wwPDB X-ray Structure Validation Summary Report (i)

Jun 25, 2024 – 11:23 AM EDT

PDB ID	:	5OKZ
Title	:	Crystal Strucrure of the Mpp6 Exosome complex
Authors	:	Falk, S.; Ebert, J.; Conti, E.
Deposited on	:	2017-07-26
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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

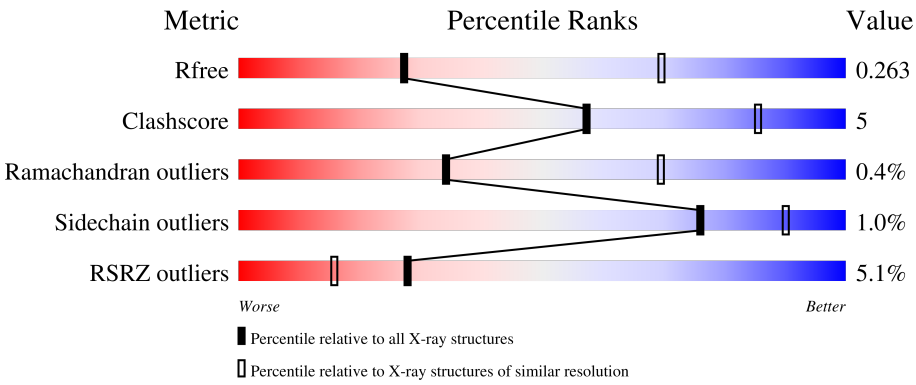
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.20 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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	27% 52% 8% 40%
1	S	295	35% 64% 6% 29%
1	c	295	26% 67% 33%
1	m	295	20% 64% 36%
2	A	305	86% 10% • •

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Mol	Chain	Length	Quality of chain
2	K	305	%, 86%, 11%
2	U	305	2%, 85%, 11%
2	e	305	95%
3	B	249	2%, 84%, 14%
3	L	249	85%, 11%
3	V	249	%, 86%, 11%
3	f	249	94%, 5%
4	C	394	%, 70%, 10%, 21%
4	M	394	69%, 10%, 21%
4	W	394	%, 69%, 11%, 19%
4	g	394	%, 80%, 20%
5	D	226	83%, 14%
5	N	226	84%, 14%
5	X	226	82%, 16%
5	h	226	97%
6	E	268	%, 78%, 18%
6	O	268	84%, 13%
6	Y	268	84%, 14%
6	i	268	96%
7	F	250	%, 74%, 9%, 17%
7	P	250	%, 73%, 10%, 17%
7	Z	250	3%, 74%, 9%, 17%
7	j	250	2%, 82%, 18%
8	G	244	%, 84%, 11%, 5%
8	Q	244	4%, 71%, 13%, 15%

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

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
12	CL	R	401	-	-	-	X

2 Entry composition (i)

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

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
			Total	C	N	O	S			
2	A	295	2244	1410	384	434	16	0	0	0
2	K	295	2244	1410	384	434	16	0	0	0

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

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

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

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
			Total	C	N	O	S			
4	C	313	2335	1478	404	444	9	0	0	0
			Total	C	N	O	S			
4	M	310	2283	1439	398	436	10	0	0	0
			Total	C	N	O	S			
4	W	319	2400	1518	416	455	11	0	0	0

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

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

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

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

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

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
			Total	C	N	O	S			
9	H	267	2013	1262	361	380	10	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	R	265	2019	1263	360	386	10	0	0	0
			Total	C	N	O	S			
9	b	262	1993	1250	357	375	11	0	0	0
			Total	C	N	O	S			
9	l	268	2020	1268	361	380	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
			Total	C	N	O			
10	J	20	139	89	25	25	0	0	0
			Total	C	N	O			
10	T	7	46	27	10	9	0	0	0

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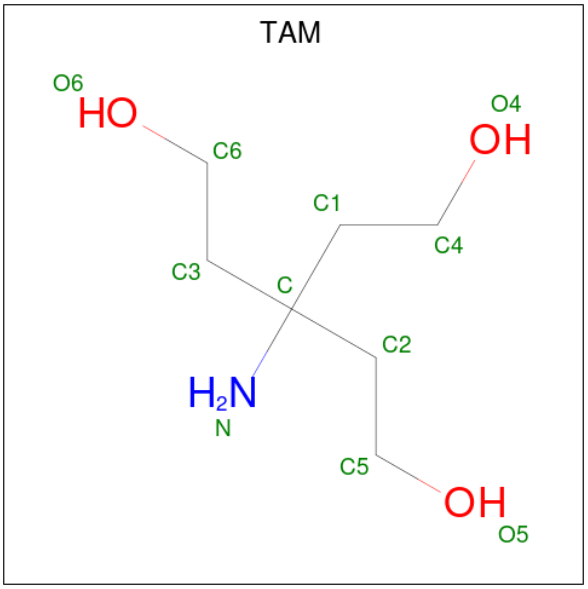
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	d	7	46	27	10	9	0	0	0
			Total	C	N	O			
10	n	10	70	44	14	12	0	0	0

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
			Total	C	N	O		
11	A	1	11	7	1	3	0	0
11	K	1	11	7	1	3	0	0
11	U	1	11	7	1	3	0	0
11	e	1	11	7	1	3	0	0

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

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

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

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

- Molecule 14 is water.

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

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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

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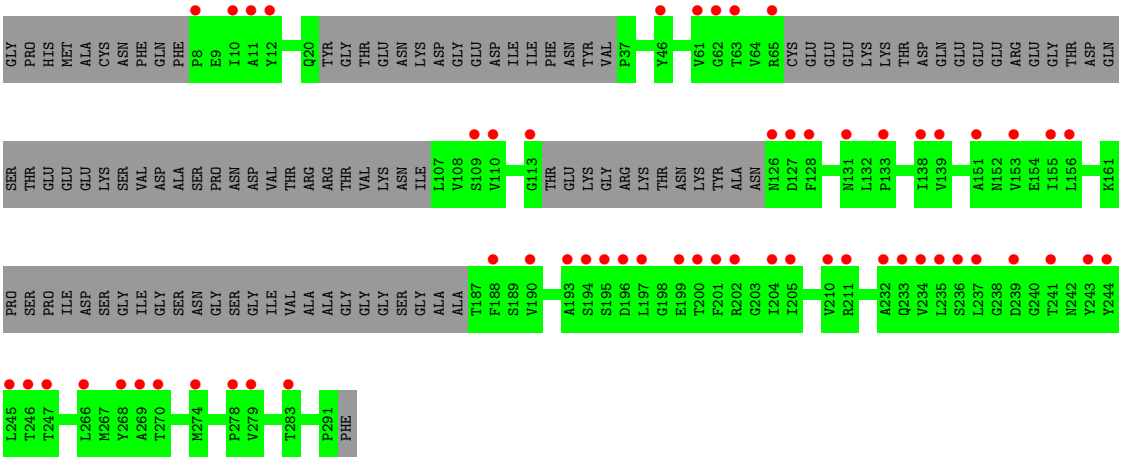
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	j	1	Total O 1 1	0	0
14	l	8	Total O 8 8	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

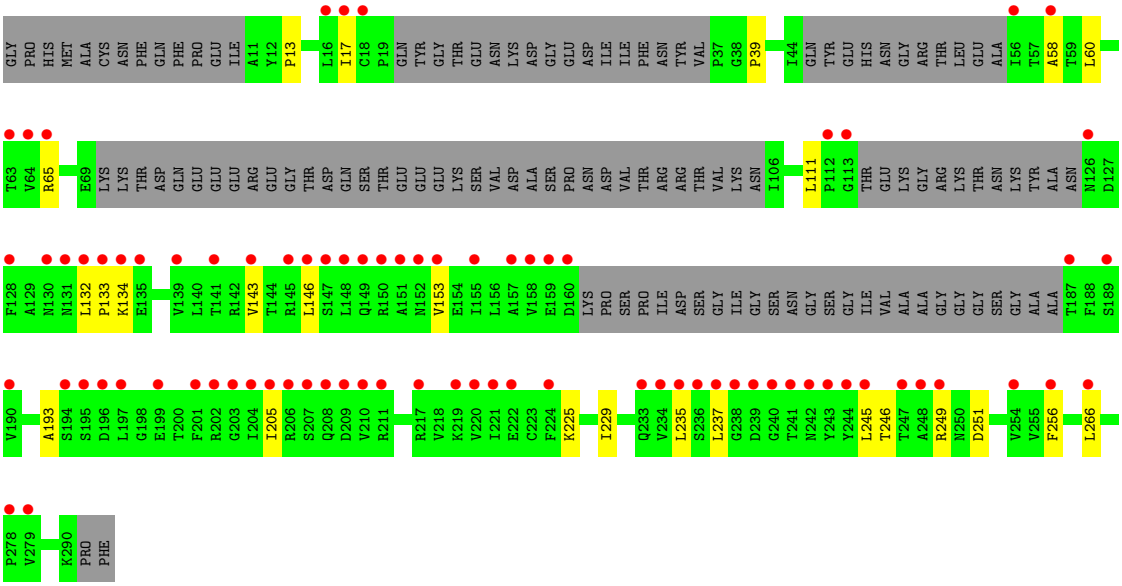
• Molecule 1: Exosome complex component CSL4

Chain m:



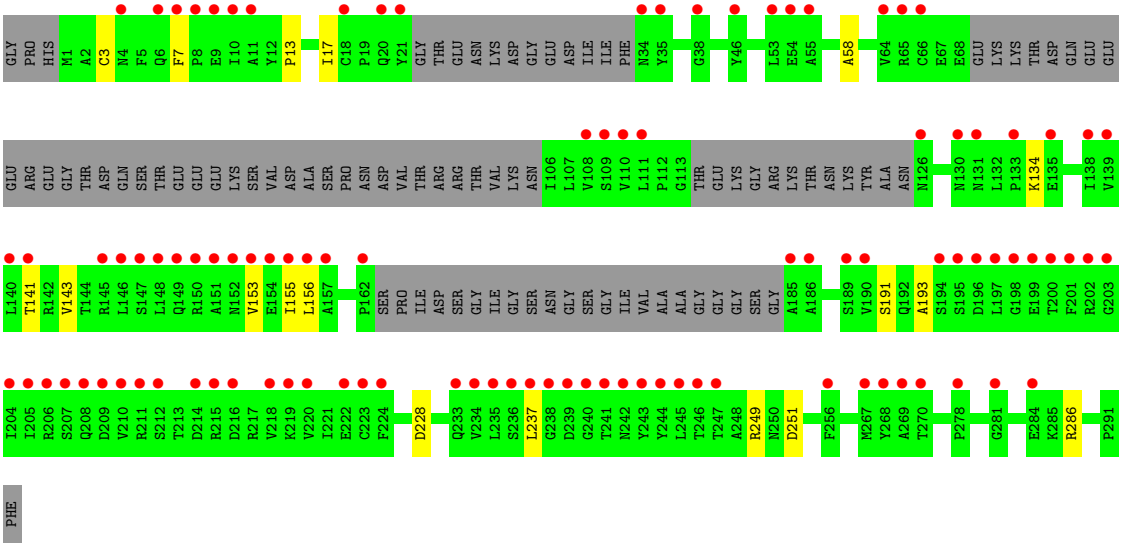
• Molecule 1: Exosome complex component CSL4

Chain I:



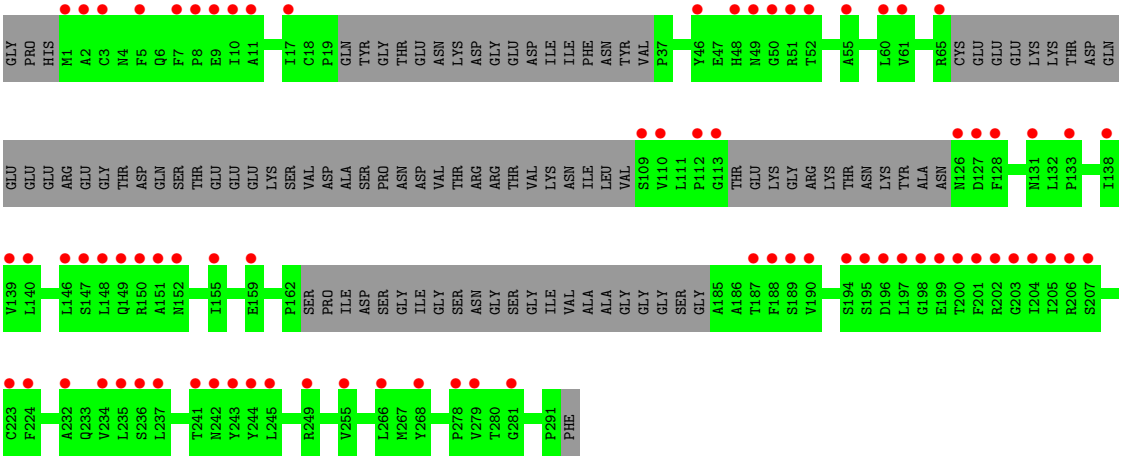
• Molecule 1: Exosome complex component CSL4

Chain S:



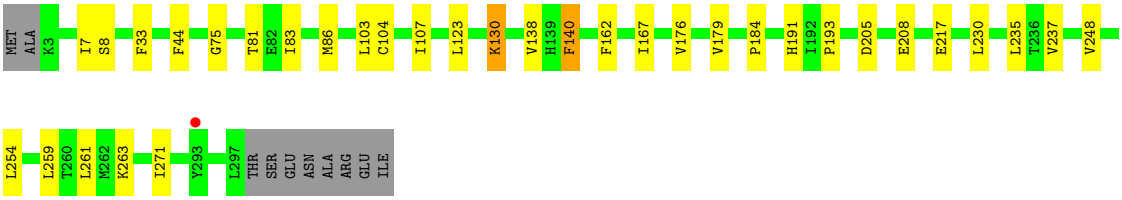
• Molecule 1: Exosome complex component CSL4

Chain c:



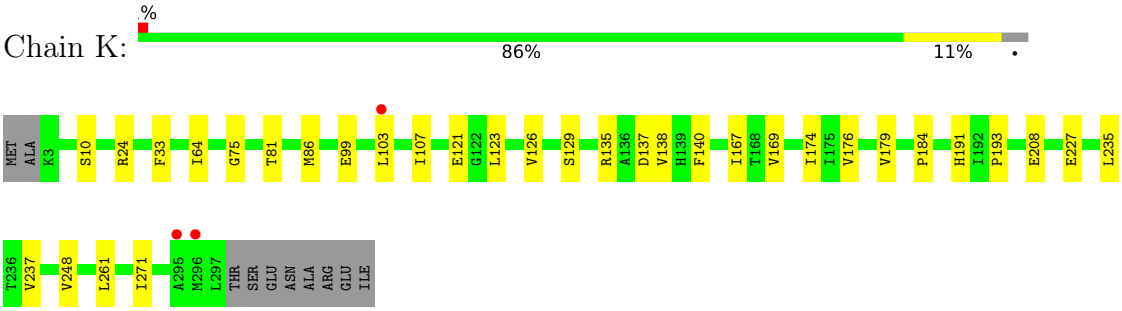
• Molecule 2: Exosome complex component RRP45

Chain A:



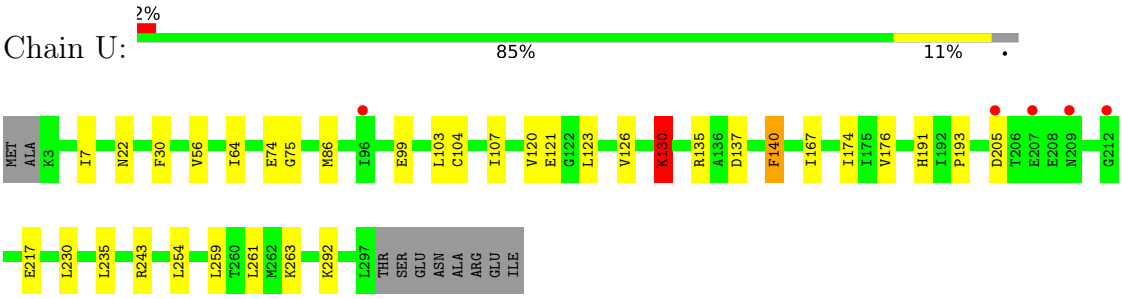
• Molecule 2: Exosome complex component RRP45

Chain K:



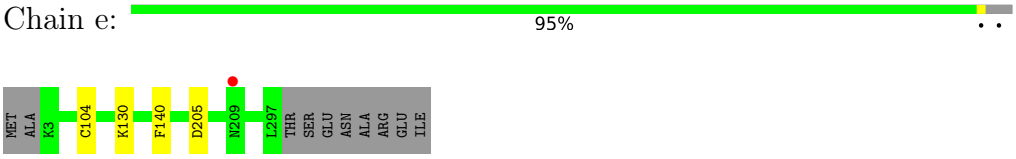
- Molecule 2: Exosome complex component RRP45

Chain U:



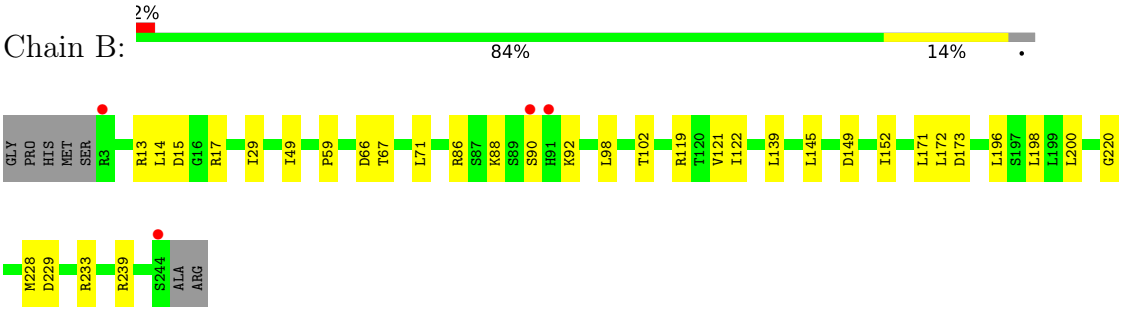
- Molecule 2: Exosome complex component RRP45

Chain e:



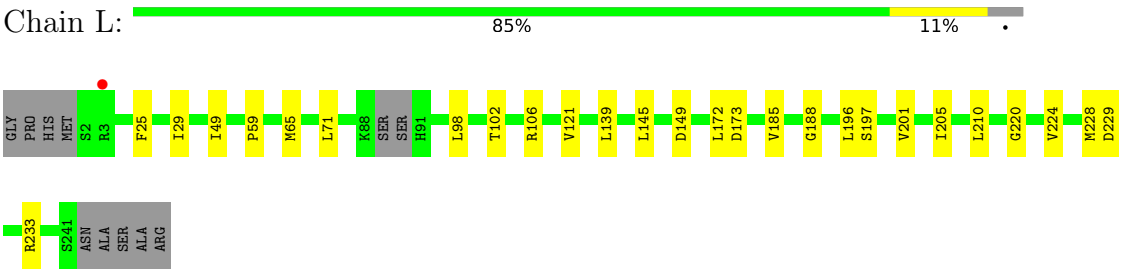
- Molecule 3: Exosome complex component SKI6

Chain B:



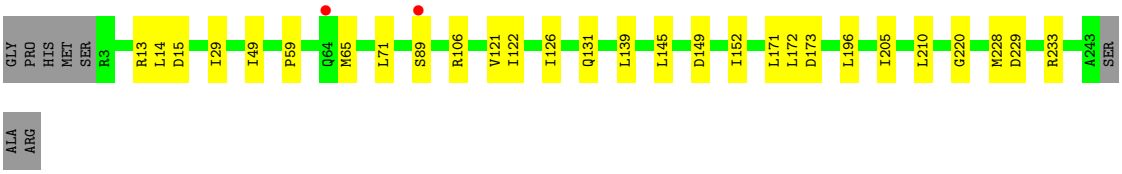
- Molecule 3: Exosome complex component SKI6

Chain L:



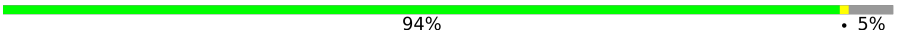
- Molecule 3: Exosome complex component SKI6

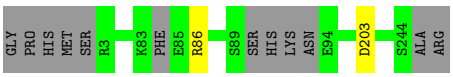
Chain V:



• Molecule 3: Exosome complex component SKI6

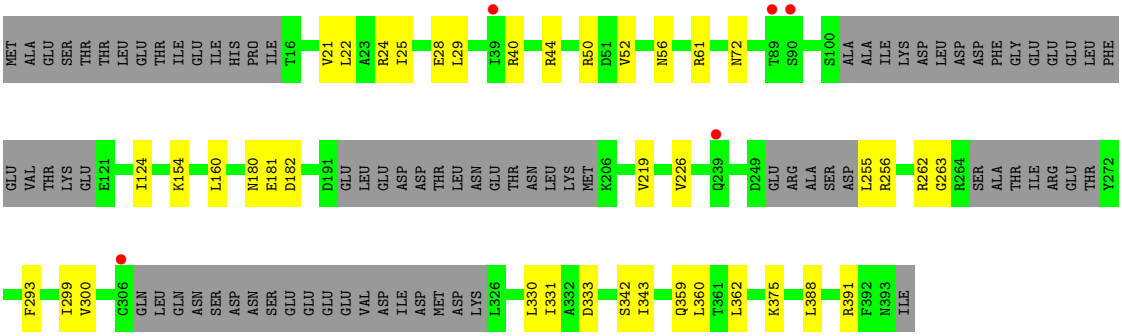
Chain f:





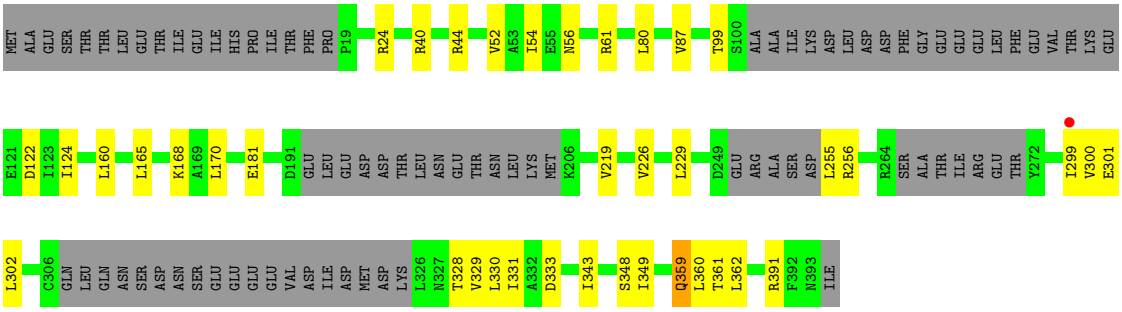
• Molecule 4: Exosome complex component RRP43

Chain C:



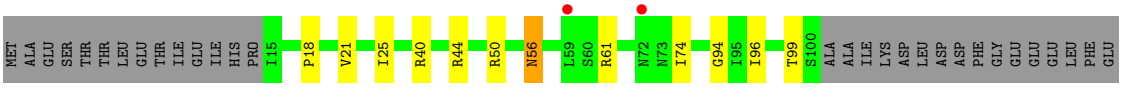
• Molecule 4: Exosome complex component RRP43

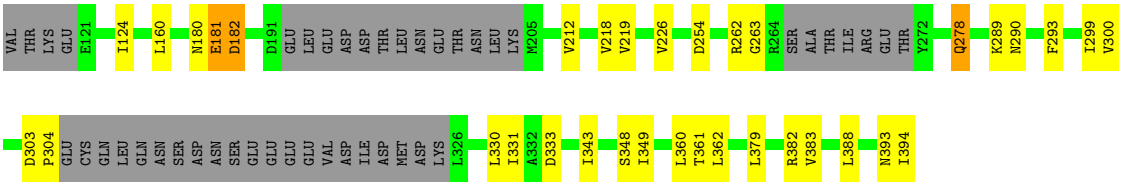
Chain M:



• Molecule 4: Exosome complex component RRP43

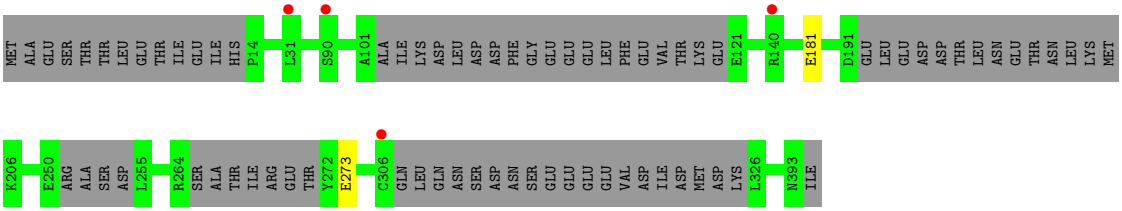
Chain W:





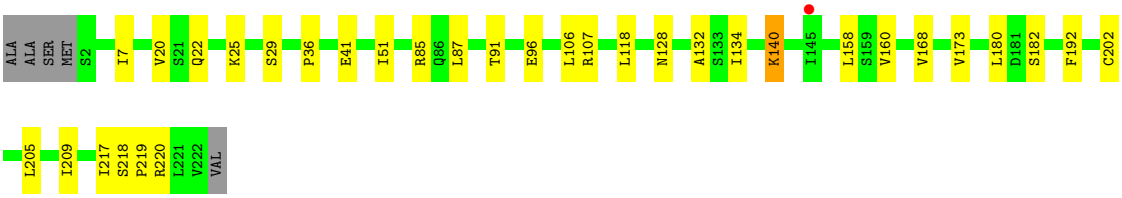
• Molecule 4: Exosome complex component RRP43

Chain g:



• Molecule 5: Exosome complex component RRP46

Chain D:

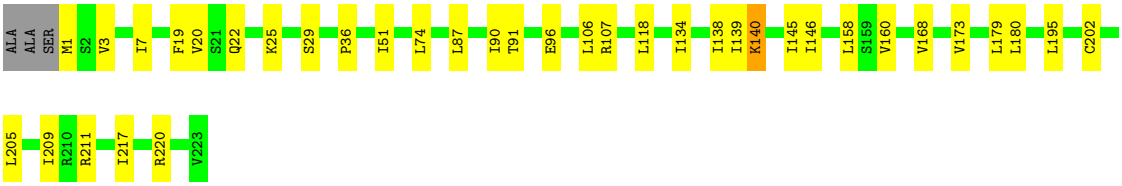


• Molecule 5: Exosome complex component RRP46

Chain N:

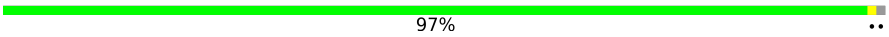
• Molecule 5: Exosome complex component RRP46

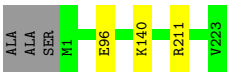
Chain X:



• Molecule 5: Exosome complex component RRP46

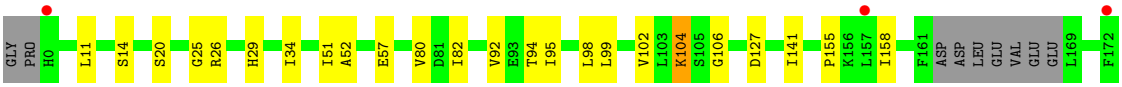
Chain h:

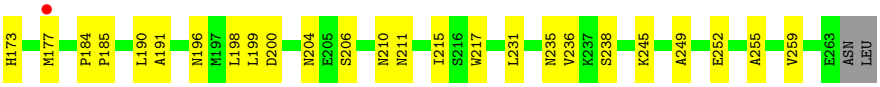




• Molecule 6: Exosome complex component RRP42

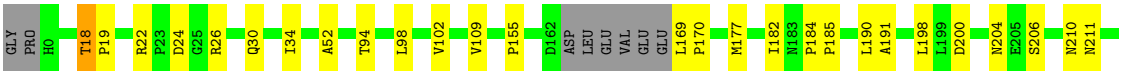
Chain E:

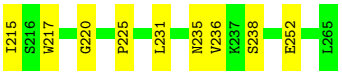




• Molecule 6: Exosome complex component RRP42

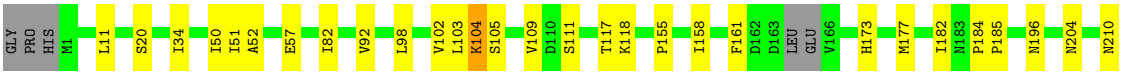
Chain O:





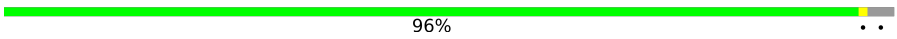
• Molecule 6: Exosome complex component RRP42

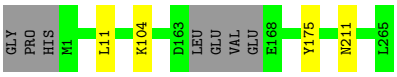
Chain Y:



• Molecule 6: Exosome complex component RRP42

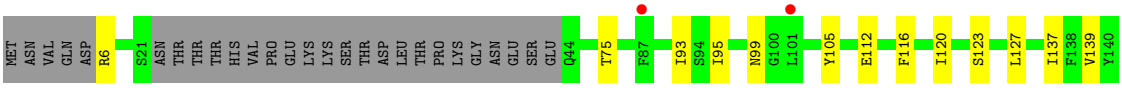
Chain i:

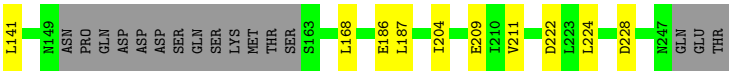




• Molecule 7: Exosome complex component MTR3

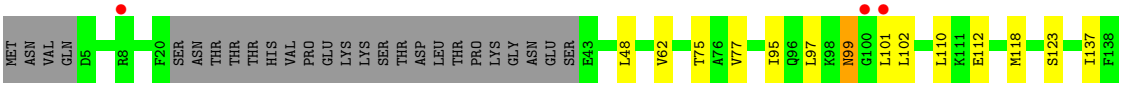
Chain F:

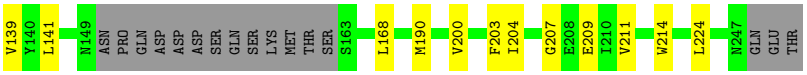




• Molecule 7: Exosome complex component MTR3

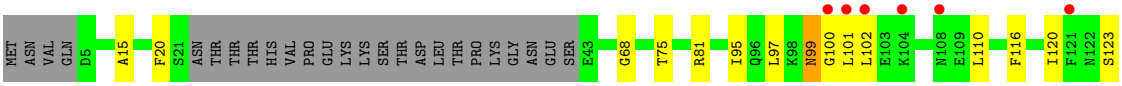
Chain P:

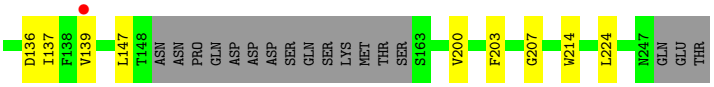




• Molecule 7: Exosome complex component MTR3

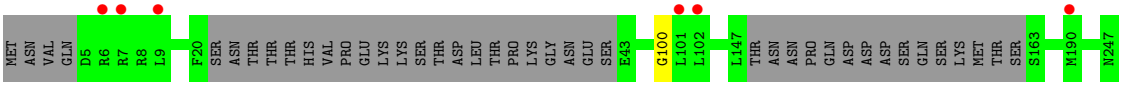
Chain Z:





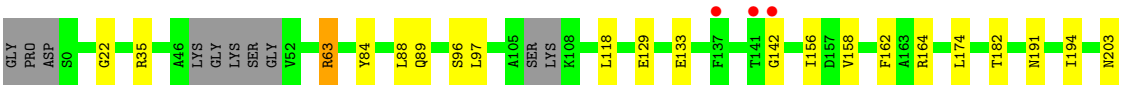
• Molecule 7: Exosome complex component MTR3

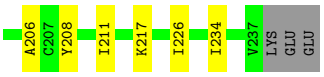
Chain j:



• Molecule 8: Exosome complex component RRP40

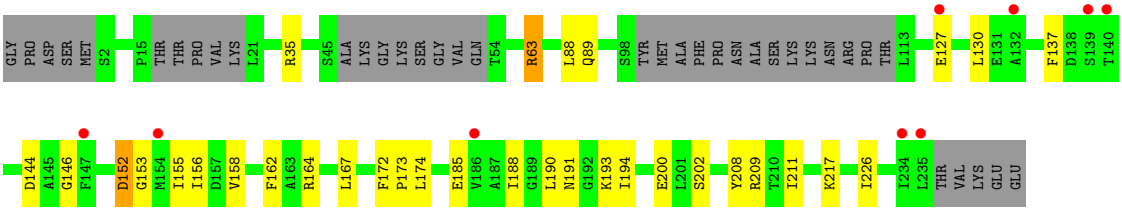
Chain G:





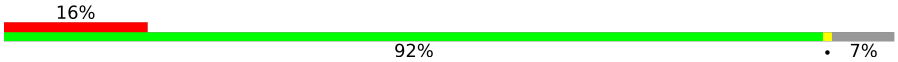
• Molecule 8: Exosome complex component RRP40

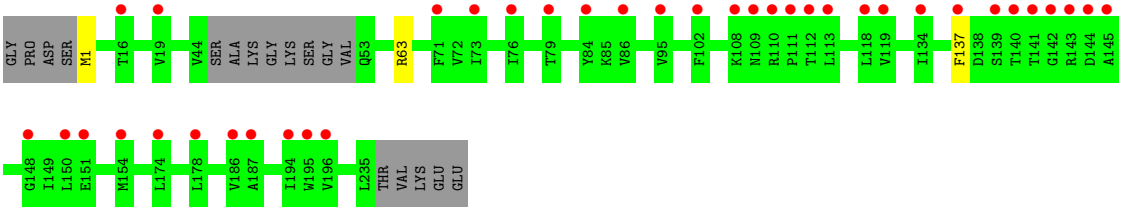
Chain Q:



• Molecule 8: Exosome complex component RRP40

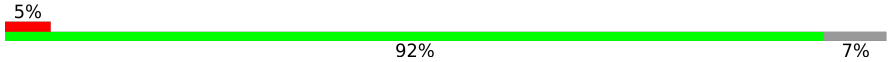
Chain a:

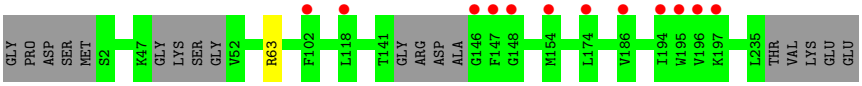




• Molecule 8: Exosome complex component RRP40

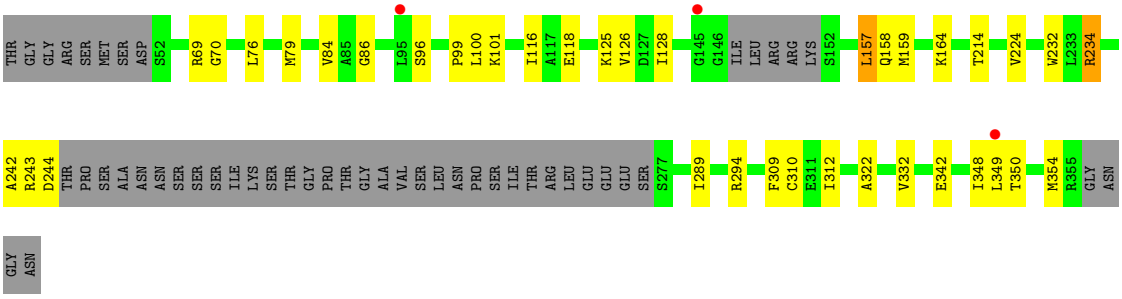
Chain k:





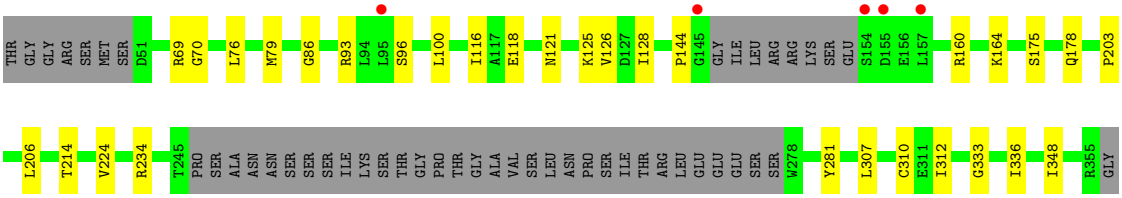
• Molecule 9: Exosome complex component RRP4

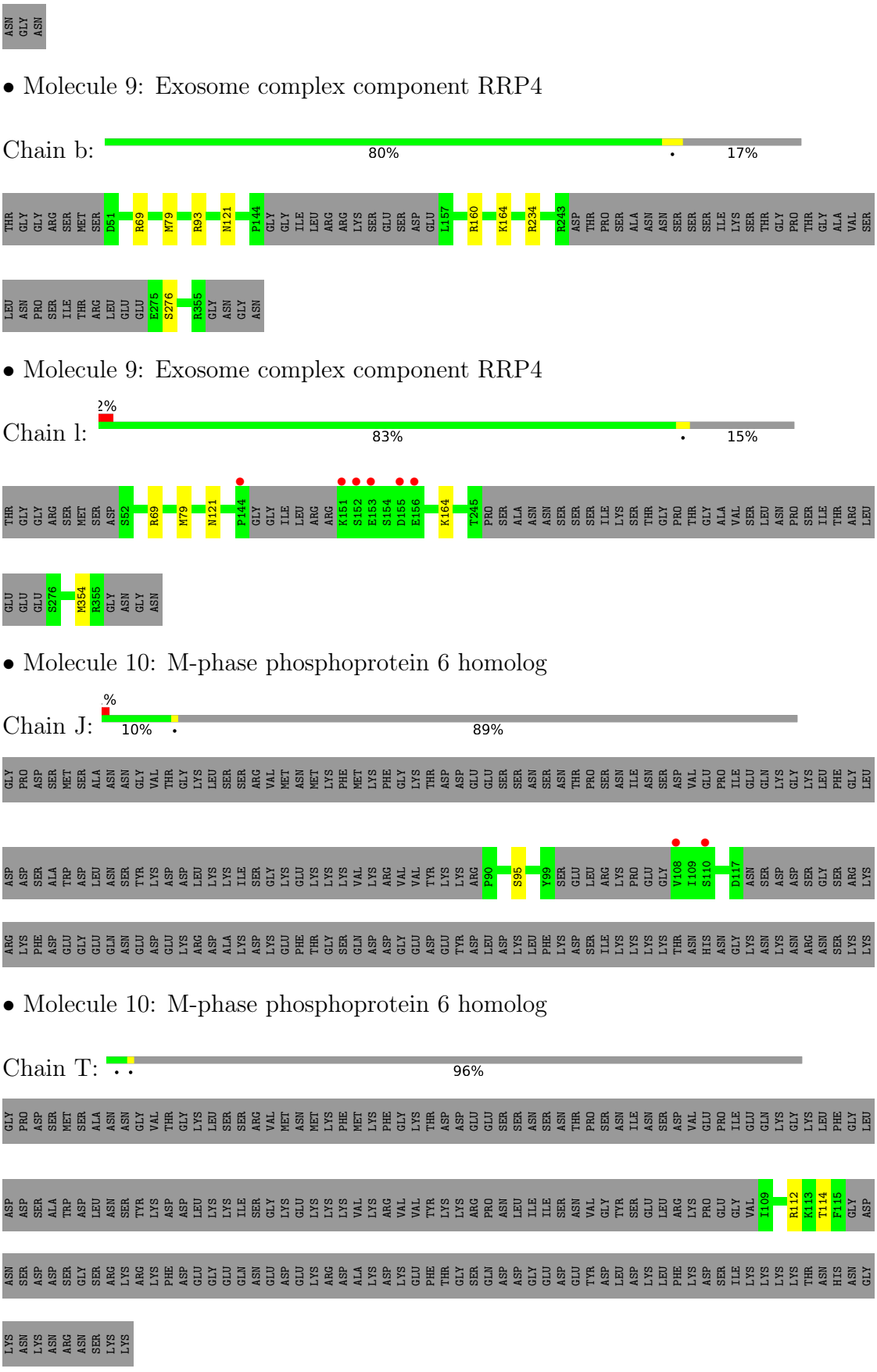
Chain H:



• Molecule 9: Exosome complex component RRP4

Chain R:




• Molecule 9: Exosome complex component RRP4
Chain b:
80%
17%
• Molecule 9: Exosome complex component RRP4
Chain l:
2%
83%
15%
• Molecule 10: M-phase phosphoprotein 6 homolog
Chain J:
%
10%
89%
• Molecule 10: M-phase phosphoprotein 6 homolog
Chain T:
96%

• Molecule 10: M-phase phosphoprotein 6 homolog

Chain d: 96%

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

ASP ASP SER ALA TRP ASP LEU ASN SER TYR LYS ASP ASP LEU LYS LYS ILE SER GLY LYS GLU LYS LYS LYS VAL LYS ARG VAL VAL TYR LYS LYS ARG PRO ASN LEU ILE ILE SER ASN VAL GLY TYR SER GLU LEU ARG LYS PRO GLU GLY VAL I109 F115 GLY ASP ASN SER ASP

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

ASN ARG ASN SER LYS LYS

• Molecule 10: M-phase phosphoprotein 6 homolog

Chain n: % 5% 95%

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

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

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

ARG ASN SER LYS LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	161.78Å 237.43Å 201.90Å 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
$< I/\sigma(I) >$ [1]	1.54 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.223 , 0.262 0.226 , 0.263	Depositor DCC
R_{free} test set	11386 reflections (4.96%)	wwPDB-VP
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]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	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 $< |L| >$, $< L^2 >$ 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

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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

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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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	166/295 (56%)	162 (98%)	3 (2%)	1 (1%)	25	64
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%)	41	74
2	K	293/305 (96%)	280 (96%)	13 (4%)	0	100	100
2	U	293/305 (96%)	279 (95%)	13 (4%)	1 (0%)	41	74
2	e	293/305 (96%)	278 (95%)	14 (5%)	1 (0%)	41	74
3	B	240/249 (96%)	225 (94%)	15 (6%)	0	100	100
3	L	234/249 (94%)	226 (97%)	7 (3%)	1 (0%)	34	69
3	V	239/249 (96%)	227 (95%)	10 (4%)	2 (1%)	19	58
3	f	234/249 (94%)	223 (95%)	10 (4%)	1 (0%)	34	69
4	C	301/394 (76%)	288 (96%)	12 (4%)	1 (0%)	41	74
4	M	298/394 (76%)	285 (96%)	12 (4%)	1 (0%)	41	74
4	W	309/394 (78%)	292 (94%)	13 (4%)	4 (1%)	12	47
4	g	306/394 (78%)	294 (96%)	11 (4%)	1 (0%)	41	74
5	D	219/226 (97%)	212 (97%)	6 (3%)	1 (0%)	29	67
5	N	220/226 (97%)	213 (97%)	6 (3%)	1 (0%)	29	67
5	X	221/226 (98%)	215 (97%)	5 (2%)	1 (0%)	29	67
5	h	221/226 (98%)	215 (97%)	5 (2%)	1 (0%)	29	67
6	E	253/268 (94%)	244 (96%)	8 (3%)	1 (0%)	34	69
6	O	256/268 (96%)	246 (96%)	10 (4%)	0	100	100
6	Y	259/268 (97%)	250 (96%)	8 (3%)	1 (0%)	34	69
6	i	257/268 (96%)	247 (96%)	9 (4%)	1 (0%)	34	69
7	F	201/250 (80%)	194 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	P	202/250 (81%)	195 (96%)	6 (3%)	1 (0%)	29	67
7	Z	202/250 (81%)	194 (96%)	7 (4%)	1 (0%)	29	67
7	j	200/250 (80%)	193 (96%)	6 (3%)	1 (0%)	29	67
8	G	225/244 (92%)	218 (97%)	6 (3%)	1 (0%)	34	69
8	Q	199/244 (82%)	192 (96%)	6 (3%)	1 (0%)	29	67
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%)	14	51
9	R	259/316 (82%)	251 (97%)	7 (3%)	1 (0%)	34	69
9	b	256/316 (81%)	244 (95%)	10 (4%)	2 (1%)	19	58
9	l	262/316 (83%)	253 (97%)	8 (3%)	1 (0%)	34	69
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%)	34	69

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	140/242 (58%)	140 (100%)	0	100	100

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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%)	62	84
2	K	243/266 (91%)	242 (100%)	1 (0%)	91	95
2	U	243/266 (91%)	239 (98%)	4 (2%)	62	84
2	e	244/266 (92%)	241 (99%)	3 (1%)	71	88
3	B	194/220 (88%)	193 (100%)	1 (0%)	88	95
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%)	88	95
4	C	244/349 (70%)	242 (99%)	2 (1%)	81	93
4	M	235/349 (67%)	231 (98%)	4 (2%)	60	83
4	W	255/349 (73%)	253 (99%)	2 (1%)	81	93
4	g	247/349 (71%)	246 (100%)	1 (0%)	91	95
5	D	182/198 (92%)	181 (100%)	1 (0%)	88	95
5	N	187/198 (94%)	186 (100%)	1 (0%)	88	95
5	X	196/198 (99%)	193 (98%)	3 (2%)	65	85
5	h	195/198 (98%)	193 (99%)	2 (1%)	76	90
6	E	208/242 (86%)	205 (99%)	3 (1%)	67	86
6	O	215/242 (89%)	214 (100%)	1 (0%)	88	95
6	Y	224/242 (93%)	220 (98%)	4 (2%)	59	82
6	i	225/242 (93%)	222 (99%)	3 (1%)	69	87
7	F	155/219 (71%)	153 (99%)	2 (1%)	69	87
7	P	150/219 (68%)	149 (99%)	1 (1%)	84	94
7	Z	156/219 (71%)	155 (99%)	1 (1%)	86	94
7	j	153/219 (70%)	153 (100%)	0	100	100
8	G	168/212 (79%)	167 (99%)	1 (1%)	86	94
8	Q	162/212 (76%)	159 (98%)	3 (2%)	57	81
8	a	191/212 (90%)	188 (98%)	3 (2%)	62	84
8	k	151/212 (71%)	150 (99%)	1 (1%)	84	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	H	212/270 (78%)	208 (98%)	4 (2%)	57	81
9	R	218/270 (81%)	213 (98%)	5 (2%)	50	78
9	b	213/270 (79%)	207 (97%)	6 (3%)	43	74
9	l	211/270 (78%)	207 (98%)	4 (2%)	57	81
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%)	76	90

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

Mol	Chain	Res	Type
2	e	104	CYS
9	l	354	MET
2	e	205	ASP
6	i	175	TYR
6	O	211	ASN

Sometimes 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 (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	e	401	-	7,10,10	0.81	0	9,12,12	1.25	1 (11%)
11	TAM	A	401	-	7,10,10	0.83	0	9,12,12	1.23	1 (11%)
11	TAM	K	401	-	7,10,10	0.82	0	9,12,12	1.22	1 (11%)
11	TAM	U	401	-	7,10,10	0.81	0	9,12,12	1.24	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	e	401	-	-	3/12/12/12	-
11	TAM	A	401	-	-	6/12/12/12	-
11	TAM	K	401	-	-	4/12/12/12	-
11	TAM	U	401	-	-	4/12/12/12	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	e	401	TAM	O5-C5-C2	-2.20	105.50	111.39
11	K	401	TAM	O5-C5-C2	-2.20	105.53	111.39
11	U	401	TAM	O5-C5-C2	-2.19	105.54	111.39
11	A	401	TAM	O5-C5-C2	-2.16	105.61	111.39

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	401	TAM	C1-C-C2-C5
11	A	401	TAM	C3-C-C2-C5
11	A	401	TAM	N-C-C2-C5
11	A	401	TAM	C1-C-C3-C6
11	A	401	TAM	N-C-C3-C6

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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	I	178/295 (60%)	1.96	81 (45%)	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%)	1.86	78 (39%)	0	0	125, 167, 214, 246	0
1	m	190/295 (64%)	1.51	59 (31%)	0	0	110, 153, 199, 232	0
2	A	295/305 (96%)	-0.07	1 (0%)	94	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%)	94	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	78	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%)	94	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%)	91	86	47, 69, 104, 126	0
5	N	222/226 (98%)	-0.14	1 (0%)	91	86	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

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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%) 45 29	61, 89, 133, 156	0
7	j	206/250 (82%)	0.11	6 (2%) 51 36	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%) 35 22	89, 142, 185, 264	0
8	a	227/244 (93%)	0.64	38 (16%) 1 1	90, 137, 211, 267	0
8	k	226/244 (92%)	0.02	12 (5%) 26 14	87, 118, 178, 226	0
9	H	267/316 (84%)	-0.04	3 (1%) 80 69	42, 85, 128, 189	0
9	R	265/316 (83%)	-0.09	5 (1%) 66 53	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%) 7 4	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%)	-0.00	0 100 100	110, 131, 137, 140	0
10	n	10/190 (5%)	0.89	1 (10%) 7 4	110, 124, 167, 178	0
All	All	8926/10948 (81%)	0.17	452 (5%) 28 16	37, 85, 174, 272	0

The worst 5 of 452 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	c	196	ASP	16.0
1	m	195	SER	14.8
1	S	196	ASP	12.1
1	c	278	PRO	12.1
1	S	238	GLY	10.6

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 monosaccharides 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(Å^2)	Q<0.9
12	CL	R	401	1/1	0.60	0.42	95,95,95,95	0
13	MG	O	301	1/1	0.66	0.35	85,85,85,85	0
13	MG	g	401	1/1	0.72	0.14	60,60,60,60	0
12	CL	b	401	1/1	0.86	0.27	86,86,86,86	0
11	TAM	e	401	11/11	0.87	0.15	75,89,96,99	0
12	CL	H	401	1/1	0.90	0.20	80,80,80,80	0
12	CL	f	301	1/1	0.90	0.29	79,79,79,79	0
11	TAM	U	401	11/11	0.91	0.18	79,98,112,119	0
11	TAM	A	401	11/11	0.92	0.17	85,96,101,103	0
11	TAM	K	401	11/11	0.92	0.19	69,86,103,111	0
12	CL	G	301	1/1	0.92	0.27	99,99,99,99	0
12	CL	l	401	1/1	0.95	0.11	75,75,75,75	0
12	CL	R	402	1/1	0.96	0.17	73,73,73,73	0

6.5 Other polymers (i)

There are no such residues in this entry.