



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:32 AM UTC

PDB ID : 5OKZ / pdb_00005okz
Title : Crystal Structure 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 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

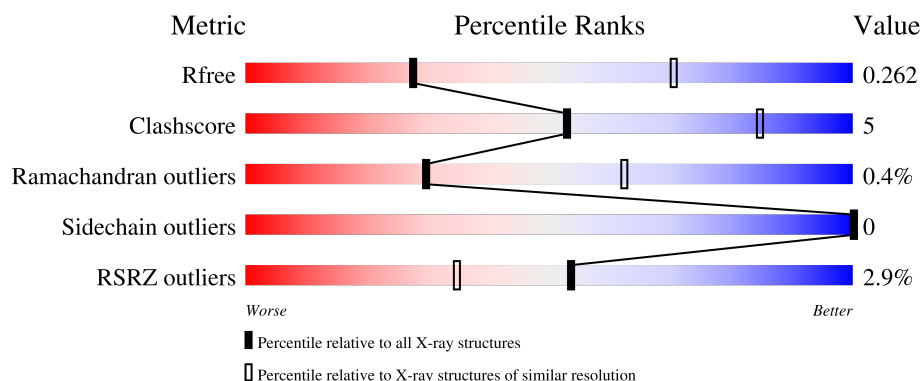
1 Overall quality at a glance

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.



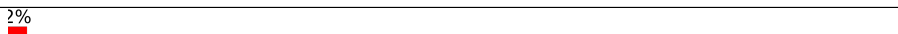
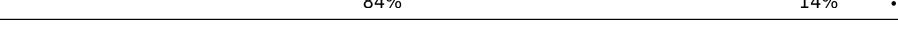
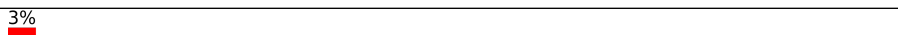
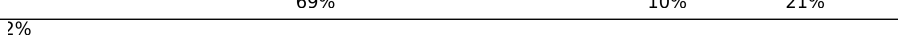
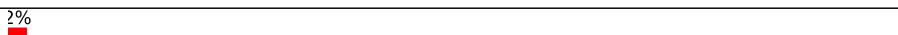
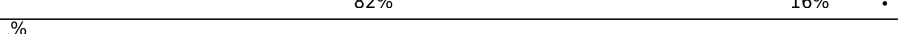
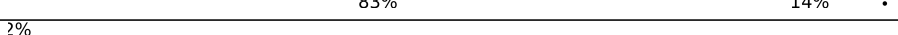
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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 $\leq 5\%$. 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	5% 52% 8% 40%
1	S	295	6% 64% 6% 29%
1	c	295	7% 61% 6% 33%
1	m	295	2% 57% 8% 36%
2	A	305	% 85% 11% .

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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	5%76%17%7%
8	k	244	12%83%9%7%
9	H	316	2%72%12%16%
9	R	316	2%75%9%16%
9	b	316	%72%11%17%
9	l	316	3%75%10%15%
10	J	190	%10%89%
10	T	190	..96%
10	d	190	%..96%
10	n	190	%..95%

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	C	N	O	S	0	0	0
			2019	1263	360	386	10			
9	b	262	Total	C	N	O	S	0	0	0
			1993	1250	357	375	11			
9	l	268	Total	C	N	O	S	0	0	0
			2020	1268	361	380	11			

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	C	N	O	0	0	0
			139	89	25	25			
10	T	7	Total	C	N	O	0	0	0
			46	27	10	9			

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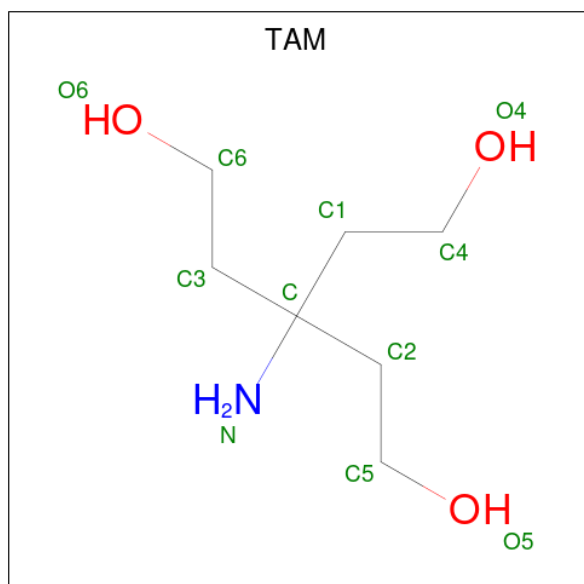
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	d	7	Total	C	N	O	0	0	0
			46	27	10	9			
10	n	10	Total	C	N	O	0	0	0
			70	44	14	12			

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 (CCD ID: 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 (CCD ID: 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	R	2	Total Cl 2 2	0	0
12	b	1	Total Cl 1 1	0	0
12	f	1	Total Cl 1 1	0	0
12	l	1	Total Cl 1 1	0	0

- Molecule 13 is MAGNESIUM ION (CCD ID: 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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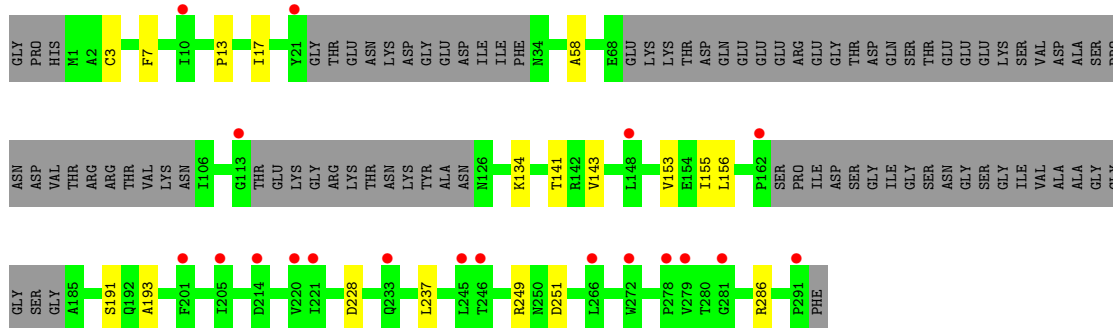
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	D	7	Total O 7 7	0	0
14	E	2	Total O 2 2	0	0
14	G	3	Total O 3 3	0	0
14	H	3	Total O 3 3	0	0
14	L	2	Total O 2 2	0	0
14	N	2	Total O 2 2	0	0
14	O	7	Total O 7 7	0	0
14	P	2	Total O 2 2	0	0
14	R	3	Total O 3 3	0	0
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

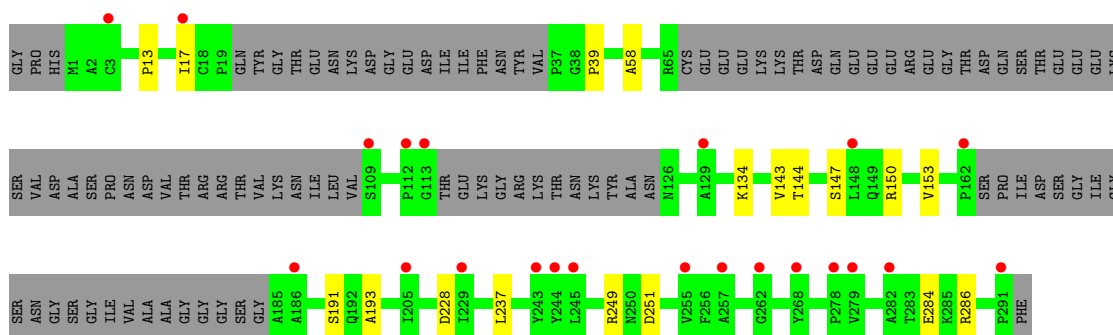
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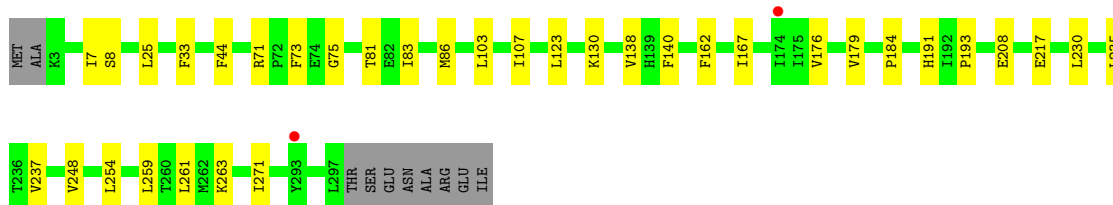
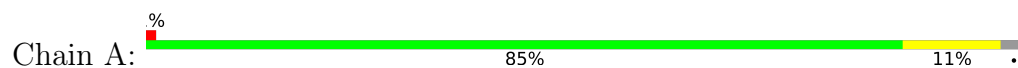
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	j	1	Total	O	0	0
			1	1		
14	l	8	Total	O	0	0
			8	8		



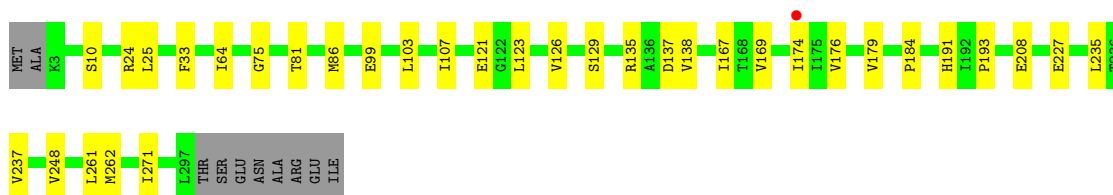
• Molecule 1: Exosome complex component CSL4



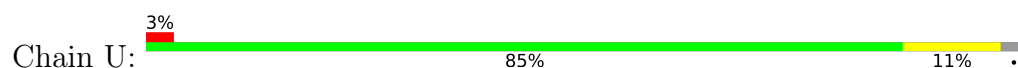
• Molecule 2: Exosome complex component RRP45

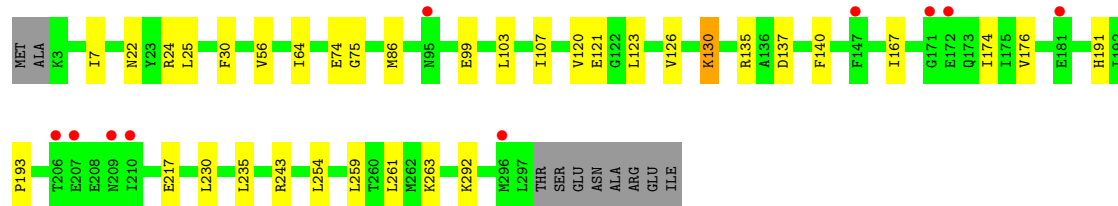


• Molecule 2: Exosome complex component RRP45

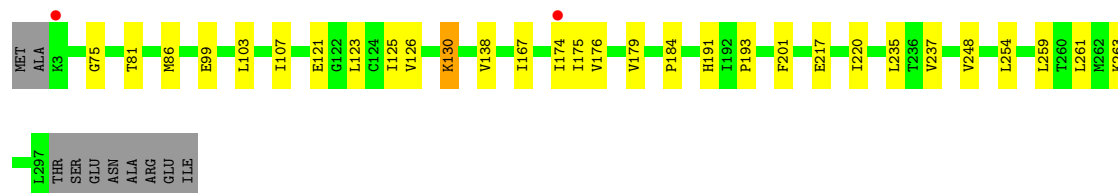
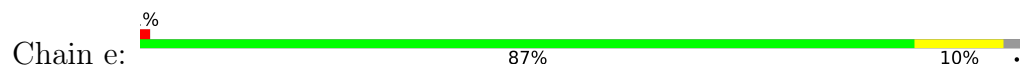


• Molecule 2: Exosome complex component RRP45

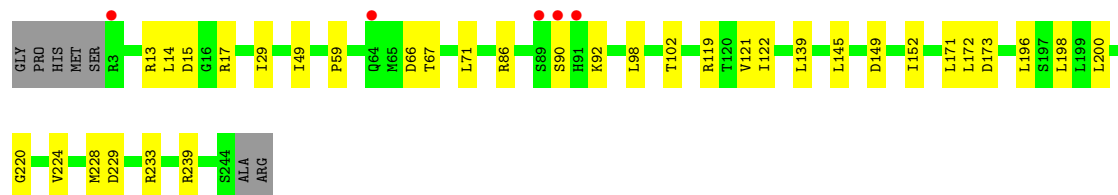
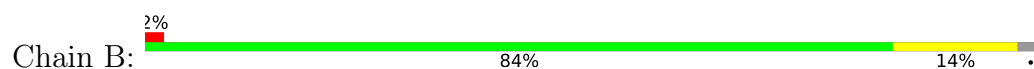




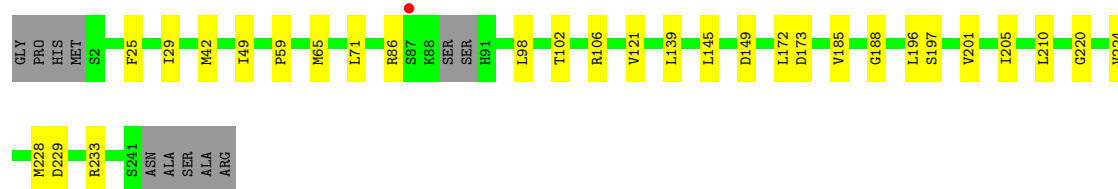
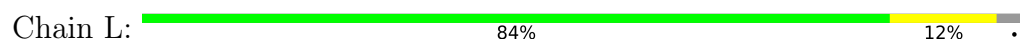
- Molecule 2: Exosome complex component RRP45



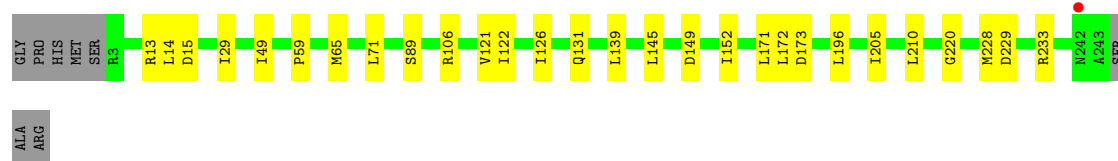
- Molecule 3: Exosome complex component SKI6



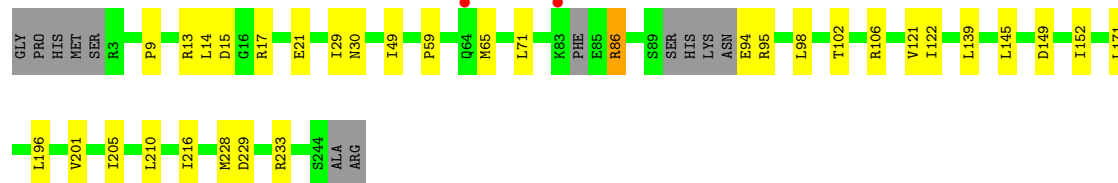
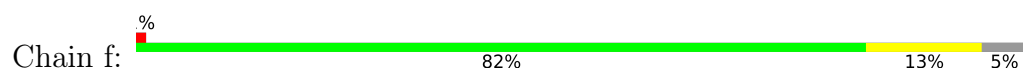
- Molecule 3: Exosome complex component SKI6



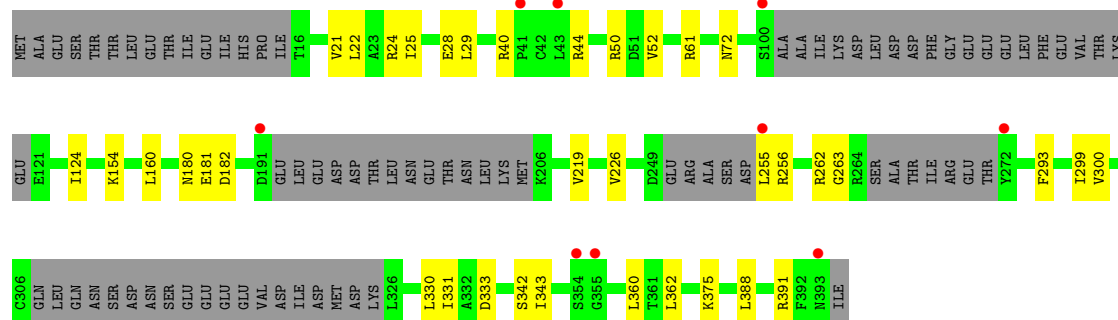
- Molecule 3: Exosome complex component SKI6



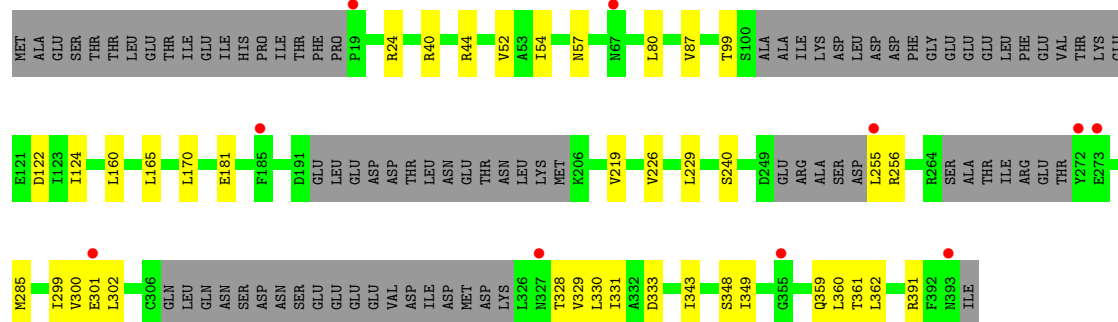
- Molecule 3: Exosome complex component SKI6



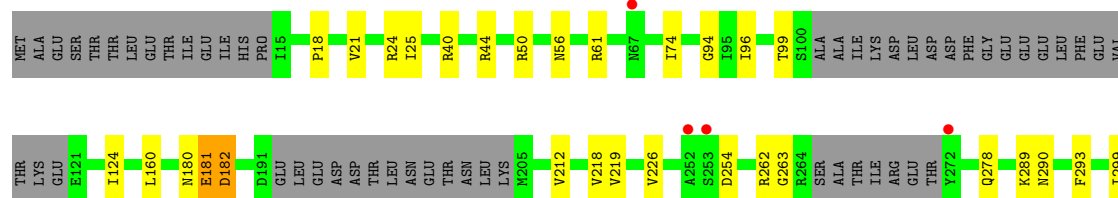
• Molecule 4: Exosome complex component RRP43



• Molecule 4: Exosome complex component RRP43

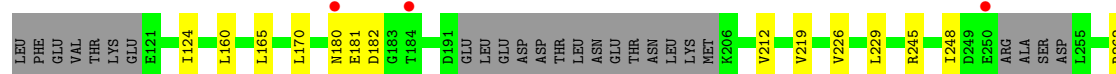


• Molecule 4: Exosome complex component RRP43

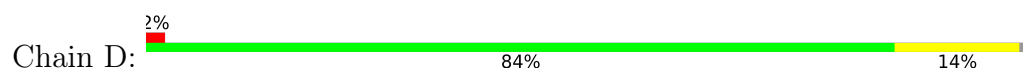




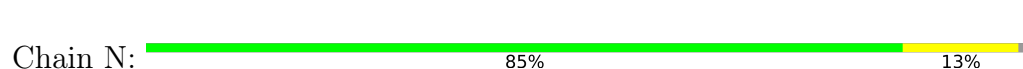
• Molecule 4: Exosome complex component RRP43



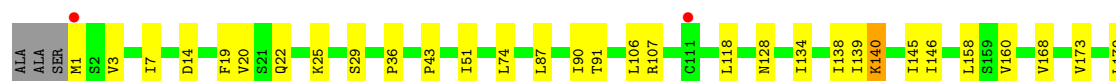
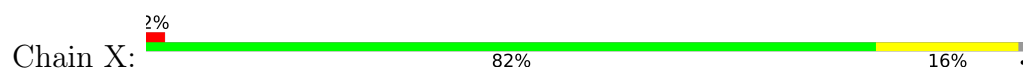
• Molecule 5: Exosome complex component RRP46



• Molecule 5: Exosome complex component RRP46

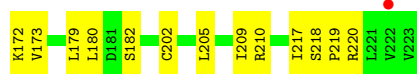
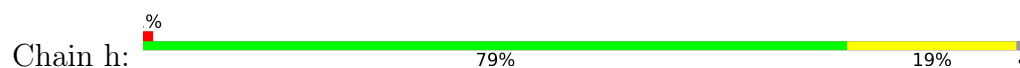


• Molecule 5: Exosome complex component RRP46

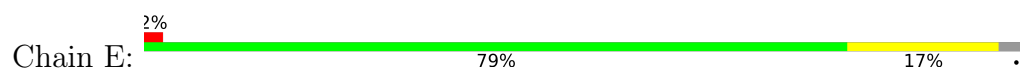




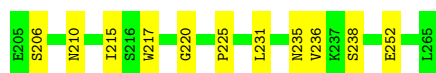
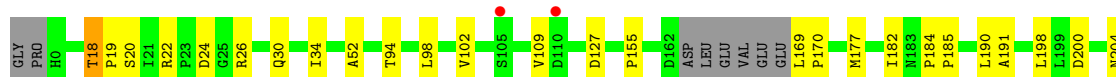
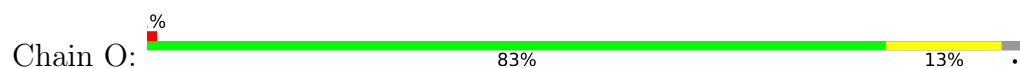
- Molecule 5: Exosome complex component RRP46



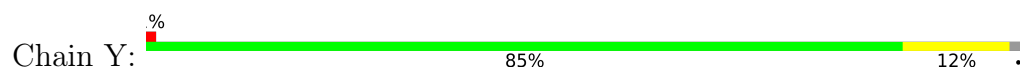
- Molecule 6: Exosome complex component RRP42



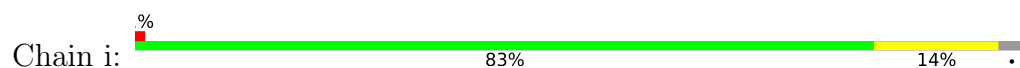
- Molecule 6: Exosome complex component RRP42

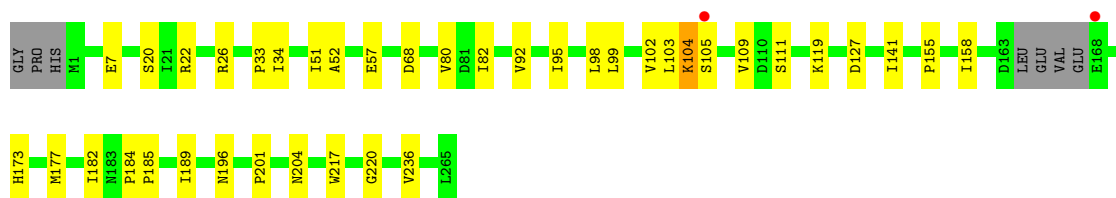


- Molecule 6: Exosome complex component RRP42

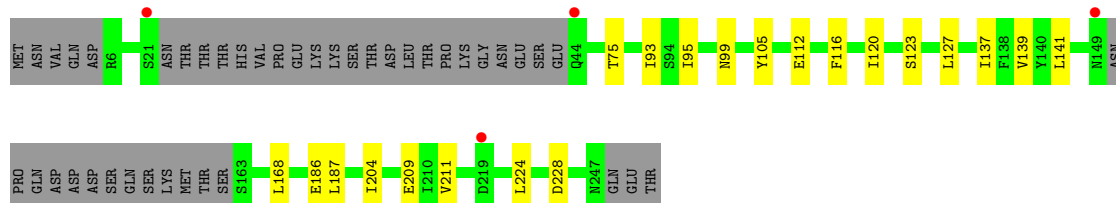
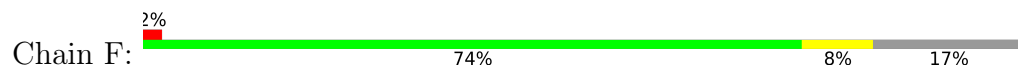


- Molecule 6: Exosome complex component RRP42

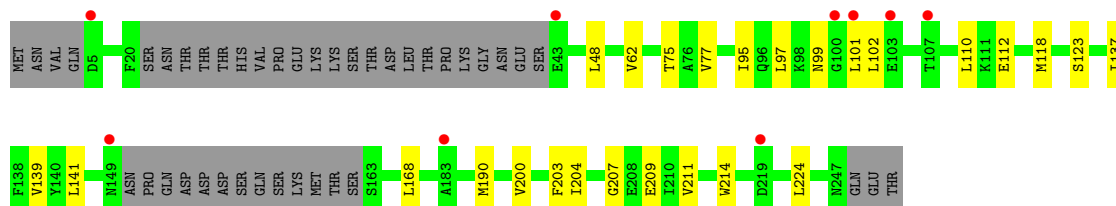
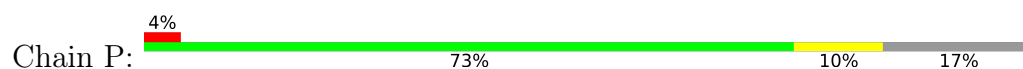




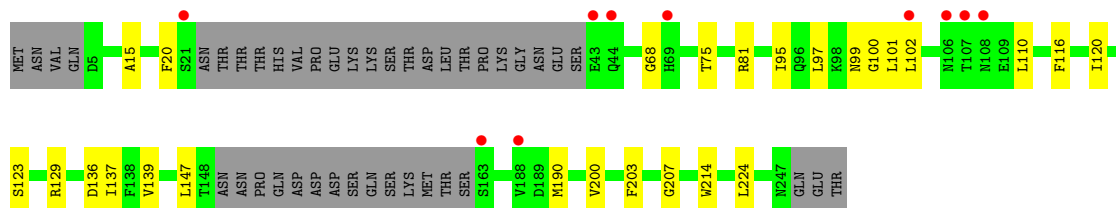
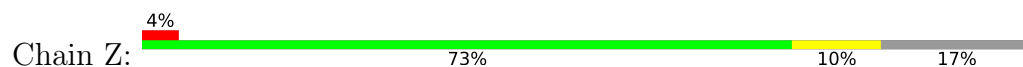
• Molecule 7: Exosome complex component MTR3



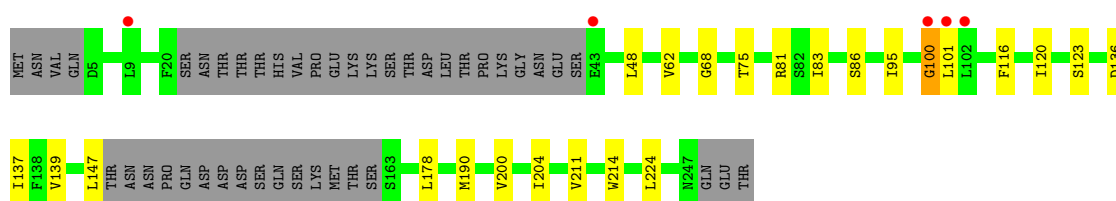
• Molecule 7: Exosome complex component MTR3



• Molecule 7: Exosome complex component MTR3

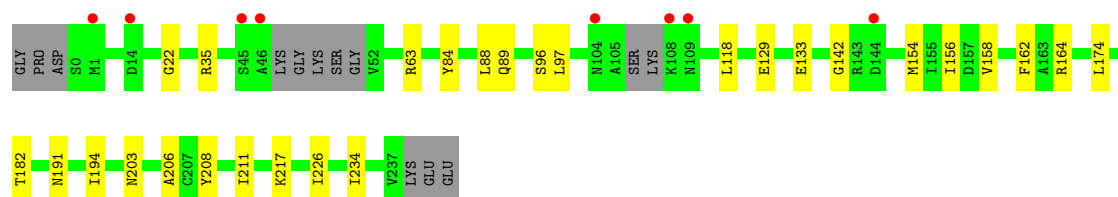


• Molecule 7: Exosome complex component MTR3



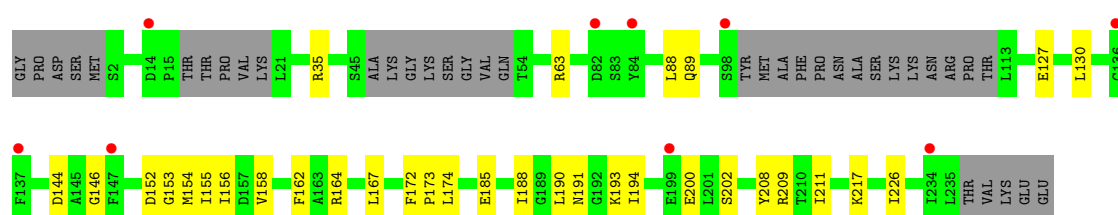
- Molecule 8: Exosome complex component RRP40

Chain G: 



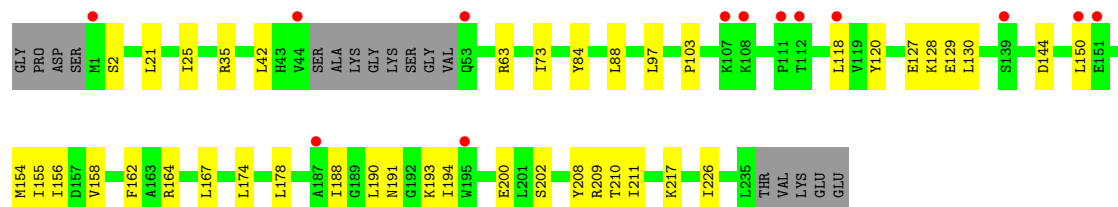
- Molecule 8: Exosome complex component RRP40

Chain Q: 



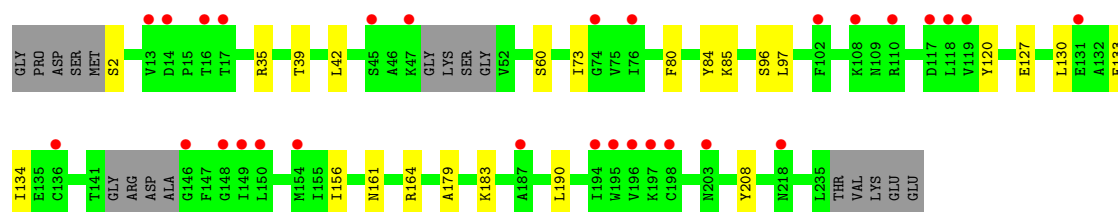
- Molecule 8: Exosome complex component RRP40

Chain a: 



- Molecule 8: Exosome complex component RRP40

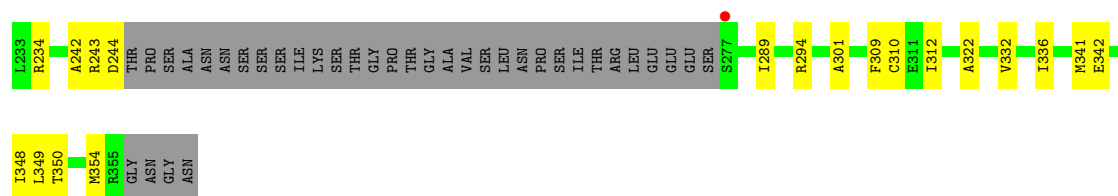
Chain k: 



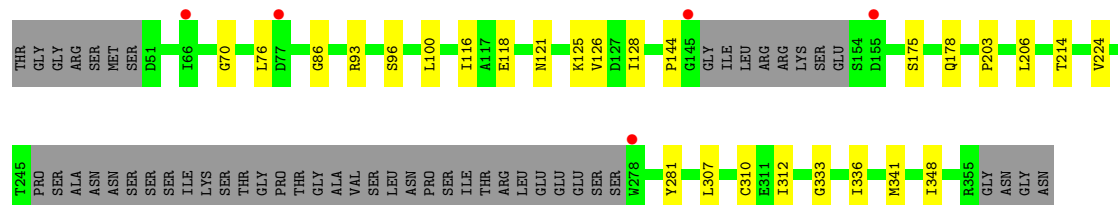
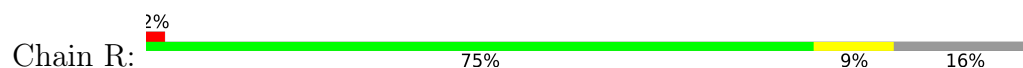
- Molecule 9: Exosome complex component RRP4

Chain H: 

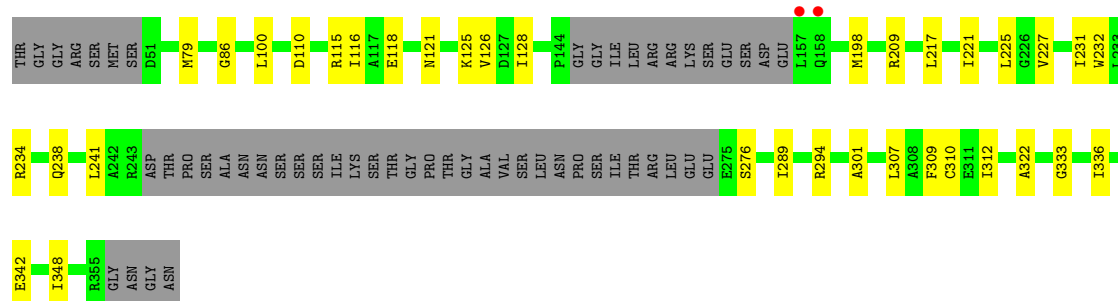




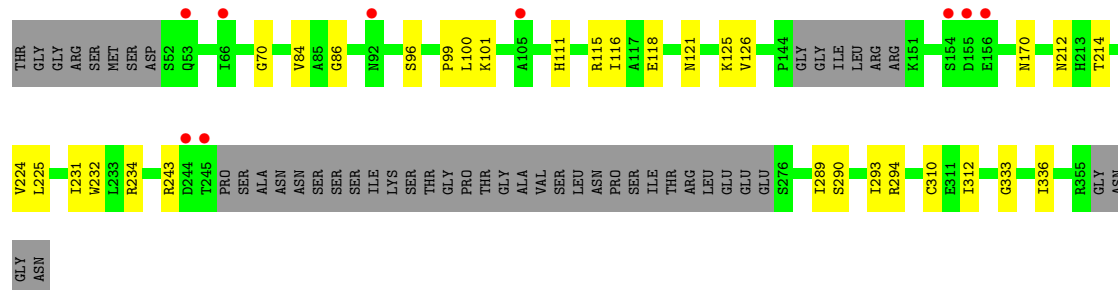
• Molecule 9: Exosome complex component RRP4



• Molecule 9: Exosome complex component RRP4

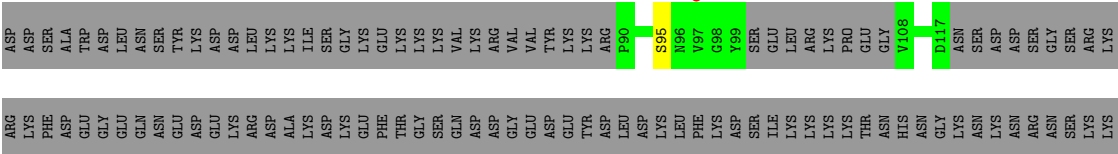


• Molecule 9: Exosome complex component RRP4

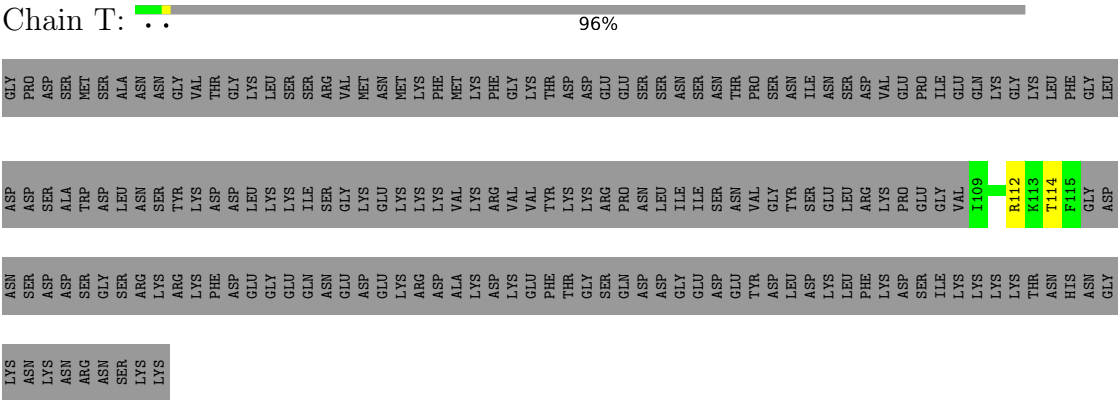


• Molecule 10: M-phase phosphoprotein 6 homolog

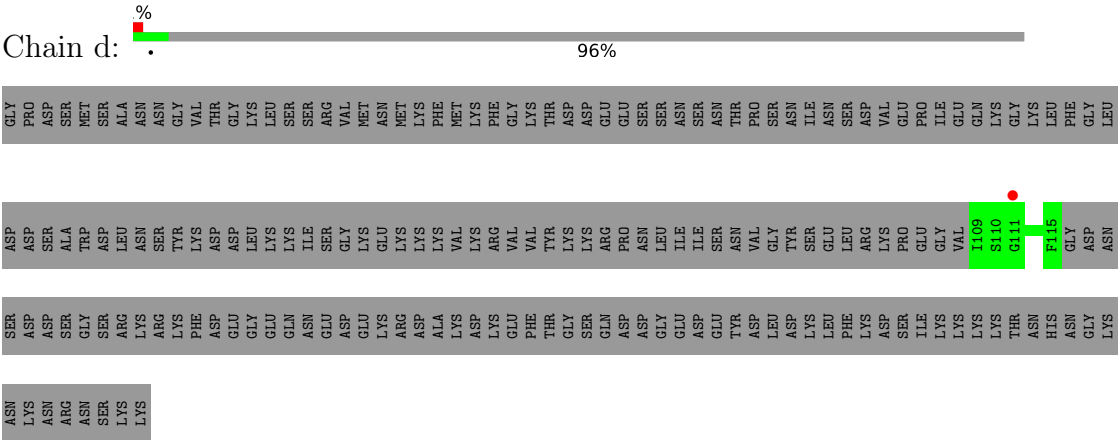




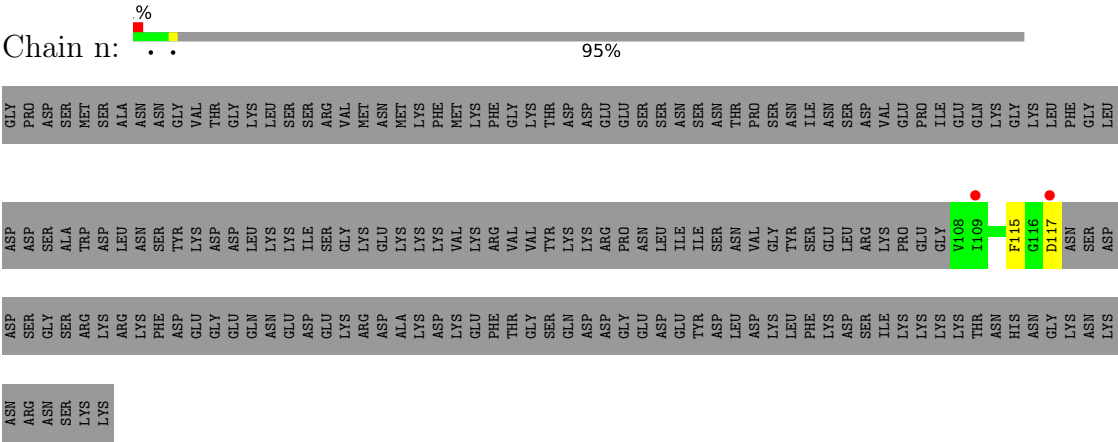
● Molecule 10: M-phase phosphoprotein 6 homolog



● Molecule 10: M-phase phosphoprotein 6 homolog



● Molecule 10: M-phase phosphoprotein 6 homolog



4 Data and refinement statistics

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 80.76 – 3.20	Depositor EDS
% Data completeness (in resolution range)	95.8 (80.76-3.20) 97.7 (80.76-3.20)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.223 , 0.262 0.226 , 0.262	Depositor DCC
R_{free} test set	11386 reflections (4.71%)	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)	0.29 , 69.2	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	0.92	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, TAM, 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	0.08	0/1330	0.26	0/1798
1	S	0.08	0/1576	0.25	0/2138
1	c	0.08	0/1483	0.27	0/2009
1	m	0.08	0/1443	0.26	0/1952
2	A	0.09	0/2279	0.28	0/3083
2	K	0.10	0/2279	0.27	0/3083
2	U	0.09	0/2279	0.28	0/3083
2	e	0.09	0/2283	0.27	0/3087
3	B	0.10	0/1852	0.33	0/2506
3	L	0.10	0/1818	0.30	0/2459
3	V	0.09	0/1873	0.29	0/2529
3	f	0.10	0/1854	0.33	0/2502
4	C	0.10	0/2365	0.31	0/3209
4	M	0.12	0/2312	0.35	0/3138
4	W	0.11	0/2432	0.32	0/3297
4	g	0.10	0/2408	0.30	0/3263
5	D	0.10	0/1667	0.30	0/2269
5	N	0.10	0/1684	0.29	0/2291
5	X	0.10	0/1722	0.30	0/2336
5	h	0.09	0/1721	0.29	0/2335
6	E	0.11	0/1928	0.31	0/2631
6	O	0.23	1/1978 (0.1%)	0.30	0/2698
6	Y	0.11	0/2010	0.30	0/2741
6	i	0.11	0/2019	0.30	0/2748
7	F	0.09	0/1538	0.29	0/2084
7	P	0.10	0/1537	0.30	0/2084
7	Z	0.09	0/1552	0.30	0/2101
7	j	0.09	0/1527	0.30	0/2070
8	G	0.10	0/1731	0.29	0/2361
8	Q	0.09	0/1576	0.28	0/2138
8	a	0.09	0/1780	0.27	0/2420
8	k	0.10	0/1649	0.28	0/2254

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
9	H	0.09	0/2046	0.30	0/2773
9	R	0.09	0/2050	0.29	0/2777
9	b	0.09	0/2026	0.30	0/2744
9	l	0.08	0/2052	0.30	0/2779
10	J	0.13	0/140	0.38	0/186
10	T	0.09	0/45	0.29	0/59
10	d	0.10	0/45	0.44	0/59
10	n	0.08	0/70	0.25	0/91
All	All	0.10	1/67959 (0.0%)	0.29	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	8.89	1.54	1.33

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	12	0
1	m	1425	0	1432	14	0
2	A	2244	0	2190	23	0
2	K	2244	0	2190	25	0
2	U	2244	0	2190	23	0
2	e	2248	0	2201	19	0
3	B	1830	0	1813	23	0
3	L	1797	0	1781	19	0
3	V	1851	0	1866	20	0
3	f	1832	0	1840	26	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	27	0
4	W	2400	0	2400	34	0
4	g	2376	0	2375	31	0
5	D	1649	0	1663	20	0
5	N	1666	0	1689	18	0
5	X	1704	0	1759	23	0
5	h	1703	0	1756	26	0
6	E	1894	0	1869	28	0
6	O	1941	0	1913	26	0
6	Y	1974	0	1960	22	0
6	i	1981	0	1987	22	0
7	F	1517	0	1441	14	0
7	P	1515	0	1420	16	0
7	Z	1531	0	1461	16	0
7	j	1506	0	1436	15	0
8	G	1696	0	1558	21	0
8	Q	1550	0	1463	21	0
8	a	1744	0	1688	25	0
8	k	1615	0	1456	16	0
9	H	2013	0	1965	23	0
9	R	2019	0	1990	16	0
9	b	1993	0	1960	19	0
9	l	2020	0	1967	17	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	2	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	1	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	670	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 (670) 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
1:m:191:SER:O	4:g:24:ARG:NH1	2.14	0.79
9:H:157:LEU:O	9:H:159:MET:N	2.15	0.79
5:h:121:VAL:HG13	8:k:39:THR:HG21	1.64	0.77
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
4:g:52:VAL:HG22	4:g:391:ARG:HH21	1.54	0.72
3:f:59:PRO:HG2	3:f:65:MET:HG3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:W:24:ARG:NH1	1:c:193:ALA:O	2.24	0.71
1:S:249:ARG:NH1	1:S:251:ASP:OD1	2.25	0.70
8:a:127:GLU:HB2	8:a:130:LEU:HB2	1.72	0.69
6:O:155:PRO:HA	6:O:177:MET:HG2	1.74	0.69
3:L:145:LEU:HG	3:L:228:MET:HE3	1.74	0.69
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
3:f:71:LEU:HB2	3:f:121:VAL:HG22	1.75	0.68
2:K:10:SER:HB3	8:Q:153:GLY:H	1.58	0.68
4:g:248:ILE:HG23	4:g:274:ILE:HD12	1.74	0.68
4:g:362:LEU:HB2	5:h:180:LEU:HB3	1.75	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
3:f:145:LEU:HG	3:f:228:MET:HE3	1.77	0.66
3:B:224:VAL:HG12	3:B:228:MET:HE2	1.77	0.66
2:K:174:ILE:HD11	4:M:99:THR:HG22	1.77	0.66
7:j:81:ARG:NH2	7:j:136:ASP:OD2	2.24	0.66
9:b:118:GLU:HG2	9:b:125:LYS:HB2	1.77	0.66
8:k:127:GLU:HB2	8:k:130:LEU:HB2	1.75	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
1:m:249:ARG:NH1	1:m:251:ASP:OD1	2.30	0.65
3:f:94:GLU:OE2	3:f:94:GLU:N	2.29	0.65
3:V:145:LEU:HG	3:V:228:MET:HE3	1.78	0.64
5:X:1:MET:HE1	5:X:205:LEU:HD13	1.78	0.64
7:Z:81:ARG:NH2	7:Z:136:ASP:OD2	2.26	0.64
3:B:66:ASP:O	3:B:67:THR:OG1	2.13	0.64
1:c:249:ARG:NH1	1:c:251:ASP:OD1	2.30	0.64
8:a:200:GLU:HG3	8:a:202:SER:H	1.63	0.63
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
9:l:118:GLU:HG2	9:l:125:LYS:HB2	1.80	0.63
4:C:24:ARG:NH1	1:I:193:ALA:O	2.22	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:7:ILE:HD11	5:D:118:LEU:HB3	1.80	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
3:f:30:ASN:OD1	9:l:101:LYS:NZ	2.29	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
6:i:34:ILE:HG22	6:i:52:ALA:HA	1.82	0.61
3:f:29:ILE:HD11	3:f:145:LEU:HB3	1.81	0.61
6:i:236:VAL:HG12	7:j:123:SER:HB3	1.82	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
9:b:198:MET:HE1	9:b:301:ALA:HB2	1.83	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
9:l:86:GLY:HA2	9:l:100:LEU:HG	1.84	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
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:174:LEU:HD21	8:Q:211:ILE:HG12	1.83	0.59
8:Q:185:GLU:HA	10:T:114:THR:HG22	1.84	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
5:X:128:ASN:OD1	8:a:35:ARG:NH2	2.36	0.59
8:G:174:LEU:HD21	8:G:211:ILE:HG12	1.85	0.58
5:h:22:GLN:HB2	5:h:107:ARG:HH12	1.68	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:g:79:VAL:HG22	4:g:88:ILE:HG23	1.85	0.58
7:P:141:LEU:HD11	7:P:168:LEU:HD21	1.86	0.58
3:f:14:LEU:HD12	3:f:14:LEU:H	1.66	0.58
5:h:36:PRO:HB3	5:h:87:LEU:HB2	1.85	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
6:i:7:GLU:OE2	9:l:115:ARG:NH1	2.36	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
6:i:155:PRO:HA	6:i:177:MET:HG2	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
6:i:109:VAL:HB	6:i:182:ILE:HD11	1.86	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
5:h:168:VAL:HG23	5:h:173:VAL:HB	1.87	0.56
2:e:259:LEU:HD22	2:e:263:LYS:HE3	1.88	0.56
4:g:219:VAL:HG11	4:g:226:VAL:HG21	1.88	0.56
2:A:71:ARG:HH22	3:f:9:PRO:HA	1.71	0.56
3:f:29:ILE:HD12	3:f:149:ASP:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:l:333:GLY:O	9:l:336:ILE:HG12	2.05	0.55
6:Y:34:ILE:HG22	6:Y:52:ALA:HA	1.87	0.55
1:m:134:LYS:HD2	1:m:237:LEU:HD21	1.88	0.55
4:C:124:ILE:HD11	4:C:160:LEU:HG	1.88	0.55
2:U:86:MET:HG3	5:X:29:SER:HB3	1.88	0.55
2:U:235:LEU:HD22	2:U:261:LEU:HD22	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
4:W:218:VAL:HG22	7:Z:101:LEU:HD21	1.89	0.55
5:X:168:VAL:HG23	5:X:173:VAL:HB	1.88	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
3:f:13:ARG:HD3	3:f:171:LEU:HD13	1.89	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
8:a:88:LEU:HB3	8:a:191:ASN:HD22	1.71	0.54
4:W:219:VAL:HG11	4:W:226:VAL:HG21	1.89	0.54
1:c:17:ILE:HD11	1:c:58:ALA:HB2	1.88	0.54
5:N:74:LEU:HD13	5:N:90:ILE:HD13	1.90	0.54
2:e:175:ILE:HA	4:g:101:ALA:HB2	1.89	0.54
9:l:111:HIS:NE2	9:l:170:ASN:OD1	2.40	0.54
5:D:20:VAL:HG22	5:D:25:LYS:HG3	1.87	0.54
5:h:128:ASN:OD1	8:k:35:ARG:NH2	2.40	0.54
5:h:139:ILE:HD13	5:h:146:ILE:HD13	1.88	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
3:f:49:ILE:HD13	3:f:139:LEU:HD23	1.89	0.54
5:X:139:ILE:HD13	5:X:146:ILE:HD13	1.88	0.54
7:j:95:ILE:HG12	7:j:137:ILE:HB	1.90	0.54
9:b:110:ASP:HB3	9:b:227:VAL:HG21	1.90	0.53
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
1:m:13:PRO:HB2	7:j:190:MET:HE3	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:e:237:VAL:HG23	2:e:248:VAL:HG22	1.91	0.53
2:K:25:LEU:HD21	8:Q:154:MET:HE2	1.89	0.53
1:S:134:LYS:HD2	1:S:237:LEU:HD21	1.91	0.53
8:a:217:LYS:HD2	8:a:226:ILE:HD11	1.90	0.52
7:j:75:THR:HG22	7:j:139:VAL:HG22	1.90	0.52
2:e:167:ILE:HG22	2:e:176:VAL:HA	1.91	0.52
2:K:86:MET:HG3	5:N:29:SER:HB3	1.91	0.52
5:h:20:VAL:HG22	5:h:25:LYS:HG3	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
9:b:86:GLY:HA2	9:b:100:LEU:HG	1.91	0.52
5:D:132:ALA:HB1	5:D:205:LEU:HD23	1.91	0.52
6:i:98:LEU:O	6:i:102:VAL:HG23	2.10	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
9:b:217:LEU:HD12	9:b:221:ILE:HD11	1.92	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
9:H:116:ILE:HD13	9:H:126:VAL:HG22	1.92	0.52
9:H:336:ILE:HA	9:H:341:MET:HE3	1.91	0.52
3:B:239:ARG:HH12	9:H:101:LYS:HE2	1.75	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
9:H:198:MET:HE1	9:H:301:ALA:HB2	1.91	0.52
2:U:126:VAL:HG22	2:U:130:LYS:HB2	1.92	0.52
6:i:33:PRO:HD3	9:l:336:ILE:HD12	1.90	0.52
4:W:180:ASN:O	4:W:182:ASP:N	2.43	0.52
8:a:158:VAL:HG21	8:a:194:ILE:HD12	1.92	0.52
1:I:65:ARG:HH11	1:I:111:LEU:HD12	1.74	0.51
6:i:20:SER:HB2	6:i:196:ASN:HD22	1.74	0.51
9:l:214:THR:HG23	9:l:224:VAL:HG22	1.93	0.51
8:a:103:PRO:HG3	8:a:144:ASP:HB3	1.92	0.51
7:j:100:GLY:O	7:j:101:LEU:HB2	2.11	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:e:121:GLU:OE1	11:e:401:TAM:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:h:7:ILE:HD11	5:h:118:LEU:HB3	1.91	0.51
2:K:235:LEU:HD22	2:K:261:LEU:HD22	1.93	0.51
4:W:24:ARG:NH1	1:c:191:SER:O	2.43	0.51
5:N:7:ILE:HD11	5:N:118:LEU:HB3	1.93	0.51
4:g:300:VAL:HG22	4:g:343:ILE:HG12	1.91	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
6:i:158:ILE:HD11	6:i:173:HIS:HA	1.93	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
2:e:235:LEU:HD22	2:e:261:LEU:HD22	1.92	0.51
5:h:132:ALA:HB1	5:h:205:LEU:HD23	1.93	0.51
2:A:208:GLU:HA	9:H:76:LEU:HD22	1.92	0.50
6:E:190:LEU:HD13	6:E:215:ILE:HD12	1.93	0.50
4:W:181:GLU:HG2	4:W:182:ASP:H	1.76	0.50
8:k:73:ILE:HG12	8:k:120:TYR:HD1	1.77	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
3:f:59:PRO:HG3	3:f:121:VAL:HG23	1.93	0.50
7:j:200:VAL:HB	7:j:214:TRP:HB3	1.93	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
7:j:190:MET:HE2	7:j:190:MET:HA	1.94	0.50
1:m:143:VAL:HA	1:m:153:VAL:HG12	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:f:86:ARG:HH12	6:i:127:ASP:CG	2.20	0.49
4:g:285:MET:HA	4:g:285:MET:HE3	1.94	0.49
6:i:105:SER:O	6:i:111:SER:HB3	2.13	0.49
8:G:156:ILE:HG12	8:G:208:TYR:CD1	2.48	0.49
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
8:a:84:TYR:HB2	8:a:97:LEU:HB3	1.94	0.49
5:h:62:ARG:NH2	5:h:108:GLU:OE1	2.41	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
6:i:22:ARG:HD3	6:i:26:ARG:HB3	1.95	0.49
1:m:263:ALA:HB2	5:h:81:HIS:CG	2.48	0.49
5:N:129:SER:OG	5:N:166:GLU:OE1	2.31	0.49
5:h:217:ILE:HA	5:h:220:ARG:HD2	1.94	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
2:e:191:HIS:CE1	2:e:193:PRO:HG3	2.48	0.49
3:f:205:ILE:HG21	3:f:210:LEU:HD13	1.95	0.49
5:X:43:PRO:HB3	1:c:144:THR:O	2.13	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
8:a:21:LEU:HD22	8:a:25:ILE:HG21	1.95	0.48
8:a:118:LEU:HB3	8:a:150:LEU:HB2	1.94	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
6:O:238:SER:OG	7:P:209:GLU:OE1	2.28	0.48
2:e:217:GLU:HG2	2:e:254:LEU:HD21	1.95	0.48
2:K:24:ARG:O	8:Q:209:ARG:NH2	2.47	0.48
5:N:138:ILE:HG12	5:N:145:ILE:HG12	1.95	0.48
4:W:300:VAL:HG22	4:W:343:ILE:HG12	1.95	0.48
9:l:70:GLY:HA3	9:l:96:SER:HB3	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:m:17:ILE:HD11	1:m:58:ALA:HB2	1.95	0.48
2:e:75:GLY:HA3	2:e:123:LEU:HB2	1.95	0.48
2:e:130:LYS:HG2	2:e:174:ILE:HG21	1.95	0.48
4:g:44[A]:ARG:NH2	4:g:333:ASP:HB3	2.28	0.48
2:e:86:MET:HG3	5:h:29:SER:HB3	1.95	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
9:R:336:ILE:HA	9:R:341:MET:HE3	1.95	0.47
3:V:172:LEU:HD11	3:V:220:GLY:HA3	1.96	0.47
8:a:178:LEU:HD21	8:a:210:THR:HG21	1.95	0.47
8:k:156:ILE:HG12	8:k:208:TYR:CD1	2.49	0.47
8:k:183:LYS:HE3	10:n:117:ASP:HA	1.94	0.47
6:Y:98:LEU:O	6:Y:102:VAL:HG23	2.15	0.47
9:l:310:CYS:HB2	9:l:312:ILE:HG12	1.97	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
9:b:322:ALA:HB2	9:b:348:ILE:HD11	1.96	0.47
3:f:94:GLU:HG2	3:f:95:ARG:N	2.29	0.47
4:g:348:SER:HB2	4:g:361:THR:HB	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
8:a:164:ARG:HG2	8:a:190:LEU:HD22	1.95	0.47
9:b:79:MET:SD	9:b:79:MET:N	2.87	0.47
9:l:84:VAL:HG21	9:l:99:PRO:HG3	1.96	0.47
9:l:116:ILE:HD13	9:l:126:VAL:HG22	1.97	0.47
2:A:83:ILE:HD11	2:A:140:PHE:HD2	1.79	0.47
6:E:190:LEU:HG	6:E:199:LEU:HD23	1.97	0.47
2:U:24:ARG:O	8:a:209:ARG:NH2	2.47	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
6:Y:7:GLU:OE2	9:b:115:ARG:NH1	2.47	0.47
4:g:245:ARG:HD2	4:g:280:LYS:HD3	1.97	0.47
3:L:172:LEU:HD11	3:L:220:GLY:HA3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD12	7:Z:224:LEU:H	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
5:h:169:ASN:O	5:h:172:LYS:HG2	2.15	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
2:e:103:LEU:O	2:e:107:ILE:HG12	2.14	0.46
6:i:99:LEU:HD11	6:i:141:ILE:HG21	1.97	0.46
6:i:217:TRP:CZ2	6:i:220:GLY:HA2	2.51	0.46
9:H:242:ALA:C	9:H:244:ASP:H	2.24	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
9:b:110:ASP:OD2	9:b:209:ARG:NH2	2.49	0.46
1:c:134:LYS:HD2	1:c:237:LEU:HD21	1.98	0.46
1:c:147:SER:OG	1:c:150:ARG:HG2	2.15	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
9:b:225:LEU:HD23	9:b:231:ILE:HG12	1.97	0.46
5:D:106:LEU:HD13	5:D:160:VAL:HB	1.97	0.46
6:E:29:HIS:HA	6:E:199:LEU:HD12	1.98	0.46
6:E:184:PRO:HA	6:E:185:PRO:HD3	1.85	0.46
9:R:310:CYS:HB2	9:R:312:ILE:HG12	1.98	0.46
2:e:81:THR:HG22	2:e:138:VAL:HB	1.97	0.46
3:f:17:ARG:HB3	3:f:21:GLU:HB3	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
8:a:127:GLU:HG3	8:a:130:LEU:HD12	1.96	0.46
5:h:218:SER:OG	5:h:219:PRO:HD3	2.16	0.46
4:C:50:ARG:HD3	4:C:333:ASP:OD2	2.15	0.46
4:C:262:ARG:HA	4:C:263:GLY:HA2	1.57	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
8:k:164:ARG:HG2	8:k:190:LEU:HD22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:e:261:LEU:HD12	3:f:196:LEU:HD12	1.98	0.45
3:f:94:GLU:HG2	3:f:95:ARG:H	1.81	0.45
1:m:134:LYS:HE2	1:m:237:LEU:HD11	1.98	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
8:a:174:LEU:HD21	8:a:211:ILE:HG12	1.98	0.45
5:h:13:VAL:HG11	5:h:29:SER:HB2	1.98	0.45
1:m:65:ARG:HD2	1:m:111:LEU:HD12	1.97	0.45
5:N:132:ALA:HB1	5:N:205:LEU:HD23	1.98	0.45
6:O:204:ASN:OD1	6:O:204:ASN:N	2.49	0.45
7:P:95:ILE:HB	7:P:118:MET:HG3	1.98	0.45
3:B:17:ARG:HD2	4:g:262:ARG:HD2	1.97	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
2:e:99:GLU:HB3	3:f:106:ARG:HH12	1.81	0.45
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
7:Z:129:ARG:NH1	1:c:39:PRO:HA	2.32	0.45
9:l:225:LEU:HD23	9:l:231:ILE:HG12	1.97	0.45
1:I:146:LEU:HD11	1:I:225:LYS:HA	1.99	0.45
8:a:73:ILE:HG12	8:a:120:TYR:HD1	1.81	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
2:A:25:LEU:HD21	8:G:154:MET:HE2	1.99	0.45
7:F:228:ASP:OD1	2:U:292:LYS:HD2	2.16	0.45
7:j:224:LEU:HD12	7:j:224:LEU:H	1.82	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:a:156:ILE:HG12	8:a:208:TYR:CD2	2.51	0.45
4:g:262:ARG:HA	4:g:263:GLY:HA2	1.45	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
3:f:201:VAL:HG13	3:f:205:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:i:82:ILE:HD12	6:i:92:VAL:HG22	1.99	0.44
7:j:48:LEU:HD22	7:j:62:VAL:HG22	2.00	0.44
7:j:83:ILE:HB	7:j:86:SER:HB2	1.99	0.44
4:C:180:ASN:O	4:C:182:ASP:N	2.50	0.44
2:U:25:LEU:HD21	8:a:154:MET:HE2	1.99	0.44
8:a:128:LYS:HG3	8:a:129:GLU:OE1	2.17	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:HD13	9:R:128:ILE:HA	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
9:b:128:ILE:HD13	9:b:128:ILE:HA	1.84	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
2:A:73:PHE:HZ	3:f:216:ILE:HD11	1.83	0.44
9:R:175:SER:HB3	4:W:383:VAL:HG21	2.00	0.44
3:V:229:ASP:O	3:V:233:ARG:HG3	2.18	0.44
5:X:14:ASP:OD2	8:a:63:ARG:HD2	2.18	0.44
6:i:68:ASP:OD1	6:i:119:LYS:HG2	2.18	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
8:G:129:GLU:OE2	1:I:225:LYS:HE3	2.18	0.44
1:I:132:LEU:HD12	1:I:133:PRO:HD2	2.00	0.44
4:W:50:ARG:HD3	4:W:333:ASP:OD2	2.18	0.44
4:g:180:ASN:O	4:g:182:ASP:N	2.50	0.44
4:g:353:PRO:C	4:g:355:GLY:H	2.25	0.44
2:K:33:PHE:HB2	2:K:271:ILE:HD13	1.99	0.44
4:M:54:ILE:HG22	4:M:80:LEU:HD13	2.00	0.44
4:M:87:VAL:HG21	4:M:229:LEU:HB3	2.00	0.44
8:Q:164:ARG:HG2	8:Q:190:LEU:HD22	2.00	0.44
4:g:94:GLY:O	4:g:212:VAL:N	2.46	0.44
5:X:140:LYS:HA	5:X:158:LEU:HD13	1.98	0.43
8:k:97:LEU:HD13	8:k:134:ILE:HG13	2.00	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
9:H:84:VAL:HG21	9:H:99:PRO:HG3	2.00	0.43
3:f:122:ILE:HD13	3:f:152:ILE:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:h:170:GLY:HA2	5:h:210:ARG:CZ	2.48	0.43
8:k:84:TYR:HB2	8:k:97:LEU:HB3	2.01	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
8:a:162:PHE:CZ	8:a:174:LEU:HD22	2.53	0.43
1:c:228:ASP:OD2	1:c:286:ARG:NE	2.50	0.43
4:g:40:ARG:HD2	4:g:331:ILE:HD12	1.99	0.43
6:i:204:ASN:OD1	6:i:204:ASN:N	2.51	0.43
6:i:103:LEU:O	6:i:104:LYS:O	2.36	0.43
8:k:179:ALA:HB2	10:n:115:PHE:HB3	1.99	0.43
6:E:104:LYS:O	6:E:106:GLY:N	2.52	0.43
4:g:293:PHE:HB3	4:g:388:LEU:HD12	2.00	0.43
7:j:116:PHE:CE2	7:j:120:ILE:HD11	2.53	0.43
8:k:80:PHE:CE2	8:k:85:LYS:HB2	2.53	0.43
8:k:96:SER:HB3	8:k:133:GLU:HG2	2.00	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
4:g:61:ARG:HB3	4:g:72:ASN:HB3	2.01	0.43
5:h:51:ILE:HB	5:h:91:THR:HG23	2.00	0.43
1:m:141:THR:HG22	1:m:155:ILE:HA	1.99	0.43
6:E:51:ILE:HG12	6:E:57:GLU:HG3	2.00	0.43
6:E:204:ASN:OD1	6:E:204:ASN:N	2.52	0.43
8:Q:144:ASP:OD1	8:Q:144:ASP:N	2.50	0.43
4:W:289:LYS:NZ	4:W:290:ASN:OD1	2.51	0.43
4:g:87:VAL:HG21	4:g:229:LEU:HB3	2.00	0.43
6:E:14:SER:OG	9:H:294:ARG:NH1	2.49	0.43
4:M:57:ASN:CG	4:M:240:SER:HB2	2.44	0.43
9:b:309:PHE:HE2	9:b:342:GLU:HG3	1.84	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:H61	11:K:401:TAM:H21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
9:b:116:ILE:HD13	9:b:126:VAL:HG22	2.01	0.42
9:b:238:GLN:HA	9:b:241:LEU:HD12	2.01	0.42
6:i:184:PRO:HA	6:i:185:PRO:HD3	1.86	0.42
8:k:156:ILE:HG12	8:k:208:TYR:HD1	1.84	0.42
1:m:37:PRO:HD3	1:m:56:ILE:HD12	2.01	0.42
1:m:284:GLU:OE1	1:m:286:ARG:NH1	2.46	0.42
7:P:224:LEU:HD12	7:P:224:LEU:H	1.84	0.42
4:g:21:VAL:O	4:g:25:ILE:HG13	2.20	0.42
9:l:289:ILE:HG22	9:l:294:ARG:HG3	2.02	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
3:f:229:ASP:O	3:f:233:ARG:HG3	2.20	0.42
7:j:204:ILE:HG12	7:j:211:VAL:HG13	2.02	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
9:H:123:ARG:N	9:H:159:MET:HE1	2.35	0.42
4:M:285:MET:HA	4:M:285:MET:HE2	2.01	0.42
9:b:289:ILE:HG22	9:b:294:ARG:HG3	2.02	0.42
4:g:61:ARG:HG2	4:g:74:ILE:O	2.19	0.42
6:i:189:ILE:HG23	6:i:201:PRO:HD2	2.00	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
4:W:353:PRO:C	4:W:355:GLY:H	2.27	0.42
1:c:143:VAL:HA	1:c:153:VAL:HG12	2.01	0.42
2:e:201:PHE:HE1	2:e:220:ILE:HG12	1.84	0.42
8:k:73:ILE:HG12	8:k:120:TYR:CD1	2.53	0.42
9:l:232:TRP:NE1	9:l:234:ARG:HB3	2.35	0.42
9:H:350:THR:O	9:H:354:MET:HG2	2.20	0.42
9:b:232:TRP:NE1	9:b:234:ARG:HB3	2.35	0.42
9:b:333:GLY:O	9:b:336:ILE:HG12	2.20	0.42
1:I:235:LEU:HD11	1:I:246:THR:HB	2.02	0.42
2:K:262:MET:HE2	2:K:262:MET:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:g:53:ALA:C	4:g:54:ILE:HD12	2.45	0.42
9:l:290:SER:H	9:l:293:ILE:HD12	1.85	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: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:HD2	9:R:93:ARG:HA	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
4:g:362:LEU:O	5:h:179:LEU:HA	2.20	0.41
5:h:106:LEU:HD13	5:h:160:VAL:HB	2.02	0.41
5:h:205:LEU:O	5:h:209:ILE:N	2.48	0.41
6:i:51:ILE:HG12	6:i:57:GLU:HG3	2.01	0.41
8:k:2:SER:HA	8:k:42:LEU:O	2.20	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
6:O:19:PRO:O	6:O:20:SER:C	2.63	0.41
4:W:18:PRO:HB2	4:W:21:VAL:HG23	2.01	0.41
9:b:310:CYS:HB2	9:b:312:ILE:HG12	2.02	0.41
2:e:125:ILE:HG22	2:e:126:VAL:HG13	2.02	0.41
3:f:98:LEU:O	3:f:102:THR:HG23	2.20	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:HD13	3:V:29:ILE:HA	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
7:Z:190:MET:HG2	1:c:13:PRO:O	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OE1	9:R:178:GLN:N	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
4:W:362:LEU:O	5:X:179:LEU:HA	2.21	0.41
5:X:138:ILE:HG12	5:X:145:ILE:HG12	2.01	0.41
2:e:126:VAL:HG22	2:e:130:LYS:HB2	2.02	0.41
8:k:60:SER:HA	8:k:161:ASN:OD1	2.21	0.41
3:B:13:ARG:HD3	3:B:171:LEU:HD13	2.01	0.41
5:D:7:ILE:HD13	5:D:7:ILE:HA	1.97	0.41
6:E:158:ILE:HD11	6:E:173:HIS:HA	2.01	0.41
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
3:f:15:ASP:OD2	3:f:17:ARG:NE	2.53	0.41
4:g:165:LEU:HD21	4:g:170:LEU:HD11	2.01	0.41
5:h:74:LEU:HD13	5:h:90:ILE:HD13	2.03	0.41
7:j:48:LEU:HD13	7:j:178:LEU:HD11	2.01	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
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
1:c:284:GLU:OE1	1:c:286:ARG:NH1	2.50	0.41
2:K:24:ARG:NH2	2:K:227:GLU:OE2	2.50	0.41
9:l:212:ASN:HD21	9:l:243:ARG:NH2	2.19	0.41
6:E:80:VAL:HG21	6:E:95:ILE:HG22	2.02	0.41
1:I:134:LYS:HD2	1:I:134:LYS:HA	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
8:a:162:PHE:HZ	8:a:174:LEU:HD22	1.85	0.41
2:e:179:VAL:HG23	2:e:184:PRO:HD3	2.03	0.41
4:g:299:ILE:HG13	4:g:330:LEU:HD12	2.01	0.41
1:m:10:ILE:HG13	1:m:11:ALA:H	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
8:a:2:SER:HA	8:a:42:LEU:O	2.21	0.41
8:a:155:ILE:HD11	8:a:193:LYS:HB3	2.03	0.41
9:b:307:LEU:HD21	9:b:348:ILE:HD12	2.03	0.41
4:g:50:ARG:HD3	4:g:333:ASP:OD2	2.21	0.41
4:g:302:LEU:HD21	4:g:329:VAL:HG13	2.03	0.41
5:h:134:ILE:HG12	5:h:202:CYS:SG	2.60	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:278:GLN:HG2	7:Z:20:PHE:HB3	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
1:m:275:MET:HG3	1:m:288:CYS:SG	2.61	0.40
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
8:a:167:LEU:HD13	8:a:188:ILE:HB	2.02	0.40
4:g:124:ILE:HD11	4:g:160:LEU:HG	2.03	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
3:L:86:ARG:HH12	6:O:127:ASP:CG	2.29	0.40
6:O:18:THR:HB	6:O:19:PRO:HD3	2.03	0.40
7:j:68:GLY:O	7:j:147:LEU:N	2.54	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
3:f:29:ILE:HD13	3:f:29:ILE:HA	1.95	0.40
9:H:309:PHE:HE2	9:H:342:GLU:HG3	1.86	0.40
3:L:25:PHE:CE2	3:L:42:MET:HE1	2.57	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
4:g:360:LEU:HB3	5:h:182:SER:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:h:30:VAL:HA	5:h:89:GLN:O	2.22	0.40
6:i:80:VAL:HG21	6:i:95:ILE:HG22	2.03	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%)	21	56
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%)	36	68
2	K	293/305 (96%)	280 (96%)	13 (4%)	0	100	100
2	U	293/305 (96%)	279 (95%)	13 (4%)	1 (0%)	36	68
2	e	293/305 (96%)	278 (95%)	14 (5%)	1 (0%)	36	68
3	B	240/249 (96%)	225 (94%)	15 (6%)	0	100	100
3	L	234/249 (94%)	226 (97%)	7 (3%)	1 (0%)	30	62
3	V	239/249 (96%)	227 (95%)	10 (4%)	2 (1%)	16	50
3	f	234/249 (94%)	223 (95%)	10 (4%)	1 (0%)	30	62
4	C	301/394 (76%)	288 (96%)	12 (4%)	1 (0%)	36	68
4	M	298/394 (76%)	285 (96%)	12 (4%)	1 (0%)	36	68
4	W	309/394 (78%)	292 (94%)	13 (4%)	4 (1%)	9	40
4	g	306/394 (78%)	294 (96%)	11 (4%)	1 (0%)	36	68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	D	219/226 (97%)	212 (97%)	6 (3%)	1 (0%)	24	59
5	N	220/226 (97%)	213 (97%)	6 (3%)	1 (0%)	24	59
5	X	221/226 (98%)	215 (97%)	5 (2%)	1 (0%)	24	59
5	h	221/226 (98%)	215 (97%)	5 (2%)	1 (0%)	24	59
6	E	253/268 (94%)	244 (96%)	8 (3%)	1 (0%)	30	62
6	O	256/268 (96%)	246 (96%)	10 (4%)	0	100	100
6	Y	259/268 (97%)	250 (96%)	8 (3%)	1 (0%)	30	62
6	i	257/268 (96%)	247 (96%)	9 (4%)	1 (0%)	30	62
7	F	201/250 (80%)	194 (96%)	7 (4%)	0	100	100
7	P	202/250 (81%)	195 (96%)	6 (3%)	1 (0%)	24	59
7	Z	202/250 (81%)	194 (96%)	7 (4%)	1 (0%)	24	59
7	j	200/250 (80%)	193 (96%)	6 (3%)	1 (0%)	24	59
8	G	225/244 (92%)	218 (97%)	6 (3%)	1 (0%)	30	62
8	Q	199/244 (82%)	192 (96%)	6 (3%)	1 (0%)	24	59
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%)	11	43
9	R	259/316 (82%)	251 (97%)	7 (3%)	1 (0%)	30	62
9	b	256/316 (81%)	244 (95%)	10 (4%)	2 (1%)	16	50
9	l	262/316 (83%)	253 (97%)	8 (3%)	1 (0%)	30	62
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%)	30	62

All (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

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Mol	Chain	Res	Type
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	243 (100%)	0	100	100
2	K	243/266 (91%)	243 (100%)	0	100	100
2	U	243/266 (91%)	243 (100%)	0	100	100
2	e	244/266 (92%)	244 (100%)	0	100	100
3	B	194/220 (88%)	194 (100%)	0	100	100
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%)	199 (100%)	0	100	100
4	C	244/349 (70%)	244 (100%)	0	100	100
4	M	235/349 (67%)	235 (100%)	0	100	100
4	W	255/349 (73%)	255 (100%)	0	100	100
4	g	247/349 (71%)	247 (100%)	0	100	100
5	D	182/198 (92%)	182 (100%)	0	100	100
5	N	187/198 (94%)	187 (100%)	0	100	100
5	X	196/198 (99%)	196 (100%)	0	100	100
5	h	195/198 (98%)	195 (100%)	0	100	100
6	E	208/242 (86%)	208 (100%)	0	100	100
6	O	215/242 (89%)	215 (100%)	0	100	100
6	Y	224/242 (93%)	224 (100%)	0	100	100
6	i	225/242 (93%)	225 (100%)	0	100	100
7	F	155/219 (71%)	155 (100%)	0	100	100
7	P	150/219 (68%)	150 (100%)	0	100	100
7	Z	156/219 (71%)	156 (100%)	0	100	100
7	j	153/219 (70%)	153 (100%)	0	100	100
8	G	168/212 (79%)	168 (100%)	0	100	100
8	Q	162/212 (76%)	162 (100%)	0	100	100
8	a	191/212 (90%)	191 (100%)	0	100	100
8	k	151/212 (71%)	151 (100%)	0	100	100
9	H	212/270 (78%)	212 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	R	218/270 (81%)	218 (100%)	0	100	100
9	b	213/270 (79%)	213 (100%)	0	100	100
9	l	211/270 (78%)	211 (100%)	0	100	100
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%)	7146 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	m	126	ASN
1	m	152	ASN
1	m	242	ASN
1	m	273	GLN
4	C	57	ASN
4	C	78	ASN
4	C	239	GLN
5	D	214	GLN
6	E	150	ASN
7	F	96	GLN
7	F	106	ASN
7	F	233	GLN
9	H	133	HIS
9	H	316	GLN
1	I	242	ASN
2	K	66	GLN
4	M	239	GLN
5	N	214	GLN
6	O	30	GLN
6	O	45	ASN
6	O	150	ASN
7	P	49	HIS
7	P	99	ASN
7	P	233	GLN
8	Q	230	GLN

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Mol	Chain	Res	Type
9	R	295	GLN
9	R	316	GLN
1	S	126	ASN
1	S	152	ASN
1	S	242	ASN
5	X	45	GLN
5	X	89	GLN
5	X	214	GLN
7	Z	106	ASN
8	a	53	GLN
8	a	230	GLN
9	b	316	GLN
1	c	126	ASN
1	c	242	ASN
2	e	266	HIS
4	g	327	ASN
5	h	183	ASN
5	h	214	GLN
6	i	30	GLN
6	i	77	GLN
6	i	115	GLN
6	i	150	ASN
6	i	219	ASN
7	j	171	HIS
8	k	159	ASN
9	l	133	HIS
9	l	212	ASN
9	l	316	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 9 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	TAM	A	401	-	10,10,10	0.92	0	12,12,12	1.31	2 (16%)
11	TAM	K	401	-	10,10,10	0.92	0	12,12,12	1.30	2 (16%)
11	TAM	e	401	-	10,10,10	0.91	0	12,12,12	1.30	2 (16%)
11	TAM	U	401	-	10,10,10	0.91	0	12,12,12	1.30	2 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	TAM	A	401	-	-	6/12/12/12	-
11	TAM	K	401	-	-	4/12/12/12	-
11	TAM	e	401	-	-	3/12/12/12	-
11	TAM	U	401	-	-	4/12/12/12	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	401	TAM	C4-C1-C	-2.21	113.36	115.97
11	U	401	TAM	C4-C1-C	-2.12	113.47	115.97
11	e	401	TAM	O5-C5-C2	-2.08	105.50	111.33
11	e	401	TAM	C4-C1-C	-2.07	113.52	115.97
11	K	401	TAM	O5-C5-C2	-2.07	105.53	111.33
11	K	401	TAM	C4-C1-C	-2.07	113.53	115.97
11	U	401	TAM	O5-C5-C2	-2.07	105.54	111.33
11	A	401	TAM	O5-C5-C2	-2.04	105.61	111.33

There are no chirality outliers.

All (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
11	K	401	TAM	C3-C-C2-C5
11	K	401	TAM	N-C-C2-C5
11	U	401	TAM	C-C2-C5-O5
11	e	401	TAM	C3-C-C2-C5
11	U	401	TAM	C-C1-C4-O4
11	A	401	TAM	C2-C-C3-C6
11	K	401	TAM	C1-C-C2-C5
11	K	401	TAM	C-C3-C6-O6
11	e	401	TAM	C1-C-C2-C5
11	e	401	TAM	N-C-C2-C5
11	U	401	TAM	C2-C-C1-C4
11	U	401	TAM	C3-C-C1-C4

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	K	401	TAM	3	0
11	e	401	TAM	1	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%)	0.75	14 (7%) 18 12	100, 161, 215, 252	0
1	S	208/295 (70%)	0.78	19 (9%) 15 9	111, 190, 246, 272	0
1	c	197/295 (66%)	0.90	22 (11%) 10 7	125, 167, 214, 246	0
1	m	190/295 (64%)	0.42	6 (3%) 50 31	110, 153, 199, 232	0
2	A	295/305 (96%)	-0.25	2 (0%) 84 69	51, 71, 133, 178	0
2	K	295/305 (96%)	-0.20	1 (0%) 90 81	48, 78, 137, 219	0
2	U	295/305 (96%)	-0.08	10 (3%) 48 30	50, 74, 144, 218	0
2	e	295/305 (96%)	-0.22	2 (0%) 84 69	56, 76, 140, 200	0
3	B	242/249 (97%)	-0.32	5 (2%) 63 43	45, 66, 120, 174	0
3	L	238/249 (95%)	-0.29	1 (0%) 88 79	37, 57, 101, 133	0
3	V	241/249 (96%)	-0.32	1 (0%) 88 79	41, 61, 107, 154	0
3	f	237/249 (95%)	-0.21	2 (0%) 82 67	41, 68, 115, 160	1 (0%)
4	C	313/394 (79%)	-0.02	9 (2%) 53 35	57, 85, 147, 224	0
4	M	310/394 (78%)	0.00	10 (3%) 50 31	55, 84, 141, 208	0
4	W	319/394 (80%)	-0.08	6 (1%) 66 46	50, 79, 140, 208	0
4	g	317/394 (80%)	-0.00	10 (3%) 50 31	40, 85, 135, 207	1 (0%)
5	D	221/226 (97%)	-0.36	5 (2%) 61 41	47, 69, 104, 126	0
5	N	222/226 (98%)	-0.29	1 (0%) 87 76	50, 85, 123, 173	0
5	X	223/226 (98%)	-0.35	4 (1%) 67 48	46, 75, 111, 164	0
5	h	223/226 (98%)	-0.30	2 (0%) 81 64	59, 78, 111, 132	0
6	E	257/268 (95%)	-0.13	6 (2%) 61 41	56, 83, 134, 157	0
6	O	260/268 (97%)	-0.26	2 (0%) 82 67	49, 77, 125, 171	0
6	Y	263/268 (98%)	-0.29	3 (1%) 78 61	43, 72, 123, 149	0
6	i	261/268 (97%)	-0.25	2 (0%) 82 67	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%)	-0.04	4 (1%) 66 46	58, 90, 137, 166	0
7	P	208/250 (83%)	0.14	9 (4%) 40 24	62, 94, 133, 159	0
7	Z	208/250 (83%)	-0.02	10 (4%) 35 22	61, 89, 133, 156	0
7	j	206/250 (82%)	-0.13	5 (2%) 59 40	61, 89, 136, 160	0
8	G	231/244 (94%)	0.00	8 (3%) 47 29	58, 91, 150, 217	0
8	Q	207/244 (84%)	0.36	9 (4%) 40 24	89, 142, 185, 264	0
8	a	227/244 (93%)	0.33	13 (5%) 29 19	90, 137, 211, 267	0
8	k	226/244 (92%)	0.64	29 (12%) 7 6	87, 118, 178, 226	0
9	H	267/316 (84%)	-0.10	6 (2%) 62 42	42, 85, 128, 189	0
9	R	265/316 (83%)	-0.28	5 (1%) 66 46	40, 71, 114, 158	0
9	b	262/316 (82%)	-0.26	2 (0%) 82 67	49, 82, 135, 160	0
9	l	268/316 (84%)	0.01	9 (3%) 48 30	59, 93, 144, 196	0
10	J	20/190 (10%)	0.90	1 (5%) 34 22	88, 118, 157, 157	0
10	T	7/190 (3%)	0.59	0 100 100	131, 137, 142, 163	0
10	d	7/190 (3%)	0.66	1 (14%) 6 5	110, 131, 137, 140	0
10	n	10/190 (5%)	0.91	2 (20%) 3 2	110, 124, 167, 178	0
All	All	8926/10948 (81%)	-0.04	258 (2%) 53 35	37, 85, 174, 272	2 (0%)

All (258) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	293	TYR	6.0
9	l	156	GLU	5.8
4	g	393	ASN	5.7
8	a	112	THR	5.6
6	E	105	SER	5.0
7	F	21	SER	5.0
5	X	223	VAL	5.0
8	k	195	TRP	4.8
1	I	148	LEU	4.8
1	c	278	PRO	4.7
8	k	118	LEU	4.6
8	G	46	ALA	4.5
4	M	393	ASN	4.4
1	I	69	GLU	4.4
6	Y	163	ASP	4.4

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Mol	Chain	Res	Type	RSRZ
3	B	91	HIS	4.2
7	Z	44	GLN	4.1
8	k	196	VAL	4.0
4	W	304	PRO	4.0
4	g	37	LEU	4.0
1	c	109	SER	3.9
1	m	148	LEU	3.9
9	l	245	THR	3.9
8	G	109	ASN	3.9
1	c	113	GLY	3.8
4	C	100	SER	3.8
1	S	278	PRO	3.8
3	B	90	SER	3.8
9	l	155	ASP	3.8
1	I	151	ALA	3.7
7	Z	108	ASN	3.7
9	R	278	TRP	3.7
7	j	100	GLY	3.6
8	k	154	MET	3.6
1	S	148	LEU	3.6
8	a	44	VAL	3.6
7	P	43	GLU	3.6
7	Z	43	GLU	3.6
7	P	101	LEU	3.6
8	G	14	ASP	3.5
1	c	129	ALA	3.5
2	U	210	ILE	3.4
8	k	131	GLU	3.4
8	k	74	GLY	3.4
8	k	146	GLY	3.4
5	X	1	MET	3.4
3	B	64	GLN	3.4
8	k	14	ASP	3.4
4	W	253	SER	3.3
8	k	110	ARG	3.3
8	Q	199	GLU	3.3
4	C	355	GLY	3.3
6	E	0	HIS	3.3
8	a	151	GLU	3.3
7	Z	102	LEU	3.3
4	C	393	ASN	3.3
2	U	181	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
7	P	100	GLY	3.3
6	Y	166	VAL	3.2
8	k	148	GLY	3.2
2	A	174	ILE	3.2
1	S	113	GLY	3.2
4	W	272	TYR	3.2
6	E	1	MET	3.2
7	Z	106	ASN	3.2
3	f	83	LYS	3.1
7	j	102	LEU	3.1
2	U	147	PHE	3.1
8	Q	84	TYR	3.1
10	n	117	ASP	3.1
8	k	149	ILE	3.1
9	R	66	ILE	3.1
4	C	191	ASP	3.1
4	M	272	TYR	3.1
8	k	16	THR	3.0
2	U	207	GLU	3.0
9	l	244	ASP	3.0
8	k	102	PHE	3.0
3	B	3	ARG	3.0
8	k	150	LEU	3.0
9	R	155	ASP	3.0
4	W	394	ILE	3.0
8	a	118	LEU	3.0
1	c	243	TYR	2.9
3	L	87	SER	2.9
5	X	222	VAL	2.9
4	g	101	ALA	2.9
4	g	250	GLU	2.9
5	N	222	VAL	2.9
3	B	89	SER	2.9
1	c	112	PRO	2.8
8	a	139	SER	2.8
1	m	129	ALA	2.8
1	S	245	LEU	2.8
7	F	149	ASN	2.8
8	k	203	ASN	2.8
4	C	272	TYR	2.8
7	Z	21	SER	2.8
2	U	206	THR	2.8

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Mol	Chain	Res	Type	RSRZ
4	M	255	LEU	2.8
7	F	219	ASP	2.8
8	k	108	LYS	2.8
1	S	281	GLY	2.7
8	a	107	LYS	2.7
8	a	187	ALA	2.7
4	C	255	LEU	2.7
8	a	108	LYS	2.7
1	m	278	PRO	2.7
9	l	154	SER	2.7
8	k	187	ALA	2.7
1	c	282	ALA	2.7
1	c	148	LEU	2.7
7	j	101	LEU	2.7
1	S	205	ILE	2.6
1	c	279	VAL	2.6
8	Q	98	SER	2.6
1	c	162	PRO	2.6
9	H	91	VAL	2.6
6	E	111	SER	2.6
1	I	278	PRO	2.6
1	S	162	PRO	2.6
2	U	296	MET	2.6
9	H	96	SER	2.6
6	O	110	ASP	2.6
4	g	38	GLY	2.6
5	D	142	THR	2.6
2	K	174	ILE	2.6
2	e	174	ILE	2.6
8	Q	234	ILE	2.6
8	G	45	SER	2.6
9	R	145	GLY	2.6
7	P	149	ASN	2.6
9	l	92	ASN	2.6
9	l	53	GLN	2.5
8	Q	137	PHE	2.5
1	c	245	LEU	2.5
8	G	104	ASN	2.5
1	I	266	LEU	2.5
8	k	198	CYS	2.5
10	d	111	GLY	2.5
9	R	77	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
9	l	66	ILE	2.5
1	I	19	PRO	2.5
4	M	19	PRO	2.5
8	a	111	PRO	2.5
1	I	192	GLN	2.5
3	f	64	GLN	2.5
8	a	53	GLN	2.5
4	g	36	SER	2.5
6	O	105	SER	2.5
6	E	73	ASN	2.5
7	P	103	GLU	2.4
1	S	201	PHE	2.4
1	c	268	TYR	2.4
1	c	205	ILE	2.4
8	a	1	MET	2.4
4	C	354	SER	2.4
1	m	216	ASP	2.4
7	P	219	ASP	2.4
7	F	44	GLN	2.4
8	a	195	TRP	2.4
5	D	141	ASP	2.4
8	k	117	ASP	2.4
1	c	229	ILE	2.4
5	D	4	GLN	2.4
6	i	105	SER	2.4
9	H	66	ILE	2.4
2	e	3	LYS	2.4
6	i	168	GLU	2.4
4	g	306	CYS	2.4
1	I	44	ILE	2.3
4	g	180	ASN	2.3
6	E	157	LEU	2.3
4	M	301	GLU	2.3
5	X	111	CYS	2.3
7	j	9	LEU	2.3
8	Q	147	PHE	2.3
8	G	144	ASP	2.3
9	b	157	LEU	2.3
1	S	220	VAL	2.3
7	j	43	GLU	2.3
7	P	183	ALA	2.3
3	V	242	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
4	M	327	ASN	2.3
1	S	233	GLN	2.3
8	G	108	LYS	2.3
5	D	144	ASP	2.3
8	Q	82	ASP	2.3
1	S	246	THR	2.2
8	k	119	VAL	2.2
1	I	112	PRO	2.2
9	H	95	LEU	2.2
4	g	184	THR	2.2
1	c	255	VAL	2.2
4	M	67	ASN	2.2
4	C	43	LEU	2.2
1	I	187	THR	2.2
4	g	39	ILE	2.2
8	k	76	ILE	2.2
1	I	131	ASN	2.2
8	k	218	ASN	2.2
9	l	105	ALA	2.2
8	k	13	VAL	2.2
1	I	106	ILE	2.2
7	Z	163	SER	2.2
8	k	45	SER	2.2
9	H	277	SER	2.2
4	C	41	PRO	2.2
8	Q	136	CYS	2.2
7	Z	69	HIS	2.2
4	W	252	ALA	2.1
1	c	291	PRO	2.1
1	c	3	CYS	2.1
8	Q	14	ASP	2.1
9	H	77	ASP	2.1
1	m	234	VAL	2.1
7	Z	188	VAL	2.1
1	S	10	ILE	2.1
4	M	273	GLU	2.1
4	M	355	GLY	2.1
2	U	95	ASN	2.1
1	S	214	ASP	2.1
6	Y	162	ASP	2.1
10	J	97	VAL	2.1
1	S	21	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	S	266	LEU	2.1
8	a	150	LEU	2.1
8	k	47	LYS	2.1
1	S	291	PRO	2.1
2	U	172	GLU	2.1
2	U	209	ASN	2.1
4	W	67	ASN	2.1
1	S	279	VAL	2.1
5	h	222	VAL	2.1
1	S	221	ILE	2.1
7	P	5	ASP	2.1
8	k	194	ILE	2.1
7	Z	107	THR	2.1
1	c	257	ALA	2.1
4	M	185	PHE	2.1
1	I	17	ILE	2.1
1	c	244	TYR	2.1
7	P	107	THR	2.1
8	k	17	THR	2.1
8	k	136	CYS	2.1
9	b	158	GLN	2.1
5	D	222	VAL	2.0
8	k	197	LYS	2.0
5	h	2	SER	2.0
10	n	109	ILE	2.0
1	S	272	TRP	2.0
1	I	113	GLY	2.0
1	c	262	GLY	2.0
1	m	8	PRO	2.0
1	c	17	ILE	2.0
8	G	1	MET	2.0
1	c	186	ALA	2.0
2	U	171	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 oligosaccharides 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
11	TAM	A	401	11/11	0.70	0.18	85,96,101,103	0
11	TAM	e	401	11/11	0.72	0.15	75,89,96,99	0
11	TAM	K	401	11/11	0.75	0.20	69,86,103,111	0
11	TAM	U	401	11/11	0.78	0.20	79,98,112,119	0
12	CL	R	401	1/1	0.80	0.22	95,95,95,95	0
13	MG	g	401	1/1	0.87	0.23	60,60,60,60	0
12	CL	G	301	1/1	0.88	0.11	99,99,99,99	0
12	CL	l	401	1/1	0.90	0.09	75,75,75,75	0
12	CL	f	301	1/1	0.91	0.27	79,79,79,79	0
12	CL	H	401	1/1	0.94	0.10	80,80,80,80	0
12	CL	R	402	1/1	0.94	0.08	73,73,73,73	0
13	MG	O	301	1/1	0.94	0.10	85,85,85,85	0
12	CL	b	401	1/1	0.94	0.11	86,86,86,86	0

6.5 Other polymers [i](#)

There are no such residues in this entry.