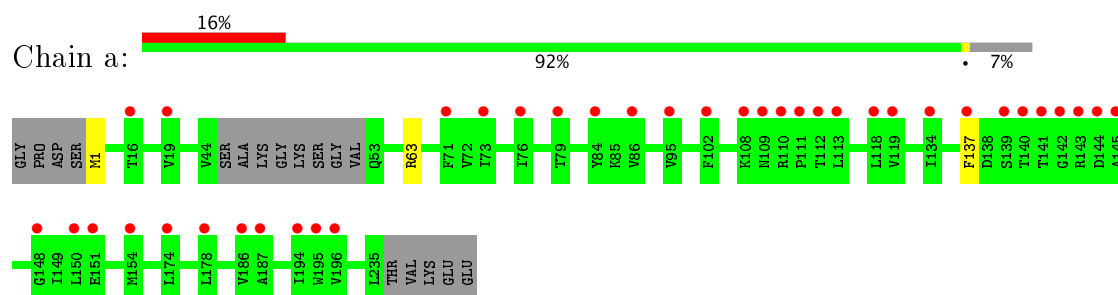
- Molecule 8: Exosome complex component RRP40



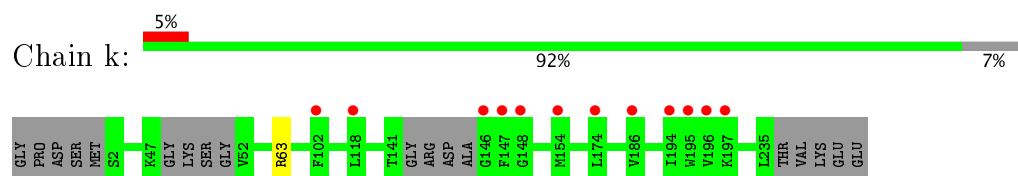
- Molecule 8: Exosome complex component RRP40



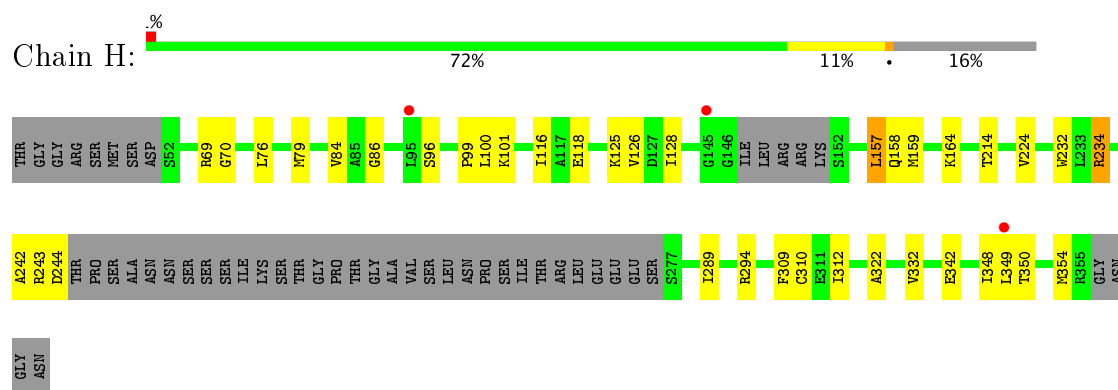
- Molecule 8: Exosome complex component RRP40



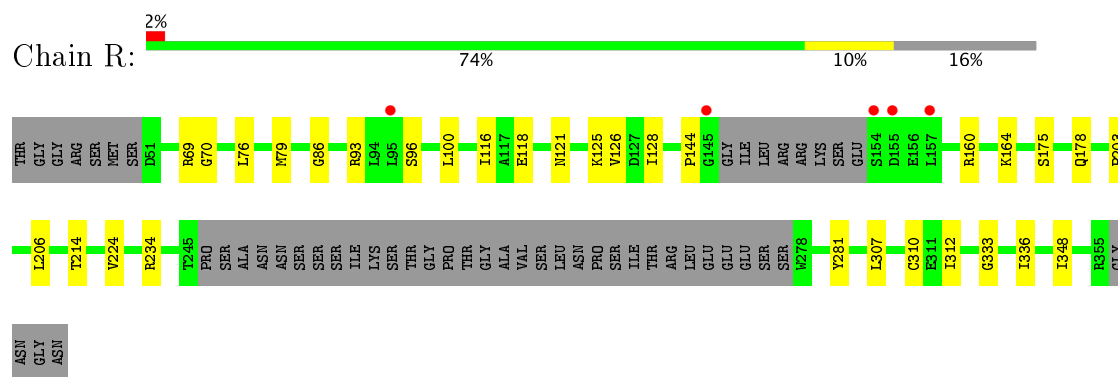
- Molecule 8: Exosome complex component RRP40



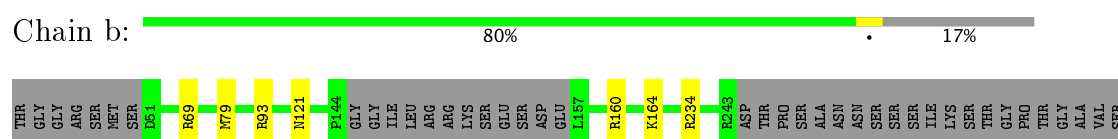
- Molecule 9: Exosome complex component RRP4

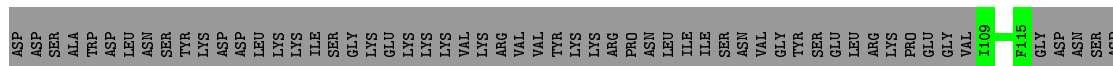


- Molecule 9: Exosome complex component RRP4



- Molecule 9: Exosome complex component RRP4





ASP
SER
GLY
SER
SER
SER
ARG
LYS
ARG
LYS
PHE
ASP
GLU
GLY
GLY
GLN
ASN
GLU
ASP
GLU
LYS
ARG
ASP
ALA
LYS
ASP
LYS
GLU
PHE
THR
GLY
SER
GLN
ASP
ASP
GLY
GLU
ASP
GLU
TYR
ASP
LEU
ASP
LYS
LYS
PHE
LEU
PHE
LYS
SER
SER
ILE
LYS
LYS
LYS
LYS
LYS
THR
ASN
GLY
LYS

ASN
ARG
ASN
SER
LYS
LYS

- Molecule 10: M-phase phosphoprotein 6 homolog



GLY
PRO
ASP
SER
SER
MET
SER
ALA
ASN
ASN
GLY
VAL
THR
GLY
LYS
LEU
SER
SER
ARG
VAL
MET
ASN
MET
LYS
LYS
PHE
MET
LYS
PHE
GLY
LYS
THR
ASP
ASP
GLU
PRO
SER
SER
ASN
SER
SER
ASN
PRO
GLY
SER
ASN
ILE
ASN
ASN
THR
THR
PRO
SER
GLY
ASN
ILE
ASN
ASP
THR
GLN
LYS
GLY
LYS
LEU
PHE
GLY
LEU

ASP
ASP
SER
SER
ALA
TRP
ASP
LEU
ASN
SER
TYR
LYS
ASP
ASP
LEU
LYS
LYS
ILE
SER
GLY
GLY
LYS
PRO
GLY
GLY
V108
F115
G116
D117
ASN
SER
ASP
ASP

SER
GLY
SER
ARG
LYS
ARG
LYS
PHE
ASP
GLY
GLY
GLY
GLN
ASN
GLU
ASP
GLU
LYS
LYS
ARG
THR
GLY
SER
GLN
ASP
ASP
GLY
GLU
ASP
GLY
LEU
ASP
LYS
PHE
LYS
ASP
GLU
ILE
LYS
LYS
LYS
LYS
LYS
THR
ASN
HIS
ASN
GLY
LYS
ASN
LYS
ASN

ARG
ASN
SER
LYS
LYS

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	161.78 Å 237.43 Å 201.90 Å 90.00° 110.37° 90.00°	Depositor
Resolution (Å)	80.76 – 3.20 151.66 – 3.20	Depositor EDS
% Data completeness (in resolution range)	95.8 (80.76-3.20) 97.7 (151.66-3.20)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 3.19 Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.223 , 0.262 0.212 , 0.250	Depositor DCC
R_{free} test set	11369 reflections (4.96%)	DCC
Wilson B-factor (Å ²)	72.8	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 53.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	67168	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.58 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.1430e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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: TAM, MG, 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	I	0.23	0/1330	0.44	0/1798
1	S	0.24	0/1576	0.43	0/2138
1	c	0.24	0/1483	0.44	0/2009
1	m	0.24	0/1443	0.44	0/1952
2	A	0.24	0/2279	0.41	0/3083
2	K	0.24	0/2279	0.40	0/3083
2	U	0.24	0/2279	0.41	0/3083
2	e	0.23	0/2283	0.41	0/3087
3	B	0.23	0/1852	0.43	0/2506
3	L	0.23	0/1818	0.43	0/2459
3	V	0.23	0/1873	0.42	0/2529
3	f	0.23	0/1854	0.43	0/2502
4	C	0.24	0/2365	0.43	0/3209
4	M	0.24	0/2312	0.44	0/3138
4	W	0.24	0/2432	0.43	0/3297
4	g	0.24	0/2408	0.41	0/3263
5	D	0.23	0/1667	0.44	0/2269
5	N	0.24	0/1684	0.43	0/2291
5	X	0.24	0/1722	0.43	0/2336
5	h	0.23	0/1721	0.43	0/2335
6	E	0.24	0/1928	0.43	0/2631
6	O	0.34	1/1978 (0.1%)	0.41	0/2698
6	Y	0.24	0/2010	0.42	0/2741
6	i	0.24	0/2019	0.42	0/2748
7	F	0.24	0/1538	0.43	0/2084
7	P	0.24	0/1537	0.43	0/2084
7	Z	0.24	0/1552	0.44	0/2101
7	j	0.24	0/1527	0.43	0/2070
8	G	0.25	0/1731	0.41	0/2361
8	Q	0.24	0/1576	0.42	0/2138
8	a	0.25	0/1780	0.41	0/2420
8	k	0.25	0/1649	0.41	0/2254

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
9	H	0.24	0/2046	0.42	0/2773
9	R	0.23	0/2050	0.42	0/2777
9	b	0.24	0/2026	0.42	0/2744
9	l	0.24	0/2052	0.43	0/2779
10	J	0.24	0/140	0.41	0/186
10	T	0.20	0/45	0.35	0/59
10	d	0.20	0/45	0.44	0/59
10	n	0.25	0/70	0.37	0/91
All	All	0.24	1/67959 (0.0%)	0.42	0/92165

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	O	18	THR	C-N	10.73	1.54	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	1317	0	1323	18	0
1	S	1554	0	1536	13	0
1	c	1463	0	1454	0	0
1	m	1425	0	1432	0	0
2	A	2244	0	2190	20	0
2	K	2244	0	2190	23	0
2	U	2244	0	2190	21	0
2	e	2248	0	2201	0	0
3	B	1830	0	1813	21	0
3	L	1797	0	1781	16	0
3	V	1851	0	1866	19	0
3	f	1832	0	1840	0	0
4	C	2335	0	2314	24	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	M	2283	0	2232	25	0
4	W	2400	0	2400	31	0
4	g	2376	0	2375	0	0
5	D	1649	0	1663	20	0
5	N	1666	0	1689	18	0
5	X	1704	0	1759	19	0
5	h	1703	0	1756	0	0
6	E	1894	0	1869	28	0
6	O	1941	0	1913	24	0
6	Y	1974	0	1960	22	0
6	i	1981	0	1987	0	0
7	F	1517	0	1441	14	0
7	P	1515	0	1420	16	0
7	Z	1531	0	1461	14	0
7	j	1506	0	1436	0	0
8	G	1696	0	1558	20	0
8	Q	1550	0	1463	20	0
8	a	1744	0	1688	0	0
8	k	1615	0	1456	0	0
9	H	2013	0	1965	20	0
9	R	2019	0	1990	15	0
9	b	1993	0	1960	0	0
9	l	2020	0	1967	0	0
10	J	139	0	130	1	0
10	T	46	0	42	2	0
10	d	46	0	42	0	0
10	n	70	0	67	0	0
11	A	11	0	17	0	0
11	K	11	0	17	3	0
11	U	11	0	17	1	0
11	e	11	0	17	0	0
12	G	1	0	0	0	0
12	H	1	0	0	0	0
12	R	2	0	0	0	0
12	b	1	0	0	0	0
12	f	1	0	0	0	0
12	l	1	0	0	0	0
13	O	1	0	0	0	0
13	g	1	0	0	0	0
14	A	4	0	0	0	0
14	B	9	0	0	0	0
14	C	8	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	D	7	0	0	0	0
14	E	2	0	0	0	0
14	G	3	0	0	1	0
14	H	3	0	0	0	0
14	L	2	0	0	0	0
14	N	2	0	0	0	0
14	O	7	0	0	0	0
14	P	2	0	0	0	0
14	R	3	0	0	0	0
14	U	13	0	0	1	0
14	V	12	0	0	1	0
14	W	6	0	0	0	0
14	X	7	0	0	0	0
14	Y	6	0	0	0	0
14	Z	2	0	0	0	0
14	b	11	0	0	0	0
14	e	8	0	0	0	0
14	f	4	0	0	0	0
14	g	5	0	0	0	0
14	h	3	0	0	0	0
14	i	2	0	0	0	0
14	j	1	0	0	0	0
14	l	8	0	0	0	0
All	All	67168	0	65887	429	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 5.

The worst 5 of 429 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)
7:Z:99:ASN:ND2	7:Z:102:LEU:O	1.97	0.97
9:H:157:LEU:O	9:H:159:MET:N	2.15	0.79
4:M:24:ARG:NH1	1:S:193:ALA:O	2.19	0.75
5:N:139:ILE:HD13	5:N:146:ILE:HD13	1.67	0.74
4:W:180:ASN:ND2	4:W:181:GLU:OE1	2.23	0.72

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	I	166/295 (56%)	162 (98%)	3 (2%)	1 (1%)	28	72
1	S	198/295 (67%)	193 (98%)	5 (2%)	0	100	100
1	c	187/295 (63%)	183 (98%)	4 (2%)	0	100	100
1	m	180/295 (61%)	176 (98%)	4 (2%)	0	100	100
2	A	293/305 (96%)	279 (95%)	13 (4%)	1 (0%)	44	81
2	K	293/305 (96%)	280 (96%)	13 (4%)	0	100	100
2	U	293/305 (96%)	279 (95%)	13 (4%)	1 (0%)	44	81
2	e	293/305 (96%)	278 (95%)	14 (5%)	1 (0%)	44	81
3	B	240/249 (96%)	225 (94%)	15 (6%)	0	100	100
3	L	234/249 (94%)	226 (97%)	7 (3%)	1 (0%)	38	77
3	V	239/249 (96%)	227 (95%)	10 (4%)	2 (1%)	22	65
3	f	234/249 (94%)	223 (95%)	10 (4%)	1 (0%)	38	77
4	C	301/394 (76%)	288 (96%)	12 (4%)	1 (0%)	44	81
4	M	298/394 (76%)	285 (96%)	12 (4%)	1 (0%)	44	81
4	W	309/394 (78%)	292 (94%)	13 (4%)	4 (1%)	14	55
4	g	306/394 (78%)	294 (96%)	11 (4%)	1 (0%)	44	81
5	D	219/226 (97%)	212 (97%)	6 (3%)	1 (0%)	32	74
5	N	220/226 (97%)	213 (97%)	6 (3%)	1 (0%)	32	74
5	X	221/226 (98%)	215 (97%)	5 (2%)	1 (0%)	32	74
5	h	221/226 (98%)	215 (97%)	5 (2%)	1 (0%)	32	74
6	E	253/268 (94%)	244 (96%)	8 (3%)	1 (0%)	38	77
6	O	256/268 (96%)	246 (96%)	10 (4%)	0	100	100
6	Y	259/268 (97%)	250 (96%)	8 (3%)	1 (0%)	38	77
6	i	257/268 (96%)	247 (96%)	9 (4%)	1 (0%)	38	77
7	F	201/250 (80%)	194 (96%)	7 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	P	202/250 (81%)	195 (96%)	6 (3%)	1 (0%)	32	74
7	Z	202/250 (81%)	194 (96%)	7 (4%)	1 (0%)	32	74
7	j	200/250 (80%)	193 (96%)	6 (3%)	1 (0%)	32	74
8	G	225/244 (92%)	218 (97%)	6 (3%)	1 (0%)	38	77
8	Q	199/244 (82%)	192 (96%)	6 (3%)	1 (0%)	32	74
8	a	223/244 (91%)	217 (97%)	6 (3%)	0	100	100
8	k	220/244 (90%)	213 (97%)	7 (3%)	0	100	100
9	H	261/316 (83%)	249 (95%)	9 (3%)	3 (1%)	17	58
9	R	259/316 (82%)	251 (97%)	7 (3%)	1 (0%)	38	77
9	b	256/316 (81%)	244 (95%)	10 (4%)	2 (1%)	22	65
9	l	262/316 (83%)	253 (97%)	8 (3%)	1 (0%)	38	77
10	J	16/190 (8%)	14 (88%)	2 (12%)	0	100	100
10	T	5/190 (3%)	4 (80%)	1 (20%)	0	100	100
10	d	5/190 (3%)	4 (80%)	1 (20%)	0	100	100
10	n	8/190 (4%)	7 (88%)	1 (12%)	0	100	100
All	All	8714/10948 (80%)	8374 (96%)	306 (4%)	34 (0%)	38	77

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	130	LYS
5	D	140	LYS
6	E	104	LYS
9	H	158	GLN
8	Q	152	ASP

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	I	140/242 (58%)	140 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	S	163/242 (67%)	163 (100%)	0	100	100
1	c	153/242 (63%)	153 (100%)	0	100	100
1	m	152/242 (63%)	152 (100%)	0	100	100
2	A	243/266 (91%)	239 (98%)	4 (2%)	68	89
2	K	243/266 (91%)	242 (100%)	1 (0%)	93	97
2	U	243/266 (91%)	239 (98%)	4 (2%)	68	89
2	e	244/266 (92%)	241 (99%)	3 (1%)	75	91
3	B	194/220 (88%)	193 (100%)	1 (0%)	91	97
3	L	192/220 (87%)	192 (100%)	0	100	100
3	V	200/220 (91%)	200 (100%)	0	100	100
3	f	199/220 (90%)	198 (100%)	1 (0%)	91	97
4	C	244/349 (70%)	242 (99%)	2 (1%)	85	95
4	M	235/349 (67%)	231 (98%)	4 (2%)	66	88
4	W	255/349 (73%)	253 (99%)	2 (1%)	85	95
4	g	247/349 (71%)	246 (100%)	1 (0%)	93	97
5	D	182/198 (92%)	181 (100%)	1 (0%)	91	97
5	N	187/198 (94%)	186 (100%)	1 (0%)	91	97
5	X	196/198 (99%)	193 (98%)	3 (2%)	70	90
5	h	195/198 (98%)	193 (99%)	2 (1%)	80	93
6	E	208/242 (86%)	205 (99%)	3 (1%)	71	90
6	O	215/242 (89%)	214 (100%)	1 (0%)	91	97
6	Y	224/242 (93%)	220 (98%)	4 (2%)	64	87
6	i	225/242 (93%)	222 (99%)	3 (1%)	73	91
7	F	155/219 (71%)	153 (99%)	2 (1%)	73	91
7	P	150/219 (68%)	149 (99%)	1 (1%)	87	96
7	Z	156/219 (71%)	155 (99%)	1 (1%)	89	96
7	j	153/219 (70%)	153 (100%)	0	100	100
8	G	168/212 (79%)	167 (99%)	1 (1%)	89	96
8	Q	162/212 (76%)	159 (98%)	3 (2%)	62	86
8	a	191/212 (90%)	188 (98%)	3 (2%)	68	89
8	k	151/212 (71%)	150 (99%)	1 (1%)	87	96

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	H	212/270 (78%)	208 (98%)	4 (2%)	62	86
9	R	218/270 (81%)	213 (98%)	5 (2%)	56	84
9	b	213/270 (79%)	207 (97%)	6 (3%)	49	81
9	l	211/270 (78%)	207 (98%)	4 (2%)	62	86
10	J	13/171 (8%)	13 (100%)	0	100	100
10	T	4/171 (2%)	4 (100%)	0	100	100
10	d	4/171 (2%)	4 (100%)	0	100	100
10	n	6/171 (4%)	6 (100%)	0	100	100
All	All	7146/9556 (75%)	7074 (99%)	72 (1%)	80	93

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	R	164	LYS
5	X	1	MET
6	i	211	ASN
9	R	234	ARG
2	U	140	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
9	l	212	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 9 are monoatomic - leaving 4 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	$\# Z > 2$
11	TAM	A	401	-	7,10,10	0.82	0	9,12,12	1.21	1 (11%)
11	TAM	K	401	-	7,10,10	0.81	0	9,12,12	1.20	1 (11%)
11	TAM	U	401	-	7,10,10	0.80	0	9,12,12	1.22	1 (11%)
11	TAM	e	401	-	7,10,10	0.80	0	9,12,12	1.22	1 (11%)

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
11	TAM	A	401	-	-	0/12/12/12	0/0/0/0
11	TAM	K	401	-	-	0/12/12/12	0/0/0/0
11	TAM	U	401	-	-	0/12/12/12	0/0/0/0
11	TAM	e	401	-	-	0/12/12/12	0/0/0/0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	e	401	TAM	O5-C5-C2	-2.06	105.50	111.33
11	K	401	TAM	O5-C5-C2	-2.05	105.53	111.33
11	U	401	TAM	O5-C5-C2	-2.05	105.54	111.33
11	A	401	TAM	O5-C5-C2	-2.02	105.61	111.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	K	401	TAM	3	0
11	U	401	TAM	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	I	178/295 (60%)	1.95	80 (44%) 0 0	100, 161, 215, 252	0
1	S	208/295 (70%)	2.46	102 (49%) 0 0	111, 190, 246, 272	0
1	c	197/295 (66%)	1.85	78 (39%) 0 0	125, 167, 214, 246	0
1	m	190/295 (64%)	1.51	59 (31%) 0 1	110, 153, 199, 232	0
2	A	295/305 (96%)	-0.06	1 (0%) 93 92	51, 71, 133, 178	0
2	K	295/305 (96%)	0.08	3 (1%) 82 72	48, 78, 137, 219	0
2	U	295/305 (96%)	0.07	5 (1%) 70 57	50, 74, 144, 218	0
2	e	295/305 (96%)	-0.01	1 (0%) 93 92	56, 76, 140, 200	0
3	B	242/249 (97%)	0.03	4 (1%) 70 57	45, 66, 120, 174	0
3	L	238/249 (95%)	-0.01	1 (0%) 92 89	37, 57, 101, 133	0
3	V	241/249 (96%)	0.09	2 (0%) 86 77	41, 61, 107, 154	0
3	f	237/249 (95%)	0.10	0 100 100	50, 68, 115, 160	0
4	C	313/394 (79%)	0.01	5 (1%) 72 59	57, 85, 147, 224	0
4	M	310/394 (78%)	-0.03	1 (0%) 93 92	55, 84, 141, 208	0
4	W	319/394 (80%)	0.04	2 (0%) 89 83	50, 79, 140, 208	0
4	g	317/394 (80%)	0.14	4 (1%) 77 65	60, 85, 135, 207	0
5	D	221/226 (97%)	-0.15	1 (0%) 90 85	47, 69, 104, 126	0
5	N	222/226 (98%)	-0.14	1 (0%) 90 85	50, 85, 123, 173	0
5	X	223/226 (98%)	-0.01	0 100 100	46, 75, 111, 164	0
5	h	223/226 (98%)	-0.19	0 100 100	59, 78, 111, 132	0
6	E	257/268 (95%)	-0.05	4 (1%) 72 59	56, 83, 134, 157	0
6	O	260/268 (97%)	-0.17	0 100 100	49, 77, 125, 171	0
6	Y	263/268 (98%)	-0.13	0 100 100	43, 72, 123, 149	0
6	i	261/268 (97%)	-0.13	0 100 100	51, 76, 123, 172	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
7	F	207/250 (82%)	0.05	2 (0%) 82 72	58, 90, 137, 166	0
7	P	208/250 (83%)	-0.09	3 (1%) 75 63	62, 94, 133, 159	0
7	Z	208/250 (83%)	0.22	7 (3%) 46 30	61, 89, 133, 156	0
7	j	206/250 (82%)	0.11	6 (2%) 52 37	61, 89, 136, 160	0
8	G	231/244 (94%)	-0.09	3 (1%) 77 65	58, 91, 150, 217	0
8	Q	207/244 (84%)	0.08	9 (4%) 36 23	89, 142, 185, 264	0
8	a	227/244 (93%)	0.64	38 (16%) 2 1	90, 137, 211, 267	0
8	k	226/244 (92%)	0.02	12 (5%) 27 15	87, 118, 178, 226	0
9	H	267/316 (84%)	-0.04	3 (1%) 80 68	42, 85, 129, 189	0
9	R	265/316 (83%)	-0.09	5 (1%) 67 52	40, 71, 114, 158	0
9	b	262/316 (82%)	-0.17	0 100 100	49, 82, 135, 160	0
9	l	268/316 (84%)	-0.11	6 (2%) 62 48	59, 93, 144, 196	0
10	J	20/190 (10%)	0.31	2 (10%) 8 5	88, 118, 157, 157	0
10	T	7/190 (3%)	-0.60	0 100 100	131, 137, 142, 163	0
10	d	7/190 (3%)	-0.01	0 100 100	110, 131, 137, 140	0
10	n	10/190 (5%)	0.89	1 (10%) 8 5	111, 124, 167, 178	0
All	All	8926/10948 (81%)	0.17	451 (5%) 29 16	37, 85, 174, 272	0

The worst 5 of 451 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	c	196	ASP	16.1
1	m	195	SER	14.8
1	S	196	ASP	12.2
1	c	278	PRO	12.0
1	S	238	GLY	10.6

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 [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
12	CL	G	301	1/1	0.92	0.28	0.88	99,99,99,99	0
11	TAM	K	401	11/11	0.92	0.19	0.86	69,86,103,111	0
11	TAM	U	401	11/11	0.91	0.18	-0.34	79,98,112,119	0
11	TAM	A	401	11/11	0.92	0.17	-0.38	85,96,101,103	0
13	MG	g	401	1/1	0.73	0.14	-1.12	60,60,60,60	0
11	TAM	e	401	11/11	0.86	0.15	-1.87	75,89,96,99	0
13	MG	O	301	1/1	0.66	0.36	-	85,85,85,85	0
12	CL	R	401	1/1	0.59	0.43	-	95,95,95,95	0
12	CL	l	401	1/1	0.95	0.11	-	75,75,75,75	0
12	CL	f	301	1/1	0.90	0.29	-	79,79,79,79	0
12	CL	b	401	1/1	0.86	0.27	-	86,86,86,86	0
12	CL	R	402	1/1	0.96	0.17	-	73,73,73,73	0
12	CL	H	401	1/1	0.90	0.20	-	80,80,80,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.