



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 10, 2017 – 01:13 PM EDT

PDB ID : 5OKZ
Title : Crystal Structure of the Mpp6 Exosome complex
Authors : Falk, S.; Ebert, J.; Conti, E.
Deposited on : unknown
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

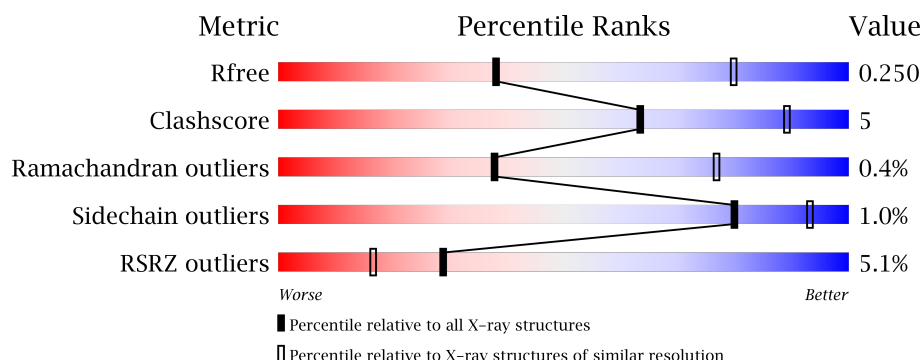
1 Overall quality at a glance

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.



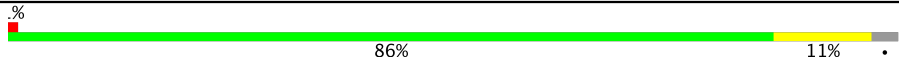

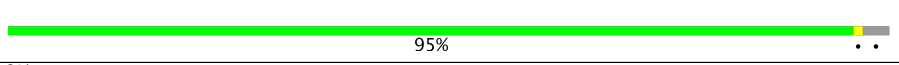

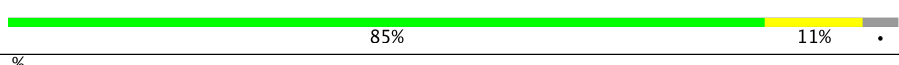
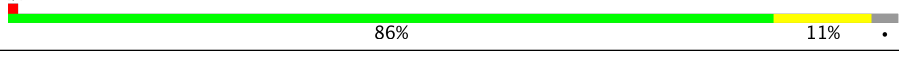
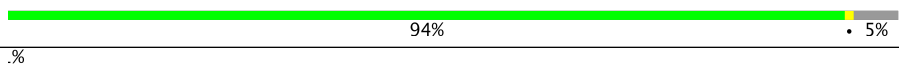

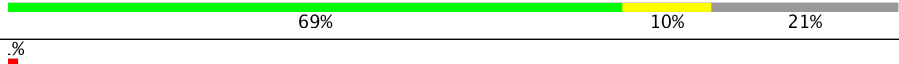


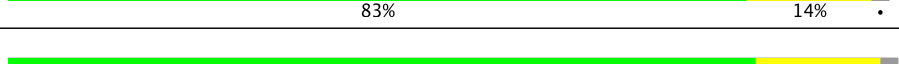
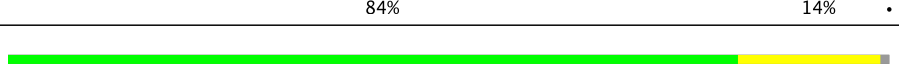
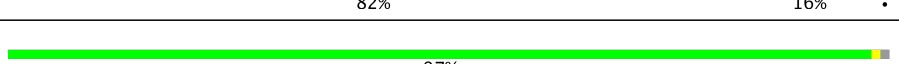
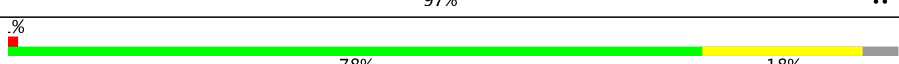
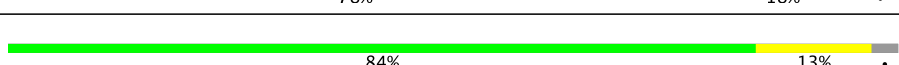
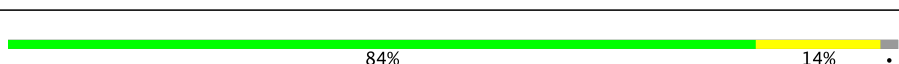
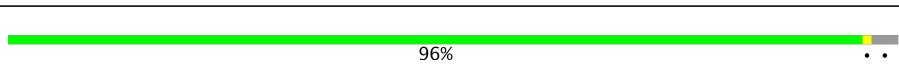
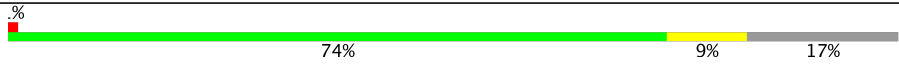


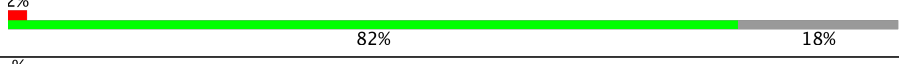
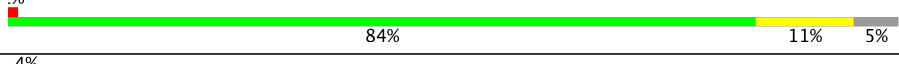


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)

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

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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	

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

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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			

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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			

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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

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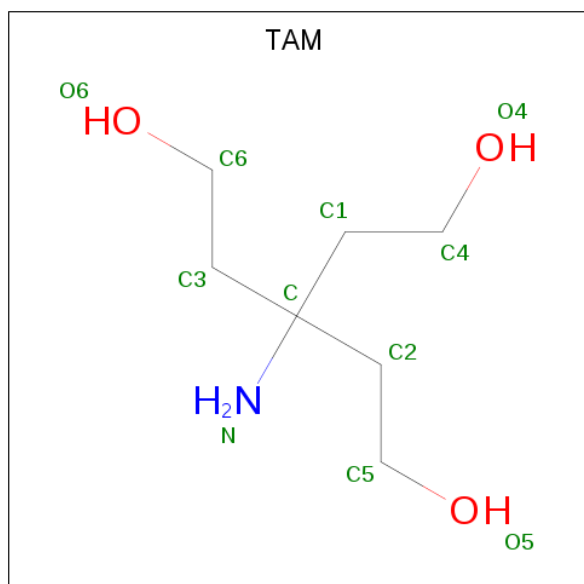
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	d	7	Total	C	N	O	0	0	0
			46	27	10	9			
10	n	10	Total	C	N	O	0	0	0
			70	44	14	12			

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

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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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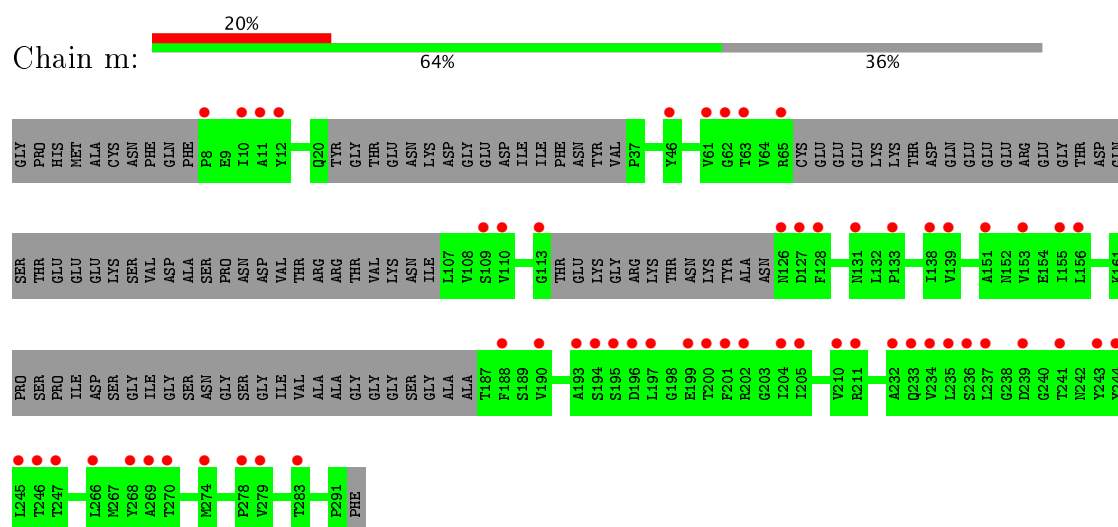
Continued from previous page...

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

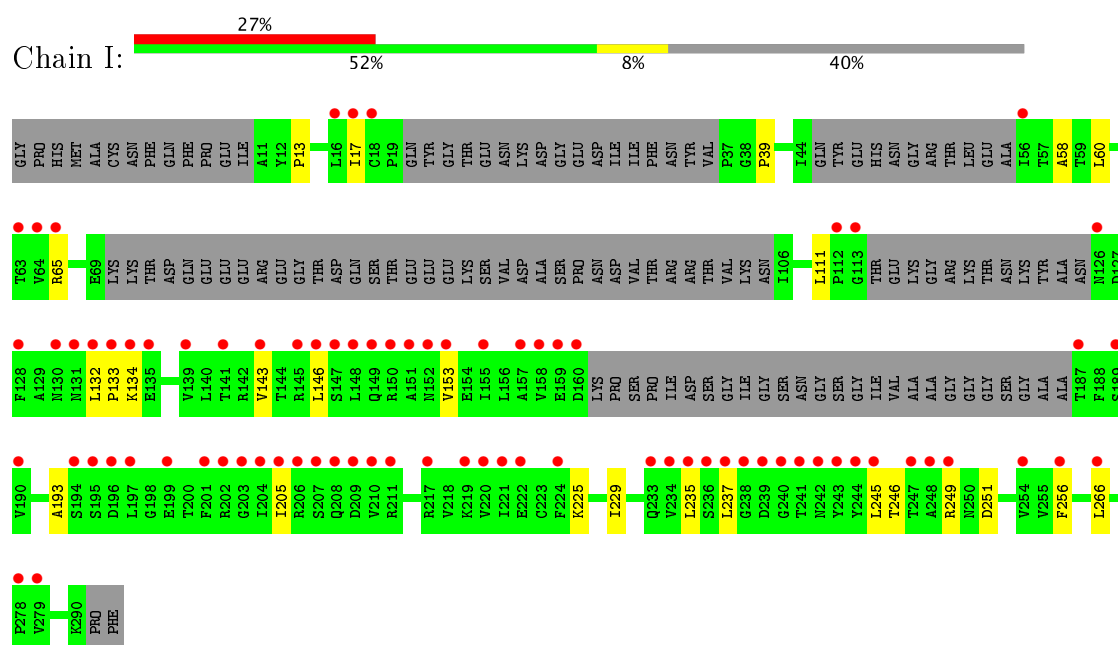
3 Residue-property plots

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.

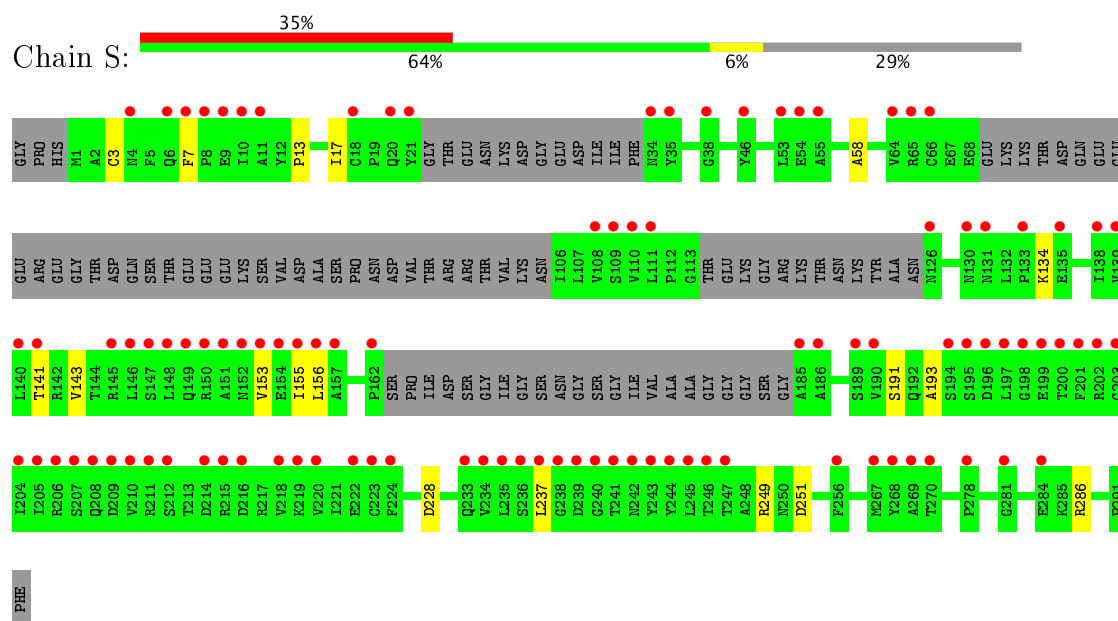
• Molecule 1: Exosome complex component CSL4



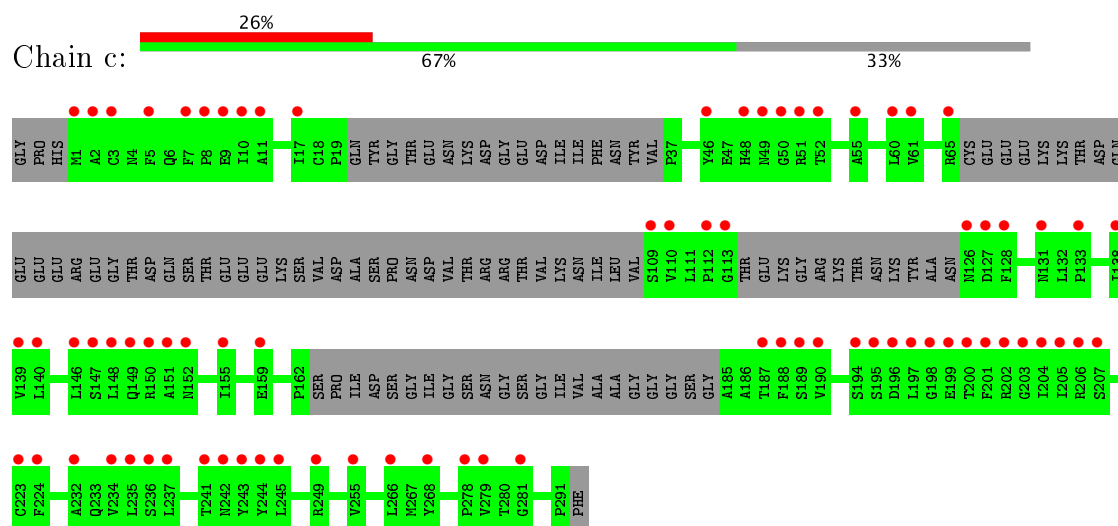
• Molecule 1: Exosome complex component CSL4



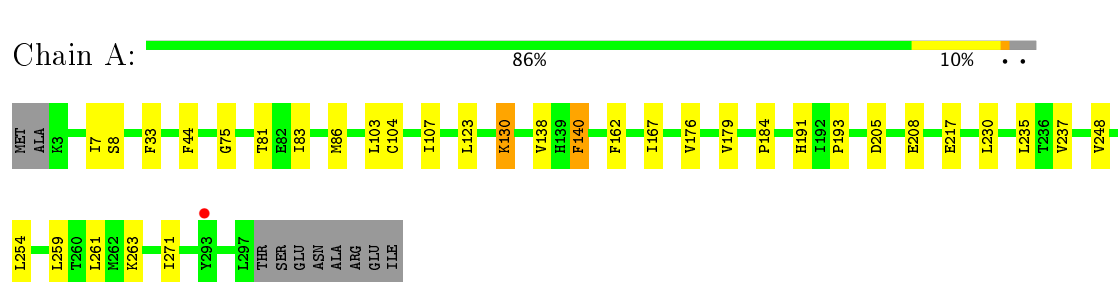
• Molecule 1: Exosome complex component CSL4



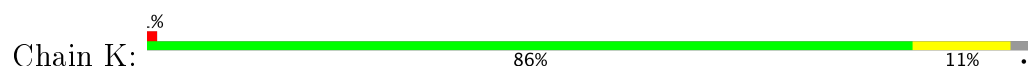
- Molecule 1: Exosome complex component CSL4



- Molecule 2: Exosome complex component RRP45

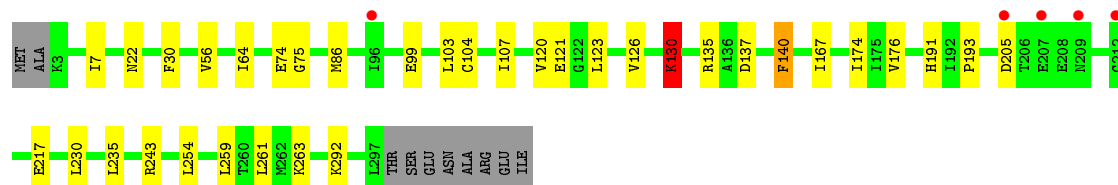
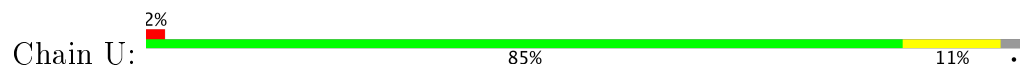


- Molecule 2: Exosome complex component RRP45

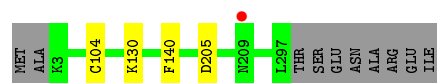




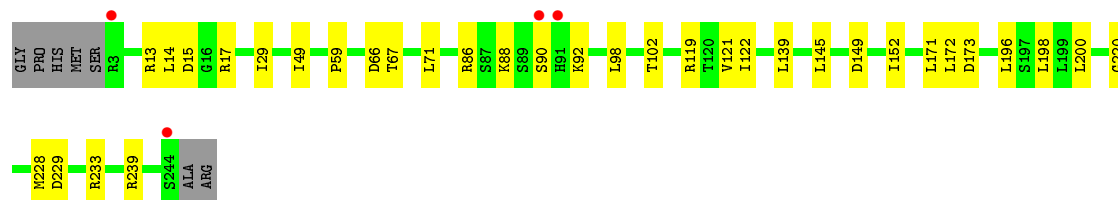
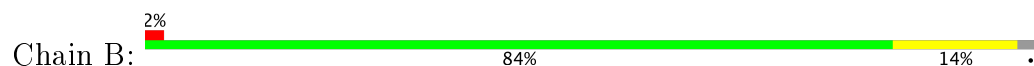
- Molecule 2: Exosome complex component RRP45



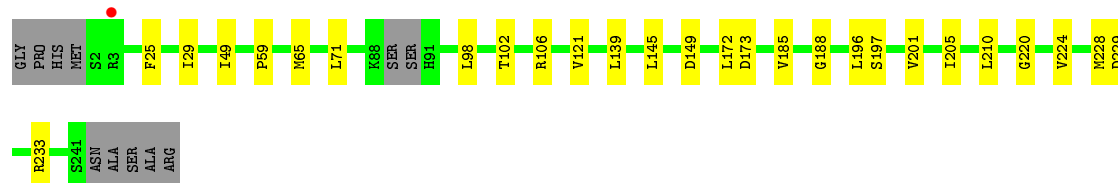
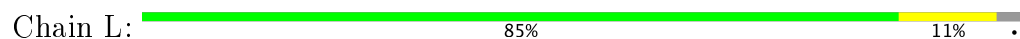
- Molecule 2: Exosome complex component RRP45



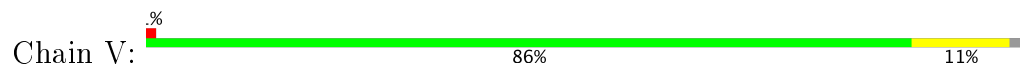
- Molecule 3: Exosome complex component SKI6

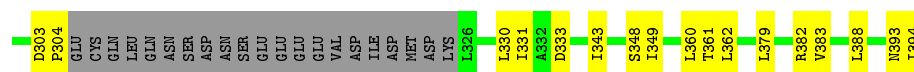


- Molecule 3: Exosome complex component SKI6

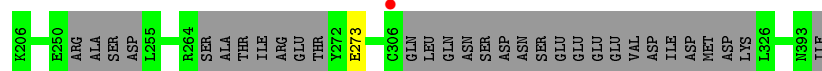
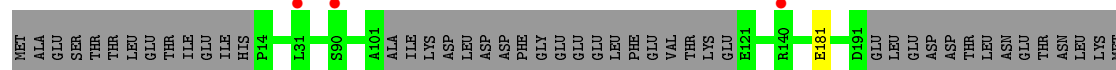
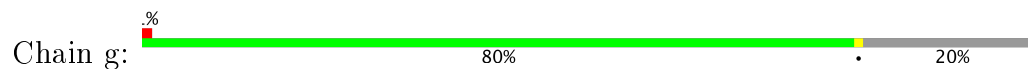


- Molecule 3: Exosome complex component SKI6

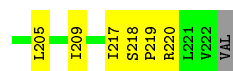
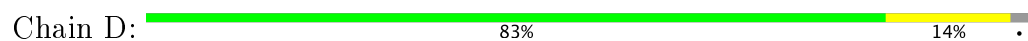




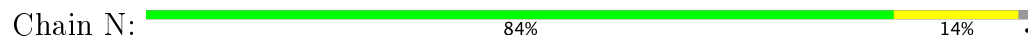
- Molecule 4: Exosome complex component RRP43



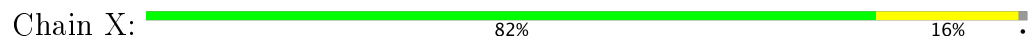
- Molecule 5: Exosome complex component RRP46



- Molecule 5: Exosome complex component RRP46



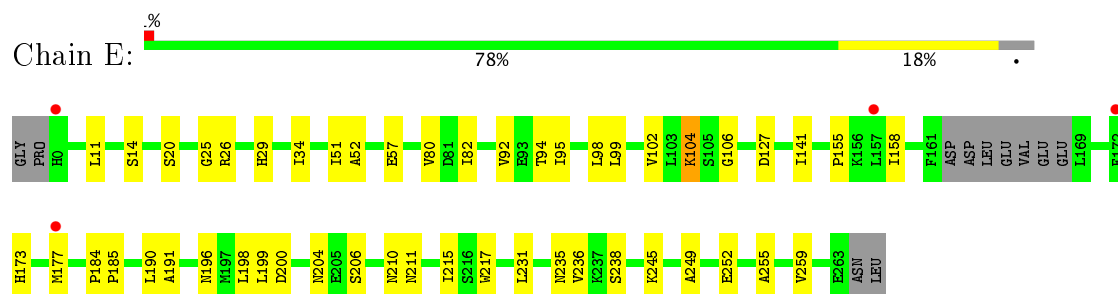
- Molecule 5: Exosome complex component RRP46



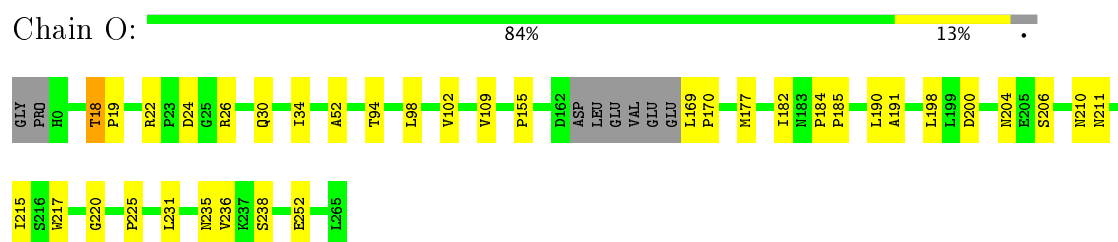
- Molecule 5: Exosome complex component RRP46



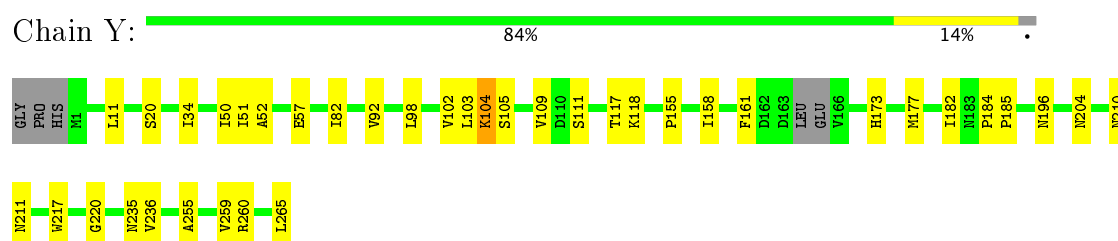
- Molecule 6: Exosome complex component RRP42



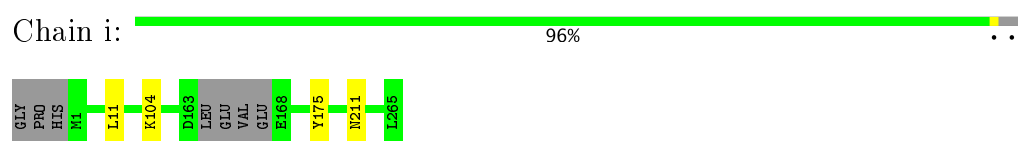
- Molecule 6: Exosome complex component RRP42



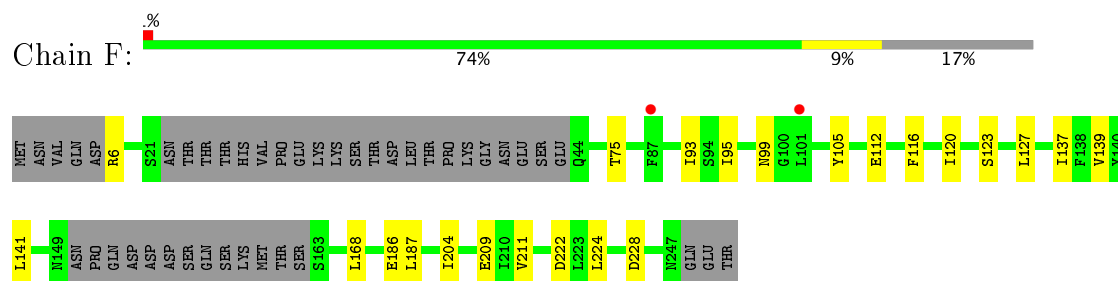
- Molecule 6: Exosome complex component RRP42



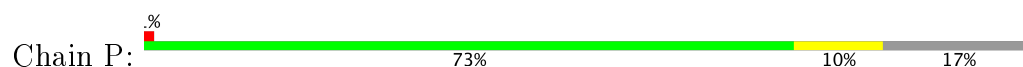
- Molecule 6: Exosome complex component RRP42



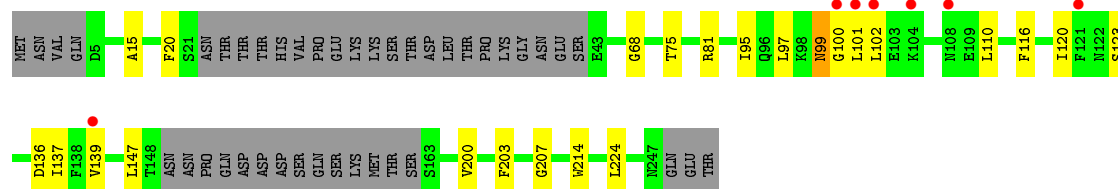
- Molecule 7: Exosome complex component MTR3



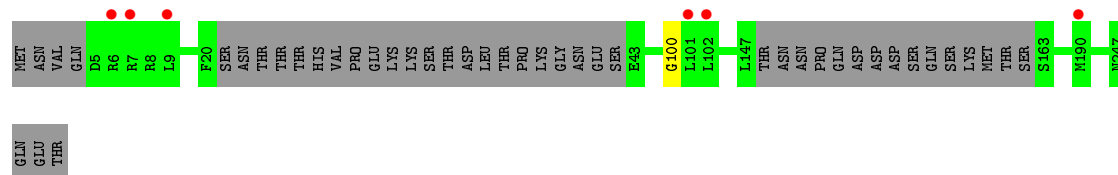
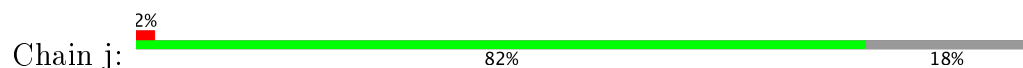
- Molecule 7: Exosome complex component MTR3



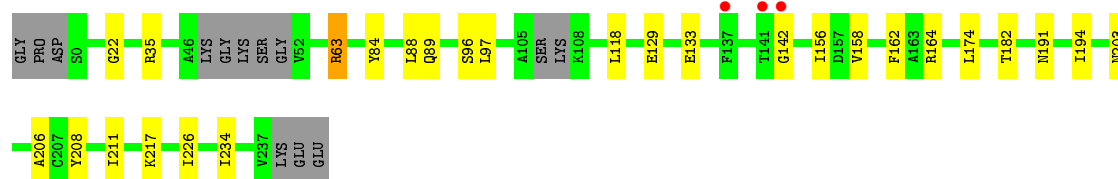
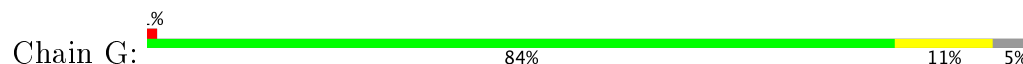
- Molecule 7: Exosome complex component MTR3



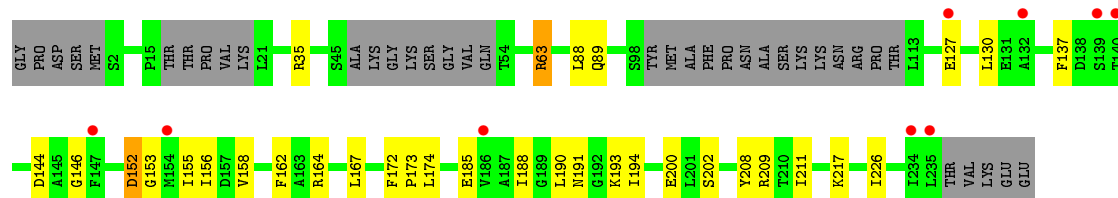
- Molecule 7: Exosome complex component MTR3



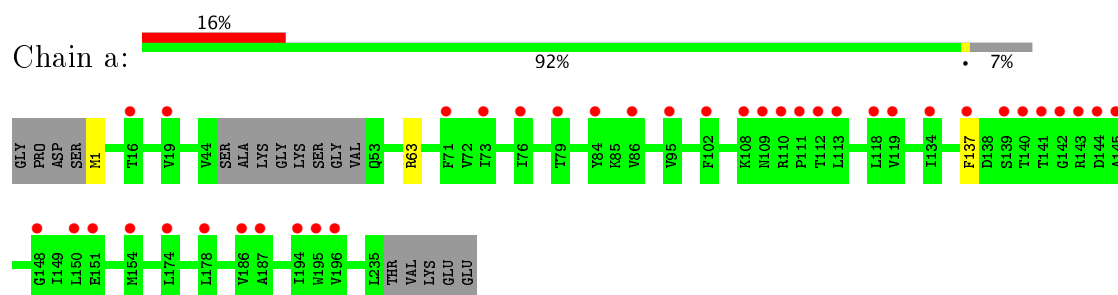
- Molecule 8: Exosome complex component RRP40



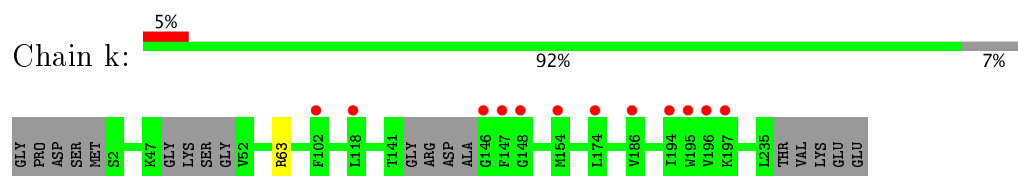
- Molecule 8: Exosome complex component RRP40



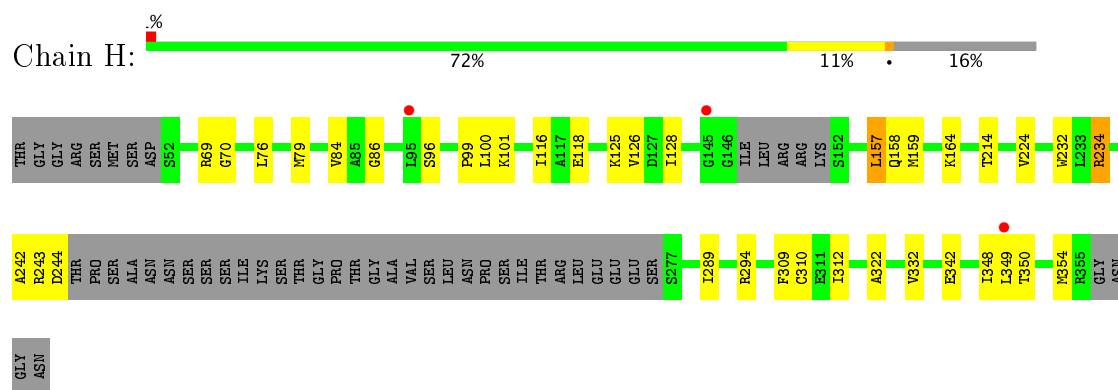
- Molecule 8: Exosome complex component RRP40



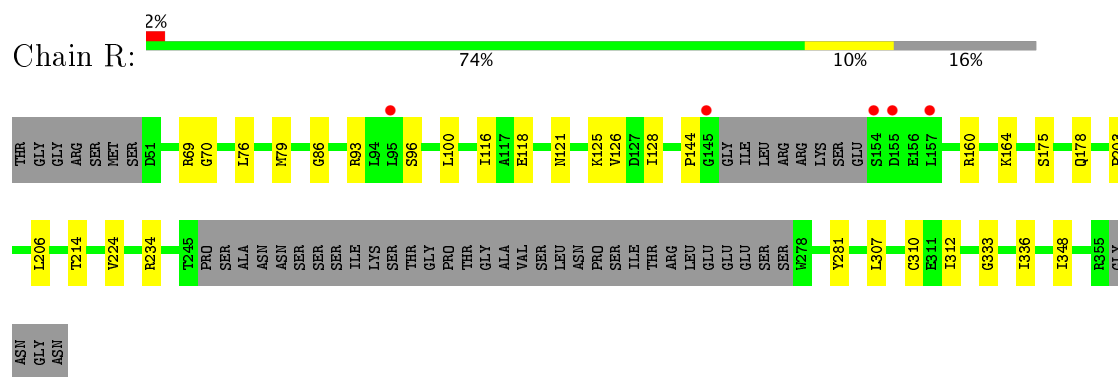
- Molecule 8: Exosome complex component RRP40



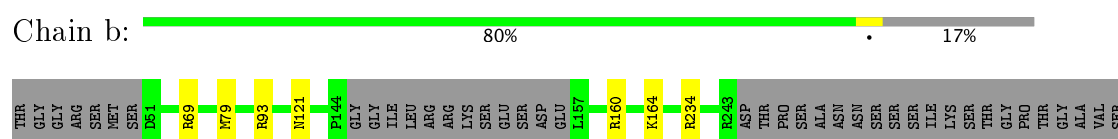
- Molecule 9: Exosome complex component RRP4



- Molecule 9: Exosome complex component RRP4



- Molecule 9: Exosome complex component RRP4



ASP	SER	GLY	ARG	LYS	ARG	LYS	PHE	ASP	GLU	GLY	GLU	GLN	ASN	GLU	ASP	ALA	LYS	ASP	LYS	GLY	SER	GLN	ASP	ASP	GLY	THR	THR	GLY	LEU	ASP	LYS	PHE	TYP	GLU
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

ASN
ARG
ASN
SER
LYS
LYS

- Molecule 10: M-phase phosphoprotein 6 homolog



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

[illegible]

SER	GLY	SER	ARG	ARG	PHE	ASP	GLU	GLY	GLU	GLN	ASN	GLU	GLY	ASP	GLU	LYS	ANG	ASP	ALA	LYS	LYS	ASP	LYS	GLY	GLY	SER	GLN	ASP	ASP	GLY	GLY	ASP	GLU	TYR	ASP	LEU	LYS	LYS	LYS	THR	ASN	HIS	ASN	LYS	LYS	LYS	LYS	GLN
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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 ⓘ

5.1 Standard geometry ⓘ

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.

All (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
5:X:22:GLN:HB2	5:X:107:ARG:HH12	1.55	0.72
3:L:59:PRO:HG2	3:L:65:MET:HG3	1.72	0.71
2:K:121:GLU:OE1	11:K:401:TAM:N	2.24	0.71
1:S:249:ARG:NH1	1:S:251:ASP:OD1	2.25	0.70
6:O:155:PRO:HA	6:O:177:MET:HG2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:O:24:ASP:OD2	6:O:26:ARG:NH1	2.25	0.69
6:E:26:ARG:NH2	6:E:200:ASP:O	2.25	0.68
2:K:10:SER:HB3	8:Q:153:GLY:H	1.58	0.68
5:N:36:PRO:HB3	5:N:87:LEU:HB2	1.74	0.68
2:A:8:SER:HB2	8:G:118:LEU:HD11	1.76	0.68
4:W:362:LEU:HB2	5:X:180:LEU:HB3	1.76	0.67
4:C:362:LEU:HB2	5:D:180:LEU:HB3	1.75	0.67
3:L:71:LEU:HB2	3:L:121:VAL:HG22	1.77	0.67
5:D:36:PRO:HB3	5:D:87:LEU:HB2	1.76	0.66
2:K:174:ILE:HD11	4:M:99:THR:HG22	1.77	0.66
5:X:36:PRO:HB3	5:X:87:LEU:HB2	1.77	0.66
3:V:71:LEU:HB2	3:V:121:VAL:HG22	1.78	0.65
9:H:118:GLU:HG2	9:H:125:LYS:HB2	1.78	0.65
8:Q:217:LYS:HD2	8:Q:226:ILE:HD11	1.79	0.65
3:B:66:ASP:O	3:B:67:THR:OG1	2.13	0.64
7:Z:81:ARG:NH2	7:Z:136:ASP:OD2	2.26	0.64
3:L:29:ILE:HD12	3:L:149:ASP:HB2	1.80	0.63
4:W:181:GLU:HG2	4:W:182:ASP:N	2.14	0.63
5:D:7:ILE:HD11	5:D:118:LEU:HB3	1.80	0.63
4:C:24:ARG:NH1	1:I:193:ALA:O	2.22	0.63
3:B:71:LEU:HB2	3:B:121:VAL:HG22	1.80	0.63
4:M:52:VAL:HG22	4:M:391:ARG:HH21	1.63	0.62
6:O:26:ARG:HG2	6:O:30:GLN:HB3	1.82	0.62
2:K:99:GLU:HB3	3:L:106:ARG:HH12	1.65	0.62
5:X:7:ILE:HD11	5:X:118:LEU:HB3	1.82	0.62
8:G:206:ALA:HB2	8:G:234:ILE:HG13	1.81	0.62
6:E:155:PRO:HA	6:E:177:MET:HG2	1.81	0.62
2:U:75:GLY:HA3	2:U:123:LEU:HB2	1.82	0.61
8:Q:200:GLU:HG3	8:Q:202:SER:H	1.64	0.61
6:O:236:VAL:HG12	7:P:123:SER:HB3	1.83	0.61
5:D:217:ILE:HA	5:D:220:ARG:HD2	1.83	0.61
9:R:118:GLU:HG2	9:R:125:LYS:HB2	1.83	0.60
3:B:145:LEU:HD11	3:B:228:MET:HG2	1.83	0.60
9:R:86:GLY:HA2	9:R:100:LEU:HG	1.84	0.60
5:D:128:ASN:OD1	8:G:35:ARG:NH2	2.35	0.60
2:U:167:ILE:HG22	2:U:176:VAL:HA	1.82	0.60
6:E:236:VAL:HG12	7:F:123:SER:HB3	1.84	0.60
8:G:182:THR:HG21	8:G:203:ASN:HB3	1.82	0.60
9:H:86:GLY:HA2	9:H:100:LEU:HG	1.83	0.60
4:M:219:VAL:HG11	4:M:226:VAL:HG21	1.82	0.60
3:V:59:PRO:HG2	3:V:65:MET:HG3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:127:GLU:HB2	8:Q:130:LEU:HB2	1.83	0.59
3:B:29:ILE:HD11	3:B:145:LEU:HB3	1.84	0.59
8:Q:185:GLU:HA	10:T:114:THR:HG22	1.84	0.59
8:Q:174:LEU:HD21	8:Q:211:ILE:HG12	1.83	0.59
8:G:96:SER:HB3	8:G:133:GLU:HG2	1.84	0.59
3:V:49:ILE:HD13	3:V:139:LEU:HD23	1.85	0.59
8:G:217:LYS:HD2	8:G:226:ILE:HD11	1.84	0.59
5:N:128:ASN:OD1	8:Q:35:ARG:NH2	2.36	0.59
8:G:174:LEU:HD21	8:G:211:ILE:HG12	1.85	0.58
4:M:348:SER:HB2	4:M:361:THR:HB	1.85	0.58
7:P:99:ASN:ND2	7:P:102:LEU:O	2.36	0.58
2:A:167:ILE:HG22	2:A:176:VAL:HA	1.84	0.58
4:M:362:LEU:HB2	5:N:180:LEU:HB3	1.85	0.58
7:P:141:LEU:HD11	7:P:168:LEU:HD21	1.86	0.58
2:A:8:SER:CB	8:G:118:LEU:HD11	2.33	0.58
4:M:24:ARG:NH1	1:S:191:SER:O	2.37	0.58
2:A:7:ILE:HG21	2:A:230:LEU:HD21	1.86	0.58
5:D:22:GLN:HB2	5:D:107:ARG:HH22	1.68	0.58
3:B:67:THR:HA	3:B:119:ARG:HG3	1.86	0.58
4:C:219:VAL:HG11	4:C:226:VAL:HG21	1.85	0.58
7:P:75:THR:HG22	7:P:139:VAL:HG22	1.85	0.58
3:L:145:LEU:HD11	3:L:228:MET:HG2	1.86	0.57
4:W:40:ARG:HD2	4:W:331:ILE:HD12	1.86	0.57
4:C:154:LYS:NZ	14:C:401:HOH:O	2.37	0.57
2:K:126:VAL:HG23	2:K:129:SER:HB2	1.86	0.57
3:L:49:ILE:HD13	3:L:139:LEU:HD23	1.86	0.57
3:B:14:LEU:HD12	3:B:14:LEU:H	1.69	0.57
3:V:14:LEU:HD12	3:V:14:LEU:H	1.68	0.57
6:Y:236:VAL:HG12	7:Z:123:SER:HB3	1.87	0.57
1:I:143:VAL:HA	1:I:153:VAL:HG12	1.87	0.57
3:V:29:ILE:HD11	3:V:145:LEU:HB3	1.86	0.57
3:V:131:GLN:NE2	14:V:301:HOH:O	2.36	0.57
3:B:29:ILE:HD12	3:B:149:ASP:HB2	1.87	0.56
8:Q:155:ILE:HD11	8:Q:193:LYS:HB3	1.87	0.56
8:G:88:LEU:HB3	8:G:191:ASN:HD22	1.70	0.56
6:Y:155:PRO:HA	6:Y:177:MET:HG2	1.87	0.56
4:C:300:VAL:HG22	4:C:343:ILE:HG12	1.87	0.56
3:B:49:ILE:HD13	3:B:139:LEU:HD23	1.88	0.56
8:G:158:VAL:HG21	8:G:194:ILE:HD12	1.88	0.56
2:U:7:ILE:HG21	2:U:230:LEU:HD21	1.87	0.56
7:Z:200:VAL:HB	7:Z:214:TRP:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Y:34:ILE:HG22	6:Y:52:ALA:HA	1.87	0.55
4:C:124:ILE:HD11	4:C:160:LEU:HG	1.88	0.55
2:U:235:LEU:HD22	2:U:261:LEU:HD22	1.88	0.55
2:U:86:MET:HG3	5:X:29:SER:HB3	1.88	0.55
7:Z:75:THR:HG22	7:Z:139:VAL:HG22	1.86	0.55
2:K:167:ILE:HG22	2:K:176:VAL:HA	1.87	0.55
5:X:168:VAL:HG23	5:X:173:VAL:HB	1.88	0.55
4:W:218:VAL:HG22	7:Z:101:LEU:HD21	1.89	0.55
3:L:29:ILE:HD11	3:L:145:LEU:HB3	1.89	0.55
2:U:174:ILE:HD11	4:W:99:THR:HG22	1.87	0.55
6:Y:117:THR:HG23	6:Y:161:PHE:HA	1.87	0.55
4:M:300:VAL:HG22	4:M:343:ILE:HG12	1.88	0.54
4:C:40:ARG:HD2	4:C:331:ILE:HD12	1.90	0.54
4:M:52:VAL:HB	4:M:80:LEU:HD11	1.88	0.54
4:W:303:ASP:HB3	4:W:304:PRO:HD3	1.89	0.54
4:W:219:VAL:HG11	4:W:226:VAL:HG21	1.89	0.54
5:N:74:LEU:HD13	5:N:90:ILE:HD13	1.90	0.54
5:D:20:VAL:HG22	5:D:25:LYS:HG3	1.87	0.54
4:M:255:LEU:HD23	4:M:256:ARG:H	1.72	0.54
6:O:190:LEU:HD13	6:O:215:ILE:HD12	1.90	0.54
3:V:29:ILE:HD12	3:V:149:ASP:HB2	1.89	0.54
5:X:139:ILE:HD13	5:X:146:ILE:HD13	1.88	0.54
3:B:17:ARG:NH2	3:B:173:ASP:O	2.36	0.53
6:O:109:VAL:HB	6:O:182:ILE:HD11	1.90	0.53
6:Y:109:VAL:HB	6:Y:182:ILE:HD11	1.91	0.53
2:A:75:GLY:HA3	2:A:123:LEU:HB2	1.91	0.53
6:O:206:SER:HB3	6:O:231:LEU:HB3	1.91	0.53
4:W:44:ARG:NH2	4:W:333:ASP:HB3	2.24	0.53
8:G:84:TYR:HB2	8:G:97:LEU:HB3	1.91	0.53
8:G:63:ARG:HH21	8:G:89:GLN:HG2	1.74	0.53
2:K:75:GLY:HA3	2:K:123:LEU:HB2	1.91	0.53
1:S:134:LYS:HD2	1:S:237:LEU:HD21	1.91	0.53
2:K:86:MET:HG3	5:N:29:SER:HB3	1.91	0.52
2:A:103:LEU:O	2:A:107:ILE:HG12	2.10	0.52
2:K:261:LEU:HD12	3:L:196:LEU:HD12	1.92	0.52
4:M:122:ASP:H	5:N:140:LYS:HE3	1.73	0.52
5:D:132:ALA:HB1	5:D:205:LEU:HD23	1.91	0.52
5:N:134:ILE:HG12	5:N:202:CYS:SG	2.49	0.52
7:P:203:PHE:HB3	7:P:207:GLY:HA2	1.90	0.52
7:F:141:LEU:HD11	7:F:168:LEU:HD21	1.92	0.52
5:N:106:LEU:HD13	5:N:160:VAL:HB	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:116:ILE:HD13	9:H:126:VAL:HG22	1.92	0.52
5:D:168:VAL:HG23	5:D:173:VAL:HB	1.91	0.52
7:F:95:ILE:HG12	7:F:137:ILE:HB	1.92	0.52
3:B:239:ARG:HH12	9:H:101:LYS:HE2	1.75	0.52
2:U:126:VAL:HG22	2:U:130:LYS:HB2	1.92	0.52
4:W:180:ASN:O	4:W:182:ASP:N	2.43	0.52
1:I:65:ARG:HH11	1:I:111:LEU:HD12	1.74	0.51
5:D:140:LYS:HA	5:D:158:LEU:HD13	1.92	0.51
9:H:214:THR:HG23	9:H:224:VAL:HG22	1.91	0.51
4:M:40:ARG:HD2	4:M:331:ILE:HD12	1.91	0.51
2:A:8:SER:HB2	8:G:118:LEU:CD1	2.41	0.51
2:K:191:HIS:CE1	2:K:193:PRO:HG3	2.46	0.51
1:S:17:ILE:HD11	1:S:58:ALA:HB2	1.92	0.51
2:U:103:LEU:O	2:U:107:ILE:HG12	2.11	0.51
6:Y:158:ILE:HD11	6:Y:173:HIS:HA	1.93	0.51
2:K:235:LEU:HD22	2:K:261:LEU:HD22	1.93	0.51
5:N:7:ILE:HD11	5:N:118:LEU:HB3	1.93	0.51
1:I:17:ILE:HD11	1:I:58:ALA:HB2	1.93	0.51
8:Q:146:GLY:O	10:T:112:ARG:NH1	2.44	0.51
2:U:135:ARG:NH1	2:U:137:ASP:OD1	2.42	0.51
4:C:22:LEU:HD11	4:C:29:LEU:HD13	1.92	0.51
4:M:24:ARG:HH21	1:S:156:LEU:HD22	1.76	0.51
6:E:190:LEU:HD13	6:E:215:ILE:HD12	1.93	0.50
2:A:208:GLU:HA	9:H:76:LEU:HD22	1.92	0.50
4:W:181:GLU:HG2	4:W:182:ASP:H	1.76	0.50
7:F:204:ILE:HG12	7:F:211:VAL:HG13	1.93	0.50
2:K:169:VAL:HG22	2:K:174:ILE:HG22	1.91	0.50
2:U:259:LEU:HD22	2:U:263:LYS:HE3	1.92	0.50
2:A:259:LEU:HD22	2:A:263:LYS:HE3	1.93	0.50
4:C:25:ILE:HG23	1:I:229:ILE:HG13	1.93	0.50
5:X:74:LEU:HD13	5:X:90:ILE:HD13	1.94	0.50
2:A:86:MET:HG3	5:D:29:SER:HB3	1.93	0.50
6:O:102:VAL:HG22	6:O:225:PRO:HD2	1.94	0.50
1:I:249:ARG:NH1	1:I:251:ASP:OD1	2.45	0.50
2:K:237:VAL:HG23	2:K:248:VAL:HG22	1.94	0.50
3:L:25:PHE:CE2	3:L:224:VAL:HG13	2.47	0.50
6:O:26:ARG:NH2	6:O:200:ASP:O	2.44	0.50
2:U:191:HIS:CE1	2:U:193:PRO:HG3	2.46	0.49
7:F:75:THR:HG22	7:F:139:VAL:HG22	1.92	0.49
2:U:261:LEU:HD12	3:V:196:LEU:HD12	1.94	0.49
8:G:156:ILE:HG12	8:G:208:TYR:CD1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:255:LEU:HD22	4:C:256:ARG:H	1.78	0.49
9:R:333:GLY:O	9:R:336:ILE:HG12	2.11	0.49
6:E:82:ILE:HD12	6:E:92:VAL:HG22	1.94	0.49
6:E:94:THR:HG23	7:F:112:GLU:HG3	1.95	0.49
5:N:129:SER:OG	5:N:166:GLU:OE1	2.31	0.49
6:E:191:ALA:HB3	6:E:198:LEU:HB2	1.93	0.49
6:E:238:SER:OG	7:F:209:GLU:OE1	2.30	0.49
2:K:135:ARG:NH1	2:K:137:ASP:OD1	2.39	0.49
3:L:229:ASP:O	3:L:233:ARG:HG3	2.13	0.49
4:M:255:LEU:HD23	4:M:256:ARG:N	2.28	0.49
7:P:77:VAL:HG22	7:P:137:ILE:HG12	1.95	0.49
5:X:51:ILE:HB	5:X:91:THR:HG23	1.94	0.49
6:Y:20:SER:HB2	6:Y:196:ASN:HD22	1.77	0.49
4:C:52:VAL:HG22	4:C:391:ARG:HH21	1.78	0.48
5:N:20:VAL:HG22	5:N:25:LYS:HG3	1.93	0.48
9:R:116:ILE:HD13	9:R:126:VAL:HG22	1.95	0.48
4:C:44:ARG:NH2	4:C:333:ASP:O	2.45	0.48
2:A:235:LEU:HD22	2:A:261:LEU:HD22	1.95	0.48
3:B:229:ASP:O	3:B:233:ARG:HG3	2.13	0.48
5:N:138:ILE:HG12	5:N:145:ILE:HG12	1.95	0.48
2:K:24:ARG:O	8:Q:209:ARG:NH2	2.47	0.48
4:W:300:VAL:HG22	4:W:343:ILE:HG12	1.95	0.48
4:C:299:ILE:HG13	4:C:330:LEU:HD12	1.96	0.48
2:K:103:LEU:O	2:K:107:ILE:HG12	2.13	0.48
4:M:124:ILE:HD11	4:M:160:LEU:HG	1.96	0.48
2:U:99:GLU:HB3	3:V:106:ARG:HH12	1.79	0.48
3:V:145:LEU:HD11	3:V:228:MET:HG2	1.96	0.48
6:Y:105:SER:O	6:Y:111:SER:HB3	2.14	0.48
4:M:359:GLN:OE1	4:M:361:THR:OG1	2.27	0.47
3:V:172:LEU:HD11	3:V:220:GLY:HA3	1.96	0.47
6:Y:98:LEU:O	6:Y:102:VAL:HG23	2.15	0.47
1:I:134:LYS:HE2	1:I:237:LEU:HD11	1.96	0.47
5:N:168:VAL:HG23	5:N:173:VAL:HB	1.95	0.47
6:E:217:TRP:CZ3	6:E:252:GLU:HA	2.50	0.47
9:H:70:GLY:HA3	9:H:96:SER:HB3	1.96	0.47
2:K:208:GLU:HA	9:R:76:LEU:HD22	1.96	0.47
3:V:59:PRO:HG3	3:V:121:VAL:HG23	1.96	0.47
6:Y:82:ILE:HD12	6:Y:92:VAL:HG22	1.95	0.47
4:W:262:ARG:HA	4:W:263:GLY:HA2	1.50	0.47
6:Y:51:ILE:HG12	6:Y:57:GLU:HG3	1.95	0.47
2:A:83:ILE:HD11	2:A:140:PHE:HD2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:190:LEU:HG	6:E:199:LEU:HD23	1.97	0.47
4:W:44:ARG:HH22	4:W:333:ASP:HB3	1.79	0.47
5:X:134:ILE:HG12	5:X:202:CYS:SG	2.54	0.47
3:L:172:LEU:HD11	3:L:220:GLY:HA3	1.97	0.47
6:O:22:ARG:HD3	6:O:26:ARG:HB3	1.97	0.47
2:U:243:ARG:NH2	14:U:501:HOH:O	2.36	0.47
4:W:94:GLY:O	4:W:212:VAL:N	2.42	0.47
7:Z:224:LEU:H	7:Z:224:LEU:HD12	1.80	0.47
3:B:172:LEU:HD11	3:B:220:GLY:HA3	1.97	0.46
5:D:51:ILE:HB	5:D:91:THR:HG23	1.97	0.46
4:M:301:GLU:HA	4:M:328:THR:HG22	1.97	0.46
1:I:134:LYS:HD2	1:I:237:LEU:HD21	1.97	0.46
3:L:205:ILE:HG21	3:L:210:LEU:HD13	1.97	0.46
1:S:143:VAL:HA	1:S:153:VAL:HG12	1.98	0.46
3:V:126:ILE:HG21	3:V:139:LEU:HD22	1.97	0.46
5:D:134:ILE:HG12	5:D:202:CYS:SG	2.55	0.46
1:S:228:ASP:OD2	1:S:286:ARG:NE	2.48	0.46
5:X:3:VAL:HG11	5:X:19:PHE:CZ	2.50	0.46
5:D:106:LEU:HD13	5:D:160:VAL:HB	1.97	0.46
6:E:184:PRO:HA	6:E:185:PRO:HD3	1.85	0.46
6:E:29:HIS:HA	6:E:199:LEU:HD12	1.98	0.46
9:R:310:CYS:HB2	9:R:312:ILE:HG12	1.98	0.46
3:B:15:ASP:OD2	3:B:17:ARG:HD3	2.15	0.46
7:P:200:VAL:HB	7:P:214:TRP:HB3	1.98	0.46
4:C:262:ARG:HA	4:C:263:GLY:HA2	1.57	0.46
4:C:50:ARG:HD3	4:C:333:ASP:OD2	2.15	0.46
6:E:98:LEU:O	6:E:102:VAL:HG23	2.16	0.46
8:G:22:GLY:HA2	10:J:95:SER:O	2.16	0.46
4:M:165:LEU:HD21	4:M:170:LEU:HD11	1.98	0.46
7:P:204:ILE:HG12	7:P:211:VAL:HG13	1.98	0.46
6:Y:182:ILE:O	6:Y:184:PRO:HD3	2.16	0.46
3:B:198:LEU:HD11	3:B:200:LEU:HD13	1.98	0.45
6:E:20:SER:HB2	6:E:196:ASN:HD22	1.80	0.45
2:A:217:GLU:HG2	2:A:254:LEU:HD21	1.98	0.45
6:O:34:ILE:HG22	6:O:52:ALA:HA	1.98	0.45
5:N:132:ALA:HB1	5:N:205:LEU:HD23	1.98	0.45
6:O:204:ASN:N	6:O:204:ASN:OD1	2.49	0.45
7:P:95:ILE:HB	7:P:118:MET:HG3	1.98	0.45
8:Q:63:ARG:HH21	8:Q:89:GLN:HG2	1.81	0.45
9:R:203:PRO:HD2	9:R:206:LEU:HD12	1.98	0.45
2:U:121:GLU:OE1	11:U:401:TAM:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:34:ILE:HG22	6:E:52:ALA:HA	1.97	0.45
8:G:162:PHE:CZ	8:G:174:LEU:HD22	2.51	0.45
3:L:185:VAL:HG22	3:L:201:VAL:HG22	1.98	0.45
2:U:217:GLU:HG2	2:U:254:LEU:HD21	1.98	0.45
1:I:146:LEU:HD11	1:I:225:LYS:HA	1.99	0.45
2:A:81:THR:HG22	2:A:138:VAL:HB	1.99	0.45
4:C:21:VAL:HG12	4:C:25:ILE:HD11	1.99	0.45
5:D:218:SER:OG	5:D:219:PRO:HD3	2.17	0.45
7:F:224:LEU:HD12	7:F:224:LEU:H	1.82	0.45
5:N:8:GLY:HA3	5:N:220:ARG:HH22	1.82	0.45
7:F:228:ASP:OD1	2:U:292:LYS:HD2	2.16	0.45
9:H:289:ILE:HG22	9:H:294:ARG:HG3	1.99	0.45
4:W:299:ILE:HG13	4:W:330:LEU:HD12	1.98	0.45
8:G:164:ARG:NH2	14:G:401:HOH:O	2.50	0.44
8:Q:88:LEU:HB3	8:Q:191:ASN:HD22	1.82	0.44
4:C:180:ASN:O	4:C:182:ASP:N	2.50	0.44
6:E:255:ALA:O	6:E:259:VAL:HG23	2.18	0.44
2:U:22:ASN:HA	2:U:30:PHE:CZ	2.53	0.44
3:V:205:ILE:HG21	3:V:210:LEU:HD13	2.00	0.44
3:L:201:VAL:HG13	3:L:205:ILE:HD12	2.00	0.44
8:Q:158:VAL:HG21	8:Q:194:ILE:HD12	2.00	0.44
9:R:128:ILE:HA	9:R:128:ILE:HD13	1.83	0.44
5:X:20:VAL:HG22	5:X:25:LYS:HG3	1.98	0.44
6:Y:117:THR:HG22	6:Y:118:LYS:N	2.33	0.44
3:B:59:PRO:HG3	3:B:121:VAL:HG23	2.00	0.44
1:S:141:THR:HG22	1:S:155:ILE:HG13	1.99	0.44
7:Z:95:ILE:HG12	7:Z:137:ILE:HB	2.00	0.44
3:V:229:ASP:O	3:V:233:ARG:HG3	2.18	0.44
9:R:175:SER:HB3	4:W:383:VAL:HG21	2.00	0.44
3:B:90:SER:O	3:B:92:LYS:N	2.41	0.44
4:C:255:LEU:CD2	4:C:256:ARG:H	2.30	0.44
1:I:132:LEU:HD12	1:I:133:PRO:HD2	2.00	0.44
8:G:129:GLU:OE2	1:I:225:LYS:HE3	2.18	0.44
4:W:50:ARG:HD3	4:W:333:ASP:OD2	2.18	0.44
2:K:33:PHE:HB2	2:K:271:ILE:HD13	1.99	0.44
4:M:87:VAL:HG21	4:M:229:LEU:HB3	2.00	0.44
4:M:54:ILE:HG22	4:M:80:LEU:HD13	2.00	0.44
8:Q:164:ARG:HG2	8:Q:190:LEU:HD22	2.00	0.44
5:X:140:LYS:HA	5:X:158:LEU:HD13	1.98	0.43
2:A:44:PHE:HB3	2:A:162:PHE:HA	2.00	0.43
4:C:375:LYS:HG3	5:D:192:PHE:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:84:VAL:HG21	9:H:99:PRO:HG3	2.00	0.43
6:O:238:SER:OG	7:P:209:GLU:OE1	2.28	0.43
6:E:249:ALA:HA	6:E:252:GLU:HG2	2.00	0.43
9:H:128:ILE:HD12	9:H:128:ILE:HA	1.85	0.43
9:H:322:ALA:HB2	9:H:348:ILE:HD11	2.00	0.43
6:O:191:ALA:HB3	6:O:198:LEU:HB2	1.99	0.43
3:V:13:ARG:HD3	3:V:171:LEU:HD13	2.00	0.43
4:M:299:ILE:HG13	4:M:330:LEU:HD12	2.00	0.43
6:O:217:TRP:CZ3	6:O:252:GLU:HA	2.53	0.43
9:R:70:GLY:HA3	9:R:96:SER:HB3	2.00	0.43
2:U:74:GLU:HG2	2:U:120:VAL:HB	2.00	0.43
4:W:56:ASN:HB2	4:W:394:ILE:HD13	1.99	0.43
6:E:104:LYS:O	6:E:106:GLY:N	2.52	0.43
6:O:210:ASN:HA	6:O:235:ASN:O	2.18	0.43
8:Q:167:LEU:HD13	8:Q:188:ILE:HB	2.01	0.43
6:E:204:ASN:N	6:E:204:ASN:OD1	2.52	0.43
6:E:51:ILE:HG12	6:E:57:GLU:HG3	2.00	0.43
8:Q:144:ASP:OD1	8:Q:144:ASP:N	2.50	0.43
6:E:14:SER:OG	9:H:294:ARG:NH1	2.49	0.43
3:B:122:ILE:HD13	3:B:152:ILE:HD13	2.01	0.42
6:E:210:ASN:HA	6:E:235:ASN:O	2.19	0.42
11:K:401:TAM:H21	11:K:401:TAM:H61	1.91	0.42
4:W:21:VAL:O	4:W:25:ILE:HG13	2.19	0.42
4:W:293:PHE:HB3	4:W:388:LEU:HD12	2.01	0.42
6:Y:217:TRP:CZ2	6:Y:220:GLY:HA2	2.54	0.42
5:D:41:GLU:OE2	5:D:85:ARG:NE	2.48	0.42
5:X:217:ILE:HA	5:X:220:ARG:HD2	2.01	0.42
7:P:224:LEU:H	7:P:224:LEU:HD12	1.84	0.42
2:A:179:VAL:HG23	2:A:184:PRO:HD3	2.01	0.42
2:K:64:ILE:HD13	2:K:174:ILE:HD12	2.01	0.42
7:P:190:MET:HG2	1:S:13:PRO:O	2.19	0.42
4:W:124:ILE:HD11	4:W:160:LEU:HG	2.02	0.42
6:Y:34:ILE:HD12	6:Y:50:ILE:HD11	2.00	0.42
7:Z:116:PHE:CE2	7:Z:120:ILE:HD11	2.54	0.42
2:A:261:LEU:HD12	3:B:196:LEU:HD12	2.01	0.42
7:F:93:ILE:HG13	7:F:127:LEU:HD21	2.02	0.42
6:O:182:ILE:O	6:O:184:PRO:HD3	2.19	0.42
6:O:217:TRP:HZ3	6:O:252:GLU:HA	1.84	0.42
7:P:97:LEU:HD22	7:P:110:LEU:HD22	2.01	0.42
1:S:3:CYS:HB3	1:S:7:PHE:CD2	2.55	0.42
9:H:350:THR:O	9:H:354:MET:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:235:LEU:HD11	1:I:246:THR:HB	2.02	0.42
8:Q:156:ILE:HG12	8:Q:208:TYR:CD2	2.55	0.42
1:S:141:THR:HG22	1:S:155:ILE:HA	2.01	0.42
3:V:122:ILE:HD13	3:V:152:ILE:HD13	2.02	0.42
6:Y:210:ASN:HA	6:Y:235:ASN:O	2.19	0.42
2:A:191:HIS:CE1	2:A:193:PRO:HG3	2.55	0.42
7:F:186:GLU:HG2	1:I:60:LEU:HG	2.02	0.42
3:L:98:LEU:O	3:L:102:THR:HG23	2.19	0.42
4:W:289:LYS:NZ	4:W:290:ASN:OD1	2.51	0.42
4:W:61:ARG:HG2	4:W:74:ILE:O	2.20	0.42
6:Y:184:PRO:HA	6:Y:185:PRO:HD3	1.86	0.42
7:F:99:ASN:HD21	7:F:105:TYR:H	1.67	0.42
2:K:81:THR:HG22	2:K:138:VAL:HB	2.02	0.42
3:L:188:GLY:O	3:L:197:SER:N	2.50	0.42
9:R:93:ARG:HA	9:R:93:ARG:HD2	1.88	0.42
6:Y:117:THR:HG22	6:Y:118:LYS:H	1.84	0.42
2:K:121:GLU:OE2	11:K:401:TAM:H42	2.20	0.41
4:W:349:ILE:HG12	4:W:360:LEU:HD13	2.01	0.41
3:B:86:ARG:NH1	6:E:127:ASP:OD1	2.53	0.41
6:E:99:LEU:HD11	6:E:141:ILE:HG21	2.02	0.41
7:F:116:PHE:CE2	7:F:120:ILE:HD11	2.55	0.41
2:K:179:VAL:HG23	2:K:184:PRO:HD3	2.02	0.41
4:M:302:LEU:HD21	4:M:329:VAL:HG13	2.01	0.41
4:W:18:PRO:HB2	4:W:21:VAL:HG23	2.01	0.41
4:C:29:LEU:HD12	1:I:256:PHE:CZ	2.56	0.41
4:C:61:ARG:HB3	4:C:72:ASN:HB3	2.03	0.41
3:V:29:ILE:HA	3:V:29:ILE:HD13	1.95	0.41
4:W:379:LEU:HD12	4:W:382:ARG:HH12	1.86	0.41
7:Z:68:GLY:O	7:Z:147:LEU:N	2.54	0.41
4:C:293:PHE:HB3	4:C:388:LEU:HD12	2.01	0.41
6:O:184:PRO:HA	6:O:185:PRO:HD3	1.87	0.41
7:P:95:ILE:HG12	7:P:137:ILE:HB	2.02	0.41
8:Q:162:PHE:CZ	8:Q:174:LEU:HD22	2.56	0.41
9:R:178:GLN:N	9:R:178:GLN:OE1	2.50	0.41
9:R:214:THR:HG23	9:R:224:VAL:HG22	2.02	0.41
2:U:56:VAL:HG12	2:U:140:PHE:CD1	2.55	0.41
5:X:138:ILE:HG12	5:X:145:ILE:HG12	2.01	0.41
4:W:362:LEU:O	5:X:179:LEU:HA	2.21	0.41
3:B:13:ARG:HD3	3:B:171:LEU:HD13	2.01	0.41
5:D:7:ILE:HA	5:D:7:ILE:HD13	1.97	0.41
6:E:158:ILE:HD11	6:E:173:HIS:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:64:ILE:HD13	2:U:174:ILE:HD12	2.02	0.41
5:X:180:LEU:HD22	5:X:195:LEU:HD21	2.01	0.41
5:X:205:LEU:O	5:X:209:ILE:N	2.49	0.41
2:A:33:PHE:HB2	2:A:271:ILE:HD13	2.02	0.41
3:B:98:LEU:O	3:B:102:THR:HG23	2.21	0.41
7:F:187:LEU:O	1:I:13:PRO:HB3	2.21	0.41
9:H:242:ALA:C	9:H:244:ASP:H	2.24	0.41
6:O:98:LEU:O	6:O:102:VAL:HG23	2.20	0.41
6:O:217:TRP:CZ2	6:O:220:GLY:HA2	2.56	0.41
8:Q:172:PHE:HA	8:Q:173:PRO:HD3	1.94	0.41
6:Y:204:ASN:N	6:Y:204:ASN:OD1	2.52	0.41
2:K:24:ARG:NH2	2:K:227:GLU:OE2	2.50	0.41
6:E:80:VAL:HG21	6:E:95:ILE:HG22	2.02	0.41
1:I:134:LYS:HA	1:I:134:LYS:HD2	1.90	0.41
1:I:256:PHE:HE1	1:I:266:LEU:HD22	1.85	0.41
4:M:44:ARG:NH2	4:M:333:ASP:HB3	2.35	0.41
9:R:144:PRO:HD3	9:R:281:TYR:HE2	1.85	0.41
5:X:106:LEU:HD13	5:X:160:VAL:HB	2.01	0.41
7:Z:203:PHE:HB3	7:Z:207:GLY:HA2	2.02	0.41
4:C:28:GLU:HG3	4:C:342:SER:HB3	2.03	0.41
9:H:312:ILE:HD12	9:H:349:LEU:HD21	2.03	0.41
6:O:94:THR:HG23	7:P:112:GLU:HG3	2.03	0.41
7:P:48:LEU:HD22	7:P:62:VAL:HG22	2.03	0.41
4:W:96:ILE:HB	7:Z:15:ALA:HB2	2.03	0.41
2:A:237:VAL:HG23	2:A:248:VAL:HG22	2.03	0.41
8:Q:63:ARG:HA	8:Q:89:GLN:HE22	1.85	0.41
1:S:134:LYS:HE2	1:S:237:LEU:HD11	2.03	0.41
4:W:348:SER:HB2	4:W:361:THR:HB	2.02	0.41
6:Y:103:LEU:O	6:Y:109:VAL:HG22	2.21	0.41
7:Z:97:LEU:HD22	7:Z:110:LEU:HD22	2.03	0.41
4:W:278:GLN:HG2	7:Z:20:PHE:HB3	2.03	0.41
4:C:360:LEU:HB3	5:D:182:SER:HB2	2.02	0.40
1:I:205:ILE:HG12	1:I:245:LEU:HB2	2.02	0.40
5:N:30:VAL:HA	5:N:89:GLN:O	2.21	0.40
6:E:25:GLY:HA3	9:H:332:VAL:HB	2.03	0.40
8:G:162:PHE:HZ	8:G:174:LEU:HD22	1.85	0.40
9:H:310:CYS:HB2	9:H:312:ILE:HG12	2.04	0.40
6:O:18:THR:HB	6:O:19:PRO:HD3	2.03	0.40
6:E:206:SER:HB3	6:E:231:LEU:HB3	2.03	0.40
8:G:156:ILE:HG12	8:G:208:TYR:HD1	1.86	0.40
4:M:362:LEU:O	5:N:179:LEU:HA	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:309:PHE:HE2	9:H:342:GLU:HG3	1.86	0.40
4:M:349:ILE:HG12	4:M:360:LEU:HD13	2.02	0.40
6:O:169:LEU:HA	6:O:170:PRO:HD3	1.93	0.40
9:R:307:LEU:HD21	9:R:348:ILE:HD12	2.03	0.40
3:V:15:ASP:OD1	3:V:15:ASP:N	2.51	0.40
6:Y:103:LEU:O	6:Y:104:LYS:O	2.38	0.40
6:Y:255:ALA:O	6:Y:259:VAL:HG23	2.21	0.40
5:D:205:LEU:O	5:D:209:ILE:N	2.49	0.40
9:H:232:TRP:NE1	9:H:234:ARG:HB3	2.36	0.40

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	130	LYS

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Mol	Chain	Res	Type
5	D	140	LYS
6	E	104	LYS
9	H	158	GLN
8	Q	152	ASP
2	U	130	LYS
4	W	181	GLU
4	W	393	ASN
5	X	140	LYS
6	Y	104	LYS
2	e	130	LYS
5	h	140	LYS
6	i	104	LYS
9	l	121	ASN
4	C	181	GLU
8	G	142	GLY
5	N	140	LYS
9	R	121	ASN
4	g	181	GLU
7	j	100	GLY
4	M	181	GLU
7	P	101	LEU
9	H	157	LEU
9	H	243	ARG
3	V	89	SER
4	W	254	ASP
9	b	121	ASN
9	b	276	SER
3	f	86	ARG
3	L	173	ASP
3	V	173	ASP
4	W	182	ASP
7	Z	100	GLY
1	I	39	PRO

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
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

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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

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	104	CYS
2	A	130	LYS
2	A	140	PHE
2	A	205	ASP
3	B	88	LYS
4	C	56	ASN
4	C	359	GLN
5	D	96	GLU
6	E	11	LEU
6	E	211	ASN
6	E	245	LYS
7	F	6	ARG
7	F	222	ASP
8	G	63	ARG
9	H	69	ARG
9	H	79	MET
9	H	164	LYS
9	H	234	ARG
2	K	140	PHE
4	M	56	ASN
4	M	61	ARG
4	M	168	LYS
4	M	359	GLN
5	N	111	CYS
6	O	211	ASN
7	P	99	ASN

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Mol	Chain	Res	Type
8	Q	63	ARG
8	Q	137	PHE
8	Q	152	ASP
9	R	69	ARG
9	R	79	MET
9	R	160	ARG
9	R	164	LYS
9	R	234	ARG
2	U	104	CYS
2	U	130	LYS
2	U	140	PHE
2	U	205	ASP
4	W	56	ASN
4	W	278	GLN
5	X	1	MET
5	X	96	GLU
5	X	211	ARG
6	Y	11	LEU
6	Y	211	ASN
6	Y	260	ARG
6	Y	265	LEU
7	Z	99	ASN
8	a	1	MET
8	a	63	ARG
8	a	137	PHE
9	b	69	ARG
9	b	79	MET
9	b	93	ARG
9	b	160	ARG
9	b	164	LYS
9	b	234	ARG
2	e	104	CYS
2	e	140	PHE
2	e	205	ASP
3	f	203	ASP
4	g	273	GLU
5	h	96	GLU
5	h	211	ARG
6	i	11	LEU
6	i	175	TYR
6	i	211	ASN
8	k	63	ARG

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Mol	Chain	Res	Type
9	1	69	ARG
9	1	79	MET
9	1	164	LYS
9	1	354	MET

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

Mol	Chain	Res	Type
9	1	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 carbohydrates 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	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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	TAM	e	401	-	7,10,10	0.80	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

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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%) 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

All (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
1	S	126	ASN	9.9
1	S	185	ALA	9.8
1	m	196	ASP	9.7
1	S	195	SER	9.6
8	a	139	SER	9.5
1	S	236	SER	9.4
1	S	202	ARG	8.9
1	I	135	GLU	8.7
8	a	112	THR	8.6
1	c	195	SER	8.6

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Mol	Chain	Res	Type	RSRZ
1	S	240	GLY	8.2
1	I	151	ALA	8.2
1	I	134	LYS	8.0
1	S	8	PRO	7.7
1	S	237	LEU	7.5
1	S	278	PRO	7.1
1	S	241	THR	7.1
1	I	237	LEU	7.1
1	S	244	TYR	6.8
1	c	245	LEU	6.8
1	S	245	LEU	6.8
1	I	243	TYR	6.7
1	I	240	GLY	6.7
1	S	243	TYR	6.7
1	S	153	VAL	6.6
1	S	219	LYS	6.6
1	c	49	ASN	6.6
1	S	212	SER	6.5
1	S	205	ILE	6.4
1	S	206	ARG	6.4
1	c	65	ARG	6.3
1	S	200	THR	6.2
1	S	220	VAL	6.2
1	c	243	TYR	6.1
1	c	126	ASN	6.1
1	S	21	TYR	6.1
1	c	205	ILE	6.0
8	a	111	PRO	5.9
1	c	204	ILE	5.9
8	Q	235	LEU	5.9
1	S	130	ASN	5.8
1	I	201	PHE	5.7
1	S	151	ALA	5.7
7	P	101	LEU	5.6
2	K	295	ALA	5.6
1	S	208	GLN	5.5
1	I	160	ASP	5.5
1	c	3	CYS	5.4
1	c	202	ARG	5.3
1	m	241	THR	5.3
8	a	108	LYS	5.2
1	S	194	SER	5.2

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Mol	Chain	Res	Type	RSRZ
9	l	155	ASP	5.2
1	m	235	LEU	5.1
1	m	199	GLU	5.1
9	l	156	GLU	5.0
9	l	151	LYS	5.0
1	m	236	SER	5.0
1	I	126	ASN	5.0
1	I	210	VAL	5.0
1	S	201	PHE	5.0
1	S	203	GLY	4.9
1	S	156	LEU	4.9
1	S	140	LEU	4.9
8	a	102	PHE	4.8
1	c	109	SER	4.8
1	m	245	LEU	4.8
1	c	241	THR	4.8
1	S	133	PRO	4.8
1	I	242	ASN	4.7
8	a	113	LEU	4.7
1	I	207	SER	4.7
8	a	110	ARG	4.7
1	m	11	ALA	4.7
1	S	235	LEU	4.7
1	c	8	PRO	4.7
4	g	306	CYS	4.6
1	S	247	THR	4.6
1	c	223	CYS	4.6
1	S	199	GLU	4.5
8	a	174	LEU	4.5
1	I	155	ILE	4.5
7	Z	101	LEU	4.5
1	m	155	ILE	4.5
1	I	17	ILE	4.5
1	S	218	VAL	4.5
8	a	140	THR	4.5
1	S	204	ILE	4.5
1	I	133	PRO	4.5
6	E	157	LEU	4.5
6	E	0	HIS	4.4
1	I	234	VAL	4.4
1	m	202	ARG	4.4
8	Q	234	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
1	S	224	PHE	4.3
8	k	154	MET	4.3
1	m	244	TYR	4.3
1	S	46	TYR	4.3
1	S	150	ARG	4.3
7	F	101	LEU	4.3
8	k	146	GLY	4.3
1	c	139	VAL	4.2
1	I	209	ASP	4.2
1	m	62	GLY	4.2
9	R	155	ASP	4.2
1	S	155	ILE	4.2
1	I	235	LEU	4.2
1	m	205	ILE	4.2
1	S	233	GLN	4.2
1	S	246	THR	4.2
1	I	153	VAL	4.2
1	S	7	PHE	4.2
1	c	113	GLY	4.1
1	S	20	GLN	4.1
1	I	205	ILE	4.1
1	S	138	ILE	4.1
9	l	144	PRO	4.1
1	S	242	ASN	4.0
1	c	224	PHE	4.0
1	m	269	ALA	4.0
1	m	234	VAL	4.0
1	I	208	GLN	4.0
1	c	48	HIS	4.0
8	k	196	VAL	4.0
8	a	187	ALA	4.0
2	U	209	ASN	3.9
1	c	151	ALA	3.9
1	m	197	LEU	3.9
8	a	151	GLU	3.9
1	I	56	ILE	3.9
1	I	112	PRO	3.9
8	a	137	PHE	3.9
1	m	243	TYR	3.9
10	n	115	PHE	3.9
1	S	55	ALA	3.9
1	c	2	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
9	l	152	SER	3.9
7	Z	102	LEU	3.8
1	S	190	VAL	3.8
8	a	144	ASP	3.8
1	I	221	ILE	3.8
1	S	108	VAL	3.8
1	m	237	LEU	3.8
1	c	133	PRO	3.8
1	m	247	THR	3.8
1	I	196	ASP	3.7
1	S	210	VAL	3.7
1	S	215	ARG	3.7
1	I	241	THR	3.7
2	K	296	MET	3.7
1	c	138	ILE	3.6
1	c	199	GLU	3.6
1	S	154	GLU	3.6
8	a	118	LEU	3.6
3	B	90	SER	3.6
1	c	7	PHE	3.6
1	S	6	GLN	3.6
1	I	64	VAL	3.6
2	U	205	ASP	3.5
1	I	148	LEU	3.5
8	G	141	THR	3.5
1	c	10	ILE	3.5
1	m	194	SER	3.5
1	c	150	ARG	3.5
8	Q	140	THR	3.5
1	I	278	PRO	3.5
1	S	131	ASN	3.4
1	c	235	LEU	3.4
1	m	113	GLY	3.4
7	P	100	GLY	3.4
1	I	248	ALA	3.4
1	I	238	GLY	3.4
1	I	150	ARG	3.4
1	m	61	VAL	3.4
1	S	214	ASP	3.4
1	c	244	TYR	3.4
8	a	143	ARG	3.4
1	m	10	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
9	R	154	SER	3.4
1	c	197	LEU	3.4
1	c	140	LEU	3.4
1	S	269	ALA	3.4
1	I	199	GLU	3.4
1	I	247	THR	3.4
1	I	16	LEU	3.3
1	S	10	ILE	3.3
8	a	195	TRP	3.3
1	c	206	ARG	3.3
1	I	187	THR	3.3
8	k	102	PHE	3.3
1	S	186	ALA	3.3
1	S	53	LEU	3.3
1	c	17	ILE	3.3
1	m	131	ASN	3.3
1	m	201	PHE	3.3
1	I	224	PHE	3.3
1	I	131	ASN	3.2
1	I	204	ILE	3.2
8	a	194	ILE	3.2
1	I	63	THR	3.2
1	S	270	THR	3.2
1	c	131	ASN	3.2
1	I	244	TYR	3.2
8	a	141	THR	3.2
1	I	146	LEU	3.2
1	c	148	LEU	3.2
1	m	190	VAL	3.2
1	c	152	ASN	3.2
6	E	177	MET	3.1
1	m	138	ILE	3.1
1	c	61	VAL	3.1
8	a	145	ALA	3.1
1	S	239	ASP	3.1
1	S	207	SER	3.1
1	m	283	THR	3.1
8	a	19	VAL	3.1
1	m	232	ALA	3.1
1	m	278	PRO	3.1
7	j	101	LEU	3.1
1	S	223	CYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	m	233	GLN	3.1
1	c	51	ARG	3.1
8	a	148	GLY	3.1
1	I	202	ARG	3.0
1	m	266	LEU	3.0
8	k	195	TRP	3.0
1	c	234	VAL	3.0
3	B	3	ARG	3.0
1	c	50	GLY	3.0
8	Q	147	PHE	3.0
1	c	159	GLU	3.0
1	m	65	ARG	3.0
1	I	211	ARG	3.0
1	c	198	GLY	2.9
8	a	196	VAL	2.9
1	m	133	PRO	2.9
1	m	200	THR	2.9
7	Z	139	VAL	2.9
1	S	209	ASP	2.9
1	S	267	MET	2.9
1	S	146	LEU	2.9
3	B	244	SER	2.9
8	G	142	GLY	2.9
8	k	148	GLY	2.9
1	I	220	VAL	2.9
8	k	118	LEU	2.9
1	S	11	ALA	2.9
1	c	46	TYR	2.9
7	Z	108	ASN	2.9
1	S	234	VAL	2.9
1	I	195	SER	2.9
2	e	209	ASN	2.9
1	c	9	GLU	2.9
8	a	84	TYR	2.8
2	A	293	TYR	2.8
1	I	236	SER	2.8
8	Q	154	MET	2.8
1	I	222	GLU	2.8
1	c	237	LEU	2.8
1	S	149	GLN	2.8
1	c	268	TYR	2.8
1	c	155	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	S	222	GLU	2.8
7	j	102	LEU	2.8
1	m	188	PHE	2.8
1	I	141	THR	2.8
8	a	150	LEU	2.8
1	S	139	VAL	2.8
1	S	65	ARG	2.8
8	Q	139	SER	2.8
1	m	109	SER	2.7
1	c	266	LEU	2.7
7	P	8	ARG	2.7
1	m	127	ASP	2.7
1	I	132	LEU	2.7
1	c	1	MET	2.7
1	I	130	ASN	2.7
1	m	46	TYR	2.7
1	S	35	TYR	2.7
1	S	109	SER	2.7
1	m	139	VAL	2.7
1	S	135	GLU	2.7
4	C	306	CYS	2.7
3	L	3	ARG	2.7
2	K	103	LEU	2.7
1	c	128	PHE	2.7
1	c	203	GLY	2.7
1	m	153	VAL	2.7
1	S	157	ALA	2.7
1	m	63	THR	2.7
1	I	219	LYS	2.7
8	a	142	GLY	2.7
1	I	159	GLU	2.7
1	m	268	TYR	2.6
9	H	349	LEU	2.6
1	m	274	MET	2.6
1	c	190	VAL	2.6
8	Q	186	VAL	2.6
1	S	189	SER	2.6
1	S	211	ARG	2.6
8	a	79	THR	2.6
1	S	4	ASN	2.6
1	S	198	GLY	2.6
1	c	255	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
8	a	109	ASN	2.6
1	m	270	THR	2.6
8	Q	132	ALA	2.6
1	m	151	ALA	2.6
1	I	239	ASP	2.6
1	S	34	ASN	2.6
1	I	206	ARG	2.5
1	m	156	LEU	2.5
1	I	245	LEU	2.5
3	B	91	HIS	2.5
1	m	193	ALA	2.5
1	I	279	VAL	2.5
8	a	119	VAL	2.5
8	a	73	ILE	2.5
1	c	55	ALA	2.5
8	k	147	PHE	2.5
8	k	194	ILE	2.5
8	a	95	VAL	2.5
1	S	197	LEU	2.5
1	I	147	SER	2.5
1	S	162	PRO	2.5
1	S	281	GLY	2.5
1	c	242	ASN	2.5
1	c	194	SER	2.5
8	a	178	LEU	2.5
10	J	108	VAL	2.5
1	I	194	SER	2.5
8	G	137	PHE	2.5
1	S	54	GLU	2.5
8	a	154	MET	2.5
1	c	5	PHE	2.5
9	H	95	LEU	2.4
1	S	145	ARG	2.4
7	Z	104	LYS	2.4
4	C	239	GLN	2.4
1	I	18	CYS	2.4
9	l	153	GLU	2.4
4	g	90	SER	2.4
1	c	127	ASP	2.4
1	I	139	VAL	2.4
1	I	189	SER	2.4
1	S	9	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
4	W	59	LEU	2.4
4	g	31	LEU	2.4
1	I	190	VAL	2.4
2	U	96	ILE	2.4
1	I	128	PHE	2.3
1	c	188	PHE	2.3
1	S	111	LEU	2.3
4	C	39	ILE	2.3
1	I	143	VAL	2.3
1	I	254	VAL	2.3
1	c	187	THR	2.3
3	V	89	SER	2.3
1	I	149	GLN	2.3
3	V	64	GLN	2.3
1	c	112	PRO	2.3
1	c	236	SER	2.3
1	m	126	ASN	2.3
1	S	216	ASP	2.3
1	I	152	ASN	2.3
6	E	172	PHE	2.3
9	R	157	LEU	2.3
1	c	201	PHE	2.3
9	R	145	GLY	2.3
1	c	189	SER	2.3
1	S	152	ASN	2.3
1	S	38	GLY	2.3
1	c	200	THR	2.3
1	I	266	LEU	2.3
1	m	210	VAL	2.3
1	S	141	THR	2.3
2	U	207	GLU	2.3
4	M	299	ILE	2.3
1	c	207	SER	2.3
1	I	65	ARG	2.2
5	D	145	ILE	2.2
8	k	197	LYS	2.2
1	c	232	ALA	2.2
1	c	60	LEU	2.2
1	S	147	SER	2.2
1	S	64	VAL	2.2
1	m	8	PRO	2.2
9	R	95	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
8	a	16	THR	2.2
1	m	128	PHE	2.2
1	I	256	PHE	2.2
1	c	249	ARG	2.2
1	m	279	VAL	2.2
1	c	279	VAL	2.2
7	j	190	MET	2.2
8	a	186	VAL	2.2
8	k	186	VAL	2.2
4	C	90	SER	2.2
1	I	113	GLY	2.2
1	m	12	TYR	2.2
1	S	18	CYS	2.2
8	a	134	ILE	2.2
1	c	52	THR	2.2
7	j	9	LEU	2.1
1	I	158	VAL	2.1
1	I	233	GLN	2.1
1	S	66	CYS	2.1
7	j	6	ARG	2.1
1	m	204	ILE	2.1
1	c	110	VAL	2.1
1	m	239	ASP	2.1
1	m	211	ARG	2.1
1	m	246	THR	2.1
5	N	140	LYS	2.1
1	S	110	VAL	2.1
7	Z	100	GLY	2.1
2	U	212	GLY	2.1
1	S	148	LEU	2.1
1	S	284	GLU	2.1
1	c	149	GLN	2.1
4	W	72	ASN	2.1
1	I	157	ALA	2.1
7	j	7	ARG	2.1
7	F	87	PHE	2.1
1	S	268	TYR	2.1
10	J	110	SER	2.1
1	I	197	LEU	2.1
9	H	145	GLY	2.1
4	C	89	THR	2.1
8	Q	127	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	c	146	LEU	2.1
8	k	174	LEU	2.1
1	I	249	ARG	2.1
1	m	110	VAL	2.1
8	a	76	ILE	2.1
1	S	256	PHE	2.0
1	I	145	ARG	2.0
8	a	86	VAL	2.0
1	I	203	GLY	2.0
1	I	217	ARG	2.0
4	g	140	ARG	2.0
8	a	71	PHE	2.0
1	c	147	SER	2.0
1	c	11	ALA	2.0
7	Z	121	PHE	2.0
1	c	281	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
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.