



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 07:22 am BST

PDB ID : 5OKZ
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

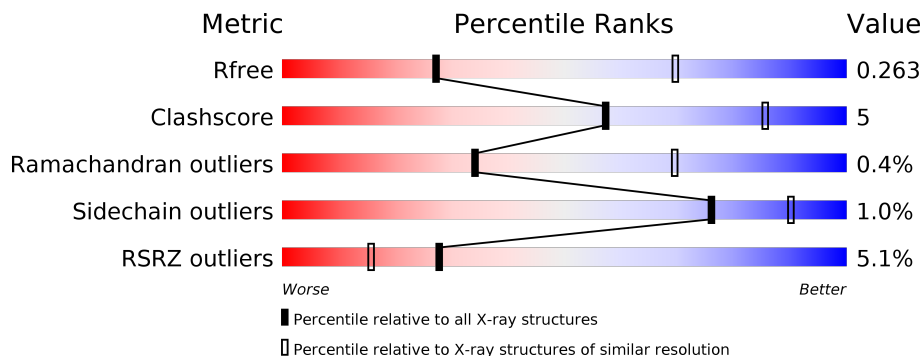
1 Overall quality at a glance

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.




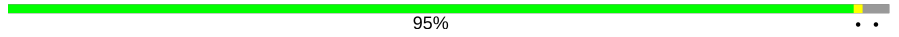

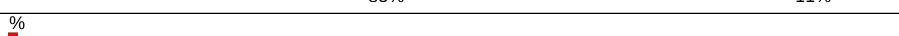
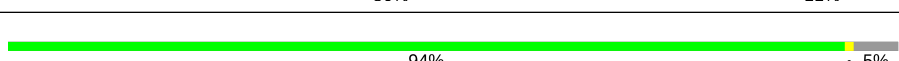


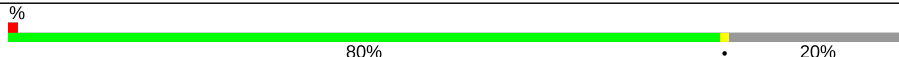
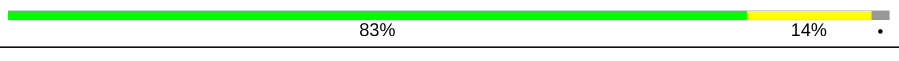
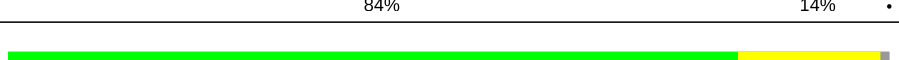
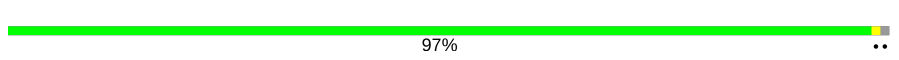

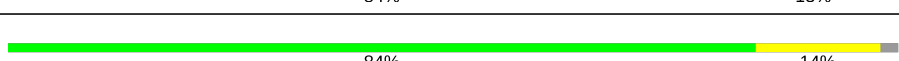
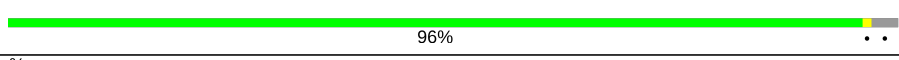

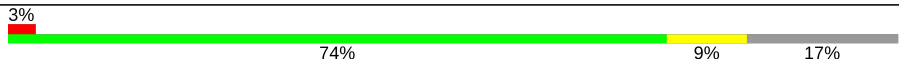
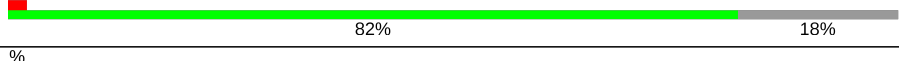

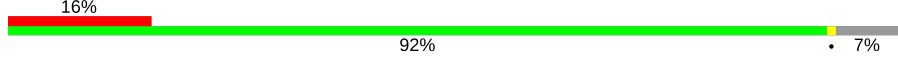



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	
1	S	295	
1	c	295	
1	m	295	
2	A	305	
2	K	305	

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Mol	Chain	Length	Quality of chain
2	U	305	 2% 85% 11%
2	e	305	 95%
3	B	249	 2% 84% 14%
3	L	249	 85% 11%
3	V	249	 1% 86% 11%
3	f	249	 94% 5%
4	C	394	 1% 70% 10% 21%
4	M	394	 69% 10% 21%
4	W	394	 1% 69% 11% 19%
4	g	394	 1% 80% 20%
5	D	226	 83% 14%
5	N	226	 84% 14%
5	X	226	 82% 16%
5	h	226	 97%
6	E	268	 1% 78% 18%
6	O	268	 84% 13%
6	Y	268	 84% 14%
6	i	268	 96%
7	F	250	 1% 74% 9% 17%
7	P	250	 1% 73% 10% 17%
7	Z	250	 3% 74% 9% 17%
7	j	250	 2% 82% 18%
8	G	244	1% 84% 11% 5%
8	Q	244	4% 71% 13% 15%
8	a	244	16% 92% 7%

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Mol	Chain	Length	Quality of chain
8	k	244	
9	H	316	
9	R	316	
9	b	316	
9	l	316	
10	J	190	
10	T	190	
10	d	190	
10	n	190	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CL	R	401	-	-	-	X

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 67168 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Exosome complex component CSL4.

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

There are 12 discrepancies between the modelled and reference sequences:

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

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

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

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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
			Total	C	N	O	S			
4	g	317	2376	1508	417	441	10	0	1	0

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

There are 12 discrepancies between the modelled and reference sequences:

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

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

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

There are 16 discrepancies between the modelled and reference sequences:

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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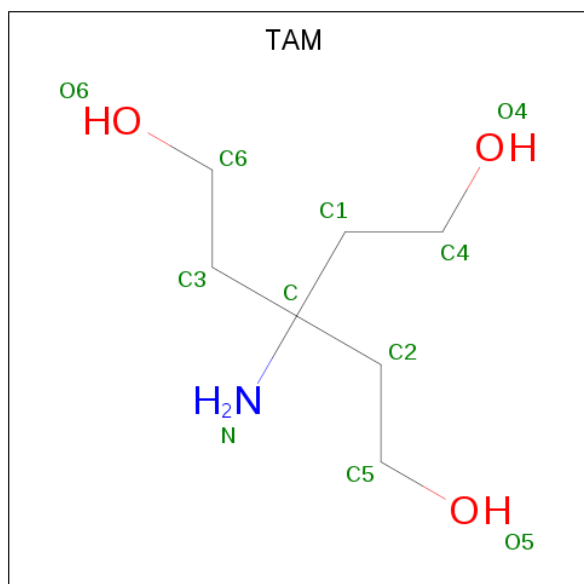
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	d	7	Total	C	N	O	0	0	0
			46	27	10	9			
10	n	10	Total	C	N	O	0	0	0
			70	44	14	12			

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 (three-letter code: TAM) (formula: C₇H₁₇NO₃).



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

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

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

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

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

- Molecule 14 is water.

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

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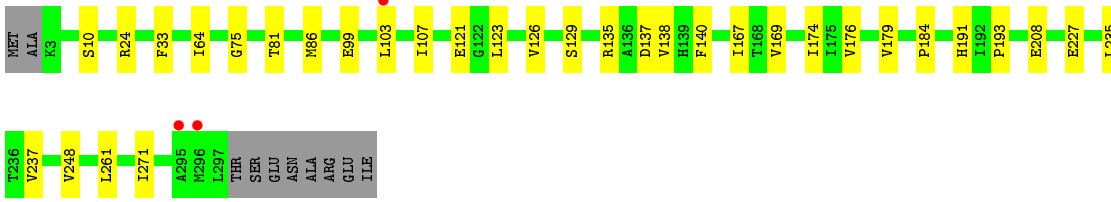
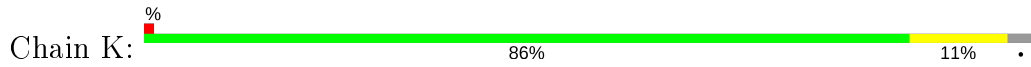
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	D	7	Total O 7 7	0	0
14	E	2	Total O 2 2	0	0
14	G	3	Total O 3 3	0	0
14	H	3	Total O 3 3	0	0
14	L	2	Total O 2 2	0	0
14	N	2	Total O 2 2	0	0
14	O	7	Total O 7 7	0	0
14	P	2	Total O 2 2	0	0
14	R	3	Total O 3 3	0	0
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

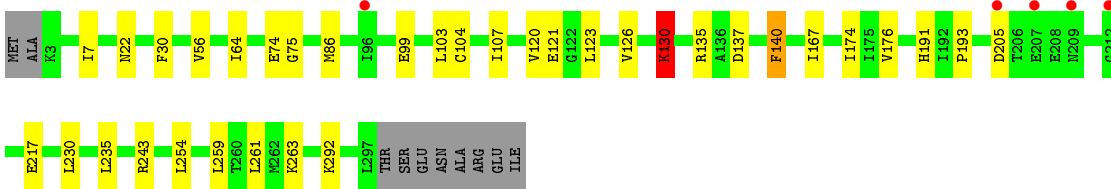
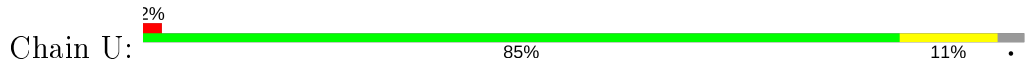
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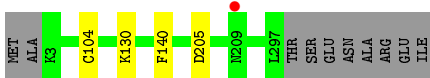
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	j	1	Total O 1 1	0	0
14	l	8	Total O 8 8	0	0



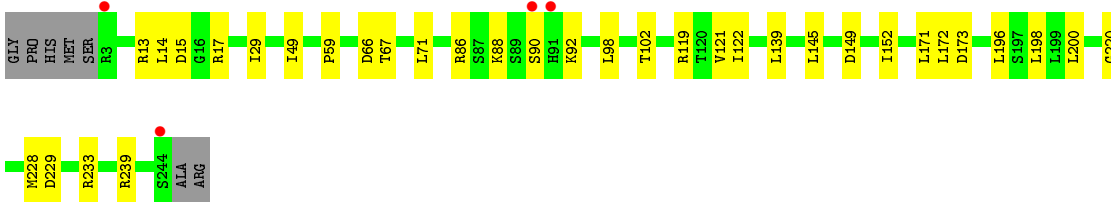
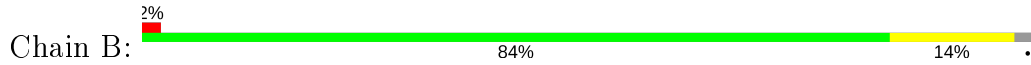
- Molecule 2: Exosome complex component RRP45



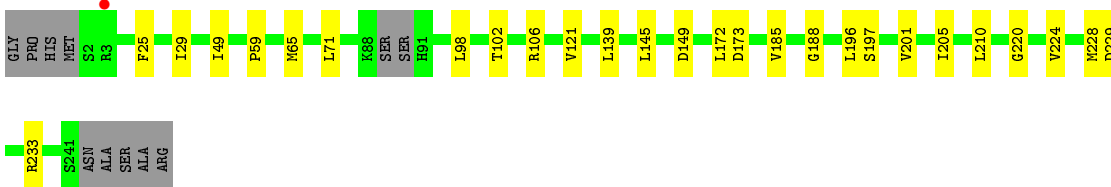
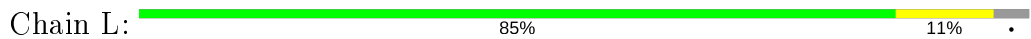
- Molecule 2: Exosome complex component RRP45



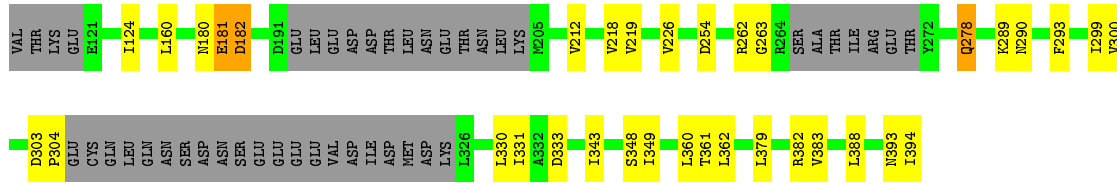
- Molecule 3: Exosome complex component SKI6



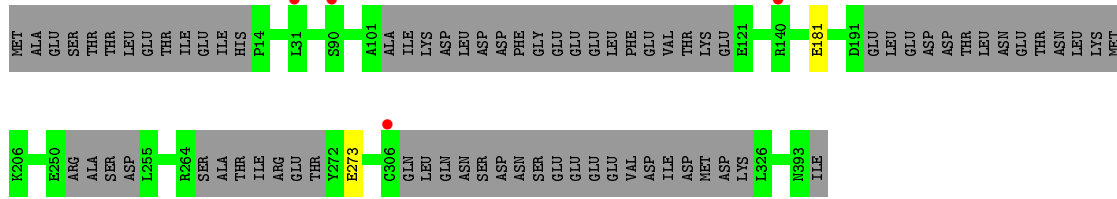
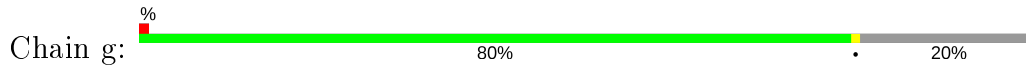
- Molecule 3: Exosome complex component SKI6



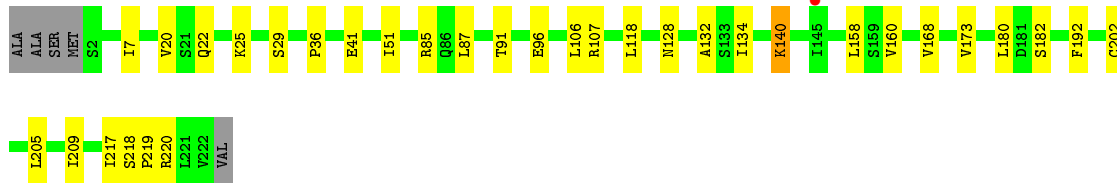
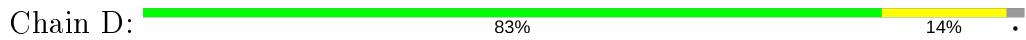
- Molecule 3: Exosome complex component SKI6



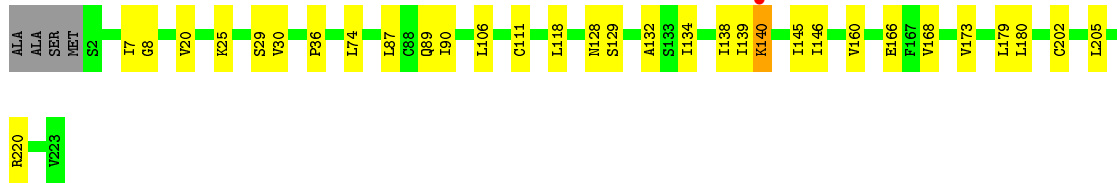
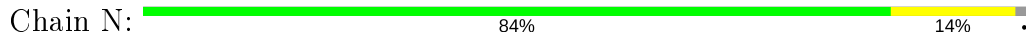
• Molecule 4: Exosome complex component RRP43



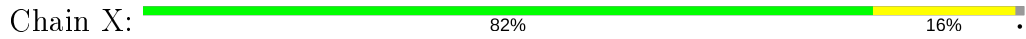
• Molecule 5: Exosome complex component RRP46



• Molecule 5: Exosome complex component RRP46

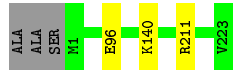


• Molecule 5: Exosome complex component RRP46




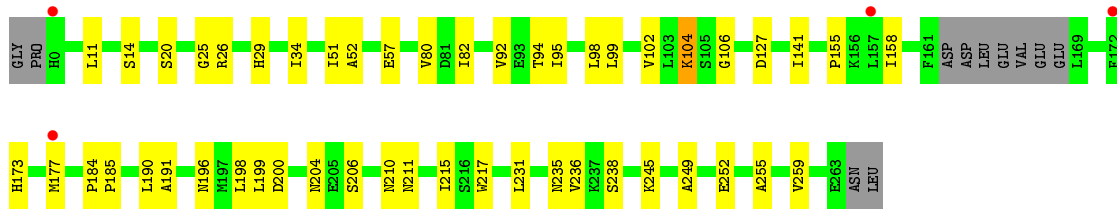
• Molecule 5: Exosome complex component RRP46

Chain h:  97%




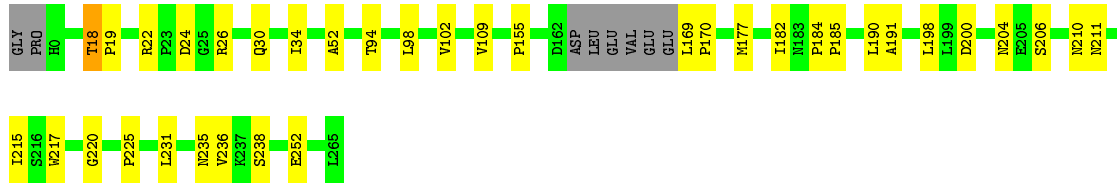
• Molecule 6: Exosome complex component RRP42

Chain E:  78%




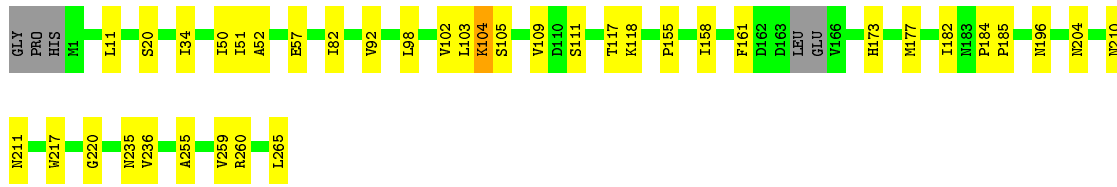
• Molecule 6: Exosome complex component RRP42

Chain O:  84%



• Molecule 6: Exosome complex component RRP42

Chain Y:  84%




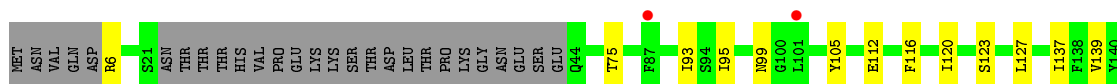
• Molecule 6: Exosome complex component RRP42

Chain i:  96%



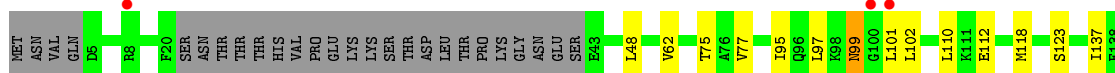
• Molecule 7: Exosome complex component MTR3

Chain F:  74%

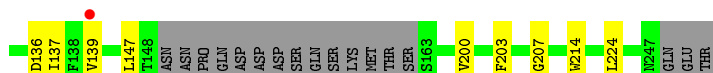
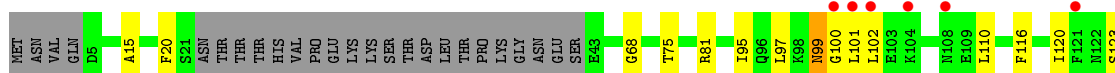
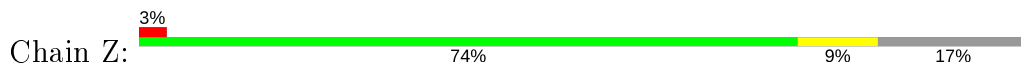




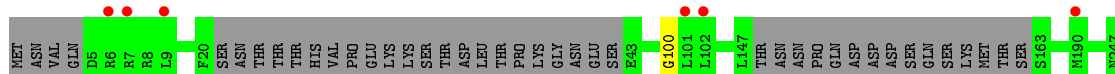
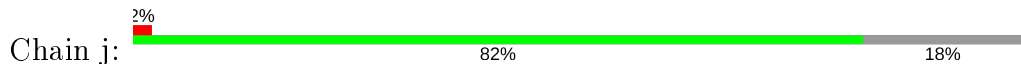
• Molecule 7: Exosome complex component MTR3



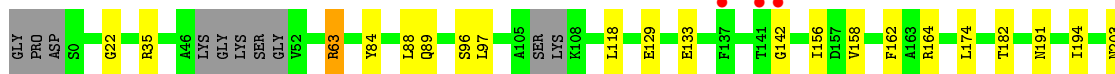
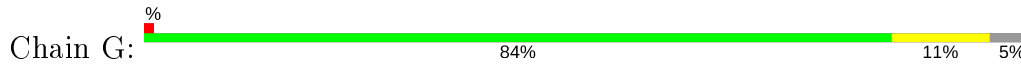
• Molecule 7: Exosome complex component MTR3



• Molecule 7: Exosome complex component MTR3

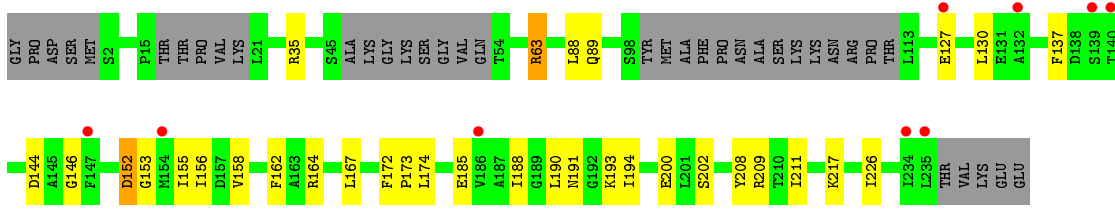


• Molecule 8: Exosome complex component RRP40

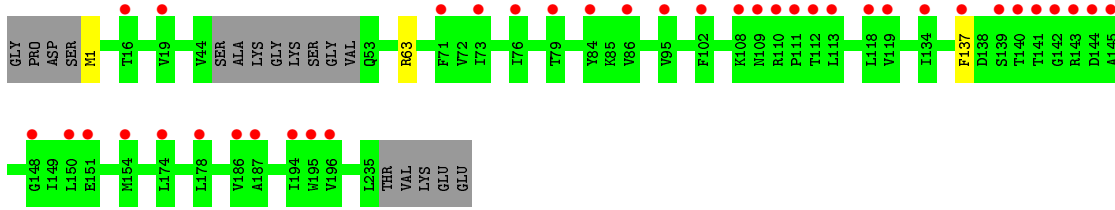
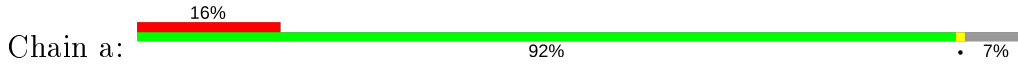


• Molecule 8: Exosome complex component RRP40

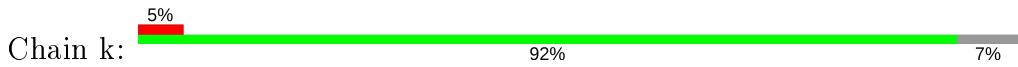




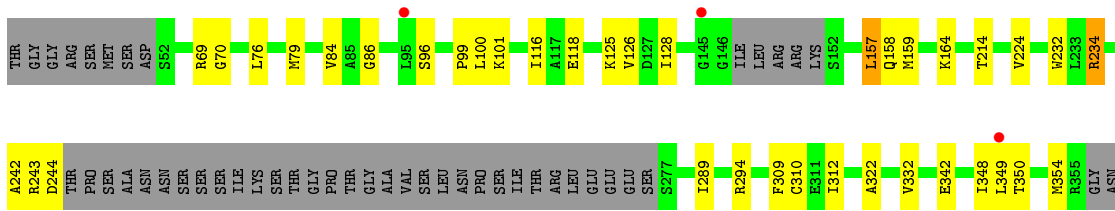
• Molecule 8: Exosome complex component RRP40



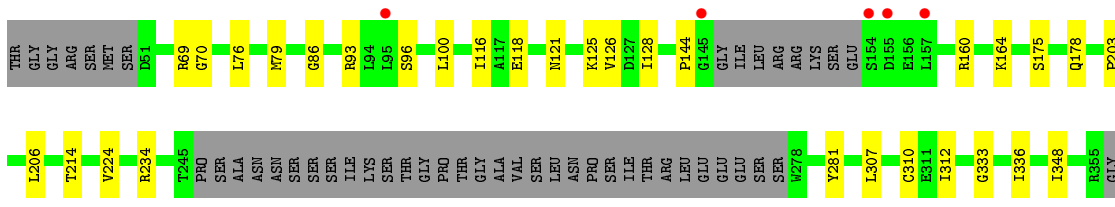
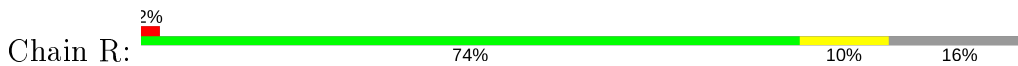
• Molecule 8: Exosome complex component RRP40



• Molecule 9: Exosome complex component RRP4



• Molecule 9: Exosome complex component RRP4



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 – 3.20 151.66 – 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 3.19Å)	Xtrriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.223 , 0.262 0.226 , 0.263	Depositor DCC
R_{free} test set	11386 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	72.8	Xtrriage
Anisotropy	0.351	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 53.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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: 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: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
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
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
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
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
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
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
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
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
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:61:ARG:HB3	4:C:72:ASN:HB3	2.03	0.41
4:C:29:LEU:HD12	1:I:256:PHE:CZ	2.56	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
9:H:242:ALA:C	9:H:244:ASP:H	2.24	0.41
7:F:187:LEU:O	1:I:13:PRO:HB3	2.21	0.41
6:O:217:TRP:CZ2	6:O:220:GLY:HA2	2.56	0.41
6:O:98:LEU:O	6:O:102:VAL:HG23	2.20	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
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:E:25:GLY:HA3	9:H:332:VAL:HB	2.03	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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	166/295 (56%)	162 (98%)	3 (2%)	1 (1%)	25	64
1	S	198/295 (67%)	193 (98%)	5 (2%)	0	100	100
1	c	187/295 (63%)	183 (98%)	4 (2%)	0	100	100
1	m	180/295 (61%)	176 (98%)	4 (2%)	0	100	100
2	A	293/305 (96%)	279 (95%)	13 (4%)	1 (0%)	41	74
2	K	293/305 (96%)	280 (96%)	13 (4%)	0	100	100
2	U	293/305 (96%)	279 (95%)	13 (4%)	1 (0%)	41	74
2	e	293/305 (96%)	278 (95%)	14 (5%)	1 (0%)	41	74
3	B	240/249 (96%)	225 (94%)	15 (6%)	0	100	100
3	L	234/249 (94%)	226 (97%)	7 (3%)	1 (0%)	34	69
3	V	239/249 (96%)	227 (95%)	10 (4%)	2 (1%)	19	58
3	f	234/249 (94%)	223 (95%)	10 (4%)	1 (0%)	34	69
4	C	301/394 (76%)	288 (96%)	12 (4%)	1 (0%)	41	74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	M	298/394 (76%)	285 (96%)	12 (4%)	1 (0%)	41	74
4	W	309/394 (78%)	292 (94%)	13 (4%)	4 (1%)	12	47
4	g	306/394 (78%)	294 (96%)	11 (4%)	1 (0%)	41	74
5	D	219/226 (97%)	212 (97%)	6 (3%)	1 (0%)	29	67
5	N	220/226 (97%)	213 (97%)	6 (3%)	1 (0%)	29	67
5	X	221/226 (98%)	215 (97%)	5 (2%)	1 (0%)	29	67
5	h	221/226 (98%)	215 (97%)	5 (2%)	1 (0%)	29	67
6	E	253/268 (94%)	244 (96%)	8 (3%)	1 (0%)	34	69
6	O	256/268 (96%)	246 (96%)	10 (4%)	0	100	100
6	Y	259/268 (97%)	250 (96%)	8 (3%)	1 (0%)	34	69
6	i	257/268 (96%)	247 (96%)	9 (4%)	1 (0%)	34	69
7	F	201/250 (80%)	194 (96%)	7 (4%)	0	100	100
7	P	202/250 (81%)	195 (96%)	6 (3%)	1 (0%)	29	67
7	Z	202/250 (81%)	194 (96%)	7 (4%)	1 (0%)	29	67
7	j	200/250 (80%)	193 (96%)	6 (3%)	1 (0%)	29	67
8	G	225/244 (92%)	218 (97%)	6 (3%)	1 (0%)	34	69
8	Q	199/244 (82%)	192 (96%)	6 (3%)	1 (0%)	29	67
8	a	223/244 (91%)	217 (97%)	6 (3%)	0	100	100
8	k	220/244 (90%)	213 (97%)	7 (3%)	0	100	100
9	H	261/316 (83%)	249 (95%)	9 (3%)	3 (1%)	14	51
9	R	259/316 (82%)	251 (97%)	7 (3%)	1 (0%)	34	69
9	b	256/316 (81%)	244 (95%)	10 (4%)	2 (1%)	19	58
9	l	262/316 (83%)	253 (97%)	8 (3%)	1 (0%)	34	69
10	J	16/190 (8%)	14 (88%)	2 (12%)	0	100	100
10	T	5/190 (3%)	4 (80%)	1 (20%)	0	100	100
10	d	5/190 (3%)	4 (80%)	1 (20%)	0	100	100
10	n	8/190 (4%)	7 (88%)	1 (12%)	0	100	100
All	All	8714/10948 (80%)	8374 (96%)	306 (4%)	34 (0%)	34	69

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	140/242 (58%)	140 (100%)	0	100	100
1	S	163/242 (67%)	163 (100%)	0	100	100
1	c	153/242 (63%)	153 (100%)	0	100	100
1	m	152/242 (63%)	152 (100%)	0	100	100
2	A	243/266 (91%)	239 (98%)	4 (2%)	62	84
2	K	243/266 (91%)	242 (100%)	1 (0%)	91	95
2	U	243/266 (91%)	239 (98%)	4 (2%)	62	84
2	e	244/266 (92%)	241 (99%)	3 (1%)	71	88
3	B	194/220 (88%)	193 (100%)	1 (0%)	88	95
3	L	192/220 (87%)	192 (100%)	0	100	100
3	V	200/220 (91%)	200 (100%)	0	100	100
3	f	199/220 (90%)	198 (100%)	1 (0%)	88	95
4	C	244/349 (70%)	242 (99%)	2 (1%)	81	93
4	M	235/349 (67%)	231 (98%)	4 (2%)	60	83
4	W	255/349 (73%)	253 (99%)	2 (1%)	81	93
4	g	247/349 (71%)	246 (100%)	1 (0%)	91	95
5	D	182/198 (92%)	181 (100%)	1 (0%)	88	95
5	N	187/198 (94%)	186 (100%)	1 (0%)	88	95
5	X	196/198 (99%)	193 (98%)	3 (2%)	65	85
5	h	195/198 (98%)	193 (99%)	2 (1%)	76	90
6	E	208/242 (86%)	205 (99%)	3 (1%)	67	86
6	O	215/242 (89%)	214 (100%)	1 (0%)	88	95
6	Y	224/242 (93%)	220 (98%)	4 (2%)	59	82
6	i	225/242 (93%)	222 (99%)	3 (1%)	69	87
7	F	155/219 (71%)	153 (99%)	2 (1%)	69	87
7	P	150/219 (68%)	149 (99%)	1 (1%)	84	94
7	Z	156/219 (71%)	155 (99%)	1 (1%)	86	94
7	j	153/219 (70%)	153 (100%)	0	100	100
8	G	168/212 (79%)	167 (99%)	1 (1%)	86	94
8	Q	162/212 (76%)	159 (98%)	3 (2%)	57	81
8	a	191/212 (90%)	188 (98%)	3 (2%)	62	84
8	k	151/212 (71%)	150 (99%)	1 (1%)	84	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	H	212/270 (78%)	208 (98%)	4 (2%)	57	81
9	R	218/270 (81%)	213 (98%)	5 (2%)	50	78
9	b	213/270 (79%)	207 (97%)	6 (3%)	43	74
9	l	211/270 (78%)	207 (98%)	4 (2%)	57	81
10	J	13/171 (8%)	13 (100%)	0	100	100
10	T	4/171 (2%)	4 (100%)	0	100	100
10	d	4/171 (2%)	4 (100%)	0	100	100
10	n	6/171 (4%)	6 (100%)	0	100	100
All	All	7146/9556 (75%)	7074 (99%)	72 (1%)	76	90

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	0.83	0	9,12,12	1.23	1 (11%)
11	TAM	K	401	-	7,10,10	0.82	0	9,12,12	1.22	1 (11%)
11	TAM	e	401	-	7,10,10	0.81	0	9,12,12	1.25	1 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	TAM	U	401	-	7,10,10	0.81	0	9,12,12	1.24	1 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	TAM	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 (4) bond angle outliers are listed below:

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

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	K	401	TAM	C3-C-C2-C5
11	K	401	TAM	N-C-C2-C5
11	e	401	TAM	C3-C-C2-C5
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	U	401	TAM	C-C2-C5-O5
11	K	401	TAM	C1-C-C2-C5
11	A	401	TAM	C2-C-C3-C6
11	U	401	TAM	C-C1-C4-O4
11	e	401	TAM	C1-C-C2-C5
11	K	401	TAM	C-C3-C6-O6

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Mol	Chain	Res	Type	Atoms
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.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	K	401	TAM	3	0
11	U	401	TAM	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	I	178/295 (60%)	1.96	81 (45%) 0 0	100, 161, 215, 252	0
1	S	208/295 (70%)	2.46	102 (49%) 0 0	111, 190, 246, 272	0
1	c	197/295 (66%)	1.86	78 (39%) 0 0	125, 167, 214, 246	0
1	m	190/295 (64%)	1.51	59 (31%) 0 0	110, 153, 199, 232	0
2	A	295/305 (96%)	-0.07	1 (0%) 94 92	51, 71, 133, 178	0
2	K	295/305 (96%)	0.08	3 (1%) 82 72	48, 78, 137, 219	0
2	U	295/305 (96%)	0.07	5 (1%) 70 57	50, 74, 144, 218	0
2	e	295/305 (96%)	-0.01	1 (0%) 94 92	56, 76, 140, 200	0
3	B	242/249 (97%)	0.03	4 (1%) 70 57	45, 66, 120, 174	0
3	L	238/249 (95%)	-0.01	1 (0%) 92 89	37, 57, 101, 133	0
3	V	241/249 (96%)	0.09	2 (0%) 86 78	41, 61, 107, 154	0
3	f	237/249 (95%)	0.10	0 100 100	50, 68, 115, 160	0
4	C	313/394 (79%)	0.01	5 (1%) 72 59	57, 85, 147, 224	0
4	M	310/394 (78%)	-0.03	1 (0%) 94 92	55, 84, 141, 208	0
4	W	319/394 (80%)	0.04	2 (0%) 89 83	50, 79, 140, 208	0
4	g	317/394 (80%)	0.14	4 (1%) 77 65	60, 85, 135, 207	0
5	D	221/226 (97%)	-0.15	1 (0%) 91 86	47, 69, 104, 126	0
5	N	222/226 (98%)	-0.14	1 (0%) 91 86	50, 85, 123, 173	0
5	X	223/226 (98%)	-0.01	0 100 100	46, 75, 111, 164	0
5	h	223/226 (98%)	-0.19	0 100 100	59, 78, 111, 132	0
6	E	257/268 (95%)	-0.05	4 (1%) 72 59	56, 83, 134, 157	0
6	O	260/268 (97%)	-0.17	0 100 100	49, 77, 125, 171	0
6	Y	263/268 (98%)	-0.13	0 100 100	43, 72, 123, 149	0
6	i	261/268 (97%)	-0.13	0 100 100	51, 76, 123, 172	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
7	F	207/250 (82%)	0.05	2 (0%) 82 72	58, 90, 137, 166	0
7	P	208/250 (83%)	-0.09	3 (1%) 75 63	62, 94, 133, 159	0
7	Z	208/250 (83%)	0.22	7 (3%) 45 29	61, 89, 133, 156	0
7	j	206/250 (82%)	0.11	6 (2%) 51 36	61, 89, 136, 160	0
8	G	231/244 (94%)	-0.09	3 (1%) 77 65	58, 91, 150, 217	0
8	Q	207/244 (84%)	0.08	9 (4%) 35 22	89, 142, 185, 264	0
8	a	227/244 (93%)	0.64	38 (16%) 1 1	90, 137, 211, 267	0
8	k	226/244 (92%)	0.02	12 (5%) 26 14	87, 118, 178, 226	0
9	H	267/316 (84%)	-0.04	3 (1%) 80 69	42, 85, 129, 189	0
9	R	265/316 (83%)	-0.09	5 (1%) 66 53	40, 71, 114, 158	0
9	b	262/316 (82%)	-0.17	0 100 100	49, 82, 135, 160	0
9	l	268/316 (84%)	-0.11	6 (2%) 62 48	59, 93, 144, 196	0
10	J	20/190 (10%)	0.31	2 (10%) 7 4	88, 118, 157, 157	0
10	T	7/190 (3%)	-0.60	0 100 100	131, 137, 142, 163	0
10	d	7/190 (3%)	-0.00	0 100 100	110, 131, 137, 140	0
10	n	10/190 (5%)	0.89	1 (10%) 7 4	111, 124, 167, 178	0
All	All	8926/10948 (81%)	0.17	452 (5%) 28 16	37, 85, 174, 272	0

All (452) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	c	196	ASP	16.0
1	m	195	SER	14.8
1	S	196	ASP	12.1
1	c	278	PRO	12.1
1	S	238	GLY	10.6
1	S	126	ASN	10.0
1	S	185	ALA	9.7
8	a	139	SER	9.7
1	m	196	ASP	9.6
1	S	195	SER	9.5
1	S	236	SER	9.4
1	S	202	ARG	8.9
1	I	135	GLU	8.6
8	a	112	THR	8.6
1	c	195	SER	8.5

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Mol	Chain	Res	Type	RSRZ
1	I	151	ALA	8.2
1	S	240	GLY	8.1
1	I	134	LYS	8.1
1	S	8	PRO	7.6
1	S	237	LEU	7.5
1	S	278	PRO	7.1
1	S	241	THR	7.1
1	I	237	LEU	7.0
1	c	245	LEU	6.9
1	S	244	TYR	6.8
1	S	245	LEU	6.8
1	I	243	TYR	6.7
1	I	240	GLY	6.7
1	S	243	TYR	6.6
1	S	219	LYS	6.6
1	S	212	SER	6.6
1	S	153	VAL	6.6
1	c	49	ASN	6.6
1	S	206	ARG	6.4
1	S	205	ILE	6.4
1	c	65	ARG	6.3
1	S	200	THR	6.2
1	S	220	VAL	6.2
1	c	243	TYR	6.2
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	5.8
1	S	151	ALA	5.6
1	I	160	ASP	5.6
1	S	208	GLN	5.6
2	K	295	ALA	5.6
7	P	101	LEU	5.6
1	c	3	CYS	5.4
1	c	202	ARG	5.3
1	m	241	THR	5.3
8	a	108	LYS	5.2
9	l	155	ASP	5.2

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Mol	Chain	Res	Type	RSRZ
1	S	194	SER	5.2
1	m	235	LEU	5.1
9	l	156	GLU	5.1
1	m	199	GLU	5.1
9	l	151	LYS	5.0
1	I	210	VAL	5.0
1	m	236	SER	5.0
1	I	126	ASN	5.0
1	S	201	PHE	4.9
1	S	203	GLY	4.9
1	S	140	LEU	4.9
1	S	156	LEU	4.9
1	c	109	SER	4.9
1	c	241	THR	4.8
8	a	102	PHE	4.8
1	m	245	LEU	4.8
1	S	133	PRO	4.8
1	I	207	SER	4.8
1	I	242	ASN	4.7
8	a	110	ARG	4.7
8	a	113	LEU	4.7
1	c	8	PRO	4.7
1	m	11	ALA	4.7
1	S	235	LEU	4.7
1	c	223	CYS	4.6
1	S	247	THR	4.6
4	g	306	CYS	4.6
8	a	174	LEU	4.6
1	S	199	GLU	4.5
1	I	155	ILE	4.5
6	E	0	HIS	4.5
1	I	17	ILE	4.5
1	S	218	VAL	4.5
7	Z	101	LEU	4.5
6	E	157	LEU	4.5
1	m	155	ILE	4.5
1	S	204	ILE	4.5
1	I	133	PRO	4.5
1	I	234	VAL	4.4
8	a	140	THR	4.4
1	m	202	ARG	4.4
1	m	244	TYR	4.4

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Mol	Chain	Res	Type	RSRZ
8	Q	234	ILE	4.4
8	k	154	MET	4.3
1	S	224	PHE	4.3
1	S	46	TYR	4.3
1	c	139	VAL	4.3
1	S	150	ARG	4.3
1	I	209	ASP	4.3
1	m	62	GLY	4.3
9	R	155	ASP	4.2
8	k	146	GLY	4.2
1	m	205	ILE	4.2
7	F	101	LEU	4.2
1	I	153	VAL	4.2
1	S	155	ILE	4.2
1	I	235	LEU	4.2
1	S	246	THR	4.2
1	S	233	GLN	4.1
1	S	20	GLN	4.1
1	I	205	ILE	4.1
1	S	138	ILE	4.1
1	S	7	PHE	4.1
1	c	113	GLY	4.1
1	m	269	ALA	4.0
1	c	224	PHE	4.0
9	l	144	PRO	4.0
8	a	187	ALA	4.0
1	S	242	ASN	4.0
1	I	208	GLN	4.0
1	c	48	HIS	4.0
8	k	196	VAL	4.0
1	m	234	VAL	4.0
2	U	209	ASN	4.0
1	I	56	ILE	3.9
1	c	151	ALA	3.9
1	I	112	PRO	3.9
8	a	151	GLU	3.9
1	m	197	LEU	3.9
10	n	115	PHE	3.9
1	m	243	TYR	3.9
8	a	144	ASP	3.9
1	S	55	ALA	3.9
8	a	137	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
9	l	152	SER	3.9
1	I	221	ILE	3.8
1	S	190	VAL	3.8
1	c	2	ALA	3.8
7	Z	102	LEU	3.8
1	c	133	PRO	3.8
1	S	108	VAL	3.8
1	m	247	THR	3.8
1	m	237	LEU	3.7
1	S	215	ARG	3.7
1	I	241	THR	3.7
1	S	210	VAL	3.7
1	I	196	ASP	3.7
1	c	138	ILE	3.7
2	K	296	MET	3.7
1	c	199	GLU	3.7
3	B	90	SER	3.6
8	a	118	LEU	3.6
1	S	154	GLU	3.6
1	c	7	PHE	3.6
1	I	64	VAL	3.6
2	U	205	ASP	3.5
1	I	278	PRO	3.5
1	c	10	ILE	3.5
1	I	148	LEU	3.5
1	S	6	GLN	3.5
1	m	194	SER	3.5
1	c	235	LEU	3.5
1	c	150	ARG	3.5
1	S	131	ASN	3.5
8	G	141	THR	3.5
8	Q	140	THR	3.4
1	I	238	GLY	3.4
7	P	100	GLY	3.4
1	I	150	ARG	3.4
1	I	248	ALA	3.4
1	m	61	VAL	3.4
1	S	269	ALA	3.4
1	c	244	TYR	3.4
1	m	113	GLY	3.4
1	S	214	ASP	3.4
1	c	197	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	m	10	ILE	3.4
9	R	154	SER	3.4
1	I	199	GLU	3.4
1	c	140	LEU	3.4
8	a	195	TRP	3.4
1	I	16	LEU	3.3
1	I	187	THR	3.3
1	I	247	THR	3.3
1	c	206	ARG	3.3
8	a	143	ARG	3.3
1	S	10	ILE	3.3
1	c	17	ILE	3.3
1	S	53	LEU	3.3
1	m	131	ASN	3.3
1	I	63	THR	3.3
1	I	224	PHE	3.3
8	k	102	PHE	3.3
1	I	204	ILE	3.3
1	S	186	ALA	3.3
1	I	131	ASN	3.3
1	S	270	THR	3.2
1	c	148	LEU	3.2
1	I	244	TYR	3.2
1	m	201	PHE	3.2
1	c	131	ASN	3.2
8	a	194	ILE	3.2
1	c	152	ASN	3.2
1	I	146	LEU	3.2
1	m	190	VAL	3.2
1	m	283	THR	3.2
8	a	141	THR	3.2
1	S	207	SER	3.2
6	E	177	MET	3.2
8	a	145	ALA	3.2
1	m	138	ILE	3.1
1	c	61	VAL	3.1
1	c	51	ARG	3.1
1	S	239	ASP	3.1
8	a	19	VAL	3.1
1	m	278	PRO	3.1
7	j	101	LEU	3.1
1	m	232	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	m	233	GLN	3.1
8	a	148	GLY	3.1
1	S	223	CYS	3.1
1	I	202	ARG	3.0
1	m	266	LEU	3.0
1	c	198	GLY	3.0
1	c	234	VAL	3.0
8	k	195	TRP	3.0
1	I	211	ARG	3.0
3	B	3	ARG	3.0
8	a	196	VAL	3.0
1	c	159	GLU	3.0
8	Q	147	PHE	3.0
1	c	50	GLY	3.0
1	m	133	PRO	3.0
1	m	65	ARG	2.9
1	m	200	THR	2.9
7	Z	139	VAL	2.9
1	S	11	ALA	2.9
1	S	267	MET	2.9
7	Z	108	ASN	2.9
1	S	209	ASP	2.9
2	e	209	ASN	2.9
8	k	118	LEU	2.9
1	I	220	VAL	2.9
1	S	146	LEU	2.9
3	B	244	SER	2.9
1	S	234	VAL	2.9
1	c	46	TYR	2.9
1	c	9	GLU	2.9
1	I	195	SER	2.9
8	a	84	TYR	2.9
8	k	148	GLY	2.9
1	S	149	GLN	2.8
8	G	142	GLY	2.8
2	A	293	TYR	2.8
1	I	236	SER	2.8
1	c	237	LEU	2.8
7	j	102	LEU	2.8
1	m	188	PHE	2.8
1	c	155	ILE	2.8
1	I	222	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
8	a	150	LEU	2.8
8	Q	154	MET	2.8
1	c	268	TYR	2.8
1	c	266	LEU	2.8
1	S	139	VAL	2.8
1	S	222	GLU	2.8
7	P	8	ARG	2.8
1	I	141	THR	2.8
8	Q	139	SER	2.8
1	m	127	ASP	2.8
1	I	130	ASN	2.8
1	S	109	SER	2.7
1	S	65	ARG	2.7
1	m	109	SER	2.7
1	m	46	TYR	2.7
1	S	135	GLU	2.7
1	c	128	PHE	2.7
1	c	203	GLY	2.7
1	m	139	VAL	2.7
1	S	35	TYR	2.7
4	C	306	CYS	2.7
1	I	132	LEU	2.7
2	K	103	LEU	2.7
1	c	1	MET	2.7
3	L	3	ARG	2.7
1	I	219	LYS	2.7
1	S	157	ALA	2.7
1	I	159	GLU	2.7
1	m	268	TYR	2.7
1	m	63	THR	2.7
1	m	153	VAL	2.7
9	H	349	LEU	2.6
1	m	274	MET	2.6
1	c	190	VAL	2.6
8	a	142	GLY	2.6
1	S	189	SER	2.6
8	a	79	THR	2.6
8	Q	186	VAL	2.6
1	S	211	ARG	2.6
1	S	198	GLY	2.6
1	I	239	ASP	2.6
3	B	91	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
8	a	109	ASN	2.6
1	m	270	THR	2.6
1	I	245	LEU	2.6
1	m	151	ALA	2.6
1	c	255	VAL	2.6
8	a	119	VAL	2.6
1	I	206	ARG	2.6
1	I	279	VAL	2.6
1	S	162	PRO	2.6
1	m	193	ALA	2.5
8	Q	132	ALA	2.5
1	m	156	LEU	2.5
1	c	55	ALA	2.5
8	k	147	PHE	2.5
1	S	4	ASN	2.5
1	S	34	ASN	2.5
8	a	73	ILE	2.5
8	k	194	ILE	2.5
1	I	147	SER	2.5
1	S	281	GLY	2.5
1	c	242	ASN	2.5
8	a	95	VAL	2.5
8	a	178	LEU	2.5
1	I	194	SER	2.5
1	S	197	LEU	2.5
10	J	108	VAL	2.5
9	H	95	LEU	2.5
1	c	194	SER	2.5
1	S	54	GLU	2.5
8	G	137	PHE	2.5
7	Z	104	LYS	2.4
1	c	5	PHE	2.4
8	a	154	MET	2.4
1	S	145	ARG	2.4
1	I	18	CYS	2.4
1	c	236	SER	2.4
9	l	153	GLU	2.4
1	I	189	SER	2.4
4	g	90	SER	2.4
4	C	239	GLN	2.4
1	I	139	VAL	2.4
1	c	127	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	128	PHE	2.4
1	c	188	PHE	2.4
4	W	59	LEU	2.4
4	g	31	LEU	2.4
1	I	190	VAL	2.4
1	I	149	GLN	2.4
3	V	64	GLN	2.4
1	S	9	GLU	2.4
1	c	187	THR	2.4
2	U	96	ILE	2.4
1	I	254	VAL	2.3
3	V	89	SER	2.3
1	m	126	ASN	2.3
1	S	111	LEU	2.3
1	I	143	VAL	2.3
1	c	112	PRO	2.3
4	C	39	ILE	2.3
1	I	152	ASN	2.3
1	S	216	ASP	2.3
1	c	201	PHE	2.3
1	c	207	SER	2.3
1	S	152	ASN	2.3
9	R	157	LEU	2.3
1	c	189	SER	2.3
6	E	172	PHE	2.3
9	R	145	GLY	2.3
1	I	266	LEU	2.3
1	S	38	GLY	2.3
1	c	200	THR	2.3
2	U	207	GLU	2.3
4	M	299	ILE	2.3
1	m	210	VAL	2.3
1	S	141	THR	2.3
1	m	8	PRO	2.2
1	c	60	LEU	2.2
1	I	65	ARG	2.2
5	D	145	ILE	2.2
1	c	232	ALA	2.2
8	k	197	LYS	2.2
1	S	147	SER	2.2
1	I	256	PHE	2.2
1	S	64	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
9	R	95	LEU	2.2
1	m	128	PHE	2.2
8	a	16	THR	2.2
8	a	186	VAL	2.2
4	C	90	SER	2.2
1	c	249	ARG	2.2
1	c	52	THR	2.2
1	c	279	VAL	2.2
8	k	186	VAL	2.2
1	m	12	TYR	2.2
1	S	18	CYS	2.2
1	m	239	ASP	2.2
1	m	279	VAL	2.2
7	j	190	MET	2.2
1	I	233	GLN	2.1
1	m	204	ILE	2.1
1	c	110	VAL	2.1
8	a	134	ILE	2.1
1	m	246	THR	2.1
7	j	9	LEU	2.1
1	m	211	ARG	2.1
1	I	158	VAL	2.1
7	j	6	ARG	2.1
1	I	113	GLY	2.1
2	U	212	GLY	2.1
1	S	284	GLU	2.1
1	S	110	VAL	2.1
7	j	7	ARG	2.1
1	S	66	CYS	2.1
7	Z	100	GLY	2.1
5	N	140	LYS	2.1
4	W	72	ASN	2.1
1	S	148	LEU	2.1
7	F	87	PHE	2.1
1	I	157	ALA	2.1
1	c	149	GLN	2.1
4	C	89	THR	2.1
9	H	145	GLY	2.1
1	m	110	VAL	2.1
1	I	217	ARG	2.1
10	J	110	SER	2.1
1	I	197	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
8	k	174	LEU	2.1
1	I	249	ARG	2.1
8	a	76	ILE	2.1
1	S	256	PHE	2.1
8	a	86	VAL	2.1
1	S	268	TYR	2.0
1	I	203	GLY	2.0
1	I	145	ARG	2.0
4	g	140	ARG	2.0
8	a	71	PHE	2.0
1	I	58	ALA	2.0
1	c	11	ALA	2.0
1	c	146	LEU	2.0
1	c	281	GLY	2.0
8	Q	127	GLU	2.0
1	c	147	SER	2.0
7	Z	121	PHE	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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	CL	R	401	1/1	0.60	0.42	95,95,95,95	0
13	MG	O	301	1/1	0.66	0.35	85,85,85,85	0
13	MG	g	401	1/1	0.72	0.14	60,60,60,60	0
12	CL	b	401	1/1	0.86	0.27	86,86,86,86	0
11	TAM	e	401	11/11	0.87	0.15	75,89,96,99	0
12	CL	f	301	1/1	0.90	0.29	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
12	CL	H	401	1/1	0.90	0.20	80,80,80,80	0
11	TAM	U	401	11/11	0.91	0.18	79,98,112,119	0
11	TAM	K	401	11/11	0.92	0.19	69,86,103,111	0
12	CL	G	301	1/1	0.92	0.27	99,99,99,99	0
11	TAM	A	401	11/11	0.92	0.17	85,96,101,103	0
12	CL	I	401	1/1	0.95	0.11	75,75,75,75	0
12	CL	R	402	1/1	0.96	0.17	73,73,73,73	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.